
Extended Reservoir Approach for Quantum Transport and non-Markovian Dynamics

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by

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To those who know that I just don't know.

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Streszczenie

Transport kwantowy jest przykładem procesu nierówno-wagowego, w którym przepływ cząstek lub energii między nieskończonymi otoczeniami generuje prąd przez złącze. Tematyka transportu kwantowego pojawia się między innymi w kontekście charakterystyki urządzeń nanoelektronicznych, symulatorów kwantowych, oraz termodynamiki kwantowej. Problem stanowi istotne wyzwanie numeryczne ze względu na wykładniczo rosnący rozmiar przestrzeni Hilberta oraz konieczność uwzględnienia wpływu nieskończonych otoczeń.

Niniejsza praca zawiera przegląd podejść użytecznych do badania transportu kwantowego w układach fermionowych. W szczególności, omówione zostało podejście rozszerzonych otoczeń (ang. extended reservoir approach, ERA), które pozwala na numerycznie kontrolowalne przybliżenie niemarkowskich rezerwuarów. W tym podejściu są one przybliżane przez skończony system, w którym zmiany spowodowane przepływem cząstek kompensowane są przez relaksację obsadzeń. Podejście to ma na celu odtworzenie właściwości spektralnych rzeczywistego rezerwuaru a w konsekwencji też rzeczywistego transportu przez złącze.

Kluczem do efektywnej symulacji jest optymalny wybór parametrów modelu, tak by stan stacjonarny nie nosił artefaktów przybliżenia. W pracy zostały omówione jak wybór rozszerzonego rezerwuaru wpływa na stan stacjonarny, mechanizmy niefizycznych artefaktów w ERA, oraz sposoby ich unikania. Ponadto, zestawiono standardowe podejście Lindblada dyskretnym podejściem, gdzie koherentna ewolucja i relaksacja działają naprzemiennie w czasie.

Symulacja dowolnego układu kwantowego wymaga użycia specjalistycznych narzędzi numerycznych takich jak sieci tensorowe. W pracy przedstawiono zalety i wady dostępnych rozwiązań, w tym sposobu reprezentacji macierzy gęstości oraz znajdowania stanu stacjonarnego. Na podstawie analizy struktury splątania omówiono jak przez manipulację sieci można obniżyć koszt numeryczny.

Połączenie podejścia rozszerzonych otoczeń i sieci tensorowych tworzy wydajną, skalowalną i numerycznie dokładną platformę zdolną do symu-

Streszczenie

lacji transportu kwantowego i niemarkowskiej dynamiki.

Abstract

Quantum transport is an example of a non-equilibrium process where an imbalance between macroscopic reservoirs induces particle or energy current through a junction. This phenomenon is relevant in various fields, including nanoelectronic devices, quantum simulators, and quantum thermodynamics. However, simulating quantum transport numerically remains a challenging task since it requires handling exponentially large Hilbert spaces and including the influence of infinite environments. For fermionic systems, the non-Markovian character of reservoirs necessitates incorporating the dynamics of infinite reservoirs, which remains one of the main challenges.

This thesis presents novel approaches to simulate and optimize quantum transport. Our main focus is on the extended reservoir approach (ERA), which provides a controllable platform for non-Markovian quantum transport through many-body junction. In ERA, we approximate the infinite reservoir by a finite system that is subject to dissipation, compensating for the particle flow during time evolution. By reproducing the spectral properties of the true reservoir, we achieve a precise description of the steady-state quantum transport.

Efficient simulation relies on optimal microscopic models for extended reservoirs. In this thesis, we study how the choice of finite system and dissipation influences the steady state and comment on how certain choices may lead to artifacts that substantially distort the physical current. Moreover, we present procedures to avoid unwanted effects and compare the standard Lindblad approach to the periodic formulation, where coherent evolution and dissipation act interchangeably in time.

Quantum simulation requires powerful toolboxes such as tensor networks (TNs). In this thesis, we discuss possible approaches to implement TNs and obtain a steady state. However, the applicability of TNs remains limited by entanglement. Therefore, based on the scattering structure for ERA, we design a representation that minimizes the numerical cost of the simulation.

By combining the extended reservoir approach with tensor networks, we are able to create an efficient, scalable, and numerically exact platform

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capable of handling arbitrary many-body quantum transport.

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Abbreviations

ARC Accumulative reservoir construction

DOS Density of states

DMRG Density matrix renormalization group

ERA Extended reservoir approach

GF Green's function

NEGF Non-equilibrium Green's function

NESS Non-equilibrium steady state

MPS Matrix product state

MPO Matrix product operator

OSEE Operator-space entanglement entropy

TEBD Time-evolving block decimation

TDVP Time-dependent variational principle

TN Tensor network

Symbols

e elementary charge

h Planck's constant, $\hbar = h/2\pi$

i imaginary unit

$*$ complex conjugation

^{T} transpose

† conjugate transpose, Hermitian transpose

$\otimes$ Kronecker product, tensor product

$\circ$ scalar product

Preface

The non-equilibrium states provide new and exciting phenomena which help us to understand the dynamical aspects of quantum matter. One of them is quantum transport where the imbalance between macroscopic environments induces a current through a small quantum system. Many-body interaction in that model results in some exciting designs of devices that harvest on quantum principles, such as efficient quantum-dot heat engines [10] or graphene-based single-electron transistors [11]. Recently, there are also new ideas to design a quantum simulator based on doped semiconductors [12], [13]. While the technology is still under development there is a growing need to have an efficient numerical simulation to study these kinds of problems. This requires solving quantum transport for an arbitrary many-body quantum system in contact with non-interacting but infinite environments. Studying non-equilibrium properties for electron transport is particularly challenging due to the long time-correlation for the reservoirs. Simulating non-Markovian dynamics requires incorporating the effects of the evolution of the infinite reservoirs which is difficult to do.

For that reason, numerical treatment of the quantum transport is generally hard, apart from special cases such as non-interacting models. In Chpt. 1 and Chpt. 2 we give an overview of standard approaches to studying quantum transport. These methods enable simulation for some classes of systems but are not useful for general non-Markovian and many-body cases. These can be targeted using the *extended reservoirs approach*, where an infinite environment is replaced by a finite system coupled to dissipation which maintains a thermal distribution and a steady state.

My thesis is dedicated to the development of that numerical approach and consists of five publications:

- [1] G. Wójtowicz, J. E. Elenewski, M. M. Rams, *et al.*, “Open-system tensor networks and Kramers’ crossover for quantum transport,” *Phys. Rev. A*, vol. 101, 050301(R), 2020. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevA.101.050301>

[org/doi/10.1103/PhysRevA.101.050301](https://doi.org/10.1103/PhysRevA.101.050301),

- [2] G. Wójtowicz, J. E. Elenewski, M. M. Rams, *et al.*, “Dual current anomalies and quantum transport within extended reservoir simulations,” *Phys. Rev. B*, vol. 104, p. 165 131, 2021. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.104.165131>,
- [3] J. E. Elenewski, G. Wójtowicz, M. M. Rams, *et al.*, “Performance of reservoir discretizations in quantum transport simulations,” *J. Chem. Phys.*, vol. 155, p. 124 117, 2021. [Online]. Available: <https://aip.scitation.org/doi/10.1063/5.0065799>,
- [4] G. Wójtowicz, A. Purkayastha, M. Zwolak, *et al.*, “Accumulative reservoir construction: Bridging continuously relaxed and periodically refreshed extended reservoirs,” *Phys. Rev. B*, vol. 107, p. 035 150, 2023. [Online]. Available: <https://link.aps.org/doi/10.1103/PhysRevB.107.035150>,
- [5] B. De, G. Wojtowicz, J. Zakrzewski, *et al.*, “Transport in a periodically-driven tilted lattice via the extended reservoir approach: Stability criterion for recovering the continuum limit,” *arXiv:2303.04160*, 2023. [Online]. Available: <https://arxiv.org/abs/2303.04160>.

Based on Ref. [2], [3], [5], in Chpt. 4 we explain the origin of common artifacts of the approximations and we design an effective approach to avoid them. In addition, in Chpt. 5 we compare the standard Lindblad approach to a novel periodic formulation [4] where coherent evolution and dissipation are applied interchangeably in time.

Since we ultimately aim to study many-body models we develop a numerical implementation based on *tensor networks*, which provide a controllable toolbox for quantum systems. The description in Chpt. 6 is mainly based on Ref. [1] which significantly shaped our numerical approaches to implement ERA. After a short introduction, we describe how the implementation we choose permits us to omit some of the common limitations. Some of the understanding developed from directly working with the implementation of tensor networks. Therefore, the thesis is directly related to the open-source tensor network library

- [6] M. M. Rams, J. Hasik, G. Wojtowicz, *et al.*, *Yet Another Symmetric Tensor Network*, <https://github.com/yastn/yastn>, 2023.

The *extended reservoir approach* combined with *tensor networks* provide an efficient, scalable, and systematically converging platform to simulate non-Markovian and many-body quantum transport. This thesis summarizes the publications listed above and expands on some aspects which

have not been extensively covered in the published versions. Writing it I hope to give a comprehensive introduction to the subject and systematize all conclusions I obtained during my doctoral studies. The theoretical discussion is supplemented with practical guidelines which can be useful while implementing the ERA numerically. Given the novelty of that topic, this thesis is likely one of the first to discuss that specific field in such detail.

In the course of my studies, I also co-authored the following articles, that however are not part of this thesis:

- [7] A. Jochim, M. Rams, T. Neumann, *et al.*, “Structural Diversity in Ni Chain Coordination Polymers: Synthesis, Structures, Isomerism and Magnetism,” *European Journal of Inorganic Chemistry*, vol. 2018, no. 44, pp. 4779–4789, 2018, ISSN: 1434-1948, 1099-0682. DOI: [10.1002/ejic.201800939](https://doi.org/10.1002/ejic.201800939). [Online]. Available: <https://onlinelibrary.wiley.com/doi/10.1002/ejic.201800939>,
- [8] W. Piskorz, F. Zasada, G. Wójtowicz, *et al.*, “Attaching titania clusters of various size to reduced graphene oxide and its impact on the conceivable photocatalytic behavior of the junctions—a DFT/D + U and TD DFTB modeling,” *Journal of Physics: Condensed Matter*, vol. 31, no. 40, p. 404 001, 2019, ISSN: 0953-8984, 1361-648X. DOI: [10.1088/1361-648X/ab2bc8](https://doi.org/10.1088/1361-648X/ab2bc8). [Online]. Available: <https://iopscience.iop.org/article/10.1088/1361-648X/ab2bc8>,
- [9] P. Dąbczyński, G. Wójtowicz, and J. Rysz, “Mutual Diffusion of Model Acceptor/Donor Bilayers under Solvent Vapor Annealing as a Novel Route for Organic Solar Cell Fabrication,” *Energies*, vol. 15, no. 3, p. 1033, 2022, ISSN: 1996-1073. DOI: [10.3390/en15031033](https://doi.org/10.3390/en15031033). [Online]. Available: <https://www.mdpi.com/1996-1073/15/3/1033>.

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1. Quantum transport

Condensed matter is a fundamental area of research that develops an understanding of material properties based on microscopic description. Consequently, we know how to control them and potentially use them for material science, engineering, and technology. They also exhibit some exciting phenomena such as e.g., superconductivity [14] and topologically protected states [15] which are interesting from the perspective of fundamental science. Some of the most intriguing phenomena in condensed matter physics are observed in materials with a strong correlation between electrons. The strongly correlated particles often respond collectively under external forces and make the material sensitive to small changes in internal or external parameters. Contrary to weakly correlated materials, they can't be approximated by free-electron theories [16] and physicists and chemists work to understand that complex behavior based on theory and experiment.

The equilibrium state properties of a quantum system are relatively well-studied and understood. However, the character of non-equilibrium phases can be drastically different from equilibrium [17] and still hold many open questions. This is particularly true for strongly correlated materials where the collective nature of particles is reflected in time-correlation and non-equilibrium dynamics.

Among many non-equilibrium processes, there is a *quantum transport*, dealing with a quantum system coupled to infinite reservoirs. In quantum transport, the imbalance between the reservoirs generates a directional flow of particles or energy, i.e. a current, across the quantum system. The phenomena is considered in the context of nanophotonics and nanoelectronics [11], [18], quantum thermodynamics [10], [19], and quantum simulation [12], [13].

In this chapter, we introduce the problem of quantum transport in fermionic systems. In Sec. 1.1 we outline a typical model which will be central to the whole discussion and analysis in this thesis. In Sec. 1.2 we discuss the time-evolution of a quantum system and introduce open-

system description. Later, in Sec. 1.3 and 1.4 we use the typical model and an open-system description to write the master equation for the evolution of a system weakly coupled to reservoirs. There we explain how the evolution of the environment enters the master equation and we present common approximations for the short time-correlated (Markovian) cases. The chapter aims to discuss the nature of quantum transport, including coupling strength and time-correlation for the reservoirs. The common approaches provide an introduction to non-Markovian aspects of electron quantum transport and the analytical and numerical difficulties.

1.1 Quantum Transport

A paradigm model to study quantum transport consists of a finite system $\mathcal{S}$ which is coupled to one or many reservoirs. The imbalance in the system induces a transport that can be measured as particle or energy current between the constituents. Generally, the reservoirs are not coupled to each other but are connected to $\mathcal{S}$. Therefore the transport between them is controlled by $\mathcal{S}$ quantum system.

A Hamiltonian for a typical model takes two reservoirs $\mathcal{L}$ and $\mathcal{R}$ often acting as a source and a drain, and finite, but otherwise arbitrary, system $\mathcal{S}$. For the composite $\mathcal{L}\mathcal{S}\mathcal{R}$ system the Hamiltonian is

$$H = H_{\mathcal{S}} + H_{\mathcal{L}} + H_{\mathcal{R}} + H_{\mathcal{I}}, \quad (1.1)$$

where $H_{\mathcal{L}(\mathcal{R})}$ is the Hamiltonian of the reservoir $\mathcal{L}(\mathcal{R})$, $H_{\mathcal{S}}$ is the Hamiltonian of the system $\mathcal{S}$, and $H_{\mathcal{I}}$ is the interaction between $\mathcal{L}\mathcal{R}$ and $\mathcal{S}$. The model in Eq. (1.1) can be generalized to an arbitrary number of reservoirs and bosonic and fermionic modes. Nonetheless, in this text, we focus on fully fermionic models and only two reservoirs as in Fig. 1.1.

The system $\mathcal{S}$ is a quantum system described by the Hamiltonian $H_{\mathcal{S}}$ which is finite but otherwise arbitrary and may include many-body interactions¹.

The reservoirs $\mathcal{L}\mathcal{R}$ are macroscopic and, in practice, infinite quantum systems. They can have arbitrary geometry and spatial dimension but typically they are chosen to be non-interacting. This choice can be motivated by the experimental setup where the reservoirs are often metallic contacts or 2D free-electron gas formed in doped material, both described by the Fermi liquid theory [20]. Reservoirs are typically thermalized to a state with well-defined temperature and chemical potential.

The reservoir Hamiltonian can always be diagonalized and expressed in

¹Throughout this thesis we use the term *non-interacting* for models described by a Hamiltonian which is at most quadratic in creation/annihilation operators. Any term which is outside this category is regarded as an *interacting* or a *many-body*.

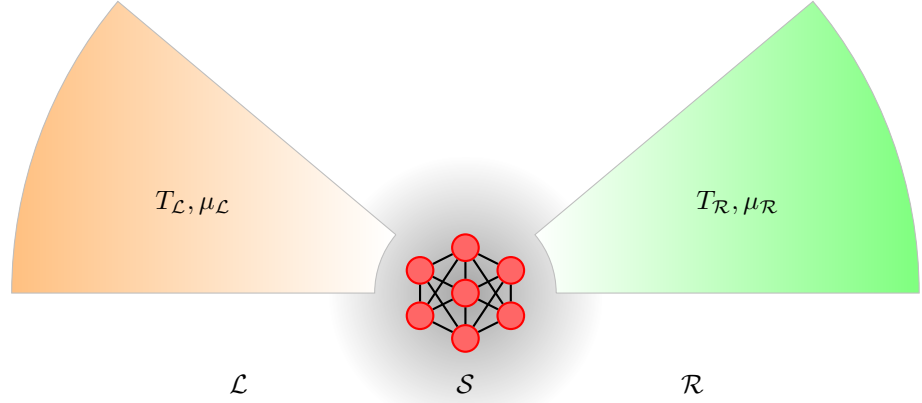


Figure 1.1. Typical model for quantum transport. A small system $\mathcal{S}$ is coupled to macroscopic reservoirs $\mathcal{L}$ and $\mathcal{R}$. The $\mathcal{L}(\mathcal{R})$ reservoir are infinite thermal systems of a temperature $T^{\mathcal{L}(\mathcal{R})}$ and chemical potential $\mu^{\mathcal{L}(\mathcal{R})}$. The imbalance in $\mathcal{L}\mathcal{S}\mathcal{R}$ induces currents between the reservoirs which are controlled by $\mathcal{S}$ at the junction.

terms of energies

$$H_{\mathcal{L}(\mathcal{R})} = \sum_{k \in \mathcal{L}(\mathcal{R})} \omega_k c_k^\dagger c_k, \quad (1.2)$$

where $c_k^\dagger (c_k)$ is a fermionic creation (annihilation) operator for eigenstate of frequency ω_k ².

The interaction between $\mathcal{S}$ and $\mathcal{L}\mathcal{R}$ is a hopping described by the interaction Hamiltonian

$$H_{\mathcal{S}} = \sum_{k \in \mathcal{L}\mathcal{R}} \sum_{j \in \mathcal{S}} v_{kj} c_k^\dagger a_j + v_{kj}^* a_j^\dagger c_k, \quad (1.3)$$

where v_{kj} is a hopping amplitude between a reservoir mode $k \in \mathcal{L}\mathcal{R}$ and an mode $j \in \mathcal{S}$. The operators $a_j^\dagger (a_j)$ in Eq. (1.3) are creation (annihilation) operator for $j \in \mathcal{S}$.

The amplitudes v_{kj} depend on the geometry of the reservoir and its coupling to $\mathcal{S}$. It is often more convenient to characterize this coupling using a *spectral function*³. A spectral function for a reservoir α linearly coupled to a single mode in $\mathcal{S}$ is

$$J^\alpha(\omega) = 2\pi \sum_{k \in \alpha} |v_k|^2 \delta(\omega - \omega_k), \quad (1.4)$$

where $v_k = v_{kj}$ is a coupling to the designated site, and $\delta(x)$ is the Dirac delta function. If the reservoir couples to more than one mode in $\mathcal{S}$ the

²Notice that the Hamiltonian is in frequency, not energy units. This choice is motivated by convenience and doesn't influence physics. We apply this systematically throughout this thesis. One can always go back to energy units by multiplying by a factor of $\hbar$.

³It is often referred to as a *spectral density*. Terminology depends on the community.

spectral function is generalized to a matrix [21], [22]

$$\Gamma_{i,j}^\alpha(\omega) = 2\pi \sum_{k \in \alpha} v_{ik} v_{jk}^* \delta(\omega - \omega_k), \quad (1.5)$$

where $i, j \in \mathcal{S}$. Notice that diagonal elements correspond to the formula in Eq. (1.4). For an infinite fermionic reservoir, the spectral function becomes a continuous function having non-zero values for energies within a bandwidth $\mathcal{W}$ and zero outside.

The interaction described by Eq. (1.4) and Eq. (1.5) is fundamental for transport properties. It can be obtained straightforwardly from a microscopic model after we diagonalize the reservoirs. For models where the first principle approach can't be done, the spectral function can be obtained from experimental data [23], [24].

The quantum system is prepared in some initial state which is generally not an equilibrium for $\mathcal{L}\mathcal{S}\mathcal{R}$. Then it evolves with the Hamiltonian in Eq. (1.1) resulting in currents between system constituents. The transport of particles through the junction in Fig. 1.1 can be characterized by the current from $\mathcal{L}$ to $\mathcal{S}$ given by a formula

$$I = \frac{ie}{\hbar} \sum_{k \in \mathcal{L}} \sum_{j \in \mathcal{S}} v_{ki} \langle c_k^\dagger a_j \rangle - v_{ki}^* \langle a_j^\dagger c_k \rangle \quad (1.6)$$

where $\langle a_j^\dagger c_k \rangle$ is a two-point correlator which represents a hopping from the reservoir mode $k \in \mathcal{L}$ to the system mode $j \in \mathcal{S}$, and $\langle c_k^\dagger a_j \rangle$ describes a situation in reversed direction.

For late times, a finite $\mathcal{L}\mathcal{S}\mathcal{R}$ tends to a global equilibrium⁴ which stops all transport. Formally this is achieved in the limit of an infinite time but the time to equilibrate depends on the system size and the imbalance in the initial state. In $\mathcal{L}\mathcal{S}\mathcal{R}$ with infinite reservoirs, the equilibration is effectively never established and the system reaches *non-equilibrium steady state* (NESS)⁵ instead. The imbalance can be quantified by a temperature and chemical potential difference calculated between the source and the drain⁶.

1.2 Time evolution

The quantum system can be in a *pure state* when it shares no information with the environment. The pure state is fully characterized by a *wavevector*

⁴In the classical world, the equilibration is well understood. However, in a quantum system, the equilibration is generally less obvious [25], [26].

⁵In this work, we focus on cases where a unique steady state exists, however, generally the existence and uniqueness of NESS is non-trivial.

⁶Another source of imbalance can be associated with external forces acting on $\mathcal{L}\mathcal{S}\mathcal{R}$. In Ref. [5], we it is induced by a periodic driving of $\mathcal{S}$ even when there is no imbalance between $\mathcal{L}$ and $\mathcal{R}$.

$|\Psi\rangle$. The evolution of a wavevector is described by the standard *time-dependent Schrödinger equation* which gives differential relation

$$\iota \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle, \quad (1.7)$$

where $H(t)$ is a general time-dependent Hamiltonian ⁷.

Integrating the equation over time we obtain the state evolved from time t' to t

$$|\Psi(t)\rangle = U(t, t') |\Psi(t')\rangle, \quad (1.8)$$

where the propagator in time is given by the unitary

$$U(t, t') = \mathcal{T} \exp \left(-\iota \int_{t'}^t ds H(s) \right), \quad (1.9)$$

where $\mathcal{T}$ indicates time ordering. For time-independent Hamiltonian, the propagator simplifies to $U(t, t') = e^{-\iota(t-t')H}$.

In general, a quantum system is rarely in a pure state. For most cases the system develops correlations to the environment and becomes a *mixed state* which is described by a density matrix

$$\rho(t) = \sum_{i,j} \rho_{i,j} |\Psi_i(t)\rangle \langle \Psi_j(t)| \quad (1.10)$$

where $|\Psi_i(t)\rangle$ are vectors spanning the local Hilbert space. The density matrix for a pure state is $\rho(t) = |\Psi(t)\rangle \langle \Psi(t)|$. A valid density matrix is:

- positive semidefinite: $\forall_{|x\rangle \in \mathcal{H}} \langle x | \rho | x \rangle \geq 0$, where $|x\rangle$ is a vector from the Hilbert space $\mathcal{H}$ (it is equivalent to having non-negative eigenvalues),
- Hermitian: $\rho^\dagger = \rho$,
- normalized: $\text{tr } \rho = 1$.

Time evolution of a closed system under the Hamiltonian is governed by the *Liouville-Von Neumann equation* ⁸

$$\frac{d}{dt} \rho(t) = -\iota [H(t), \rho(t)] \quad (1.11)$$

⁷Notice that in Eq. (1.7) we omitted $\hbar$ factor. This is because throughout the text we consistently write all Hamiltonians in terms of frequencies instead of energies. The Schrödinger equation for the Hamiltonian in units of energy is $\iota \hbar \frac{d}{dt} |\Psi(t)\rangle = H(t) |\Psi(t)\rangle$.

⁸Due to similar form one might easily mistake the Liouville-Von Neumann equation, Eq. (1.11), with the Heisenberg equation. However, the Heisenberg equation uses the Heisenberg picture where states are time-independent and operators are time-evolved. This is different from the Liouville-Von Neumann equation which is in the Schrödinger picture.

where $[A, B] = AB - BA$ is a commutator. Integrating the Eq. (1.11) formally leads to time evolved density matrix

$$\rho(t) = \rho(t') - i \int_{t'}^t ds [H(s), \rho(s)] \quad (1.12)$$

The density matrix is propagated from time t' to t by the unitary evolution

$$\rho(t) = U(t, t') \rho(t') U^\dagger(t, t'), \quad (1.13)$$

where the unitary is given by the expression in Eq. (1.9).

If the system evolves together with the environment, the subsystem's evolution is not necessarily generated by a unitary operator and it is called an *open quantum system*. In general, the system and the environment can still follow a global unitary evolution, however, now the evolution of a subsystem $\mathcal{S}$ is governed by a *dynamical map*

$$\rho_{\mathcal{S}}(t) = \Phi(t, t')[\rho(t')]. \quad (1.14)$$

The dynamical map can be obtained starting from a global unitary evolution and then tracing out the environment. For the $\mathcal{S}$ interacting with the environment $\mathcal{E}$ that is

$$\Phi(t, t')[\rho(t')] = \text{tr}_{\mathcal{E}} (U(t, t') \rho(t') U^\dagger(t, t')), \quad (1.15)$$

where $\text{tr}_{\mathcal{E}}$ is a partial trace over $\mathcal{E}$ and the state evolves under the Hamiltonian

$$H = H_{\mathcal{S}} + H_{\mathcal{E}} + H_{\mathcal{J}}, \quad (1.16)$$

where $H_{\mathcal{S}}$ describes the system $\mathcal{S}$, $H_{\mathcal{E}}$ describes the environment $\mathcal{E}$, and $H_{\mathcal{J}}$ gives the interaction between $\mathcal{S}$ and $\mathcal{E}$. If $\mathcal{S}$ and $\mathcal{E}$ evolve separately then the dynamical map reduces to Eq. (1.13) but becomes non-unitary for all other cases.

Although Eq. (1.15) gives the exact dynamics, its explicit form can be very complicated. This is because it directly depends on the global state including the evolution inside the macroscopic environment. In Sec. 1.3 we simplify the dynamical map by applying the Born and Markov approximations.

1.3 Born and Markov approximation

It turns out that for some cases of modes, the environment damps the perturbation induced by the coupling to $\mathcal{S}$ much faster than any relevant timescale for $\mathcal{S}$. In these cases, the reservoir appears unperturbed at the relevant timescale allowing us to ignore the internal evolution inside it.

Depending on the damping rate we can classify environments as *Markovian* and *non-Markovian*. A Markovian environment is always in equilibrium with itself which physically corresponds to immediate damping of all possible perturbations. If everything is processed at a very fast rate, the environment is effectively “memoryless” and thus Markovian. In contrast, the non-Markovian environment has a finite correlation time and requires considering the evolution explicitly. As a result, the non-Markovian cases are generally much harder to study both analytically and numerically.

In this section, we illustrate the meaning of reservoirs’ timescales by deriving the *Born-Markov master equation*. The approximation is an illustrative example that allows us to understand the meaning of the reservoir’s timescales. In the process, we also discuss what are non-Markovian and Markovian aspects of time evolution and how it affects the master equation.

We start by introducing the *interaction picture*. Operator $\hat{O}$ in an interaction picture with respect to the Hamiltonian H_0 is

$$\hat{O}(t) = e^{+itH_0} \hat{O} e^{-itH_0} \quad (1.17)$$

where we use time dependence to indicate the interaction picture of otherwise time-independent $\hat{O}$. In the interaction picture, we absorb the coherent evolution under the Hamiltonian H_0 into the operator. This is in contrast to the Schrödinger picture which keeps absorbing the evolution to a state of a system, not the operator. In practice, the interaction picture allows rotating-out of any trivial evolution and focusing only on the relevant part.

In quantum transport, we focus on the interaction between reservoirs and $\mathcal{S}$. We use the interaction picture to rotate out any trivial evolution happening locally on $\mathcal{L}$, $\mathcal{S}$, and $\mathcal{R}$, i.e., $H_0 = H_{\mathcal{L}} + H_{\mathcal{R}} + H_{\mathcal{S}}$. For this derivation let us forget about $H_{\mathcal{S}}$. The von Neumann equation in the interaction picture is

$$\frac{d}{dt} \rho^I(t) = -i [V(t), \rho^I(t)] \quad (1.18)$$

where $\rho^I(t)$ indicates a density matrix in the interaction picture, and $V(t)$ is the interaction Hamiltonian which is also in the interaction picture and now is time-dependent.

Formally integrating the Eq. (1.18) yields

$$\rho^I(t) = \rho^I(0) - i \int_0^t d\tau [V(\tau), \rho^I(\tau)]. \quad (1.19)$$

Inserting Eq. (1.19) back to Eq. (1.18) we obtain integro-differential equation approximating time evolution up to a second order in interaction strength

$$\frac{d}{dt} \rho^I(t) = -i [V(t), \rho^I(0)] - \int_0^t d\tau [V(t), [V(\tau), \rho^I(\tau)]]. \quad (1.20)$$

After taking a trace over the environment $\mathcal{E}$ and choosing the initial state such that $\text{tr}_{\mathcal{E}}[V(t), \rho^I(0)] = 0$ we write the evolution for the $\mathcal{S}$ as

$$\frac{d}{dt}\rho_{\mathcal{S}}^I(t) = - \int_0^t d\tau \text{tr}_{\mathcal{E}} [V(t), [V(\tau), \rho^I(\tau)]] . \quad (1.21)$$

For weak coupling $V(t)$ it is enough to reproduce the evolution correctly. This is true for weak coupling and time up to time on the order of $1/\|V(t)\|$. Notice that in Eq. (1.21) the evolution in $\mathcal{S}$ depends explicitly on the dynamics of the whole system up to time t and, in principle, can be very non-Markovian.

In *Born approximation* we assume fast relaxation of the system under perturbation induced by coupling to $\mathcal{S}$. The Born approximation assumes that at all times the state of a composite system factorizes to

$$\rho(t) \approx \rho_{\mathcal{S}}(t) \otimes \rho_{\mathcal{E}} \quad (1.22)$$

where the environment always remains in the equilibrium $\rho_{\mathcal{E}}(t) = \rho_{\mathcal{E}} = \rho_{\mathcal{L}} \otimes \rho_{\mathcal{R}}$.

Physically, this approximation corresponds to a weak system–environment interaction with a sufficiently large environment. A large environment can damp all correlations at a scale much smaller than the evolution of $\mathcal{S}$. From the perspective of $\mathcal{S}$ the environment appears to be always in equilibrium and can be considered time-independent.

However, with the Born approximation the evolution is still hard to solve since the state $\rho_{\mathcal{S}}^I(t)$ always depends on the past snapshots $\rho_{\mathcal{S}}^I(\tau)$. This can be circumvented in *Markov approximation*. Physically, this approximation requires that the reservoir memory timescale, understood as a correlation time or time over which the information is preserved in the environment, is much shorter than any relevant timescale for the $\mathcal{S}$ dynamics. First, we assume that the master equation is local in time for the density matrix by making a substitution $\rho_{\mathcal{S}}^I(\tau) \rightarrow \rho_{\mathcal{S}}^I(t)$. Now, the master equation becomes

$$\frac{d}{dt}\rho_{\mathcal{S}}^I(t) = - \int_0^t d\tau \text{tr}_{\mathcal{E}} [V(t), [V(\tau), \rho^I(t)]] , \quad (1.23)$$

which is also called the *Redfield equation* [27], [28].

The master equation in Eq. (1.23) still depends on time. To achieve a fully Markovian form we require that the integrand decays very quickly. For convenience, we substitute $\tau \rightarrow t - s$ which doesn't change the integration limits giving the master equation

$$\frac{d}{dt}\rho_{\mathcal{S}}^I(t) = - \int_0^t ds \text{tr}_{\mathcal{E}} [V(t), [V(t-s), \rho^I(t)]] . \quad (1.24)$$

Now the time s measures the distance backward in time tracing back the memory effects. If the memory effects are visible back to $s = \tau_B$ then the

τ_B is memory time for the reservoir, i.e., a time necessary for the reservoir correlation function to decay. If the integrand decays sufficiently fast then we have no penalty of taking the integral limits to ∞ in the Eq. (1.24). This gives the final Markovian master equation⁹

$$\frac{d}{dt}\rho_{\mathcal{S}}^I(t) = - \int_0^\infty ds \operatorname{tr}_{\mathcal{E}} [V(t), [V(t-s), \rho^I(t)]] . \quad (1.25)$$

giving the course-grained evolution on timescales $t \gg \tau_B$. The approximation is justified only if the correlation decays quickly. This requires that the timescale over which the $\mathcal{S}$ state appreciably varies is large compared to the timescale τ_B . This cannot be done for all other cases.

The Eq. (1.25) allows us to formulate the evolution of an open system for weak coupling, however, it still needs writing a global state before we take the trace. In Sec. 1.4 we expand the evolution to an explicit form of the master equation for a subsystem $\mathcal{S}$.

1.4 Gorini-Kossakowski-Sudarshan-Lindblad master equation

The celebrated *Gorini-Kossakowski-Sudarshan-Lindblad master equation* (also referred to as *Lindblad master equation* or *Lindbladian* for short) gives the evolution in a general form

$$\frac{d}{dt}\rho = -i[H, \rho] + \sum_i \sum_j \gamma_{ij} \left(L_i \rho L_j^\dagger - \frac{1}{2} \{L_j^\dagger L_i, \rho\} \right), \quad (1.26)$$

where L_j is a Lindblad operator (also called a *jump operator*), and γ_{ij} are damping rates that form a positive semidefinite matrix of coefficients, and $\{A, B\} = AB + BA$ is an anticommutator. In general, for a system of N sites, there are at most $N^2 - 1$ Lindblad operators. The matrix γ_{ij} can be diagonalized and the evolution can be rewritten in a diagonal form for dissipation

$$\frac{d}{dt}\rho = -i[H, \rho] + \sum_j \gamma_j \left(L_j \rho L_j^\dagger - \frac{1}{2} \{L_j^\dagger L_j, \rho\} \right), \quad (1.27)$$

where now γ_j and L_j are linear combinations of those appearing in Eq. (1.26), and γ_j are non-negative coefficients.

We will derive the Lindblad form for the Born approximation assuming that the reservoirs are in thermal equilibrium

$$\rho_{\mathcal{LR}} = \prod_{k \in \mathcal{LR}} Z_k^{-1} e^{-\beta(\omega_k - \mu)n_k}, \quad (1.28)$$

⁹Notice that the same can be formulated for an open system. When the evolution of large system has additional dissipation $D[\cdot]$ the Born-Markov for reduced system is $\frac{d}{dt}\rho_{\mathcal{S}}^I(t) = - \int_0^\infty ds \operatorname{tr}_{\mathcal{E}} [V(t), e^{D(s)} \circ [V(t-s), \rho^I(t)]]$.

where $Z_k = \text{tr} (e^{-\beta(\omega_k - \mu)n_k})$ is partition function, $n_k = c_k^\dagger c_k$ is particle number operator, and $\beta = \hbar/k_B T$ is an inverse temperature¹⁰. The Boltzmann constant is k_B , the absolute temperature is T , and the chemical potential is μ .

The thermal state of the reservoirs is a Kronecker product of states occupied according to *Fermi-Dirac distribution*

$$f(\omega_k) = \frac{1}{e^{(\omega_k - \mu)\beta} + 1}. \quad (1.29)$$

The interaction between $\mathcal{S}$ and reservoirs $\mathcal{LR}$ is governed by the hopping Hamiltonian Eq. (1.3). We go to the interaction picture with respect to $\mathcal{LR}$ evolution and rewrite the fermionic operators as

$$c_k(t) = e^{-i\omega_k t} c_k \quad (1.30)$$

and

$$c_k^\dagger(t) = e^{+i\omega_k t} c_k^\dagger. \quad (1.31)$$

Plugging it to the interaction Hamiltonian we obtain

$$V(t) = \sum_{k \in \mathcal{LR}} \sum_{j \in \mathcal{S}} v_{kj} e^{i\omega_k t} c_k^\dagger a_j + v_{kj}^* e^{-i\omega_k t} a_j^\dagger c_k. \quad (1.32)$$

Now, we take the Eq. (1.32) and insert it into Redfield master equation in Eq. (1.23). Next, we expand the sum and trace over thermal reservoirs. For thermal reservoirs, the only non-zero quadratic correlation is $\langle c_k^\dagger c_k \rangle$. After the simplification we arrive with the master equation

$$\begin{aligned} \frac{d}{dt} \rho_{\mathcal{S}}^I(t) = & \sum_{k \in \mathcal{LR}} \sum_{j, j' \in \mathcal{S}} \int_0^t ds \Gamma_{j, j'}(\omega_k) [1 - f(\omega_k)] e^{i\omega_k s} \left(\rho_{\mathcal{S}}^I(t) a_{j'}^\dagger a_j - a_j \rho_{\mathcal{S}}^I(t) a_{j'}^\dagger \right) + h.c. \\ & + \sum_{k \in \mathcal{LR}} \sum_{j, j' \in \mathcal{S}} \int_0^t ds \Gamma_{j, j'}(\omega_k) f(\omega_k) e^{i\omega_k s} \left(a_j a_{j'}^\dagger \rho_{\mathcal{S}}^I(t) - a_{j'}^\dagger \rho_{\mathcal{S}}^I(t) a_j \right) + h.c. \end{aligned} \quad (1.33)$$

For a continuous reservoir, the sum is taken to an integral. The time-correlation of the interaction depends on the *memory kernels*

$$\mathcal{K}_{j, j'}^{+, \alpha}(s) = \int_{-\mathcal{W}/2}^{\mathcal{W}/2} d\omega \Gamma_{j, j'}^\alpha(\omega) f^\alpha(\omega) e^{i\omega s}, \quad (1.34)$$

and

$$\mathcal{K}_{j, j'}^{-, \alpha}(s) = \int_{-\mathcal{W}/2}^{\mathcal{W}/2} d\omega \Gamma_{j, j'}^\alpha(\omega) [1 - f^\alpha(\omega)] e^{i\omega s}, \quad (1.35)$$

¹⁰Note that for consistency we absorbed the factor $\hbar$ into the definition of inverse temperature. Typically, the inverse temperature is $\beta = 1/k_B T$.

that enter the master equation

$$\begin{aligned} \frac{d}{dt}\rho_{\mathcal{S}}^I(t) = & \sum_{\alpha \in \{\mathcal{L}, \mathcal{R}\}} \sum_{j, j' \in \mathcal{S}} \int_0^\infty ds \left(\mathcal{K}_{j, j'}^{-, \alpha}(s) \left(\rho_{\mathcal{S}}^I(t) a_{j'}^\dagger a_j - a_j \rho_{\mathcal{S}}^I(t) a_{j'}^\dagger \right) + h.c. \right. \\ & \left. + \mathcal{K}_{j, j'}^{+, \alpha}(s) \left(a_j a_{j'}^\dagger \rho_{\mathcal{S}}^I(t) - a_{j'}^\dagger \rho_{\mathcal{S}}^I(t) a_j \right) + h.c. \right). \end{aligned} \quad (1.36)$$

If the memory kernels decay instantaneously then there is no memory effect of the interaction. In this case, the Eq. (1.36) reduces to time-independent dissipation as in Eq. (1.26). Instantaneous decay is similar to the delta function which is defined as $2\pi\delta(s) = \int_{-\infty}^{\infty} d\omega e^{i\omega s}$. That suggests a trivial example for Markovian evolution which is obtained when both $\Gamma(\omega)$ and $f(\omega)$ are constant and supported on the infinite bandwidth $\mathcal{W}$. Physically, Fermi–Dirac distribution is constant only when the reservoir is completely full, completely empty, or at infinite temperature.

In general, the memory kernels decay at some finite rates. Then, the upper limit for integration shouldn't be extended and the master equation remains time-dependent. Sometimes, due to the existing memory effect coming from the interaction, we call this evolution non-Markovian. Notice, that the evolution is non-Markovian for any finite bandwidth, finite temperature, finite chemical potential, and 'colored' spectral function (where some energies are coupled stronger than others).

The profound memory effects in quantum transport in fermionic systems generally forbid us to use the Born–Markov approximation. In Sec. 2 we will review Green's function methods which enable us to study transport properties exactly for more general cases. The method can be applied to any quantum transport model but may not be efficacious for interacting models. The discussion in this and the next chapter motivate the approximation based on the *extended reservoir approach* which is introduced in Chpt. 3.

2. Green's functions for quantum transport

Quantum transport through scattering region $\mathcal{S}$ depends on transmission probability. The dynamics of the model can be conveniently formulated in terms of the *Green's functions*. Green's functions are spatiotemporal correlation functions that provide an alternative formulation of the evolution replacing the state wavefunction or density matrix. In this chapter, we review some basic properties of Green's functions for condensed matter theory and discuss their application for quantum transport.

2.1 Green's functions

The time evolution of a quantum state introduced in Sec. 1.2 can be alternatively described in terms of *Green's functions* (GFs). They are defined as a propagator

$$|\Psi(t)\rangle = \mathbf{G}(t, t') |\Psi(t')\rangle, \quad (2.1)$$

where $\mathbf{G}(t, t')$ is the Green's function which depends on initial and final time and generates the evolution of a quantum state $|\Psi(t)\rangle$.

Schrödinger equation for the Green's function reads

$$\left(\iota \frac{d}{dt} - H \right) \mathbf{G}(t, t') = \delta(t - t'), \quad (2.2)$$

and it is equivalent to the Eq. (1.7).

The Green's functions carry information about the propagation of the excitation under the evolution with the Hamiltonian H . In condensed matter theory, they are defined as two-point correlators. For fermionic systems¹ we define the *lesser* Green's function

$$\mathbf{G}_{mn}^<(t, t') = \iota \langle c_n^\dagger(t') c_m(t) \rangle, \quad (2.3)$$

¹For Green's function for bosonic systems we replace an anticommutator with a commutator.

the *greater* Green's function

$$\mathbf{G}_{mn}^>(t, t') = -\iota \langle c_n(t) c_m^\dagger(t') \rangle, \quad (2.4)$$

the *retarded* Green's function

$$\mathbf{G}_{mn}^r(t, t') = -\iota \Theta(t - t') \langle \{ c_n^\dagger(t'), c_m(t) \} \rangle \quad (2.5)$$

and the *advanced* Green's function

$$\mathbf{G}_{mn}^a(t, t') = \iota \Theta(t' - t) \langle \{ c_n^\dagger(t'), c_m(t) \} \rangle, \quad (2.6)$$

where $\Theta(x)$ is Heaviside step function². The retarded and advanced Green's function are related by $[\mathbf{G}_{nm}^a(t, t')]^* = \mathbf{G}_{mn}^r(t', t)$, so having determined one of them, we can immediately write the other one.

Physically, Green's functions correspond to a fermionic excitation at some time and position, which is later detected by fermionic operator action at another time and position. For example, the retarded Green's function is non-zero for $t > t'$ and physically can be interpreted as a probability of observing a particle on a site m and at time t after it was injected into the system at time t' and at position n . Therefore, it describes the propagation of the system excitation. Notice that the lesser Green's function for $t = t'$ is proportional to single-particle correlation matrix at time t , precisely $\mathcal{C}(t) = -\iota \mathbf{G}^<(t, t)$.

So far, we reviewed Green's functions in a time domain. In some cases, it is more convenient to work with their spectral representation. As we will see later in this text, the Fourier transform of Eq. (2.4) is related to the momentum-dependent spectral function Eq. (1.5) describing the coupling to reservoirs. The spectral representation can be obtained for an equilibrium and a non-equilibrium steady state. Both states don't change in time and therefore depend only on the time-difference $t - t'$. To obtain a spectral representation we switch to the frequency domain using Fourier transform

$$\mathbf{G}(\omega) = \int_{-\infty}^{\infty} dt \mathbf{G}(t) e^{-\iota \omega t}. \quad (2.8)$$

For non-interacting systems, the Fourier transform of the retarded Green's function Eq. (2.5) takes a particularly simple form. It can be written in

²The Heaviside step function $\Theta(x)$ is defined by

$$\Theta(x) = \begin{cases} 0, & x > 0, \\ 1, & x < 0. \end{cases} \quad (2.7)$$

The function has discontinuity at $x = 0$ where it typically is taken as $\Theta(0) = 1/2$. The derivative of $\Theta(x)$ is the Dirac delta function $\delta(x)$.

single-particle formulation³ as the matrix

$$\mathbf{G}^r(\omega) = \frac{1}{\omega \mathbb{1} - \bar{\mathbf{H}}}, \quad (2.10)$$

where $\bar{\mathbf{H}}_{ij}$ is single-particle Hamiltonian $H = \sum_{ij} \bar{\mathbf{H}}_{ij} c_i^\dagger c_j$, and $\mathbb{1}$ is an identity matrix of the same dimension as $\bar{\mathbf{H}}$.

The Eq. (2.10) can be derived starting from Schrödinger equation for a single-particle Hamiltonian H such that

$$i\partial_t \mathbf{G}_{ij}^r(t) - \sum_k H_{ik} \mathbf{G}_{kj}^r(t) = \delta(t) \delta_{ij}. \quad (2.11)$$

Applying the Fourier transform we write it in spectral representation

$$\sum_k (\omega \delta_{ik} - H_{ik}) \mathbf{G}_{kj}^r(\omega) = \delta_{ij}, \quad (2.12)$$

which is exactly the relation in Eq. (2.10).

The dynamical aspect of Green's function can be used to calculate the transport properties through $\mathcal{LSR}$ junction as in Sec. 1.1. In the sections below we discuss non-equilibrium Green's function for $\mathcal{LSR}$ focusing on steady-state properties.

2.2 Non-equilibrium Green's functions

The *non-equilibrium Green's function* (NEGF) formalism is a theoretical framework for modeling electron quantum transport out-of-equilibrium. Electron transport in $\mathcal{LSR}$ system, described in Sec. 1.1, is a coherent scattering process where the particles from $\mathcal{LR}$ scatter on the $\mathcal{S}$ region generating currents through the junction. In NEGF formalism, we aim to compute the transmission function, which describes the rate at which electrons of energy ω are transmitted across the scattering region $\mathcal{S}$. From the transmission function, we calculate the electric current defined in Eq. (1.6).

In a steady-state, it is convenient to use Green's functions in spectral representation. Now, Green's function for $\mathcal{S}$ includes the influence of the coupling to the $\mathcal{LR}$ reservoirs. The NEGF is obtained from GF of isolated $\mathcal{S}$ using the *Dyson equation* [29], [30]

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \Sigma \mathbf{G}, \quad (2.13)$$

³The Eq. (2.10) uses the matrix inverse. Notice, that inverse is not defined for ω equal to eigenvalues of H . There, the inverse is formally taken as the limit

$$\mathbf{G}^r(\omega) = \lim_{\eta \rightarrow 0^+} \frac{1}{\omega \mathbb{1} - H - i\eta \mathbb{1}}. \quad (2.9)$$

where $\mathbf{G}_0$ is bare Green's function for $\mathcal{S}$ and Σ is a self-energy. The reservoir's influence is included via the kernel given by the self-energy Σ .

For non-interacting systems the self-energy is given in single-particle representation as $\Sigma_{ij} = \sum_{k \in \mathcal{LR}} v_{ik} v_{jk} g_k$. For $\Sigma^<, \Sigma^r, \Sigma^a$ we use $g_k = g_k^<, g_k^r, g_k^a$ which are Green's functions for an isolated reservoir mode $k \in \mathcal{LR}$.

The retarded GF for the non-interacting $\mathcal{LSR}$ is

$$\mathbf{G}_{\mathcal{S}}^r = \frac{1}{\omega \mathbb{1} - \bar{\mathbf{H}}_{\mathcal{S}} - \Sigma^r}, \quad (2.14)$$

where the $\bar{\mathbf{H}}_{\mathcal{S}}$ is single particle Hamiltonian for $\mathcal{S}$

$$\bar{\mathbf{H}}_{\mathcal{S}} = \sum_{m,n \in \mathcal{S}} \bar{\mathbf{H}}_{mn} a_m^\dagger a_n, \quad (2.15)$$

and Σ^r is the retarded self-energy

$$\Sigma_{\alpha}^r = \sum_{k \in \alpha} g_k^r |v_k\rangle \langle v_k|, \quad (2.16)$$

where $|v_k\rangle$ means the couplings v_{ki} arranged in a vector such that $\langle i | v_k \rangle = v_{ik}$, and $g_k^r = 1/(\omega - \omega_k + i\eta)$ is retarded Green's function for an isolated reservoir mode $k \in \mathcal{LR}$.

The advanced and retarded Green's functions are related by $\mathbf{G}^r(\omega) = [\mathbf{G}^a(\omega)]^\dagger$ and the retarded self-energy relates to the advanced self-energy by $\Sigma^a = (\Sigma^r)^*$. For non-interacting models they relate to the lesser Green's function by the *Keldysh equation* [31]

$$\mathbf{G}^< = \mathbf{G}^r \Sigma^< \mathbf{G}^a, \quad (2.17)$$

where $\Sigma^<$ is lesser self-energy. The last missing NEGF is the greater GF which can be obtained from the relation $\mathbf{G}^> - \mathbf{G}^< = \mathbf{G}^r - \mathbf{G}^a$ [29].

Having defined all the NEGFs, we can calculate various expectation values including the current through the $\mathcal{LSR}$ junction. In Sec. 2.3 and Sec. 2.4 we give the expressions for NESS current in non-interacting and interacting scattering regions, respectively.

2.3 Landauer formula

The *Landauer formalism* is well-known for describing quantum transport for time-independent, non-interacting models⁴. The *Landauer formula* is proportional to transmission through scattering region $T(\omega) =$

⁴For the revision on Green's function approach for non-interacting time-dependent models see Refs. [32]–[34].

$\text{tr} [\Gamma^{\mathcal{L}} \mathbf{G}^r(\omega) \Gamma^{\mathcal{R}} \mathbf{G}^a(\omega)]$ and the imbalance between $\mathcal{L}$ and $\mathcal{R}$ occupation [22], [35], [36].

The Landauer formula for the particle current reads

$$I = e \int \frac{d\omega}{2\pi} (f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)) \text{tr} [\Gamma^{\mathcal{L}} \mathbf{G}^r(\omega) \Gamma^{\mathcal{R}} \mathbf{G}^a(\omega)], \quad (2.18)$$

where e is the electron charge, $\mathbf{G}^{r(a)}$ is the retarded (advanced) NEGF of the $\mathcal{S}$, and $\Gamma^{\mathcal{L}(\mathcal{R})}$ is the spectral function in Eq. (1.5).

The spectral function Γ^a , which describes the interaction to the reservoirs, is related to the retarded self-energy by

$$\Gamma^a = \imath(\Sigma_{\alpha}^r - \Sigma_{\alpha}^a) = -2\text{Im} \Sigma_{\alpha}^r, \quad (2.19)$$

where the Σ_{α}^r (Σ_{α}^a) is retarded (advanced) self-energy for the reservoir α .

The Landauer formula takes particularly simple form for $\mathcal{S}$ proportionally coupled to $\mathcal{L}$ and $\mathcal{R}$ reservoirs, i.e., $\Gamma^{\mathcal{L}} \sim \Gamma^{\mathcal{R}}$, and is

$$I = \imath e \int \frac{d\omega}{2\pi} (f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)) \text{tr} [\Gamma \{\mathbf{G}^r(\omega) - \mathbf{G}^a(\omega)\}], \quad (2.20)$$

where the first term is symmetrized spectral function $\Gamma = \frac{\Gamma^{\mathcal{L}} \Gamma^{\mathcal{R}}}{\Gamma^{\mathcal{L}} + \Gamma^{\mathcal{R}}}$ and we use that $\mathbf{G}^r(\omega) - \mathbf{G}^a(\omega) = 2\text{Im} \mathbf{G}^r(\omega)$.

Since $\mathbf{G}^a = (\mathbf{G}^r)^*$, the Landauer formula in Eq. (2.18) requires only retarded NEGF, which for non-interacting systems has a very simple form in Eq. (2.14). The Landauer formula gives an exact steady-state current for arbitrary non-interacting scattering region $\mathcal{S}$. In contrast to the Born-Markov approximation, Sec. 1.3, it is exact for any reservoir- $\mathcal{S}$ coupling strength and general non-Markovian reservoirs. In Sec. 2.4 we describe the generalization of the Landauer formula for interacting scattering region provided by the *Meir-Wingreen formula*.

2.4 Meir-Wingreen formula

The *Meir-Wingreen formalism* gives the exact transport through an interacting scattering region $\mathcal{S}$ coupled to non-interacting reservoirs. The formula takes a similar approach to Landauer's, expressing transport in terms of NEGFs.

The *Meir-Wingreen formula* reads [22], [37]

$$I = \frac{\imath e}{2} \int \frac{d\omega}{2\pi} \text{tr} \left[\{ \Gamma^{\mathcal{L}} - \Gamma^{\mathcal{R}} \} G^< + \{ \tilde{\Gamma}^{\mathcal{L}} - \tilde{\Gamma}^{\mathcal{R}} \} \{ \mathbf{G}^r - \mathbf{G}^a \} \right], \quad (2.21)$$

where $\tilde{\Gamma}^{\mathcal{R}}$ is weighted spectral function. For non-interacting system $\tilde{\Gamma}^{\mathcal{R}} = \imath(\tilde{\Sigma}_{\alpha}^r - \tilde{\Sigma}_{\alpha}^a)$ is weighted spectral function which takes weighted self

energies $\tilde{\Sigma}_\alpha^r = \sum_{k \in \alpha} f^\alpha(\omega) g_k^r |v_k\rangle \langle v_k|$. When $\mathcal{L}\mathcal{S}\mathcal{R}$ system is fully non-interacting then the Dyson equation implies $-\imath \mathbf{G}^< = \mathbf{G}^r \tilde{\Gamma}^{\mathcal{L}} \mathbf{G}^a + \mathbf{G}^r \tilde{\Gamma}^{\mathcal{R}} \mathbf{G}^a$ and $\mathbf{G}^r - \mathbf{G}^a = -\imath \mathbf{G}^r (\Gamma^{\mathcal{L}} + \Gamma^{\mathcal{R}}) \mathbf{G}^a$ [38], and the Meir-Wingreen formula reduces to the Landauer formula Eq. (2.18).

It is already apparent that Eq. (2.21) is much harder to evaluate than its non-interacting counterpart in Eq. (2.18). This is because it takes a retarded, advanced, and lesser NEGFs. These don't have simple forms, similar to fully non-interacting systems, because the single-particle picture is not applicable for a many-body system (e.g., we can't use the Eq. (2.14)).

Green's function for a general interacting system can be obtained from the definition in Sec. 2.1. The approach is mainly based on the diagonalization of the Hamiltonian or the time evolution. Both approaches are challenging both analytically and numerically. The latter can be understood when we consider the size of full Hilbert space which scales exponentially with system size⁵. Additionally, the exact Green's function requires obtaining an infinite-time evolution. The truncation of the time evolution introduces features for low frequencies which are often the most relevant for transport properties. Due to the numerical intensity of the problem we require approximate methods.

In Chpt. 3 we will introduce the *extended reservoir approach* where the reservoirs are treated approximately. The approximation allows us to solve for a steady state for any interacting scattering region $\mathcal{S}$, arbitrary spectral function, and non-Markovian dynamics. The next chapter starts a discussion about the approach which is the main thread of this thesis. The summary of the research related to that topic is included in Chpts. 4 and 5. This is followed by the discussion about the numerical implementation with many-body techniques in Chpt. 6.

⁵The Hilbert space is a Kronecker product of local Hilbert spaces so the total dimension grows exponentially with system size. For fermionic systems, the local dimension is $d = 2$, which means that N -mode system requires matrices of dimension 2^N .

3. Extended reservoir approach for steady state

In Chpts. 1 and 2, we gave an overview of quantum transport and standard approaches to simulate it. The Born and Markov approximation introduced in Chpt. 1 provides an efficient method for weak coupling and short timescales for the environment. More general problems can be studied with Green's function approach discussed in Chpt. 2. The Landauer and Meir-Wingreen formulas give a prescription for general non-Markovian transport through the non-interacting and interacting junctions respectively. Green's function approach can be used efficiently for fully non-interacting systems but remain challenging when many-body interactions are present. The above-mentioned motivates a necessity to develop efficient approximate methods capable of describing quantum transport for the general non-Markovian and many-body models.

The evolution up to a finite time can be simulated quantum transport using finite environments. The approach gives a correct description when the size of the environment includes all sites contributing to the current. The finite reservoirs are sufficient because the particles from further distances travel too slowly to arrive at the junction. The size of required environments can be estimated from the quantum speed limit [39]. If the evolution is long enough, we can extract quasi-steady state from the intermediate time [40]. However, the size of the reservoirs necessary to capture the dynamics correctly grows systematically with time and soon the simulation becomes impractical.

Here, we introduce the *extended reservoir approach* (ERA) which is state of the art method to study steady-state quantum transport. The ERA originates in the relaxation time approximation [41]–[47] that later evolved into a framework that describes reservoirs in terms of broadened energy modes [48]–[51]. In ERA we take advantage of the fact that all microscopic models of the reservoirs leading to the same spectral properties give the same steady-state. This fact allows us to approximate the reservoir by a finite-size system in open-system treatment. Finite representation systematically accumulates essential features of the true infinite reservoir when increasing the number of reservoir modes [3], [52]–[54] ultimately

converging to the thermodynamic limit. Therefore, we can control the error of the approximation by allowing for a larger numerical cost.

In this chapter, we define and characterize ERA. We discuss the validity and features of the approximation. In Sec. 3.1 we define the approach, and in Sec. 4.1.1 and Sec. 3.3 we describe the spectral properties of ERA. Finally, in Sec. 3.4 we outline standard regimes of ERA and discuss where it describes the physical scenario. The discussion concentrates on the main model with two reservoirs and a finite quantum system $\mathcal{S}$ introduced in Sec. 1.1.

Although the ERA is dedicated to studying interacting quantum systems we illustrate its properties based on non-interacting models and later we generalize it for many-body. Using fully non-interacting models we can develop a good intuition about the extended reservoirs (which are non-interacting anyways) without error introduced by many-body machinery (see Chpt. 6). The non-interacting models can be studied efficiently using Green's function (see Chpt. 2) and correlation matrix approach (see App. B).

3.1 Extended reservoir approach

The *extended reservoir approach* (ERA) builds up on the fact that we can have a good approximation of a non-equilibration steady state when the reservoirs' spectral properties are captured correctly.

To define ERA we choose a finite collection of modes, i.e., a discretization, which is a representation of the true reservoir. In principle, ERA allows for an arbitrary distribution of modes, however, depending on that we have different quality of the approximation for a fixed size as discussed in Sec. 3.3 and Sec. 3.4. The couplings for the discretization are determined based on a microscopic model [40] or using coarse-graining of the spectral function [3].

To study NESS we define the problem as an open system. The finite $\mathcal{LR}$ representation is coupled to external reservoirs acting implicitly and restoring the equilibrium Fermi-Dirac distribution maintaining the temperature and chemical potential of the true reservoir. Additionally, the dissipation broadens discrete modes such that, together, they reproduce the spectral function in the continuum.

The evolution is governed by the Lindblad master equation (for an overview on Lindblad see Sec. 1.4)

$$\frac{d}{dt}\rho = -\imath[H, \rho] + \gamma\mathcal{D}[\rho]. \quad (3.1)$$

where H is the $\mathcal{LSR}$ Hamiltonian in Eq. (1.1), and $\mathcal{D}[\cdot]$ is the dissipation acting on the $\mathcal{LR}$ reservoirs.

In the next sections we focus on the dissipative contribution

$$\begin{aligned} \mathcal{D}[\rho] = & \sum_{k \in \mathcal{LR}} f^{\alpha_k}(\omega_k) \left(c_k^\dagger \rho c_k - \frac{1}{2} \{ c_k c_k^\dagger, \rho \} \right) \\ & + \sum_{k \in \mathcal{LR}} (1 - f^{\alpha_k}(\omega_k)) \left(c_k \rho c_k^\dagger - \frac{1}{2} \{ c_k^\dagger c_k, \rho \} \right), \end{aligned} \quad (3.2)$$

which, without the coupling to $\mathcal{S}$, relaxes each reservoir occupation to thermal equilibrium set by the temperature T_α and chemical potential μ_α of the reservoir α . The dissipator in Eq. (3.2) becomes physical for weak coupling γ or at least broadening γ which is smaller than thermal such that $\hbar\gamma < k_B T$ [55].

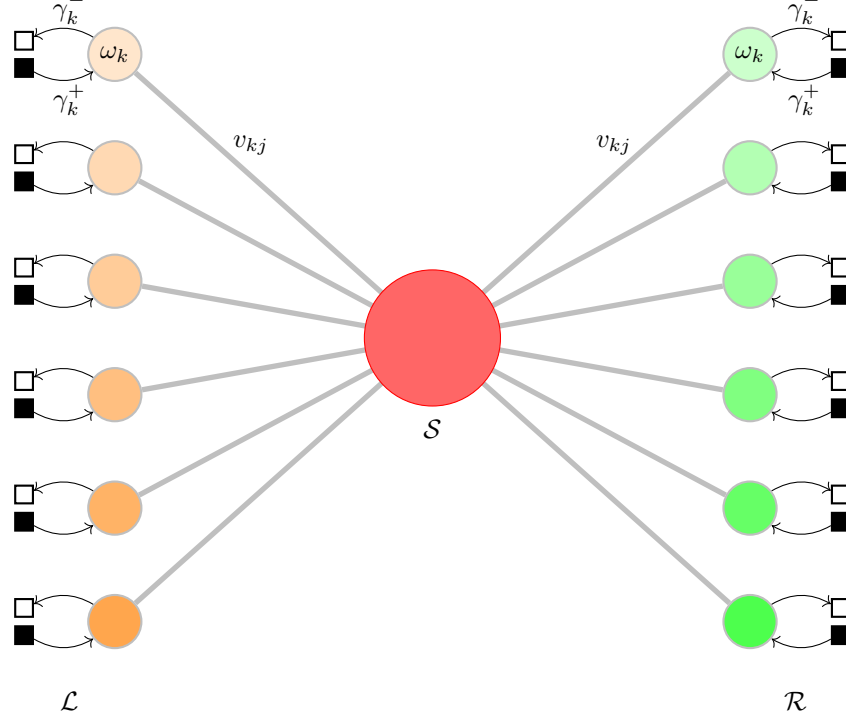


Figure 3.1. Schematic model of an extended reservoir approach. The reservoirs are approximated by finite $\mathcal{LR}$ systems (orange and green circles) represented explicitly in the $\mathcal{LSR}$ Hamiltonian. Discrete $\mathcal{LR}$ modes are coupled to $\mathcal{S}$ with the hopping amplitude v_{kj} (gray lines) such that the spectral function is approximately recovered. The reservoir modes are coupled to implicit reservoirs (black and white squares) restoring thermal distribution in the reservoirs. The implicit reservoirs act on ERA modes by a dissipation (black lines) with the injection rate $\gamma_k^+ = \gamma f^{\alpha_k}(\omega_k)$ and depletion rate $\gamma_k^- = \gamma(1 - f^{\alpha_k}(\omega_k))$. The approach can be understood as two-parameter family of open-system approaches parameterized by the discretization and the relaxation rates.

In Eq. (3.2) we assume that the relaxation happens on a homogeneous relaxation rate γ . This assumption can be relaxed to have inhomogeneous relaxation rates but it makes little difference to the general outcome [3]. Related techniques aim to minimize the number of reservoir modes by

introducing *intermode* transitions during relaxation. More complex models can be leveraged to achieve a given level of approximation [56]–[59] but they are usually more computationally intensive.

The Lindblad master equation in Eq. (3.1) represents an open system where each reservoir mode is damped continuously in time by a Markovian dissipator. The microscopic origin of continuous relaxation can be understood as a coupling of each mode ω_k to the full and empty reservoir of infinite bandwidth and flat spectral function $J^-(\omega) = \gamma_k^-/2\pi$ and $J^+(\omega) = \gamma_k^+/2\pi$ respectively [55]. A schematic model of an ERA is presented in Fig. 3.1.

An alternative formulation of open-system approaches is discussed in Chpt. 5. Note that Eq. (3.2) is Markovian for $\mathcal{L}\mathcal{S}\mathcal{R}$ since the reservoirs $\mathcal{L}\mathcal{R}$ are coupled to Markovian environments. However, the dynamics for $\mathcal{S}$ alone is non-Markovian due to non-Markovian nature of the evolution of finite $\mathcal{L}\mathcal{R}$ representation undergoing a coherent evolution together with the $\mathcal{S}$. The master equation simulates the internal dynamics of the reservoirs, where the relaxation rate γ should be proportional to the timescale of the reservoir. A more detailed description of the meaning of γ is included in Sec. 3.4 and Chpt. 4.

The ERA as defined in Eq. (3.1) has two free parameters. One of them is a discretization, and the other is a relaxation rate γ . In the next sections, we will continue to discuss ERA. In particular, we will develop an understanding of discretization schemes and relaxation rates in the context of recovering accurate transport properties.

3.2 Relation to spectral function

The first aspect we should consider when choosing discretization is the ability to reproduce the spectral function of a true reservoir. The spectral function of a finite representation undergoing an evolution in Eq. (3.1) is equivalent to a sum of contributions from each reservoir mode. The contribution from a mode ω_k dissipated at rate γ , is proportional to the imaginary part of its retarded Green's function

$$g_k(\omega) = \frac{1}{\omega - \omega_k + i\frac{\gamma}{2}}. \quad (3.3)$$

Therefore, the spectral function for ERA is a sum of Lorentzian peaks

$$J_\alpha(\omega) = -2 \sum_{k \in \alpha} |v_k|^2 \frac{\gamma/2}{(\omega - \omega_k)^2 + \left(\frac{\gamma}{2}\right)^2}, \quad (3.4)$$

where ω_k energies and v_k couplings belongs to the reservoir mode $k \in \alpha$. Each Lorentzian peak has an amplitude $2/\gamma$ and full width at half maximum γ . The broadening of a mode can be interpreted as a finite timescale.

In that sense, the Lorentzian peak corresponds to a finite memory time of reservoir mode. In ERA we optimize the parameters to fit the spectral function in Eq. (3.4) to the continuum.

The ERA by construction converges to a continuum in the limit of $N_{\mathcal{W}} \rightarrow \infty$ and then $\gamma \rightarrow 0$ [21], resulting in the memory time going to infinity and capturing the full character of a true reservoir. The formal limit provides the guarantee of convergence for both non-interacting and many-body systems [21], [22], [55], [60], [61], as well as bounds on parameters to ensure the validity of Markovian relaxation in Eq. (3.1) [21], [55]. Yet, the goal of ERA is to introduce a platform that allows obtaining accurate and physically meaningful results at finite $\mathcal{L}\mathcal{S}\mathcal{R}$ given limited computational resources. For optimal performance, we would like to adjust the discretization and γ such that transport properties are captured correctly.

3.3 Discretization

While ERA doesn't specify the discretization method it should be chosen such that it converges to spectral properties of a continuum reservoir. This flexibility has spawned a variety of methods, including discretizations that

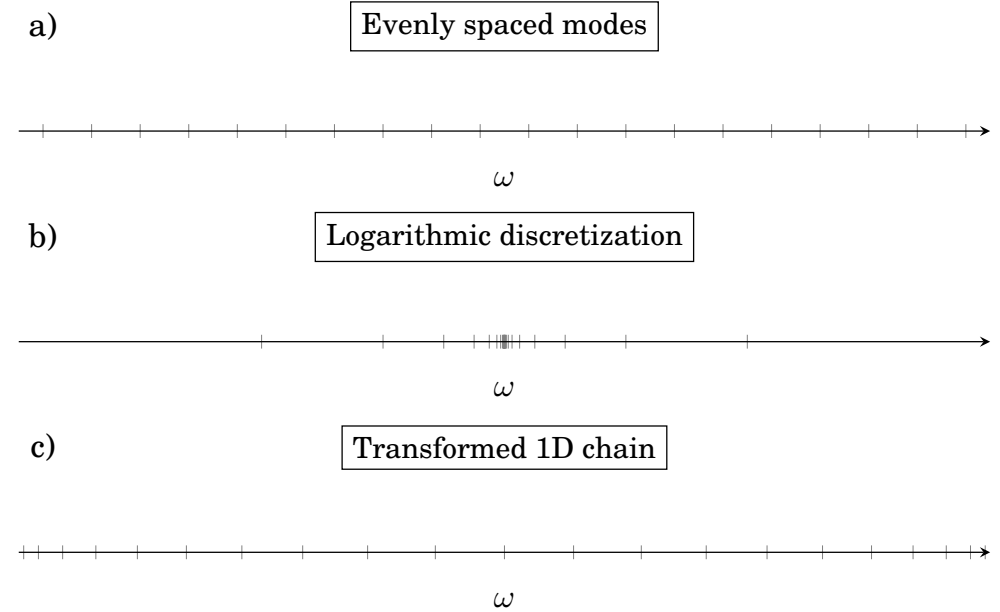


Figure 3.2. Common discretization schemes. ERA allows the choice of any discretization that leads to a continuum in the limit of an infinite number of modes. The discretization should be adjusted to the studied case. Among the most popular choices, there is a discretization (a) with modes evenly distributed in the bandwidth, (b) with modes distributed logarithmically around the Fermi level, and (c) a discretization obtained directly from the microscopic model (here for uniform one-dimensional chain with nearest-neighbor hopping).

place modes evenly across the bandwidth, assign modes from canonical transforms of finite tight-binding lattices, distribute them evenly inside the bias window and logarithmically outside [62]–[65], or use an influence-based approach to give a linear spacing across the bias window and an inverse spacing outside [3], [52]. Some of them are schematically represented in Fig. 3.2. The discretization should be optimized to allow for the best convergence at finite N_W modes per reservoir.

The Lorentzian form of the spectral function in Eq. (3.4) suggests putting more modes around the relevant frequencies according to the spectral function in the continuum (for more see Sec. 4.1.1). The discretization can be exactly equivalent to the thermodynamic limit if the spectral function in the continuum is a collection of a finite number of Lorentzians. Otherwise, it is not ideal and requires increasing N_W to improve the approximation. In particular, for many cases, the spectral function has a broad background, e.g., semicircle or flat spectral function, which makes it hard to fit with a small number of modes.

Another deciding factor is related to the regime contributing to the current (for more see Sec. 4.1.2). For elastic scattering, the relevant measure is $f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)$ giving a region of imbalance between $\mathcal{L}$ and $\mathcal{R}$ ¹. For low-temperature the relevant $f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)$ is equivalent to the bias window. In Ref. [3] we show that the convergence of the current depends mainly on the discretization within the bias window. The discretization outside the bias window weakly affects the current and can be sparser if needed. Simultaneously, the computational cost for the implementation with many-body machinery (described in Chpt. 6) is dominated by the contribution from the bias window. All of that permits using any convenient discretization outside the bias window. In Ref. [3] we show that by choosing an appropriate basis the cost of representing the states outside of the bias window is a minor contribution and the cost and convergence depend on the discretization inside the bias window. This contradicts the approach in Ref. [64] where they use separate treatment for states within and outside the relevant regime. The states outside are processed with special care by applying the renormalization-group method.

In fact, there are other relevant mechanisms relevant for a discretization choice and, in general, it depends on $\mathcal{S}$ (see Chpt. 4 for more).

In Sec. 3.4 we will characterize transport properties as a function of γ for an arbitrary discretization scheme. This starts the discussion about the domain of confidence for fixed discretization which allows us to recover physical current at fixed N_W .

¹This is straightforward when you compare it to the Landauer formula Eq. (2.18) for non-interacting systems.

3.4 Kramers' turnover

Regardless of a discretization scheme the steady-state current of ERA exhibits the same character in the function of the relaxation rate γ . In this section, we treat ERA as a one-parameter family of open-system approaches with γ as a free parameter. This allows us to investigate how NESS depends on γ dismissing a concern whether it is physical or not. The discussion gives an explanation of why and when the ERA can approximate physical transport through the junction.

The plot of the current versus γ is also regarded as the *Kramer's turnover* [66] in similarity to the Kramers' turnover in the rate of condensed-phase reactions [67]. Instead of a turnover versus the solution friction, the electronic transport depends on the external relaxation [68]–[70], which is a dependence also found in thermal transport [71]–[75].

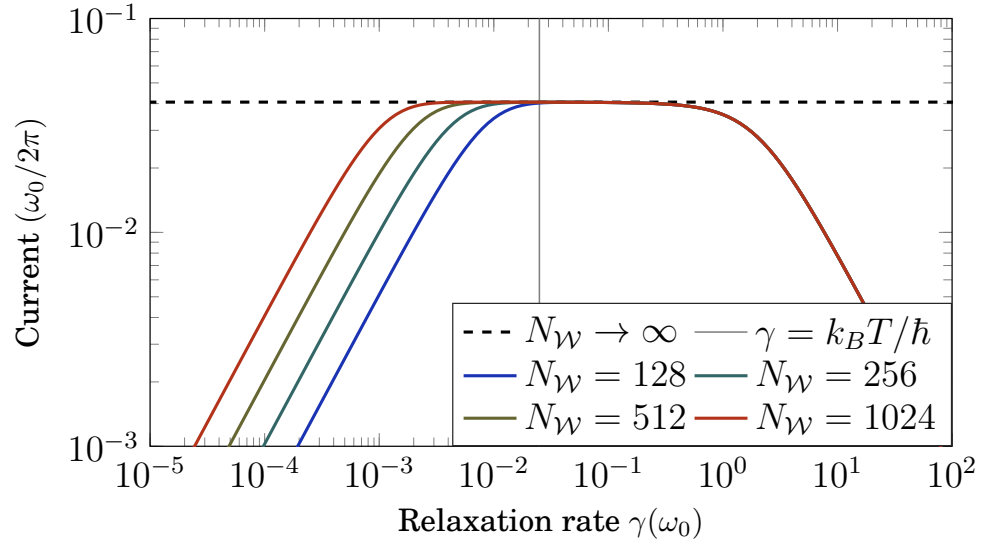


Figure 3.3. Kramers' turnover. Steady-state current for $\mathcal{L}\mathcal{S}\mathcal{R}$ system as a function of relaxation rate γ . There are three distinct regimes of behavior: the underdamped regime for weak γ with current $I \propto \gamma$, the overdamped regime for large γ when $I \propto 1/\gamma$, and the physical regime for intermediate γ when current is independent on γ in the leading order. The physical plateau extends to smaller γ as the number of modes per reservoir N_W increases. The ERA approximation becomes exact for the plateau extending down to $\gamma \leq k_B T$ (marked with a gray vertical line). The data shows $\mathcal{L}\mathcal{S}\mathcal{R}$ with the single site impurity of the Hamiltonian $H_{\mathcal{S}} = \omega_0 n_1$ which is proportionally coupled to 1D chains with strength $v_0 = \omega_0/2$. Between reservoirs, we apply a bias $\mu = \omega_0/2$, and both have inverse temperature $\beta = 40\hbar/k_B\omega_0$.

Generally, the Kramers' turnover for $\mathcal{L}\mathcal{S}\mathcal{R}$ has three distinct regimes [21], [66].

Small- γ or underdamped regime.

In this regime, the particle current is limited by the relaxation strength

since the supply of particles by the implicit environments is too small compared to the natural current through $\mathcal{S}$. The current is proportional to the total replenishing rate $(\gamma N_{\mathcal{W}})^{-1}$. Therefore the current grows linearly in γ and shifts to smaller γ as $N_{\mathcal{W}}$ increases.

Intermediate- γ or physical regime.

In this regime, the supply rate is sufficiently strong to support the intrinsic, physical current without disturbing it significantly. In this regime, a plateau in the current develops and increases its width with growing $N_{\mathcal{W}}$ as the relaxation-limited regime is pushed down in γ . It is in this regime that we capture physically relevant NESS current and also full density matrix [3]. Extending this plateau, we approach the exact solution which is finally achieved by taking a limit of $N_{\mathcal{W}} \rightarrow \infty$ and then $\gamma \rightarrow 0$.

Large- γ or overdamped regime.

In this regime, the effects of relaxation dominate NESS. Too strong relaxation damps the coherence between the extended reservoir and $\mathcal{S}$ and that suppresses the current $\propto 1/\gamma$ as currents are just coherences. Strong relaxation effectively decouples the extended reservoirs, localizing particles within extended reservoirs. The situation is analogous to the Zeno effect where frequent/strong measurement slows down the dynamics. One can also cast this regime into a series of resistors. The overdamped regime generalizes directly to many-body models. This can be understood by Green's functions in the time domain which are dominated by the exponential decay. The current Eq. (1.6) is proportional to $\text{Im} \mathbf{G}_{mn}^<$ which is now suppressed like $e^{-\gamma t/2}$.

While the overdamped regime is independent of $N_{\mathcal{W}}$, the underdamped regime shifts to smaller γ as $N_{\mathcal{W}}\gamma$ gives a collectively greater replenishing rate. This shifts the lower bound to a plateau regime roughly $\propto N_{\mathcal{W}}^{-1}$ developing a wider physical regime. This property generalizes to any many-body model ensuring the convergence below $\hbar\gamma < k_B T$ which ensures that the broadening is smaller than the thermal broadening natural for the reservoir and evolution Eq. 3.1 is physical. Increasing $N_{\mathcal{W}}$, the plateau current converges to the thermodynamic limit which makes the number of modes the parameter controlling the convergence and cost in ERA.

In reality, the intermediate regime is not entirely independent of γ . Depending on $\mathcal{S}$ there may be additional features [2], [3] that distort the physical current. In Chpt. 4 we review the physical origin of some common features in ERA. Ultimately, the features depend on $\mathcal{S}$ which is also the reason why standard approaches for the optimal γ may lead to unphysical

current even if the number of reservoir modes increases [2], [5]. In Chpt. 4 we develop a strategy to determine the optimal relaxation rate based on the stability of Kramers' turnover under perturbation of extended reservoirs. Since the Kramers' turnover is general for any many-body system, the approach also can be used for any model.

4. Features of Extended Reservoir Approach

The *extended reservoir approach*, introduced in Chpt. 3, is a strategy useful to simulate non-Markovian quantum transport through a general many-body quantum system. To ensure an efficient convergence the extended reservoirs, i.e., discretization and dissipation, should be chosen such that they give a good approximation of the reservoir's spectral properties. Taking the approximation we shall analyze how they influence the results and when they are least invasive.

In this chapter, we review properties relevant to determining the optimal extended reservoir. In Sec. 4.1.1 we analyze it in relation to the spectral function, in Sec. 4.1.2 the reservoir occupation, and in Sec. 4.1.3 the unphysical features of ERA. This chapter is a natural extension of Chpt. 3, where we introduced Kramers' turnover, i.e., a plot for a fixed discretization showing current versus dissipation rate. The physical scenario should be recovered for an intermediate- γ regime where the current is mainly controlled by the transmission through $\mathcal{S}$.

Starting from Ref. [1] we realized that there are additional regimes that hide the physical scenario in the intermediate- γ plateau. In Ref. [2], [3], [5] we studied the physical origin of the features and the convergence when they are present. The projects lead to the conclusion that choosing the discretization solely based on the spectral function is not sufficient, possibly leading to systematic errors. Instead, we found that the optimal choice depends on the impurity $\mathcal{S}$. In Sec. 4.1.4 and 4.1.5, we summarize our findings about transitions leading to unphysical artifacts, and in Sec. 4.2 we outline the effective strategies to avoid them. We solve the problem of determining an optimal relaxation by introducing the stability test which probes the Kramers' turnover for potential resonances. We mark, that the test may not give the best transport properties but ensures stable convergence to the thermodynamic limit with increasing N_W .

4.1 Spectral properties in ERA

While any discretization should converge to the thermodynamic limit with $N_{\mathcal{W}} \rightarrow \infty$ and $\gamma \rightarrow 0$, it is important to ask what is the best estimation at finite $N_{\mathcal{W}}$ which gives the most physical results. The standard approach to determining an optimal relaxation rate is based on the spectral function. Below we discuss other relevant properties one should take into account. We focus on one of the most difficult cases where the spectral function has a wide continuous background, such as a flat or semicircle spectral function, and sharp features, such as a finite bandwidth or bias.

4.1.1 Relation to spectral function

The spectral function for ERA in Eq. (3.4) is equivalent to a sum of Lorentzian peaks. Each peak is proportional to $\text{Im} g_k^r$, where g_k is the retarded Green's function for isolated mode ω_k broadened by a dissipation γ . The full half maximum width of $\text{Im} g_k$ is equal to γ and the maximum is $1/\gamma$.

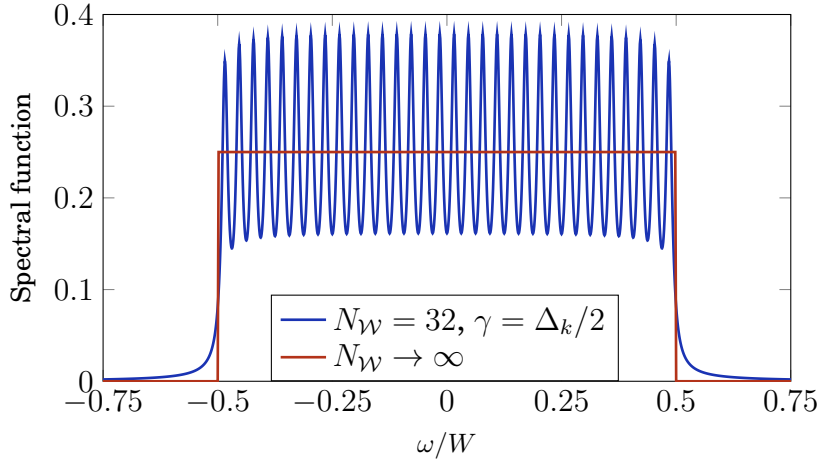


Figure 4.1. Spectral density for ERA with too weak γ . Finite representation fails to reproduce a wide continuous background of the true spectral function. The relaxation rate γ is too small and the discretization is not dense enough. The flat spectral function $J(\omega) = v_0^2/\mathcal{W}$, with bandwidth $\mathcal{W} = 4\omega_0$ and coupling amplitude $v_0 = \omega_0$, is approximated by the ERA with $N_{\mathcal{W}} = 32$ evenly spaced modes dissipated with rate $\gamma = \Delta_k/2$, where $\Delta_k = \mathcal{W}/N_{\mathcal{W}}$ is the spacing between reservoir modes.

For a very small γ , the peak is sharp and centered around ω_k . If $\gamma \ll \Delta_k$, where Δ_k is a gap between neighboring energy modes, then the spectral function appears as a collection of well-separated peaks. The weakly damped mode is perfect to represent fine features in the spectral function but if $\gamma \ll \Delta_k$ it requires a dense discretization to reproduce the wide continuous background as visible in Fig. 4.1. Alternatively, we say that for finite $N_{\mathcal{W}}$ the relaxation rate γ is too weak to capture the continuum.

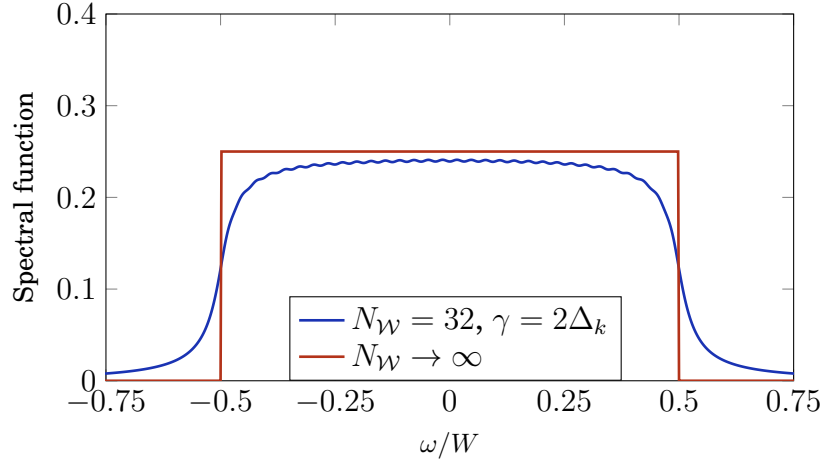


Figure 4.2. Spectral density for ERA with too strong γ . Finite representation fails to reproduce the sharp features, rounds DOS on the edges of the bandwidth, and allows some states outside $\mathcal{W}$. The flat spectral function $J(\omega) = v_0^2/\mathcal{W}$, with bandwidth $\mathcal{W} = 4\omega_0$ and coupling amplitude $v_0 = \omega_0$, is approximated by the ERA with $N_{\mathcal{W}} = 32$ evenly spaced modes dissipated with rate $\gamma = 2\Delta_k$, where $\Delta_k = \mathcal{W}/N_{\mathcal{W}}$ is the spacing between reservoir modes.

As γ increases, peaks become broader spreading further from the center and filling the gap between peaks. As relaxation increases further the Lorentzian becomes smeared all over the energy scale. These are ideal to have nice continuous spectral functions but are not suitable to capture sharp features such as a finite bandwidth. An example of such a situation is plotted in Fig. 4.2 where we can see that ERA fails to reproduce a finite bandwidth by allowing states outside its range which is unphysical.

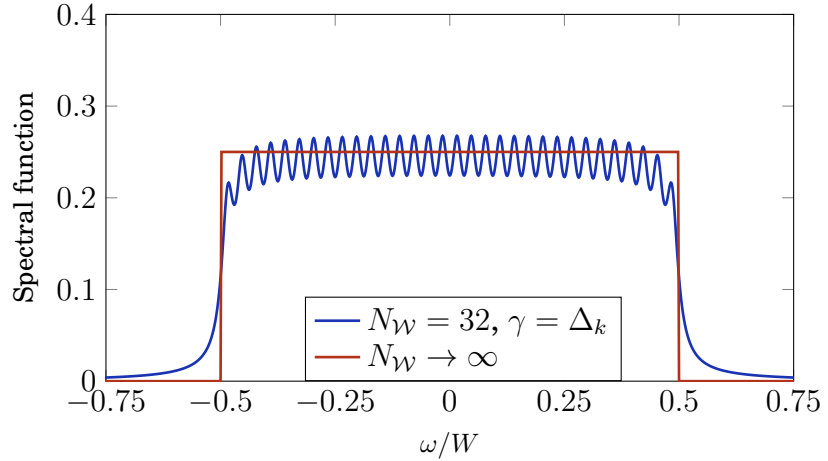


Figure 4.3. Spectral density for ERA with $\gamma = \Delta_k$. Finite representation is not able to reproduce the true reservoir but is a good approximation for finite $N_{\mathcal{W}}$. The flat spectral function $J(\omega) = v_0^2/\mathcal{W}$, with bandwidth $\mathcal{W} = 4\omega_0$ and coupling amplitude $v_0 = \omega_0$, is approximated by the ERA with $N_{\mathcal{W}} = 32$ evenly spaced modes dissipated with rate $\gamma = 2\Delta_k$, where $\Delta_k = \mathcal{W}/N_{\mathcal{W}}$ is the spacing between reservoir modes.

It is a standard approach to choose γ depending on mode separation Δ_k

with γ proportional, and typically equal, to the level spacing [63], [76]–[79]. As visible in Fig. 4.3 that doesn't necessarily ensure a featureless representation of spectral function but it is often used as a rule of thumb to achieve a compromise between features of the too-weak and too-strong relaxation.

The choice of extended reservoirs affects the density of states for $\mathcal{S}$. In Fig. 4.4 we show the illustrative example showing how the relaxation rate influences the density of states for $\mathcal{S}$. If the relaxation is too weak then the DOS is not smooth having peaks shattering the actual density of states. On the other hand, once the relaxation becomes too strong it decouples the $\mathcal{L}\mathcal{R}$, and DOS sharpens more than natural broadening due to the coupling.

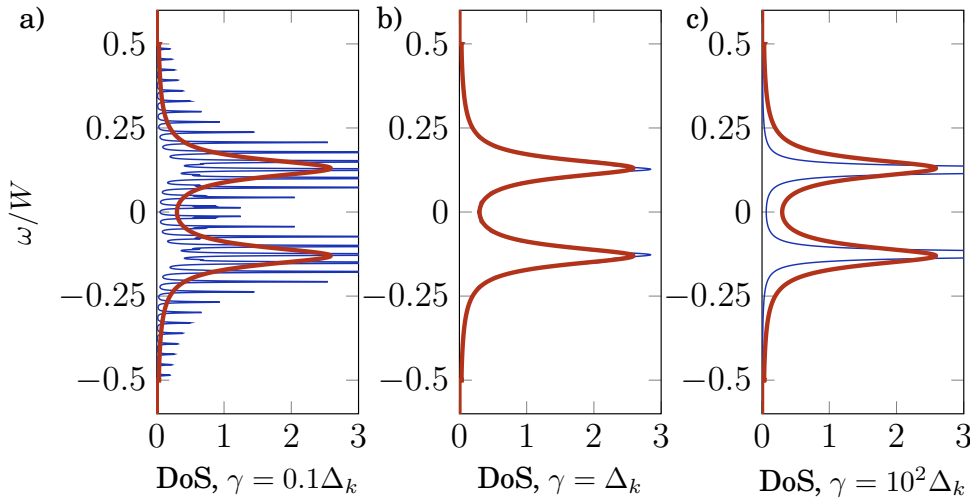


Figure 4.4. Density of states for $\mathcal{S}$ impurity. Density of states $\text{DOS}(\omega) = -\frac{1}{\pi} \text{Im tr} \mathbf{G}^r(\omega)$ carries over features due to finite representation of reservoirs. The blue line shows DOS for (a) weak relaxation, (b) moderate relaxation, and (c) strong relaxation rate with $N_{\mathcal{W}} = 32$ modes per reservoir and flat spectral function (shown in red). The Hamiltonian for the scattering region is $H_{\mathcal{S}} = \frac{\omega_0}{2} a_1^\dagger a_2 + h.c.$.

To determine the relaxation rate one can also compute γ from the self-energies of explicit reservoir modes in contact with the implicit infinite environment [80]. Such reasoning, however, considers the reservoir in isolation from the rest of the setup. As we comment below, due to the presence of $\mathcal{S}$, this may not be sufficient and leads to systematic errors thus always requiring further validation.

4.1.2 Relation to reservoir's occupation

The master equation in Eq. (3.1) assumes the dissipation which occupies each mode according to the Fermi–Dirac distribution at each mode. The mode broadened by the relaxation spreads outside ω_k therefore dissipation also occupies energies across the spectrum. This should make us suspicious

of whether we reproduce the true Fermi–Dirac distribution. Now, the relevant measure is the weighted (occupied) spectral function,

$$\tilde{J}_\alpha(\omega) = -2 \sum_{k \in \alpha} f(\omega_k) |v_k|^2 \frac{\gamma/2}{(\omega - \omega_k)^2 + (\gamma/2)^2}, \quad (4.1)$$

where $f(\omega)$ is Fermi–Dirac distribution at frequency ω . In Fig. 4.5 we plot the occupied spectral function for Fig. 4.1 and 4.2 the features of too–weak and too–strong relaxation rate.

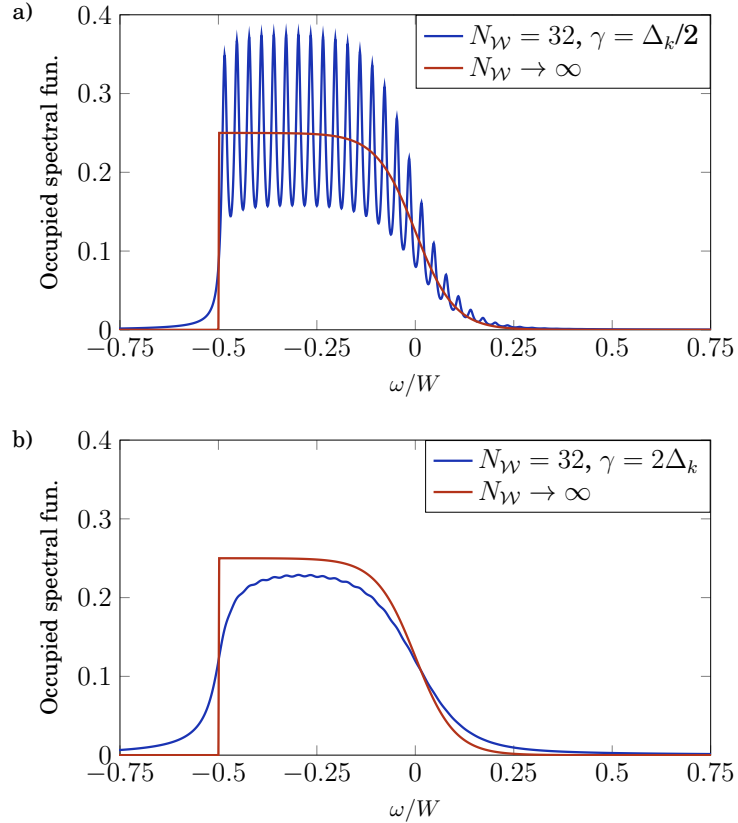


Figure 4.5. Occupied spectral function for ERA. The reservoir of temperature $\beta = 5/\omega_0$, a chemical potential $\mu = 0$, and a flat spectral function is approximated by the ERA with $N_W = 32$ evenly spaced modes. The dissipation rate (a) $\gamma = \Delta_k/2$, and (b) $\gamma = 2\Delta_k$, where $\Delta_k = W/N_W$, influences the occupied spectral function in Eq. (4.1). Similarly as in Fig. 4.1 and Fig. 4.2 the ERA fails to reproduce reservoirs occupation. In panel (a) the γ is too small and the occupation is not a valid Fermi–Dirac distribution, and in (b) the dissipation occupies energies outside the bandwidth and artificially broadens the Fermi–Dirac around the Fermi level. The data obtained for the same model as in Fig. 4.1.

For weak γ we don't reproduce any valid Fermi–Dirac distribution. For large γ the dissipation has a similar effect as temperature, smoothing the distribution around the Fermi level. As stated in another way, the broadening due to relaxation has replaced temperature in determining the effective bias window. In addition, the ERA populates extended tails of the Lorentzian, which may lead to unphysical occupation outside the bandwidth.

The feature of the Markovian dissipator in Eq. (3.2) can be cured by allowing to choose a set of γ_k depending on ω_k such that together they give appropriate occupation. However, with a coupling to $\mathcal{S}$ this problem becomes time-dependent. It can be solved self-consistently, however, this makes the calculation much more convoluted compared to standard Markovian relaxation in Eq. (3.1).

4.1.3 Features on the Kramers' turnover

The disparities of a spectral function and an occupation for finite $N_{\mathcal{W}}$ described above lead to some unphysical features in Kramers' turnover. In this section, we use previously developed intuition to explain the physical mechanisms behind the most common features visible in Fig. 4.6.

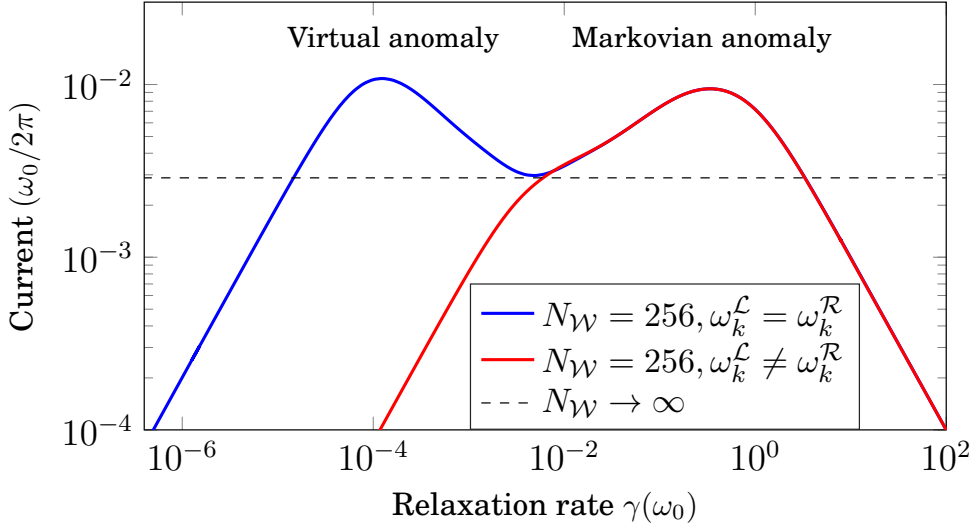


Figure 4.6. Kramers' turnover with the Markovian and virtual anomaly. The *Markovian anomaly* is enhanced current due to the artificial broadening of reservoirs occupation. The dissipation occupies energies outside the Fermi-Dirac distribution creating additional transport channels. The *virtual anomaly* occurs due to virtual transitions between resonant transitions from $\mathcal{L}$ to $\mathcal{R}$. The anomalies are located on both sides of the physical regime covering natural current for $\mathcal{S}$. Growing $N_{\mathcal{W}}$ the plateau expands and the current saturates on the thermodynamic limit solution (dashed line). The standard case (blue line) represents the case when the reservoirs have identical discretizations. The virtual transitions can be suppressed by shifting $\mathcal{L}\mathcal{R}$ out of resonance (red line). The data obtained ERA with $N_{\mathcal{W}} = 256$ evenly spaced modes. The impurity is described by the Hamiltonian $H_{\mathcal{S}} = 5/16\omega_0 a_1^\dagger a_2 + h.c.$, reservoirs of the temperature $T_{\mathcal{L}} = T_{\mathcal{R}} = \omega_0/40$, the bias $\mu = \omega_0/2$, bandwidth $\mathcal{W} = 4\omega_0$, and coupling to reservoirs $v_0 = \omega_0/20$.

The standard setting for $\mathcal{L}\mathcal{S}\mathcal{R}$ is to have $\mathcal{L}$ and $\mathcal{R}$ with identical mode distributions and uniform relaxation rates. There we find that the current can be artificially enhanced leading typically to two anomalies [2]. The anomalies branch the plateau regime with *virtual* anomaly located on low-to-moderate γ and *Markovian* anomaly located on moderate-to-large γ . The former originates from a resonance between modes in $\mathcal{L}$ and $\mathcal{R}$

leading to unphysical current from virtual transitions, and the latter is a result of the improper representation of reservoirs' occupation when modes are broadened too much by Markovian relaxation.

4.1.4 Markovian anomaly

Markovian anomaly is enhanced current due to the unphysical broadening of reservoirs' modes. The broadening leads to misrepresentation of reservoir occupation and puts the occupied (unoccupied) DOS from $\mathcal{L}(\mathcal{R})$ "in resonance" with the system $\mathcal{S}$. Improper occupation opens additional channels contributing to the total current. These increase with γ in moderate-to-large regime typically between the plateau and overdamped regime.

As the relaxation becomes stronger the full system's Green's function Eq. (2.14) is getting sharper and sharper (as in Fig. 4.4), and rapid decoherence effectively decouples the reservoirs from the system $\mathcal{S}$ lowering the overall current. Now the modes are so broad that all $\mathcal{S}$'s states are within its body and the current decays as the Lorentzian amplitude $1/\gamma$ due to further broadening.

Due to its nature, the anomaly is present for any N_W even in the thermodynamic limit. It can be removed by going beyond Markovian relaxation [2] to cure reservoirs occupation as mentioned in Sec. 4.1. Unfortunately, this requires non-Markovian relaxation and this comes at a cost: while easy to solve for non-interacting systems, this does not yield a time-local Lindblad master equation that is amenable to many-body simulations. However, keeping Markovian dissipation the anomaly has a minor contribution for small γ which is more important given that we want $\hbar\gamma \leq k_B T$.

4.1.5 Virtual anomaly and resonances

Virtual anomaly is enhanced current which originates from virtual transitions between resonant modes. It is situated on small-to-moderate relaxation rates typically between underdamped and plateau regimes. Handling the virtual anomaly is essential since it lies in a physical regime of low γ . The anomaly may lead to systematic error even when N_W is large [5]. In the next chapter, we focus on the physics of virtual anomaly to design an effective approach able to determine physical current at finite N_W .

The virtual anomaly originates from virtual transitions between resonant modes. The probability or effective tunneling rate of a particle from a reservoir through the $\mathcal{S}$ is inversely proportional to the energy barrier to the conducting mode in $\mathcal{S}$. For elastic scattering, the particle tunnels between reservoir modes of the same energy. If the relaxation rate is too small the virtual transitions are mitigated by a small supply rate

turning the anomaly into the underdamped regime where the current is proportional to γ . This happens for γ much smaller than the level spacing in the reservoirs and also much smaller than the effective coupling to $\mathcal{S}$ energy levels. On the other hand, as the relaxation rate increases and the relaxation rate becomes stronger than the effective coupling rate, the virtual transitions are suppressed as $1/\gamma$ in a similar way as in the large- γ regime.

The virtual anomaly depends on the coupling to $\mathcal{S}$, the reservoir size, and the density of states of $\mathcal{S}$. As the $N_{\mathcal{W}}$ increases it shifts to smaller γ together with an underdamped regime revealing the plateau of physical current. Note that for $\hbar\gamma \leq k_B T$ Markovian and non-Markovian relaxation are identical [21] so the virtual anomaly can't be cured by switching to non-Markovian [21] description.

A special case of virtual transition happens when the transmission happens through a resonant $\mathcal{S}$ mode. There the resonance with $\mathcal{S}$ happens in addition to the virtual anomaly for $\mathcal{L}$ -to- $\mathcal{R}$ transitions. Resonances with $\mathcal{S}$ are hard to predict since we don't know *a priori* the $\mathcal{S}$ DOS.

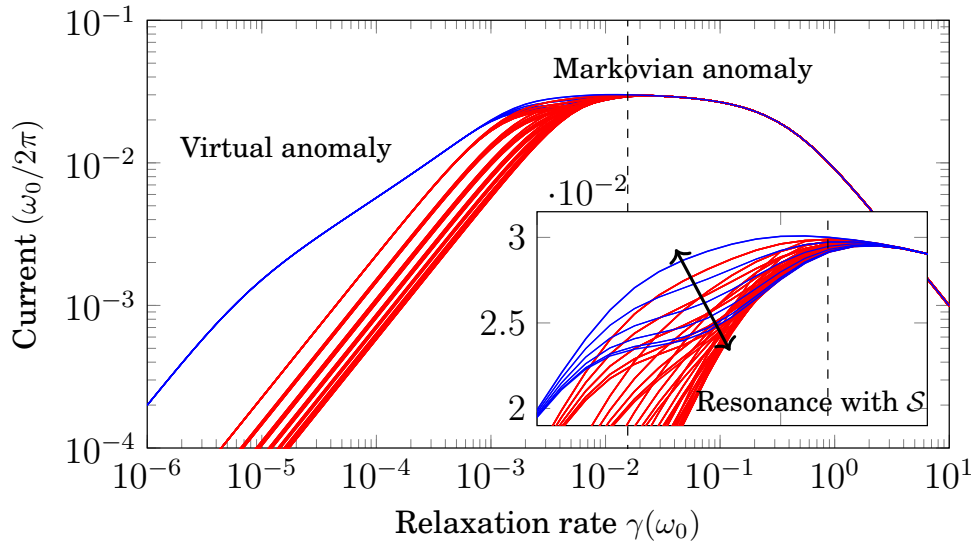


Figure 4.7. Stability test of Kramers' turnover. We test the stability of the current by applying small global shifts to $\mathcal{L}$ and $\mathcal{R}$ modes. If matching $\mathcal{L}\mathcal{R}$ distributions are shifted against $\mathcal{S}$ (blue lines) the current is enhanced by resonance with $\mathcal{S}$ (see the inset). For these cases, we always observe the virtual anomaly in low-to-moderate γ coming from virtual transitions between $\mathcal{L}$ and $\mathcal{R}$. The virtual transitions are mitigated by shifting $\mathcal{L}\mathcal{R}$ against each other (red lines). Different red lines correspond to applying shifts to $\mathcal{L}\mathcal{R}$ for different blue lines. There we have both symmetric and asymmetric shifts of $\mathcal{L}\mathcal{R}$ modes. The bigger the shift the smaller the virtual anomaly and overdamped regime moves to stronger γ . The test shows that standard choice $\gamma = \Delta_k$ (dashed line) is not stable against perturbations giving the variation of the order of 10% of the current. The stability test can be used to determine the optimal γ which is the lowest γ that is affected by perturbations up to a small variation. The data obtained for the model in Fig. 4.6 but with $v_0 = \omega_0/2$ coupling.

Notice, that the virtual anomaly is very prominent for weak coupling

when DOS of $\mathcal{S}$ is sharp. Also there, it quickly decays when modes are slightly off the resonance. This suggests that avoiding anomalies can be done by destroying the resonance between them [2], [5]. In order to do that we apply a perturbation to reservoir modes such that the $\mathcal{LR}$ modes are not matching. This modification is allowed in ERA as it doesn't assume a discretization scheme as long as the spectral function is well approximated.

In Fig. 4.6 we show the result of perturbation relying on asymmetric and symmetric shifts applied to $\mathcal{LR}$. An asymmetric shift moves all modes in one reservoir up and the other one down [2]. Also, the resonance with $\mathcal{S}$ can be also avoided by shifting reservoirs together with respect to $\mathcal{S}$. The most complete set of perturbations is presented in Fig. 4.7 where the current for asymmetric shifts is in red and for symmetric shifts in blue. Both of these modifications should remove any resonances revealing unphysical features on the Kramers' turnover by testing the stability.

4.2 Strategies for optimal relaxation rate

In previous sections, we showed that determining the optimal extended reservoir is a task requiring consideration of various aspects related to reservoir spectral function, reservoir occupation, and the unphysical current due to coupling to $\mathcal{S}$. It is apparent that the task is non-trivial even for choosing the optimal relaxation rate for a fixed discretization.

Instead of using standard approaches, we determine optimal γ based on the Kramers' turnover. Based on a physical understanding of the features in previous sections, we introduce a procedure based on the perturbation of reservoir modes. If the current is not stable against these perturbations we say that the current is unphysical. For examples of the effect of perturbations see Fig. 4.6 and Fig. 4.7 mentioned in the last section.

More generally, to test the stability we can also vary the discretization scheme and number of reservoir modes. In an abstract form, the convergence will be quantified by

$$\partial_{\{\omega_k\}_{\mathcal{LR}}, N_{\mathcal{W}}, \gamma} I(\{\omega_k\}_{\mathcal{LR}}, N_{\mathcal{W}}, \gamma), \quad (4.2)$$

which requires that the current I is largely unaffected by the construction of extended reservoirs, including discretization scheme $\{\omega_k\}_{\mathcal{LR}}$, number of modes per reservoir $N_{\mathcal{W}}$, and the dissipation rate γ .

In the physical regime, this saturates to zero at the plateau in the limit of infinite reservoirs and $\gamma \rightarrow 0$. For the Kramers' turnover, we evaluate the condition in Eq. (4.2) with respect to small perturbation to mode distribution for each point γ . In Ref. [2] and Ref. [5] we define a simple stability test based on perturbations to the $\mathcal{LR}$ mode distribution. Note that, the stability trivially improves with growing γ because for large γ the reservoir's spectral function appears flat and infinite so any perturbation

doesn't affect that situation. However, this is not a regime we are interested in. In order to make the physical estimate we have to find the relaxation rate which is the closest to satisfying $\hbar\gamma < k_B T$. This adds a physical criterion on top of the stability criterion in Eq. (4.2).

In reality, the perturbation always gives some effect on the current. That is why we define the optimal relaxation rate as the smallest γ which is ϵ -stable under the perturbation, where ϵ is a small number. This ensures that we are the closest to the physical condition for Markovian relaxation. In Ref. [5] we show that the transition from stable and unstable γ is sharp which is a result of the Lorentzian form of the mode's density of states. This simplifies the strategy for optimal relaxation rate to finding the lowest γ that is within ϵ stability, preferably at the transition to the highly-unstable regime.

Note that the optimal γ is not necessarily the closest to the thermodynamic limit. Instead, it is the most reliable and free of features of ERA. Alternatively, the stability test can be understood as a measure of instability and can be used to quantify that error.

In Ref. [5] we show that for periodically driven lattice the standard γ leads to systematic error which remains even if the N_W increases. This stress the necessity to perform the stability test to remove these features. Finally, let us mention that there are still many open questions related to that approach. In particular, how to define the best stability test, and how to extract representative current and associated error from the stability test. The first step towards the latter has been done in Ref. [5] where we notice that the median current gives a good estimate of the current (there it was better current than for γ determined from the stability test) even when we take the highly-unstable standard choice of γ . We leave that discussion for future projects.

5. Accumulative reservoir construction

The *extended reservoir approach* we discuss in Chpt. 3 and Chpt. 4 approximate the infinite reservoir by a finite collection of modes dissipated by external environments. There the dissipator in Eq. (3.2) acts continuously in time restoring thermal distribution and maintaining NESS. An alternative formulation of ERA takes the master equation as a cyclic process where coherent evolution and dissipation act independently and interchangeably in time.

The idea for a discrete master equation is similar to having a collection of collisions that accumulate the character of the infinite environment over time. The idea is analogous to the collision model [81]–[83]. There, a collision takes place between sites from a reservoir and from a system. An environment site approaches a system and interacts with it for a finite time. After this time, the site is traced out and the process is repeated. The evolution reduces to Lindblad master equation for infinitesimal interaction time [82]–[84].

This idea can be implemented for ERA [81]–[83] where the collisions are replaced by an iterative refresh of the finite environments [85]. The approach has been introduced in Ref. [85] in the context of the convergence of transport properties but didn't provide sufficient data to compare it to the standard Lindblad approach. One of the biggest benefits of the periodic refresh is to get rid of the Markovian dissipation which truncates the coherence time in extended reservoirs. A longer time for coherent evolution in the periodic refresh approach suggests that it may develop more natural coherences as in an increasing number of modes for Lindblad but it wasn't clear how they compare on the computational cost.

This chapter bases on Ref. [4] where we investigate convergence and computational cost for these approaches. In order to compare them systematically we developed the *accumulative reservoir construction* (ARC) which provides a unified framework interpolating between continuous relaxation and periodic refresh. Here, the evolution is defined as a two-step cycle where in the first step we perform a coherent evolution for a time τ , and after that, the $\mathcal{LR}$ are disconnected from $\mathcal{S}$ and dissipated for a time τ .

Time evolution is schematically depicted in Fig. 5.1.

The evolution can be written as,

$$\rho(n\tau + \tau) = e^{\gamma\tau\mathcal{D}[\cdot]} \circ e^{-i\tau H} \rho(n\tau) e^{i\tau H}. \quad (5.1)$$

In contrast to the periodic refresh, the reservoirs are only partially dissipated maintaining some correlation from the previous step.

In discrete formulation, the steady-state should be understood as a steady state in a periodically driven model when we look at the system only at the stroboscopic time before we apply relaxation.

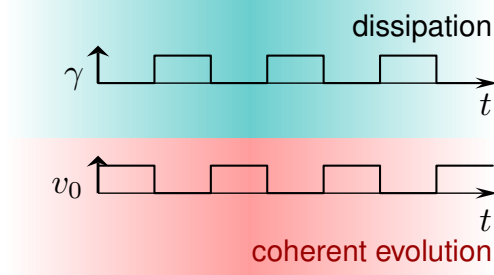


Figure 5.1. Time evolution in accumulative reservoir construction. First, for a time τ the system evolves fully coherently with the $\mathcal{LSR}$ Hamiltonian. After that, the reservoirs are decoupled from $\mathcal{S}$ (having $v_0 = 0$) and dissipated to thermal with a rate γ for a time τ . The process is repeated until the state reaches steady-state on the stroboscopic time.

ARC can be treated as two-parameter family of open-system approaches. In Ref. [4] we show that the parameter space can be separated into distinct regimes demarcated based on the timescales in $\mathcal{LSR}$. Similar to Trotter decomposition, the evolution appears to be continuous if the time for coherent evolution is lower than any relevant timescale. This separates the parameter space into continuous-like and periodic-like regimes. Both of these show under-damped, over-damped, and physical regimes similar to those in Kramers' turnover in Sec. 3.4. We found that the periodic refresh approach always gives better transport properties than continuous relaxation for the same number of discretized modes in the reservoirs. This is, as we predicted, due to more natural coherence developing in time evolution. It is better than continuous relaxation because it always has a correction due to unphysical Markovian relaxation. On the other hand, periodic refresh is more prone to exhibit finite-size effects due to the scattering of particles at the boundaries.

In Ref. [4] we investigate the computational cost for tensor network implementation (for details see Chpt. 6). We concluded that a large collection of modes and a long time for coherent evolution can increase the fidelity of the reservoir representation but come at a substantial computational cost when included in numerical many-body techniques. We found that the benefit of periodic refresh is overshadowed by high computational cost. On the other hand, the standard relaxation rate exhibits a smaller cost for the cost of the slowest convergence.

We found that continuous-like and periodic-like regimes have distinct rates of errors-to-cost scaling. The points exhibiting continuous-like regime have slow convergence but moderate cost, and those in the periodic-like regime give better convergence for a higher cost. Surprisingly, we found that the best-performing ARC strategy lies in the intermediate point of the phase diagram right after exceeding the natural timescales for $\mathcal{S}$. These points are, in principle, the most efficient to numerically study quantum transport. An example error-to-cost scaling is presented in Fig. 5.2.

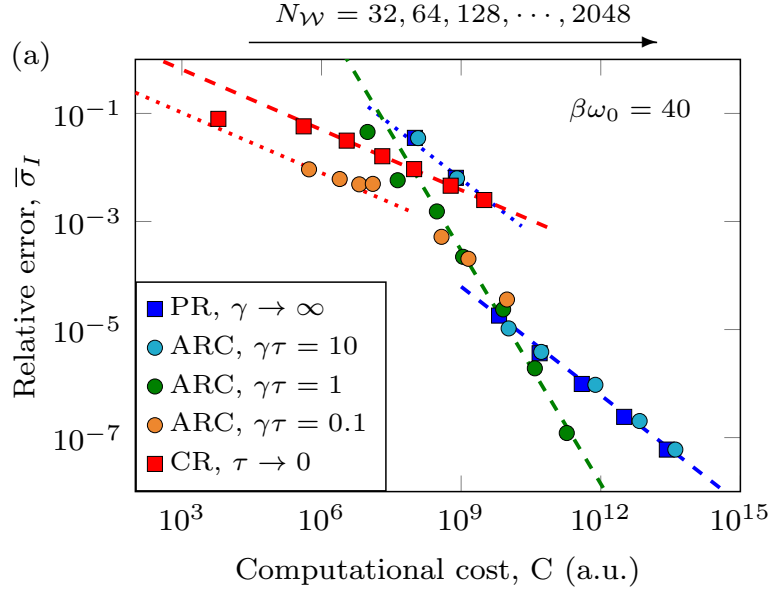


Figure 5.2. Error-cost scaling for ARC. The convergence error gives the relative error of a steady-state current achievable by the ARC with fixed $\gamma\tau$ to the thermodynamic limit. The computational cost quantifies the time of convergence and numerical insensitivity of tensor network implementation (see Chpt. 6). Inside the continuous-like regime, the convergence is slow with increasing N_W but the computational cost is moderate (red line). On the other hand, inside the periodic-like regime, the current is described much better at finite N_W but the computational cost grows substantially (blue line). The best error-to-cost trade-off is achieved for the intermediate case (green line). The figure is taken from Ref. [4]. See there for a more detailed discussion.

The discussion in Ref. [4] sparked an intriguing observation about the connection between natural timescales for ERA and convergence. This is the periodic nature of ARC exposes these natural $\mathcal{LSR}$ features. In particular, the phase diagram for ARC can be fully understood by analyzing the timescales. Most important timescales for the $\mathcal{LSR}$ system can be derived from quantum speed limits e.g., based on the Lieb-Robinson bound. In order to find a good approximation of the transport the ERA should enable reproducing coherences exceeding the $\mathcal{S}$ timescales such that the correlation across the junction can develop. Simultaneously, to avoid the finite-system effects the coherent time shouldn't be longer than the natural timescale for finite $\mathcal{LR}$ environments. Besides, the coherent evolution

it also relates to timescales associated with the dissipation and thermal reservoirs.

The discussion in Ref. [4] provides a comprehensive understanding of conditions needed to converge in ERA. However, there are still many open questions about the applicability of ARC for other models for quantum transport.

6. Tensor Networks for quantum transport

Quantum transport is generally very hard to study both analytically and numerically. The approaches introduced in Chpts. 1, 2, and 3 with the advantages and limitations associated with each one of them illustrate the challenges of studying quantum transport. Among them, the *extended reservoir approach*, introduced in Chpt. 3, is the most general method, capable of describing quantum transport through the many-body scattering region and with very non-Markovian reservoirs.

In ERA we approximate the (infinite) reservoir by a finite system coupled to implicit reservoirs which restore thermal distribution and maintain NESS. The model is described by the master equation Eq. 3.1 (alternatively Eq. 5.1 which takes the same coherent and dissipative terms applied interchangeably). The steady state is obtained in direct simulation using many-body machinery. Although many exist, *tensor networks* leverage the structure of correlations and entanglement to provide a local, numerically controllable many-body description.

This chapter gives an overview of tensor networks and algorithms useful to implement ERA. In particular, based on the experience gained in the preparation of Ref. [1], and additional investigation in the process of formatting other research projects, we describe strategies to implement an open system, optimize tensor network ansatz, and solve for a steady-state. The practical aspects of working with tensor networks were developed while working on the *YASTN* tensor network package [6]¹.

6.1 Tensor Networks

Tensor network (TN) is a construction where a multidimensional dataset is represented as a product of interconnected tensors. The decomposition

¹The YASTN is a Python library for differentiable linear algebra with block-sparse tensors, supporting abelian symmetries. It is an open-source project that is available on *GitHub* platform.

into TN can be understood as a separation of variables where each tensor holds information about selected variables and shared dimensions encode correlation to all others. The connection through shared dimension forms a network that can be contracted to recover the original dataset. For some classes of problems, the TN decomposition can be more efficient than the original formulation. This is true for some classes of quantum systems.

The Hilbert space for a quantum system scales exponentially with system size. The numerical representation for L particles with local dimension d requires matrices of dimension d^L . To put that in numbers, the Hamiltonian of a 10-particle system with local dimensions 2 is a 1024×1024 matrix but system 2 times larger takes matrices $1,048,576 \times 1,048,576$. Obviously, this quickly becomes inefficient forbidding large-scale simulations.

TNs have been proven to be a convenient tool to study low-dimensional quantum systems. They give the description of a quantum state and they provide a scalable and numerically exact tool to target models with many-body interactions [86]–[88]. Among many TN geometries, there are one-dimensional tensor networks [87], [88]. There, the state vector of the quantum system is described as a *matrix product state* (MPS) which is one-dimensional tensor network with open boundaries.

The matrix product state can be constructed starting from a state vector

$$|\Psi\rangle = \sum_{\sigma_1, \dots, \sigma_L} \theta_{\sigma_1, \dots, \sigma_L} |\sigma_1, \dots, \sigma_L\rangle, \quad (6.1)$$

which describes the state of a quantum system with L sites and local dimension d_j . The labels $\sigma_j = \{1, \dots, d\}$ indexes the physical dimension of a site j , $\theta_{\sigma_1, \dots, \sigma_L}$ are numerical coefficients associated with the basis vector $|\sigma_1, \dots, \sigma_L\rangle$ spanning the Hilbert space.

6.1.1 Schmidt decomposition

The separation of variables can be performed using the *Schmidt decomposition*²

$$|\Psi\rangle = \sum_j \lambda_j |\sigma_1\rangle \otimes |\sigma_2, \dots, \sigma_L\rangle, \quad (6.2)$$

where λ_j are called *Schmidt values* and are the amplitudes associated with $|\sigma_1\rangle \otimes |\sigma_2, \dots, \sigma_L\rangle$ product state. Here, there are at most d Schmidt values and the normalization of $|\Psi\rangle$ requires that $\sum_{j=1}^d |\lambda_j|^2 = 1$.

The Schmidt values carry information about the correlations between site 1 and the rest of the system. In the MPS the number of non-zero Schmidt values is equivalent to a *virtual dimension* (also called *bond dimension*). For example, the state $\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$ which can be decomposed

²For a multidimensional dataset separation of variables can be done using the *singular value decomposition*, the *QR-decomposition*, and *principal component analysis*.

to $|0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ has only one non-zero Schmidt value therefore the bond dimension is 1. On the other hand, the Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ has two non-trivial Schmidt values and therefore bond dimension is 2.

Physically, the Schmidt decomposition can be connected to the entanglement shared across bipartition. The entanglement can be quantified by the *von Neumann entropy*. The entropy of a subsystem A in AB composite system is defined as

$$S_A = -\text{tr}_A (\rho_A \log \rho_A), \quad (6.3)$$

where $\rho_A = \text{tr}_B (\rho)$ is a reduced density matrix for a subsystem A after tracing out B and $\log_2$ is a matrix logarithm with base 2 (to have value in bits of entanglement). The Eq. (6.4) is also known as the *entanglement entropy* which is zero for a product state and maximal for a maximally-entangled state.

Having access to Schmidt values we can define the von Neumann entropy as

$$S = -\sum_j |\lambda_k|^2 \log_2 |\lambda_k|^2. \quad (6.4)$$

For the previous examples, we find that for $\frac{1}{\sqrt{2}}(|00\rangle + |01\rangle)$ which is a product state the entanglement between the first and second site is $S_1 = S_2 = 0$, and for the Bell state $\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ it is maximally entangled with $S_1 = S_2 = 1$.

6.1.2 Matrix Product State

To decompose the wavevector in Eq. (6.1) to MPS we perform subsequent Schmidt decomposition at each bipartition forming MPS tensors one site after another. At the end we can finally write the state as a *matrix product state* (MPS)

$$|\Psi\rangle = \sum_{\sigma_1, \dots, \sigma_L} A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_{L-1}} A^{\sigma_L} |\sigma_1\rangle \dots |\sigma_L\rangle, \quad (6.5)$$

where A^{σ_j} is a tensor associated with a local variable σ_j associated with a site j . Notice that $\theta_{\sigma_1, \sigma_2, \dots, \sigma_L}$ is recovered after contracting the product $A^{\sigma_1} A^{\sigma_2} \dots A^{\sigma_L}$ along shared indices. In Eq. (6.5), each tensor has one physical and two virtual indices having total size $D_{j-1} \times d_j \times D_j$ size. The MPS tensor is pictorially depicted in Fig. 6.1.

The MPS in Fig. 6.2 is formed by arranging tensors in Fig. 6.1 into one-dimensional network.

The MPS decomposition can always be performed, but the crux of the methods, though, is that there needs to be limited entanglement so that the simulation requires MPS of small virtual dimensions. In practice, we rarely perform top-to-bottom construction but rather impose an ansatz with fixed bond dimension. This restricts us to a subspace of the total

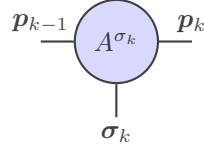


Figure 6.1. Graphical representation of an MPS tensor. Physical index (vertical protruding line) encodes local basis, e.g., $|0\rangle$ and $|1\rangle$ for fermions. Two virtual indices (horizontal lines) correspond to the correlations to the left and right to the designated tensor.

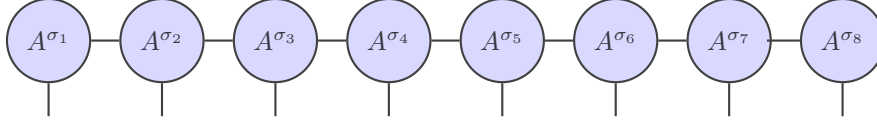


Figure 6.2. Graphical representation of an MPS state. The tensors in Fig. 6.1 are arranged into the one-dimensional network with open boundaries.

Hilbert space which are the moderately-entangled cases. We enlarge the achievable subspace by allowing larger and larger bond dimensions. This makes the bond dimension a single control parameter for the TN representation.

In Sec. 6.2, we introduce a tensor network toolbox to study open systems. This will be useful to finally implement the ERA for a general interacting model.

6.2 Open system tensor networks

The state of an open system is generally described by the mixed-state density matrix. Similar as in Eq. (6.1) we write it as

$$\rho = \sum_{\sigma_1, \dots, \sigma_L} \mathcal{R}_{\sigma_1, \bar{\sigma}_1, \dots, \sigma_L, \bar{\sigma}_L} |\sigma_1, \dots, \sigma_L\rangle \langle \bar{\sigma}_1, \dots, \bar{\sigma}_L|, \quad (6.6)$$

where $R_{\sigma_1, \bar{\sigma}_1, \dots, \sigma_L, \bar{\sigma}_L}$ is $d^L \times d^L$ coefficient matrix.

The density matrix can be decomposed to one-dimensional tensor network which, in similarity to MPS, we call the *matrix product operator* (MPO)³. A single MPO tensor is graphically represented in Fig. 6.3.

The same applies to any operator. The tensors are interconnected via two virtual dimensions as for the MPS in Fig. 6.2 but have two physical dimensions, one for *ket* and one for *bra* dimension of the density matrix.

³In the context of density matrix MPO decomposition is also called *matrix product density operator* (MPDO).

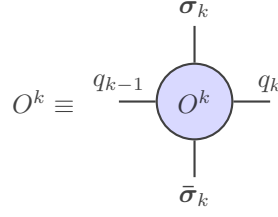


Figure 6.3. Graphical representation of an MPO tensor. Physical indices (vertical protruding lines) encode the local Hilbert space. Two virtual indices (horizontal lines) encode correlation to the left and right to the designated tensor.

6.2.1 Tensor networks for mixed states

The tensor networks promote working with pure states and, therefore, over the years the toolbox for pure states became immense [86]. All of these are not directly applicable to mixed states which require dedicated treatment.

One way to represent a mixed state as a tensor network is by implementing it in *vectorization* [89], [90]. In vectorization, a matrix M is mapped to a vector $|M\rangle\rangle$ on a higher dimensional Hilbert space. The mapping is always defined with the interpretation which is used to recover a matrix from vector elements. Later in Sec. 6.5 we show how the gauge freedom on vectorization can be used to design more efficient simulations.

The vectorization has an inner product defined as *Hilbert-Schmidt inner product*

$$\langle\langle A|B\rangle\rangle = \text{tr}(A^\dagger B), \quad (6.7)$$

where $|A\rangle\rangle$ and $|B\rangle\rangle$ are vectorizations of the operators A and B respectively. The *left-multiplication* of the operator A on ρ is

$$(A \otimes \mathbb{1})|\rho\rangle\rangle = |A\rho\rangle\rangle, \quad (6.8)$$

and the *right-multiplication* is

$$(\mathbb{1} \otimes A^T)|\rho\rangle\rangle = |\rho A\rangle\rangle, \quad (6.9)$$

where we use the notation $\mathcal{O}|\rho\rangle\rangle = |\mathcal{O}\rho\rangle\rangle$ and ^{T} denotes a transposition. Notice that from the above we have

$$|A\rangle\rangle = (\mathbb{1} \otimes A^T)|\mathbb{1}\rangle\rangle = (A^T \otimes \mathbb{1})|\mathbb{1}\rangle\rangle, \quad (6.10)$$

where $|\mathbb{1}\rangle\rangle$ is a vectorization of identity matrix $\mathbb{1}$.

Using vectorization enables using the MPS structure with an already broad range of MPS techniques. This comes with the cost of working with $\langle\langle \rho || \rho \rangle\rangle = \rho^2$ normalization of the MPS. This in turn leads to less natural truncation compared to ρ -norm. In addition, vectorization doesn't necessarily ensure the positivity of a density matrix under truncation, and checking for that is generally a very nontrivial task. However, we note

that the vectorization still gives a correct description as long as we keep the truncation error low.

Besides the vectorization, we can also write the problem as a purification which by construction always gives a valid density matrix [91], [92]. The *purification* of a density matrix [91], [92] is constructed by expanding the Hilbert space to include an auxiliary system (typically a copy of the original problem) such that together they form a pure state. The original mixed state is obtained after taking a trace over the auxiliary degrees of freedom. Although many benefits, purification often suffers from uncontrolled growth of entanglement generated between the original and auxiliary system. For more comments about this in relation to ERA see Sec. 6.6.

Before, we use vectorization to implement the open-system evolution for ERA. The Lindblad superoperator $\mathbb{L}$ is written in the MPO form as discussed in Sec. 6.5. In Sec. 6.3 we analyze the structure of correlations in quantum transport and define the most efficient ansatz for the MPS. Understanding the scattering process in the $\mathcal{L}\mathcal{S}\mathcal{R}$ system allows designing the ansatz that localized the entanglement spread mitigating the computational cost.

6.3 Scattering in quantum transport

Quantum transport is generally hard to simulate using tensor networks due to the fast growth of entanglement generated by scattering on the $\mathcal{S}$ junction. In this section, we discuss the scattering in the $\mathcal{L}\mathcal{S}\mathcal{R}$ model introduced in Sec. 1.1 and explain how the entanglement dominates the cost of TNs. Based on the physical understanding of the process we design the optimal tensor network ansatz which mitigates the computational cost.

We make this description illustrative by focusing on transport in one-dimensional chain with nearest-neighbor hopping. The infinite chain with hopping amplitude ω_0 is interrupted by an impurity $\mathcal{S}$ which separates the chain into two semi-infinite chains. Here, all sites on the left to $\mathcal{S}$ form the reservoir $\mathcal{L}$, and all sites on the right to $\mathcal{S}$ form the reservoir $\mathcal{R}$. The reservoirs are coupled to $\mathcal{S}$ by their terminal sites by hopping of the amplitude v_0 . The model can be directly implemented in the MPS using ansatz pictorially presented in Fig. 6.4.

Although the model is a simple one-dimensional nearest-neighbor chain, it suffers from very non-local correlations when the system is out of equilibrium. The imbalance in the $\mathcal{L}\mathcal{S}\mathcal{R}$ system pushes particles from reservoirs across the system $\mathcal{S}$. Arriving at the junction the particle tunnels through the impurity with some probability p . If the tunneling is not perfect a part

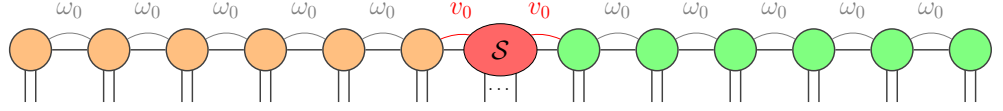


Figure 6.4. Position basis ansatz for MPS. The reservoirs $\mathcal{L}$ (orange) and $\mathcal{R}$ (green) are uniform chains with nearest-neighbor coupling ω_0 . The reservoirs are coupled to the impurity $\mathcal{S}$ (red) with hopping amplitude v_0 . The ansatz suffers a rapid increase of the entanglement due to scattering on $\mathcal{S}$. In open-system ERA, the dissipation, Eq. (3.2), relaxed the reservoirs to their thermal state which has non-zero bond dimension for the MPS.

of the particle is reflected generating a particle-hole pair shared between $\mathcal{L}$ and $\mathcal{R}$ and propagating in opposite directions [40], [93], [94]

$$\sqrt{p}|0_{\mathcal{L}}1_{\mathcal{R}}\rangle + \sqrt{1-p}|1_{\mathcal{L}}0_{\mathcal{R}}\rangle, \quad (6.11)$$

where $|0_{\mathcal{L}}1_{\mathcal{R}}\rangle$ represents a situation when the particle is transmitted from $\mathcal{L}$ to $\mathcal{R}$, and $|1_{\mathcal{L}}0_{\mathcal{R}}\rangle$ represents a case when the particle is reflected staying in $\mathcal{L}$ reservoir. Notice that if a particle is fully transmitted (or reflected), i.e., $p = 1$ or 0 then there is no entanglement shared between $\mathcal{L}$ and $\mathcal{R}$. On the other hand, if $p = 1/2$ the entanglement is maximal.

Inside the reservoirs, the particle propagates with the Fermi velocity $v_F = 2\omega_0$ estimated from *Lieb–Robinson bound* [39]. That stretches the entanglement across the lattice. As time goes on, more and more particles arrive at $\mathcal{S}$ and each scattering event generates a new entangled pair overlapping with those already present. This generates a light cone of entanglement growing around the scattering region and becoming greater and wider as time increases. In Fig. 6.4 the entanglement grows linearly in time, which typically corresponds to exponentially growing bond dimension, prohibiting long-time simulation with tensor networks [40].

It is interesting to notice that although the limitation of TN is a result of entanglement growth, which is physical, that effect can be mitigated by applying an appropriate MPS ansatz. That is because the entanglement in MPS chain depends on the way it is calculated. As we explained in Sec. 6.1 the entanglement depends on the bipartition calculated on virtual bonds. To lower the overall entanglement we adjust the MPS ansatz such that generated particle-hole pairs do not overlap. By doing that we lower overall entanglement and, in turn, lower the computational cost.

For the elastic scattering on $\mathcal{S}$ the particle-hole pair is shared between reservoir modes of the same energy. Then, the entangled pair is

$$\sqrt{T(\omega_k)}|0_{\mathcal{L}}1_{\mathcal{R}}\rangle(\omega_k) + \sqrt{1-T(\omega_k)}|1_{\mathcal{L}}0_{\mathcal{R}}\rangle(\omega_k), \quad (6.12)$$

where $T(\omega_k)$ is a transmission function for the energy ω_k , and $|\dots\rangle(\omega_k)$ indicates the state.

The Eq. (6.12) suggests working in the energy-space and minimizing the bipartitions which separate modes of the same energy. That geometry is

compatible with so-called *star geometry* where the reservoirs are in energy basis and each of them couples to the $\mathcal{S}$ modes that are central to the graph as in Fig. 3.1. To localize the entanglement we also order the $\mathcal{LR}$ modes by increasing energies, placing $\mathcal{L}$ and $\mathcal{R}$ modes of the same energy adjacent in MPS ansatz as in Fig. 6.5. The ordered ansatz is called a *mixed basis*. For simplicity, the $\mathcal{S}$ tensors are placed in the middle at $\omega = 0$ as depicted in Fig. 6.5. Notice, that there are still some correlations developing to the impurity $\mathcal{S}$, however, the mixed basis allows us to lower the entanglement associated with scattering inside $\mathcal{LR}$. For pure states, the change of basis mitigates the entropy growth from linear in time [95] for position basis (in Fig. 6.4) to logarithmic [40] for mixed basis (in Fig. 6.5).

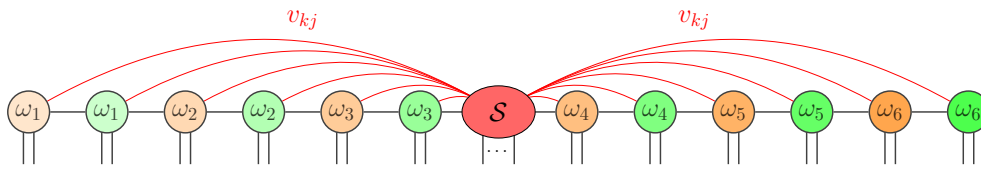


Figure 6.5. Mixed basis ansatz for matrix product state. The reservoirs (orange/green) are represented in an energy basis, and we arrange the modes adjacent to the energies. The $\mathcal{S}$ modes (red) are kept in the middle of MPS ansatz. The ansatz reflects the natural scattering structure in the $\mathcal{LSR}$ model greatly reducing the cost of the MPS representation. The ansatz is compatible with the dissipation in Eq. (3.2) which truncates the correlations across the MPS lattice, and ultimately relaxes it to thermal $\mathcal{LR}$ state that has a trivial bond dimension in the vectorization.

6.4 Scattering structure in ERA

Knowing the preferred basis for the evolution with the $\mathcal{LSR}$ Hamiltonian in Ref. [1] we took the mixed basis and apply it to the open system in ERA. Now, the master equation takes coherent evolution with the $\mathcal{LSR}$ Hamiltonian and the dissipation in Eq. (3.2) acts diagonally in energies.

The conclusion from Sec. 6.3 about the entanglement is very similar to the closed system discussed above. Still the mixed basis in Fig. 6.4 is much more efficient than the position basis in Fig. 6.5. This is because it minimizes the entanglement generated by the coherent evolution and it is compatible with the dissipation in Eq. (3.2) that relaxed the reservoirs to thermal state which has a trivial bond dimension for the vectorization. In the evolution the dissipation destroys all coherences inter- and intra-reservoir modes generated by coherent evolution lowering the MPS cost. Notice that in position ansatz even the thermal state has non-zero bond dimension between $\mathcal{LR}$ sites, so it is incompatible with both coherent and dissipative terms.

As with pure states, the computational cost of MPS for mixed states also

depends on the entanglement structure. For states, such as degenerate ground states or thermal states, the entanglement entropy Eq. (6.3) is no longer physically meaningful to quantify the entanglement. However, it still can be used to quantify the correlations in the vectorized density matrix. In this context, instead of the entropy, we study the *operator space entanglement entropy* (OSEE). More information about OSEE and its relation to the correlation matrix for non-interacting systems is discussed in Sec. A. In Sec. 6.3 we study the entanglement structure and compute the OSEE for vectorization.

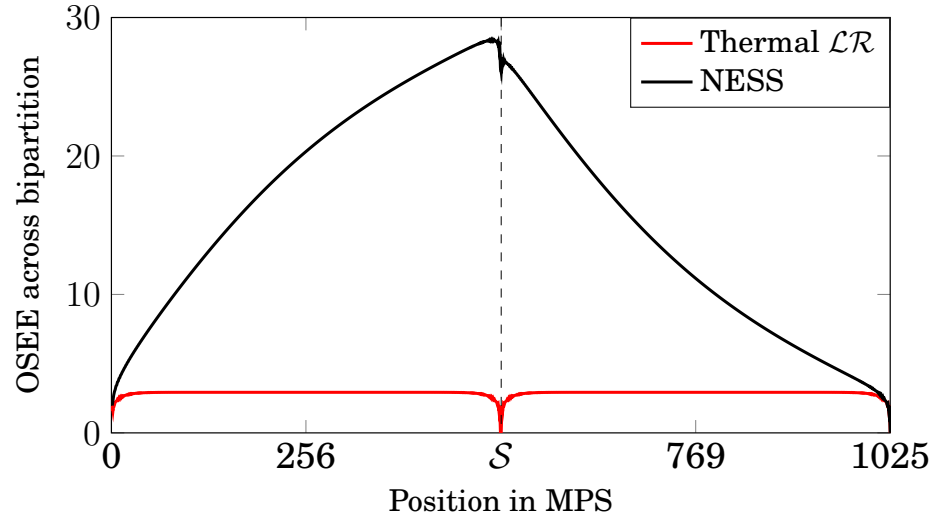


Figure 6.6. OSEE in position basis ansatz. The position basis ansatz, in Fig. 6.4, suffers from a large OSEE for ERA. That prohibits large-scale simulations using tensor networks. The basis has to encode the particle-hole pairs generated by scattering on the impurity $\mathcal{S}$. This is visible by having a large steady-state OSEE. Furthermore, the basis is not compatible with the dissipator relaxing $\mathcal{LR}$ reservoirs to the thermal state. In the ansatz, the thermal state also has non-zero OSEE. The data is obtained for $N_{\mathcal{W}} = 512$ modes per reservoir.

The success of mixed basis for open-system is visualized in Fig. 6.6 and Fig. 6.7 where we show OSEE across the MPS chain.

In the steady-state the OSEE in a mixed basis is 10× smaller than for a position basis. The position ansatz gives significant OSEE even for a thermal state while there is no OSEE for the mixed basis. In the mixed basis, the computational cost is mainly associated with the scattering of particles contributing to the current and thus is localized within the bias window⁴.

The scattering structure is richer than elastic scattering described in

⁴For a finite temperature the relevant region is determined by $|f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)|$. The region grows outside the bias window together with the temperature. However, then the state also becomes closer to infinite-temperature which has a trivial bond dimension for the vectorization of the density matrix.

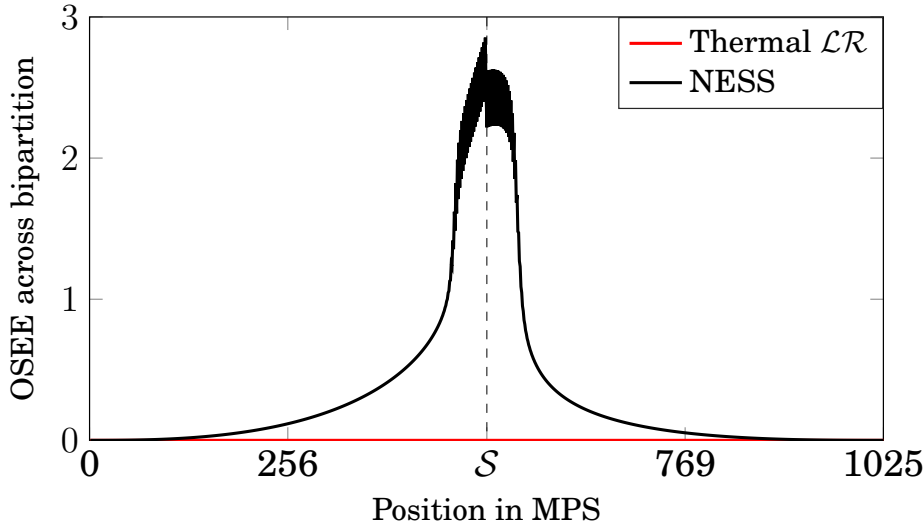


Figure 6.7. OSEE in mixed basis ansatz. The mixed basis ansatz, in Fig. 6.5, localizes the entanglement spread by using the ordered energy basis for $\mathcal{LR}$. This localizes the correlations between $\mathcal{L}$ and $\mathcal{R}$ reservoirs lowering the computational cost and enabling efficient tensor network simulation. The relevant region of the steady-state OSEE corresponds to sites contributing to the current, i.e., to the bias window. The basis has to encode the particle-hole pairs generated by scattering on the impurity $\mathcal{S}$. The dissipation in ERA relaxes the state to a thermal state which has a trivial bond dimension, i.e., OSEE is zero. The data is obtained for $N_{\mathcal{W}} = 512$ modes per reservoir.

Sec. 6.3, and the broadening due to dissipation results in additional correlations developing between modes of different energies. Despite that, the correlation still decays with the energy difference which promotes the ordering we imposed in a mixed basis.

The rich structure of correlations can be studied using the correlation matrix. In Fig. 6.8 we plot the correlation matrix for NESS in ERA calculated for the optimal relaxation rate. The correlation structure confirms that the correlations are the strongest for sites within the bias window. In addition, we can see that correlations inside $\mathcal{LR}$ decay with increasing energy distance. This further justifies the energy ordering imposed in a mixed basis.

Notice that the correlation matrix in Fig. 6.8 is visibly asymmetric with respect to $(0,0)$. In particular, the correlations are stronger for the energies around the self-energy for $\mathcal{S}$. That is reflected in Fig. 6.6 and Fig. 6.7 where OSEE is asymmetric. Although mixed basis gives an enormous advantage over position basis, their ansatz can be further improved. In particular, we can take the permutation of mixed basis such that the position of $\mathcal{S}$ tensors is closer to higher contributing modes. However, this requires knowledge about the $\mathcal{S}$ state which is not unknown *a priori*. The discussion above confirms that the mixed basis ansatz we imposed is a good compromise between lowering the spread of entanglement and the simplicity of a design.

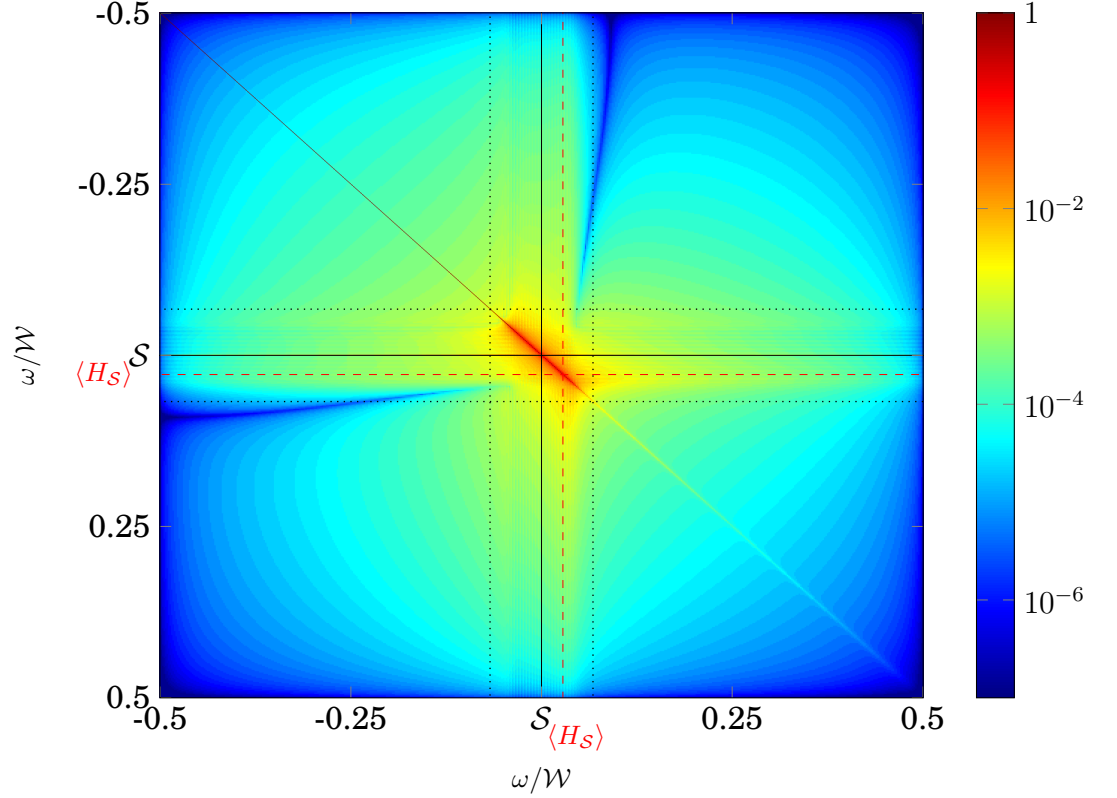


Figure 6.8. Correlation matrix for NESS. The correlation structure in the $\mathcal{LSR}$ system exhibits some typical features. This can be visualized using the correlation matrix defined as $|\mathcal{C}_{i,j}| = |\langle c_i^\dagger c_j \rangle|$. For a mixed basis, we analyze the $\mathcal{C}$ in the ordered energy basis, where the impurity mode is marked by $\mathcal{S}$ (similar as in Fig. 6.5). The $\mathcal{LSR}$ system typically exhibits the strongest correlations within the bias window (boundaries marked with black dotted lines). The $\mathcal{LR}$ modes have strong correlations to $\mathcal{S}$ (marked by a red dashed line) and between resonant reservoir modes (first off-diagonal entries $\mathcal{C}_{j,j\pm 1}$). In NESS, the correlations between reservoir modes decay with increasing energy differences. This justifies the ordering of energies in a mixed basis. Data obtained for $N_{\mathcal{W}} = 512$ modes per reservoir, bias $\mu = \omega_0/2$, temperature $T_{\mathcal{L}} = T_{\mathcal{R}} = \omega_0/40$, and coupling $v_0 = \omega_0/20$. The $\mathcal{S}$ Hamiltonian is $H_{\mathcal{S}} = \omega_0/2 a_1^\dagger a_1$.

The discussion in this section allowed us to define the mixed basis ansatz and, from now on, we fix the ansatz and implement the problem using tensor networks. In Sec. 6.5 we discuss more details of the tensor network implementation including some practical aspects of defining the tensors and solving for a steady-state.

6.5 Encoding ERA in vectorization

We implement the ERA in one-dimensional tensor network using vectorization. This section serves as insider information for the practical implementation of the problem. That includes an explicit form of MPS and

MPO and comments on the benefits of manipulating the local bases for vectorization.

The evolution of ERA is generated by a superoperator which in vectorized form is

$$\begin{aligned} \mathbb{L} = & -\imath(H \otimes \mathbb{1} - \mathbb{1} \otimes H^T) + \sum_{k \in \mathcal{LR}} \gamma_k^+ \left(c_k^\dagger \otimes c_k^T - \frac{1}{2} \left\{ c_k c_k^\dagger \otimes \mathbb{1} + \mathbb{1} \otimes (c_k c_k^\dagger)^T \right\} \right) \\ & + \sum_{k \in \mathcal{LR}} \gamma_k^- \left(c_k \otimes c_k^{\dagger T} - \frac{1}{2} \left\{ c_k^\dagger c_k \otimes \mathbb{1} + \mathbb{1} \otimes (c_k^\dagger c_k)^T \right\} \right), \end{aligned}$$

where $\gamma_k^+ = \gamma f^{\alpha_k}(\omega_k)$ and $\gamma_k^- = \gamma(1 - f^{\alpha_k}(\omega_k))$ are injection and depletion rates respectively, and $c_k^\dagger$ and c_k are normal fermionic operators.

We map fermionic operators to spin- $\frac{1}{2}$ Pauli operators by applying *Jordan-Wigner transformation*

$$c_j^\dagger = \prod_{i < j} \hat{z}_i f_j^\dagger \quad \text{and} \quad c_j = \prod_{i < j} \hat{z}_i f_j, \quad (6.13)$$

where on-site fermion operators are

$$f_j^\dagger = \frac{\hat{x}_j + \imath \hat{y}_j}{2}, \quad f_j = \frac{\hat{x}_j - \imath \hat{y}_j}{2}, \quad f_j^\dagger f_j = \frac{\hat{z}_j + \mathbb{1}_j}{2}, \quad (6.14)$$

where $\hat{x}_j$, $\hat{y}_j$, and $\hat{z}_j$ are Pauli operators for a site j . For simplicity, we omit the site indexing later in this section.

Transformation preserves fermionic anticommutation relation by introducing non-local $\hat{z}$ -string for $i < j$ for an operator acting on the site j . The indexing method is arbitrary as long as it remains consistent for all operators. We impose indexing increasing from left to right. Notice, that although the fermionic operators are very non-local, they square to identity. After the transformation, the $\hat{z}$ -strings survive in the Hamiltonian only for long-range hopping, and in the dissipator for $c_k^\dagger \rho c_k$ and $c_k \rho c_k^\dagger$ terms which are linear in fermionic operators applied to *bra* and *ket* dimensions separately.

The vectorization of the superoperator can be implemented using a *matrix product operator* (MPO) compatible with the vectorization of density matrix that is written as a *matrix product state* (MPS).

For a fermionic system, the density matrix is 2×2 at each site. These can be written as a superposition of at least four matrices. Below, we review possible vectorization bases and the corresponding MPO representing the Lindblad superoperator. Depending on local bases we can implement the problem using tensors with different embedded symmetries that keep only relevant blocks that include non-zero values. This allows us to lower the computational cost and improve the stability of the simulation compared to dense tensors that have all blocks included.

6.5.1 Vectorization in fermionic basis

Standard vectorization scheme where matrix elements are arranged into a vector can be understood as a superposition of matrices

$$f^\dagger f = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, f f^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, f = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, f^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad (6.15)$$

which can be understood in terms of fermionic operators f and $f^\dagger$ in Eq. (6.14). The vectorization maps a single matrix element to a single value in vectorization placed at the position corresponding to the basis matrix with non-zero value on the same position as mapped.

The physical index is defined by the basis vector

$$\mathcal{Q} = [f^\dagger f, f f^\dagger, f, f^\dagger], \quad (6.16)$$

which fixes the vectorization. Given the local basis we write a tensor $T = [a_0, a_1, a_2, a_3]$ which is interpreted as

$$[a_0, a_1, a_2, a_3] \circ \mathcal{Q} = \begin{pmatrix} a_1 & a_2 \\ a_3 & a_0 \end{pmatrix}, \quad (6.17)$$

where $\circ$ is a scalar product and $a_j \in \mathbb{C}$. This can be used to write any 2×2 matrix and we use it for a density matrix.

The operator acting on the vectorization generates a state within $\mathcal{Q}$ vectorization. To obtain MPO representation of the operation we calculate how it transforms $\mathcal{Q}$ basis vector in Eq. (6.16). For example, for the operator $(f \otimes \mathbb{1})$

$$(f \otimes \mathbb{1}) \mathcal{Q} = [f, 0, 0, f f^\dagger], \quad (6.18)$$

which can be written as the MPO tensor

$$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (6.19)$$

where columns represent input (bra) and rows output (ket) both respecting ordering in $\mathcal{Q}$. The operator Eq. (6.19) is the MPO tensor with two physical dimensions 4×4 and trivial virtual dimensions 1×1 .

In the first step towards writing the Lindblad superoperator as an MPO, we calculate all necessary operators as in Eq. (6.19). After that, the superoperator is constructed by blocking these operators into the MPO tensor with higher bond dimension. The MPO tensor at each site is constructed such that the Lindblad Eq. (6.13) is recovered upon contraction along the virtual bond.

Although the mixed basis in Fig. 6.5 has many long-range interactions, we can write the MPO of a small bond dimension. Below we explicitly write the MPO tensors representing the Hamiltonian for reservoirs in Eq. (1.2), and the interaction in Eq. (1.3) describing a coupling to a single site in $\mathcal{S}$.

The MPO tensor on site $k < j$ where $k \in \mathcal{LR}$ and $j \in \mathcal{S}$ is

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & \hat{z} \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ 0 & 0 & \mathbb{1} \otimes \hat{z} & 0 & 0 & 0 \\ 0 & 0 & 0 & \hat{z} \otimes \mathbb{1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbb{1} \otimes \hat{z} & 0 \\ -i\omega_k(n \otimes \mathbb{1} - \mathbb{1} \otimes n) & -iv_k f \otimes \mathbb{1} & iv_k \mathbb{1} \otimes f^\text{T} & -iv_k f^\dagger \otimes \mathbb{1} & iv_k \mathbb{1} \otimes f^{\dagger\text{T}} & \mathbb{1}_4 \end{pmatrix}, \quad (6.20)$$

where $n = f^\dagger f$ is particle number operator and $\mathbb{1}_4 = \mathbb{1} \otimes \mathbb{1}$. The Eq. (6.20) blocks local operators which act on the MPS into a larger structure. The MPO for coupling to a single site in $\mathcal{S}$ has physical dimensions 4×4 (dimension of blocked operators) and virtual dimensions 6×6 (matrix dimensions of blocked structure as in Eq. (6.20)). The dimension is independent of reservoir size $N_{\mathcal{H}}$ and grows linearly with a number of coupled sites in $\mathcal{S}$.

The tensor in Eq. (6.20) defines on-site potential for the mode k and opens a channel for a coupling of the mode to the $\mathcal{S}$ such that the hopping amplitude is $v_k = v_{kj}$. The diagonal elements carry over the $\hat{z}$ -strings for the hopping from modes $k' < k$. This is necessary for $k > 1$ since all reservoir modes are coupled to $\mathcal{S}$ in the middle of the MPS ansatz.

The hopping operator is terminated at site $j \in \mathcal{S}$ by the first column in

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ f^\dagger \otimes \mathbb{1} & 0 & 0 & 0 & 0 & 0 \\ \mathbb{1} \otimes f^{\dagger\text{T}} & 0 & 0 & 0 & 0 & 0 \\ f \otimes \mathbb{1} & 0 & 0 & 0 & 0 & 0 \\ \mathbb{1} \otimes f^\text{T} & 0 & 0 & 0 & 0 & 0 \\ 0 & f \otimes \mathbb{1} & \mathbb{1} \otimes f^\text{T} & f^\dagger \otimes \mathbb{1} & \mathbb{1} \otimes f^{\dagger\text{T}} & \mathbb{1}_4 \end{pmatrix}. \quad (6.21)$$

Notice that in Eq. (6.21) there are none $\hat{z}$ -operators from Jordan-Wigner transformation. This is because the hopping is between $\mathcal{LR}$ and $\mathcal{S}$ not across $\mathcal{S}$. The last column of the MPO tensor in Eq. (6.21) opens the hopping term to the modes $k > j$. The operator is later terminated on the

reservoir site $k > j$

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ -\imath v_k f^\dagger \otimes \mathbb{1} & \hat{z} \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ \imath v_k \mathbb{1} \otimes f^{\dagger T} & 0 & \mathbb{1} \otimes \hat{z} & 0 & 0 & 0 \\ -\imath v_k f \otimes \mathbb{1} & 0 & 0 & \hat{z} \otimes \mathbb{1} & 0 & 0 \\ \imath v_k \mathbb{1} \otimes f^T & 0 & 0 & 0 & \mathbb{1} \otimes \hat{z} & 0 \\ -\imath \omega_k (n \otimes \mathbb{1} - \mathbb{1} \otimes n) & 0 & 0 & 0 & 0 & \mathbb{1}_4 \end{pmatrix}. \quad (6.22)$$

A compact form of the MPO is possible because $\sum_k \sum_j v_k c_k^\dagger a_j = \left(\sum_k v_k c_k^\dagger \right) \left(\sum_j a_j \right)$. As mentioned above, this allows us to write a compact MPO that has a bond-dimension independent of $N_{\mathcal{W}}$ and scales linearly with a number of $\mathcal{S}$ modes coupled to the reservoirs.

The dissipator Eq. (3.2) acts locally on each $k \in \mathcal{LR}$, however, the Jordan-Wigner transformation maps them to very non-local. Despite that, we can still write the MPO in a compact form with bond dimension 3. Here, the MPO bond dimension is independent of $N_{\mathcal{W}}$ and $N_{\mathcal{S}}$.

The MPO tensor is

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 \\ \gamma_k^- f \otimes f^{\dagger T} + \gamma_k^+ f^\dagger \otimes f^T & \hat{z} \otimes \hat{z} & 0 \\ \gamma_k^- (f^\dagger f \otimes \mathbb{1} + \mathbb{1} \otimes (f^\dagger f)^T) + \gamma_k^+ (f f^\dagger \otimes \mathbb{1} + \mathbb{1} \otimes (f f^\dagger)^T) & 0 & \mathbb{1}_4 \end{pmatrix}, \quad (6.23)$$

where diagonal element carries over the $\hat{z}$ -strings from $c_k^\dagger \rho c_k$ and $c_k \rho c_k^\dagger$ which are terminated by $\gamma_k^- f \otimes f^{\dagger T} + \gamma_k^+ f^\dagger \otimes f^T$ in the first column of MPO tensor.

The density matrix consists of uncorrelated sectors of different particle numbers and can be described by symmetric tensors [6] with $U(1)$ symmetry. Symmetric tensors store only non-zero blocks, which significantly reduces the numerical cost of implementation.

6.5.2 Vectorization in Pauli basis

Alternatively, the local basis can be written in terms of spin- $\frac{1}{2}$ Pauli matrices

$$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \hat{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \hat{y} = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \hat{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (6.24)$$

which in similarity to the fermionic basis in Eq. (6.16) can be interpreted as Majorana basis.

The vectorization is fixed by fixed basis vector

$$\mathcal{Q} = [\mathbb{1}, \hat{x}, \hat{y}, \hat{z}]. \quad (6.25)$$

The vectorization written as a vector $T = [a_0, a_1, a_2, a_3]$ is interpreted as

$$[a_0, a_1, a_2, a_3] \circ \mathcal{Q} = \begin{pmatrix} a_0 + a_3 & a_1 - \iota a_2 \\ a_1 + \iota a_2 & a_0 - a_3 \end{pmatrix}. \quad (6.26)$$

As in the previous example, the set of Pauli matrices is enough to describe any 2×2 matrix thus to encode the density matrix. To obtain the MPO tensor representing the operation on a local basis we consider the transformation of $\mathcal{Q}$ under the action of the operator. For example for the operator $(f \otimes \mathbb{1})$ we have

$$(f \otimes \mathbb{1}) \mathcal{Q} = \frac{1}{2} [\hat{x} - \iota \hat{y}, -\hat{x} + \iota \hat{y}, \mathbb{1} - \hat{z}, -\iota \mathbb{1} + \iota \hat{z}]. \quad (6.27)$$

which gives the MPO tensor

$$\begin{pmatrix} 0 & 0 & 1 & -\iota \\ 0 & 0 & -1 & \iota \\ 1 & -1 & 0 & 0 \\ \iota & \iota & 0 & 0 \end{pmatrix}. \quad (6.28)$$

In tensor network language Eq. (6.28) is an MPO tensor with physical dimensions 4×4 and trivial virtual dimensions 1×1 .

We write the Lindblad superoperator Eq. (6.13) in the MPO form. The MPO for site $k < j$ with $k \in \mathcal{LR}$ and $j \in \mathcal{S}$

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & \text{Re}[\hat{z} \otimes \mathbb{1}] & \text{Im}[\hat{z} \otimes \mathbb{1}] & 0 & 0 & 0 \\ 0 & -\text{Im}[\hat{z} \otimes \mathbb{1}] & \text{Re}[\hat{z} \otimes \mathbb{1}] & 0 & 0 & 0 \\ 0 & 0 & 0 & \text{Re}[\hat{z} \otimes \mathbb{1}] & \text{Im}[\hat{z} \otimes \mathbb{1}] & 0 \\ 0 & 0 & 0 & -\text{Im}[\hat{z} \otimes \mathbb{1}] & \text{Re}[\hat{z} \otimes \mathbb{1}] & 0 \\ -\iota \omega_k (n \otimes \mathbb{1} - \mathbb{1} \otimes n) & v_k \text{Re}[\hat{x} \otimes \mathbb{1}] & v_k \text{Im}[\hat{x} \otimes \mathbb{1}] & v_k \text{Re}[\hat{y} \otimes \mathbb{1}] & v_k \text{Im}[\hat{y} \otimes \mathbb{1}] & \mathbb{1}_4 \end{pmatrix}, \quad (6.29)$$

where $n = (\mathbb{1} - \hat{z})/2$ is particle number operator. Each MPO tensor describes on-site energy for reservoir mode and opens a channel for the coupling to $j \in \mathcal{S}$. The hopping term is closed by the MPO tensor on $j \in \mathcal{S}$

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ \text{Im}[\hat{x} \otimes \mathbb{1}] & 0 & 0 & 0 & 0 & 0 \\ \text{Re}[\hat{x} \otimes \mathbb{1}] & 0 & 0 & 0 & 0 & 0 \\ \text{Im}[\hat{y} \otimes \mathbb{1}] & 0 & 0 & 0 & 0 & 0 \\ \text{Re}[\hat{y} \otimes \mathbb{1}] & 0 & 0 & 0 & 0 & 0 \\ 0 & \text{Re}[\hat{x} \otimes \mathbb{1}] & \text{Im}[\hat{x} \otimes \mathbb{1}] & \text{Re}[\hat{y} \otimes \mathbb{1}] & \text{Im}[\hat{y} \otimes \mathbb{1}] & \mathbb{1}_4 \end{pmatrix}, \quad (6.30)$$

which also opens a hopping term to $k > j$ with $k \in \mathcal{LR}$ and $j \in \mathcal{S}$. The latter is later terminated by the MPO tensor at reservoir mode $k > j$

$$\begin{pmatrix} \mathbb{1}_4 & 0 & 0 & 0 & 0 & 0 \\ v_k \text{Im}[\hat{x} \otimes \mathbb{1}] & \text{Re}[\hat{z} \otimes \mathbb{1}] & \text{Im}[\hat{z} \otimes \mathbb{1}] & 0 & 0 & 0 \\ v_k \text{Re}[\hat{x} \otimes \mathbb{1}] & -\text{Im}[\hat{z} \otimes \mathbb{1}] & \text{Re}[\hat{z} \otimes \mathbb{1}] & 0 & 0 & 0 \\ v_k \text{Im}[\hat{y} \otimes \mathbb{1}] & 0 & 0 & \text{Re}[\hat{z} \otimes \mathbb{1}] & \text{Im}[\hat{z} \otimes \mathbb{1}] & 0 \\ v_k \text{Re}[\hat{y} \otimes \mathbb{1}] & 0 & 0 & -\text{Im}[\hat{z} \otimes \mathbb{1}] & \text{Re}[\hat{z} \otimes \mathbb{1}] & 0 \\ -i\omega_k(n \otimes \mathbb{1} - \mathbb{1} \otimes n) & 0 & 0 & 0 & 0 & \mathbb{1}_4 \end{pmatrix}. \quad (6.31)$$

Similar as for previous basis the MPO for coupling to a single site gives the superoperator with a virtual dimensions 6×6 and physical dimensions 4×4 . The virtual dimension is independent of reservoir size $N_{\mathcal{W}}$ and grows linearly with number of coupled sites $N_{\mathcal{S}}$.

The vectorization can be implemented using real-valued tensors and by construction ensures the hermiticity of the density matrix. This comes with a cost of reducing tensor symmetry to $\mathbb{Z}_2$. However, the combination of a block-sparse tensors and restriction to real-valued datasets still reduces the computational cost of the tensor network representation.

After writing the MPO generating the master equation in Eq. (3.1) we solve it for a steady state. In Sec. 6.6 we discuss the numerical approaches to obtain the non-equilibrium steady state focusing on the ERA.

6.6 Solving for steady state

Having prepared the Lindblad superoperator in the MPO form we solve the master equation for a steady state which is determined by the condition

$$\mathbb{L}[\rho] = 0, \quad (6.32)$$

and in the vectorization is

$$\langle \langle \mathbb{1} | \mathbb{L} | \rho \rangle \rangle = 0. \quad (6.33)$$

The superoperator $\mathbb{L}$ is generally non-hermitian with the complex eigenvalues. The problem can be solved variationally using *density matrix renormalization group* (DMRG) algorithm, however, the standard DMRG [96] works with hermitian matrices. This problem can be circumvented by solving the variational problem for $\mathbb{L}^\dagger \mathbb{L}$ [97]–[99] which now has all eigenvalues non-negative and the smallest one is the steady state. However, if the gap between the steady state and excitations is too small, the DMRG is prone to end up in local minima which makes the convergence problematic. We found that this approach fails already for an intermediate number of reservoir modes for our problem. While some modifications of DMRG for

non-hermitian problems are available [100]–[102], their potential applicability to particularly challenging problems, like our NESS, remains to be seen.

Note that the excitation to the NESS does not satisfy the Eq. (6.32) and therefore completely disappears after a long time. Motivated by this, we obtain a steady state through the time evolution [103]–[106], where we evolve long enough for all excitations to decay.

Solving for a steady state by time evolution is advantageous because there is no problem with getting stuck in local minima. However, it may be problematic due to the scattering process described in Sec. 6.3 which may generate a highly entangled intermediate state. The time to reach a steady state is inversely proportional to the rate of the slowest decaying excitation. The slowest decay rate for the Lindblad master equation in Eq. (3.1), shown in Fig. 6.9, is proportional to γ in the relevant regime.

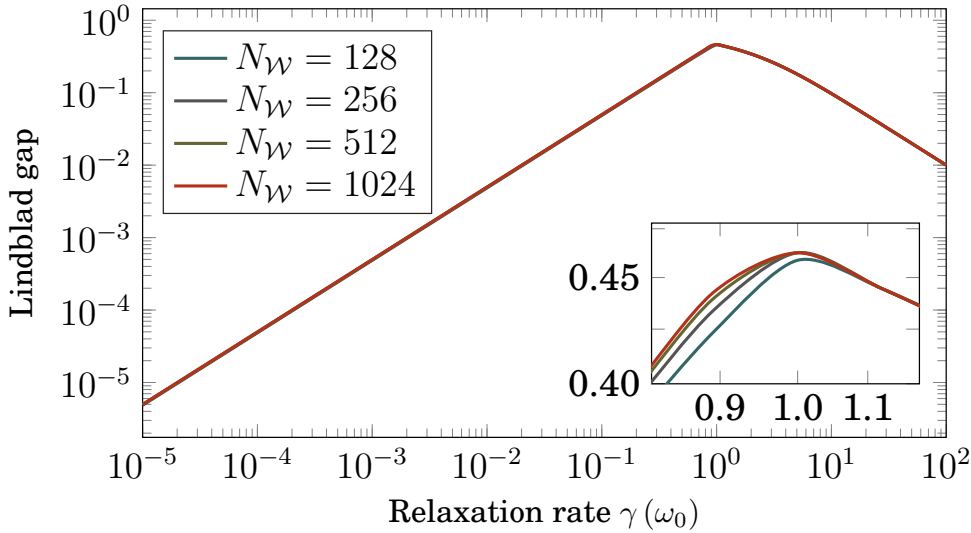


Figure 6.9. Amplitude of slowest decaying excitation to NESS. The time to reach a steady state is proportional to the decay rate of the excitation to NESS. The gap in the low and moderate relaxation rate is proportional to γ and is largely independent of reservoir discretization. The timescales for $\mathcal{L}\mathcal{S}\mathcal{R}$ are manifested for large- γ regime where the dissipation converges quickly. The data extracted for a model in Fig. 3.3.

While a variety of tensor network techniques exist in Ref. [1]–[4] we obtain the steady-state using *time-dependent variational principle* (TDVP) [107]. We note that *time-evolving block decimation* (TEBD) may also be efficacious [108] and leave open the question of an optimal implementation. The nearest-neighbor gates in TEBD can be applied by swapping the sites to neighboring positions in the MPS [77] to apply local gates. However, this poses a serious problem when working with the energy basis as in Sec. 6.3, where couplings are long-range. In addition, it complicates when reservoirs couple to more than one $\mathcal{S}$ mode. Furthermore, the swapping process leads to swapping the entanglement across the MPS chain and

prohibits using efficient ordering as discussed in Sec. 6.4. This contrasts TEBD with TDVP, where the TDVP can be applied for any long-range operator directly and can be implemented already in the efficient MPS ansatz.

In our studies, we found that solving for a steady state using time evolution using TDVP is the most efficient and stable approach. We evolve the initial state (in most cases we choose it to have thermal explicit reservoirs which are not correlated to $\mathcal{S}$) under the Lindblad superoperator, as described in Ref. [1]. An example of the evolution of the current is plotted in Fig. 6.10. After initial oscillations, the system steadily converges to NESS. The initial oscillations can be understood by analyzing timescales for the $\mathcal{LSR}$ model as introduced in Chpt. 5. A similar ERA approach was simultaneously discussed in Ref. [77], which however retained the less efficient $\mathcal{LSR}$ ansatz for MPS without energy ordering and using TEBD integrator, limiting it in practice to small reservoir representation and high temperatures.

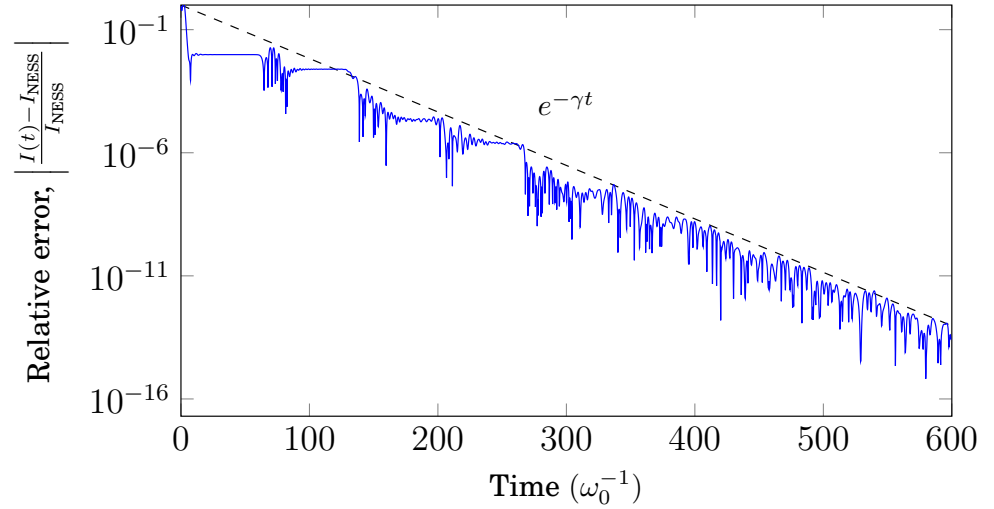


Figure 6.10. Convergence to NESS through time-evolution. The state prepared with thermal extended reservoirs evolves under the master equation in Eq. (3.1). After initial oscillations, the state systematically converges to a steady state I_{NESS} with a rate proportional to the relaxation rate γ . Data obtained for a model in Fig. 3.3 for $N_{\mathcal{W}} = 64$ modes per reservoir and dissipation rate $\gamma = \omega_0/20$.

Finally, the evolution can be also performed using the *purification* of density matrix [91], [92]. In the preparation to Ref. [1] we found that the correlation between the original and ancilla modes results in rapidly growing entanglement across the MPS chain which prohibits large-scale simulation. The gauge freedom of the ancillary modes can be used to lower the entanglement in the MPS by applying a unitary rotation. For example, the ancilla can be improved iteratively by solving the variational problem for the entanglement [109]. However, we found that this approach does not properly converge and is not applicable to our problem, apart from some

simple cases. In preparation for Ref. [1] we found that the entanglement can be efficiently reduced when applying a global evolution on the ancillary copy of the system [110]. There, the time-reversed physical Hamiltonian applied to the auxiliary sites renders the time evolution undoing the mixing done on the original system. We found that mirroring the evolution on ancilla is the most effective for high-temperature density matrix where two copies are correlated the strongest.

Despite all of that, we observed that the purification does not provide a scalable simulation approach that could be used to study quantum transport beyond small test cases.

A. Operator–space entanglement entropy

To define OSEE, one treats a density matrix as a vector in an enlarged Hilbert space that is a tensor product of local operator spaces [111], [112]. This maps a density matrix to a pure state in the enlarged space containing auxiliary fermionic operators. Hence, for each site $m \in \mathcal{L}\mathcal{S}\mathcal{R}$ we will have two fermionic species with annihilation operators c_m and $\tilde{c}_m$ for *ket* and auxiliary, *bra*, fermion. The normalized pure state is

$$|\rho\rangle \sim \rho|I\rangle, \quad (1.1)$$

where we take $|I\rangle = \prod_{m \in \mathcal{L}\mathcal{S}\mathcal{R}} (c_m^\dagger - \tilde{c}_m^\dagger)|0\rangle$ as a product of maximally entangled singlets in each local space.

A Gaussian density matrix is fully determined by its correlation matrix $\mathcal{C}$. In that case, a Gaussian $|\rho\rangle$ is described by the correlation matrix $\tilde{\mathcal{C}}$ in a block form

$$\tilde{\mathcal{C}}_{mn} = \langle \rho | \begin{bmatrix} c_n^\dagger c_m & c_n^\dagger \tilde{c}_m \\ \tilde{c}_n^\dagger c_m & \tilde{c}_n^\dagger \tilde{c}_m \end{bmatrix} | \rho \rangle. \quad (1.2)$$

The OSEE is an entanglement entropy of bipartition of $|\rho\rangle$. It is calculated in a standard way [113] from eigenvalues ϵ_i of a submatrix of $\tilde{\mathcal{C}}_{mn}$ including $m, n \in \mathcal{A}$,

$$\text{OSEE}_{\mathcal{A}} = - \sum_i \epsilon_i \log_2 \epsilon_i - \sum_i (1 - \epsilon_i) \log_2 (1 - \epsilon_i), \quad (1.3)$$

where $\mathcal{A}$ is the group of modes defining bipartition.

To obtain $\tilde{\mathcal{C}}$, one rotates fermionic operators to a diagonal basis of $\mathcal{C}$, where $d_i = \sum_{m \in \mathcal{L}\mathcal{S}\mathcal{R}} \mathcal{U}_{im}^\dagger c_m$ (similarly we will have $\tilde{d}_i = \sum_{m \in \mathcal{L}\mathcal{S}\mathcal{R}} \mathcal{U}_{im}^\dagger \tilde{c}_m$). Here $\mathcal{U}$ is a matrix of eigenvectors, and ϵ_i are eigenvalues, of $\mathcal{C}$. In that basis, a correlation matrix is block diagonal with

$$\langle \rho | \begin{bmatrix} d_i^\dagger d_i & d_i^\dagger \tilde{d}_i \\ \tilde{d}_i^\dagger d_i & \tilde{d}_i^\dagger \tilde{d}_i \end{bmatrix} | \rho \rangle = \begin{bmatrix} \alpha_i^2 & \alpha_i \beta_i \\ \alpha_i \beta_i & \beta_i^2 \end{bmatrix}, \quad (1.4)$$

where $\alpha_i = \frac{\epsilon_i}{\sqrt{(1-\epsilon_i)^2 + \epsilon_i^2}}$, and $\beta_i = -\frac{1-\epsilon_i}{\sqrt{(1-\epsilon_i)^2 + \epsilon_i^2}}$. The correlation matrix $\tilde{\mathcal{C}}$ in the original basis of interest is obtained by rotating back to c_m and $\tilde{c}_m$.

B. Correlation matrix approach for quantum transport

B.1 Correlation matrix approach for ERA

The evolution generated by Eq. (3.1) with the quadratic Hamiltonian, Eq. (1.1), retains the Gaussianity of the state. As a result, the evolution (which is also particle conserving) can be formulated via the correlation matrix,

$$\mathcal{C}_{mn} = \text{tr} (c_n^\dagger c_m \rho), \quad (2.1)$$

with $m, n \in \mathcal{L}\mathcal{S}\mathcal{R}$. In this form, we have [55]

$$\dot{\mathcal{C}} = -\imath[\tilde{\mathbf{H}}, \mathcal{C}] + \gamma \mathcal{D}[\mathcal{C}], \quad (2.2)$$

with the dissipation in Eq. (3.2) translating to

$$\mathcal{D}[\mathcal{C}]_{mn} = f^{\alpha_m}(\omega_m) \delta_{mn} \delta_{m \in \mathcal{L}\mathcal{R}} - \mathcal{C}_{mn} \frac{\delta_{m \in \mathcal{L}\mathcal{R}} + \delta_{n \in \mathcal{L}\mathcal{R}}}{2}. \quad (2.3)$$

Here, the δ_{mn} is the normal Kronecker delta, and $\delta_{m \in \mathcal{L}\mathcal{R}}$ is 1 for the mode in one of the reservoirs and 0 otherwise, i.e., relaxation occurs only for $m \in \mathcal{L}\mathcal{R}$.

Consequently, for purely unitary evolution over a time τ (without dissipation), the evolution is

$$e^{-\imath\tau\tilde{\mathbf{H}}} \mathcal{C} e^{\imath\tau\tilde{\mathbf{H}}}. \quad (2.4)$$

For pure dissipation for a time τ (without the action of the Hamiltonian), integrating Eq. (2.3) leads to an update

$$\mathcal{G}\mathcal{C}\mathcal{G}^\dagger + \mathcal{P}, \quad (2.5)$$

where the dissipative matrices are

$$\mathcal{G}_{mn} = \delta_{mn} e^{-\gamma\tau\delta_{m \in \mathcal{L}\mathcal{R}}/2} \quad (2.6)$$

and

$$\mathcal{P}_{mn} = \delta_{mn} (1 - e^{-\gamma\tau\delta_{m \in \mathcal{L}\mathcal{R}}}) f^{\alpha_m}(\omega_m). \quad (2.7)$$

B.2 Correlation matrix approach for ARC

For *accumulative reservoir construction* (ARC), introduced in Chpt. 5, the evolution in Eq. (5.1) is a two-step process with coherent evolution and dissipation performed by a finite time τ . The cycle p of this process is

$$\mathcal{C}(p\tau + \tau) = \mathbf{M}\mathcal{C}(p\tau)\mathbf{M}^\dagger + \mathcal{P}, \quad (2.8)$$

with

$$\mathbf{M} = \mathcal{G}e^{-i\tau\tilde{H}}. \quad (2.9)$$

These results hold for any Gaussian system, i.e, in absence of many-body interactions. The system can be a lattice of arbitrary dimension and geometry. It can be generalized to cases with an arbitrary number of reservoirs attached to an arbitrary number of sites in $\mathcal{S}$.

On reaching the NESS, $\mathcal{C}(p\tau + \tau) = \mathcal{C}(p\tau)$. This makes Eq. (2.8) exactly in the form of a discrete-time Lyapunov equation that can be solved directly, allowing us to find the NESS without carrying out the time evolution. The convergence time can be extracted from the spectrum of the largest magnitude eigenvalue of propagator $\mathbf{M}$. When all eigenvalues have a magnitude less than one, the steady state is unique.

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Publication I

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Open-system tensor networks and Kramers' crossover for quantum transport

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Tensor networks are a powerful tool for many-body ground states with limited entanglement. These methods can, nonetheless, fail for certain time-dependent processes—such as quantum transport or quenches—where entanglement growth is linear in time. Matrix-product-state decompositions of the resulting out-of-equilibrium states require a bond dimension that grows exponentially, imposing a hard limit on simulation timescales. However, in the case of transport, if the reservoir modes of a closed system are arranged according to their scattering structure, the entanglement growth can be made logarithmic. Here, we apply this ansatz to open systems via extended reservoirs that have explicit relaxation. This enables transport calculations that can access steady states, time dynamics and noise, and periodic driving (e.g., Floquet states). We demonstrate the approach by calculating the transport characteristics of an open, interacting system. These results open a path to scalable and numerically systematic many-body transport calculations with tensor networks.

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Many-body quantum systems are characterized by complex ground and dynamic states, reflecting the emergence of phenomena from superconductivity to exotic magnetism. Furthermore, for nonequilibrium properties, systematic excitations can yield a response that diverges markedly from the ground state [1]. The analytical treatment of many-body systems is thus challenging. This situation has driven the development of numerical methods such as quantum Monte Carlo [2,3], dynamical mean-field theory (DMFT) [4,5], and tensor networks [6–11], which now lie at the forefront of many-body theory. Among these, tensor networks leverage the structure of correlations and entanglement to provide a local, numerically controllable many-body description-limiting computation to a submanifold of Hilbert space that captures the underlying state.

While tensor networks, such as matrix product states (MPSs), are extremely successful for correlated ground states, their application to time-dependent behavior can be stifled by a rapid growth of entropy [12,13]. In the context of quantum transport, this is due to scattering, which generates entangled electron-hole pairs in the adjacent contact regions [14]. For a pair of electrodes, $\mathcal{L}$ and $\mathcal{R}$, held at a bias μ , the attempt frequency for scattering events is $\mu/2\pi$ [15]. The bipartite entanglement entropy S between them then grows linearly as $S \approx H[T(0)]\mu t/2\pi$, where $H[T(\omega=0)]$ is the binary entropy of the transmission probability $T(\omega)$ evaluated at the Fermi level (and μ is taken to be small) [16–18]. Described qualitatively, a simulation will fail when S saturates the entanglement entropy permitted by a MPS with dimension D —a condition that is met when $S \approx \log_2 D$. Increasing the

simulation duration requires an exponentially larger D and thus exponentially larger computational requirements (see, e.g., Ref. [14]).

This exponential barrier can be mitigated by a basis that reflects the scattering structure of current-carrying states [14]: An incoming particle at energy $\hbar\omega_k$ will be transmitted from one reservoir, through the system, and into an outgoing state at the same energy (up to some characteristic spread in energy). A mixed energy-spatial basis, where (nearly) isoenergetic modes in $\mathcal{L}$ and $\mathcal{R}$ are adjacent on a one-dimensional (1D) lattice, captures the highly local entanglement structure in the energy domain. We recently leveraged this observation to develop a time-dependent MPS approach for closed systems. This approach shifts the temporal growth of entanglement from *linear* to *logarithmic* [14]. The energy basis, also known in the literature as the “star geometry,” has been employed in MPS impurity solvers for nonequilibrium DMFT [19,20] and in the study of quenched and Floquet states in the Anderson impurity model [21,22], leading to suppression of entanglement [22]. Nonetheless, our method is unique in pairing the reservoir modes according to the actual entanglement structure, giving accurate, extensive simulations of previously entanglement limited nonequilibrium problems.

Here, we demonstrate that the mixed energy-spatial basis naturally permits open MPS simulations where implicit reservoirs offset carrier depletion in the explicit leads (reservoirs) $\mathcal{L}$ and $\mathcal{R}$ (Fig. 1). We first show that this method is numerically stable in the physical regime that reflects transport in the infinite reservoir limit (see Refs. [23,24]). We then apply our approach to a nontrivial example of transport through a two-site, interacting many-body impurity. The open-system framework is critical for directly targeting steady states, including at finite temperature. In doing so, it provides a unified framework for addressing driven systems or those subject to

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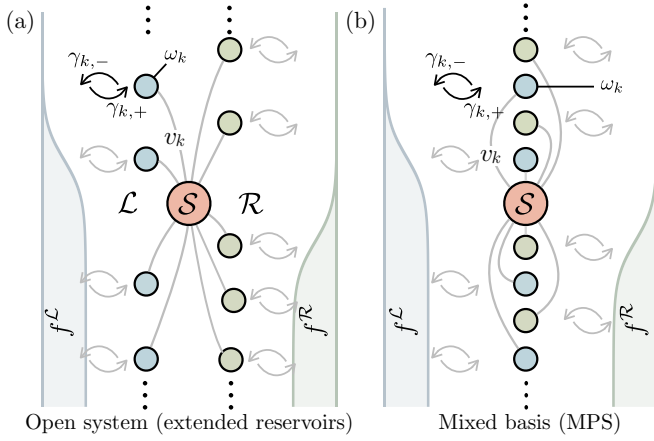


FIG. 1. Open-system transport. (a) An “extended-reservoir” approach for transport through a many-body system $\mathcal{S}$. The system is flanked by explicit left, $\mathcal{L}$, and right, $\mathcal{R}$, reservoir modes of frequency ω_k and coupling v_k to $\mathcal{S}$. Implicit reservoirs relax the modes towards a Fermi-Dirac distribution via distinct injection ($\gamma_{k,+}$) and depletion ($\gamma_{k,-}$) rates tied to $f^{\mathcal{L}/\mathcal{R}}(\omega_k)$. (b) The mixed energy-spatial basis has $\mathcal{L}$ and $\mathcal{R}$ modes arranged according to their energy $\hbar\omega_k$ [14].

time-dependent perturbations, such as Floquet dynamics and external noise on top of otherwise stationary states. These scenarios are generally difficult—and sometimes impossible—to access using existing methods.

Quantum transport is typically modeled using a composite system, containing noninteracting left ($\mathcal{L}$) and right ($\mathcal{R}$) reservoirs that drive transport through an “impurity” region [the system $\mathcal{S}$; see Fig. 1(a)] [25]. The Hamiltonian takes the form

$$H = H_{\mathcal{S}} + H_{\mathcal{L}} + H_{\mathcal{R}} + H_{\mathcal{I}}, \quad (1)$$

where $H_{\mathcal{S}}$ is the (many-body) Hamiltonian for $\mathcal{S}$, $H_{\mathcal{L}} \text{ or } \mathcal{R} = \sum_{k \in \mathcal{L}/\mathcal{R}} \hbar\omega_k a_k^\dagger a_k$ are the explicit reservoir Hamiltonians composed of $N_{\mathcal{L}(\mathcal{R})}$ modes, and $H_{\mathcal{I}} = \sum_{k \in \mathcal{L}, \mathcal{R}} \sum_{i \in \mathcal{S}} \hbar v_{k,i} (c_i^\dagger a_k + a_k^\dagger c_i)$ is the interaction Hamiltonian that couples $\mathcal{S}$ to $\mathcal{L}\mathcal{R}$. The $c_i^\dagger$ (c_i) and $a_k^\dagger$ (a_k) are fermionic creation (annihilation) operators in $\mathcal{S}$ and $\mathcal{L}\mathcal{R}$, respectively. We take the index k to implicitly include relevant reservoir labels (state, spin, etc.), while ω_k and $v_{k,i}$ are the reservoir mode frequencies and system-reservoir coupling frequencies.

While steady states can form if each reservoir contains an infinite number of explicit modes [25], only a finite reservoir can be simulated. This will never give an actual steady state, making some parameter regimes and protocols (e.g., dynamic driving) difficult to access. Implicit reservoirs offer a remedy, relaxing explicit modes to equilibrium distributions at different chemical potentials and/or temperatures [26]. Simulating this requires an evolution for the density matrix ρ of the $\mathcal{L}\mathcal{S}\mathcal{R}$ composite system. A particularly useful approach is the Markovian master equation

$$\begin{aligned} \dot{\rho} = & -\frac{i}{\hbar} [H, \rho] + \sum_k \gamma_{k,+} \left(a_k^\dagger \rho a_k - \frac{1}{2} \{a_k a_k^\dagger, \rho\} \right) \\ & + \sum_k \gamma_{k,-} \left(a_k \rho a_k^\dagger - \frac{1}{2} \{a_k^\dagger a_k, \rho\} \right), \end{aligned} \quad (2)$$

where $\{\cdot, \cdot\}$ is the anticommutator. The first term gives the Hamiltonian evolution of ρ (which includes explicit reservoirs), while the remaining terms inject and deplete particles into and from modes k at a rate $\gamma_{k,+}$ and $\gamma_{k,-}$, respectively. To ensure that explicit reservoirs relax to equilibrium in the absence of $\mathcal{S}$, these rates are $\gamma_{k,+} \equiv \gamma f^\alpha(\omega_k)$ and $\gamma_{k,-} \equiv \gamma [1 - f^\alpha(\omega_k)]$, where $f^\alpha(\omega_k)$ is the Fermi-Dirac distribution in the $\alpha \in \{\mathcal{L}, \mathcal{R}\}$ reservoir [27].

When the reservoirs are at different chemical potentials μ_α (or temperatures), the bias $\mu = \mu_{\mathcal{L}} - \mu_{\mathcal{R}}$ will drive a current [28]. We call the reservoirs that are contained explicitly in the dynamics the *extended reservoirs*. This particular Markovian master equation has been widely employed (see Ref. [24]) to describe transport in noninteracting systems [23,24,29–38]. It also follows naturally from the generic approach (explicit reservoir or bath states with Markovian broadening to represent the spectral function) suggested in Ref. [39] for open-system dynamics. While it is provably correct in noninteracting and many-body cases [23,24], the extended reservoir size and γ must lie in a certain regime [23,24] to avoid unphysical relaxation artifacts. A related DMFT method uses an equation similar to Eq. (2) but optimizes relaxation (including *intermode* relaxation) to represent the reservoir spectral function [40–44]. While intermode relaxation can represent the spectral function more effectively, it increases the computational cost of the MPS simulation (we leave this for a later contribution).

In order to demonstrate the stability and behavior of tensor networks applied to the extended reservoir framework, we solve Eq. (2) with the time-dependent variational principle (TDVP) [45,46], where the density matrix is vectorized to represent it within an MPS [47,48]. While a variety of tensor network techniques exist [49–51], we use TDVP as it is highly effective, accommodating a direct time evolution for any Hamiltonian or Lindbladian that may be represented as a matrix product operator (MPO). We note that time-evolving block decimation may also be efficacious [52] and leave open the question of an optimal implementation (via purification schemes [53,54], etc.; see also Refs. [55,56] for a review). For details of our setup, refer to the note in [57].

Our approach uses the reservoirs’ energy (or momentum) bases, and thus, there is, in principle, *no requirement* for their spatial dimensionality: They can be of arbitrary dimension and have long-range hopping both within the reservoirs and to $\mathcal{S}$. The reservoirs only need to be noninteracting, without a direct coupling between left and right regions (both requirements can be relaxed [14], albeit with a loss of efficiency). As an example, we consider a system composed of two sites with the Hamiltonian

$$H_{\mathcal{S}} = \hbar v_{\mathcal{S}} (c_1^\dagger c_2 + c_2^\dagger c_1) + \hbar U n_1 n_2, \quad (3)$$

where n_i is the number operator at site i , U is the interaction strength, and $N_{\mathcal{R}} = N_{\mathcal{L}} = N$ spinless reservoir modes defined by frequencies $\omega_k = 2\omega_0 \cos[k\pi/(N+1)]$ and couplings $v_{k,i} = v\sqrt{2/(N+1)} \sin[k\pi/(N+1)]$ for $(k, i) \in \{(\mathcal{L}, 1), (\mathcal{R}, 2)\}$, where k carries a numerical (1 to N) and reservoir label. This is the single-particle eigenbasis for spatially one-dimensional reservoirs, with the left reservoir connected only to site 1 of $\mathcal{S}$ and the right connected to site 2 of $\mathcal{S}$, of hopping frequency ω_0 . Physically, this is

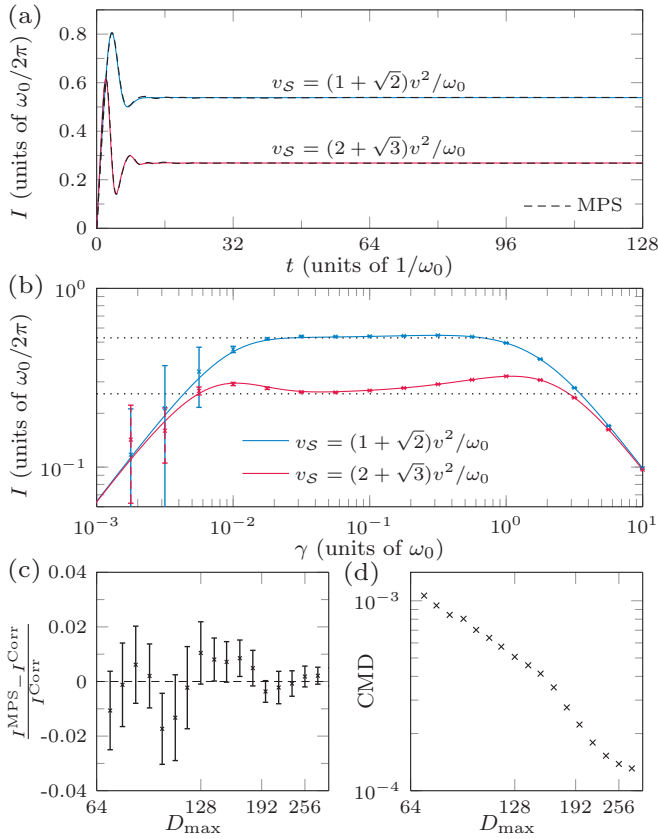


FIG. 2. Noninteracting benchmark. (a) Transient current for a noninteracting ($U = 0$), spinless, two-site system. Data are given for two values of v_S at fixed relaxation $\gamma = 0.1 \omega_0$. Mixed-basis MPS dynamics (black dashed line) match the exact result (solid colored lines) even at a modest $D_{\text{max}} = 256$. (b) Steady-state current $I(t = \infty)$ versus γ from diagonalizing the exact Lindbladian (solid lines) and the long-time limit, up to time t_{max} , of MPS propagation (data points). Exact and MPS data compare well, with deviations only in the small- γ regime. The currents for infinite reservoirs without relaxation, computed using nonequilibrium Green's functions [23,25], are shown as dotted lines. (c) Relative deviation of the current $(I^{\text{MPS}} - I^{\text{Corr}})/I^{\text{Corr}}$ and (d) relative trace distance (CMD) at the last time of the simulation between the MPS and exact results as a function of D_{max} (the relative trace distance divides the trace distance by the trace of the exact correlation matrix). (c) and (d) show the convergence in D_{max} at $\gamma = 0.1 \omega_0$ and $v_S = (1 + \sqrt{2})v^2/\omega_0$. All calculations have a bias of $\mu = \omega_0/2$ across implicit reservoirs of $N = 128$ modes each, starting from Fermi-Dirac occupations ($k_B T = \hbar\omega_0/40$), and a system-reservoir coupling $v = \omega_0/2$. The steady-state current from MPS simulations is taken as an average over the last $\Delta t = t_{\text{max}}/10$. The error bars are $\pm\sigma$, with $\sigma^2 = \sigma_1^2 + \sigma_2^2$, where σ_1 is the fluctuations of I in Δt and $\sigma_2^2 = \sum_i |I_i - I|^2/3$ is the mismatch of currents at different interfaces i . The latter likely captures the bulk of the error from truncating the bond dimension D —the dominant source of errors here.

the time-independent version of a model for photoconductive molecular devices where spin plays no role [58].

Figure 2 shows benchmark calculations of the current at $U = 0$ that compare the exact solution to the MPS simulations [59]. We calculate the current as the average across three interfaces $I = \langle I_i \rangle$, with $i \in \{\mathcal{LS}, \mathcal{SS}, \mathcal{RR}\}$, where, at the $\mathcal{LS}$

interface, $I_{\mathcal{LS}}(t) = -4 \sum_{k \in \mathcal{L}} v_k \text{Im} \langle a_k^\dagger c_1 \rangle$, with similar notation for the others [60]. In the steady state, these currents should be identical and constant. Thus, their variation in time and variance in i quantify errors within the calculation.

The transient current $I(t)$, in Fig. 2(a), rapidly reaches a steady state at intermediate reservoir relaxation and is in tight correspondence with simulations that employ the exact correlation matrix. The required D is also modest, and time evolution does not break down like closed-system approaches in the spatial basis (see Ref. [14]). Rather, once in the steady state, the current remains constant up to small, easily quantifiable errors. Prior to reaching the steady state, there are oscillations that are a manifestation of the Gibbs phenomenon [61] and its interplay with the initial state and other interactions. The rise time to a quasisteady state is set by the reservoir bandwidth ($\propto 1/\omega_0$), but ultimately, the time to reach the steady state—where all oscillations, which can be both persistent [14,62] and algebraically decaying [61], disappear—will be set by the relaxation time γ^{-1} .

The relaxation, however, also gives rise to distinct regimes of conduction, as seen in Fig. 2(b) [63]: The current initially increases linearly with γ , plateaus, and then decreases as $1/\gamma$ [64]. The three distinct regimes reflect a simulation analog of Kramers' turnover in the rate of condensed-phase reactions [65]. Instead of a turnover versus the solution friction, the electronic conductance depends on the external relaxation [23,24,37], which is a dependence also found in thermal transport [66–70]. In this context, the steady state at small γ resembles a reactive system that is rate limited by how quickly equilibrium is restored among reactants after a subset of them proceeds to products. For transport, this gives a linear dependence in γ (and N), as this gives the rate at which particles and holes are replenished in the reservoirs. At large γ , transport parallels reactions that are controlled by rapid environmental processes (e.g., solvent dynamics), which redirect intermediates along the reactive pathway back to reactants. For transport, the rapid relaxation suppresses the development of coherence, which is a necessary condition for current to flow. The intrinsic rate, when friction and relaxation are absent, is the dominant factor between small and large γ limits. Physical behavior corresponding to infinite, relaxation-free reservoirs occurs only in this intermediate regime [23,24].

In addition to performing simulations for intermediate relaxation, there are additional requirements to properly represent transport. Markovian relaxation is inherently *not physical* [23,24], as it occupies modes according to their frequencies in isolation rather than those properly broadened by contact with the implicit reservoirs. Thus, γ must be sufficiently lower than the thermal broadening, $\gamma \ll k_B T/\hbar$. The current should also be on the plateau, which occurs at $\gamma \approx W/N$, where W is the reservoir bandwidth ($W = 4\omega_0$ in our example). This requires that $N \gg \hbar W/k_B T$ for physical simulations [23,24]. In practice, we take values of γ to be on the plateau for a given N and compute errors due to the variation of N and γ . The MPS simulations work very well from large γ down to the plateau edge [Fig. 2(b)]. As γ leaves the plateau ($\gamma < W/N$), long-time coherence of particles flowing back and forth in the $\mathcal{LSR}$ system make MPS simulations difficult, albeit in a turnover regime that is uninteresting from both physical and

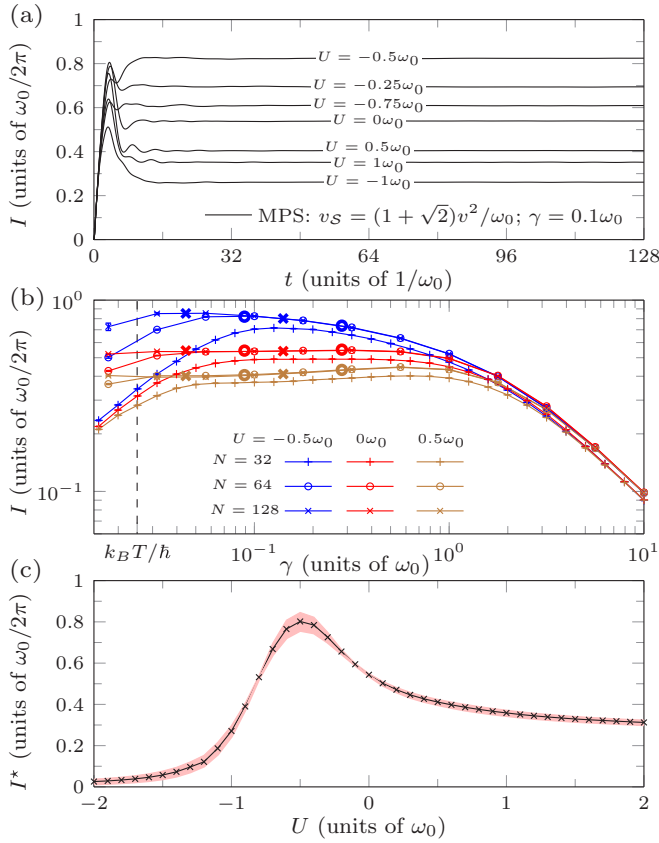


FIG. 3. Transport in an interacting, two-site system. (a) Current versus time showing the initial transient oscillations and the rapid approach to the steady state for several U and $N = 128$ with $D_{\max} = 256$. (b) Steady-state current versus γ for several values of U and at $N = 32, 64$, and 128 and $D_{\max} = 256$. This demonstrates the same regimes as the noninteracting case. Simulations are truncated at $\gamma = 0.015 \omega_0$, as converging this unphysical regime to the same accuracy as for larger γ is exceptionally costly. (c) Steady-state current in the thermodynamic limit I^* versus the many-body coupling U using $N = 128$, $\gamma^* = 10^{-3/4} 32\omega_0/N$, and $D_{\max} = 256$. All parameters are identical to those in Fig. 2 unless otherwise indicated. The error bars in (b) are the same as in Fig. 2. The error bands in (c) also include error due to improper plateau formation, σ_3^2 , which is the variance of the four bold data points in (b) (at $\gamma = 10^{-1/4} 32\omega_0/N$ and $10^{-3/4} 32\omega_0/N$ for both $N = 64$ and 128).

practical standpoints [71]. The error in the current, arising from MPS truncation, decays steadily, but nonmonotonically, with D in the plateau regime [see Fig. 2(c)]. The convergence of the state itself is monotonic in D (truncation gives the dominant source of error at fixed N and γ). We quantify this using the relative trace distance between the exact and MPS-based single-particle correlation matrices [see Fig. 2(d)].

The well-behaved nature of the simulations carries over to the many-body case. Figure 3(a) shows $I(t)$ for several values of the interaction strength U . Just as with $U = 0$, the current rapidly approaches its steady state and remains there. A modest D converges the results regardless of U . Figure 3(b) shows the current versus γ , demonstrating the existence of a many-body simulation analog to Kramers' turnover. This behavior is expected, as the junction plays only a tangential

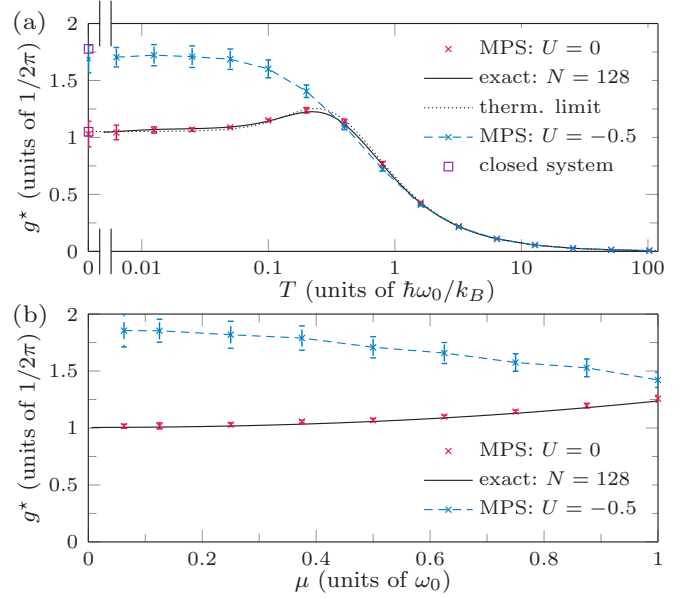


FIG. 4. Conductance versus temperature and bias. (a) Conductance versus the temperature T at $\mu = \omega_0/2$. Closed-system calculations follow Ref. [14] and use $N = 128$. (b) Conductance versus bias μ at $k_B T = \hbar\omega_0/40$. The setup for the simulations and the determination of $I^* = \sigma^* \mu$ and its error are identical to Fig. 3(c).

role in the mechanism of transport in the small- and large- γ regimes. Nonetheless, the many-body interaction does influence convergence to a smooth plateau. Moreover, the small- γ regime remains difficult for MPS but does take on a linear relationship where $I \propto \gamma$.

Using the Kramers' turnover in Fig. 3(b), we can find the best estimator I^* for the current in the thermodynamic limit and estimate its error. We take I^* to be at $\gamma^* = 10^{-3/4} 32\omega_0/N$, which is on the plateau just before the turnover to the small- γ regime. Error estimates incorporate the effect of a finite bond dimension (see σ_1 and σ_2 in Fig. 2) and plateau formation (see σ_3 in Fig. 3). In this case, incomplete plateau formation is the main contribution to the error. Figure 3(c) shows I^* versus U , which exhibits an enhanced conductance at $U = -0.5\omega_0$. There are two eigenstates in S at $\pm v_S$ when $U = 0$. When U is sufficiently large and negative, there is a bound state of two fermions in S lying outside the bias window, blocking the current (i.e., it will decay to zero as $U \rightarrow -\infty$). When U approaches but remains less than zero, the system mode at $-v_S$ is nearly occupied, and the higher-energy mode is effectively pulled down in energy by the many-body interaction. Neglecting the lower-energy mode, other than a mean-field effect on the higher-energy mode, gives a peak current at $U = -4v_S/3$. This is in reasonable agreement with the full many-body result. As U becomes repulsive, the system will begin to have only a single particle present. Nevertheless, this can sustain a finite current (half the current when $U = 0$) even as $U \rightarrow \infty$, giving rise to the asymmetry between very attractive and very repulsive interactions.

The approach can be employed in both linear response and out-of-linear response, at finite temperature, and for time-dependent processes (e.g., Floquet states or noise). Figure 4(a)

shows the conductance σ^* across a range of temperatures and biases for both interacting and noninteracting cases. There is a robust correspondence in σ^* among extended reservoir MPSs, exact correlation matrix simulations, and the thermodynamic limit from nonequilibrium Green's functions [23,25]. The magnitude of error becomes significant only when T is near zero as in Fig. 4(a). Even then, it is suitable for practical calculations. There is also good agreement with closed-system MPSs at $T = 0$ [14], with the latter being within the error estimate, confirming that our protocol is reliable. To fully approach the thermodynamic limit, N should be enlarged and γ should be diminished. Nonetheless, these data indicate that our open-system method may be applied across a broad range of parameters with no modification.

While MPS approaches have previously been employed to study transport in real time for spatially 1D models [47,62,72–79], with a numerical renormalization group approach to the reservoirs [80], and in linear response [81,82], our mixed-basis approach eliminates constraints on accessible time and spatial scales while also not requiring a one-dimensional or quasi-one-dimensional lattice for the noninteracting reservoirs [14]. The open system method here enables the direct computation of steady-state currents, making their determination comparable to finding ground states (i.e., finding a stationary state). Our approach will also be useful for find-

ing Floquet states and studying the effect of artificial gauge fields, examining time-dependent processes that perturb the system around its stationary state, handling transport when long timescales appear (e.g., due to many-body interactions), and giving the right framework for coarse-graining reservoir modes [83], all at a finite temperature that will help in the study of thermoelectrics and determining many-body temperature scales. It may also help in solving other boundary-driven problems (e.g., 1D lattices driven by Markovian processes only at the ends). Overall, this scheme will permit the accurate simulation of challenging many-body systems, where larger and more complex impurity physics gives rise to intricate behavior.

Note added. Recently, related work appeared that implemented the extended reservoir approach with MPS simulations but with different underlying machinery [84,85].

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Publication II

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Quantum transport simulations are rapidly evolving and now encompass well-controlled tensor network techniques for many-body limits. One powerful approach combines matrix product states with extended reservoirs. In this method, continuous reservoirs are represented by explicit, discretized counterparts and a chemical potential or temperature drop is maintained by external relaxation. Currents are strongly influenced by relaxation when it is very weak or strong, resulting in a simulation analog of Kramers turnover for solution-phase chemical reactions. At intermediate relaxation, the intrinsic conductance, that given by the Landauer or Meir-Wingreen expressions, moderates the current. We demonstrate that strong impurity scattering (i.e., a small steady-state current) reveals anomalous transport regimes within this methodology at weak-to-moderate and moderate-to-strong relaxation. The former is due to virtual transitions and the latter to unphysical broadening of the populated density of states. Thus, the turnover analog has *five* standard transport regimes, further constraining the parameters that lead to recovery of the intrinsic conductance. In the worst case, the common strategy of choosing a relaxation strength proportional to the reservoir level spacing can prevent convergence to the continuum limit. This advocates a simulation strategy where one utilizes the current versus relaxation turnover profiles to identify simulation parameters that most efficiently reproduce the intrinsic physical behavior.

DOI: [10.1103/PhysRevB.104.165131](https://doi.org/10.1103/PhysRevB.104.165131)**I. INTRODUCTION**

The accurate simulation of many-body transport is essential to understanding nanoscale electronics and quantum dots [1–3], quantum dynamics and control [4–7], spintronic phenomena [8–10], and the development of “atomtronic” platforms for physical simulation [11–20]. Recent developments have delivered increasingly rigorous and well-controlled numerical tools to pursue this goal. One approach employs a canonical transformation to a *mixed basis*, where energy or momentum modes are paired according to their natural scattering structure, to perform tensor network simulations that are extensive in space and time [21]. This is a substantial advance for matrix product state calculations, which are otherwise limited by the linear growth of entanglement entropy [14,20,22–30] (though some operate in linear response via the Kubo formula [31,32]). Alternative strategies have also been presented, including those that introduce a linear-logarithmic reservoir discretization and reorganize reservoir modes to improve performance [33]. All of these techniques assume closed systems, which only give quasi-steady-state currents when starting from a density or chemical potential imbalance [34,35].

The mixed-basis approach reflects a natural scattering structure, making it ideal for simulating open systems.

Notably, it can directly target steady and Floquet states, or simulate real-time noise around a stationary state [36]. Related methods have also been applied to describe quantum thermal machines [37]. These developments employ “extended” or “mesoscopic” reservoirs, where finite collections of fermionic modes are broadened by external environments to yield an effective continuum.

The extended reservoir approach (ERA) has a lengthy history, originating in the relaxation time approximation [38–44]. These early developments have evolved into a framework that describes reservoirs in terms of broadened modes [45–48]. Within this framework, nonequilibrium Green’s functions yield the exact, formal solution for both noninteracting and interacting many-body systems [49–53]. These results provide a foundation to the overall approach but are limited for *practical* many-body calculations. Consequently, most simulations have been for transport through noninteracting systems [54–65] (summarized in Ref. [50]) or classical thermal energy propagation [66–70]. However, recent developments in tensor networks deliver a general strategy for many-body calculations within the ERA and related methods. These methods have enabled large-scale simulations of many-body impurity systems [36,37,71], delivered solvers for dynamical mean-field theory [72–77], and offered new perspectives for open system dynamics [78]. The theory of extended reservoirs is thus extensive.

The ERA yields a simulation analog of Kramers turnover [49–53], where different transport behaviors are regulated by the strength of relaxation. This leads to “friction-controlled”

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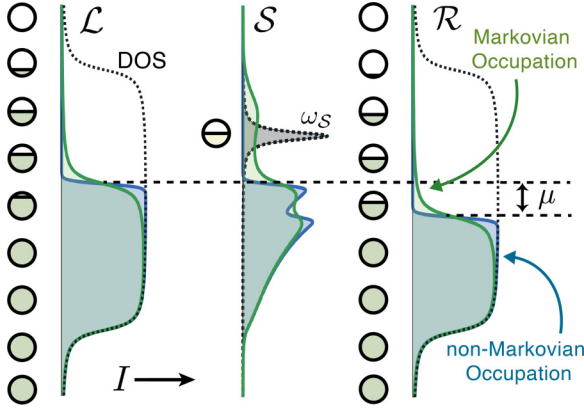


FIG. 1. Extended reservoir occupied density of states. The extended reservoir approach represents the left ($\mathcal{L}$) and right ($\mathcal{R}$) reservoirs of a device $\mathcal{S}$ using a finite collection of modes. An external environment broadens these modes through Markovian or non-Markovian relaxation, which we depict using the occupied density of states for thermodynamic limit (green or blue, respectively). Transport is then driven by a chemical potential difference μ across $\mathcal{L}/\mathcal{R}$, affording a current I through $\mathcal{S}$. We show a single mode ω_S in isolation (gray, dotted line assuming a small broadening) and depict its occupied DOS when hybridized with Markovian or non-Markovian reservoirs (green or blue, respectively). Practical calculations generally require Markovian relaxation. This can anomalously broaden the populated DOS, necessitating judicious parametrization. Data are from the single-site impurity model in Eq. (14) with $\omega_S = \omega_0$, system-reservoir hopping $v = \omega_0/8$, $N_W = 128$ equally spaced reservoir modes, and $\gamma = \omega_0/5$, lying on the low- γ side of a Markovian anomaly.

currents at very weak (contact-limited) and strong (over-damped) relaxation, with the physically relevant conductance moderating the current at some point between these limits. Here, we go beyond prior developments and demonstrate that additional transport regimes are unveiled for strong impurity scattering. One of these is a *virtual anomaly* associated with tunneling processes and the other a *Markovian anomaly* that emerges from the unphysical Markovian broadening of the occupied density of states (DOS). These regimes become pronounced at weak system-reservoir coupling, revealing very large currents relative to the continuum limit (i.e., the physically relevant current given by the Landauer or Meir-Wingreen expressions for noninteracting and many-body impurities, respectively). Additional features can emerge due to unrelated processes (e.g., strongly off-resonant tunneling) but the five regimes we discuss appear to be universal, persisting even for weak scattering [36] and are enhanced when destructive interference is present in the impurity [65].

II. BACKGROUND

We will focus on transport through a central system $\mathcal{S}$ driven by a chemical potential or temperature drop across noninteracting left ($\mathcal{L}$) and right ($\mathcal{R}$) reservoirs (see Fig. 1) [79–81]. The full Hamiltonian is

$$H = H_S + H_{\mathcal{L}} + H_{\mathcal{R}} + H_{\mathcal{I}}, \quad (1)$$

where the system Hamiltonian H_S may contain many-body interactions, including electron-electron, electron-photon, and electron-vibration couplings. Furthermore, the reservoir Hamiltonians $H_{\mathcal{L}(\mathcal{R})} = \sum_{k \in \mathcal{L}(\mathcal{R})} \hbar \omega_k c_k^\dagger c_k$ describe a collection of explicit, noninteracting modes of frequencies ω_k ($\hbar$ is the reduced Planck's constant). A quadratic Hamiltonian $H_{\mathcal{I}} = \sum_{k \in \mathcal{L}\mathcal{R}} \sum_{i \in \mathcal{S}} \hbar (v_{ki} c_k^\dagger c_i + v_{ik} c_i^\dagger c_k)$ couples $\mathcal{S}$ to $\mathcal{L}\mathcal{R}$ with strength $v_{ik} = v_{ki}^*$, where c_m ($c_m^\dagger$) are fermionic annihilation (creation) operators for a level $m \in \mathcal{L}\mathcal{S}\mathcal{R}$. We take the index of sites in $\mathcal{L}\mathcal{S}\mathcal{R}$ to include all relevant labels (state, spin, reservoir, or system, etc.) and sum over all states in a given region.

Finite reservoirs only support a stationary current when external reservoirs are present. Thus, we will solve the (Markovian) Lindblad master equation

$$\begin{aligned} \dot{\rho} = & -\frac{i}{\hbar} [H, \rho] + \sum_{k \in \mathcal{L}\mathcal{R}} \gamma_{k+} \left(c_k^\dagger \rho c_k - \frac{1}{2} \{c_k c_k^\dagger, \rho\} \right) \\ & + \sum_{k \in \mathcal{L}\mathcal{R}} \gamma_{k-} \left(c_k \rho c_k^\dagger - \frac{1}{2} \{c_k^\dagger c_k, \rho\} \right) \end{aligned} \quad (2)$$

for the $\mathcal{L}\mathcal{S}\mathcal{R}$ system with Markovian relaxation in $\mathcal{L}\mathcal{R}$ ($\{\cdot, \cdot\}$ is the anticommutator) and a corresponding scenario for non-Markovian relaxation. Throughout this work, we use the term Markovian relaxation when it follows from a time-local Lindblad master equation as in Eq. (2). Non-Markovian relaxation corresponds to evolution with similar retarded and advanced Green's functions, but instead with proper occupations as described in Sec. II A; that would, however, follow from an inherently non-time-local master equation. Reference [49] shows the Hamiltonian for the $\mathcal{L}\mathcal{S}\mathcal{R}$ system and environment that gives rise to the non-Markovian equation of motion when the environment is integrated out.

The first term in Eq. (2) gives the evolution of the full, many-body density matrix ρ according to the Hamiltonian H in Eq. (1). Open dynamics arise from the Lindbladian terms, which inject or deplete particles to or from the modes k at rates γ_{k+} and γ_{k-} , respectively. If we adopt a convention where these rates are $\gamma_{k+} \equiv \gamma_k f^\alpha(\omega_k)$ and $\gamma_{k-} \equiv \gamma_k [1 - f^\alpha(\omega_k)]$, the $\mathcal{L}\mathcal{R}$ reservoir modes will relax to an equilibrium Fermi-Dirac distribution $f^\alpha(\omega_k)$ (with $\alpha \in \{\mathcal{L}, \mathcal{R}\}$) when decoupled from $\mathcal{S}$. The chemical potential μ_α of each reservoir is included in $f^\alpha(\omega_k)$, where we take $\mu_{\mathcal{L}} = -\mu_{\mathcal{R}} = \mu/2$ for the potential bias between reservoirs μ . The result is a pseudoequilibrium state, as it does not incorporate relaxation-induced broadening of the extended reservoirs' modes. We will show how this leads to a transport anomaly at moderate to strong γ .

Reference [49] provides the formal solution for the steady-state current corresponding to Eq. (2), which is valid both for interacting and noninteracting many-body systems $\mathcal{S}$ (see Refs. [52,53] for a unified derivation and fully analytic solutions for proportional coupling). It was also proven that the formal solution limits to either the Meir-Wingreen expression or the Landauer formula. These expressions require us to find the single-particle Green's function in a system with many-body interactions. This can be complicated and often requires many approximations. Alternatively, one can solve Eq. (2) numerically using established techniques such as tensor networks (as recently applied to transport in Refs. [36,37,71]).

We begin by addressing systems that are proportionally coupled to the electrodes. This requires identical distributions of mode frequencies and relaxation strengths in each finite, extended reservoir. The distribution of the system-reservoir coupling constants must also be the same up to some overall proportionality constant. We will show that if we apply a small level shift between reservoirs, we can effectively “turn off” the virtual anomaly. This general observation will carry over to nonproportionally coupled and interacting setups. Even if the continuum limit has such a symmetry, there can be finite representations that limit to proportional coupling yet have it formally broken. In fact, breaking proportional coupling and using non-Markovian relaxation results in a three-regime Kramer turnover, which is more well behaved, with both anomalies removed.¹

A. Steady-state current

The steady-state current associated with Eq. (2) has an exact solution for arbitrary noninteracting systems and reservoirs [49,52,53]

$$I = e \int \frac{d\omega}{2\pi} \text{tr}[\tilde{\Gamma}^{\mathcal{L}} \mathbf{G}^a \Gamma^{\mathcal{R}} \mathbf{G}^r - \Gamma^{\mathcal{L}} \mathbf{G}^r \tilde{\Gamma}^{\mathcal{R}} \mathbf{G}^a], \quad (3)$$

encompassing both Markovian and non-Markovian relaxation. Here, e is the electron charge, $\mathbf{G}^{r(a)}$ is the retarded (advanced) Green’s function of the full system, and $\Gamma^{\mathcal{L}(\mathcal{R})}$ ($\tilde{\Gamma}^{\mathcal{L}(\mathcal{R})}$) are the unweighted (weighted) spectral functions (we note to the reader that in some contexts the spectral function is also known as a “hybridization function”), which all depend on the frequency ω . We employ notation where bold symbols indicate matrices with standard matrix multiplication assumed. For non-Markovian (nM) relaxation, this formula reduces to

$$I^{\text{nM}} = e \int \frac{d\omega}{2\pi} (f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)) \text{tr}[\Gamma^{\mathcal{L}} \mathbf{G}^r \Gamma^{\mathcal{R}} \mathbf{G}^a], \quad (4)$$

where we indicate specific conditions for the equation by labeling the equality (i.e., here “nM” indicates that this expression is for non-Markovian relaxation). The explicit forms for the underlying Green’s functions are $\mathbf{G}^{r(a)} = 1/(\omega - \tilde{\mathbf{H}}_{\mathcal{S}} - \Sigma^{r(a)})$ with self-energies $\Sigma^{r(a)} = \sum_{k \in \mathcal{LR}} g_k^{r(a)} |v_k\rangle \langle v_k|$. These expressions are identical for Markovian and non-Markovian relaxation. We use $|v_k\rangle$ to denote the coupling vector between mode $k \in \mathcal{LR}$ and all sites $i \in \mathcal{S}$, i.e., $\langle i | v_k \rangle = v_{ik}$, and write $g_k^{r(a)} = 1/(\omega - \omega_k \pm i\gamma_k/2)$ for the retarded (advanced) Green’s function with $k \in \mathcal{LR}$. These latter quantities have $\gamma_k > 0$ but are isolated from the system. The single-particle Hamiltonian describing $\mathcal{S}$ is $\tilde{\mathbf{H}}_{\mathcal{S}}$, where $\mathbf{H}_{\mathcal{S}} = \sum_{i,j \in \mathcal{S}} [\tilde{\mathbf{H}}_{\mathcal{S}}]_{i,j} c_i^\dagger c_j$. General and exact results for the steady-state current with many-body impurities, in the presence of Markovian and non-Markovian relaxation, can be found in Refs. [49,53]. We study many-body systems numerically, and provide analytic results for noninteracting systems.

¹Breaking proportional coupling is much more reflective of physical reality, where defects and other inhomogeneities in structure will break such a strong symmetry.

As a final component, one also needs the spectral density $\Gamma^{\mathcal{L}(\mathcal{R})} = i(\Sigma_{\mathcal{L}(\mathcal{R})}^r - \Sigma_{\mathcal{L}(\mathcal{R})}^a) = -2 \text{Im} \Sigma_{\mathcal{L}(\mathcal{R})}^r$,

$$\Gamma^{\mathcal{L}(\mathcal{R})}(\omega) = i \sum_{k \in \mathcal{L}(\mathcal{R})} [g_k^r(\omega) - g_k^a(\omega)] |v_k\rangle \langle v_k|. \quad (5)$$

The population-weighted counterpart is

$$\tilde{\Gamma}^{\mathcal{L}(\mathcal{R})}(\omega) = i \sum_{k \in \mathcal{L}(\mathcal{R})} \tilde{f}_k [g_k^r(\omega) - g_k^a(\omega)] |v_k\rangle \langle v_k|. \quad (6)$$

Based on this, Markovian and non-Markovian relaxation only differ in how we evaluate the Fermi-Dirac occupations $\tilde{f}_k$,

$$\tilde{f}_k = \begin{cases} f^\alpha(\omega) & \text{non-Markovian,} \\ f^\alpha(\omega_k) & \text{Markovian} \end{cases} \quad (7)$$

for reservoir $\alpha \in \{\mathcal{L}, \mathcal{R}\}$ and $f^\alpha(\omega)$ having bias μ_α . These distributions set mode occupations to an inherently unphysical Markovian equilibrium or to a physical non-Markovian equilibrium. The latter occupies modes to give an appropriate broadening and thus gives a proper Fermi level as shown in Fig. 1.

For systems that are proportionally coupled yet otherwise arbitrary (e.g., in structure, with or without many-body interactions, and for Markovian or non-Markovian relaxation), the steady-state current is [52,53]

$$I \stackrel{\lambda}{=} i e \frac{\lambda}{1+\lambda} \int \frac{d\omega}{2\pi} \text{tr}[\Delta \tilde{\Gamma} \{\mathbf{G}^r - \mathbf{G}^a\}], \quad (8)$$

where we use label “ λ ” to indicate proportional coupling. Stated formally, this means that [80,81]

$$\Gamma^{\mathcal{R}} = \lambda \Gamma^{\mathcal{L}} \equiv \lambda \Gamma \quad (9)$$

for some positive constant λ . The current $I = \frac{\lambda}{1+\lambda} I_{\mathcal{L}} + \frac{1}{1+\lambda} I_{\mathcal{R}}$ is then an average over the left, $I_{\mathcal{L}}$, and right, $I_{\mathcal{R}}$, currents to/from $\mathcal{S}$. The current in Eq. (8) also contains a difference in weighted spectral densities

$$\Delta \tilde{\Gamma} \stackrel{\lambda}{=} i \sum_{k \in \mathcal{L}} (\tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}}) [g_k^r(\omega) - g_k^a(\omega)] |v_k\rangle \langle v_k|, \quad (10)$$

where the sum only runs over states k in the left reservoir. As per the proportional coupling requirements, the left and right reservoirs are equivalent in their mode placement and relaxation, with couplings related by $v_{k'i} = v_{ki} \sqrt{\lambda} \delta_{kk'}$ with $k' \in \mathcal{R}$, $k \in \mathcal{L}$. The factor of λ does not appear in Eq. (10), as averaging brings it out front in Eq. (8).

We may simplify this further for Markovian (M) relaxation. The occupation factors in Eq. (8) are then evaluated at ω_k , removing them from the ω integration and giving an analytic expression [52,53]

$$I \stackrel{\lambda, \text{M}}{=} \frac{-2e\lambda}{1+\lambda} \sum_{k \in \mathcal{L}} (\tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}}) \langle v_k | \text{Im} [\mathbf{G}^r(\omega_k + i\gamma_k/2)] | v_k \rangle. \quad (11)$$

The integral in Eq. (8) cannot be evaluated for the non-Markovian case due to the appearance of $f^\alpha(\omega)$.

B. Kramers turnover

In the presence of relaxation, particle and thermal transport yield behavior analogous to Kramers turnover for condensed-phase chemical reaction rates [49,68]. Stated succinctly,

Kramers problem describes reactants that must overcome a free-energy barrier to become products, while also being subject to friction and noise due to the encapsulating solvent [82,83]. When friction is weak, the reaction rate will be linearly proportional to the strength of this friction. This quantity defines the rate at which equilibrium is reestablished, restoring the proportion of reactants that possess sufficient free energy to overcome the barrier. For large friction, this restoration process is rapid. However, strong friction can localize reactants in the initial state, decreasing the reaction rate in inverse proportion to the frictional strength. Between these limits there is a region where the intrinsic, transition state rate is dominant.

A similar phenomenon occurs for transport simulations. At weak relaxation (friction, noise), the current is limited by coupling to the external (implicit) environments, which control the rate of particle injection and depletion in the reduced $\mathcal{LSR}$ system. This regime is characterized by a current [49,52,53]

$$I \approx^{\lambda, M} \frac{2e\lambda}{(1+\lambda)^2} \sum_{k \in \mathcal{L}} \gamma_k (\tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}}), \quad (12)$$

where factors γ_k contribute proportionally.

Conversely, at strong relaxation, coherence with the central region is destroyed, localizing particles in the extended reservoir modes. This results in the current [49,52,53]

$$I \approx^{\lambda, M} \frac{4e\lambda}{1+\lambda} \sum_{k \in \mathcal{L}} \frac{|v_k|^2}{\gamma_k} (\tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}}), \quad (13)$$

with $|v_k|^2 = \langle v_k | v_k \rangle$, and the factors γ_k giving inversely proportional contributions.

Equations (12) and (13) give the asymptotic limits of Eq. (11) for Markovian relaxation and proportional coupling, with a linear regime for weak relaxation and an inverse regime at strong. The primary objective of this paper is to extend prior developments [49] by accounting for additional regimes that occur for weak coupling and nonresonant conditions. We will show that these linear and inverse regimes flank a pair of anomalous transport regimes. These anomalous regimes, in turn, flank the physical regime corresponding to continuum reservoirs (where relaxation is not present).

C. Example models

For demonstrative purposes, we will focus on two central systems $\mathcal{S}$: a single-site (noninteracting) impurity and a two-site (interacting) impurity. For the single-site case,

$$H_{\mathcal{S}} = \hbar \omega_{\mathcal{S}} c_1^\dagger c_1, \quad (14)$$

with onsite mode frequency $\omega_{\mathcal{S}}$. As a representative many-body model, we take

$$H_{\mathcal{S}} = \hbar v_{\mathcal{S}} (c_1^\dagger c_2 + c_2^\dagger c_1) + \hbar U n_1 n_2, \quad (15)$$

where the hopping frequency between sites is $v_{\mathcal{S}}$, the number operator is $n_j = c_j^\dagger c_j$, the density-density interaction strength is U , and onsite mode frequencies are fixed at zero.

We consider a setup, where the central region $\mathcal{S}$ is situated between spatially one-dimensional (1D) reservoirs i.e., one-dimensional chains with hopping of frequency ω_0 between nearest-neighbor lattice sites. The last site of each reservoir

is attached to a single site of $\mathcal{S}$ via hopping frequency v . This makes for a unique arrangement in the single-site model.

For the two-site model, we address two variants of attachment. First, we consider the destructive interference model of Ref. [65] (but with a many-body interaction U), where the first site is connected to both reservoirs and the second to neither (i.e., it is proportionally coupled). In the second variant, the sites form a serial junction with the first site connected only to $\mathcal{L}$ and the second only to $\mathcal{R}$, as in Ref. [36]. There is no proportional coupling in this case since each site is coupled to a single reservoir.

In the continuum limit, when each reservoir chain extends to infinity, each of our reservoirs contributes to retarded self-energy of the system site it is attached to so that (see, e.g., Ref. [49])

$$\Sigma^r = \frac{8v^2}{W^2} \left(\omega + i\frac{\gamma}{2} - i\sqrt{\frac{W^2}{4} - \left(\omega + i\frac{\gamma}{2} \right)^2} \right), \quad (16)$$

where $W = 4\omega_0$ is the reservoir bandwidth. Equation (16) is sufficient to derive the Green's functions and spectral densities. This choice will minimally impact most of the results. This also holds for the performance of numerical simulations, where we employ the reservoirs' energy bases instead of their chain representations. Nonetheless, our numerical results will be specific to this setup and some equations will be specific to the 1D DOS.

The reservoirs can be discretized in a number of ways, provided that they reproduce the continuum in the asymptotic limit. We will present equations for “evenly spaced” (ES) reservoir modes as well as “transformed spacing” (TS). TS is defined by the eigenfrequencies of a finite, spatially one-dimensional chain of $N_{\mathcal{W}}$ sites. These can be found using the canonical transformation $c_k = \sum_{j \in \alpha} \mathcal{U}_{kj}^\dagger c_j$ with $\mathcal{U}_{kj}^\dagger = \sqrt{2/(N_{\mathcal{W}} + 1)} \sin[jk\pi/(N_{\mathcal{W}} + 1)]$ and $k = 1, \dots, N_{\mathcal{W}}$. This yields frequencies $\omega_k = 2\omega_0 \cos[k\pi/(N_{\mathcal{W}} + 1)]$ and couplings $v_{ki} = v_k = v\sqrt{2/(N_{\mathcal{W}} + 1)} \sin[k\pi/(N_{\mathcal{W}} + 1)]$. We note that k carries both a numerical index and a reservoir index α . This discretization gives the system-reservoir coupling at the Fermi level ($\hbar\omega_F = 0$)

$$|v_F|^2 \stackrel{\text{TS}}{=} |v|^2 \Delta_F / (\pi\omega_0), \quad (17)$$

as well as the level spacing

$$\Delta_F = 2\omega_0\pi/(N_{\mathcal{W}} + 1). \quad (18)$$

These quantities will be used below. Similar expressions hold for the evenly spaced discretization, where we have

$$|v_F|^2 \stackrel{\text{ES}}{=} |v|^2 \Delta_0 / (\pi\omega_0) \quad (19)$$

and

$$\Delta_0 = W/N_{\mathcal{W}} = 4\omega_0/N_{\mathcal{W}}, \quad (20)$$

where reservoir modes ω_k are placed in midpoints of each of the $N_{\mathcal{W}}$ bins of size Δ_0 (thus filling in the bandwidth). We employ the midpoint approximation to set coupling constants to the reservoirs in our MPS calculations, and ensure that they properly limit to the continuum, i.e., $v_{kj} = 2v[\Delta_k/(\pi W)\sqrt{1 - (2\omega_k/W)^2}]^{1/2}$ for the interval $\omega_k \pm \Delta_0/2$. This coupling method performs comparably to the integrated

coupling for common reservoir discretization methods [84], where one integrates the spectral density over a symmetric frequency range $\omega_k \pm \Delta_0/2$ about the finite reservoir mode ω_k . This integrated quantity allows one to define an equivalent coupling for ω_k that maintains the total weight from the continuum reservoir in this spectral region, given by $v_{kj} = v\pi^{1/2}[K(\omega_k + \Delta_k/2) - K(\omega_k - \Delta_k/2)]^{1/2}$ where $K(\omega) = 2\omega/W(1 - 4\omega^2/W^2)^{1/2} + \csc^{-1}[W/(2\omega)]$. We use these integrated couplings for our exact, noninteracting calculations.

III. RESULTS

Figure 1 depicts a typical extended reservoir and its weighted spectral functions (i.e., the occupied density of states in the reservoirs). The DOS and occupied DOS are taken from continuum limit expressions for a single site coupled to a pair of one-dimensional reservoirs (transformed to the energy basis). It is clear that non-Markovian relaxation results in an actual Fermi level, while Markovian relaxation gives unphysical broadening.² This broadening is responsible for the anomaly observed at moderate-to-strong relaxation strength, as well as for the zero-bias currents associated with asymmetric (nonproportionally coupled) reservoirs [49].

Figure 2 shows the steady-state current for Markovian relaxation, Eq. (11), for the single-site model in Eq. (14). When the coupling is strong ($v \approx \omega_0$), the current assumes a well-defined plateau as a function of the relaxation rate γ . We take γ to be the same for all reservoir modes. It is here that the steady-state current generically reproduces the continuum reservoir limit. This plateau is markedly different at weak coupling ($v \ll \omega_0$), where large features exist at moderately small and moderately large γ (the peaks of which mark the plateau edges at strong coupling). Situated between these features is a regime that corresponds to the continuum limit (Landauer's formula for noninteracting cases), a region that increases in size for larger reservoirs.

We will address the origin of these anomalies in linear response, as the resulting expressions are easily interpreted (the same underlying phenomena occur out of linear response). Notably, the non-Markovian and Markovian relaxation have different forms, yielding distinct implications. Starting from Eq. (8), the current for non-Markovian relaxation is

$$I \approx_{\text{lr}}^{\lambda, \text{nM}} -\frac{e\mu}{\pi} \frac{\lambda}{1+\lambda} \text{tr}[\Gamma \text{Im} \mathbf{G}^r]|_{\omega=0}, \quad (21)$$

where $\mu = \mu_{\mathcal{L}} - \mu_{\mathcal{R}}$ is a symmetrically applied bias, resulting in evaluation at $\omega = 0$ (although it can be evaluated anywhere in the suitably small bias window). Here, we have also replaced the difference in the weighted spectral density with the spectral density of $\mathcal{L}$. In contrast, Markovian relaxation gives

$$I \approx_{\text{lr}}^{\lambda, \text{M}} -\frac{eN_{\mathcal{B}}}{\pi} \frac{\lambda}{1+\lambda} \int d\omega \text{tr}[\Gamma_F \text{Im} \mathbf{G}^r]. \quad (22)$$

²We note that this unphysical behavior specifically refers to applicability when describing fermions, as Lindblad master equations always give a mathematically proper quantum evolution.

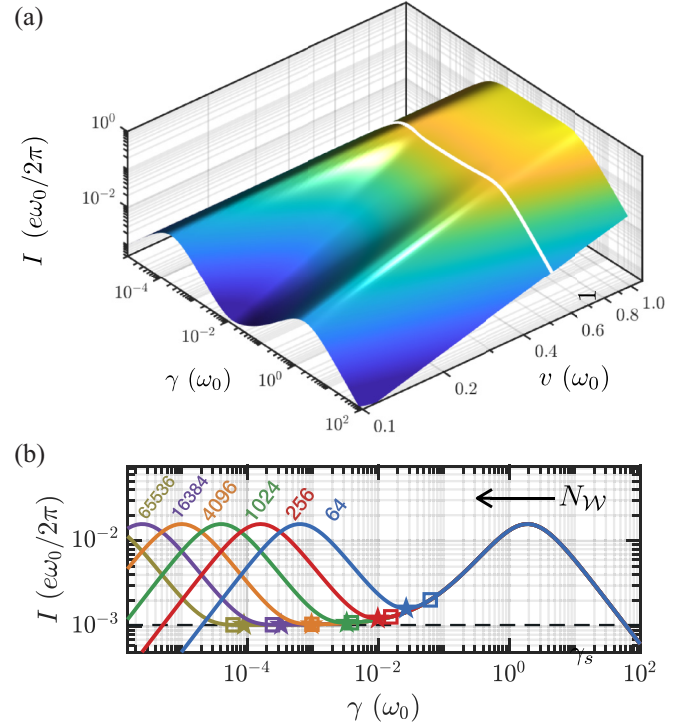


FIG. 2. Anomalous currents and Kramers turnover for a single-site impurity. (a) Kramers turnover versus relaxation γ and coupling v . Strong scattering (weak coupling) reveals two regimes: a “virtual anomaly” for weak-to-moderate relaxation and a “Markovian anomaly” for moderate-to-strong relaxation. The former is due to resonant $\mathcal{L}, \mathcal{R}$ modes which artificially increase particle currents. The respective virtual transitions through $\mathcal{S}$ are eventually overdamped and turn over. The Markovian anomaly is due to unphysical smearing of the populated DOS by the relaxation, again increasing the current. This too is ultimately overdamped at stronger relaxation. These regimes flank the intermediate γ regime where the continuum limit is best recovered. Results correspond to a single-site impurity in Eq. (14) with $\omega_{\mathcal{S}} = \omega_0$, and $N_{\mathcal{V}} = 128$ equally spaced reservoir modes. Couplings are given by the (integrated) strength within each mode bin and the bias is $\mu = \omega_0/2 = 2\mu_{\mathcal{L}} = -2\mu_{\mathcal{R}}$. The white line designates the onset of the anomaly parameter space, according to Eq. (33). (b) Kramers turnover at weak coupling versus γ for several $N_{\mathcal{V}}$. On the logarithm scale, the size of the continuum regime is proportional to $\log N_{\mathcal{V}}$, while anomalies slow its convergence to the Landauer limit (dashed black line). Parameters are the same as in (a) but at $v = \omega_0/8$ and for various $N_{\mathcal{V}}$. Stars denote the optimal relaxation γ^* while squares correspond to $\gamma^{\square}$ (a popular choice; proportional to the level spacing in the reservoirs), demonstrating a shift of $\gamma^{\square}$ from the optimum.

The integral is the key difference: this gives an overlap of the system DOS at all frequencies with the spectral density, while taking only contributions from the Fermi level modes (taken at $\omega_k = 0$ and designated F),

$$\Gamma_F = \iota[g_F^r(\omega) - g_F^a(\omega)]|v_F\rangle\langle v_F|. \quad (23)$$

Alternatively, we can start with the analytic solution (11) for Markovian relaxation, yielding

$$I \approx_{\text{lr}}^{\lambda, \text{M}} -2eN_{\mathcal{B}} \frac{\lambda}{1+\lambda} \langle v_F | \text{Im} \mathbf{G}_F^r | v_F \rangle, \quad (24)$$

which is equivalent to Eq. (22). The Green's function

$$\mathbf{G}_F^r = \mathbf{G}^r(0 + i\gamma_F/2) \quad (25)$$

is at the Fermi level (assuming a smooth γ_k there) and

$$N_B = \sum_{k \in \mathcal{L}} \tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}} \approx \begin{cases} 2N_W \frac{\mu}{\pi W} & \text{for TS,} \\ N_W \frac{\mu}{W} & \text{for ES} \end{cases} \quad (26)$$

is the effective number of modes in the bias window, which is typically not an integer (though it will be at zero temperature and for particular arrangements of modes). Linear response requires that $\tilde{f}_k^{\mathcal{L}} - \tilde{f}_k^{\mathcal{R}}$ is negligible except around the Fermi level or, more broadly, non-negligible only in the region where there is little variation for the other factors present in Eq. (24). The approximate equality in Eq. (26) reflects that the level spacing varies in the bias window and that modes can cover more than just the bias window (e.g., μ/Δ_F is not always an integer).³

The non-Markovian and Markovian expressions (21) and (22) converge when relaxation is weak. The difference between these is nonetheless pronounced at strong relaxation, where non-Markovian effects give an overlap between the spectral density and system DOS around the Fermi level. Conversely, Markovian relaxation gives an overlap over all frequencies. This issue originates in the violation of the fluctuation-dissipation theorem and has important consequences.

We will examine this behavior in detail for a single-site impurity. Its Green's function is

$$\mathbf{G}^r \stackrel{\lambda}{\approx} \frac{1}{\omega - \omega_S - (1 + \lambda) \sum_{k \in \mathcal{L}} \frac{|v_k|^2}{\omega - \omega_k + i\gamma_k/2}}, \quad (27)$$

where ω_S is onsite frequency for the impurity and v_k is a scalar since there is only one site in $\mathcal{S}$. In the following, we will take equally spaced reservoir modes that are finite realizations of a one-dimensional lattice with real-space hopping frequency ω_0 . Nonetheless, all of our analytic results will apply to arbitrary, proportionally coupled reservoirs (see Sec. II C). For simplicity we assume a homogeneous relaxation rate, i.e., $\gamma_k = \gamma$.

Employing Eq. (27) in Eq. (24) allows us to interpolate between all regimes for weak system-reservoir coupling (WC). At very small γ , the contribution from the self-energy becomes dominant and $\mathbf{G}^r$ scales proportional to γ , yielding $I \propto \gamma$. Conversely, for very large γ , the self-energy contribution is small. However, since Eq. (24) is evaluated at $\omega_k + i\gamma/2$, the dominant factor in $\mathbf{G}^r$ is inversely proportional to relaxation rate leading to $I \propto 1/\gamma$. Approximating the self-energy with the dominant contribution at small γ , the current is

$$I \stackrel{\lambda, \text{M, WC}}{\approx}_{\text{lr}} \frac{2e\lambda N_B |v_F|^2}{1 + \lambda} \frac{\gamma/2 + (1 + \lambda)|v_F|^2/\gamma}{\omega_S^2 + (\gamma/2 + (1 + \lambda)|v_F|^2/\gamma)^2}, \quad (28)$$

where the reservoir size is embedded in both N_B [see Eq. (26)] and $|v_F|^2 \propto v^2/N_W$. This approximate interpolation breaks down at large system-reservoir coupling but becomes exact

as the coupling goes to zero for off-resonant tunneling (e.g., ω_S outside of the bias window). It nonetheless captures the physics of different turnover regimes, as well as their quantitative behavior when coupling is weak. For finite reservoirs, this expression converges to the exact *finite reservoir* result, not the Landauer formula, as $|v|^2/\omega_S$ drops below the finite level spacing. Here, v is the total, real-space coupling and not v_k which already depends on $1/\sqrt{N_W}$. Due to this, the order of limits is important, as we will discuss later.

As a point of reference, we introduce I° to denote the continuum (Landauer) result

$$I^\circ \stackrel{\lambda}{\approx}_{\text{lr}} \frac{e}{2\pi} \frac{4\lambda|v|^4}{(1 + \lambda)^2|v|^4 + \omega_0^2\omega_S^2} \mu. \quad (29)$$

This expression is given in linear response. Nonetheless, the correspondence with the extended reservoir approach also becomes exact for nonlinear response and arbitrary $\mathcal{S}$ as the reservoirs approach the continuum and relaxation limits to zero [49,52,53].

A. Duality between current anomalies

We can isolate specific aspects of turnover by rewriting Eq. (28) in a Lorentzian form for the weak-to-moderate and moderate-to-strong anomalies,

$$I \stackrel{\lambda, \text{M, WC}}{\approx}_{\text{lr}} \frac{2e\lambda N_B |v_F|^2}{1 + \lambda} \frac{\tilde{\gamma}}{\omega_S^2 + \tilde{\gamma}^2}. \quad (30)$$

This expression permits an easy separation of relaxation regimes,

$$\tilde{\gamma} \Rightarrow (1 + \lambda)|v_F|^2/\gamma \Leftrightarrow \begin{matrix} \text{small } \gamma \\ \tilde{\gamma} \Rightarrow (1 + \lambda)|v_F|^2/\gamma \end{matrix} \Leftrightarrow \begin{matrix} \text{large } \gamma \\ \tilde{\gamma} \Rightarrow \gamma/2 \end{matrix} \quad (31)$$

which are distinguished by the parameter $\tilde{\gamma}$.⁴ We immediately find some useful results. First and foremost, the anomalous current maximum $I^\top$ is the same for both anomalies, *independent* of N_W , and is given by

$$I^\top \approx \frac{e\lambda N_B |v_F|^2}{1 + \lambda} \frac{1}{\omega_S} \stackrel{\text{ES}}{\approx} \frac{e\lambda|v|^2\mu}{(1 + \lambda)\pi\omega_0\omega_S}. \quad (32)$$

The second expression assumes evenly spaced modes (that represent a one-dimensional spectral function). In linear response, this implies that the current anomaly will surpass the Landauer value by a factor of

$$\frac{I^\top}{I^\circ} \stackrel{\text{ES}}{=} \frac{\omega_0\omega_S}{2(1 + \lambda)|v|^2}, \quad (33)$$

where the Landauer current I° is in Eq. (29). This relation diverges as the coupling decreases, implying that the anomalies progressively dwarf the Landauer current. If we take $I^\top = I^\circ$ at weak coupling, Eq. (33) yields the parameter values where the anomalous regime is revealed [see the white turnover curve in Fig. 2(a)].

³For closed systems, one will get systematic errors when the mode “bins” do not exactly fill the bias window [34].

⁴While we expect some other models will show such a strong duality, it will not be general. However, we expect the qualitative discussion to apply beyond the one-site impurity and that some of the quantitative expressions for weak coupling will hold.

At weak coupling, the current (28) will not develop a well-defined plateau, but will instead give a distinct minimum between anomalies. Due to the nature of this arrangement, this minimum will occur at the *geometric* midpoint between the anomalies. This will not hold for strong coupling, as the minimum will be distorted by nonperturbative effects. Note that additional features may appear in this region, such as an additional nonlinear dip for strongly off-resonant tunneling.

The duality (30) also indicates that the maximum of both anomalies will be found at $\tilde{\gamma} = \omega_S$, as defined by the two particular $\tilde{\gamma}$.⁵ The *optimal* relaxation γ^* for estimating the current is at their geometric mean

$$\gamma^* \stackrel{\text{WC}}{\approx} |v_F| \sqrt{2(1+\lambda)} \stackrel{\text{ES}}{=} 2|v| \sqrt{\frac{2(1+\lambda)}{\pi N_W}} \quad (34)$$

in the weak-coupling limit. By this, we mean that it gives the best estimate for the Landauer limit while excluding the “accidental” crossings within the $I \propto \gamma$ and the $I \propto 1/\gamma$ regimes. We write Eq. (34) as an approximate expression since it only becomes exact when we take $v \rightarrow 0$.⁶ Figure 3 shows how the optimal estimator behaves across coupling regimes when we go to very large N_W . We indeed find consistency with Eq. (34) when N_W is small and coupling is weak, observing a γ^* that scales as $N_W^{-1/2}$. However, this shifts to different asymptotic behavior as N_W is increased. The origin of this discrepancy lies in how we take limits for Eq. (28) and subsequent results. That is, our analytical solution is predicated on limiting to $v \rightarrow 0$ at a fixed N_W , while the procedure used in Fig. 3 effectively limits to $N_W \rightarrow \infty$ at fixed v . Despite this caveat, Eq. (34) will still hold at small and moderate N_W and thus for most practical simulations.

Equation (34) is peculiar. Folklore suggests that an appropriate γ should be comparable to the level spacing in the reservoirs. Indeed, this assumption is used in most of the literature. For large coupling, this is correct: the linear in γ region terminates upon reaching the Landauer plateau near a transition point at $\gamma \propto 1/N_W$ [49]. The same behavior also occurs for the case discussed above. However, owing to the anomaly, it overshoots the Landauer plateau (while both cases end at $\gamma \propto 1/N_W$, the numerical prefactor is different, with one being the bandwidth and the other containing the real-space system-reservoir coupling). As such, this choice can increase errors when coupling is weak. In other words, the relaxation defined by the level spacing $\gamma^\square = W/N_W$ only coincides with the optimum relaxation when $N_W = \frac{2\pi\omega_0^2}{v^2(1+\lambda)}$. For a smaller number of modes, γ^* will be weaker than $\gamma^\square$. For a larger number of modes, γ^* will be stronger than $\gamma^\square$. While changing the prefactor in $\gamma^\square$ can improve accuracy for finite N_W , it does not fundamentally alter this behavior. The relaxation $\gamma^\square$ will be offset from the optimum and this can result in a saturation of the relative current error at a magnitude

⁵One can also take the point where the two Lorentzian turnovers intersect, which gives the same value.

⁶Note that, even as coupling becomes weak, the current at γ^* in Eq. (34) will not yield Landauer’s result as noted in the main text after Eq. (28), as that equation becomes exact only when the effective real-space coupling is less than the finite level spacing.

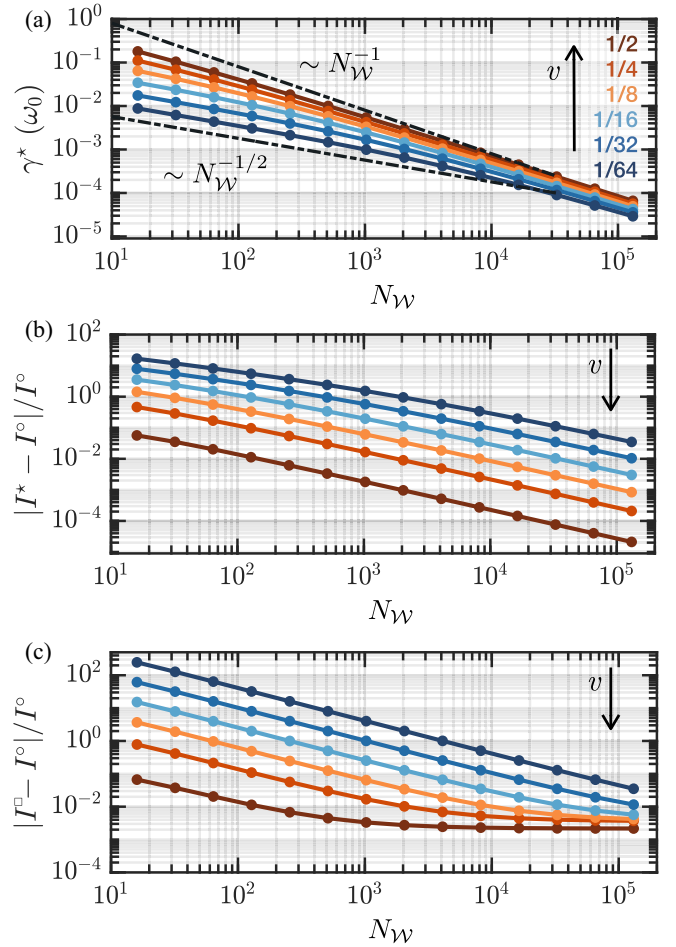


FIG. 3. Optimal relaxation and accurate simulation. Extended reservoir simulations typically employ a relaxation γ proportional to the level spacing ($\gamma \propto 1/N_W$). However, the dual anomalies, present for Markovian reservoirs and weak coupling, indicate that the optimal estimator should be proportional to the inverse square root of modes ($\gamma \propto 1/\sqrt{N_W}$). (a) The actual optimal estimator γ^* (found numerically by comparing turnover to the continuum limit I^o) transitions from scaling as $1/\sqrt{N_W}$ to $1/N_W$ as the coupling approaches unity. Deviations are seen for large N_W at weak coupling, as explained in the text. Best fits to A/N_W^p scaling give parameters $(A, p) = (1.72, -0.81), (0.87, -0.74), (0.41, -0.69), (0.18, -0.59), (0.08, -0.55),$ and $(0.04, -0.52)$ for v from large to small (couplings v are labeled in units of ω_0 and increase between curves as denoted by the arrows). The standard deviation for all fitting parameters is ± 0.01 . (b) Relative error $|I^* - I^o|/I^o$ versus N_W for the current $I^* = I(\gamma^*)$ for the γ^* from (a) compared to the continuum limit value. (c) Relative error $|I^\square - I^o|/I^o$ for the estimate $I^\square = I(\gamma^\square)$, where the relaxation $\gamma^\square = W/N_W$ is equal to the level spacing. This current estimate misses the plateau by a fixed amount as $N_W \rightarrow \infty$ and $\gamma \rightarrow 0$ (taken together) and *will not converge to the continuum limit*. Model parameters are the same as Fig. 2(b), except where specified.

comparable with the accuracy obtainable with tensor network simulations [see Fig. 3(c)].

Our observations demonstrate that, barring additional knowledge about a transport problem, one should always

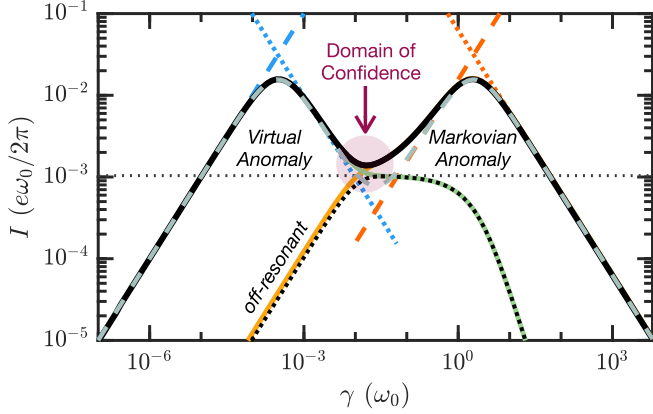


FIG. 4. Domain of confidence. Turnover behavior (black solid line) generically gives rise to five regimes: (1) a region linear in γ where the current is limited by the contact to external environment (dashed blue line); (2) a regime where virtual transitions connect resonant reservoir modes, leading to a “virtual anomaly” with overdamped turnover (dotted blue line); (3) a domain of confidence where calculations most closely represent the continuum limit; (4) a regime where unphysical broadening, “the Markovian anomaly,” creates overlap between reservoir and system states (dashed orange line); and (5) an overdamped regime where the current is inversely proportional to the relaxation (dotted orange line). The straight lines are the approximate analytic expressions for the currents in these different regimes, the dotted gray line is the Landauer limit, and the dashed gray line the “dual” anomalies, Eq. (28), at weak coupling. The calculation has the same parameters as Fig. 2(b) with $N_W = 128$ evenly spaced reservoir modes. Also shown are three other calculations: one (yellow solid line) with shifted Markovian reservoirs so that all $\mathcal{L}$ modes are off resonant with $\mathcal{R}$ modes, removing the virtual anomaly; a second simulation (green solid line) with non-Markovian relaxation, which contains the virtual anomaly but not the Markovian anomaly since there is a well-defined Fermi level. The third (black dashed line) has shifted, non-Markovian reservoirs, removing both anomalies. Note that the non-Markovian relaxation often displays different scaling in the large- γ regime (here $\propto 1/\gamma^2$ since ω_S is outside the bias window, whereas it would give $1/\gamma$ otherwise [49]).

scan the current versus relaxation strength, as in Ref. [36]. This will indicate if anomalous behavior is present, as shown in Fig. 4 where the anomalies flank a “domain of confidence.” One should obtain a plateau (see Fig. 2) in this intermediate relaxation regime and extend past $k_B T/\hbar$, with k_B Boltzmann’s constant and T the temperature. This thermal relaxation strength marks the onset of convergence between Markovian dynamics, with an improper equilibrium, and non-Markovian dynamics, with a proper Fermi level [49].

The preceding results constitute an overview of anomalies for the single-site impurity, which encapsulate general implications that extend beyond this analytically tractable case. We now will discuss their physical origin and derive some approximate expressions for the current.

B. Small- γ (virtual) anomaly

For very small γ we can expand Eq. (28) to obtain

$$I \stackrel{\lambda, \text{M, WC}}{\approx}_{\text{lr}} \frac{2e\lambda}{(1+\lambda)^2} N_B \gamma \stackrel{\text{ES}}{\approx} \frac{2e\mu\lambda}{W(1+\lambda)^2} N_W \gamma, \quad (35)$$

which is the weak relaxation expression when limited to linear response and weak coupling [49,52,53] [the second equality invokes the approximation in Eq. (26) and the bandwidth for a 1D DOS] [see Eq. (12)]. This expression assumes that both $|v_F|^2/\gamma \gg \gamma$ and $|v_F|^2/\gamma \gg |\omega_S|$. Furthermore, since $|v_F|^2 \propto |v|^2/N_W$, the second condition will define the start of the linear regime for nonresonant tunneling at weak coupling. This implies that γ must be much smaller than the level spacing in the reservoirs and also much smaller than the effective coupling $|v_F|^2/\omega_S$ (i.e., perturbatively from one reservoir mode to the system state). One can, however, satisfy the first inequality yet have a case where $|v_F|^2/\gamma \ll |\omega_S|$. This yields a second expression for the current,

$$I \stackrel{\lambda, \text{M, WC}}{\approx}_{\text{lr}} 2e\lambda N_B \frac{|v_F|^4}{\omega_S^2} \frac{1}{\gamma} \stackrel{\text{ES}}{\approx} \frac{8e\mu\lambda |v|^4}{\pi^2 \omega_S^2 \omega_0} \frac{1}{N_W \gamma}, \quad (36)$$

corresponding to an additional $1/\gamma$ regime where virtual tunneling between individual pairs of reservoir states is suppressed. That is, we now have an effective coupling of $|v_F|^2/\omega_S$ between the system and $\mathcal{L}$ (and $\lambda|v_F|^2/\omega_S$ for $\mathcal{R}$). While coherence is suppressed in this regime, similar to its large- γ counterpart, this suppression now occurs for virtual processes. It depends on $|v|^4$, the reservoir size, and the system’s ω_S^2 , i.e., to the perturbative coupling squared $(|v|^2/\omega_S)^2$. Figure 4 shows where these approximations fit on the full turnover profile.

The origin of this process immediately suggests how we can remove the anomaly. We need only shift the $\mathcal{L}$ and $\mathcal{R}$ modes out of alignment, and thus out of resonance, so that the virtual tunneling events are suppressed by an additional factor of the level spacing [for the equally spaced case, the shift can be at most $W/(2N_W)$]. Figure 4 also shows the turnover profile with suppressed virtual tunneling, leaving a $I \propto \gamma$ region that transitions into the large- γ anomaly directly through the intermediate, physical regime.

If $\gamma \ll k_B T/\hbar$, the non-Markovian and Markovian relaxation will have similar behavior in the weak-to-moderate γ regime [49]. This implies that non-Markovian relaxation will have the same virtual anomaly, and thus we do not discuss it separately.

C. Large- γ (Markovian) anomaly

For very large γ , we can expand Eq. (28) to obtain

$$I \stackrel{\lambda, \text{M, WC}}{\approx}_{\text{lr}} \frac{4e\lambda}{1+\lambda} N_B \frac{|v_F|^2}{\gamma} \stackrel{\text{ES}}{\approx} \frac{4e\mu\lambda}{(1+\lambda)\pi\omega_0} \frac{|v|^2}{\gamma}, \quad (37)$$

which is the strong relaxation expression limited to linear response [49,52,53] [again, the second equality uses the approximation in Eq. (26) and the bandwidth for a 1D DOS] [see Eq. (13)]. In contrast to small- γ approximation, this expression now assumes that $\gamma/2 \gg (1+\lambda)|v_F|^2/\gamma$ and $\gamma/2 \gg |\omega_S|$. Since $|v_F|^2 \propto |v|^2/N_W$, the second condition will define the start of the $1/\gamma$ regime for nonresonant tunneling at weak coupling. For moderate-to-strong coupling, broadening of the system mode due to system-reservoir coupling will determine where the transition happens. For the cases when the first inequality is satisfied but the second is violated, i.e., we have

$\gamma/2 \ll |\omega_S|$, the following relation is established:

$$I \underset{\text{lr}}{\approx}^{\lambda, \text{M, WC}} \frac{e\lambda}{1+\lambda} N_B \frac{|v_F|^2}{\omega_S^2} \gamma \overset{\text{ES}}{\approx} \frac{e\mu\lambda}{(1+\lambda)\pi\omega_0} \frac{|v|^2}{\omega_S^2} \gamma, \quad (38)$$

corresponding to another $I \propto \gamma$ regime. In this case, reservoir states at the Fermi level (precisely, within the bias window, which is assumed to be small) are broadened to give increased spectral weight around the system's DOS. While the mathematical origin for this is clear, the behavior is unphysical since the broadened tail of the reservoir modes should not be occupied. This region is improperly populated due to the Markovian relaxation. The expressions derived for moderate-to-strong and strong relaxation are also plotted in Fig. 4.

Markovian and non-Markovian relaxation give different behavior in the moderate-to-strong γ regime. If we compare Eqs. (21) and (22) in linear response, we see that non-Markovian relaxation gives a current from the overlap between the reservoir DOS at the Fermi level and the (broadened) system DOS at the Fermi level, $\omega = 0$. Conversely, for Markovian relaxation, the current is the total overlap between broadened Fermi level modes in the reservoir and the system's density of states. These Lorentzian broadened modes have long tails, which give large anomalous currents when coupling to the central region is weak. This is compounded when broadened reservoir modes at the Fermi level reach the highly peaked system DOS. This effectively puts the occupied (unoccupied) DOS from $\mathcal{L}(\mathcal{R})$ “in resonance” with the system level(s). Stated in another way, the broadening due to relaxation has replaced temperature in determining the effective bias window.

The origin of this anomaly indicates that it can be removed by using non-Markovian relaxation. Figure 4 shows this, confirming the absence of the Markovian anomaly at large γ . While our off-resonant example gives a large- γ turnover that scales as $I \propto 1/\gamma^2$, we would get $I \propto 1/\gamma$ for non-Markovian relaxation when the system mode is in resonance (this is an example of system-induced asymptotics). The benefits from using non-Markovian relaxation do come at a cost: while easy to solve for noninteracting systems, this does not yield a time-local Lindblad master equation that is amenable to many-body simulations.

To further explore this moderate-to-strong γ anomaly, we can do a separate calculation at weak coupling v . In this case, we may ignore reservoir-induced broadening in the system if the relaxation is moderate to large. Such maneuvers are possible since the explicit reservoir modes become progressively disconnected from the system due to rapid decoherence at large γ (a fact related to the Zeno paradox). This is not possible at weak relaxation where strong coherence remains even at weak coupling (i.e., a strong hybridization of modes).

In this weak-coupling limit at strong relaxation, the current from Eq. (22) becomes

$$I \underset{\text{lr}}{\approx}^{\lambda, \text{M, WC}} -\frac{eN_B}{\pi} \frac{\lambda}{1+\lambda} \int d\omega \text{tr}[\Gamma_F \text{Im } G_0^r], \quad (39)$$

where G_0^r is the bare system's Green's function [i.e., for a single-site system $G_0^r = 1/(\omega - \omega_S + i\eta)$ with $\eta \rightarrow 0$ at the end of calculation]. If the system has a strong peak in the DOS

around ω_S , we get the overlap integral

$$I \underset{\text{lr}}{\approx}^{\lambda, \text{M, WC}} eN_B \frac{\lambda}{1+\lambda} |v_F|^2 \frac{\gamma}{\omega_S^2 + \gamma^2/4}, \quad (40)$$

which is equivalent to Eq. (30) for large γ . This derivation underscores that an unphysical spread of the occupied (and unoccupied) DOS for extended reservoir modes is causing the anomaly.

This approach generalizes to more complex systems. For instance, we can discuss multiple noninteracting system states coupled to environments with a proportionality factor λ :

$$I \underset{\text{lr}}{\approx}^{\lambda, \text{M, WC}} eN_B \frac{\lambda}{1+\lambda} \sum_{i \in \mathcal{S}} |v_{iF}|^2 \frac{\gamma}{\omega_i^2 + \gamma^2/4}. \quad (41)$$

It is immediately apparent that the behavior for moderate-to-strong and strong relaxation is not markedly different from that of a single impurity. The only difference is that $|v_F|^2/\omega_S$ is replaced by a sum over all sites in the moderate-to-strong case $\sum_{j \in \mathcal{S}} |v_{jF}|^2/\omega_j$, and furthermore that $|v_F|^2$ is replaced with $\sum_{j \in \mathcal{S}} |v_{jF}|^2$ for the large- γ limit. Note that the current in these expressions scales with number of sites N_S in the central region. If we imagine that $\mathcal{S}$ is an array of identical sites which are decoupled from each other so that $v_{jF} = v_F$ and $\omega_j = \omega_S$, we will find a large- γ anomaly that grows linearly with N_S .

D. Continuum limit

The Markovian anomaly will persist even as we approach the continuum limit $N_W \rightarrow \infty$. Conversely, the virtual anomaly will be completely suppressed, as a finite γ is always sufficient to “turn over” the infinitesimal coupling from individual reservoir modes to the system. However, the level spacing will not impact moderate-to-strong relaxation, provided that it is sufficient to have anomalies separated from each other. Since compact expressions are readily derived in the continuum limit, we can also examine behavior outside of weak coupling. The only quantity we need is the retarded self-energy in Eq. (16), which is sufficient to derive the Green's functions $\mathbf{G}^r = [\omega - \omega_S - (1+\lambda)\mathbf{\Sigma}^r]^{-1} = (\mathbf{G}^a)^\dagger$ and spectral densities $\mathbf{\Gamma} = -2 \text{Im } \mathbf{\Sigma}^r$. In a formal sense, this allows us to obtain expressions in nonlinear response by integrating Eq. (8).

Nonproportional coupling may also be addressed using the more general expressions provided in Ref. [49]. For instance, one may assume that both reservoirs are one dimensional with a shifted DOS, as previously derived for flat-band reservoirs [49], to show the existence of zero-bias currents due to the Markovian anomaly.

In linear response, we can apply Eq. (16) to Eq. (22), yielding a straightforward expression

$$I \underset{\text{lr}}{\approx}^{\lambda, \text{M}} \frac{2e|v|^2\mu\lambda}{\pi\omega_0(1+\lambda)} \frac{\Upsilon}{\omega_S^2 + \Upsilon^2}, \quad (42)$$

where

$$\Upsilon = \frac{\gamma}{2} + \frac{|\tilde{v}|^2}{2\omega_0^2} (-\gamma + \sqrt{\gamma^2 + 4\omega_0^2}). \quad (43)$$

This result includes incoherent processes due to relaxation from implicit environments alongside coherent processes

from extended environments $\mathcal{L}(\mathcal{R})$. For convenience, we defined a modified coupling constant $|\tilde{v}|^2 = (1 + \lambda)|v|^2$. When γ is still weak compared to the total hybridization strength $|v|^2/\omega_0$, we expect a linear increase in the current versus γ . This arises from Lorentzian broadening of the Fermi level mode in the reservoir, which increases its weight near the system DOS (this is essentially static). The current, with its linear in γ correction, is given by

$$I \stackrel{\lambda, M}{\approx}_{lr} I^\circ + \gamma \frac{2e\lambda|v|^2\mu}{\pi(1+\lambda)\omega_0} \frac{(|\tilde{v}|^2 - \omega_0^2)(|\tilde{v}|^4 - \omega_0^2\omega_S^2)}{(|\tilde{v}|^4 + \omega_0^2\omega_S^2)^2}, \quad (44)$$

which converges to Eq. (38) for weak coupling. This correction can be positive or negative depending on the alignment of the system level and the given coupling strength. For weak coupling it is a linear increase away from the Landauer limit, which will subsequently reach a maximum and decrease as $1/\gamma$.

To see the sign of the correction, we can examine the extremum in the current for $|\tilde{v}|^2 > \omega_0^2$, occurring at

$$\gamma = \frac{2|\tilde{v}|^2 - 2\omega_0^2}{\sqrt{2|\tilde{v}|^2 - \omega_0^2}}. \quad (45)$$

The value of the current is given by Eq. (42) with $\Upsilon^2 = 2|\tilde{v}|^2 - \omega_0^2$. This is a maximum when $\omega_S^2 < \Upsilon^2$ [i.e., when $|\tilde{v}|^2 > (\omega_0^2 + \omega_S^2)/2$], but a minimum when $\omega_S^2 > \Upsilon^2$ [i.e., when $|\tilde{v}|^2 < (\omega_0^2 + \omega_S^2)/2$, with this condition yielding a negative sign in Eq. (44)⁷]. For increasing relaxation rate, the minimum will be followed by a subsequent maximum with current

$$I^\top = \frac{e\lambda|v|^2\mu}{\pi(1+\lambda)\omega_0\omega_S} \quad (46)$$

at

$$\gamma = \omega_S + \frac{-\omega_0^2\omega_S + 2|\tilde{v}|^2\sqrt{-2|\tilde{v}|^2 + \omega_0^2 + \omega_S^2}}{2|\tilde{v}|^2 - \omega_0^2}. \quad (47)$$

Equation (46) is the same as Eq. (32) for weak coupling.

When $|\tilde{v}|^2 < \omega_0^2$, there will be a maximum in the current with value given by Eq. (46) provided that $|\tilde{v}|^2 < \omega_0\omega_S$. This comes at Eq. (47) except when $|\tilde{v}|^2 = \omega_0^2/2$ where $\gamma = (4\omega_S^2 - \omega_0^2)/(2\omega_S)$. These results show a wide range of behavior for Markovian relaxation, even for a simple, single-site model. Thus, when performing practical simulations, it is imperative to increase $N_{\mathcal{V}}$ and decrease γ in a manner that avoids this behavior. For any given system of interest, one should also scan the current versus γ to ensure formation of a Landauer plateau.

Moving beyond these features, the current will decrease as γ becomes stronger. In effect, the Lorentzian is now so broad that the full system's state(s) are within its body, with a decay of $1/\gamma$ due to further broadening. This occurs as the full

system's Green's function is getting sharper and sharper since the rapid decoherence due to γ effectively cuts the system off from the reservoirs.

E. Landauer's regime

We can use the preceding results to constrain the required reservoir size and relaxation strength. The prior work demonstrated, in Ref. [49], that $\gamma \ll k_B T/\hbar$ must hold for the Markovian approximation (which has an ill-defined Fermi level) to converge to the non-Markovian relaxation (which has a well-defined Fermi level). This is a useful condition since neither the proof nor the expression rely on the system architecture, the reservoir band structure, or any other details, just the nature of the relaxation. Here, we give more precise conditions for our reference impurity problem, which are generally helpful for understanding the extended reservoir approach.

We begin from the large- γ side. To fully remove the Markovian anomaly, we require a γ small enough that the linear component of Eq. (44) is negligible. Taking the ratio of the linear component to I° to obtain an upper bound on γ yields

$$\gamma \ll \frac{|\tilde{v}|^2\omega_0(|\tilde{v}|^4 + \omega_0^2\omega_S^2)}{||\tilde{v}|^2 - \omega_0^2|||\tilde{v}|^4 - \omega_0^2\omega_S^2} \xrightarrow{v \rightarrow 0} \frac{|\tilde{v}|^2}{\omega_0}. \quad (48)$$

Once again, the linear correction can be negative due to different behavior in different parameter regimes. Similarly, we can find where the virtual anomaly turnover, Eq. (36), equals I° to provide a lower bound on γ . In the weak-coupling limit,

$$\gamma \gg \frac{4\omega_0}{\pi N_{\mathcal{V}}} \stackrel{\text{ES}}{=} \frac{\Delta_0}{\pi}, \quad (49)$$

where Δ_0 is the level spacing.

There is no contradiction between this result and the square-root result. Putting the two inequalities, Eqs. (48) and (49), together and maximally satisfying the constraints will yield the same $N_{\mathcal{V}}$ dependence of the optimal estimator in Eq. (34). As we discussed earlier, Fig. 3 shows that the optimal estimator behaves as $1/\sqrt{N_{\mathcal{V}}}$ for strong scattering (weak coupling) and shifts to $1/N_{\mathcal{V}}$ for weak scattering.

F. Many body $\mathcal{S}$

The considerations in this work carry over to more complicated noninteracting systems, as well as to interacting many-body systems. Here, we present data for the two-site systems of Eq. (15) and Sec. II C in a weak-coupling regime. In doing so, we compare limits with and without a density-density interaction U . These data are for (i) a proportional coupling case, where both reservoirs are coupled to the same system site, and none coupled to the other system site [Fig. 5(a)] and (ii) for a nonproportional coupling case, where each reservoir is connected to a different site of the system [Fig. 5(b)]. The reservoirs themselves are identical in both cases.

To address many-body interactions, we employ the extended reservoir tensor network approach of Ref. [36]. In this case, the density matrix of the $\mathcal{LSR}$ system is vectorized and expanded as a matrix product state (MPS) using local

⁷We have two conditions for the minimum, $|\tilde{v}|^2 > \omega_0^2$ and $|\tilde{v}|^2 < (\omega_0^2 + \omega_S^2)/2$, which together give that $|\tilde{v}|^4 < \omega_0^2\omega_S^2$. The former condition also gives that $|\tilde{v}|^2 - \omega_0^2 > 0$. Thus, the linear term is negative.

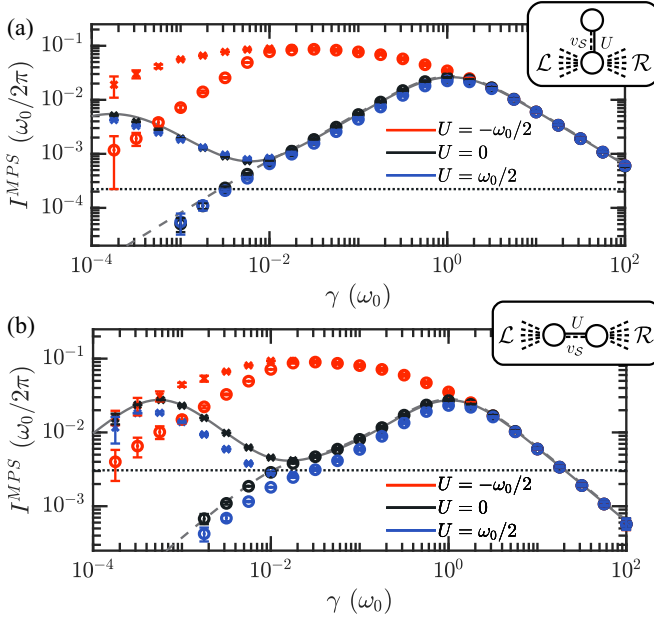


FIG. 5. Anomalies in interacting systems. Current for the spinless, interacting two-site system in Eq. (15), where the insets indicate how the system is connected to the reservoirs. The anomalous regions are apparent and we refer to the main text for further discussion. Profiles with resonant and off-resonant modes are marked with open circles and crosses, respectively, with the latter always removing the virtual anomaly. The setup follows Sec. II C with $N_V = 128$ evenly spaced reservoir modes. Our reservoir-impurity coupling is weak, $v = \omega_0/8$, and the interimpurity coupling is $v_S = (1 + \sqrt{2})\omega_0/4$. We apply a symmetric bias $\mu = \omega_0/2$ between $\mathcal{L}$ and $\mathcal{R}$ and assume a temperature $k_B T = \hbar\omega_0/40$. The density-density interaction strength is $U = -\omega_0/2$ (red), $U = 0$ (black), and $U = \omega_0/2$ (blue). The black lines indicate the reference (exact) solution for the noninteracting case with the horizontal line marking the Landauer limit in this case. The error bars at $\pm\sigma$ show an estimate of the MPS convergence, where $\sigma^2 = \sigma_1^2 + \sigma_2^2$. Here, σ_1 is a standard deviation reflecting fluctuations of the current in a time window of $\Delta t = 50/\omega_0$ at long times after reaching the steady state. The current I is defined as $I = \sum_i I_i/n_i$ [with i iterating over $n_i = 2$ possible interfaces for (a) and 3 for (b)] and $\sigma_2^2 = \sum_i |I_i - I|^2/n_i$ quantifies the mismatch of currents at different interfaces. The errors are associated with the finite MPS bond dimension, where we fix $D_{\max} = 256$ (or 352 for low- γ slopes) and truncate the MPS Schmidt values below 10^{-6} (whichever gives a smaller bond dimension at a given cut).

operator bases. These are formed by operators appearing in the Lindbladian from Eq. (2) when using an energy representation [23]. This arrangement is configured in the *mixed basis*, where we order modes in a manner that localizes correlations to the bias window and thus minimizes entanglement along the chain [21]. It should be noted that the Lindbladian does not mix different particle sectors. We enforce the resulting block structure of the density matrix by forming MPS from $U(1)$ -symmetric (particle-number-preserving) tensors [85], speeding up and stabilizing the simulations.

The superoperator $\mathbb{L}$ encoding the action of the Lindbladian on the vectorized density matrix is represented as a matrix product operator. This allows us to simulate Eq. (2) efficiently using the time-dependent variational principle for

MPS [86,87], despite the complicated long-range coupling structure in that setup (and Jordan-Wigner strings). We note that standard approaches to target the steady state directly, e.g., variationally minimizing $\mathbb{L}^\dagger \mathbb{L}$ with the help of the density-matrix renormalization group algorithm, prove to be unstable. This behavior is due to a gap that rapidly vanishes with decreasing γ and nontrivial entanglement that persists in the optimized basis. Nevertheless, simulating the time evolution is a viable strategy to reach the desired steady state. We illustrate this in Fig. 5 where, for $U = 0$, we compare the exact values of the current (black lines) with the MPS results (black symbols). These data overlap tightly across several orders of magnitude in γ , and only in the limit of very low γ do errors from the MPS become noticeable. A similar comparison cannot be made for the interacting case, as exact results are inaccessible. Thus, we must rely solely on our MPS simulations.

The results for a repulsive interaction ($U = \omega_0/2$, blue points in Fig. 5) closely mimic the turnover structure of the noninteracting case: both anomalies are clearly visible for unshifted modes (crosses) and only the Markovian anomaly remains when modes in $\mathcal{L}(\mathcal{R})$ are brought out of alignment (circles). Conversely, when the interaction is attractive ($U = -\omega_0/2$, red points in Fig. 5), the system is close to resonance is enhanced in both setups. There is now an effective impurity mode that is pushed into the bias window, hiding the two anomalies under a larger intrinsic current. We nonetheless retain a signature of the low- γ anomaly if the mode energies are taken out of alignment, as shown by the departure of the red crosses and red circles around $\gamma \approx \omega_0/100$.

A comparison of transport profiles when reservoirs modes are on and off resonant can be used to estimate an optimal γ^* . In particular, the Landauer regime may be found by seeking the intersection between turnover profiles with on-resonant and off-resonant modes, guiding convergence to the Landauer limit for finite- N_V simulations. We explore this possibility in detail in Ref. [84] while quantifying the impact of different reservoir discretization on simulation efficiency.

IV. CONCLUSIONS

The conclusions herein, together with prior results on quantum electron [49–53] and classical thermal [68,69] transport, provide a global perspective on the factors for accurate extended reservoir simulations:

(i) The Markovian relaxation strength must be weaker than the thermal relaxation $k_B T/\hbar$, at least around the Fermi level, to approximate proper reservoir equilibria [49]. This requirement can be relaxed on occasion since transport properties do not necessarily change when passing below a given effective temperature scale. Thus, accurate conductance values will still result if $\gamma < k_B T^*/\hbar$, with T^* the lowest of these temperature scales. This behavior is observed for common models (see, e.g., Ref. [36] where below about $k_B T^* \approx \omega_0/10$ the conductance does not change). If there are no features, whether in the density of states, the transmission function, or due to many-body interactions (e.g., the Kondo temperature [88]), then there is no reason to have an excessively small γ . This is heuristic and should be employed with care, especially when considering other observables such as noise.

It should be noted that there is a fundamental pathology of the Markovian Lindblad master equation [89], which is due to improper equilibrium (i.e., the Markovian equation relaxes the modes to the occupation of the equilibrium state for isolated reservoirs). However, it can be rigorously proven that with appropriate choice of parameters an approach based on the Lindblad equation limits to the correct results. The approach based on an extended reservoirs and a Redfield master equation is a promising alternative which might potentially help convergence to the thermodynamic limit for some cases.

(ii) Other energy scales appear within the Markovian extended reservoir framework. In particular, we have shown that the reservoir spacing Δ and the coupling $|v|^2/\omega_0$ (or its more complicated version), set important energy scales for simulation. These bound the domain of confidence for γ from below and above, respectively. The former suppresses virtual transitions and thus helps to identify an upper bound for the virtual anomaly. The latter ensures that broadening is under control and that the simulation result lies prior to the Markovian anomaly.

(iii) Certain features, such as the band structure and gap states [51,69], can collectively give rise to a range of behavior. Many-body interactions may *sometimes* help in this regard (though they may also be detrimental) by smearing sharp features in the DOS, particularly those that support interference or effects that give rise to anomalous currents.

The only generally effective approach for extended reservoir transport simulations is to scan physical observables versus relaxation strength and reservoir size. This consideration also holds for other applications, such as nonequilibrium thermodynamics. Weak-coupling cases are particularly troublesome due to the anomalies studied here and the complexity

resulting from five distinct transport regimes. Other methods, such as perturbative treatments of the system-reservoir coupling, can address parameter regions where extended reservoirs may be numerically difficult to apply.⁸ It remains to be seen if these factors influence alternative implementations with intermode relaxation in the reservoirs.

Our results provide a comprehensive perspective for extended reservoir simulations, while refining the Kramers turnover picture for open transport simulations. We likewise establish a domain of confidence where Markovian relaxation can provide accurate transport profiles. This will advance the practical use of these methods and help usher in the era of ERAs.

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⁸If one desires to simulate cases where contact is weak, or where it fluctuates between weak and strong regimes (such as Floquet states that are modulated by a harmonic function), then one needs to resolve this issue and have a verified and validated simulation approach throughout the range of parameters (e.g., large enough reservoir size, small enough gamma that one remains on the plateau). Similar concerns arise when discussing electronic sensing and junction configurations [90–98].

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Publication III

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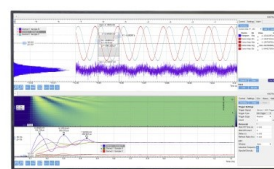
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ABSTRACT

Quantum transport simulations often use explicit, yet finite, electronic reservoirs. These should converge to the correct continuum limit, albeit with a trade-off between discretization and computational cost. Here, we study this interplay for extended reservoir simulations, where relaxation maintains a bias or temperature drop across the system. Our analysis begins in the non-interacting limit, where we parameterize different discretizations to compare them on an even footing. For many-body systems, we develop a method to estimate the relaxation that best approximates the continuum by controlling virtual transitions in Kramers turnover for the current. While some discretizations are more efficient for calculating currents, there is little benefit with regard to the overall state of the system. Any gains become marginal for many-body, tensor network simulations, where the relative performance of discretizations varies when sweeping other numerical controls. These results indicate that typical reservoir discretizations have little impact on numerical costs for certain computational tools. The choice of a relaxation parameter is nonetheless crucial, and the method we develop provides a reliable estimate of the optimal relaxation for finite reservoirs.

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I. INTRODUCTION

The design of new electronic materials and nanoelectronic devices requires scalable, high-fidelity approaches to simulate transport. Modern methods can accurately describe the atomic and band structure of many materials, often using density functional theory.^{1–3} Moreover, dedicated many-body techniques, such as quantum Monte Carlo or tensor networks, can include contributions from explicit correlations.^{4–11} The computational cost of these tools is nonetheless appreciable for large systems or long simulation timescales. These limitations are particularly onerous for tensor networks, where an explicit treatment of the reservoirs will introduce many degrees of freedom.^{7–15}

A typical transport simulation is shown in Fig. 1, where a system (device) of interest is coupled to explicit reservoirs. Transport is maintained by a bias. In a closed system, this could be introduced by a density imbalance or a time-dependent, inhomogeneous on-site potential in the reservoirs. Open systems can go a step

further by including implicit reservoirs, which drive transport by relaxing explicit reservoir modes to biased Fermi distributions.^{16–22} The *extended reservoir approach* exemplifies such an arrangement, and it has become popular in many guises,^{16–39} including those that accommodate many-body transport.^{8–11}

These computational methods employ reservoirs that are discretized. While a given discretization should converge to the spectral function of a continuum reservoir, its construction is otherwise arbitrary. This flexibility has resulted in a variety of approaches, including the placement of modes evenly across the bandwidth (linear discretization), assigning them according to the canonical transform of finite tight-binding lattices, distributing them evenly inside the bias window and logarithmically outside (linear-logarithmic),^{10,14,40,41} and using an influence-based approach that yields a linear mode spacing across the bias window and an inverse spacing outside (linear-inverse).⁴² Moreover, the deviation of finite representations from the continuum can be corrected for perturbatively.^{43,44} Related techniques aim to minimize the number of reservoir modes

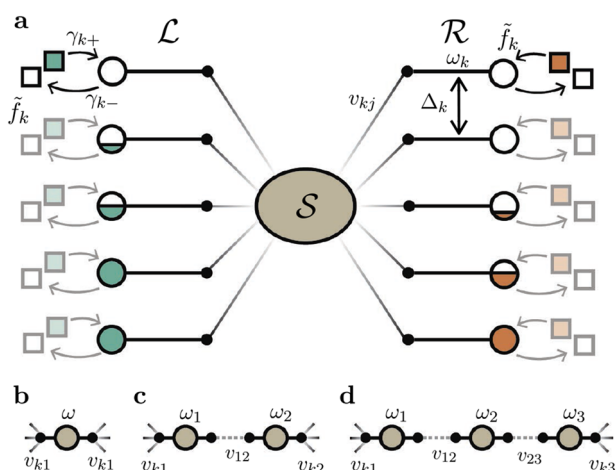


FIG. 1. Quantum transport with extended reservoirs. (a) An arbitrary impurity (S) is flanked by explicit left ($\mathcal{L}$) and right ($\mathcal{R}$) reservoirs. Each reservoir contains $N_{\mathcal{V}}$ modes of frequencies ω_k that couple to a designated system site i with constant strength v_{ki} . Implicit reservoirs relax $\mathcal{L}$ and $\mathcal{R}$ to biased Fermi distributions $\tilde{f}_k$ at a rate γ_k for the k th mode. We consider models for S that include (b) one, (c) two, and (d) three site systems with onsite frequencies ω_i . These sites couple to each other with strength v_{ij} and to the reservoirs at terminal sites (i.e., a single system mode couples to each reservoir).

by introducing *intermode* transitions during relaxation. While these additional fitting parameters provide a higher fidelity spectral density,^{12,13,15,45} they also add numerous long-range couplings from the intermode relaxations. This ultimately limits the feasible size of reservoirs. Ideally, one desires high accuracy simulations at low computational cost (and favorable scaling). It is unclear what approach performs best, as a quantitative comparison does not exist.

Here, we address one very important facet of this comparison: How does the choice of reservoir discretization influence the computational cost needed to converge transport properties to a given accuracy? We also examine how the system–reservoir coupling and implicit relaxation impact the convergence of steady-state transport. We study non-interacting systems and their many-body counterparts but only consider extended reservoirs with *intramode* Markovian relaxation.^{8,16–22} For non-interacting systems, we optimize the relaxation (e.g., discretization and coupling to implicit modes) to get the highest accuracy in steady-state currents. This procedure has limited generality since it requires knowledge of the exact, continuum reservoir solution. For the many-body case, we demonstrate how Kramers turnover can be used to estimate an optimal relaxation rate.

We find that certain discretizations can increase efficiency for non-interacting calculations, where efficiency is measured by the number of reservoir modes required to reproduce the current up to a fixed accuracy. This advantage is weak for other system observables (e.g. the impurity’s density) and its correlation matrix particularly when working at small to moderate reservoir sizes. While tensor network calculations exhibit moderate, discretization-dependent deviations in the impurity correlation matrix, we find that the overall efficiency is tied to other control parameters—most importantly,

the Schmidt cutoff. This behavior reflects the natural structure of our tensor network, which uses an energy/momentum basis for the explicit reservoirs and orders them globally according to their energies to minimize the bipartite entanglement in the numerical ansatz. While certain discretizations reduce the number of modes, they do so for energy scales that are weakly correlated. These scales contribute little to the computational cost. Thus, the choice of discretization has little practical impact on efficiency.

II. BACKGROUND AND SETUP

We follow a conventional arrangement^{46,47} that consists of non-interacting left ($\mathcal{L}$) and right ($\mathcal{R}$) reservoirs and a bias that drives transport through an impurity system (S); see Fig. 1. The associated Hamiltonian has the form $H = H_S + H_{\mathcal{L}} + H_{\mathcal{R}} + H_I$, where H_S is the (potentially many-body) Hamiltonian for S , $H_{\mathcal{L}(\mathcal{R})} = \sum_{k \in \mathcal{L}(\mathcal{R})} \hbar \omega_k c_k^\dagger c_k$ are the reservoir Hamiltonians, and $H_I = \sum_{k \in \mathcal{L}(\mathcal{R})} \sum_{i \in S} \hbar (v_{ki} c_k^\dagger c_i + v_{ik} c_i^\dagger c_k)$ is the interaction Hamiltonian that couples S to $\mathcal{L}\mathcal{R}$. The $c_m^\dagger$ (c_m) are fermionic creation (annihilation) operators for a state $m \in \mathcal{LSR}$. All indices implicitly include multiple relevant labels (such as mode number, reservoir, and spin). The frequency for the k th reservoir mode is denoted by ω_k , while $v_{ki} = v_{ik}^*$ is used for the coupling between $i \in S$ and $k \in \mathcal{L}\mathcal{R}$. For two-site impurity S , the Hamiltonian is

$$H_S = \hbar v_S (c_1^\dagger c_2 + c_2^\dagger c_1) + \hbar U n_1 n_2, \quad (1)$$

where v_S is the internal coupling in S , $n_i = c_i^\dagger c_i$ is the particle number operator for site i , and U is the many-body density–density interaction strength.⁸ The description of other models can be found in the [supplementary material](#). This model corresponds to a (time-independent) photoconductive molecular device where spin can be neglected.⁴⁸

We calculate the properties of non-interacting systems, including the impurity’s correlation matrix, using non-equilibrium Green’s functions^{16–18,20,21} and employ tensor networks for the many-body case.^{8,22} When considering the latter, we solve a Lindblad master equation

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \sum_{k \in \mathcal{L}\mathcal{R}} \gamma_{k+} \left(c_k^\dagger \rho c_k - \frac{1}{2} \{ c_k c_k^\dagger, \rho \} \right) + \sum_{k \in \mathcal{L}\mathcal{R}} \gamma_{k-} \left(c_k \rho c_k^\dagger - \frac{1}{2} \{ c_k^\dagger c_k, \rho \} \right), \quad (2)$$

for the $\mathcal{LSR}$ system with Markovian relaxation in $\mathcal{L}\mathcal{R}$ (here, $\{ \cdot, \cdot \}$ is the anticommutator). The first term gives the evolution of the many-body density matrix ρ under our Hamiltonian H , while the second and third terms give open dynamics through injection and depletion of the modes k at rates γ_{k+} and γ_{k-} , respectively. To ensure that the reservoirs relax to the fully isolated $\mathcal{L}\mathcal{R}$ state, we set these rates to $\gamma_{k+} \equiv \gamma_k f^\alpha(\omega_k)$ and $\gamma_{k-} \equiv \gamma_k [1 - f^\alpha(\omega_k)]$, where $f^\alpha(\omega_k)$ is the Fermi–Dirac distribution in the $\alpha \in \{\mathcal{L}, \mathcal{R}\}$ reservoir.

We quantify the accuracy of the steady-state current I for non-interacting models using a relative error $|I - I^o|/I^o$, where the

reference current I° is the Landauer limit for continuum reservoirs⁴⁹ (we work with the current itself for many-body cases, as I° is not known exactly). Furthermore, we quantify the combined error in occupancy and correlations using the correlation matrix of $\mathcal{S}$, i.e., $C_S = C_{ij} = \langle c_i^\dagger c_j \rangle$, with $i, j \in \mathcal{S}$. The quantity C_S completely characterizes all equal time correlations for non-interacting systems and includes the information on densities (occupancy) $n_i = C_{ii}$. A natural metric for the convergence of the system state is the normalized trace distance, $\|C_S - C_S^\circ\|_* = \|C_S - C_S^\circ\| / 2 [\text{tr } C_S + \text{tr } C_S^\circ]$, defined in terms of the trace norm $\|M\| = \text{tr} \sqrt{M^\dagger M}$ and the exact correlation matrix C_S° for continuum reservoirs.

Discretizations are compared by maintaining a common set of modes within the bias window $\mathcal{B}$ while distributing modes outside the bias window $\mathcal{W} \setminus \mathcal{B}$ according to a designated arrangement (here, $\mathcal{W}$ denotes both the reservoir band and its bandwidth). We formalize this by associating an abstract influence scale $\chi(\omega)$ with each discretization, which we use to specify mode placement within the reservoir bandwidth. In this manner, the functional form of $\chi(\omega)$ completely specifies a given discretization. Mode placement begins by defining integrated weights for modes inside $X_B = \int_B \chi(\omega) d\omega$ and outside $X_{W \setminus B} = \int_{W \setminus B} \chi(\omega) d\omega$ the bias window. We also introduce an integrated influence per mode x (a target weight per mode) that specifies $N_B = \lceil X_B/x \rceil$ modes in the bias window and $N_{W \setminus B} = \lceil X_{W \setminus B}/x \rceil$ modes outside the bias window. The region $\mathcal{B}$ is then divided into N_B bins Δ_k with boundaries satisfying $\int_{\Delta_k} \chi(\omega) d\omega = X_B/N_B$ and $\cup_{k \in B} \Delta_k = \mathcal{B}$ (similarly for the complement of $\mathcal{B}$). We choose values of x so that there is always an even number of symmetrically distributed modes in both $\mathcal{B}$ and $\mathcal{W} \setminus \mathcal{B}$. This accommodation ensures that there is never a mode at the Fermi level. Reservoir modes are then placed at the midpoint ω_k of each bin.

We compare three reservoir discretizations: (i) a linear case, with modes spaced evenly throughout the bandwidth; (ii) a linear-logarithmic discretization (motivated by energy scale separation under the numerical renormalization group⁵⁰); and (iii) a linear-inverse arrangement following the influence approach of Ref. 42. The influence scales for these discretizations are

$$\chi_{\text{lin}}(\omega) = 1, \quad (3)$$

$$\chi_{\text{log}}(\omega) = \theta\left(\frac{\mu}{2} - |\omega|\right) + \frac{\mu}{2|\omega|} \theta\left(|\omega| - \frac{\mu}{2}\right), \quad (4)$$

$$\chi_{\text{inv}}(\omega) = \theta\left(\frac{\mu}{2} - |\omega|\right) + \left(\frac{\mu}{2\omega}\right)^2 \theta\left(|\omega| - \frac{\mu}{2}\right), \quad (5)$$

which are nonzero within the reservoir bandwidth and zero outside, as depicted in Fig. 2(a). Here, $\theta(x)$ is the Heaviside step function. All three measures give evenly spaced modes within $\mathcal{B}$ yet differ in $\mathcal{W} \setminus \mathcal{B}$, acknowledging that bias window modes contribute significantly to the current. Our terminology reflects a measure of influence that is given by the integral of χ .

Using these, we compare simulations with the reservoir relaxation rate γ_k , a fixed multiple of the mean level spacing in the bias window $\langle \Delta_k \rangle_B$ (this is equal to μ/N_B for all cases herein), to the relaxation defined by the mode-dependent level spacing Δ_k . We also compare system-reservoir couplings that are defined by the midpoint between two discrete reservoir modes to couplings defined

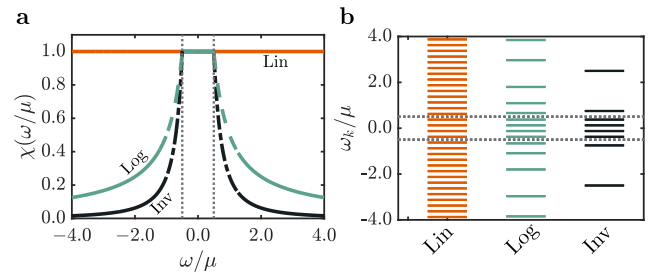


FIG. 2. Influence scales and discretizations. (a) Influence scales that induce linear [$\chi_{\text{lin}}(\omega)$: orange solid line], linear-logarithmic [$\chi_{\text{log}}(\omega)$: green dashed line], and linear-inverse [$\chi_{\text{inv}}(\omega)$: black dashed-dotted line] discretizations. (b) The resulting minimal mode distributions ω_k , calculated at the same integrated influence per mode x . Thin dotted lines in both plots demarcate the bias window edge. Data are at a bias $\mu = \omega_0/2$ and reservoir bandwidth $\mathcal{W} = 4\omega_0$, where ω_0 is the real-space hopping in the reservoir. Modes near the band edges of the linear-logarithmic discretization are a consequence of the chosen influence scale, bias, and bandwidth—they are not necessarily present for denser distributions.

by the integrated coupling over an interval of width Δ_k about a mode ω_k (which is placed at the center of the bin).⁵¹

III. KRAMERS TURNOVER

The composite $\mathcal{LSR}$ system exhibits distinct transport regimes in the presence of relaxation,¹⁶ which mimic Kramers turnover for chemical reaction rates; see Fig. 3(a)⁵² (a similar result holds for thermal transport^{53–57}). When relaxation is weak, transport is determined by the rate at which particles and holes are replenished in the extended reservoirs. In this regime, the current will rise proportionally with the mode-dependent relaxation rate γ_k , analogous to chemical systems where environmental friction controls the equilibration of reacting species. When the relaxation is strong, phase coherence is suppressed and the current decays as γ_k^{-1} . Here, transport emulates reactions where strong friction redirects partially formed products back to the reactants (i.e., recrossings). The intermediate region contains a plateau-like region where the continuum limit current is reproduced, analogous to reactions that are controlled by the transition state rate. As we will emphasize later, the system state does not necessarily reflect the exact model on the whole plateau. The width of the plateau—and convergence to this limit—is dominated by the number and distribution of explicit reservoir modes. The natural transport rate only predominates in the intermediate region.¹⁶

The formation of the plateau as $N_W \rightarrow \infty$ and $\gamma_k \rightarrow 0$ (in that order) is sufficient to determine the continuum current, although not all points on the plateau will correspond to a fully converged system state (e.g., local electronic densities). Moreover, this regime is not guaranteed to be unambiguous. There may be additional features due to the underlying Hamiltonian^{8,18} or the presence of specific anomalies that exist on either side of the plateau [Figs. 3(a) and 3(b)].²² For large relaxation, a Markovian anomaly is associated with an unphysical broadening of reservoir modes and the lack of a well-defined Fermi level.¹⁶ This is a direct consequence of Markovian relaxation, which fills a reservoir mode according to its bare frequency ω_k rather than accounting for its broadening. Such

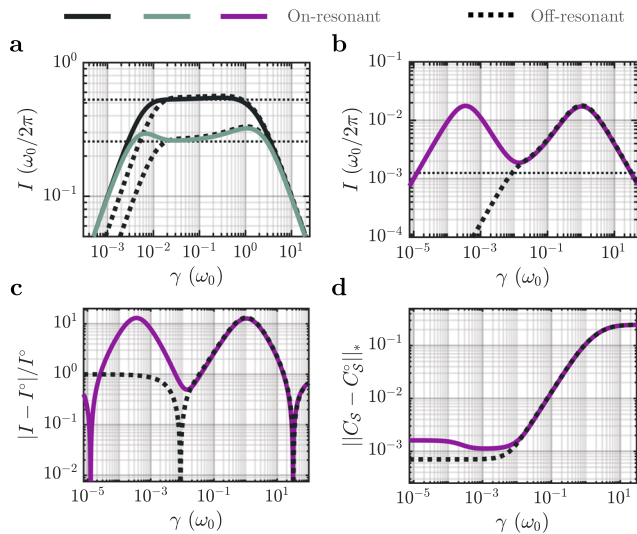


FIG. 3. Kramers turnover and accuracy. Steady-state transport for a two-site model and discrete reservoirs with mode-independent reservoir relaxation $\gamma_k = \gamma$. Data are presented for on-resonant reservoir modes (solid lines) and those made off-resonant via a frequency shift $\langle \Delta_k \rangle_B/2$ between isoenergetic modes (dotted lines). (a) Current turnover $I(\gamma)$ at strong system–reservoir coupling $v_0 = \omega_0/2$ and for two system–site couplings, $v_S = (1 + \sqrt{2})\omega_0/4$ (black) and $v_S = (2 + \sqrt{3})\omega_0/4$ (green), showing different plateau topographies at different intrasite coupling scales. (b) Current turnover at small system–reservoir coupling, $v_0 = \omega_0/10$, reveals anomalies on either side of an interstitial Landauer regime ($v_S = (1 + \sqrt{2})\omega_0/4$).²² (c) Relative current error with respect to the continuum limit I^0 for the model in (b). (d) Convergence of the system state via the normalized trace distance between finite C_S and continuum C_S^0 correlation matrices, illustrating that no conditions are uniformly optimal for all observables (the current impacts this convergence in a limited manner; see the [supplementary material](#)). The continuum (Landauer) limit is denoted by the dotted horizontal line. All calculations use $N_W = 128$ explicit reservoir modes, spaced evenly between $\pm W/2$ and integrated couplings (see Ref. 49). We apply a symmetric bias $\mu = \omega_0/2$ between reservoirs both held at temperature $T = \omega_0/40$.

behavior can lead to zero bias currents in some cases.¹⁶ These concerns are irrelevant for non-Markovian relaxation, where reservoir modes are properly occupied according to their broadened density of states.

For weak relaxation, a *virtual anomaly* occurs due to virtual transitions through the system, specifically between on-resonant $\mathcal{L}$ and $\mathcal{R}$ modes. This leads to excess transport, as previously seen in Refs. 8 and 38 and explained in Ref. 22. The virtual anomaly can be suppressed by shifting the relative energy of $\mathcal{L}$ and $\mathcal{R}$ by half the level spacing, $\Delta_k/2$, disrupting the resonant structure. While anomalous regimes can be difficult to distinguish at strong system–reservoir coupling (e.g., $v_0 \approx \omega_0/2$), they become prominent when the coupling is weak (e.g., $v_0 \approx \omega_0/10$); see Fig. 3(b).

Various factors, including the finite distribution of reservoir modes and the specific Hamiltonian, can influence the turnover architecture (e.g., weak and strong coupling can have a different optimal relaxation as a function of N_W).²² Thus, we need a method that compares discretizations while not placing any given discretization at a disadvantage *a priori*. We obtain this for non-interacting systems by choosing a relaxation that most accurately

reflects the steady-state current of continuum reservoirs. For many-body cases, we estimate the optimal relaxation as described later in the manuscript.

IV. OPTIMAL RELAXATION

We can obtain the exact, continuum-limit current of non-interacting systems using established methods. For finite reservoirs, there is an optimal relaxation located in the intermediate, physical turnover regime that best estimates this current (see Fig. 3; we exclude incidental crossovers at weak and strong relaxation). To proceed, we must quantify this optimum for reservoirs with an inhomogeneous mode spacing. We begin by introducing a relaxation $\gamma_k = \alpha\eta(\omega_k)$, where $\alpha > 0$ is a real scaling constant and $\eta(\omega_k)$ is a function of the level spacing within the extended reservoirs. Using this convention, we examine $\eta(\omega_k)$ as either (i) a constant independent of k (in some cases, we set this constant to the average bias window level spacing) or (ii) that set to the k -dependent level spacing. We then seek α^* in the intermediate region that minimizes the relative current error $\alpha^* = \arg \min(|I[\gamma_k(\alpha)] - I^0|/I^0)$ with respect to the continuum limit I^0 . This α^* completely defines the optimal relaxation for both equally and unequally spaced cases (with a single $\gamma^* = \gamma_k$ for equally spaced modes). In some cases, we could also derive an optimal relaxation using the normalized trace distance between correlation matrices [see Fig. 3(d)] although we do not take this approach. Convergence of this quantity would ensure convergence of all other (time-local) system observables,⁵⁸ including the current if there is a boundary that divides the impurity into left and right parts. This relaxation would not necessarily coincide with γ^* as defined above.⁵⁹

When the exact, continuum limit current I^0 is unknown, as is the case for most interacting systems, there is no obvious way to optimize $I[\gamma_k(\alpha)]$. This point is critical in practical calculations. Optimization can also fail when the plateau is featureless, e.g., at strong-coupling in Fig. 3(a), when many plateau features are present,¹⁸ or if convergence occurs from below the Landauer limit (see the [supplementary material](#)). We can, however, estimate an optimal regime by applying a relative shift of $\langle \Delta_k \rangle_B/2$ between isoenergetic states in $\mathcal{L}$ and $\mathcal{R}$ reservoirs. That is, we shift the modes in $\mathcal{L}$ and $\mathcal{R}$ by plus/minus a quarter of the level spacing. As noted earlier, this eliminates the virtual anomaly associated with resonant transitions.²² The shifted profile should intersect the unshifted profile at a point γ_s near the physical regime γ^* .⁶⁰ A second estimate is given by extrapolating the linear, small- γ regime of the shifted case and finding the point γ_ℓ where this intersects the unshifted profile. This γ_ℓ will typically lie prior to γ^* .

Figure 4(a) shows these two estimators. Since the region between anomalies expands into an almost flat profile with an increasing number of reservoir sites, we expect these estimators to bound γ^* on either side for large N_W . This is indeed the case here. Moreover, the intersection estimator γ_s tightly reproduces the optimal point $I[\gamma_k(\alpha^*)]$ starting at moderate N_W . In contrast, the extrapolation estimator γ_ℓ moves away from the optimum as N_W increases [see Fig. 4(c) and the [supplementary material](#)]. This is a consequence of the plateau topography. That is, the estimator γ_ℓ scales with $1/N_W$ and rides the edge of the virtual anomaly as $N_W \rightarrow \infty$. However, there is a duality between virtual and Markovian anomalies, which can make the optimal relaxation scale as $1/\sqrt{N_W}$ in the moderate

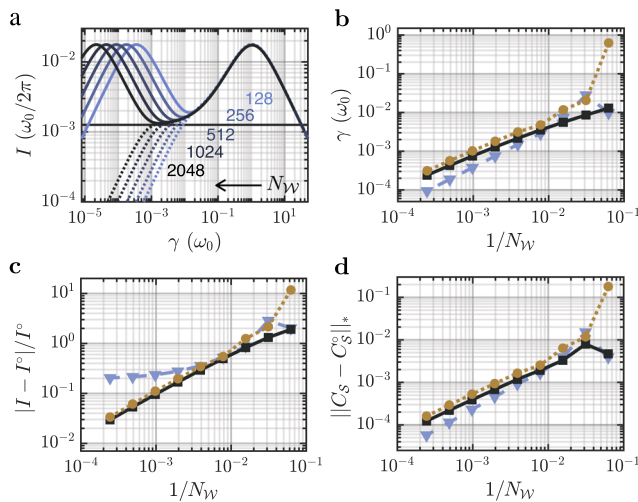


FIG. 4. Optimal relaxation and estimators. (a) Elongation of the region between anomalies as the number of reservoir modes N_W is increased. Turnover profiles are shown with (dotted line) and without (solid line) a frequency shift of $\langle \Delta_k \rangle_B/2$ between isoenergetic modes in $\mathcal{L}$ and $\mathcal{R}$, defined by the mean level spacing in the bias window. (b) Determination of the best estimator for the Landauer regime $I[\gamma^*] = I[\gamma_k(\alpha^*)]$ (black squares). Estimators are based on either γ_ℓ (blue triangles)—the linear extrapolation of the small- γ regime of the shifted model (off-resonant; blue dashed line) into the unshifted (on-resonant) profile—or γ_s (tan circles)—the intersection between shifted and unshifted profiles. (c) Convergence of the relative current error $|I - I^0|/I^0$ and (d) the trace norm $\|C_S - C_S^0\|_*$ with respect to N_W . All scaling profiles correspond to $\gamma^* = \gamma_k(\alpha^*)$ (black squares), the linear extrapolation estimator (blue triangles), and the intersection of shifted/unshifted turnover profiles (tan circles). All panels reflect a linear reservoir discretization for the weak coupling model of Fig. 3(b). (d) Scaling of relaxation associated with γ_ℓ and γ_s estimators.

N_W regime.²² Thus, in this moderate regime, the γ_ℓ departs from the optimal relaxation and its error saturates.

The intersection estimator γ_s is also robust when examining the overall state of the system [Fig. 4(e)]. However, the extrapolation estimator γ_ℓ actually outperforms both the optimal and intersection estimators for this case [see Fig. 4(e) and the [supplementary material](#)]. We consider this incidental as it is due to the fact that smaller relaxation often results in a more accurate system correlation matrix; see Fig. 3(d).⁶¹ Despite this, the intersection estimator is better behaved. Thus, to find the Landauer limit, we only need to calculate turnover profiles with on-resonant and off-resonant reservoir modes and find their intersection γ_s —an approach that is borne out for other models and in the strong coupling limit (see the [supplementary material](#)). While Hamiltonian parameters can change the plateau architecture, the intersection between turnover profiles will invariably remain a useful estimator of the physical (continuum) regime.

V. RESULTS

Having established a framework to compare different discretizations, we now examine both non-interacting and many-body transport. As a first step, we compare different system–reservoir coupling methods and different choices of $\eta(\omega_k)$ for the non-interacting case.

A. Non-interacting systems

The behavior of a reservoir discretization may be influenced by the system–reservoir coupling and the assignment of relaxation rates γ_k to each reservoir mode. We present this behavior for the linear–inverse discretization in Fig. 5. The more significant factor is the choice of relaxation, which nontrivially moderates convergence to the continuum limit with increasing N_W . The error in I is smaller when the relaxation is a multiple of the mean level spacing in the bias window, $\gamma_k = \alpha \langle \Delta_k \rangle_B$ (which, in the cases here, is equal to μ/N_B). This situation is more variable for convergence of C_S , where we see better performance at small N_W if the relaxation is a multiple of the level spacing $\gamma_k = \alpha \Delta_k$ [Figs. 5(a) and 5(b)]. Nonetheless, this behavior crosses over to favor the mean-spacing approach at modest N_W . We note that convergence is minimally impacted by the coupling method—the integrated and mean methods do not differ appreciably at any N_W scale. From here on, we employ mode-independent relaxation $\gamma_k = \gamma$ and the integrated coupling constants.

Figure 6 shows the performance of different discretizations when converging a transport calculation. We find the full linear discretization $\chi_{\text{lin}}(\omega)$ to behave more poorly in terms of either the relative error in current I or that in the system-site density n_i [Figs. 6(a) and 6(b)]. Notably, the error in the steady-state current is uniformly higher than the other discretizations for all values of N_W . Using the same criteria, the linear–inverse influence measure $\chi_{\text{inv}}(\omega)$ outperforms the linear–logarithmic discretization $\chi_{\text{log}}(\omega)$. This implies a lower degree of error at fewer reservoir sites, providing better convergence in a regime with decreased computational cost. The performance gain when moving between these methods is nonetheless smaller than the gain when moving to them from the full linear discretization.

Any advantage is less clear-cut for the overall state of the system, where all three discretizations exhibit comparable performance at large N_W . Nonetheless, the linear–inverse discretization performs more poorly when N_W is small—a region where convergence can oscillate due to the placement of states outside the bias window edge. Similar conclusions may be drawn for models containing one

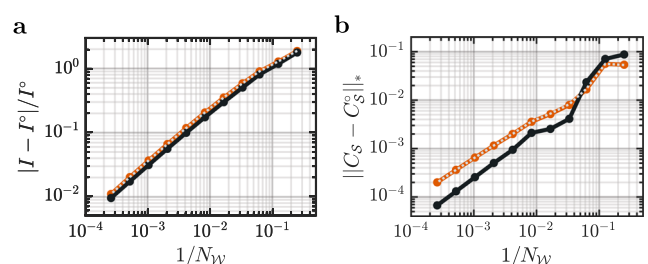


FIG. 5. Coupling and relaxation methods. Convergence of the steady-state current $I[\gamma_k(\alpha^*)]$ using integrated couplings and mode-dependent relaxation. Error in I is shown for (a) integrated couplings with relaxation defined by the mean bias window spacing $\gamma_k = \alpha^* \langle \Delta_k \rangle_B$ (black solid line) or by the level spacing $\gamma_k = \alpha^* \Delta_k$ (orange dashed line), where α^* is the optimal prefactor. (b) Convergence of the system state, as reflected by the normalized trace distance $\|C_S - C_S^0\|_*$ between correlation matrices, for the same methods as (a). The gray dotted line in (a) and (b) has $\gamma_k = \alpha^* \Delta_k$ but with couplings from the midpoint of the discretization intervals. The model is otherwise that of Fig. 3(b) with a linear–inverse discretization.

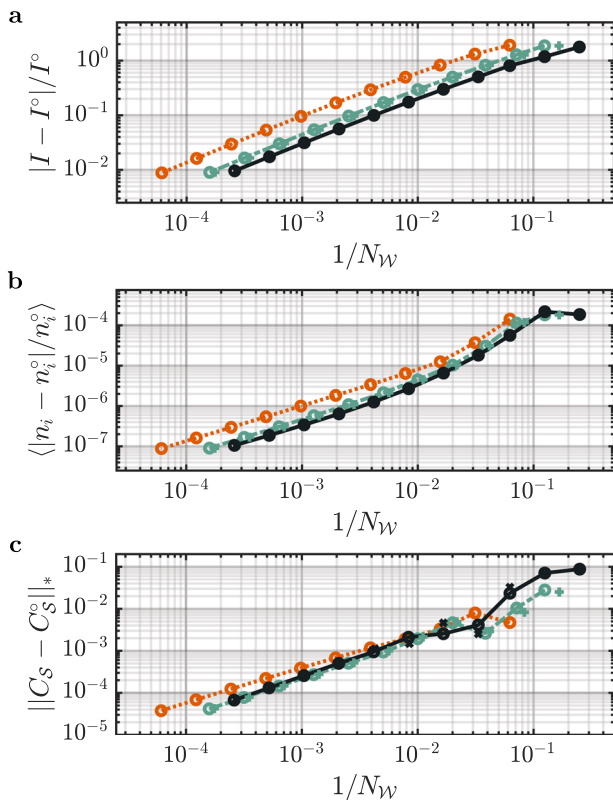


FIG. 6. Error and discretization. Convergence of reservoir discretizations when increasing the number N_W of explicit reservoir sites. This behavior is quantified through (a) relative error in the steady-state current $I[\gamma_k(\alpha^*)]$, (b) the mean relative error of the on-site densities n_i within S , and (c) the normalized trace distance between the correlation matrix C_S for S and its infinite reservoir counterpart C_S^0 . Discretizations correspond to the standard linear (orange dotted line), the linear-logarithmic (green dashed line), and the linear-inverse (black solid line) arrangements. Results are also provided for modified linear-logarithmic and linear-inverse discretizations that incorporate the 1D spectral density into the influence scale (this pinches off the influence at the band edge) (green and black crosses, respectively). Profiles from (a) fit to A/N_W^p with $[A, p] = [11 \pm 1, 0.65 \pm 0.02]$, $[8.5 \pm 0.2, 0.72 \pm 0.01]$, and $[4.4 \pm 0.2, 0.64 \pm 0.18]$ for the main discretizations. All data are from the non-interacting, two-site Hamiltonian of Fig. 3(b) at weak-coupling ($v_0 = \omega_0/10$), with integrated system-reservoir couplings, and relaxations $\gamma = \alpha\langle\Delta_k\rangle_B$ determined by the mean mode spacing within the bias window B .

or three sites [Figs. 1(b) and 1(d); see the [supplementary material](#)]. These methods are roughly equivalent for the number of states used in typical many-body transport simulations (i.e., N_W in the 100's).

A parallel analysis can be done in terms of the number of reservoir modes N_B within the bias window (Fig. 7). This region is particularly important when representing the current, and the accuracy of a representation correlates with N_B . Working from this perspective, we find uniform scaling across discretizations with respect to the current error. This observation simply reflects that transport is dominated by bias window modes and one needs to accurately represent the spectral density in that window. The occupations also scale uniformly at large N_B , albeit with discrepancies when this parameter is small. Correlation matrices have more sporadic behavior,

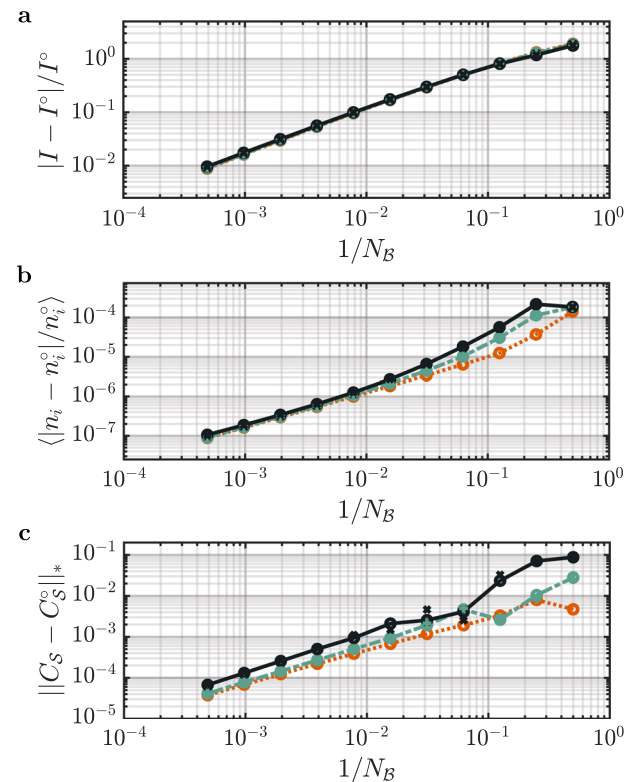


FIG. 7. Error and discretization in the bias window. Convergence of the reservoir discretizations from Fig. 6, now parameterized in terms of the number of states N_B in the bias window. Scaling is quantified through (a) relative error in the steady-state current $I[\gamma_k(\alpha^*)]$, (b) the mean relative error of the on-site densities n_i within S , and (c) the normalized trace distance between correlation matrix C_S for S and its infinite reservoir counterpart C_S^0 . Colors and symbols follow from Fig. 6. Profiles from (a) fit to A/N_B^p with $[A, p] = [4.1 \pm 0.1, 0.76 \pm 0.02]$, $[4.0 \pm 0.2, 0.76 \pm 0.02]$, and $[3.8 \pm 0.3, 0.74 \pm 0.03]$ for the main discretizations while restricting to $N_B > 4$ to mitigate finite size effects. These results indicate that, for the current, it is the convergence of the spectral density in the bias window that matters. If arbitrary observables are desired, however, the spectral density at higher frequencies is relevant.

though the linear-inverse arrangement reproduces the system state most poorly at a given N_B . This reflects a lower fidelity spectral density outside of the bias window. The performance gap for the linear-inverse is nonetheless offset by the overall reduction in N_W at a given integrated influence per mode, as seen in Fig. 6(c).

B. Many-body impurities

To study complex, interacting models, we require sophisticated numerical methods, such as tensor networks. We adopt a typical approach for open quantum systems, where the density matrix is vectorized and approximated as a one-dimensional tensor network, also called a matrix product state (MPS).^{63,64} While the MPS has a one dimensional structure, this does not require that the Hamiltonian have only local interactions. The MPS may also tolerate long-range couplings, particularly when a judicious state ordering is imposed for the reservoirs (as in our ordering for the mixed basis in Fig. 8). These give a small, fixed MPO dimension. This construction

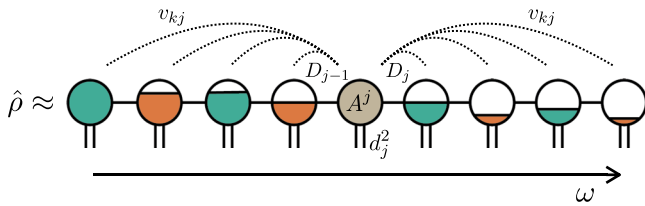


FIG. 8. Matrix product state ansatz. The reservoirs (orange/green) are represented in the energy basis (similar to the so-called star geometry⁶²), where we mix the modes from the two reservoirs along the one-dimensional MPS lattice, ordering them globally according to their energies and keeping the impurity sites (brown) in the middle. This order reflects the natural scattering structure of the current-carrying states,^{7,8} greatly reducing the bipartite entanglement in the lattice and the MPS bond dimension needed to achieve a given level of precision. The color-coding follows Fig. 1.

is represented diagrammatically in Fig. 8, where we have ordered the combined $\mathcal{LR}$ modes (green/orange) according to their energies, reflecting the resonant nature of the current-carrying states^{7,8} (the color-coding follows Fig. 1). The system $\mathcal{S}$ (gray) is positioned in the middle at $\omega = 0$. Following this notation, d_j is the local Hilbert space dimension at site j and D_j is the MPS bond dimension to the right of site j . The latter determines the size $D_{j-1} \times d_j^2 \times D_j$ of each tensor A^j constituting the MPS. The computational cost will depend on both N_W and the structure of the correlations, which set the minimal D_j needed to reach a given level of accuracy. Our choice of reservoir mode ordering has been shown to minimize this bond dimension by mitigating the spread of entanglement.^{7,8} We obtain steady-states by using the time-dependent variational principle⁶⁵ to evolve an MPS under the Lindblad superoperator, as described in Ref. 8 (see Ref. 9 for a similar approach with a different state ordering). Since the accuracy of this approach depends on the bond dimension, we can adjust the latter using a cutoff $\epsilon_{\min}$. That is, we only retain the singular values that are above this cutoff for each bipartition of the lattice in Fig. 8.

We quantify the convergence of our MPS calculations via the steady-state current, which is expected to have consistently larger error than other measures. Our analysis will focus on the weakly coupled, two-site impurity model from Fig. 6 in both non-interacting and interacting limits. To assess the consistency of our methods, we first confirm that the current and correlation matrix from the non-interacting MPS can reproduce the exact solution for all three discretizations (Fig. 9). This confidence allows us to focus on a particular level of discretization-related error, indicated by the red band in Fig. 9(a). By fixing the number N_W of sites in each reservoir to a value within this band, we can determine how the singular value threshold $\epsilon_{\min}$ controls the convergence of the current and the system state at a given accuracy. This accommodation also fixes the number of bias window sites N_B to be the same for each discretization—an important point that we will address later. To proceed, we measure error with respect to the exact (i.e., with no truncation), finite-size current I^R associated with a given N_W and discretization of a non-interacting system. We find a numerical solution that slowly approaches the exact current as $\epsilon_{\min}$ is decreased; however, this convergence is not uniform [Fig. 10(a)]. The choice of discretization has little impact on convergence (and its numerical cost) even though the number of MPS sites is quite different.

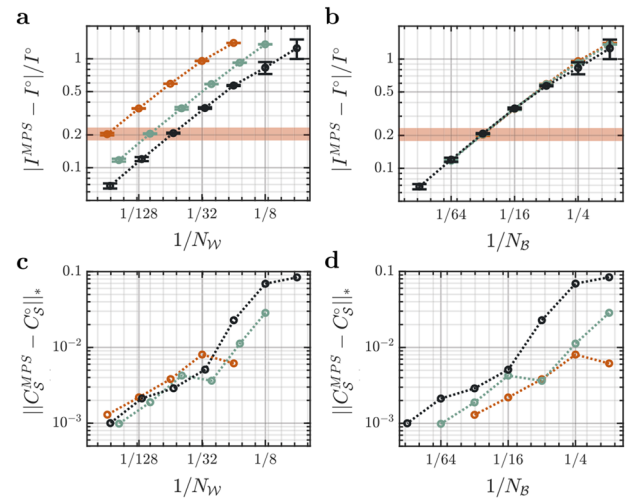


FIG. 9. Error and discretization for non-interacting MPS. Convergence of reservoir discretizations for the non-interacting two-site system $\mathcal{S}$ of Fig. 6, obtained using MPS with a fixed Schmidt cutoff $\epsilon_{\min} = 10^{-6}$. Scaling is quantified with respect to the number of modes in each reservoir N_W and the number of modes within the bias window N_B . Data correspond to [(a) and (b)] the relative error in the steady-state current $I^{\text{MPS}} = I[\gamma^*]$ vs the Landauer limit I^0 and [(c) and (d)] the normalized trace distance between the correlation matrix C_S^{MPS} for $\mathcal{S}$ and its infinite reservoir counterpart C_S^C . Discretizations follow linear (orange), the linear-logarithmic (green), and the linear-inverse (black) arrangements. The red band in (a) and (b) is at relative error scale (0.20), for which N_W is 256, 100, and 60, respectively, and N_B is 32. The current I^{MPS} is an average from $\mathcal{LS}$, $\mathcal{S}_1\mathcal{S}_2$, and $\mathcal{SR}$ interfaces. Uncertainties $\sigma = \pm \sqrt{\sigma_1^2 + \sigma_2^2}$ reflect fluctuations σ_1 of the current over a temporal window $\Delta t = 50 \omega_0^{-1}$, as well as the mismatch $\sigma_2^2 = \sum_j |I_j - I^{\text{MPS}}|^2 / 3$ of currents at the interfaces $j \in \{\mathcal{LS}_1, \mathcal{S}_1\mathcal{S}_2, \mathcal{S}_2\mathcal{R}\}$. The designated C_S^{MPS} is representative of the final simulation time step. Parameters are identical to Fig. 6 but with a system-reservoir coupling $v_0 = \omega_0/8$.

This behavior can be understood by using the quantity $F = \sum_j D_j^3$ to estimate the relative cost of MPS simulations for a given $\epsilon_{\min}$. This metric encapsulates the scaling of computational time with bond dimension, as other parameters contributing to the cost (e.g., bond dimensions for the Lindbladian MPO and local Hilbert space dimensions) are the same for all discretizations. Our discretizations differ in the total number of reservoir sites N_W that are needed to reproduce a given level of accuracy. However, an analysis based on F suggests that the degree of correlation is determined by the number of states within the bias window N_B , which is the same for each discretization at a given accuracy level (Fig. 10). Thus, we cannot specify a discretization that will yield a clear increase in computational performance for MPS simulations. The only benefit to having a smaller N_W is having fewer modes outside the bias window. This has little computational impact, as our ordering places these modes near the ends of the MPS, where they require a small D_j and contribute weakly to F .

A related analysis can be performed for interacting systems, which we demonstrate by introducing a density-density interaction of strength $U = -\omega_0/2$ between the impurity sites. Since the exact solution is unknown, we estimate an optimal relaxation γ_s by comparing γ -dependent turnover profiles with on/off-resonant modes (Fig. 4), as validated earlier in the manuscript. This procedure is

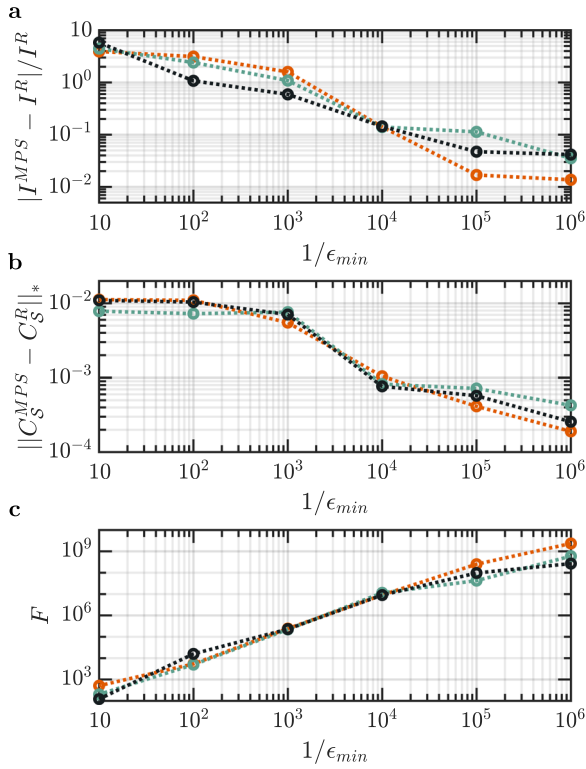


FIG. 10. Error and Schmidt cutoff for non-interacting MPS. (a) The relative error in the steady-state current I^{MPS} compared to reference values I^R [these reference currents correspond to exact, finite N_W simulations performed using values of N_W that give data points demarcated by the red band in Figs. 9(a) and 9(b), thus reflecting the $\epsilon_{\min} \rightarrow 0$ limit]. I^R is at a fixed error level with respect to the continuum current I° . The convergence is plotted vs the inverse Schmidt cutoff $1/\epsilon_{\min}$. (b) The normalized trace distance between the correlation matrix C_S^{MPS} for S and the reference C_S^R vs $1/\epsilon_{\min}$. (c) The relative, approximate numerical cost, vs $1/\epsilon_{\min}$, of a single MPS update $F = \sum_j D_j^3$, defined in terms of the MPS bond dimensions D_j at all bipartitions. Discretizations correspond to linear (orange), the linear-logarithmic (green), and the linear-inverse (black) arrangements.

executed for each discretization and set of reservoir modes, yielding the scaling behavior presented in Fig. 11(a). We again find a current that converges monotonically with increasing N_W for all discretization schemes, although the convergence of occupations is more variable.

We can also assess how simulation performance scales with $\epsilon_{\min}$ when interactions are present. To avoid finite size effects, we limit this and subsequent analysis to points with $N_B > 4$. Following our analysis for the non-interacting MPS, we define a fixed level of discretization-related error. We do so by choosing discretizations that give approximately the same current I^R [the red band in Fig. 11(a)] and thus have a similar error with respect to the continuum limit. The latter is estimated to be far from distinguished points (as discussed below), but it cannot be derived exactly. In addition, we quantify truncation-related error measured with respect to the finite-size currents I^R obtained for $\epsilon_{\min} = 10^{-6}$ at given discretization. We find that the convergence of the current and correlation matrix C_S is comparable across discretizations, as is the numerical

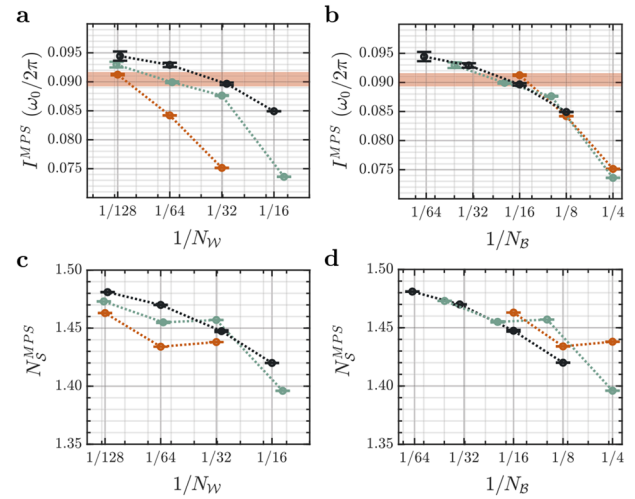


FIG. 11. Discretization effects for interacting MPS. Convergence of reservoir discretizations obtained with the MPS approach for the two-site impurity of Fig. 9 with an additional many-body interaction $U = -\omega_0/2$. The behavior is computed vs the number of modes in each reservoir N_W and the number of modes within each bias window N_B . Data correspond to [(a) and (b)] the steady-state current $I^{MPS} = I[\gamma_s]$ and [(c) and (d)] the total particle number in S , $N_S^{MPS} = N_S[\gamma_s]$, where γ_s estimates the best relaxation as described in the text. Discretizations follow linear (orange), the linear-logarithmic (green), and the linear-inverse (black) arrangements. The red band in (a) and (b) gives the reference current, I^R , which, by virtue of being approximately the same value of the current, is at the same relative error scale. The number of modes, N_W , is 128, 62, and 30, and N_B is 16, 20, and 16 for the three discretizations, respectively. Model parameters and uncertainty calculations in the current are identical to Fig. 9. Uncertainties for N_S^{MPS} are given by $\sigma = \pm\sigma_1$, reflecting fluctuations of the measurement over a temporal window $\Delta t = 50 \omega_0^{-1}$. These density uncertainties are smaller than the data point size in (c) and (d). The simulations have a Schmidt cutoff $\epsilon_{\min} = 10^{-6}$.

cost quantified through F [Fig. 12(c)]. Once again, performance is dictated by how accurately we represent the bias window (and thus by N_B), emulating the non-interacting MPS. The particular reservoir discretization, at comparable N_B , still has little impact when converging the current in tensor network simulations at practical reservoir sizes. In fact, the Schmidt cutoff $\epsilon_{\min}$ and underlying system Hamiltonian are the primary determinants of convergence and its numerical cost.

The exact, continuum-limit current is unknown for many interesting systems. Nonetheless, our extended reservoir simulations should approach this regime as the number of explicit reservoir modes is increased. This is particularly true for the current, where we have observed monotonic convergence with N_W in both non-interacting and interacting MPS simulations. Below, we propose a fitting procedure to estimate the continuum limit current using a simple scaling law. We test our procedure with non-interacting calculations and apply it to the interacting model.

The importance of bias window modes is captured by parameterizing the scaling law in terms of N_B , $I = I^\infty + A/N_B^p$, where I^∞ , A , and p are fit parameters. I^∞ provides an estimate for the continuum-limit current I° . We test the fitting procedure by applying it to MPS data for the non-interacting model in

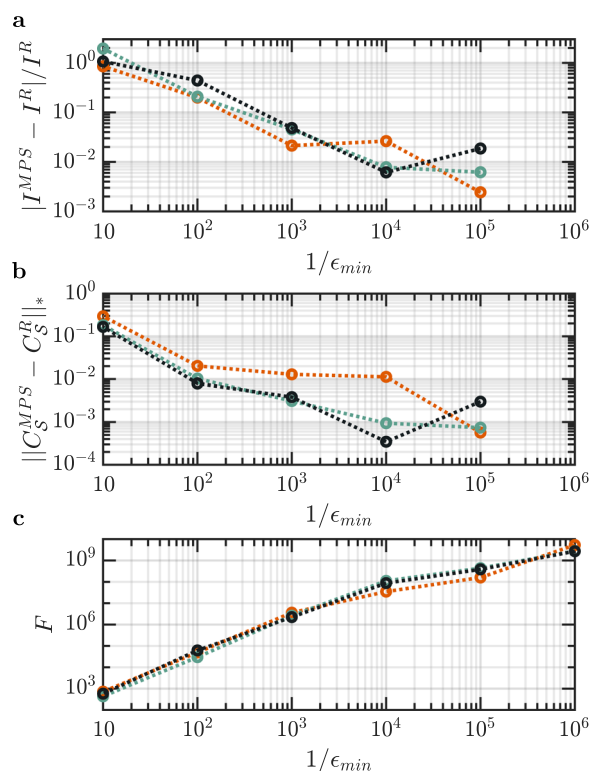


FIG. 12. Error and Schmidt cutoff for interacting MPS. (a) The relative error in the steady-state current I^{MPS} compared to the reference value I^{R} [demarcated by the red band in Figs. 11(a) and 11(b), which is at approximately the same value]. The convergence is plotted vs the inverse Schmidt cutoff $1/\epsilon_{\text{min}}$. The reference current I^{R} is at the tightest cutoff of $\epsilon_{\text{min}} = 10^{-6}$. (b) The normalized trace distance between the correlation matrix C_S^{MPS} for S and the reference C_S^{R} vs $1/\epsilon_{\text{min}}$. (c) The relative numerical cost, vs $1/\epsilon_{\text{min}}$, of a single MPS update $F = \sum_j D_j^3$, defined in terms of the MPS bond dimensions D_j at all bipartitions. Discretizations correspond to linear (orange), the linear-logarithmic (green), and the linear-inverse (black) arrangements.

Fig. 9(b). The fit for each discretization separately gives scaling exponents of $p = [0.48 \pm 0.05, 0.54 \pm 0.04, 0.67 \pm 0.02]$ and estimates for the continuum-limit current $2\pi I^\infty/\omega_0 = [0.0023 \pm 0.0003, 0.0026 \pm 0.0002, 0.0030 \pm 0.0001]$ for the linear, linear-logarithmic, and linear-inverse discretizations, respectively. These exhibit reasonable agreement with their exact counterpart $2\pi I^\circ/\omega_0 = 0.0031$, albeit with some discrepancies. The high performance of the linear-inverse arrangement is expected since bias window modes predominate for this discretization.

Given that the currents from different discretizations overlap when plotted vs $1/N_B$, we can aggregate the datasets to increase the total number of data points and also change the fit range to be $N_B > 4$. A collective fit to this aggregated data gives us a scaling exponent $p = 0.72 \pm 0.02$ and an estimate for the continuum current of $2\pi I^\infty/\omega_0 = 0.0030 \pm 0.0001$. This is in good agreement with I° . The MPS scaling exponents p can be compared to the exact finite N_W profiles in Fig. 6, which includes many more points than accessible with MPS. We assume that they give an exact estimate $I^\infty = I^\circ$. The fit for each discretization separately

gives scaling exponents of $p = [0.77 \pm 0.01, 0.77 \pm 0.01, 0.74 \pm 0.01]$ for the linear, linear-logarithmic and linear-inverse discretizations, respectively, and $p = 0.76 \pm 0.01$ for the collective fit. This suggests that the collective fit for the aggregated MPS data is yielding better results.

The same strategy can be applied to the interacting system of Fig. 11. Since we have a very limited dataset, we aggregate the data from different discretizations. The collective fit gives $p = 1.50 \pm 0.63$ and $2\pi I^\infty/\omega_0 = 0.093 \pm 0.002$. The large standard error in the exponent may be due to a few factors: non-scaling finite-size effects, other contributions to numerical uncertainty, or that modes outside the bias window have a greater influence when interactions are present. The outer modes influence densities and, in turn, affect the current, which may be increasing their importance.

VI. CONCLUSIONS

Our observations suggest a general approach when using discrete reservoirs in quantum transport simulations. In a technical sense, we find that the linear-inverse discretization is the most efficient arrangement for non-interacting cases, particularly when combined with a relaxation method based on the level spacing in the bias window. Nonetheless, the performance between discretizations is not dramatic and is effectively negligible for the N_W used in practical simulations. This is especially true for interacting MPS-based simulations, where correlations ultimately regulate the computational cost. Despite this behavior, one should remain mindful of cases where the choice of discretization can become more important—notably for small N_W or at a small bias where a large portion of the bandwidth becomes less relevant (at least for the current). The importance of this limit has been recognized by other authors, particularly in the context of numerical renormalization group calculations.^{66–70} Furthermore, there may remain some interplay between the performance of a given discretization toward a particular observable and the distribution of states within S . This consideration could be relevant in computationally taxing cases, including certain many-body limits, where N_W is strongly limited by practical constraints.

In addition, we developed a method for estimating the optimal relaxation γ^* that approximates the continuum result $I(\gamma^*) \approx I^\circ$. This is valuable when the continuum limit I° is unknown. While the turnover region will vary between model Hamiltonians and coupling regimes, we need only “switch on” a level shift between reservoirs and use the intersection γ_s between shifted and unshifted turnover profiles (or γ_ℓ from linear extrapolation) to estimate the best relaxation. This provides a practical tool for performing extended reservoir simulations with matrix product states and tensor networks.

SUPPLEMENTARY MATERIAL

The [supplementary material](#) contains turnover and scaling analyses for additional multi-site systems.

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DATA AVAILABILITY

The data that support the findings of this study are available within the article and its [supplementary material](#).

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Publication IV

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Accumulative reservoir construction: Bridging continuously relaxed and periodically refreshed extended reservoirs

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The simulation of open many-body quantum systems is challenging, requiring methods to both handle exponentially large Hilbert spaces and represent the influence of (infinite) particle and energy reservoirs. These two requirements are at odds with each other: larger collections of modes can increase the fidelity of the reservoir representation but come at a substantial computational cost when included in numerical many-body techniques. An increasingly utilized and natural approach to control the growth of the reservoir is to cast a finite set of reservoir modes themselves as an open quantum system. There are, though, many routes to do so. Here, we introduce an accumulative reservoir construction—an ARC—that employs a series of partial refreshes of the extended reservoirs. Through this series, the representation accumulates the character of an infinite reservoir. This provides a unified framework for both continuous (Lindblad) relaxation and a recently introduced periodically refresh approach (i.e., discrete resets of the reservoir modes to equilibrium). In the context of quantum transport, we show that the phase space for physical behavior separates into discrete and continuous relaxation regimes with the boundary between them set by natural, physical timescales. Both of these regimes “turnover” into regions of over- and underdamped coherence in a way reminiscent of Kramers’ crossover. We examine how the range of behavior impacts errors and the computational cost, including within tensor networks. These results provide the first comparison of distinct extended reservoir approaches, showing that they have different scaling of error versus cost (with a bridging ARC regime decaying fastest). Exploiting the enhanced scaling, though, will be challenging, as it comes with a substantial increase in (operator space) entanglement entropy.

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I. INTRODUCTION

The interplay between the dynamics of isolated quantum systems and processes induced by macroscopic reservoirs, such as dissipation and decoherence, is central to the understanding and design of quantum devices. Yet, the resulting composite systems are challenging to simulate. Overcoming this challenge will lead to more than just accurate modeling of phenomena, such as transport and many-body relaxation. It will also provide new avenues for the experimental realization of open quantum systems—ones that exploit the control and stability of ultracold atom [1–6], trapped ion [7–9], and quantum dot and other platforms [10–12]. This will, in turn, provide new insights into, e.g., quantum effects in thermodynamic machines [13] (i.e., quantum engines [14,15]) and may lead to scalable, physical simulators.

Macroscopic reservoirs are often taken as continuum, noninteracting collections of electrons or phonons. These *Gaussian environments* are exactly solvable when not in

contact with the system. However, the combination of the reservoirs and the quantum system will typically lead to analytically intractable equations of motion. Numerical techniques are thus the method of choice to benchmark approximations or to find the solution—e.g., the nonequilibrium steady state (NESS) of the system or the real-time dynamics of the current, among other quantities. Even within this simplified setting, though, simulation is difficult since it must capture both the many-body nature of the system and the non-Markovian behavior due to contact with the environment.

In order to address this challenge, there is a rapidly growing body of methods that exploit the Gaussian nature of the environment to move the system-environment boundary. Instead of a clean split between system and environment, the boundary is between the system and a finite—and, due to computational constraints, relatively modest—set of reservoir modes on one side and the remaining external environment—the “true” reservoir—on the other. We dub these *extended reservoir approaches* (ERAs) as the finite collection of modes acts as an extension of the reservoir into the system. These modes impart explicit non-Markovianity to the dynamics. This idea builds on the concept of pseudo-modes [16–19], where external, time-local (Markovian) damping broadens the

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modes into Lorentzian peaks turning a discrete reservoir into an effective continuum.

ERAs can be applied with fermionic (e.g., electronic reservoirs) or bosonic (e.g., thermal baths) environments, as well as with a variety of relaxation methods (inter- and intramode relaxation, Markovian or non-Markovian relaxation, etc.). Almost all of the approaches to date have focused on the continuous relaxation (CR) regime, where relaxation is always present in the equation of motion. This framework can handle both noninteracting and many-body systems, where the formal transport solution is given by Meir-Wingreen-like equations [20–24]. However, due to practical limitations, most simulations are of noninteracting electron [25–36] (summarized in Ref. [21]) or classical thermal transport [37–41]. Tensor networks, though, are now enabling the implementation of this framework to nonperturbatively simulate many-body impurities [42–49] and extended systems [50].

Recently, an idea was put forward to periodically refresh the reservoirs rather than provide continuous relaxation [51]. This periodic refresh (PR) approach evolves the system and the finite collection of reservoir modes coherently except at periodic intervals where the reservoir modes are reset into their initial (isolated) equilibrium. The refresh time has a firm physical basis: The Fermi velocity dictates how fast the density wavefront reaches the finite boundary of the explicit reservoir [52], which is more generally related to a Lieb-Robinson bound [51,53]. PR is recent and, as such, its accuracy as a simulation technique has not yet been carefully investigated.

Within the CR approach, the accuracy is tied to the reproduction of the continuum spectral function—particularly the weighted spectral function for quantum transport. This also provides bounds on parameters. For instance, the relaxation strength has to be less than the thermal relaxation [20,21], which yields a minimum reservoir size as well. Ultimately, though, convergence depends on details of the model. On one hand, anomalous behavior (at zero bias [20] or with interference [36] or weak coupling [54]) can hinder convergence and also modify optimal parameter selection [55]. On the other hand, saturation and smooth behavior of observables like current can enhance convergence beyond what hard bounds would suggest [49,54]. A comparison of different ERAs is thus imperative for both understanding the machinery and determining the optimal approach.

Here, we take the first step in comparing distinct ERA approaches by providing a link between CR and PR approaches through what we call the *accumulative reservoir construction* (ARC), see Fig. 1. ARC reduces to CR and PR in two different limits. The core idea of the ARC is to divide the evolution into two steps: a unitary evolution of the system in contact with finite reservoirs followed by a *partial* relaxation of the reservoir modes (as opposed to full refresh in PR). We perform an extensive numerical characterization of ARC, focusing on the NESS of a solvable example, implemented both exactly and with tensor networks. A phase diagram results, where a “cut” separates CR- and PR-like behavior. The point for the best estimate of the current jumps from the CR- to the PR-like side of the cut, creating discontinuities in the operator entanglement and other quantities. On the CR side, there is

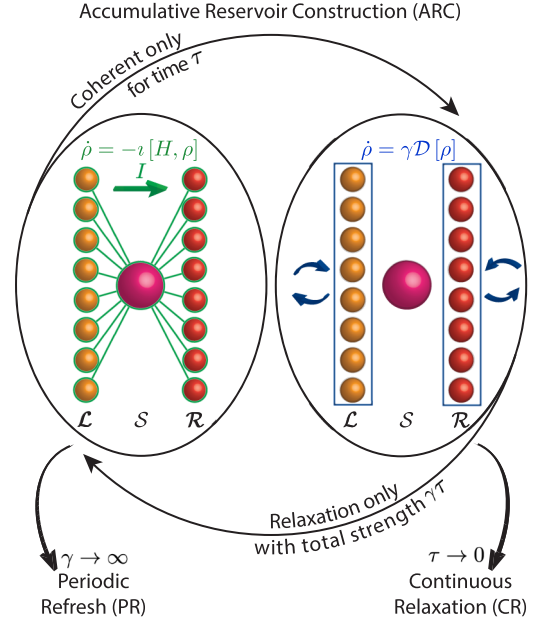


FIG. 1. Accumulative reservoir construction (ARC). ARC bridges two different approaches to simulate open quantum systems, from continuous relaxation (CR) to periodic refresh (PR). It consists of two steps of time τ . The first is a unitary evolution with the composite Hamiltonian (highlighted in green on the left) of the system S and reservoirs $\mathcal{L}\mathcal{R}$, the reservoirs being discretized into a finite number of modes N_W . The second step is a dissipative process that partially relaxes the reservoir modes towards their isolated equilibrium states (highlighted in blue on the right). In our implementation the dissipation is Lindblad damping with a homogeneous, intramode relaxation strength γ and acts only on the reservoirs. ARC is shown in the context of quantum transport, where two reservoirs at different chemical potentials and/or temperatures drive a current I through an impurity or extended system S . Depending on γ , τ , and N_W , the NESS from ARC can be a good approximation to the NESS from macroscopic reservoirs. CR corresponds to the limit $\tau \rightarrow 0$ at fixed γ , whereas PR corresponds to $\gamma \rightarrow \infty$ at fixed τ .

a modest level of entropy (i.e., low computational cost) but a moderate level of error (in current or system density matrix). On the PR side, there is a much larger entropy but much smaller errors. These regimes have different scaling behavior and thus the method of choice depends on the computational resources available. This is manifest within tensor networks, where the PR-like regime of ARC is difficult to converge.

II. OVERVIEW

We formulate the accumulative reservoir approach (ARC) as a method to numerically investigate quantum transport (Sec. III), as well as non-Markovian open quantum systems more generally. The ARC bridges two existing approaches using continuous relaxation (CR), and periodic refresh (PR). As this bridge, it has three core parameters: reservoir size, relaxation strength, and time between refresh events. We focus on the noninteracting resonant level model (Sec. IV) and extensively characterize the behavior of transport in this parameter space—i.e., we provide a phase diagram—for this model (Sec. V). This allows us to benchmark ARC against

exact results to assess the convergence of the steady-state current, as well as the impurity state. We then conclude (Sec. VI).

The phase diagram for ARC has two overarching categorizations. The first is whether the behavior is CR- or PR-like. There is a “cut” that defines the transition between the two and signifies the interplay of ARC parameters with different physical timescales. The second categorization is Kramers’ turnover. ARC broadly falls into the paradigm of this turnover. The current has over- and underdamped regions of behavior. The overdamped behavior is Zeno-like regardless of whether one is in the CR- or PR-like regime, as it is essentially constant measurement from the relaxation that dictates the current. Underdamped behavior manifests itself differently in the CR- and PR-like regimes. Except at the cut, the region between over- and underdamped behavior captures the physics of the current. This region grows as the number of reservoir modes increases and is thus the physically applicable regime that reproduces the continuum limit.

In the context of efficient simulation, CR and PR yield different error-cost scaling, with PR having a faster decay of error versus cost but it also has a larger prefactor. The larger prefactor causes convergence difficulties. With the tensor network implementation we employ, CR is thus preferable. ARC, however, has a large swath of phase space between CR and PR. The intermediate regime is refreshlike in its physics, but has even better error-cost scaling. It still is more challenging to converge than CR, but may serve as a target for more accurate simulations.

We expect the results and conclusions for ARC to generalize to more complex models, including those with many-body interactions. For CR, for instance, the overdamped regime can be derived directly from Meir-Wingreen-like equations for both noninteracting and many-body impurities [20]. Those equations also show that CR limits to the exact result. The underdamped regime has been proven for a large class of models and is expected to always hold based on physical arguments. Similarly, physical arguments suggest the turnover for PR and PR-like behavior will always hold. By construction, PR also limits to the right current in the intermediate turnover regime. Many-body interactions may change the error-cost scaling, especially its nonasymptotic behavior (i.e., smaller explicit reservoir sizes) by introducing different time and temperature scales, or power-law decaying correlations. We do not expect these will change the qualitative distinctions in the error-cost relationships between CR, PR, and intermediate regimes. These distinctions are due to balancing the reservoir representation and relaxation-induced reduction of entanglement, neither of which are system dependent.

III. FRAMEWORK

While the ERA is a general approach to handle a large class of non-Markovian open quantum systems, we will employ it here in the context of quantum transport through an impurity or junction region. In this scenario, a chemical potential (or temperature) drop between two (noninteracting) metallic electronic reservoirs $\mathcal{L}$ and $\mathcal{R}$ will drive a current through a system $\mathcal{S}$, as seen by the left schematic in Fig. 1. The total Hamiltonian,

$$H = H_S + H_{\mathcal{L}} + H_{\mathcal{R}} + H_{\mathcal{I}}, \quad (1)$$

is given by a sum of a system Hamiltonian H_S , $\alpha \in \{\mathcal{L}, \mathcal{R}\}$ reservoir Hamiltonian,

$$H_{\alpha} = \sum_{k \in \alpha} \omega_k c_k^{\dagger} c_k, \quad (2)$$

and coupling Hamiltonian between $\mathcal{S}$ and $\mathcal{LR}$,

$$H_{\mathcal{I}} = \sum_{k \in \mathcal{LR}} \sum_{i \in \mathcal{S}} (v_{ki} c_k^{\dagger} c_i + v_{ik} c_i^{\dagger} c_k). \quad (3)$$

Here, $c_m^{\dagger}$ (c_m) is the fermionic creation (annihilation) operator for mode $m \in \mathcal{LSR}$, the index m carries all necessary labels (frequency, location, spin, etc.), and all Hamiltonians are in terms of frequencies. Each reservoir is taken to have $N_{\mathcal{L}} = N_{\mathcal{R}} = N_{\mathcal{W}}$ modes, where the label $\mathcal{W}$ signifies the electronic band (the two reservoirs could have a different number of modes but we do not consider that case). The Hermitian coupling matrix $v_{ki} = v_{ik}^*$ defines the quadratic interaction between the reservoirs and the system. More generally, $H_{\mathcal{I}}$ could be taken as a coupling linear in the reservoir operators but with an arbitrary system operator. We restrict to the transport setting where there is just hopping between the reservoirs and system. The Hamiltonian H_S is also generally arbitrary, potentially having, e.g., electron-electron or electron-vibrational couplings. In our example, as described later, we take it to be quadratic so that we can compare to the exact solution.

In addition to the Hamiltonian, we must have proper boundary conditions to drive a current. There are many ways to do this, such as having an initially disconnected reservoirs $\mathcal{L}$ and $\mathcal{R}$ with a chemical potential drop between them or by turning on a chemical potential drop at an initial time where $\mathcal{LSR}$ is in equilibrium state, among others. For continuum (macroscopic) reservoirs, as well as ERA, we will take the former approach. The state at time $t = 0$ is thus

$$\rho(t = 0) = \rho_S(0) \otimes \rho_{\mathcal{L}}^{\text{eq}} \otimes \rho_{\mathcal{R}}^{\text{eq}}, \quad (4)$$

where we take $\rho_S(0)$ to be the maximally mixed state on $\mathcal{S}$ and $\rho_{\alpha}^{\text{eq}}$ the isolated equilibrium state of reservoir α . The NESS can, in principle, depend on initial conditions but the example we will examine in this work has a unique steady state. The states $\rho_{\alpha}^{\text{eq}}$ are defined by the Fermi-Dirac distribution,

$$f^{\alpha}(\omega) = \frac{1}{1 + e^{\beta_{\alpha}(\omega - \mu_{\alpha})}}, \quad (5)$$

at chemical potential μ_{α} and thermal relaxation time $\beta_{\alpha} = \hbar/k_B T_{\alpha}$, where $\hbar$ is the reduced Planck’s constant, k_B is Boltzmann’s constant, and T_{α} is the temperature. Note that, for convenience, we work with β as the inverse thermal relaxation rate, i.e., thermal relaxation time, which has a unit of time. We will take a symmetrically applied bias $\mu_{\mathcal{L}} = -\mu_{\mathcal{R}} = \mu/2$ and uniform temperature $T_{\mathcal{L}} = T_{\mathcal{R}} = T$. The ERA relaxes the reservoirs toward $\rho_{\alpha}^{\text{eq}}$ in order to maintain a chemical potential and/or temperature imbalance between the finite collection of explicit reservoir modes.

For continuum reservoirs, $N_{\mathcal{W}} \rightarrow \infty$ and $v_{ki} \sim 1/\sqrt{N_{\mathcal{W}}}$, the NESS is

$$\rho_S^{\circ} = \lim_{t \rightarrow \infty} \left(\lim_{N_{\mathcal{W}} \rightarrow \infty} \text{tr}_{\mathcal{LR}} [e^{-iH} \rho(0) e^{iH}] \right), \quad (6)$$

where $\text{tr}_{\mathcal{LR}}$ denotes the trace over $\mathcal{LR}$. A hallmark of a NESS is that there are currents flowing due to the different chemical

potentials or temperatures. The goal of ERA is to supply an efficient numerical technique to find a NESS that has a well-defined convergence to ρ_S^0 , while simultaneously enabling the numerically exact inclusion of many-body interactions. This enables determining the current-voltage relationship or energy currents, as well as other characteristics of the system.

When working with noninteracting, number-conserving reservoirs, Eq. (2), linearly coupled to the system, as in Eq. (3), the NESS is governed by the reservoir spectral functions. Commonly, the reservoirs are coupled each to only a single mode in the system, $v_{ki} \equiv v_k$ (the system mode k can be different for different α). In this case, the spectral function is

$$J_\alpha(\omega) = 2\pi \sum_{k \in \alpha} v_k^2 \delta(\omega - \omega_k). \quad (7)$$

More generally, the spectral function will be a matrix that characterizes the couplings to all $\mathcal{S}$ modes [20,24]. For the specific model we examine, each reservoir is only connected to a single boundary site on the left (for $\mathcal{L}$) and right (for $\mathcal{R}$) of the system. Thus Eq. (7) will be the relevant quantity. All microscopic models of the reservoirs that lead to the same macroscopic ($N_W \rightarrow \infty$) spectral functions give the same dynamics and NESS. This feature is often used to obtain finite-size reservoirs that systematically accumulate essential features of these functions when increasing the number of reservoir modes [55–58]. The approaches we discuss are all based on such finite-size representations of the reservoirs.

Since ERA methods use a finite number of modes that are in turn open to implicit environments, we need to specify how these implicit environments relax the explicit modes. In addition to basic model properties (e.g., the spectral function and $\mathcal{S}$), this relaxation will dictate the NESS and how well the technique approximates ρ_S^0 . We will now describe the two limits of ARC, one with damping given by continuous, Markovian relaxation and the other with periodic, full refreshes. We then will turn to the general ARC description.

A. Continuous relaxation (CR)

For CR, each reservoir is damped continuously via a Lindblad dissipator. The equation of motion is

$$\dot{\rho} = -i[H, \rho] + \gamma \mathcal{D}[\rho], \quad (8)$$

where the dissipative contribution is

$$\begin{aligned} \mathcal{D}[\rho] = & \sum_{k \in \mathcal{LR}} f^{\alpha_k}(\omega_k) \left(c_k^\dagger \rho c_k - \frac{1}{2} \{c_k c_k^\dagger, \rho\} \right) \\ & + \sum_{k \in \mathcal{LR}} [1 - f^{\alpha_k}(\omega_k)] \left(c_k \rho c_k^\dagger - \frac{1}{2} \{c_k^\dagger c_k, \rho\} \right) \end{aligned} \quad (9)$$

and $[\cdot, \cdot]$ ($\{\cdot, \cdot\}$) is the commutator (anticommutator). This form, Eqs. (8) and (9), assumes a homogeneous relaxation strength γ (this assumption can be relaxed but it makes little difference with common discretizations of the reservoirs [55]) and only intramode relaxation. We can alternatively cast the equations in terms injection and depletion rates, $\gamma_{k+} = \gamma f^{\alpha_k}(\omega_k)$ and $\gamma_{k-} = \gamma [1 - f^{\alpha_k}(\omega_k)]$, respectively. Without the coupling to $\mathcal{S}$, each mode thermalizes to its own

equilibrium state set by the temperature T_α and chemical potential μ_α of its respective reservoir α .

We note that Eq. (9) is Markovian for $\mathcal{LSR}$ since the reservoirs $\mathcal{LR}$ are coupled to Markovian environments. The dynamics for $\mathcal{S}$ only, though, is non-Markovian. Each explicit mode in $\mathcal{L}$ or $\mathcal{R}$ that has relaxation will have a Lorentzian spectral function and thus have a memory time—i.e., non-Markovianity—of $1/\gamma$. From $\mathcal{S}$'s perspective, multiple explicit modes in $\mathcal{LR}$ add frequency dependence to the environment's response (i.e., “color”) within this $1/\gamma$ timescale. Moreover, in order to target physical dynamics, one takes the joint limit of $N_W \rightarrow \infty$ and $\gamma \rightarrow 0$, resulting in the memory time going to infinity and capturing the full character of the continuum.

While Eq. (9) can be derived for weak coupling to external environments with chemical potentials at $\pm\infty$ [21], the important aspect is that its NESS converges to the continuum, macroscopic result as $N_W \rightarrow \infty$ and then $\gamma \rightarrow 0$ [20]. The formal solution provides the guarantee of convergence for both noninteracting and many-body systems [20–24], as well as bounds on parameters (such as the aforementioned $\beta\gamma \leq 1$) [20,21]. Yet, there are still many aspects of the convergence, such as its rate and the presence of features, that need to be understood and properly handled [54,55]. The goal is to obtain accurate, physically meaningful results with minimal computational resources (often, the smallest N_W possible but other characteristics are equally important).

Toward this end, one can explore the NESS, and specifically the steady-state particle current, from Eq. (8) treating γ (and N_W) as parameters. Generally there are three basic regimes analogous to Kramers' turnover in solution-phase chemical reactions [59] as the relaxation strength varies [20] (similarly for the same ERA approach for classical thermal transport [39]):

(1) *Small- γ or relaxation-limited regime.* In this regime, the particle current is dictated by the relaxation strength. The supply of particles by the implicit environments is too small compared to the intrinsic current—the physical current—that can flow through the system. This regime can be cast as a three resistor model, with two resistors at the interfaces to the left and right external environments and one resistor for $\mathcal{LSR}$. The latter is much smaller than the former and thus the interfaces to the external environments dominate (albeit the former is proportional to $1/\gamma N_W$ and thus the transition from relaxation-limited to the intrinsic current depends on N_W). Thus there is a linear increase of the total current versus γ . This regime is also characterized by overly coherent interactions within $\mathcal{LSR}$, i.e., that there are unphysical global oscillations within all the explicit degrees of freedom. From the initial state, a wavefront transverses $\mathcal{LSR}$ with the Fermi velocity in the same way as in a closed system. This transversal and associated oscillations decays into the steady state, but they still influence the character of the NESS.

(2) *Intermediate- γ or physical regime.* In this regime, the supply rate is sufficiently strong to support the intrinsic, physical current without disturbing it significantly. As with the small γ regime, one can cast this regime within the three resistor model. However now, since γ is larger, the $\mathcal{LSR}$ resistor dominates and one obtains the physical current from calculations. In this regime, a plateau in the current develops

and increases in size with N_W . It is in this regime that the current—typically the most important observable—accurately captures the current in the true NESS. The approximate NESS will also approach ρ_S° [55]. Extending this plateau is the practical realization of the limits $N_W \rightarrow \infty$ and then $\gamma \rightarrow 0$ (i.e., as N_W increases but is still finite, adjusting γ to be sufficiently small but not so small to turn over into the small γ regime).

(3) *Large- γ or overdamped regime.* In this regime, the relaxation is too strong, suppressing the coherence between the extended reservoir and S that is necessary to carry a current (as currents are just coherences). This effectively decouples the extended reservoirs, resulting in the current decaying as $1/\gamma$. The situation here is analogous to the Zeno effect. As a consequence of the decoupling, S itself is overly coherent. As with the other two regimes, one can also cast this regime—in fact, all three regimes—into a series of resistors. One has to include two additional resistors, though, one at the interface between $\mathcal{L}S$ and one at $\mathcal{S}R$ (but with resistor proportional to γ rather than $1/\gamma$).

While the above regimes hold generally, there can also be additional regimes due to anomalous behavior [54]. For example, at finite relaxation strength, the Markovian relaxation fails to reproduce the Fermi level, increasing the transmission across $\mathcal{L}SR$ due to artificial spreading of the occupied density of states. This is related to the bound $\beta\gamma \leq 1$ and, as such, it manifests at strong relaxation (*a Markovian anomaly*). For proportionally coupled reservoirs (i.e., ones where we have the same set of modes in $\mathcal{L}$ and $\mathcal{R}$), another anomaly can occur at weak relaxation due to virtual (resonant) transitions (*a virtual anomaly*). Small intrinsic currents, e.g., for weak system-reservoir coupling, reveal these anomalies. The plateau forms between them as N_W increases. We previously proposed a heuristic approach to estimate the optimal γ to target the physical regime for a general, including many-body, S [55]. The approach removes the virtual anomaly by applying a small shift between the frequencies of $\mathcal{L}$ and $\mathcal{R}$ modes. The estimate for γ is where the turnover curve intersects the curve without this shift, i.e., it finds a domain of confidence for CR (a sweet spot for γ). We will employ this approach in this work for CR. Additional information on this procedure is in Appendix A.

B. Periodic refresh (PR)

In the PR approach [51], the system and finite-size reservoirs evolve fully unitarily for a time τ after which the reservoirs are “refreshed” (reset to their initial, isolated equilibrium state), and the process repeats periodically. At cycle $p = 0, 1, \dots$, the evolution follows:

$$\rho(p\tau + \tau) = \text{tr}_{\mathcal{LR}}[e^{-i\tau H} \rho(p\tau) e^{i\tau H}] \otimes \rho_{\mathcal{L}}^{\text{eq}} \otimes \rho_{\mathcal{R}}^{\text{eq}}. \quad (10)$$

This provides the state of $\mathcal{L}SR$ at discrete intervals $p\tau$. In order to examine the behavior of this approach, we will also sometimes make use of the state in between these discrete intervals at times $t = p\tau + \tau'$ with $\tau' < \tau$. When we do, we employ the assignment, $\rho(p\tau + \tau') = e^{-i\tau'H} \rho(p\tau) e^{i\tau'H}$ (in words, only coherent evolution is included in assigning the time). A physical realization of this process would either require multiple copies of each reservoir—a so-called collisional or repeated interaction model—or the ability to

otherwise control and reset the reservoir (e.g., turn off interactions with and in the system and “refill” the explicit reservoir modes).

The NESS in PR is a periodic state. However, if we stroboscopically look at the system at time steps of τ , $\rho_S(p\tau) = \text{tr}_{\mathcal{LR}}[\rho(p\tau)]$, then we will find an approximation to ρ_S° as $p \rightarrow \infty$. The interfacial currents (between the reservoirs and system) are often of interest, e.g., for special cases, such as impurities with only one site in contact with the reservoirs, they are the only place to obtain the overall current. In which case, one uses $\rho(p\tau - \epsilon)$ with $\epsilon \rightarrow 0^+$. This selects the full state just before the refresh. It has no bearing on the estimated ρ_S° , as $\rho_S(p\tau) = \lim_{\epsilon \rightarrow 0^+} \text{tr}_{\mathcal{LR}}[\rho(p\tau - \epsilon)]$ since the refresh does nothing to the S ’s state. It does, however, retain the system-reservoir correlations, enabling an estimate of the steady-state interfacial current.

In a similar manner to CR, as $N_W \rightarrow \infty$ and then $\tau \rightarrow \infty$, the system’s NESS will converge to the continuum, macroscopic NESS. The periodic refreshing, though, stabilizes the state into a true NESS, opposed to closed—“microcanonical”—evolution (where the system state and/or current is taken from the quasisteady state that forms at finite time [6,52,60–64]). We further note that, for a given N_W , a physically meaningful τ results from a lattice mapping of the reservoir spectral function followed by Lieb-Robinson arguments. For, e.g., a simple one-dimensional (1D) reservoir, this τ is

$$\tau_W = N_W/2\omega_0, \quad (11)$$

where $2\omega_0$ is the Fermi velocity, which is set by the (uniform) hopping frequency, ω_0 , in the 1D lattice. This τ signifies when the current wavefront has impinged of the boundary of the finite reservoir. This effectively yields only one free parameter (either N_W or τ , both increasing in tandem). Just as with CR the non-Markovian character increases as this free parameter increases. We designate τ_W the physical timescale. Additional information on PR, specifically its Kramers’ turnover-like physics that we study in this work, is in Appendix B.

C. Accumulative reservoir construction (ARC)

As with PR, the ARC also takes a periodic process starting first with a fully unitary evolution of the system and explicit reservoir modes for time τ . This is followed by a dissipative process of total strength $\gamma\tau$ with the system and system-reservoir coupling frozen. Since these processes are alternating, the relaxation can be applied for time τ with strength γ or could be an “impulse” or discrete “gate” with the same total strength $\gamma\tau$. This cyclical process is depicted in Fig. 1. At cycle $p = 0, 1, \dots$, the evolution follows the form

$$\rho(p\tau + \tau) = e^{\gamma\tau\mathcal{D}}[e^{-i\tau H} \rho(p\tau) e^{i\tau H}], \quad (12)$$

where $e^{\gamma\tau\mathcal{D}}[\cdot]$ is the evolution superoperator for the dissipation from Eq. (9). Note that there are two separate evolutions in Eq. (12) each for a time τ , yet we only increment the time of the density matrix by τ (opposed to 2τ). In other words, we do not count the dissipative evolution in the time. As with PR, we employ the assignment, $\rho(p\tau + \tau') = e^{-i\tau'H} \rho(p\tau) e^{i\tau'H}$, for intermediate times $t = p\tau + \tau'$ with $\tau' < \tau$.

For ARC, the coherent evolution is exactly as for PR. The dissipation, though, does not give a complete refresh of the reservoirs. Rather, it relaxes the reservoirs with a total strength of $\gamma\tau$. If τ is fixed, for instance, but $\gamma \rightarrow \infty$, then this performs a full refresh and thus completely recovers PR. If one fixes γ but takes $\tau \rightarrow 0$, then one recovers CR. This limit is just a first order Trotter expansion of the evolution in Eq. (8). This motivates leaving out the dissipative evolution in the assignment of intermediate times, as the two processes taken separately with a step τ is a numerical approximation to a single step τ taken jointly. As we will see, even away from the CR or PR limits, there is a wide range of parameters where the NESS approximates ρ_S° .

This discussion already makes apparent that there are three free parameters in ARC (γ , τ , and N_W). This is opposed to CR and PR, which both have an effective single parameter. Albeit, in the case of CR, imposing a single relation between γ and N_W will not be the most effective use of computational resources; Rather, one wants to make use of the existence of a domain of confidence to set the relationship between the two [55], yielding γ for a set N_W . A similar consideration holds for PR. One can use the physical τ_W , but this may not be the most effective in terms of error for a given cost, as we will discuss. For ARC, however, using γ and τ as the parameters is not always the most suitable choice. Rather, the product,

$$\gamma\tau = \text{Total relaxation}, \quad (13)$$

provides the total amount of relaxation at each cycle and is the only relevant quantity for the dissipation. For the other parameter, we choose the quantity

$$\tilde{\tau} = \left| \tau - i \frac{2}{\gamma} \right| = \text{Action}, \quad (14)$$

which is the magnitude of a complex action. This choice is motivated by the way in which the relaxation appears in the retarded Green's function, see Ref. [20]. We will numerically characterize the ARC as function of these parameters using a solvable example. We will see that the choice of parameters makes many features of the phase diagram for ARC readily apparent, as well as has the two limits (CR and PR) as ‘‘Cartesian’’ boundaries on polar opposites of the phase space. These aspects make it a good choice, but there may be other choices that are superior. For instance, the bare parameters, τ and γ , remain meaningful when interpreting aspects of the evolution, as we will discuss.

Finally, we can view ARC (and PR) as an example of a bang-bang protocol [65,66]. Such protocols appear, for instance, in the context of quantum computation as a procedure outputting the desired state through the alternating application of two (or more) noncommuting processes. In variational quantum algorithms [65,66], protocol parameters are optimized, typically to minimize some cost function, such as energy. Similarly, in ARC, the parameters should, within finite resources, best reproduce the influence of continuum reservoirs. As the latter does not admit a straightforward variational form, we approximate the optimal ARC parameters based on a physical understanding of the process. Appendix C 1 contains additional discussion on ARC.

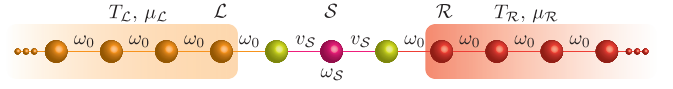


FIG. 2. Resonant-level model. The schematic shows the example—the resonant level model—used to numerically characterize ARC. We will use the parameters $\omega_S = v_S = \omega_0/2$, several different temperatures but with $T_L = T_R = T$, and the chemical potentials $\mu_L = -\mu_R = \omega_0/4$ (i.e., a total potential drop of $\omega_0/2$ applied symmetrically). By going to the single particle eigenbasis of $\mathcal{L}$ and $\mathcal{R}$, the model conforms to the setup in Fig. 1. Even within tensor networks, we simulate the reservoirs using their eigenbasis and thus their spatial dimension is not directly relevant.

IV. EXAMPLE SYSTEM

In all the results below, we consider reservoirs that are 1D lattices with a uniform nearest-neighbor hopping frequency ω_0 . The impurity region is composed of $N_S = 3$ sites also arranged in a one-dimensional configuration with Hamiltonian,

$$H_S = \omega_S a_2^\dagger a_2 + v_S (a_1^\dagger a_2 + a_2^\dagger a_3 + \text{H.c.}), \quad (15)$$

where a_i ($a_i^\dagger$) are fermionic annihilation/creation operators for site i in $\mathcal{S}$ and H.c. signifies the Hermitian conjugate terms. As the example model, we take the onsite frequency of the middle site to be $\omega_S = \omega_0/2$ and hopping amplitude $v_S = \omega_0/2$. As indicated in Fig. 2, the reservoirs $\mathcal{L}$ and $\mathcal{R}$ will both be at the initial temperature T , while the (symmetric) chemical potential imbalance of $\mu_L = -\mu_R = \omega_0/4$ drives the particle current. This model is a noninteracting resonant level model (see Refs. [67,68] for the interacting resonant level model). For the reservoirs, by choosing a finite lattice length of N_W for $\mathcal{L}$ and $\mathcal{R}$ and then diagonalizing the single-particle Hamiltonians, the reservoirs and the system-reservoir couplings are cast in the form of Eqs. (2) and (3). This process provides the finite reservoirs that we use. For $N_W \rightarrow \infty$, the reservoir spectral function for a uniform 1D lattice with hopping ω_0 (in contact with the impurity boundary with coupling also ω_0) are

$$J_{\mathcal{L}}(\omega) = J_{\mathcal{R}}(\omega) = J(\omega) = \sqrt{4\omega_0^2 - \omega^2}. \quad (16)$$

We are after the NESS of this model. Although there are no many-body interactions, we expect the qualitative nature of the results to carry over to presence of many-body interactions in the system $\mathcal{S}$.

A. Reference NESS

Since this is a noninteracting model, we can solve for all properties of the system in the continuum, macroscopic limit by employing nonequilibrium Green's functions. It is helpful to write the Hamiltonian, Eq. (1), in terms of its single-particle counterpart, $\bar{H}$,

$$H = \sum_{m,n \in \mathcal{L}\mathcal{S}\mathcal{R}} \bar{H}_{mn} c_m^\dagger c_n, \quad (17)$$

as well as the system's Hamiltonian itself,

$$H_S = \sum_{i,j \in \mathcal{S}} [\bar{H}_S]_{ij} c_i^\dagger c_j, \quad (18)$$

where $[\bar{\mathbf{H}}_S]_{ij} = \bar{\mathbf{H}}_{ij}$ is a submatrix. Using this, the retarded (advanced) Green's function of the system is

$$\mathbf{G}^{r(a)} = 1/(\omega - \bar{\mathbf{H}}_S - \Sigma_{\mathcal{L}}^{r(a)} - \Sigma_{\mathcal{R}}^{r(a)}), \quad (19)$$

with respective self-energies

$$\Sigma_{\alpha}^{r(a)} = \sum_{k \in \alpha} g_k^{r(a)} |v_k\rangle \langle v_k|. \quad (20)$$

We use $|v_k\rangle$ for the coupling vector between mode $k \in \mathcal{LR}$ and all sites $i \in \mathcal{S}$, i.e., $\langle i|v_k\rangle = v_{ik}$, and $g_k^{r(a)} = 1/(\omega - \omega_k \pm i\eta)$ for the retarded (advanced) Green's function of $k \in \mathcal{LR}$. As usual, the limit of $\eta \rightarrow 0^+$ is taken at the end of the calculation. Note that this formalism also permits the formal CR solution, including analytic in some cases, of the current and correlation matrices for $\mathcal{LSR}$ [20–24].

These quantities give the spectral densities (which are the spectral functions, the terminology depends on the community) $\Gamma^{\alpha} = i(\Sigma_{\alpha}^r - \Sigma_{\alpha}^a) = -2 \text{Im} \Sigma_{\alpha}^r$,

$$\Gamma^{\alpha}(\omega) = i \sum_{k \in \alpha} [g_k^r(\omega) - g_k^a(\omega)] |v_k\rangle \langle v_k|. \quad (21)$$

The population-weighted counterpart is

$$\tilde{\Gamma}^{\alpha}(\omega) = i \sum_{k \in \alpha} f^{\alpha}(\omega) [g_k^r(\omega) - g_k^a(\omega)] |v_k\rangle \langle v_k|. \quad (22)$$

With this, the current in the continuum, macroscopic limit is given by the Landauer expression,

$$I^{\circ} = \int \frac{d\omega}{2\pi} (f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)) \text{tr}[\Gamma^{\mathcal{L}} \mathbf{G}^r \Gamma^{\mathcal{R}} \mathbf{G}^a]. \quad (23)$$

In other words, this is the current in the true NESS, the one we are after. We designate it with the superscript $\circ$ to indicate that it is our standard, or reference, current.

Since we are considering an example with a quadratic Hamiltonian, the NESS is Gaussian state and thus can be completely characterized by the correlation matrix

$$[\mathbf{C}_S^{\circ}]_{ij} = \text{tr}[c_{j_i}^{\dagger} c_i \rho_S^{\circ}], \quad (24)$$

where $\mathbf{C}_S^{\circ}$ is the system's submatrix of the full correlation matrix. The correlation matrix is often referred to as the single-particle density matrix. It is a Hermitian, semi-positive definite matrix, although it does not have a trace equal to one. We can similarly write the system's correlation matrix in the NESS,

$$\mathbf{C}_S^{\circ} = \int \frac{d\omega}{2\pi} \mathbf{G}^r (\tilde{\Gamma}^{\mathcal{L}} + \tilde{\Gamma}^{\mathcal{R}}) \mathbf{G}^a. \quad (25)$$

Unlike the current, only the population-weighted spectral densities appear here. They are the source of particles that propagate with $\mathbf{G}^r[\cdot] \mathbf{G}^a$ into the system.

While the expressions above, Eqs. (23) and (25), for the current and correlation matrix are more general, our example only has nonzero elements of the self-energies and the spectral densities for $i = 1, j = 1$ and $i = N_S, j = N_S$. For the self-energies, these are

$$[\Sigma_{\mathcal{L}}^r(\omega)]_{11} = [\Sigma_{\mathcal{R}}^r(\omega)]_{N_S N_S} = -\frac{1}{2}(\omega + i\sqrt{4\omega_0^2 - \omega^2}). \quad (26)$$

The spectral densities (functions) readily follow, showing consistency with these quantities and Eq. (16).

B. noninteracting ARC

The evolution generated by Eq. (8) with the quadratic Hamiltonian, Eq. (1), retains the Gaussianity of the state. As a result, the evolution (which is also particle conserving) can be formulated via the correlation matrix,

$$\mathbf{C}_{mn} = \text{tr}[c_n^{\dagger} c_m \rho], \quad (27)$$

with $m, n \in \mathcal{LSR}$. In this form, we have [21]

$$\dot{\mathbf{C}} = -i[\bar{\mathbf{H}}, \mathbf{C}] + \gamma \mathcal{D}[\mathbf{C}], \quad (28)$$

with the dissipation in Eq. (9) translating to

$$\mathcal{D}[\mathbf{C}]_{mn} = f^{\alpha_m}(\omega_m) \delta_{mn} \delta_{m \in \mathcal{LR}} - \mathbf{C}_{mn} \frac{\delta_{m \in \mathcal{LR}} + \delta_{n \in \mathcal{LR}}}{2}. \quad (29)$$

Here, the δ_{mn} is the normal Kronecker delta, and $\delta_{m \in \mathcal{LR}}$ is 1 for the mode in one of the reservoirs and 0 otherwise, i.e., no relaxation occurs within the system.

Consequently, for purely unitary evolution over a time τ (without dissipation), the evolution is

$$e^{-i\tau \bar{\mathbf{H}}} \mathbf{C} e^{i\tau \bar{\mathbf{H}}}. \quad (30)$$

For pure dissipation for a time τ (without the action of the Hamiltonian), integrating Eq. (29) leads to an update

$$\mathcal{G} \mathbf{C} \mathcal{G}^{\dagger} + \mathcal{P}, \quad (31)$$

where the dissipative matrices are

$$\mathcal{G}_{mn} = \delta_{mn} e^{-\gamma \tau \delta_{m \in \mathcal{LR}}/2} \quad (32)$$

and

$$\mathcal{P}_{mn} = \delta_{mn} (1 - e^{-\gamma \tau \delta_{m \in \mathcal{LR}}}) f^{\alpha_m}(\omega_m). \quad (33)$$

For ARC in Eq. (12), the evolution is a unitary followed by a dissipation step. The cycle p of this process is

$$\mathbf{C}(p\tau + \tau) = \mathbf{M} \mathbf{C}(p\tau) \mathbf{M}^{\dagger} + \mathcal{P}, \quad (34)$$

with

$$\mathbf{M} = \mathcal{G} e^{-i\tau \bar{\mathbf{H}}}. \quad (35)$$

These results hold for any Gaussian system, i.e., in absence of many-body interactions. The system can be a lattice of arbitrary dimension and geometry. It can be generalized to cases with an arbitrary number of reservoirs attached to an arbitrary number of sites in $\mathcal{S}$.

On reaching the NESS, $\mathbf{C}(p\tau + \tau) = \mathbf{C}(p\tau)$. This makes Eq. (34) exactly of the form of a discrete-time Lyapunov equation (an equation widely studied in mathematics and engineering). The discrete-time Lyapunov equation can be solved directly, allowing to find the NESS without carrying out the time evolution. Moreover, the timescale, or the number of cycles, for reaching the NESS in an ARC process is given by the largest magnitude eigenvalue of $\mathbf{M}$. Indeed, following the standard stability analysis of the dynamical process in Eq. (34), the timescale to convergence to the NESS is

$$\tau_c = \frac{\tau}{-\ln(|m_0|)}, \quad (36)$$

where the largest magnitude eigenvalue, m_0 , of $\mathbf{M}$ dictates the number of cycles and τ is the unitary evolution for a single cycle. When all eigenvalues have magnitude less than one, the steady state is unique. In our example, the largest eigenvalue is such that $|m_0| < 1$ and uniqueness is guaranteed. Equation (36) is something we will employ to estimate one of the contributions to the computational cost in tensor networks, where explicit time evolution is currently needed to obtain the NESS.

Finally, given the correlation matrix of $\mathcal{LSR}$ at any time (or in the NESS), the particle current

$$I_{\mathcal{LS}} = 2 \sum_{k \in \mathcal{L}, i \in \mathcal{S}} \text{Im } v_{ik} \mathcal{C}_{ki} \quad (37)$$

is flowing across the $\mathcal{LS}$ interface (assuming that $\mathcal{L}$ is only connected to $\mathcal{S}$ and not directly to $\mathcal{R}$). Similar expressions apply to other interfaces.

V. RESULTS

The primary goal of this work is to extensively characterize ARC and its limits (CR and PR) in order to understand their behavior and performance (error-cost relationship), and determine the optimal approach within the confines of the example system. We will employ the approach of Sec. IV B to find the NESS, including its current, in order to compare the results with the reference (continuum, macroscopic) results of Sec. IV A. Before proceeding to the NESS properties, we first examine the full time evolution within ARC, which will elucidate the underlying processes within this framework.

A. Time dynamics

Figure 3 plots the (normalized) current $I(t)/I^\circ$ between the system and the left reservoir for the resonant level model (Sec. IV and Fig. 2). Four representative ARC parameter regimes are in the figure. In the CR limit ($\tau \rightarrow 0$ at finite γ), Fig. 3(a), there are initial oscillations but the current ultimately relaxes close to the reference value I° , as seen by the approach of the normalized current to 1. Away from this limit, the cyclic nature of the ARC becomes apparent. In Figs. 3(b) and 3(c), the intermediate values of $\gamma\tau$ show the initial oscillations, as well as oscillations after each partial refresh. The NESS defined by the periodic stroboscopic points in red shows that the current still relaxes near to I° . Figure 3(d) provides the PR limit ($\gamma \rightarrow \infty$ at finite τ). This also has oscillations but, at the end of each cycle, the current at the $\mathcal{LS}$ interface goes to zero since the correlations between the system and reservoirs are completely removed. As with the other cases (except the CR limit), the stroboscopic points define the NESS and converge to I° .

B. Phase diagram for the steady state

The steady state of ARC—specifically, the level of current that its NESS sustains—yields different phases of behavior versus the total relaxation $\gamma\tau$ and action $\tilde{\tau} = |\tau - i2/\gamma|$, see Fig. 4(a). These phases are analogous to the Kramers' turnover regimes discussed extensively in the context of ERA with continuous relaxation for quantum electron [20,21,49,54] and classical thermal [39,40] transport.

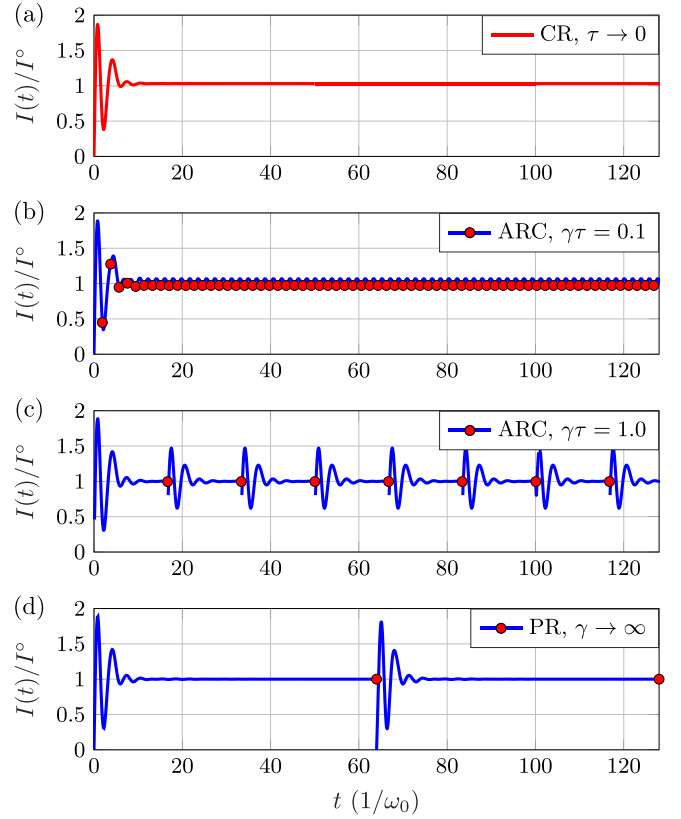


FIG. 3. Time dynamics of ARC. The plots show the current between $\mathcal{L}$ and $\mathcal{S}$ versus time for $N_{\mathcal{V}} = 128$ sites per reservoir. The ARC parameters are (a) $\tau \rightarrow 0$ at finite $\gamma \approx 0.084 \omega_0$ (i.e., in the CR regime), (b) $\gamma\tau = 0.1$ and $\tilde{\tau} \approx 37.90/\omega_0$, (c) $\gamma\tau = 1$ and $\tilde{\tau} \approx 37.30/\omega_0$, and (d) $\gamma \rightarrow \infty$ at finite $\tau = 64/\omega_0$ (i.e., in the PR regime). The red points indicate the current right before the application of dissipation, whereas CR is a continuous red line since relaxation is continuous. For all regimes of ARC except the CR limit, the stroboscopic points in red are the most relevant. The convergence of these at long times gives the estimate of the current within the exact NESS. We note that (a) γ for CR is provided by the heuristic procedure of Ref. [55], [(b) and (c)] $\tilde{\tau}$ is given by the value that best estimates the current at fixed $\gamma\tau$, and (d) τ is given by the (physical) refresh time for PR, $\tau = \tau_{\mathcal{V}} = N_{\mathcal{V}}/2\omega_0$ with $2\omega_0$ the Fermi velocity.

In Sec. III A, we introduced these phases for CR. There are relaxation-limited currents for small γ and Zeno-limited currents for large γ . In between, there is an intermediate- γ regime where the intrinsic, physical current dictates the transport behavior. This turnover is shown versus action $\tilde{\tau}$ (which depends on the inverse of γ) in Fig. 4(a), so, from left to right, the behavior goes from Zeno through the physical regime to the relaxation-limited regime. When the behavior is more like PR, there is a Zeno regime that goes to a physical regime, but the relaxation-limited regime is now characterized by overly coherent oscillations in the global $\mathcal{LSR}$ system.

The Zeno behavior for small action occurs when $\tilde{\tau}$ is shorter than any timescale in $\mathcal{LSR}$. On the PR side, this corresponds to frequent refreshes, i.e., small τ , where repeated resets of the reservoirs occur before the current fully starts to flow (i.e., before the restoration of sufficient coherence

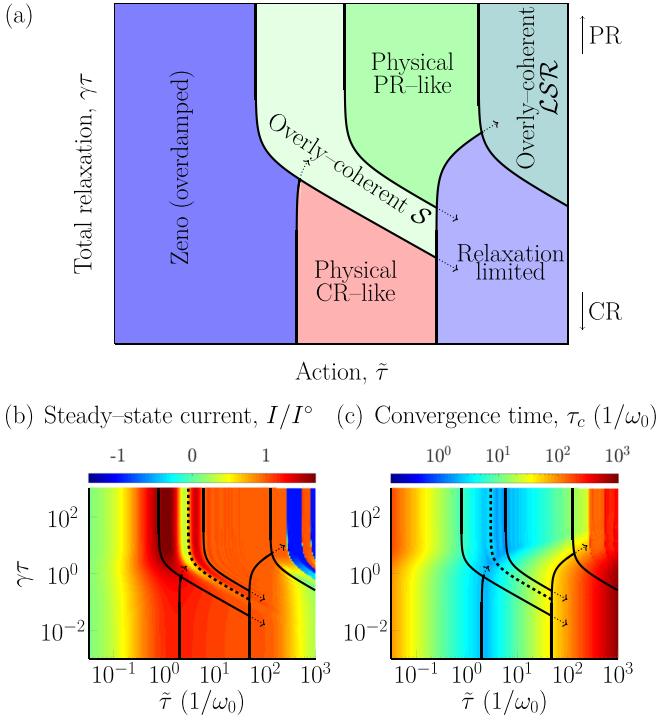


FIG. 4. Phase diagram of ARC. (a) The schematic phase diagram (of the NESS current) shows several regimes as the total relaxation $\gamma\tau$ and the action $\tilde{\tau} = |\tau - i2/\gamma|$ vary at fixed N_W . In this parametrization, the PR limit ($\gamma \rightarrow \infty$ at fixed τ) is on the upper boundary and the CR limit ($\tau \rightarrow 0$ at fixed γ) on the lower. Sweeping the action from small to large values shows three general regimes. On the left is an overdamped (Zeno) regime (i.e., large γ and small τ corresponding to a small action). On the right is an underdamped regime. The weak relaxation regime on the bottom right (i.e., with CR-like behavior) leads to currents limited by the relaxation strength. In the overly coherent regime in the top right (i.e., with PR-like behavior), there are oscillations across the $\mathcal{LSR}$ system. The middle of the diagram contains the physical regimes, with a CR-like physical regime at the bottom and PR-like at the top. The physical regimes are separated by a region of an overly coherent $\mathcal{S}$. (b) The normalized current for $N_W = 256$ on the same diagram. The lines of constant γ —the ones coming vertically from the bottom—are $\omega_0/43.3$ and ω_0 which are heuristic optimal for CR and transition to overdamped regime for CR, respectively. These are normal turnover points discussed extensively elsewhere [20,21,49,54]. The solid lines of constant τ —the ones coming vertically from the top—are from left to right, $\tau^* = \pi/\mathcal{W}$, $2\tau_S$, and τ_W . The former two define the transition regime. The dashed line is τ_S , showing it also demarcates features. The τ_W shows the transition to an overly coherent $\mathcal{LSR}$. To the right of τ_W , the current remains a good approximation until $2\tau_W$ since that is when the density wavefront returns to the system after bouncing off the finite reservoir boundary. (c) The convergence time to NESS follows from Eq. (36). For another perspective on the phase diagram, Fig. 14 shows it within the $\gamma - \tau$ parametrization.

between the system and reservoirs). This is analogous to the quantum Zeno effect in frequently measured systems [69]. For CR, the physics is similar, but now the continuous (or quasicontinuous) relaxation is strong, giving rise to the same effect. Eventually, the current will steadily decrease to zero as

the action decreases (i.e., as τ decreases and γ increases) in this regime.

In the underdamped regime, unlike the Zeno regime, there is distinct PR-like and CR-like behavior. In the former, there are global oscillations of the current as its wavefront transverses $\mathcal{LSR}$ and bounces off the finite size boundaries. The time for seeing the effect of the boundary is related to the finite speed of propagation given by the Lieb-Robinson bound. An unmistakable signature for this overcoherence is the inversion of the current when $\tau = 2\tau_W$. At twice the physical timescale τ_W , the density wavefront initiated at the time of refresh will travel to the boundary and back to the system in one cycle, reversing the current [52]. Further increasing τ by $2\tau_W$ will lead to other reversals, and so on. For CR-like behavior in the underdamped regime, such oscillations do occur and influence the character of the steady state. Yet, due to the continuous or quasicontinuous character of the relaxation, the current becomes simply linearly proportional to the relaxation strength, as the contact to the external environments is the dominant resistance.

The physically relevant regime of the current occurs at intermediate $\tilde{\tau}$. The character of intermediate phase depends on τ and γ , as the ARC cycle is the first order Trotter decomposition of the evolution superoperator generated by Eq. (8). Ignoring γ for a moment, the decomposition is exact for $\tau \rightarrow 0$ but we can still get reasonable agreement for a finite τ , i.e., quasicontinuous behavior. However, if the coherent evolution is long enough that substantial changes in $\mathcal{LSR}$ take place during the evolution τ , then the Trotterization will no longer approximate the continuous dynamics. The smallest important timescale will depend on the model. We will consider

$$\tau^* = \pi/\mathcal{W}, \quad (38)$$

which is the rise time for the formation of the steady state when the reservoir has bandwidth $\mathcal{W}$ [70]. This time is usually smaller than other relevant timescales in the $\mathcal{LSR}$ model as the bandwidth is large. In the PR limit, the time τ^* should bound the Zeno regime, as the current forms at the interface in this time. Moreover, for $\tau > \tau^*$, CR-like behavior breaks down, yet $\mathcal{LSR}$ still does not have fully formed global coherence. That coherence requires τ to be greater than the time it takes for particles to transit the system. Similar to τ_W for the reservoirs, Lieb-Robinson arguments suggest a transit time of

$$\tau_S = N_S/2v_S, \quad (39)$$

where $2v_S$ is the (effective) Fermi velocity in the system. For the parameters of our example, $N_S = 3$ and $v_S = \omega_0/2$, this is $\tau_S = 3/\omega_0$. For $\tau < \tau_S$, the system $\mathcal{S}$ accepts some particles from the reservoirs, but these are internally overly coherent (i.e., they oscillate within the system but have their coherence with the reservoirs cutoff before $\mathcal{LSR}$ coherence forms). Similarly to $\mathcal{L}$ and $\mathcal{R}$, for τ multiples of τ_S , we will see the reflection of particle front traveling from one interface to another.

All parts of a parameter space where quasicontinuity breaks down will have refresh-like physics. However, this regime of overly coherent $\mathcal{S}$ has a distinct nature, as seen in Fig. 4(b). This regime extends between τ^* and $2\tau_S$. These two times demarcate the transition region between physical CR-like and PR-like regimes. We note, though, that the upper

limit on τ is not a hard transition. In principle, one should have features at higher multiples of τ_S . Yet, their visibility will depend on details of the model, such as the probability to transmit across the system-reservoir interfaces (which depend on the system-reservoir coupling). Our example sustains a relatively high current and many reflections within $\mathcal{S}$ only give small corrections. Later we will introduce an averaging procedure to eliminate this timescale in determining the performance of ARC (see Sec. V C).

To summarize, at fixed but not too large γ , ARC remains quasicontinuous so long as τ is smaller than τ^* . On the diagram, this means following the lines of fixed γ , which start vertically from the bottom but then turn to the right. When these hit the lines of constant $\tau = \tau^*$, the behavior goes through a transition region—the overly coherent $\mathcal{S}$ region. Increasing τ beyond about $2\tau_S$ (for our example) stabilizes the current.

The physics within this diagram is further illustrated by the bottom panels of Fig. 4. Figure 4(b) shows the normalized current. This is the quantity that defines the phase diagram, showing all the regimes and features. The meaning of signature lines in γ and τ when drawing the phase diagram in terms of these parameters is in Appendix C 2. Figure 4(c) shows the timescale to reach the steady state (derived from **M**). This timescale also has signatures of the lines of constant τ and γ , but does not show all the regimes that are seen in the phase diagram. Additional information on ARC is included in Appendix C 3.

C. Convergence

Now that we have established the character of ARC, we can examine the error-cost relationship. We will characterize error in terms of two quantities. One is in terms of the steady-state current, which is often the main—or only—quantity of interest. The other will be in terms of the system’s correlation matrix. This is error-“agnostic” and captures how well one can reproduce arbitrary observables on the system (e.g., densities, etc.).

For the current, we will focus on the interfacial currents between $\mathcal{L}$ and $\mathcal{S}$, $I_{\mathcal{LS}}$, and between $\mathcal{S}$ and $\mathcal{R}$, $I_{\mathcal{SR}}$. Specifically, we will have the method (ARC with a particular set of parameters) output a current estimate

$$I = (I_{\mathcal{LS}} + I_{\mathcal{SR}})/2, \quad (40)$$

which is an average current (across the two interfaces in this case; one could take this across more partitions). The estimate of the relative error for this current, σ_I^2 , will be a combination of two independent sources that contribute to the loss of accuracy and precision,

$$\sigma_I^2 = \sigma_1^2 + \sigma_2^2. \quad (41)$$

The first contribution is just the relative accuracy,

$$\sigma_1^2 = \left(\frac{I - I^\circ}{I^\circ} \right)^2. \quad (42)$$

It is tempting to stop there when one has the exact result, I° , to compare to. However, except for the exact solution of the CR limit, one can have cases where there are mismatched currents at the interfaces, $I_{\mathcal{LS}} \neq I_{\mathcal{SR}}$, that are used to provide

the current estimator, Eq. (40). One can thus obtain the exact current but still have some underlying error where the current is not reflecting a proper stationary state (i.e., $I_{\mathcal{LS}} = I_{\mathcal{SR}}$). In PR, the mismatch can occur because $\mathcal{LSR}$ is still evolving right before the refresh. The existence of a NESS is only at the level of the state, but not at the level of the currents flowing at different partitions. Alternatively, if one does not have the exact solution but rather one uses tensor networks, the truncation of the state can make currents not match [49]. The second contribution is thus the relative mismatch,

$$\sigma_2^2 = \frac{1}{2} \left(\frac{I - I_{\mathcal{LS}}}{I^\circ} \right)^2 + \frac{1}{2} \left(\frac{I - I_{\mathcal{SR}}}{I^\circ} \right)^2 = \left(\frac{I_{\mathcal{LS}} - I_{\mathcal{SR}}}{2I^\circ} \right)^2, \quad (43)$$

which provides a measure of precision either due to numerical errors in calculations or due to refresh-induced properties of the NESS.

However, the above contributions still do not properly account for accidental crossings that can happen, e.g., when I is oscillating in the parameter space around the thermodynamic-limit value I° . This is indeed the case in PR-like phase and at an accidental crossings for small and large γ in the Kramers’ turnover in the CR limit [20,54,55]. Those are times when both the contributions are zero, $\sigma_1 = \sigma_2 = 0$, but the current is still not properly reflecting the continuum limit result.

For that reason, we quantify convergence by calculating a mean relative error,

$$\bar{\sigma}_I^2(\tilde{\tau}) = \text{mean}_{|\tilde{\tau}' - \tilde{\tau}| \leq \tau_S/2} [\sigma_I^2(\tilde{\tau}')] \quad (44)$$

at fixed $\gamma\tau$. A moving average smooths the outcome over a window of the size τ_S using Eq. (39), that corresponds to the time period of the natural oscillation in the full refresh limit due to the system, and this averaging removes this effect (and associated accidental crossings). Consequently, $\bar{\sigma}_I$ gives us a measure of consistency. An extracted current is only considered good if neighboring values of parameters are also giving good estimates. Thus accidental crossing will not be assigned zero error. Additional information on this procedure is in Appendix C 4.

Figure 5(a) shows how the mean relative error $\bar{\sigma}_I$ behaves within the parameter space of ARC. The features present reflect the phase diagram for ARC, with the lowest relative error for physical CR-like and PR-like phases. At fixed N_W , the physical PR-like phase generally performs better than physical CR-like phase due to capturing more of the non-Markovian character of the evolution. In addition, the PR-like phase has quite a large plateau, a region with low error versus $\gamma\tau$ and $\tilde{\tau}$. This is a consequence of the rapid rise of the current to the steady state in closed quantum systems [70] (i.e., the coherent evolution) together with the stabilization provided by the periodic refresh of the reservoirs. Within the figure, we also show white points. These are the points of lowest $\bar{\sigma}_I$ for a fixed $\gamma\tau$. They represent what action should be taken for a given $\gamma\tau$ in order to get the best estimate of the current. In order to compare ARC at different $\gamma\tau$, we will use the action at these points.

The convergence of the correlation matrix for $\mathcal{S}$ largely follows the convergence of the current, see Fig. 5(b), which

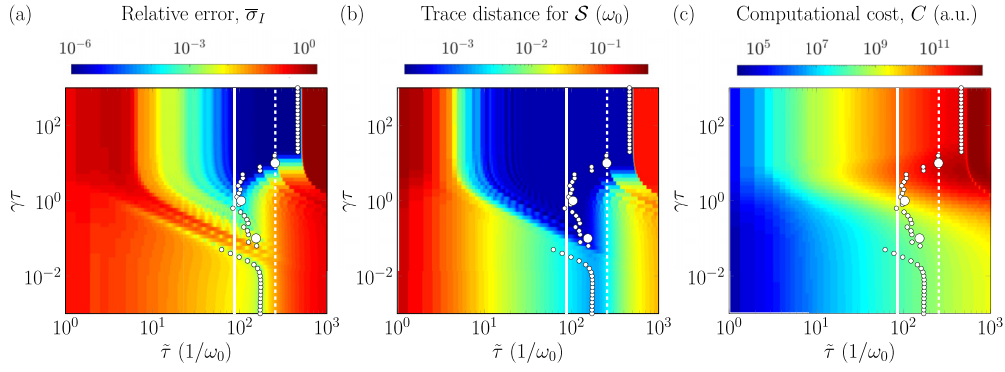


FIG. 5. Convergence and computational cost of ARC. The three panels show the (a) current error, Eq. (44), (b) the correlation matrix error, Eq. (45), and (c) the estimated computational cost, Eq. (46), for our example system and for $N_W = 512$, $\beta\omega_0 = 40$, and $\mu = \omega_0/2$. The two error plots have many of the same features as the phase diagram for ARC, Fig. 4, as we expect since the different regimes directly impact the error. Using the current error as the quantity to be optimized, the best choice of action for a fixed $\gamma\tau$ is marked by the white points in (a). These points are replicated in the other plots [(b) and (c)] to see where they fall for other quantities. These points are close to where the correlation matrix error is minimum in (b), but they do not follow any features in the computational cost in (c). As is evident, CR- and PR-like regimes have very different estimated computational costs. Within the physical regimes, this cost is correlated with the error, with cost going up for more accurate simulations. Outside of these regimes, though, there is no correlation. The white dots for $\gamma\tau = 0.1$, 1, and 10 are made thicker to guide the readers eye. Vertical solid line represents $\tilde{\tau}$ equal to heuristic choice for CR, and vertical dashed line represents $\tilde{\tau} = \tau_W$, which is the physical choice for PR. We employ these $\tilde{\tau}$ for the CR and PR limits.

shows the trace distance to the reference state,

$$\frac{1}{2}|\text{tr}[\mathcal{C}_S - \mathcal{C}_S^o]|. \quad (45)$$

Just like the current error, the plot has many of the same features as the phase diagram for ARC. There is a clear cut between physical CR-like and physical PR-like with PR-like having notably smaller error than CR-like. There is a Zeno regime on the left and underdamped regimes on the right (that split into the overly coherent $\mathcal{LSR}$ and relaxation-limited regimes, for the PR and CR sides, respectively). The site occupancies (i.e., the diagonal elements in the position basis) dominate the correlation matrix error of $\mathcal{S}$, as the current flow is only a small contribution to the total correlation matrix [55]. This is model dependent. A setup that carries a larger current may have current contributions to the error of a similar magnitude. However, we always have a bound $|\mathcal{C}_{mn}| \leq \sqrt{\mathcal{C}_{mm}\mathcal{C}_{nn}}$. This, in turn, bounds the current by the product of onsite occupancies, $\mathcal{C}_{mm}$ and $\mathcal{C}_{nn}$. Thus the current error can at most be similar in magnitude to density errors, but it can not dominate. As a consequence of the outsized importance of occupations, the trace distance does not contain all the same subtle features as the current error. Figure 5(b) also shows that the points of smallest $\bar{\sigma}_I$ (the white points) match with the regions of good convergence for the correlation matrix.

D. Estimated computational cost

Figures 5(a) and 5(b) both demonstrate that physical PR and PR-like regimes of ARC provide highly converged results, whether quantified by the current alone or the correlation matrix, at a fixed reservoir size. The results are much more accurate than the physical CR and CR-like regimes for the same reservoir size. Ultimately, however, one needs the level of error for a given computational cost and how the error scales with computational cost within some many-body method of choice.

In this section, we will estimate the computational cost, C , for a particular tensor network implementation (described in the final section before the conclusions) via quantities computed with noninteracting simulations. In the next two sections, we examine the error-cost scaling and the convergence within actual tensor network simulations. In particular, we exploit the noninteracting nature of our example and extract relevant quantities from the various tools presented in this work. The relevant quantities will be the time to reach the steady state, the lattice size (of order N_W), and the operator space entanglement entropy (OSEE) [71,72], S_O , with the latter enabling an estimate of the matrix product dimension D . We summarize the procedure to calculate S_O from the correlation matrix $\mathcal{C}$ in Appendix D.

For the tensor network techniques, we employ (see the final section before the conclusions) the estimated computational cost is

$$C \sim \tau_c \cdot N_W \cdot 2^{3 \cdot S_O}. \quad (46)$$

For the last term, we use binary entropy to define S_O , leading to base 2 exponentiation, and calculate it in the middle of the lattice as an approximation. When employing tensor networks directly, the cost is taken as

$$C^{\text{MPS}} \sim \tau_c \cdot N_W \cdot D^3. \quad (47)$$

We will explain each of these pieces in turn below.

Currently, no tensor network technique has been demonstrated to directly target the steady state for the class of problems we consider. Rather, real-time runs evolve the state until the state is stationary up to some tolerance. As introduced earlier, the quantity τ_c , Eq. (36), from the map $\mathbf{M}$ determines the convergence. A real-time run on the order of this timescale will exponentially suppress all contributions to the state except the NESS. The combination of the first two relevant factors, $\tau_c N_W$, thus gives the size of the problem. The tensor network simulation will have to iterate over a number

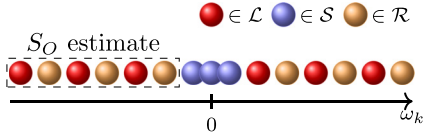


FIG. 6. Mixed basis. For MPS simulations and the calculation of OSEE, we group the modes from reservoirs $\mathcal{L}$ and $\mathcal{R}$, in the frequency basis, and ordered them according to ω_k in Eq. (2). It reflects the emergent structure of correlations in the reservoirs [73]. We place the system modes around zero frequency. We indicate the bipartition of the lattice for calculating OSEE.

of steps proportional to τ_c times a number of lattice sites proportional to $N_{\mathcal{W}}$. The latter follows from the observation that the relevant entanglement appears within the whole bias window, which contains a number of modes proportional to $N_{\mathcal{W}}$.

The remaining factor is the exponent of S_O . With matrix product states (MPS), the convergence of the state is determined by the matrix product dimension, D (other parameters, such as the Schmidt tolerance, can control convergence, but ultimately these just determine D). The time evolution within the implementation we employ (see Sec. V E) has a scaling of the computational cost with D^3 , Eq. (47). noninteracting simulations can not provide the exact D . Moreover, they can't tell us how error will depend on D . However, one can estimate the D necessary for convergence (to the exact finite $N_{\mathcal{W}}$ result) as $D \sim 2^{S_O}$. This provides the last piece in the estimate in Eq. (46). We emphasize that the cost estimates are intended to capture the scaling. There will be proportionality factors including, e.g., the inverse of the time step and the local Hilbert space dimension to the third power. Both are not changed in our case and thus they are left out.

We also note that we employ what is known as the *mixed basis* for the tensor network [73], see Fig. 6. The choice (and order) of basis has an important impact on the structure of correlations within the network that, in turn, influences the required bond dimension D . In the mixed basis, we use the frequency (or, in higher dimensions, momentum) basis and jointly order the $\mathcal{LR}$ modes according to their frequencies. This reflects natural scattering structure for elastic transport where a particle of frequency ω_k scatters from $\mathcal{S}$ and forms an entangled pair shared between modes of that frequency in $\mathcal{L}$ and $\mathcal{R}$. Placing these modes next to each other make the entangled pair localized in the MPS description, which in turn lowers the overall cost. In our implementation, the reservoirs' modes are ordered by increasing frequencies and $\mathcal{S}$ is placed in the middle of bias window. The placement of $\mathcal{S}$ is to reduce the spread of correlations across the MPS by placing $\mathcal{S}$ close to the modes that contribute to the current. This construction drastically reduces the S_O compared to working, e.g., in the spatial basis (i.e., for our case, a one-dimensional nearest-neighbor hopping model).

Figure 5(c) shows the estimated computational cost for the mixed basis. ARC has the lowest cost (with no consideration of errors) when the parameters specify frequent and strong relaxation. That relaxation brings the MPS towards a state that is a product over all reservoir modes. Veering toward this state lowers the bond dimension. However, the parameter

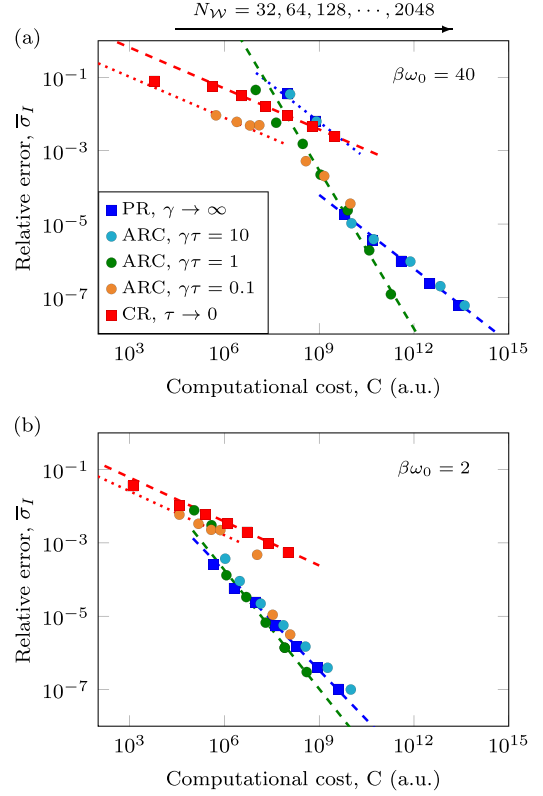


FIG. 7. Error-cost scaling for ARC. The error is shown versus the estimated computational cost, Eq. (46), for (a) a low and (b) a high temperature both with bias $\mu = \omega_0/2$. For a given $\gamma\tau$, the reservoir size $N_{\mathcal{W}}$ increases from left to right (as indicated on the top of the figure), which is the only control parameter here since the estimated computational cost comes from noninteracting simulations. For ARC, the action is taken at the white points in Fig. 5. For CR, we choose the relaxation from heuristic approach [55]. For PR, we choose $\tau = \tau_{\mathcal{W}}$. While there are some transitions in the error-cost scaling, most of the data settles into a power law behavior, Eq. (48). The dashed lines show fitted scaling for CR (red), ARC $\gamma\tau = 1$ (green), and PR (blue). Dotted lines mark related scaling laws. These are not fits but a reference lines of the same ν as their dashed counterparts. More information on the fit can be found in Sec. V E and Appendix C 5.

regimes where the state is close to a product state (for the reservoirs) is not representative of the physics that one is trying to simulate with ERAs. Rather, one needs correlations to build up between the system and reservoirs. This creates a trade-off between improving convergence and reducing computational cost. From Fig. 5, while not one-to-one, there is clearly a relation between cost and accuracy. Since we always work with limited computational resources, we would like to know how the error-cost relationship scales in different ARC regimes and whether there is an ideal regime to work in.

E. Error-cost scaling

As we discuss above, CR and PR methods converge to the continuum, macroscopic reservoir limit as $N_{\mathcal{W}} \rightarrow \infty$ (with $\gamma \rightarrow 0$ or $\tau = \tau_{\mathcal{W}}$, respectively). However, we want to know how the error scales with increasing $N_{\mathcal{W}}$. Figure 7 compares

the error-cost scalings for CR, PR, and other ARC approaches at fixed $\gamma\tau$. Here, we take CR at the heuristic point, see Sec. III A. For PR, we use the physical action $\tilde{\tau} = \tau_{\mathcal{V}}$, as described in Sec. III B. ARC regimes between these two employ the $\tilde{\tau}$ that gives the lowest current error $\bar{\sigma}_I$ (the white points in Fig. 5 and equivalent points for other $N_{\mathcal{V}}$). For each $\gamma\tau$, the reservoir size $N_{\mathcal{V}}$ increases from left to right in Fig. 7.

The error-cost scaling within the physical regimes nicely separates into three classes of behavior: physical CR-like, intermediate, and physical PR-like (the latter are both on the PR-like side of the cut in the phase diagram). The whole physical CR-like regime behaves similarly to the CR limit. We observe varying scaling in the physical PR-like regime. One is for physical PR-like, which includes the PR as a limiting case. Another for the intermediate relaxation regime that represents a case lying in the middle of the phase diagram close to the transition from PR-like regime to the overly coherent $\mathcal{S}$ regime. Here, the advantages of CR and PR reinforce each other, resulting in favorable error-cost scaling. The intermediate regime has both moderate OSEE (lowering the cost) and sufficient non-Markovianity (increasing accuracy).

Note that the borders of those three regimes follow from the phase diagram and are dependent on $N_{\mathcal{V}}$. The scaling can transition from one relation to another as $N_{\mathcal{V}}$ grows. This transition can be seen for $\gamma\tau = 0.1$, which exhibits a scaling characteristic for the physical CR-like regime for $N_{\mathcal{V}} \leq 256$, and switches to the intermediate-relaxation scaling for larger $N_{\mathcal{V}}$. The transition happens when the optimal action (the white points in the figure) jumps from the CR-like side to PR-like side, compare Fig. 16 with Fig. 5.

In Fig. 7, we show the scaling relation at low temperature $\beta\omega_0 = 40$, Fig. 7(a), and at high temperature $\beta\omega_0 = 2$, Fig. 7(b). In both plots, we determine the scaling relations using CR for the physical CR-like regime, PR for PR-like, and ARC of $\gamma\tau = 1$ for the intermediate case. We perform fits to $N_{\mathcal{V}} \geq 128$, to best capture the scaling limit.

The error of the current is typically smallest in the physical PR-like regime, which also leads to the accumulation of more non-Markovian character. However, it is the intermediate regime that has the best proportionality in terms of $N_{\mathcal{V}}$. For the physical PR-like regime, the error of the current goes down approximately as $N_{\mathcal{V}}^{-2}$ for both low and high temperatures. In the intermediate relaxation regime, we have scaling $N_{\mathcal{V}}^{-3.4 \pm 0.2}$ and $N_{\mathcal{V}}^{-2.21 \pm 0.04}$ for low and high temperature, respectively. For physical CR-like, the error of the current goes down as $N_{\mathcal{V}}^{-0.91 \pm 0.02}$ and $N_{\mathcal{V}}^{-0.87 \pm 0.02}$ for low and high temperatures, respectively.

The scaling of the computational cost goes down as the temperature increases. This is driven by the scaling of 2^{S_0} . In particular, its exponents drop by a factor of 2 to 3 times when going from low to high temperature. The decrease reflects that in the limit of infinite temperature, the MPS representation would correspond to a product state with zero OSEE. Separately, the OSEE grows fastest in the physical PR-like regime, where coherent dynamics create a lot of entanglement, and the slowest for the physical CR-like regime. The other contribution to the cost, the convergence time τ_c , grows similarly for high and low temperature, being proportional to $N_{\mathcal{V}}$ for physical CR-like, $N_{\mathcal{V}}^{0.8}$ for physical PR-like, and $N_{\mathcal{V}}^{0.66 \pm 0.04}$ to

$N_{\mathcal{V}}^{0.80 \pm 0.01}$ for low and high temperature for the intermediate case, see Appendix C 5 for details.

We fit the error-cost relationship using the form

$$\bar{\sigma}_I = AC^{-\nu}, \quad (48)$$

where A is a coefficient, ν is the scaling exponent of the decay, and C is the computational cost. Note that the contributions to ν can be delineated by looking at scaling of each component in Eq. (46) with $N_{\mathcal{V}}$, see Appendix C 5. In Fig. 7, we mark the fits by dashed lines and use dotted lines to indicate the same scaling exponent within relevant regions. At lower temperature, $\beta\omega_0 = 40$, the fits give $(\log(A), \nu)$ equal $(4.2 \pm 0.3, 0.67 \pm 0.01)$, $(21.7 \pm 1.5; 1.44 \pm 0.07)$, and $(2.14 \pm 0.06, 0.372 \pm 0.003)$ for PR, $\gamma\tau = 1$, and CR, respectively. The dotted lines show the same scaling exponent as the corresponding dashed line (of the same color) but with a different coefficient A . The red dotted line underlines the scaling relation of $\gamma\tau = 0.1$ before it transitions to intermediate ARC scaling. This stresses that it undergoes the same scaling relation as for CR-limit at heuristic γ . The dotted line is lower than for CR itself because the optimization procedure targets a different action than the CR heuristic. The blue dotted line provides the scaling relation of PR before $N_{\mathcal{V}}$ exceeds the thermal correlation length N_{th} , after which the prefactor of the fit decreases substantially. We discuss this further below. The error-cost scaling is best for $\gamma\tau = 1$ and that PR outperforms CR by about a factor of two for the exponent. Nevertheless, the prefactor is important for achieving a given error when there are constraints on available computational resources. The higher level of correlations retained in the PR approach, in particular, makes it prohibitive at low temperatures within our tensor network approach at the present level of resources.

At high temperatures, Fig. 7(b), the qualitative observations on performance carry over. However, the intermediate and PR regimes have much smaller prefactors A , with the performance of those regimes crossing the CR at smaller $N_{\mathcal{V}}$. At $\beta\omega_0 = 2$, the pairs $(\log(A), \nu)$ are $(3.7 \pm 0.4; 0.90 \pm 0.02)$, $(6.3 \pm 0.4; 1.08 \pm 0.02)$, and $(0.0 \pm 0.2; 0.40 \pm 0.01)$, for PR, $\gamma\tau = 1$, and CR, respectively. The red dotted line underlines the scaling relation of $\gamma\tau = 0.1$ before transitioning to intermediate scaling.

Finally, we already have seen the role of τ^* and $\tau_{\mathcal{S}}$ is determining the transition into the physical PR-like regime, and thus their influence on errors. There is also a sudden drop in performance in the PR limit when going from smaller $N_{\mathcal{V}}$ to larger $N_{\mathcal{V}}$ in Fig. 7(a). This is due to another length (time) scale, the thermal correlation length for the reservoirs. For a 1D uniform lattice reservoir, the thermal correlation length, calculated in isolation from the system and at half-filling, is

$$N_{\text{th}} = 2\beta\omega_0/\pi, \quad (49)$$

where, again, $\beta = \hbar/k_B T$ is the thermal relaxation time for the reservoir. This has an associated timescale

$$\tau_{\text{th}} = N_{\text{th}}/2\omega_0, \quad (50)$$

which is defined similarly to $\tau_{\mathcal{V}}$. In Fig. 8, we focus on the PR limit and show the decay of the relative current error σ_I with the number of reservoir's modes $N_{\mathcal{V}}$ for a wide range

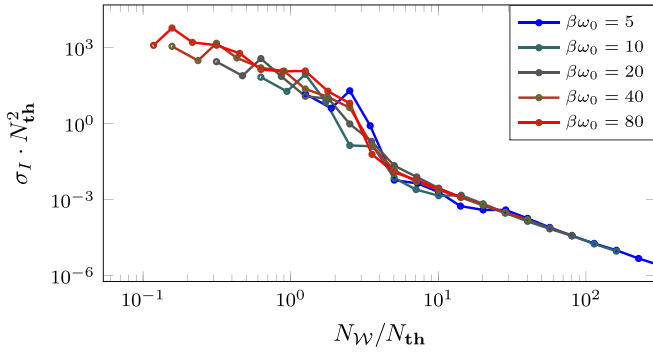


FIG. 8. Thermal correlation length in the PR regime. We show the relative current error rescaled by N_{th}^2 versus the number of reservoir modes divided by N_{th} . We observe the collapse of the data for a range of temperatures onto a single curve, that exhibits two scaling regimes, one for $N_W \lesssim N_{\text{th}}$ and the other for $N_W \gg N_{\text{th}}$. In both regimes, the error vanishes as N_W^{-2} , but with different prefactors.

of temperatures. The data collapse on a single curve when N_W is rescaled by N_{th} and the error multiplied by N_{th}^2 . The curve features a characteristic drop. It is important to note that there are also other sources of error, such as the one related to $\mathcal{S}$, which can also result in a similar drop. Nevertheless, Fig. 8 illustrates that for the best performance one may require $N_W \gg N_{\text{th}}$ in the PR limit. This is identical to a consideration for CR, which requires that $\beta\gamma \leq 1$ and yields an associated bound on the reservoir size $N_W \gtrsim \beta\omega_0$ (in the absence of other relevant factors that can mitigate the effect) [20,21].

F. Tensor network simulations

Tensor networks are a common choice in studying low-dimensional quantum systems. Those methods provide a scalable and accurate tool to target models with many-body interactions [74–76]. The crux of the methods, though, is that there needs to be limited entanglement so that the simulation can target small dimensional subspaces of the total Hilbert space. We will employ an implementation using one-dimensional tensor networks based on matrix product state (MPS) [75,76] and evolved using the time-dependent variational principle (TDVP) [77,78]. More specifically, we will employ for MPS the *mixed basis* that simulates the reservoirs in their eigenbasis with $\mathcal{L}$ and $\mathcal{R}$ modes paired in a way that makes the entanglement entropy scale logarithmically in time [73] (opposed to prohibitive linear growth in time [79] that occurs in transport due to each scattering event creating partially entangled particle-hole pair [80,81]). We include more comments on the mixed basis in Sec. V D.

This method was implemented for open system dynamics within ERAs [49] by vectorizing the density matrix [82] (so the local physical dimension is the square of the local Hilbert space dimension). It is important to note that the problem is only mapped to a 1D representation (in frequency or momentum space) for the state (the MPS). The reservoirs, though, can be any dimension so long as they are noninteracting. For TDVP, the Hamiltonian is written as matrix product operator (MPO). The geometry of the model and the mixed basis yields a very compact Hamiltonian MPO, i.e., with small virtual

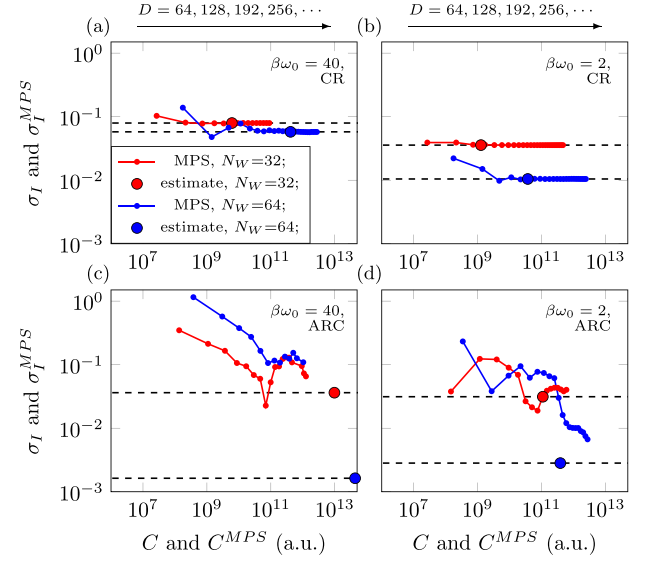


FIG. 9. Convergence with bond dimension. The plots show the error versus cost obtained using the MPS implementation as described in the main text. The data were obtained for (a) CR and (b) ARC $\gamma\tau = 1$ at low and high temperature as indicated on the panels. The matrix product dimension, D , is increased at fixed N_W (shown in the figure), starting from $D = 64$ (at the left) and increasing by 64 between consecutive points. While technically still an estimated computational cost, $C^{\text{MPS}} = \tau_c \cdot N_W \cdot D^3$, this is the actual convergence of the MPS using D from simulation (τ_c is still from the exact evolution operator). The solid circle points are from the estimated costs using a scaled version of Eq. (46), $c \cdot N_W \cdot \tau_c \cdot 2^{3 \cdot S_O}$. We take $c = 10^6$ as a uniform factor to match where the given D is sufficient to achieve convergence at a set N_W . The error of the current in MPS calculation is estimated by an average σ_I , as defined in Eq. (41), over a time window of duration $20/\omega_0$ for CR or 2 to 5 cycles for ARC. Time evolution uses an integration step of $0.125/\omega_0$. The refresh is applied in a single step rather than via time evolution.

bond dimension. Refresh operators can be applied directly on the density matrix after integrating over time, i.e., no time evolution is required. We otherwise follow the approach of Ref. [49].

It is important to emphasize that error-cost scaling and convergence with D are both intertwined and heavily dependent on the tensor network implementation (and geometry and other aspects of the physical problem). For instance, using the same implementation but ordering the reservoir modes to retain the spatial $\mathcal{L}$ - $\mathcal{S}$ - $\mathcal{R}$ structure, the cost estimate, Eq. (46), still applies. However, S_O grows linearly in time and thus the cost would be many orders of magnitude larger than for our implementation. Put more bluntly, when working in the mixed basis, $D \sim t \sim N_W$ due to the logarithmic growth of the (operator) entanglement entropy, giving a total cost growing polynomially. Retaining the spatial structure, however, gives $D \sim 2^{S^t} \sim 2^{\zeta' N_W}$ with ζ and ζ' being some positive constant. Similar considerations apply to density matrix renormalization group methods or other MPS implementations that simulate one-dimensional reservoirs with only nearest-neighbor hopping [6,64,79,82–88]. Other implementations, though, may not have the same scaling as in Eq. (47), and thus

will not use the same approximate form, Eq. (46), in terms of the operator entanglement entropy.

During the ARC process, there are two alternating processes. The step involving unitary time evolution results in the spreading of correlations and, as a result, OSEE growth. On the other hand, during the refresh step dissipation breaks some entangled pairs, making the density matrix closer to the thermal state. The thermal state is a product state with OSEE equal to zero and with trivial physical dimension $D = 1$.

Figure 9(a) shows how the current error converges versus C^{MPS} (that employs D) for CR and $\gamma\tau = 1$ at two different reservoir sizes. Truncation introduces a nontrivial level of error. This error decreases as we take $D \rightarrow \infty$ but is non-monotonic. For the CR regime, convergence is more well behaved than for ARC at $\gamma\tau = 1$, which is somewhat expected given the lower level of S_O in CR. PR has an even higher level of entropy and has higher cost in our tensor network implementation requiring an effort comparable to simulating closed systems but using a vectorized density matrix that squares the cost contribution from D . The plot also shows the full cost estimate scaled by a uniform factor (the same for all $\gamma\tau$ and N_W), showing that the estimates from noninteracting simulations (particularly, $D \sim 2^{S_O}$) are reasonable. Figure 9(b) shows the results for high temperature, which displays similar behavior but with convergence moderately improved and supporting the same conclusion.

VI. CONCLUSIONS

We introduced the *accumulative reservoir construction* (ARC) that provides a bridge between continuous relaxation (CR) and periodic refresh (PR) extended reservoir approaches. The ARC considers a periodic evolution alternating between coherent and dissipative dynamics. The duration of the coherent evolution, the strength of the relaxation, and the reservoir size yield a three parameter family that goes to CR and PR in two opposing limits. At fixed reservoir size, the phase diagram (drawn from the current) reflects aspects of Kramers' turnover, with a Zeno-like regime on one side going through an intermediate, moderate relaxation regime before the transition into an underdamped regime, as we characterized. Due to stroboscopic sampling, PR and PR-like regimes manifest underdamped behavior differently than CR and CR-like regimes. Yet, the underlying physics is the same

This turnover has been extensively investigated for CR for quantum electron transport [20–22,49,54,55] and classical thermal transport [39–41]. Examining simulation techniques across their full parameter space, rather than fixing parameters (e.g., setting γ for CR and τ for PR to functions of N_W), elucidates the underlying machinery and assesses different facets of their behavior. For CR, this has enabled the derivation of the bound $\beta\gamma \leq 1$ [20,21], which also sets a minimum reservoir size, and the discovery of anomalous regimes [20,54] that constrain how to employ the techniques, especially with modest computational resources [55]. ARC makes this readily apparent. ERA-based simulation techniques have a complex interplay of timescales and phenomena. For PR, in particular, we have seen the role of τ^* (the rise time), τ_S (the transit time across the system), and τ_{th} in determining behavior and performance. Just like CR, there is reservoir size set by

the thermal correlation length, which serves as a threshold for accurate simulations. However, there are other contributions to the errors in both cases, of which a full exploration is necessary. Our approach—the scanning of τ for PR, in particular—illuminates the role of various timescales.

The intermediate regime is the target for simulations, as it can provide accurate approximations to the steady-state current and NESS in the presence of continuum, macroscopic reservoirs. In other words, it is the physical regime of the ARC-class of techniques. It can be identified as a plateau region of almost-constant current and system density matrix. When going from CR to PR in this physical regime, there is a “cut” (complete with discontinuous quantities, such as the entanglement entropy, when following optimal parameters) when transitioning between quasicontinuous and refresh-like physics. Away from the cut, the CR- and PR-like regimes, have well-defined error-cost scaling, with the latter having approximately twice the error decay rate as the former. This more rapid decay, though, comes at a cost of a higher overall prefactor due to a larger operator entanglement entropy.

The best error-cost scaling—the best performance—for our example occurs in this transition regime (i.e., the intermediate ARC regime), right after the cut on the refresh side but well before reaching parameters that approximate the full PR. As with PR, this scaling comes at a cost (albeit, lower) in the entanglement entropy. This will be challenging to converge, as is readily apparent in the tensor network simulations. Higher temperatures reduce this barrier, bringing PR and other ARC regimes into more computationally accessible regions.

We expect many of the results for the resonant-level model to generalize to other models, including many-body problems. For continuous relaxation, the existence of overdamped, $1/\gamma$, behavior of the current has been proven to exist for all models (regardless of reservoir spectral function and impurity system, including in the presence of interactions) [20]. The underdamped—relaxation-limited—regime also has been proven for all proportionally coupled, noninteracting impurities [24]. Given the intuitive nature of this regime—that the relaxation limits the rate of particle input/output—it likely holds for all impurities, including those with many-body interactions. For PR physics, we also expect the same based on intuitive arguments. The region of the phase diagram that should change the most is the “cut” between CR- and PR-like physics. However, we only expect this to change quantitatively, not qualitatively. The behavior of entanglement entropy should also be similar and thus the trade-off of computational cost and accuracy should still hold. A full exposition of this is left for future work.

While we have focused on characterizing ARC, especially its phase diagram and performance, the discrete nature of the ARC approach makes it suitable for experimental realization, such as in ultracold atoms and ions [89]. The flexibility of these experimental approaches in controlling interactions, as well as spectral functions, temperatures, and other parameters, together with ARC may provide a route to accurate physical simulators of open, many-body quantum systems. Unlike (classical) computational simulation, entanglement generated during the dynamics is not an explicit cost. Thus ARC (and PR, in particular) may provide a promising framework to

include reservoirs [90], as well as generate novel dynamical states of matter.

ACKNOWLEDGMENTS

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In the first part of the Appendix, we will provide further discussion on Kramers’ turnover for CR and PR. Next we will discuss ARC and its phase diagram when changing reservoir and system S sizes. In the ARC section, we will further review our averaging procedure to obtain $\bar{\sigma}_I$ and scaling relations at optimal point. Finally, we describe the procedure to obtain the operator entanglement entropy for noninteracting fermions.

APPENDIX A: KRAMERS’ TURNOVER AND OPTIMAL $\tilde{\tau}$ FOR CR

The CR limit of ARC is when $\tau \rightarrow 0$, which gives the equation of motion in Eq. (8). The steady-state current is strongly influenced by the relaxation rate γ [20,21,39,49,54]. Figure 10 shows this influence versus $\tilde{\tau} = 2/\gamma$ (for CR), with the current going through the three regimes (from left to right,

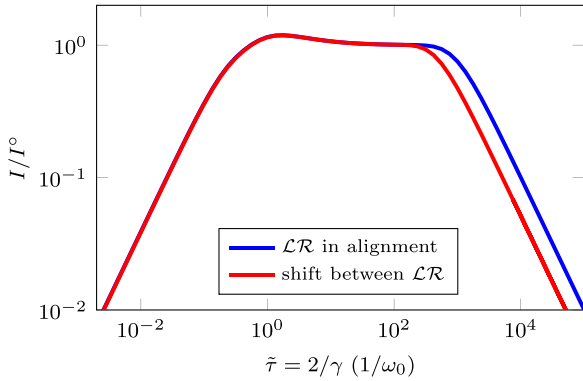


FIG. 10. CR: Kramers’ turnover and estimating the optimal γ . The relaxation rate significantly influences the steady-state current. There are always three distinct regimes of behavior [20]. Examining I/I^0 versus $\tilde{\tau}$, these are seen here as the current initially increasing linearly with $\tilde{\tau} \sim \gamma^{-1}$ (overdamped), plateauing (physical), and then decreasing as $1/\tilde{\tau} \sim \gamma$ (relaxation-limited). There also can be anomalous regimes depending on the particular model [54], for which we see here a small Markovian anomaly on the left hand side of the plateau. In order to estimate the optimal γ (or $\tilde{\tau}$), one can shift the alignment of modes in $\mathcal{L}$ and $\mathcal{R}$, which removes virtual tunneling between them. The $\mathcal{LR}$ in alignment and shifted intersection provides a good estimate of the physical current for given N_W . The heuristic approach avoids unphysical features by targeting a γ that is sufficiently large that the discreteness of the modes is not influencing the transport but allows coherence to develop [55]. The plot uses $N_W = 512$ sites per reservoir, temperature $\beta\omega_0 = 40$, and bias $\mu = \omega_0/2$.

overdamped to physical to relaxation-limited, see Sec. III A). We stress that in prior works these Kramer turnover plots showed the current versus γ rather than action $\tilde{\tau}$, so all regimes are the mirror reflection.

As a simulation approach, one wants the optimal γ to target the physical regime and be as far as possible from anomalous behavior [54,55]. While generally one expects γ to be comparable to the level spacing to optimize the representation of the spectral function, anomalous behavior in certain models can make this a poor choice for the modest number of modes simulation techniques employ.

In Ref. [55], we proposed a simple heuristic approach to estimate the optimal γ in a way that it applies not only to noninteracting systems but also many-body cases. Markovian relaxation of finite reservoirs can yield two anomalies, a Markovian anomaly (broadening of the occupied density of states rather than occupying the broadened density of states) and a virtual anomaly (alignment of reservoir modes opens unphysical channels of conductance due to the finite size of the reservoirs) [54]. Shifting the reservoir modes so that $\mathcal{L}$ and $\mathcal{R}$ modes do not align removes the latter. Finding where the Kramers’ turnover with a shift converges to the turnover with $\mathcal{LR}$ in alignment yields a γ where the current and other properties are stable with respect to small perturbations of the reservoir mode placement, and the current *should be* independent of such details. Here, this convergence occurs as a crossing of the two curves. This approach avoids the unphysical features, including both under- and overdamping, but also the Markovian and virtual anomalies. It thus provides a practical, effective approach to take the continuum limit that recognizes we are always at finite N_W and γ .

APPENDIX B: PHYSICS AND CONVERGENCE FOR PR

Just like CR, PR also goes through a turnover. Since examining this turnover is part of this work, we describe it in some detail here, similar to how we summarize prior work on CR in Sec. III A. At a fixed N_W , the (stroboscopic NESS) current exhibits the following regimes as τ varies.

(1) *Small- τ or Zeno regime.* In this regime, the refresh time is too short, suppressing coherence between the extended reservoir and S that is necessary for a current to flow. This effectively decouples the extended reservoirs, resulting in a current decreasing with τ . The situation here is the Zeno effect. It will occur when the refresh frequency is faster than the timescales for flow from/to $\mathcal{L}$ and $\mathcal{R}$. The rise time, $\tau^* = \pi/\mathcal{W}$, for an electronic reservoir of bandwidth $\mathcal{W}$, see Ref. [70], plays this role for our example. During this time, the interfacial currents increase linearly after the reservoirs are put into contact with the system. The refresh cuts off this increase. This regime is analogous to the large- γ regime for CR, as seen in Fig. 4(b).

(2) *Moderately small- τ or overly coherent- S regime.* This regime has no analog in CR. Here, particles flow into the system, but their coherence with the reservoir is destroyed by the refresh before coherence between all parts of $\mathcal{LSR}$ is sufficient to have natural current flow. The regime emerges from interplay between multiple timescales and phenomena. For smaller τ , current oscillations due to Gibbs phenomenon [70] at the system-reservoir interface influence the NESS current as

the refresh can come at points near the maximum or minimum of the oscillations. Simultaneously, this leaves excess moving particles within the $\mathcal{S}$ that oscillate—i.e., remnants of the current that are coherent in $\mathcal{S}$ but incoherent with $\mathcal{LR}$. As a result, the current will vary depending on the interplay between $\mathcal{S}$ timescales and τ . In particular, there will be a transit time across $\mathcal{S}$ of $\tau_S = N_S/2v_S$ set by the Lieb-Robinson bound. This creates oscillations in the NESS current as τ varies, as seen in Fig. 4(b), with a distinct minimum at τ_S . At larger multiples of τ_S , there are also oscillations, but their visibility will be model dependent. Additional timescales within $\mathcal{LSR}$ could potentially play a role for more complex models. When moving away from the PR into ARC, this regime defines the cut between PR-like and CR-like behavior, as we discuss extensively in the main text.

(3) *Intermediate- τ or physical regime.* In this regime, the refresh time is sufficient to support the formation of the intrinsic, physical current. That is, the coherence across $\mathcal{LSR}$ is global. A plateau in the current develops and increases in size with N_W . This plateau is a reflection of the quasisteady state that forms within microcanonical—closed $\mathcal{LSR}$ —approaches [52,60,61], of which PR is most similar. It is in this regime that the current—typically the most important observable—accurately captures the true NESS current. As well, the approximate NESS approaches ρ_S° . Extending the plateau is the limit $N_W \rightarrow \infty$.

(4) *Large- τ or overly coherent $\mathcal{LSR}$ regime.* In this regime, the particle current at the stroboscopic points is influenced by the timescale for coherent flow across the whole of $\mathcal{LSR}$. The time between refresh events is too long compared to this transit time. The wavefront of particle flow scatters off the finite boundaries of $\mathcal{LSR}$. The complete reversal of the current happens at $2\tau_W$, given by a Lieb-Robinson bound for the reservoir, when the reflected wavefront comes back to the interface. This occurs for τ larger than τ_W , although the system transit time will also play a role in the current reversal, as seen in Fig. 11. This is intuitively clear since the wavefront needs to travel across the system as well. The overly coherent oscillations that occur in this regime also occur for the relaxation-limited regime of CR, but there the relaxation strength ultimately limits the current because a global NESS develops in $\mathcal{LSR}$. In other words, the PR and PR-like current displays a glaring over coherence rather than linear dependence on $1/\tau$ (i.e., something more directly analogous to CR) because one is using stroboscopic points to provide the NESS. If one employed the average current, then the current would oscillate about $1/\tau$, still giving signatures of over coherence but also reflecting that the frequency of refresh is the rate-limiting process for the overall current.

Figure 11 shows how τ influences the stroboscopic NESS current. Figure 11(a) shows three different lengths of $\mathcal{S}$, giving distinct transit timescales, τ_S . For larger τ_S , the overly coherent $\mathcal{S}$ regime extends to larger τ . The point $\tau/\tau_S = 1$ shows a qualitative change in the curves, with strong oscillations prior to this point. Figure 11(b) shows that when the refresh time equals $2\tau_W$, the wavefront has scattered off the boundary of $\mathcal{LSR}$ and arrived back at the interface with $\mathcal{S}$. This results in reversal of the current for all $\mathcal{S}$. The system's timescale also plays a role in this reversal, showing up as oscillations before the current fully stabilizes in the reverse direction.

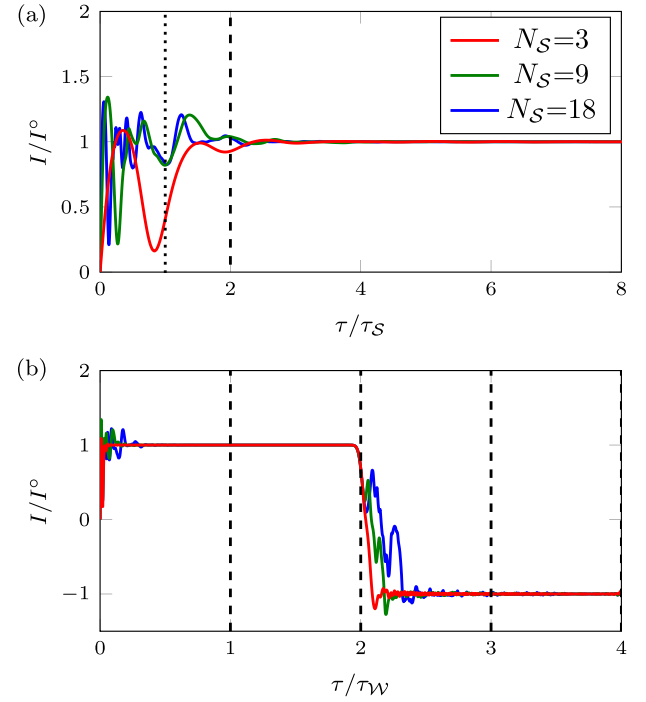


FIG. 11. Typical regimes for PR. (a) The stroboscopic steady-state current vs τ/τ_S for three system sizes (giving three different τ_S). For very small τ , the current rises to the steady-state level. If the refresh period τ is comparable to any timescale in $\mathcal{LSR}$, then coherent oscillations become apparent. For $\tau < \tau_S$, for τ_S the $\mathcal{S}$ timescale, we observe features in the steady-state current related to evolution inside $\mathcal{S}$, and distinct features for multiples of τ_S that match refresh time with wavefront traversing the $\mathcal{S}$ from one side to the other. The features become less apparent as τ increases, eventually becoming negligible. The vertical dotted and dashed lines in (a) mark τ_S and $2\tau_S$, respectively. (b) The stroboscopic steady-state current vs τ/τ_W for the same set of system sizes. The current remains stable even after reaching the reservoir timescale τ_W . It is only when the wave front returns to the interface at $2\tau_W$ that the current reverses, for which there will be further reversals at integer multiples of $2\tau_W$ (i.e., $4\tau_W$, etc.). The vertical dashed lines in (b) mark multiples of τ_W . After reversal, the timescale τ_S determine when the current stabilizes. Unlike in the main text, $\mathcal{S}$ is a uniform lattice of N_S sites with $\omega_S = 0$ and with nearest-neighbor hopping $v_S = \omega_0/2$. The data are obtained for reservoirs with $N_W = 256$ modes each, temperature $\beta\omega_0 = 40$, and symmetrically applied bias $\mu = \omega_0/2$.

Moreover, when increasing the size of reservoirs, the plateau increases between overly coherent $\mathcal{S}$ at moderate (and N_W independent) τ and overly coherent $\mathcal{LSR}$ at $\tau = 2\tau_W$. Figure 12 shows this increase in plateau size. Additionally, the larger N_W increases the accuracy of the current when compared to the continuum limit. This results in a plateau reaching lower $\bar{\sigma}_I$ error with increasing N_W , as is visible in Fig. 12.

APPENDIX C: ARC

1. Kramers' turnover analog

ARC displays behavior that is both CR-like and PR-like depending on the point on the parameter space. Generally

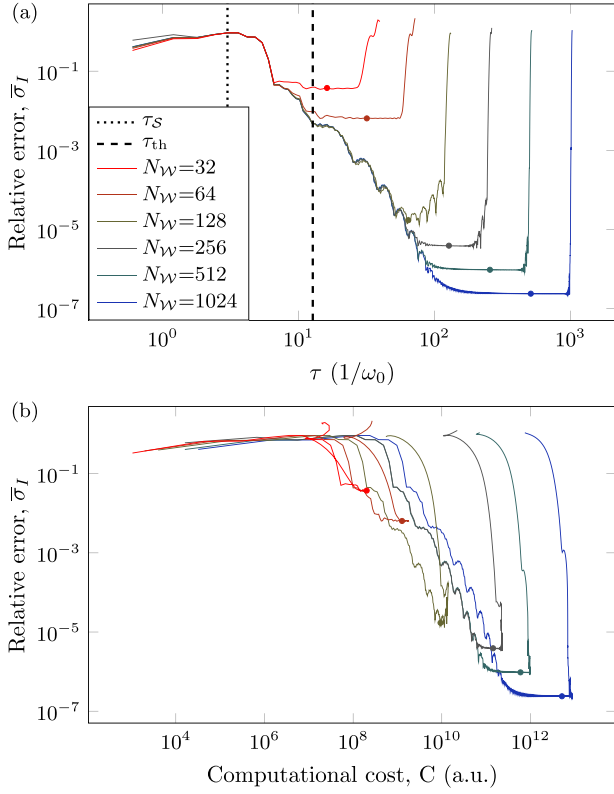


FIG. 12. PR errors for increasing N_W . (a) The curves show the relative error versus τ for many different N_W . As N_W increases, the plateau for physical behavior increases. As well, more reservoir modes increase the accuracy of the current. The vertical dotted line shows the impurity timescale τ_S and the vertical dashed line shows thermal time $\tau_{th} = N_{th}/2\omega_0$ for a reservoir with thermal relaxation time $\beta\omega_0 = 40$. (b) The curves show the same results as in (a) but versus the computational cost, Eq. (46).

speaking the separation between these two regimes happens along a line of constant τ marking the smallest $\mathcal{LSR}$ timescale to appear. Figure 13(a) shows the Kramers' turnover analog for different ARC cases. When $\gamma\tau$ line goes fully inside CR-like regime, the behavior is (by definition) directly analogous to Fig. 10. As $\gamma\tau$ increases, the curve starts to register coherent oscillations that appear on top of plateau. For low and moderate $\tilde{\tau}$, the plot registers overly coherent $\mathcal{S}$, and then enters the physical PR-like regime which is the most natural scenario for the steady state. Eventually, coherent evolution leads to the complete reversal of the current flow when entering the overly coherent $\mathcal{LSR}$ regime. Figure 13(b) shows the same data but plotted versus τ instead of $\tilde{\tau}$. This helps to see the emergence of oscillations as a result of coherent evolution. The period of coherent oscillations is roughly constant with refresh strength. This is due to the fact that the (partial) refresh incoherently adds a stationary component to the reservoir's state (e.g., the thermal equilibrium state when not connected to the junction system). The component of the state carrying the wavefront will have it continue to propagate at the same speed (dictated by the Hamiltonian and initial packet). Even in the CR and CR-like regime, the wavefront propagates at the same velocity, but, since the $\mathcal{LSR}$ state goes into a global NESS, the wavefront completely dissipates. Its

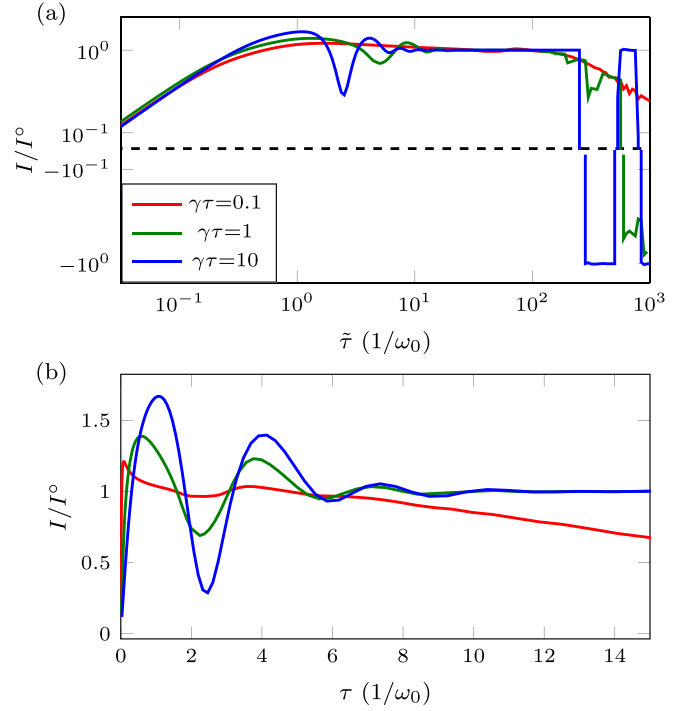


FIG. 13. Steady-state current for ARC. (a) The curves show the stroboscopic steady-state current for ARC vs $\tilde{\tau}$ for a few $\gamma\tau$. All the parameter regimes show a Kramers'-like increase and then plateau for small to moderate $\tilde{\tau}$. However, for larger $\tilde{\tau}$ and $\gamma\tau$ the curves escape the CR-like phase and coherent oscillations become apparent. For very large $\tilde{\tau}$, all curves enter the underdamped regime, which can be either directly similar to Kramers' rate-limiting process (i.e., a linear dependence on γ) or reflect the stroboscopic, PR-like current, which breaks down and eventually reverses. For $\gamma\tau = 1$, however, the underdamped regime combines these two features and the current goes down with $\tilde{\tau}$ but still undergoes some rapid oscillation and eventually reverses when the wavefront returns back to the interface. (b) The curves show ARC with the same three $\gamma\tau$ versus τ instead of $\tilde{\tau}$ (the γ is changing with τ since $\gamma\tau$ is fixed). The coherent oscillations for the two larger values of $\gamma\tau$ are seen to occur with the same frequency. Both plots take data from Fig. 4(b).

transversal, though, does influence the correlations present in the NESS.

2. Phase diagram in γ - τ space

The steady-state induced by the ARC procedure results in the phase diagram Fig. 4 which has a nice and regular structure when drawing it on $\gamma\tau$ - $\tilde{\tau}$ plane. However, the phase diagram boundaries are a consequence of γ and τ taken separately. We can see them more vividly after changing the parametrization of the phase diagram to γ - τ . In Fig. 14, the regimes are separated by vertical lines of constant τ and horizontal lines of constant γ . One can still find the limit of CR and PR, which now share a corner with the Zeno regime. Although, this point of view can be useful, it is the $\gamma\tau$ - $\tilde{\tau}$ parametrization which is more convenient and physically motivated. In Fig. 4, the phase diagram separates what is lost due to refresh, $\sim\gamma\tau$, from what remains, $\sim\tilde{\tau}$.

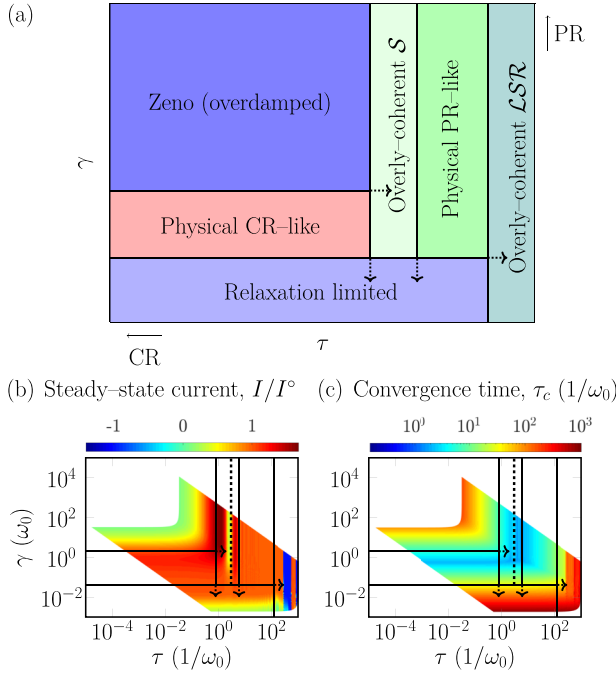


FIG. 14. ARC phase diagram in γ - τ space. (a) The abstract phase diagram for ARC. The lines of constant τ and constant γ are now vertical and horizontal, respectively. The PR and CR limits are now on the top and left, respectively. This provides a different perspective on the phase diagram in Fig. 4. [(b) and (c)] The steady-state current and convergence time both on the γ - τ space. The data and lines of constant τ and γ are at the same values as in Fig. 4.

3. Phase diagram for growing $\mathcal{S}$ and $\mathcal{L}\mathcal{R}$

The phase diagram with distinct regimes as presented in Fig. 4(a) is universal for all $\mathcal{S}$ sizes. In Fig. 15(a), we show the phase diagram for uniform $\mathcal{S}$ with no on-site energies and nearest-neighbor hopping $v_S = \omega_0/2$ coupled to reservoirs with amplitude ω_0 . The plot keeps the same regimes as for Fig. 4(b) but has wider regime of overly coherent $\mathcal{S}$ since the $\mathcal{S}$ timescale is now larger. In Fig. 15(b), we show the same case as in Fig. 15(a) but now the coupling to reservoirs is $\omega_0/2$. In Fig. 15(b), the phase diagram remains very close to Fig. 15(a) with the same upper bound for the Zeno regime.

Some boundaries in the phase diagram, Fig. 4, will depend on N_W . The transition into the Zeno regime and the transition from CR-like to PR-like both depend on intrinsic characteristics of the continuum model but not on N_W (except for some possible finite-size effects at really small N_W). When N_W increases, the transition from the physical regimes to underdamped regimes is shifted to higher $\tilde{\tau}$. This makes the physical regimes wider but otherwise maintains the structure of the phase diagram. The impact of N_W on phase diagram can be seen by comparing Fig. 16 for $N_W = 256$ to Fig. 5 for $N_W = 512$. As a consequence of growing N_W , the $\gamma\tau$ which initially had a CR-like physics at the optimum, and corresponding scaling relation, can transition to PR-like physics. For $\gamma\tau = 0.1$, the optimal point for $N_W = 256$ in the CR-like regime moves to the PR-like regime for $N_W = 512$.

One can also see the influence of the different parameter phases when examining quantities versus $\gamma\tau$. Figure 17 shows

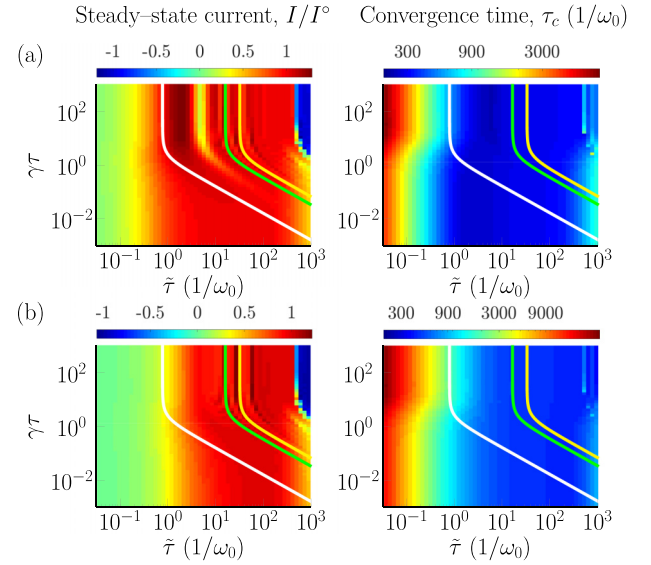


FIG. 15. Phase diagram for $N_S = 16$. The lines demarcate the boundary and some features of the overly coherent $\mathcal{S}$ regime. Unlike the main text, $\mathcal{S}$ is a uniform lattice with onsite frequencies of zero, a constant nearest-neighbor coupling $v_S = \omega_0/2$, and system-reservoir coupling of (a) ω_0 and (b) $\omega_0/2$. The line of fixed τ equal to $\tau^* = \pi/\mathcal{W}$ is plotted in white, τ_S plotted in green, and $2\tau_S$ plotted in yellow. The $\mathcal{S}$ timescale is $\tau_S = N_S/2v_S$. Both examples use $N_W = 256$ sites per reservoir, temperature $\beta\omega_0 = 40$, and bias $\mu = \omega_0/2$.

errors (in current and trace distance) and contributions to the cost (OSEE and convergence time) for the optimal points taken from Figs. 16 and 5. There is a clear distinction between points in the physical CR-like regime and those in the physical PR-like regime, as well as intermediate ARC for the cases in between. For the physical CR-like regime, the error of the current saturates at a value approximately $100\times$ larger than for the physical PR-like regime. The same happens for the trace distance, which has an approximately $10\times$ larger value (i.e., error) for physical CR-like regime. Better accuracy comes from longer coherent evolution in the physical PR-like regime that accumulates more non-Markovian character. However, it comes with a penalty: The OSEE increases by approximately 2 times. This makes the bond dimension increase quadratically when going from physical CR- to PR-like ARC. In fact, the increase of entropy dominates the overall computational cost in Eq. (46).

For the intermediate $\gamma\tau$, there a discontinuity in the trace distance, OSEE, and convergence time. This is due to the optimal $\tilde{\tau}$ jumping from the CR-like to the PR-like side of the phase diagram. Since $\bar{\sigma}_I$ is the quantity used to assign the optimal point (and it is a smooth function of $\gamma\tau$ and $\tilde{\tau}$), there will be no discontinuity in it. The convergence and cost for intermediate ARC interpolates between physical CR- and PR-like ARC.

4. Averaging procedure to get $\bar{\sigma}_I$

As we discuss extensively in the main text, an averaging procedure is taken in order to avoid assigning accidental crossings, where $I = I^\circ$, an error of zero. These crossings are due to the parameter sweep, rather than an accurate, physical

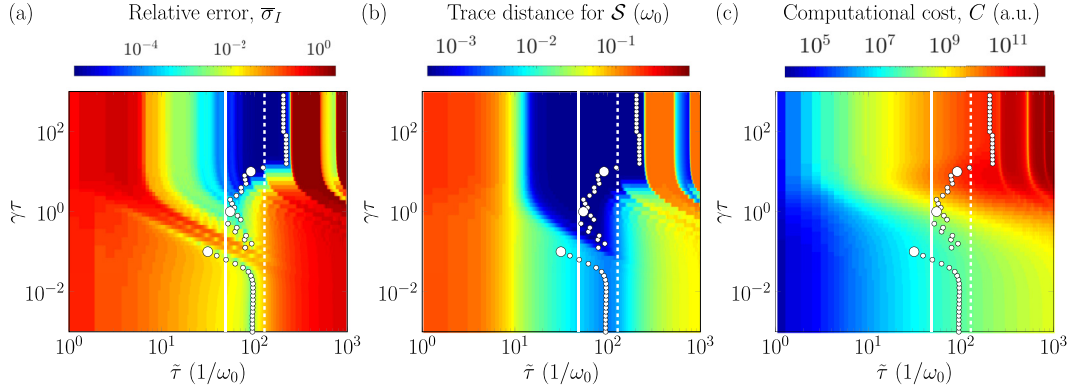


FIG. 16. Convergence and computational cost of ARC. The three panels show the (a) current error, Eq. (41), (b) the correlation matrix error, Eq. (45), and (c) the estimated computational cost, Eq. (46), for our example system and for $N_W = 256$, $\beta\omega_0 = 40$, and $\mu = \omega_0/2$. The two error plots have many of the same features as the phase diagram for ARC, Fig. 4, as we expect since the different regimes directly impact the error. Using the current error as the quantity to be optimized, the best choice of action for a fixed $\gamma\tau$ is marked by the white points in (a). These points are replicated in the plot showing the correlation matrix error (b), and estimated computational costs (c) to see where they fall for other quantities. The white dots for $\gamma\tau = 0.1, 1$, and 10 are made thicker to guide readers eye. Vertical solid line represents $\tilde{\tau}$ equal to heuristic choice for CR, and vertical dashed line represents $\tilde{\tau} = \tau_W$, which is a physical choice for PR. We employ these $\tilde{\tau}$ for the CR and PR limits.

representation of the problem. The moving average smooths out—regularizes—the error across these points, enabling the minimization procedure to choose an optimal $\tilde{\tau}$ —the minimum average error—at a fixed $\gamma\tau$, see Sec. V C. This provides an algorithmic approach to obtaining, e.g., the error-cost scaling. It is by no means, however, ideal, since the optimal point still can lie close to the crossings even if the error is more appropriately assessed. This is why for CR and PR we choose the well-defined heuristic points for setting the action instead.

We compare their scaling relations to these we obtain with the $\bar{\sigma}_I$ minimization procedure in similar ARC regimes. Figure 7 shows that this algorithmic approach is sound for delineating scaling regimes (i.e., exponents), but the error of CR-like behavior is still underestimated, as seen by the comparison with the CR limit.

To visualize the influence of the moving average, Fig. 18 presents the data from Fig. 5 without the moving average. Figure 18 has many accidental crossings with I° , albeit they are not fully visible due to the finite resolution of the plot. These

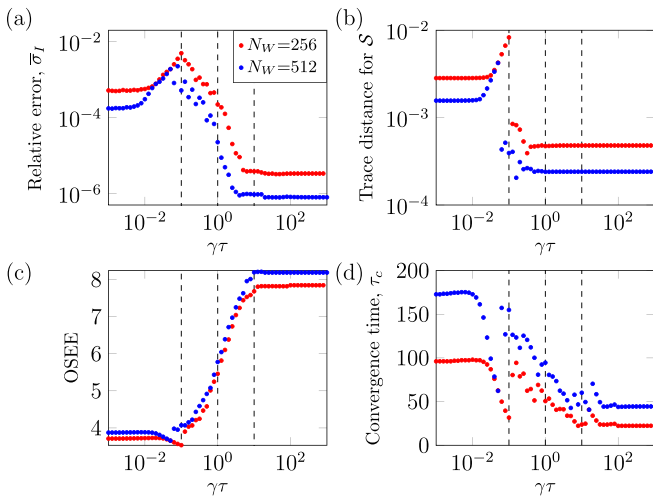


FIG. 17. Optimal estimates for ARC. The data take ARC optimal points from Fig. 16 for $N_W = 256$ and from Fig. 5 for $N_W = 512$. From the white points we extract (a) relative error $\bar{\sigma}_I$, (b) error for $\mathcal{S}$ correlation matrix, (c) operator space entanglement entropy for central cut, and (d) the convergence time to reach a steady state τ_c . The data show the transition between optimal estimates falling into CR-like regime to these which are already in PR-like regime. Vertical dashed lines are included to guide readers eye and mark $\gamma\tau = 0.1, 1$, and 10 , which are highlighted points in Figs. 16 and 5.

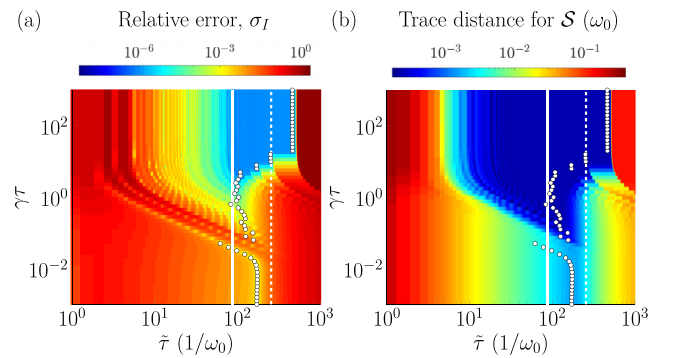


FIG. 18. Relative error without the moving average. The panels show the (a) current error, σ_I , (b) the correlation matrix error, Eq. (45), for $\mathcal{S}$ as in the main text. The reservoirs are $N_W = 512$ sites each, temperature $\beta\omega_0 = 40$, and symmetric bias $\mu = \omega_0/2$. The plot takes the data from Fig. 5 but does not apply moving average in Eq. (44) to σ_I . White points are taken from Fig. 5 and mark the position of lowest average error $\bar{\sigma}_I$ for each $\gamma\tau$. These plots demonstrate that the averaging procedure does not deform the phase diagram. They also show that the averaging itself does not bias the optimum. However, on the CR side, the optimum from $\bar{\sigma}_I$ tracks the accidental crossing. Those crossings are not fully visible on either the PR or CR side of the phase diagram due to the finite resolution of the heat map.

TABLE I. Scaling relations for low temperature, $T = \omega_0/40$. The scaling relations are for data in Fig. 7(a).

	ν	$\bar{\sigma}_I = AN_{\mathcal{W}}^{-\nu}$	$2^{S_O} = AN_{\mathcal{W}}^{\nu}$	$\tau_c = AN_{\mathcal{W}}^{\nu}$	$C = AN_{\mathcal{W}}^{\nu}$
ARC					
PR		2.03 ± 0.02	0.393 ± 0.001	0.83 ± 0.01	3.01 ± 0.09
ARC					
$\gamma\tau = 1$		3.4 ± 0.2	0.23 ± 0.01	0.66 ± 0.04	2.37 ± 0.07
CR		0.91 ± 0.02	0.171 ± 0.003	0.94 ± 0.02	2.45 ± 0.03

can lead to wrongly assigning the $\tilde{\tau}$ for capturing the physical problem when taking σ_I directly. The trace distance in both Figs. 5 and 18 does not have averaging, since regularizing the data was only necessary for determining the optimal $\tilde{\tau}$ via the current. We further note that Fig. 18 demonstrates that the averaging procedure does not significantly distort or otherwise modify the phase diagram. It also shows, however, that the optimal points from $\bar{\sigma}_I$ are influenced by the accidental crossings, especially in the CR regime. For the full CR limit, though, we use a different procedure to choose the action, one that is not influenced by the accidental crossings, as we discuss extensively in the main text and in the first Appendix. In the PR regime, the optimal points are pushed to the right on the plateau, which increases accuracy marginally but also increase the computational cost. This is not accounted when assessing the scaling for ARC. However, for the PR limit, we use the physical time scale, which shows the scaling is not significantly modified by using the optimal point. As we mention earlier, if one takes a τ smaller than the physical tau, $\tau_{\mathcal{W}}$, in the PR regime, the cost decreases without a significant loss in accuracy [see Fig. 12(b)].

5. Scaling relations

In the main text, we discussed the error-cost scaling, providing some of the extracted values for the prefactors and exponents in Fig. 7. The fits corresponds to the accuracy and performance of the ARC at fixed $\gamma\tau$ taken at the optimal point. Here, we provide the remaining values, as well as contributions to these values. Tables I and II, at low and high temperature, respectively, give the scaling relations for the individual quantities versus $N_{\mathcal{W}}$ rather than cost. For the scaling, we employ the following relations:

$$\bar{\sigma}_I = AN_{\mathcal{W}}^{-\nu} \quad (C1)$$

TABLE II. Scaling relations for high temperature, $T = \omega_0/2$. The scaling relations are for data in Fig. 7(b).

	ν	$\bar{\sigma}_I = AN_{\mathcal{W}}^{-\nu}$	$2^{S_O} = AN_{\mathcal{W}}^{\nu}$	$\tau_c = AN_{\mathcal{W}}^{\nu}$	$C = AN_{\mathcal{W}}^{\nu}$
ARC					
PR		1.96 ± 0.03	0.118 ± 0.001	0.82 ± 0.02	2.18 ± 0.02
ARC					
$\gamma\tau = 1$		2.21 ± 0.04	0.079 ± 0.002	0.80 ± 0.01	2.04 ± 0.01
CR		0.87 ± 0.02	0.074 ± 0.005	0.94 ± 0.02	2.16 ± 0.03

for the optimal $\bar{\sigma}_I$;

$$2^{S_O} = AN_{\mathcal{W}}^{\nu}, \quad (C2)$$

for operator space entanglement entropy S_O ;

$$\tau_c = AN_{\mathcal{W}}^{\nu}, \quad (C3)$$

for convergence time τ_c ; and

$$C = AN_{\mathcal{W}}^{\nu}. \quad (C4)$$

for the cost $C = N_{\mathcal{W}}\tau_c 2^{3S_O}$. The error-cost scaling relation has the form in Eq. (48). The values in the error-cost scaling can be fitted directly, see Table III, or reconstructed from scaling relations of its components. For instance, the ν from Eq. (C4) is the sum of three times ν from Eq. (C2) plus ν from Eq. (C3) plus 1. These approaches give consistent results and fit errors. Thus the delineation of the fit parameters into their components enables pinpointing how different factors influence the simulation.

APPENDIX D: OPERATOR-SPACE ENTANGLEMENT ENTROPY

For completeness, in this section, we briefly summarize the calculation of OSEE in noninteracting simulations. To define OSEE, one treats a density matrix as a vector in a Hilbert space that is a tensor product of local operator spaces [71,72]. It amounts to mapping a density matrix into a pure state in the enlarged space containing auxiliary fermionic operators, deemed as adjoint fermions in Ref. [71] or a superfermion representation in Ref. [27]. Hence, for each site $m \in \mathcal{LSR}$, we will have two fermionic species with annihilation operators c_m and $\underline{c}_m$. The normalized pure state is

$$|\rho\rangle \sim \rho|I\rangle, \quad (D1)$$

where here we take $|I\rangle = \prod_{m \in \mathcal{LSR}} (c_m^\dagger - \underline{c}_m^\dagger)|0\rangle$ as a product of maximally entangled singlets in each local space.

A Gaussian density matrix is fully determined by its correlation matrix $\mathcal{C}$. In that case, a Gaussian $|\rho\rangle$ is described by the correlation matrix $\underline{\mathcal{C}}$ in a block form

$$\underline{\mathcal{C}}_{mn} = \langle \rho | \begin{bmatrix} c_n^\dagger c_m & c_n^\dagger \underline{c}_m \\ \underline{c}_n^\dagger c_m & \underline{c}_n^\dagger \underline{c}_m \end{bmatrix} | \rho \rangle. \quad (D2)$$

The OSEE is an entanglement entropy of bipartition of $|\rho\rangle$. It is calculated in a standard way [91] from eigenvalues ϵ_i of a submatrix of $\underline{\mathcal{C}}_{mn}$ with $m, n \in \mathcal{A}$,

$$S_O = - \sum_i \epsilon_i \log_2 \epsilon_i - \sum_i (1 - \epsilon_i) \log_2 (1 - \epsilon_i). \quad (D3)$$

In this work, we consider a bipartition in the *mixed* basis, which is pictorially represented in Fig. 6, and $\mathcal{A}$ is the group of modes defining bipartition.

Finally, to obtain $\underline{\mathcal{C}}$, one rotates fermionic operators to a diagonal basis of $\mathcal{C}$, where $d_i = \sum_{m \in \mathcal{LSR}} \mathcal{U}_{im}^\dagger c_m$ (similarly we will have $\underline{d}_i = \sum_{m \in \mathcal{LSR}} \mathcal{U}_{im}^\dagger \underline{c}_m$). Here $\mathcal{U}$ is a matrix of eigenvectors, and ϵ_i are eigenvalues, of $\mathcal{C}$. In that basis, a

TABLE III. Scaling for error-cost. The scaling relations correspond to dashed lines in Figs. 7(a) and 7(b).

$\ln A, \nu$	$\beta\omega_0 = 40$	$\beta\omega_0 = 2$
ARC		
PR	$4.2 \pm 0.3, 0.67 \pm 0.01$	$3.7 \pm 0.4, 0.90 \pm 0.02$
ARC		
$\gamma\tau = 1$	$21.7 \pm 1.5, 1.44 \pm 0.07$	$6.3 \pm 0.4, 1.08 \pm 0.02$
CR	$2.14 \pm 0.06, 0.372 \pm 0.003$	$0.0 \pm 0.2, 0.40 \pm 0.01$

correlation matrix is block diagonal with

$$\langle \rho | \begin{bmatrix} d_i^\dagger d_i & d_i^\dagger \underline{d}_i \\ d_i^\dagger \underline{d}_i & \underline{d}_i^\dagger \underline{d}_i \end{bmatrix} | \rho \rangle = \begin{bmatrix} \alpha_i^2 & \alpha_i \beta_i \\ \alpha_i \beta_i & \beta_i^2 \end{bmatrix}, \quad (\text{D4})$$

where $\alpha_i = \frac{\varepsilon_i}{\sqrt{(1-\varepsilon_i)^2 + \varepsilon_i^2}}$, and $\beta_i = -\frac{1-\varepsilon_i}{\sqrt{(1-\varepsilon_i)^2 + \varepsilon_i^2}}$. The correlation matrix $\underline{\mathcal{C}}$ in the original basis of interest is obtained by rotating back to c_m and $\underline{c}_m$.

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Publication V

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Transport in a periodically-driven tilted lattice via the extended reservoir approach: Stability criterion for recovering the continuum limit

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Extended reservoirs provide a framework for capturing macroscopic, continuum environments, such as metallic electrodes driving a current through a nanoscale contact, impurity, or material. We examine the application of this approach to periodically-driven systems, specifically in the context of quantum transport. As with non-equilibrium steady states in time-independent scenarios, the current displays a Kramers' turnover including the formation of a plateau region that captures the physical, continuum limit response. We demonstrate that a simple stability criteria identifies an appropriate relaxation rate to target this physical plateau. Using this approach, we study quantum transport through a periodically-driven tilted lattice coupled to two metallic reservoirs held at a finite bias and temperature. We use this model to benchmark the extended reservoir approach and assess the stability criteria. The approach recovers well-understood physical behavior in the limit of weak system-reservoir coupling. Extended reservoirs enable addressing strong coupling and non-linear response as well, where we analyze how transport responds to the dynamics inside the driven lattice. These results set the foundations for the use of extended reservoir approach for periodically-driven, quantum systems, such as many-body Floquet states.

I. INTRODUCTION

Quantum transport plays a central role in spectroscopy for many-body quantum systems, from superconducting and hybrid interfaces [1–3] to quantum dot arrays [4–8] to cold atoms [9, 10]. Transport can also serve as a probe of time-dependent states, such as time-crystals within interacting, driven, dissipative quantum systems [11, 12]. Yet, transport properties are challenging to compute and become even more so for time-dependent driving.

We study the use of the extended reservoir approach (ERA), see Ref. 13 for an overview, in obtaining transport characteristics for time-dependent transport. ERA is a rapidly developing area of research that employs a finite collection of reservoir modes to represent the continuum environment, including environments of many-body systems [14–22]. To do so, ERA modes must be relaxed by external, implicit environments. However, one of the most useful flavors of ERA employs Markovian relaxation [23]. While being more computationally tractable, this relaxation breaks the Fluctuation-Dissipation theorem [23–25], which is only restored in an appropriate limit. The discreteness of the reservoirs also introduces anomalous virtual tunneling [26]. These make the accurate calculation of transport properties a delicate limit-

ing process, where one has to break (artificial) symmetries of the discrete model, identify an appropriate—*a moderate*—relaxation rate, and ensure the simulation is converging in a manner consistent with physical principles and continuum physics.

We demonstrate how this process plays out for time-dependent systems. These systems can introduce artificial resonances into the setup. As a model, we consider a periodically-driven tilted lattice, the closed version of which is well studied in optical systems [27–29]. Without driving, such a lattice exhibits Wannier-Stark localization for large-enough tilts [30–32] and transient Bloch oscillations [33]. Introducing interactions in that setup may result in rectification, as recently discussed for transport induced by Markovian reservoirs [34]. Driving can lead to resonance-induced transport, or obstruct transport in other scenarios, in well-studied limiting cases [35].

When simulating this model with a finite collection of (relaxed) reservoir modes, i.e., the ERA approach, artificial resonant states can form across the reservoir-system-reservoir setup. These impart anomalous behavior to the current in a way that is *a priori* more difficult to recognize than for equivalent time-independent models. Avoiding this anomaly requires a larger relaxation rate than typical approaches employ, or an additional averaging procedure. We show how a stability criteria identifies this rate and then use this approach to study the physical behavior of the driven, tilted lattice.

This paper is organized as follows: Section II outlines the general transport framework, which can include both

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impurity and extended systems. We also introduced the periodically-driven tilted lattice. Section III summarizes the extended reservoir approach with Markovian relaxation, as well as presents and assesses the stability criteria to target a physical relaxation rate. Section IV sets forth the application of the approach to the driven system, connecting the results to closed systems for weak coupling, presenting other validation procedures, and going beyond linear response. We conclude in Sec. V.

II. TRANSPORT FRAMEWORK AND MODEL

While much of what we develop is applicable to open quantum systems generally, such as those in the presence of a dissipative bosonic environment, we focus on quantum transport in this work and specifically on transport through a periodically-driven fermionic system. In this section, we first introduce the transport framework and then the particular model we study.

A. Quantum transport

The typical setup for transport has two macroscopic—i.e., continuum—reservoirs that connect to each side of a system. For time-independent scenarios, a finite bias (or temperature drop) across the reservoirs drives the system out of equilibrium and results in a current flow. Time-dependent systems can have richer behavior, as a, e.g., periodic drive can pump energy into the system and currents can flow even in the absence of an external bias.

When the system (and system only in this work) can be time dependent, the general Hamiltonian is

$$H(t) = H_S(t) + H_L + H_R + H_I. \quad (1)$$

The system S 's Hamiltonian, $H_S(t)$, is the region between the two reservoirs L and R . In addition to having time dependence, this region generally will have many-body interactions, such as electron-electron or electron-vibration interactions. In this work, we will have only a quadratic system Hamiltonian in order to benchmark the ERA without additional complications. The method we present ultimately aims at interacting models where the exact solution is not available. We can, however, develop a good understanding of ERA based on fully non-interacting models where exact reference solutions exist. Since we address issues with the reservoir representation, we expect our findings immediately generalize to many-body S in contact with the same reservoirs.

Whether for many-body or non-interacting S , the two reservoirs are both continuum, non-interacting metallic reservoirs. The Hamiltonians are

$$H_\alpha = \sum_{k \in \alpha} \omega_k c_k^\dagger c_k \quad (2)$$

for the $\alpha = L, R$ reservoirs, where ω_k is the frequency of the single-particle eigenstate $k \in \alpha$. We note that

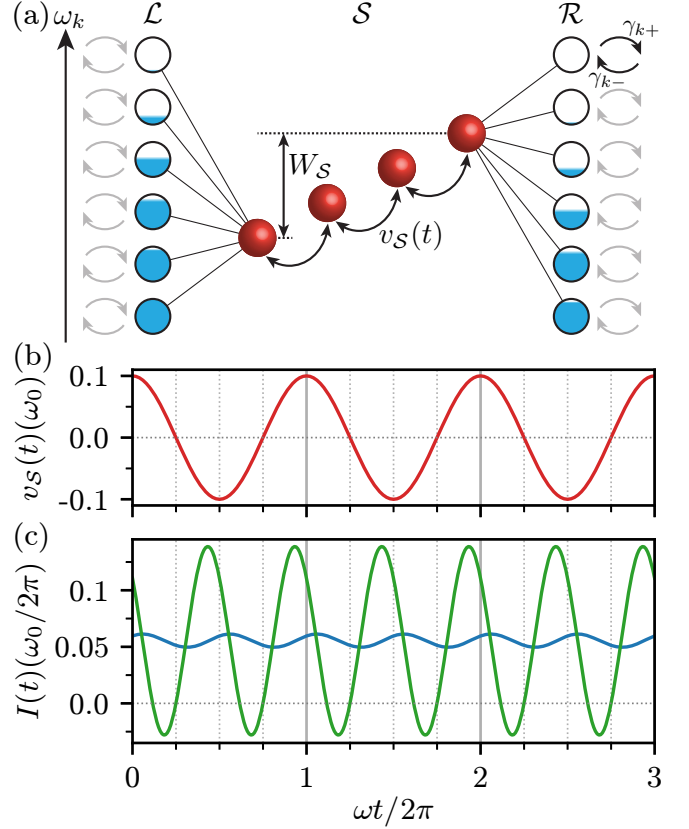


FIG. 1. **Quantum transport in the ERA.** (a) A driven tilted lattice S (red sites with total tilt W_S and hopping $v_S(t)$) between two extended reservoirs, L and R . The reservoirs are maintained at chemical potentials μ_L and μ_R , represented by different filling (blue shading), and at the same temperature for the cases we examine. Discretized modes in L and R are explicitly included in the simulation. These modes are relaxed to their (isolated) equilibrium occupancy by Markovian injection and depletion at rates γ_{k+} and γ_{k-} , respectively. (b) Periodically modulated hopping $v_S(t)$ inside system S versus time. (c) The induced particle current $I(t)$ versus time. The blue line is the current from L to S and the green line between the middle sites in S . This data is from a $N_S = 8$ site system driven at the resonant frequency $\omega = \Delta_S = \omega_0 / (N_S - 1)$, i.e., $W_S = \omega_0$. The other parameters are $V_S = v_0 = \omega_0 / 10$, $\mu = \omega_0 / 2 = 2\mu_L = -2\mu_R$, and $k_B T_L = k_B T_R = \hbar \omega_0 / 40$. The relaxation rates are set via the approach in Sec. III.

all Hamiltonians in this work are in terms of frequencies. The last contribution, H_I , is the interaction between S and L, R , which we take to be quadratic hopping only,

$$H_I = \sum_{k \in L, R} \sum_{i \in S} \left(v_{ki} c_k^\dagger c_i + v_{ik} c_i^\dagger c_k \right), \quad (3)$$

with $v_{ki} = v_{ik}^*$. This H_I is the typical paradigm whether S is non-interacting or many body. The $c_m^\dagger$ (c_m) are the fermionic creation (annihilation) operators for mode m . The index m carries all necessary mode labels, such as frequency, spin, and region (L , S , or R). We will use k 's (l 's) and i 's (j 's) to indicate single-particle eigenstates of

$\mathcal{LR}$ and spatial modes of $\mathcal{S}$, respectively.

For non-interacting reservoirs coupled linearly to the system with the number conserving interaction in Eq. (3), the behavior of the setup is determined by the reservoirs' spectral functions,

$$\mathbf{J}_\alpha(\omega) = 2\pi \sum_{k \in \alpha} |v_k\rangle \langle v_k| \delta(\omega - \omega_k), \quad (4)$$

for $\alpha = \mathcal{L}, \mathcal{R}$. The $\mathbf{J}_\alpha(\omega)$ is a square matrix of size equal to the number of sites in the system $\mathcal{S}$. To keep the notation compact, we use a coupling vector $|v_k\rangle$ between mode $k \in \mathcal{LR}$ and all sites $i \in \mathcal{S}$, i.e., $\langle i|v_k\rangle = v_{ik}$. The general aim of ERA is to recover the macroscopic limit via a finite number of broadened reservoir modes within the reservoir bandwidth $\mathcal{W}$. These modes must capture all relevant features encoded in the continuum $\mathbf{J}_\alpha(\omega)$, as well as how that spectral density is populated according to the Fermi-Dirac distribution.

We are most interested in the particle current in a Floquet state that has a periodic drive in the presence of a bias in the reservoirs' chemical potentials $\mu_{\mathcal{L}}$ and $\mu_{\mathcal{R}}$. When taken at the $\mathcal{L}$ and $\mathcal{S}$ interface, this current is

$$I_{\mathcal{LS}}(t) = 2 \text{Im} \sum_{k \in \mathcal{L}} \sum_{j \in \mathcal{S}} v_{jk} \langle c_j^\dagger c_k \rangle_t, \quad (5)$$

where $\langle \cdot \rangle_t$ indicates the quantum mechanical average at time t . The current has a similar form at the other interfaces, all following from continuity equations. Since the Hamiltonian in Eq. (1) conserves total particle number, the current between parts of the setup follows from considering time-dependence of local occupations induced by $H_{\mathcal{I}}$ in Eq. (3). While the time dependence of the current can be different for the various interfaces, we focus on the mean current. For periodic driving, the average need only be over a single oscillation period $\tau = 2\pi/\omega$,

$$I_\diamond = \frac{1}{\tau} \int_0^\tau I_{\mathcal{LS}}(t) dt, \quad (6)$$

in the Floquet state. This quantity is interface-independent in the physical limit of interest.

In all our examples, we consider a uniform, low temperature of $k_B T_{\mathcal{L}} = k_B T_{\mathcal{R}} = \hbar\omega_0/40$, where k_B is Boltzmann's constant and $\hbar$ the reduced Planck's constant. A temperature bias could also be present, but we do not consider that case. We take a symmetrically applied potential μ , with $\mu_{\mathcal{L}} = -\mu_{\mathcal{R}} = \mu/2$ and the hopping strength, ω_0 , as a reference frequency. For most examples, this is the actual hopping in the reservoirs, which are uniform one-dimensional lattices. We, however, treat these reservoirs numerically in their single-particle eigenbasis, e.g., Eq. (2), and their spatial dimensionality is not of central importance. We break the correspondence between ω_0 and the hopping only where indicated in order to further validate the ERA via the fully Markovian limit.

B. Periodically-driven tilted lattice

We consider a one-dimensional tilted lattice with $N_{\mathcal{S}}$ sites and nearest-neighbor hopping, as schematically depicted (within the ERA) in Fig. 1(a). The time-dependent Hamiltonian is

$$H_{\mathcal{S}}(t) = \sum_{i=1}^{N_{\mathcal{S}}} \omega_i(t) c_i^\dagger c_i + \sum_{i=1}^{N_{\mathcal{S}}-1} v_{\mathcal{S}}(t) (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i). \quad (7)$$

The tilt is linearly increasing with nearest-neighbor step $\Delta_{\mathcal{S}}(t)$ inside $\mathcal{S}$, giving the on-site frequencies

$$\omega_i(t) = \Delta_{\mathcal{S}}(t) \left(i - \frac{N_{\mathcal{S}} + 1}{2} \right), \quad (8)$$

for $i = 1, 2, \dots, N_{\mathcal{S}}$. This tilt is symmetric around zero frequency, following a similar choice for the reservoirs below. In all our examples, apart from Sec. IV C, we consider a static tilt $\Delta_{\mathcal{S}}(t) = \Delta_{\mathcal{S}}$, with the total tilt

$$W_{\mathcal{S}} = \Delta_{\mathcal{S}}(N_{\mathcal{S}} - 1), \quad (9)$$

and a hopping that oscillates as

$$v_{\mathcal{S}}(t) = V_{\mathcal{S}} \cos(\omega t), \quad (10)$$

with frequency ω and amplitude $V_{\mathcal{S}}$. Figure 1(b) shows the oscillation of $v_{\mathcal{S}}(t)$ along with the resulting oscillating currents (across two interfaces) in Fig. 1(c).

As already indicated, we consider $\mathcal{L}$ and $\mathcal{R}$ to be uniform one-dimensional (semi-infinite) lattices coupled, respectively, to the first and last site of $\mathcal{S}$ with hopping v_0 (i.e., $v_{ik} \neq 0$ only for $k \in \mathcal{L}$, $i = 1$ and $k \in \mathcal{R}$, $i = N_{\mathcal{S}}$). The Fermi level is at zero. This gives the continuum limit spectral functions

$$[\mathbf{J}_{\mathcal{L}}(\omega)]_{11} = [\mathbf{J}_{\mathcal{R}}(\omega)]_{N_{\mathcal{S}}N_{\mathcal{S}}} = \frac{8v_0^2}{\mathcal{W}^2} \sqrt{\mathcal{W}^2 - 4\omega^2}, \quad (11)$$

and zero otherwise. In terms of the reference frequency, ω_0 , the bandwidth is $\mathcal{W} = 4\omega_0$ unless otherwise indicated. Those exceptions will be calculations to further validate the ERA approach by showing how it converges to the fully Markovian limit.

The driven tilted lattice model provides a benchmark example for the ERA. It is well-studied in the context of closed systems, has non-trivial behavior versus the driving frequency, and allows for extended systems $\mathcal{S}$. Without driving, $v_{\mathcal{S}}(t) = V_{\mathcal{S}}$, the system is a standard tilted lattice leading to Wannier-Stark localization [30–32]. In this limit, one expects efficient transport for a small global tilt $W_{\mathcal{S}}$ and suppression of transport when the global tilt exceeds the width of the Bloch band,

$$|W_{\mathcal{S}}| \gtrsim 4|V_{\mathcal{S}}|. \quad (12)$$

This condition becomes strict for large $N_{\mathcal{S}}$. At a non-zero driving frequency, the driven system allows for effective mapping to a static setup when the coupling to the

reservoirs is weak, providing additional validation. The ERA, however, is not limited to those special cases and can be employed, for instance, also in the limit of strong or moderate system–reservoir couplings.

Moreover, this model, including the coupling to reservoirs, may be realized experimentally with a slight modification of the approaches described in Ref. [36]. Recently, similar tilted models (with interactions) gained significant attention in the studies of many-body localization without disorder [27, 28, 37–44]. Here, we consider the non-interacting lattice, however, to validate the ERA and set the foundations to simulating interacting cases with tensor networks [21].

III. EXTENDED RESERVOIR APPROACH

The exact solution for the transport problem of Sec. II A is in the macroscopic limit, where the reservoirs are a continuum and have an infinite-dimensional Hilbert space. To make the problem tractable, we employ the *extended reservoir approach* (ERA) [13, 23]. In ERA, the reservoirs are approximated by a finite collection of explicit modes/sites, which, in turn, are coupled to implicit reservoirs. The latter relax the explicit modes to an (isolated) equilibrium state to maintain set temperatures and chemical potentials. There is a long lineage of relaxation based approaches, starting from early work of Kohn and Luttinger [45] to open system approaches for semiconductors [46–48] to approximate master equations [49, 50]. The presence of implicit relaxation supports a stationary state and, within ERA, provides a limiting process to capture the influence of continuum reservoirs on transport [13, 23]. In this section, we explain the concept in detail, including both the discretization of the reservoirs and the relaxation, and introduce a stability criterion to set the main parameter of the computational approach.

A. Discretization

A standard strategy to capture the influence of the reservoirs on the system is to include them directly in the many-body calculation. For numerical simulation, this requires discretization of the continuum, approximating it by a finite collection of N_W modes. In principle, any microscopic discretization that limits to the desired macroscopic spectral function as $N_W \rightarrow \infty$ works. This leaves considerable freedom. For instance, one can employ a lattice mapping [51, 52] or an inhomogeneous placement of modes, such as lin-log (evenly distributed inside the bias window and logarithmically outside) [53] or influence-based (leading to mode density vanishing as inverse frequency squared outside of the bias window) [54, 55] distributions. At finite bias, inhomogeneous distributions will, at best, give a prefactor improvement in the number of N_W required, as the bias window requires a uniform distribution of modes (at most, one

could exploit spectral function structure in the bias window). For tensor networks, where the entanglement in the setup dictates the numerical cost rather than the bare number of modes, they may give no speedup at all [55].

We work with semi-infinite, uniform one-dimensional reservoirs. To obtain the discretized lattice for numerical simulation, we truncate this reservoir to a lattice of N_W sites. All simulations here employ these modes in the single-particle eigenbasis given by a sine transform,

$$\omega_k = \frac{W}{2} \cos\left(\frac{k\pi}{N_W + 1}\right) + \delta_\alpha, \quad (13)$$

where $k = 1, \dots, N_W$ and δ_α is a small perturbation of the discretization which globally shifts the energies in reservoir $\alpha = \mathcal{L}, \mathcal{R}$ to which k belongs. Since reservoirs are attached to terminal sites of the system $\mathcal{S}$, $v_{k1} = v_k$ for $k \in \mathcal{L}$ and $v_{kN_S} = v_k$ for $k \in \mathcal{R}$, with

$$v_k = v_0 \sqrt{\frac{2}{N_W + 1}} \sin\left(\frac{k\pi}{N_W + 1}\right) \quad (14)$$

and the other v_{kj} in Eq. (3) are equal to zero.

There is an additional class of parameters in Eq. (13) above, a set of small frequency shifts, $\delta_{\mathcal{L}}$ and $\delta_{\mathcal{R}}$. As described in the subsequent sections, we will use them as control parameters to probe the stability of the results and guide the selection of simulation parameters. The shifts are of the order of the level spacing,

$$\Delta_F \simeq \frac{\pi W}{2N_W}, \quad (15)$$

in the discretized reservoir at the Fermi level.

Now, one may initialize the setup in the desired initial state, generate a particle imbalance between reservoirs, and run the Hamiltonian evolution. However, such an approach can only support a quasi-steady state at intermediate times limited by the size of the finite reservoirs. That can make some protocols or parameter regimes hard to access. Among others, even in the time-independent setup, the Gibbs phenomena related to the finite reservoir bandwidth can result in oscillating currents in the quasi-steady state [56]. For periodic driving, the latter could interfere with the driving frequency, making the continuum limit even harder to extract.

B. Open system approach

To address such challenges, a growing number of methods augment the explicit reservoirs with a relaxation process. These go beyond closed system approaches, such as the microcanonical approach [57–61], and explicitly relax reservoir modes to their equilibrium distributions at the desired temperatures and chemical potentials. Most approaches to date employ continuous relaxation within a Markovian master equation. This has been done for classical thermal transport [62–66], for

non-interacting electrons [13, 49, 50, 53, 67–75], including for time-dependent driving [76–79], but also for interacting systems utilizing tensor network techniques in the simulations [14–22]. This builds on the original concept of pseudo-modes [80–83], where external Markovian relaxation broadens the modes into Lorentzian peaks and turns a discrete reservoir into an effective continuum. Different relaxation schemes can also be used, such as the recently introduced periodic refresh [84], which stroboscopically resets the reservoirs to their (isolated) thermal equilibrium, or a generalization that interpolates between periodic and continuous relaxations via the accumulative reservoir construction [85].

The stroboscopic refresh processes have advantages, potentially allowing for algebraically faster convergence versus N_W of physical quantities to the continuum limit [85]. However, in this work, we focus on a continuous Markovian treatment where the density matrix of $\mathcal{LSR}$ follows a Lindblad master equation,

$$\dot{\rho} = -i[H, \rho] + \mathcal{D}[\rho], \quad (16)$$

where the dissipative term is

$$\begin{aligned} \mathcal{D}[\rho] = & \sum_{k \in \mathcal{LR}} \gamma_k^+ \left(c_k^\dagger \rho c_k - \frac{1}{2} \{c_k^\dagger c_k^\dagger, \rho\} \right) + \\ & \sum_{k \in \mathcal{LR}} \gamma_k^- \left(c_k \rho c_k^\dagger - \frac{1}{2} \{c_k^\dagger c_k, \rho\} \right). \end{aligned} \quad (17)$$

The $\{\cdot, \rho\}$ gives the anticommutator with the density matrix ρ . The injection rates, $\gamma_k^+ = \gamma f^{\alpha_k}(\omega_k)$, and depletion rates, $\gamma_k^- = \gamma(1 - f^{\alpha_k}(\omega_k))$, with free parameter γ , are such that the reservoirs in isolation relax to the thermal equilibrium defined by the Fermi-Dirac distribution

$$f^\alpha(\omega) = \frac{1}{1 + e^{\beta_\alpha(\omega - \mu_\alpha)}}, \quad (18)$$

with the thermal relaxation time $\beta_\alpha = \hbar/k_B T_\alpha$. The relaxation rate γ is the central control parameter and needs to be tuned to best mimic the continuum reservoirs. We elaborate on this in the next section.

For non-interacting systems, Eq. (16) is efficiently solvable for a Floquet state utilizing standard correlation matrix techniques, see Appendix A. The Lindblad form of the master equation, Eq. (16), in principle, allows direct treatment of a general, interacting system, where the density matrix can be conveniently approximated as a matrix product state [86, 87]. However, turning matrix product states into a useful approach to tackle quantum transport requires careful selection of the computational basis and its ordering [21, 88] to avoid exponential entanglement barrier precluding successful matrix product state simulations. We focus on non-interacting systems, leaving the determination of the optimal structure of matrix product state simulations for time-dependent situations to future studies.

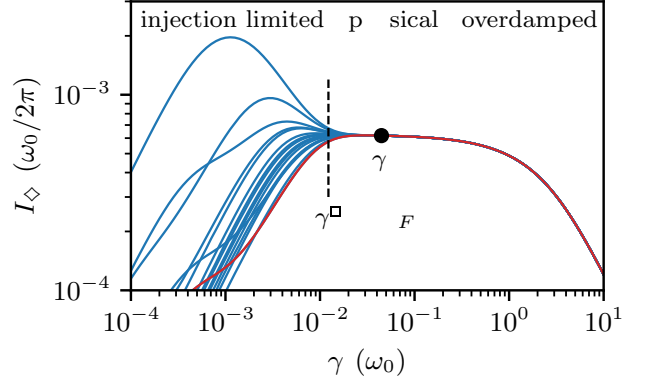


FIG. 2. Stability and discreteness. We plot Kramers’ turnover for $I_D(\gamma)$, indicating the approximate division into injection-limited, physical, and overdamped regimes. The solid lines are different combinations of small discretization shifts in Eq. (20), $s_r, s_m \in \{0, \frac{1}{3}, \frac{2}{3}, 1\}$. The red line singles out a standard choice of $s_m = s_r = 0$, i.e., no shift. For small enough γ , resonances between discrete modes artificially modify the current. The black circle shows the transition relaxation rate, $\tilde{\gamma}$, that marks the ending of the stable regime—the physical plateau—for a given reservoir size, $N_W = 512$. The dashed line marks the standard choice of $\gamma^\square = \Delta_F$, where the current noticeably varies with the shift. The data are for $N_S = 2$, a weak reservoir–system coupling $v_0 = \omega_0/100$, $\Delta_S = \omega = \omega_0\pi/16$, $V_S = \omega_0/20$, $W = 4\omega_0$, and bias $\mu \rightarrow \infty$.

C. Stability criterion and the relaxation rate

Green’s function techniques permit a formal proof [23] (for time-independent, non-interacting and interacting systems) that the steady-state of Eq. (16) converges to the continuum limit with the current given by the Meir-Wingreen formula [89, 90] (e.g., for non-interacting systems, it converges to the Landauer formula). For time-dependent non-interacting models, one can find the solution using time-dependent non-equilibrium Green’s functions [91–93], which are exact up to the truncation of the frequency expansion. We recover this limit for ERA by first taking $N_W \rightarrow \infty$ and then $\gamma \rightarrow 0$. In practical simulations, one simultaneously increases N_W while decreasing γ , but still at quite modest N_W .

A standard choice is to set γ proportional, and typically equal, to the level spacing Δ_F in Eq. (15), which should allow a sum of the discrete Lorentzians to approximately reproduce a desired spectral function, see, e.g., Refs. [22, 53, 76, 78, 79]. As well, one can approximate γ from the self-energies of explicit reservoir modes in contact with the implicit infinite environment [74], which for the reservoirs here would give $\gamma \approx 1.7\Delta_F$. Such reasoning, however, considers the reservoir in isolation from the rest of the setup, which we will show here can be poorly behaved (although even for static models, virtual resonances can dominate the current depending on trans-

mission properties of the system [26]). We will use

$$\gamma^\square = \Delta_F \quad (19)$$

as a reference relaxation rate and demonstrate that this choice can lead to systematic errors due to the presence of $\mathcal{S}$, and thus always requires further validation. We also note that one often makes γ mode dependent, but this would have marginal influence on our results. We employ a homogeneous γ here for simplicity.

It is illustrative to treat γ as a free parameter and consider its influence on the steady state. For a fixed N_W , three basic regimes appear for the steady-state current, forming a so-called Kramers' turnover [64]. The main regime of interest is a physical regime at intermediate γ where the current is independent of γ to leading order. The current is thus only weakly distorted by the reservoir approximation and it approaches the physical value of interest. This plateau regime is flanked by large- γ and small- γ regimes. In those overdamped and injection-limited regimes, respectively, the steady-state current is dominated by the relaxation rate and vanishes algebraically with that rate. This behavior is clearly visible in Fig. 2 for the periodically driven system. Such a dependence of the current on the relaxation rate mimics Kramers' turnover for chemical reaction rates [94].

A more detailed analysis reveals additional anomalous regimes that may appear at both ends of the physical regime, shifting its precise boundaries. In particular, on the low- γ end of the physical plateau, a resonance between the discrete reservoir modes in $\mathcal{L}$ and $\mathcal{R}$ can result in virtual transitions, artificially enhancing the current and masking the physical result [26]. Other conditions may also put constraints on the parameter ranges sufficient to recover physically relevant results. For instance, the γ -related broadening should be much smaller than thermal broadening, i.e., $\gamma \ll k_B T / \hbar$ [13], at the same time this provides a lower bound to the required N_W .

The above considerations have been extensively studied within time-independent setups, but should naturally generalize to time-dependent $\mathcal{S}$ since they are properties of the reservoirs (albeit, the system can impact whether anomalous features are visible in the Kramers' turnover). Time dependence of $\mathcal{S}$ only adds to the richness of phenomena. This motivates the data-driven approach here for estimating the relaxation rate that best reproduces the physical characteristics of transport.

We probe the stability of the current (or other properties) to small perturbations of the reservoir mode placement. While other options are possible, we employ small frequency shifts in Eq. (13),

$$\begin{aligned} \delta_{\mathcal{L}} &= (s_m/2 + s_r/4)\Delta_F, \\ \delta_{\mathcal{R}} &= (s_m/2 - s_r/4)\Delta_F, \end{aligned} \quad (20)$$

where the parameter $s_r \in [0, 1]$ controls the relative shift between ω_k 's in $\mathcal{L}$ and $\mathcal{R}$, and Δ_F , Eq. (15), is the mode spacing at the Fermi level. This parameter affects artifacts coming from resonance between discrete $\mathcal{L}$ and $\mathcal{R}$

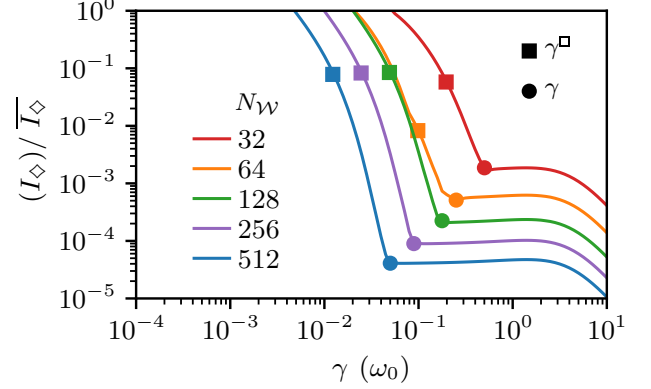


FIG. 3. **Stable and unstable relaxation.** We show the maximal deviation of the current from the median current, normalized by the median, calculated from a combination of small discretization shifts in Eq. (20): $s_r, s_m \in \{0, \frac{1}{3}, \frac{2}{3}, 1\}$ (i.e., all lines in Fig. 2). The circles indicate $\tilde{\gamma}$, which marks the transition between a stable regime with deviation proportional to the shift, and an unstable one for smaller γ 's. The squares represent a standard choice of $\gamma^\square = \Delta_F$, where the relative precision (the sensitivity to a small discretization shift) does not improve with N_W . The results are for $N_W = 32, 64, 128, 256, 512$ and other parameters as in Fig. 2.

modes. A mutual shift of both reservoirs with respect to $\mathcal{S}$ is controlled by $s_m \in [0, 1]$.

For given discretization and relaxation rate, our stability test scans over a set of (s_m, s_r) values to determine the robustness of the results against the shifts. For larger γ , see Fig. 2, small shifts do not affect the current since discrete modes are strongly broadened by coupling to implicit reservoirs. With decreasing γ , the Lorentzian broadening of ω_k gets smaller, eventually revealing discrete nature of the reservoirs as seen by the system. In this case, the overlap of the broadened levels (in both the reservoirs and system) become sensitive to small shifts, leading to potential artificial features in the current.

A systematic scan for a range of N_W 's is in Fig. 3, where we plot the normalized maximal deviation from the median current, calculated over a set of (s_m, s_r) values. It exhibits a clear transition between a stable regime for larger γ , where the small influence is proportional to the amplitude of the shift Δ_F , and a non-linear regime for smaller γ . The relaxation rate, $\tilde{\gamma}$, is at the transition between these regimes, marked with circles in Fig. 3. Still, in practical simulations, one may choose a smaller γ , provided the precision given by the stability test is satisfactory. In Fig. 3, the standard choice of $\gamma^\square$ fails the stability test, giving a systematic error that does not decrease with increasing N_W . We show a further example of such a failure in the Appendix, Fig. A1, that distorts the scan over system $\mathcal{S}$'s coupling parameter.

The stability test can be used while scanning different values of γ to help identify the range corresponding to the physical plateau (for better corroboration of a proper

convergence to the continuum limit). It can also be used without a full scan of $I_\diamond(\gamma)$ to estimate the related precision at a particular γ choice. The criterion is both intuitively appealing and mathematically necessary: So long as the reservoirs limit to the same continuum spectral function, they describe the same model. Thus, if they are providing different results (diverging curves in Fig. 2), then they do not represent continuum reservoirs.

The stability criterion naturally generalizes the procedure of Refs. [26, 55], which addressed virtual transitions between discretized reservoirs' modes as the source of instability. In that procedure, we considered two turnovers ($s_r = 0, 1$ with $s_m = 0$) and estimated the appropriate relaxation as the crossing point between them (i.e., the smallest deviation). The extension proposed here is numerically more comprehensive, recognizing artificial effects from all possible resonances. Those might be particularly hard to identify prior to the calculation for time-dependent models, as well as in interacting or otherwise complicated systems.

IV. RESULTS

We now implement this framework to study the periodically-driven tilted lattice in Sec. II B. We benchmark our results in the parameter limits where reference solutions are available and also cover cases where the simplifying approximations are no longer valid.

A. Markovian limit

In general, the evolution of $\mathcal{S}$ is inherently non-Markovian when coupled to reservoirs. However, it can become Markovian in some limits. One such case is the limit of infinite bandwidth and infinite bias, i.e., $\mathcal{W} \rightarrow \infty$ with $\mathcal{L}$ fully occupied and $\mathcal{R}$ empty [13], where the evolution of $\mathcal{S}$ is governed by the Markovian master equation

$$\dot{\rho}_S = -i[H_S, \rho_S] + \mathcal{D}_S[\rho_S] \quad (21)$$

with the dissipative term

$$\mathcal{D}_S[\rho_S] = \gamma_{\mathcal{L}}^+ \left(c_1^\dagger \rho_S c_1 - \frac{1}{2} \{ c_1 c_1^\dagger, \rho_S \} \right) + \gamma_{\mathcal{R}}^- \left(c_{N_S} \rho_S c_{N_S}^\dagger - \frac{1}{2} \{ c_{N_S}^\dagger c_{N_S}, \rho_S \} \right), \quad (22)$$

which describes particle injection at the first system site and depletion from the last site [95].

We use it to approximate a setup with finite-bandwidth reservoirs, characterized by the spectral functions in Eq. (11), and bias $\mu \rightarrow \infty$. In that case, the injection/depletion rates are

$$\gamma_{\mathcal{L}}^+ = \gamma_{\mathcal{R}}^- = 8v_0^2/\mathcal{W}, \quad (23)$$

which follows from Born-Markov approximation for weak coupling v_0 . Finite $\mathcal{W}$ will give corrections to the Markovian approximation, which, for $\mathcal{W}$ much larger than other

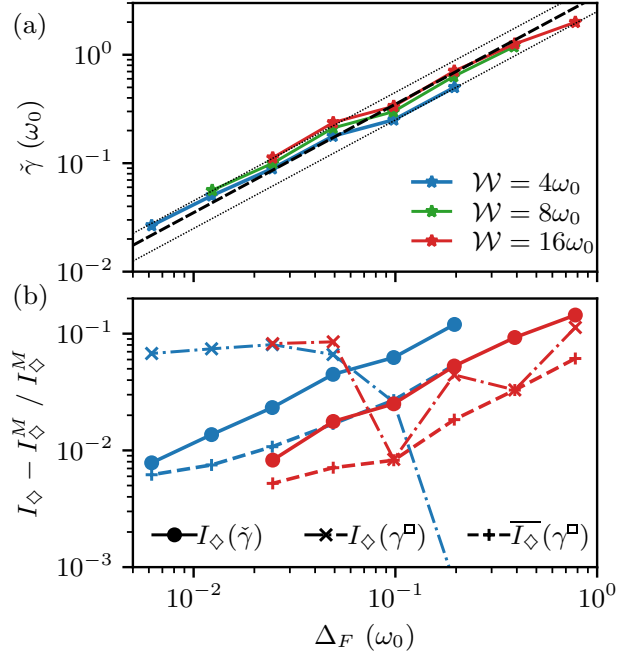


FIG. 4. **Convergence to the infinite bandwidth limit.**

(a) The $\tilde{\gamma}$ from the stability criterion, Sec. III C, versus $\Delta_F \propto \mathcal{W}/N_{\mathcal{W}}$, Eq. (15), for $N_{\mathcal{W}} = 32, 128, \dots, 1024$. Each $\tilde{\gamma}$ comes from the stability of Kramers' turnover to small perturbation of reservoir discretization, as in Fig. 3. For small enough Δ_F , $\tilde{\gamma} \simeq A\Delta_F$ (dashed line). The fit proportionality coefficient is $A = 3.5 \pm 1.0$, where the error indicates the maximal uncertainty range demarcated by the dotted lines. (b) The relative deviation from the Markovian result (infinite bandwidth and infinite bias) versus Δ_F . Circles show the current at $\tilde{\gamma}$, where ERA systematically converges to the infinite bandwidth result. Crosses show the results at $\gamma^\square$ (with no shift in the discretization), which gives rise to systematic errors with increasing $N_{\mathcal{W}}$. Finally, with pluses, we indicate a median over various shifts calculated at $\gamma^\square$, where the systematic errors are removed, and the results systematically converge. For clarity of the plot, we only show $\mathcal{W} = 4\omega_0$ (blue) and $\mathcal{W} = 16\omega_0$ (red), with $\mathcal{W} = 8\omega_0$ giving qualitatively the same results. Other parameters are as in Fig. 3.

energy scales, vanish with an extra factor of $\mathcal{W}^{-1}$, see Appendix B for the derivation.

In Fig. 4, we compare the results of the Markovian approximation in Eq. (21) to the outcome of the ERA. First, in panel (a), we show the transition $\tilde{\gamma}$ for a series of $N_{\mathcal{W}}$ and bandwidths. While it is proportional to the reservoir level spacing Δ_F to a good approximation, the proportionality coefficient takes a value 3.5 ± 1.0 in this example. In panel (b), we compare the resulting currents. The ERA results at $\tilde{\gamma}$ systematically converge with increasing $N_{\mathcal{W}}$, approaching the expected Markovian limit with growing $\mathcal{W}$. The results calculated at $\gamma^\square$ (with no shifts) are systematically shifted from the expected value, which results in the error saturating as $N_{\mathcal{W}}$ grows. We can, however, converge to the true cur-

rent at $\gamma^\square$ by taking a median over various shifts (note that this is not inconsistent with Fig. (3), which shows a maximal perturbation-related error). The convergence is less regular than at $\tilde{\gamma}$ but has a similar overall rate. Yet, the error is smaller overall for the median estimate at a given N_W , which is due to the fact that the corrections to the current from the Markovian anomaly are smaller at $\gamma^\square$ since it is a weaker relaxation (i.e., there is less distortion of the broadened modes but still a sufficient relaxation to look continuum like).

This shows that one should backup a typical choice of $\gamma^\square$ with further tests, such as assessing stability and/or scanning γ to identify the extent of a physical plateau in a particular model. These tests can be local or semi-local (stability at a fixed value of γ or varying γ in the vicinity of $\gamma^\square$) and still provide an estimate of precision.

B. Rotating wave approximation

The fully-Markovian approach in Eq. (21) is quite simple to implement and is thus frequently used in the literature. However, it cannot describe finite potential or a temperature bias, nor can it capture nontrivial reservoir features and their interplay with system dynamics. In this section, we contrast ERA results with those from a different common approximation.

Let us revisit our system $\mathcal{S}$, a tilted lattice given by Eq. (7). Recall first the time-independent system with $v_S(t) = V_S$. With a tilt, a single particle problem can yield Stark localization. Coupling the system to reservoirs with a reasonably weak coupling does not affect it, leading to an inhibition of transport for strong enough total tilt W_S , see Eq. (12).

Periodically driven tunneling $v_S(t)$ destroys localization when the driving frequency ω is close to the frequency difference Δ_S . This can be seen from Eq. (7) in an interaction picture. One can use new operators,

$$a_j \equiv e^{i\bar{w}_j t} c_j, \quad (24)$$

that are a unitary rotation $\exp(it \sum_{k \in \mathcal{LSR}} \bar{w}_k c_k^\dagger c_k)$ of the old. The original Hamiltonian with the oscillating coupling $v_S(t)$ in Eq. (10) now reads, in the rotating frame,

$$H_S(t) = \sum_{j=1}^{N_S} (w_j - \bar{w}_j) a_j^\dagger a_j + \frac{V_S}{2} \sum_{j=1}^{N_S-1} \left[a_j^\dagger a_{j+1} (1 + e^{-2i\omega t}) + \text{h.c.} \right], \quad (25)$$

when $\bar{w}_j = \omega(j - (N_S + 1)/2)$ for $j \in \mathcal{S}$, compare with Eq. (8). The gap between system sites becomes $\bar{\Delta}_S = \Delta_S - \omega$, which vanishes when $\Delta_S = \omega$ (i.e., in resonance). In the rotating wave approximation (RWA), one neglects the fast rotating terms $e^{\pm 2i\omega t}$ in the above Hamiltonian, making the approximate model time-independent.

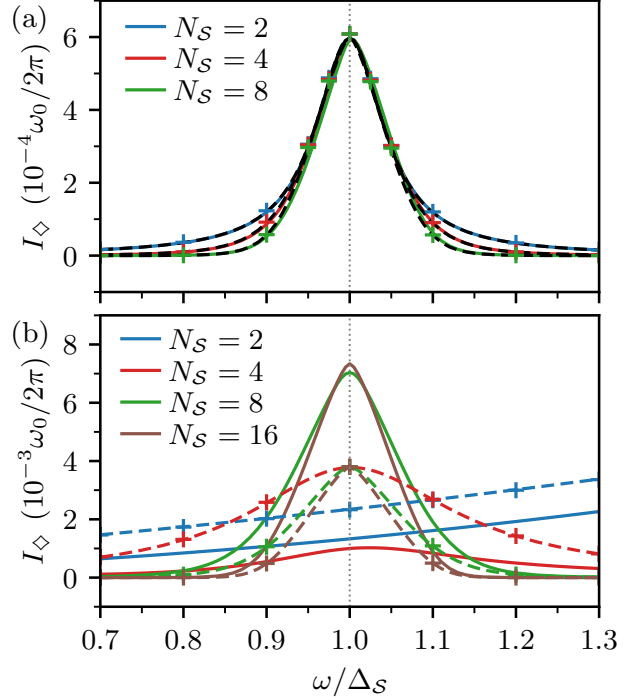


FIG. 5. **Resonant current through a tilted lattice.** (a) Current versus driving frequency showing the resonance for weak coupling to the reservoirs, $v_0 = \omega_0/100$. Time-dependent ERA results for $N_S = 2, 4, 8$ (solid lines) and time-independent RWA results (dashed lines for thermodynamic limit and symbols for ERA) follow each other closely. The resonance width is consistent with Eq. (27), reflected by the observed collapse of curves for various N_S . (b) Current versus driving frequency for strong coupling, $v_0 = \omega_0$, where the RWA provides a less accurate approximation of the time-dependent results. The RWA captures the behavior of the resonance width (for larger N_S) but poorly quantifies the current amplitude. In both panels, the inter-site tunneling, $V_S = \omega_0/20$, is weak and smaller than the driving frequency (the latter follows from the amplitude of the total tilt, $W_S = \omega_0$). Typically, one expects RWA to be a reasonable approximation of $\mathcal{S}$ in this limit. We keep the bias at zero $\mu = 0$, and the ERA results are obtained for $N_W = 512$ and $\gamma = 2\Delta_F$. We checked all points for shift-related stability, with maximal relative deviation below 0.004 (apart from time-dependent simulations for $v_0 = \omega_0$ and $N_S = 4$, where it is below 0.02). A small deviation between RWA results in the continuum limit and ERA, visible at the resonance in (a), is dominated by finite- N_W error and can be reduced by increasing N_W .

One also needs to rotate the reservoirs to keep the $\mathcal{S}$ and $\mathcal{LR}$ coupling time independent. By the coupling of $\mathcal{L}$ to left-most site of $\mathcal{S}$ the $\mathcal{L}$'s modes accumulate a shift $\omega_k \rightarrow \omega_k + \omega(N_S - 1)/2$. Similarly, the $\mathcal{R}$ reservoir's modes shift to $\omega_k \rightarrow \omega_k - \omega(N_S - 1)/2$. This effectively moves the $\mathcal{L}$ and $\mathcal{R}$ bandwidths out of alignment, and the chemical potentials follow as $\mu_{\mathcal{L}} \rightarrow \mu_{\mathcal{L}} + \omega(N_S - 1)/2$ and $\mu_{\mathcal{R}} \rightarrow \mu_{\mathcal{R}} - \omega(N_S - 1)/2$. Consequently, in the rotated

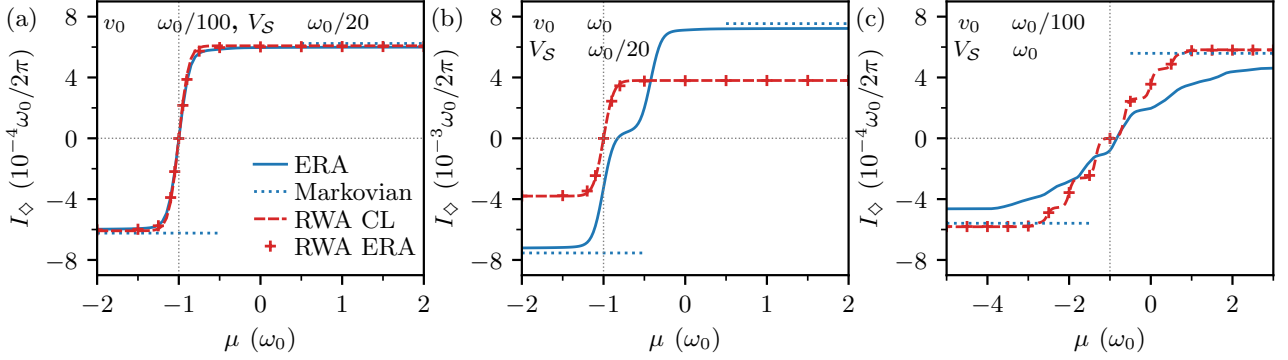


FIG. 6. **Current versus bias at resonance.** We consider various combinations of the system–reservoir coupling and hopping amplitude in $\mathcal{S}$: in (a), $v_0 = \omega_0/100$ and $V_S = \omega_0/20$; in (b), $v_0 = \omega_0$ and $V_S = \omega_0/20$; in (c), $v_0 = \omega_0/100$ and $V_S = \omega_0$. We compare the ERA results with both RWA and Markovian approximation results of Eq. (21). The latter captures the current relatively well in the limit of large biases. It is, however, unable to witness the zero crossing when the influence of periodic driving compensates for applied bias. Approximate results for the RWA are directly in the continuum limit (CL) (dashed lines) and using ERA simulations (symbols). They closely match the time-dependent simulations allowed by ERA (solid lines) in panel (a), with zero crossing for $\mu = -W_S = -\omega_0$. For strong v_0 , in (b), RWA provides a rudimentary picture where the actual current—captured by ERA—has a different amplitude and shifted position of the zero crossing. Increasing V_S in (c), the increased level spacing in finite $\mathcal{S}$ leads to current quantization within time-independent RWA, which, unlike in (a) and (b), is not washed out here by a small but finite reservoir temperature $T_L = T_R = \hbar\omega_0/40k_B$. Such steps get smoothed out in the actual periodically-driven setup. Data for a system of $N_S = 8$ sites, total tilt $W_S = \omega_0$, and the bandwidth $\mathcal{W} = 4\omega_0$. The ERA results are obtained for $N_W = 1024$ and $\gamma = 0.01$ that we checked for stability.

frame, the bias appears as

$$\bar{\mu} = \mu + \omega W_S / \Delta_S, \quad (26)$$

i.e., there is an effective bias due to the drive.

In Fig. 5, we compare the time-averaged ERA solution with the time-independent RWA predictions. The latter permits using the Landauer formula, valid for non-interacting time-independent setups, to obtain results directly in the limit of continuum reservoirs, see Appendix C. We also present ERA results applied to RWA Hamiltonian for further corroboration.

The RWA is expected to hold near resonance for driving that is much faster than other scales in the system, in particular for weak V_S and v_0 . In Fig. 5(a), we show the results for a weak coupling to reservoirs, $v_0 = 0.01\omega_0$, where we can expect RWA to work extremely well. We observe a full agreement between the two approaches. We may use RWA to estimate the width of the resonance in Fig. 5. Combining the localization/delocalization condition in Eq. (12) and RWA Hamiltonian following from Eq. (25), the resonance peak width, Γ_ω , should satisfy $\Gamma_\omega(N_S - 1) \sim V_S$. Using Eq. (9), i.e., that $W_S = \Delta_S(N_S - 1)$, this translates to

$$\frac{\Gamma_\omega}{\Delta_S} \sim \frac{4V_S}{W_S}. \quad (27)$$

Indeed, the data collapse in Fig. 5(a) for all N_S since all curves have the same V_S/W_S , and we plot the current as a function of ω/Δ_S . One expects RWA to hold around the peak of the resonance, where $\omega/\Delta_S = 1$.

In Fig. 5(b), we show the data for strong coupling to the reservoirs, $v_0 = \omega_0$. Here, the RWA approximation is no longer valid as the strong coupling to the reservoirs leads to a fast transport through the system and, at such short times, the averaging of the counter-rotating $\exp(\pm 2i\omega t)$ terms is less effective.

In Fig. 6, we focus on the resonance, $\omega = \Delta_S$, and show the current as a function of the potential bias μ . In this case, the effective bias in the rotated frame is $\bar{\mu} = \mu + W_S$. Consequently, RWA predicts that periodic driving of $v_S(t)$ leads to a non-zero current even when the applied bias is zero, $\mu = 0$, and that the direction of the current changes, crossing zero for $\mu = -W_S$. Panel (a) shows the case of weak coupling to the reservoirs when the system dynamics is dominant. The ERA approach is able to correctly recover the Fermi level in the reservoirs, and the threshold of the current precisely matches the RWA prediction. For a stronger coupling v_0 , presented in Fig. 6(b), this simple picture breaks down for the reasons explained already. The precise position of the zero crossing gets noticeably shifted from RWA prediction of $\mu = -W_S$. Also, the amplitude of the current gets underestimated by RWA. The Markovian approximation of Eq. (21) is better at recovering the current amplitude in the limit of large (negative or positive) bias. However, by its very nature, it is unable to describe the effective compensation of a finite bias by periodically driving.

Finally, in Fig. 6(c), we keep the coupling to reservoirs weak and increase V_S . This allows witnessing the presence of discrete energy levels in a finite system $\mathcal{S}$. In the RWA, $\mathcal{S}$ forms a finite lattice without a tilt,

translating to eigenfrequencies $V_S \cos(l\pi/(N_S + 1))$ with $l = 1, 2, \dots, N_S$ (analogously to Eq. (13)). Effectively, each level contributes to transport when it lies within the bias window controlled by $\bar{\mu}$. This results in visible steps in the current for the RWA, Fig. 6(c), as changing μ includes successive system eigenenergies in the bias window. Such steps are smoothed out for weak V_S in panels (a) and (b) due to thermal broadening (note that we fix $T_L = T_R = \hbar\omega_0/40k_B$). Similarly, this explains the saturation of currents in Fig. 6 for sufficiently large bias when all transition channels in S participate in transport. As discussed above, the RWA is less accurate for strong V_S and, consequently, the simulations of the actual periodically-driven system in Fig. 6(c) has a partial smoothing out of the step structure in $I_\diamond(\mu)$.

C. Periodic driving of the lattice tilt

Let us consider a second example of a periodically driven system that is well known from cold atom physics [96]. We consider a lattice with the tilt as in Eq. (7), but now we have time-independent hopping $v_S(t) = V_S$ and a periodically driven tilt $\Delta_S(t) = \Delta_S \cos(\omega t)$ in Eq. (8). As shown in Ref. 96, for sufficiently large ω , the system behaves as an effective time-independent model with no tilt, and the effective tunneling amplitude between sites equals

$$v_S^{\text{eff}} = V_S \mathcal{J}_0(\Delta_S/\omega), \quad (28)$$

where $\mathcal{J}_0(\cdot)$ is a Bessel function of the first kind and order zero. The relation holds for bosons [96] and for fermions. In effect, the tunneling is suppressed close to the zeros of the Bessel function of the first kind. For interacting bosons in an optical lattice, it has been experimentally verified, that a transition occurs from the superfluid state in the absence of driving to a Mott insulator when tunnelings are effectively eliminated [97]. Similar models for transport with $N_S = 2$ have been considered in Refs. [76, 78, 79, 98].

Here, we shall consider a one-dimensional lattice with $N_S = 8$ coupled to reservoirs. When the driving frequency is the largest scale, in Fig. 7(a), we can indeed see that the time-independent system approximation with hopping in the system given by Eq. (28) faithfully captures the behavior of the current. We observe, however, a correlation between the amplitude of the total tilt and the bias μ , i.e., an interplay between system dynamics and properties of the reservoirs. Our ERA simulations of the periodically driven system, in Fig. 7(b) and (c), illustrate that the approximation remains quantitatively valid when the amplitude of W_S fits into the bias window set by μ . With increasing Δ_S (that translates to W_S , which starts extending beyond the bias window), the current in a periodically driven system gets suppressed compared to the approximate time-independent prediction. Notwithstanding, the zeros of the current coincide well with the zeros of the Bessel function in Eq. (28) also in that limit.

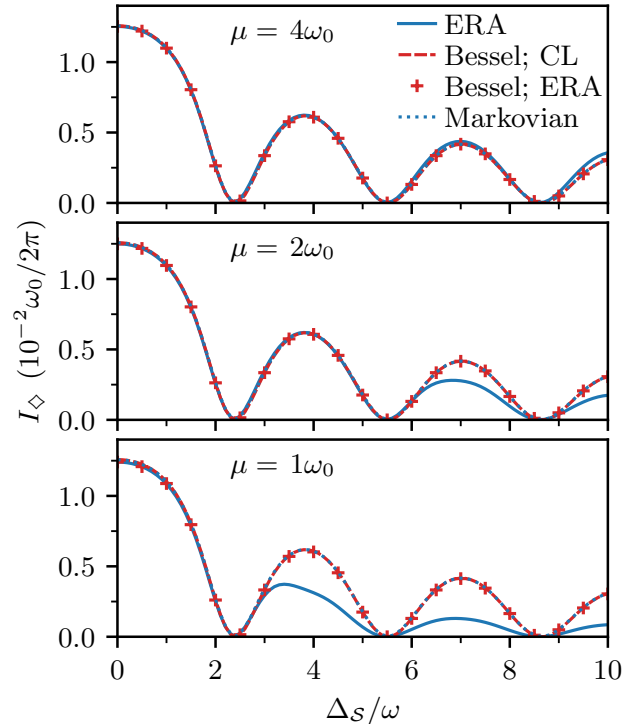


FIG. 7. **Periodically modulated tilt.** The current is shown versus the tilt. We fix the driving frequency $\omega = \omega_0/20$ to be much larger than the hopping $V_S = \omega_0/200$, allowing one to approximate a time-dependent setup with a time-independent one with the hopping modulated by a Bessel formula according to Eq. (28). The result of the latter is plotted directly in the continuum limit (dashed lines) and using ERA simulations (symbols). The approximation works exceptionally well for large enough bias and bandwidth (also captured by the Markovian limit – dotted lines). Reducing the bias μ , which becomes comparable with the amplitude of oscillating tilt for large enough Δ_S , leads to the qualitative breaking of the approximation for large tilts. The data are for $N_S = 8$, $v_0 = \omega_0/20$, and the bandwidth $\mathcal{W} = 4.0\omega_0$. ERA simulations are for $N_{\mathcal{W}} = 512$ and $\gamma = 2\Delta_F$, and checked for stability.

V. CONCLUSIONS

We benchmarked the application of ERA to simulate transport through a periodically driven system coupled to macroscopic reservoirs. We focused on a tilted fermionic lattice with periodic driving. Standard time-independent approximations of that model allow us to test proper convergence of the method in the corresponding limits. We also study the properties of the setup in the parameter limits when the approximations can no longer be faithfully applied.

Our results exemplify potential traps in simulating transport properties using ERA-like approaches, in particular for time-dependent setups. First, RWA mapping and the resulting effective shifts of the reservoir bands and bias window illustrates that discretization techniques

promoting the bias window, like linear–logarithmic strategy, should be applied only with care. A discretization strategy that distributes modes more evenly inside the whole reservoir band, like the one we use in this article, is less prone to misrepresentation of the reservoirs. Second, we introduce a stability criterion to properly tune the simulation parameters (the relaxation rates of the extended reservoirs). It provides a model–agnostic tool to systematically avoid anomalous effects within ERA due to the interplay of the discretization of the continuum reservoirs and insufficient mode broadening. Our results pave the way for faithful simulation of transport in many–body, periodically–driven quantum systems with tensor network and other techniques.

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Appendix A: Correlation matrix

For a non–interacting Hamiltonian H_S , the evolution generated by Eq. (16) preserves the Gaussianity of the density matrix. For a particle number conserving $H(t)$, the latter is fully characterized by the correlation matrix

$$\mathcal{C}_{mn} = \text{tr}[c_n^\dagger c_m \rho], \quad (\text{A1})$$

with $m, n \in \mathcal{LSR}$. The correlation matrix of a state evolved with Eq. (16) follows a dynamic equation

$$\dot{\mathcal{C}}(t) = -i [\bar{H}(t), \mathcal{C}(t)] + \mathcal{D}[\mathcal{C}(t)], \quad (\text{A2})$$

that can be efficiently integrated numerically. Above, a single–particle Hamiltonian

$$H(t) = \sum_{m,n \in \mathcal{LSR}} [\bar{H}(t)]_{mn} c_m^\dagger c_n, \quad (\text{A3})$$

and the dissipator in Eq. (17) translates to [13],

$$\mathcal{D}[\mathcal{C}(t)] = \mathcal{Z} - \mathcal{C}(t)\mathcal{G} - \mathcal{G}\mathcal{C}(t), \quad (\text{A4})$$

with matrices $\mathcal{Z} = \sum_{k \in \mathcal{LSR}} \gamma_k^+ |k\rangle\langle k|$ and $\mathcal{G} = \frac{\gamma}{2} \sum_{k \in \mathcal{LSR}} |k\rangle\langle k|$. Here, we use notation where $|k\rangle$ is a column vector with value one for mode k and zero for all other modes in $\mathcal{LSR}$.

As we are interested in a Floquet state, we consider the correlation matrix evolution over a single cycle with period $\tau = 2\pi/\omega$, which gives a map of the form

$$\mathcal{C}(t_0 + \tau) = \mathcal{M}(\tau)\mathcal{C}(t_0)\mathcal{M}^\dagger(\tau) + \mathcal{P}(\tau). \quad (\text{A5})$$

In a steady state, $\mathcal{C}(t_0 + \tau) = \mathcal{C}(t_0)$, Eq. (A5) is a discrete Lyapunov equation [85, 95, 99] that allows finding the Floquet steady state numerically efficiently. The same strategy was very recently taken in Ref. [79]. Additionally, the steady state is unique if all eigenvalues of $\mathcal{M}(\tau)$ have a magnitude smaller than one. This condition is satisfied in all our examples. However, analyzing the map in Eq. (A5) has an extra advantage, compared with a direct time evolution of some initial state, as it allows to directly probe for phenomena such as time–crystals, which would require degenerate Floquet states [100].

The equations of motion for the propagator $\mathcal{M}(\tau)$ and the source term $\mathcal{P}(\tau)$ follow directly from Eq. (A2),

$$\begin{aligned} \dot{\mathcal{P}}(t) &= -i [\bar{H}(t_0 + t), \mathcal{P}(t)] + \mathcal{D}[\mathcal{P}(t)], \\ \dot{\mathcal{M}}(t) &= [-i\bar{H}(t_0 + t) + \mathcal{G}] \mathcal{M}(t). \end{aligned} \quad (\text{A6})$$

They can be efficiently numerically integrated over time τ with the two initial conditions, $\mathcal{M}(0)$ as an identity matrix and $\mathcal{P}(0)$ as a zero matrix. We note that $\mathcal{P}(t)$ and $\mathcal{M}(t)$ also depend on the initial time t_0 that marks a conventional beginning of a single periodic cycle. We suppress it in the notation for simplicity.

Appendix B: Markovian limit

The Markovian approximation in Eq. (21) for the infinite bandwidth and infinite bias limit follows from the normal Born–Markov master equation. One considers a single system mode of frequency ω_i connected to a fully–occupied reservoir, see Ref. 13 for extended discussion. The time correlation function of the reservoir with spectral function in Eq. (11) reads

$$\begin{aligned} \mathcal{J}_+(t') &= \frac{1}{2\pi} \int_{-\mathcal{W}/2}^{\mathcal{W}/2} \frac{8v_0^2}{\mathcal{W}^2} \sqrt{\mathcal{W}^2 - 4\omega^2} e^{i\omega t'} d\omega \quad (\text{B1}) \\ &= \frac{4v_0^2 \mathcal{J}_1(t' \mathcal{W}/2)}{t' \mathcal{W}}, \end{aligned}$$

where $\mathcal{J}_1(\cdot)$ is the Bessel function of the first kind and order one. The effective relaxation is

$$\begin{aligned} \gamma_{\mathcal{L}}^+ &= \int_0^\infty 2\mathcal{J}_+(t') e^{-i\omega_i t'} dt' \quad (\text{B2}) \\ &= \frac{8v_0^2}{\mathcal{W}} \left(\sqrt{1 - 4\omega_i^2/\mathcal{W}^2} + i\omega_i/\mathcal{W} \right) \end{aligned}$$

for system mode inside the bandwidth, $2|\omega_i| < \mathcal{W}$. Expanding to the leading order in the system frequency ω_i

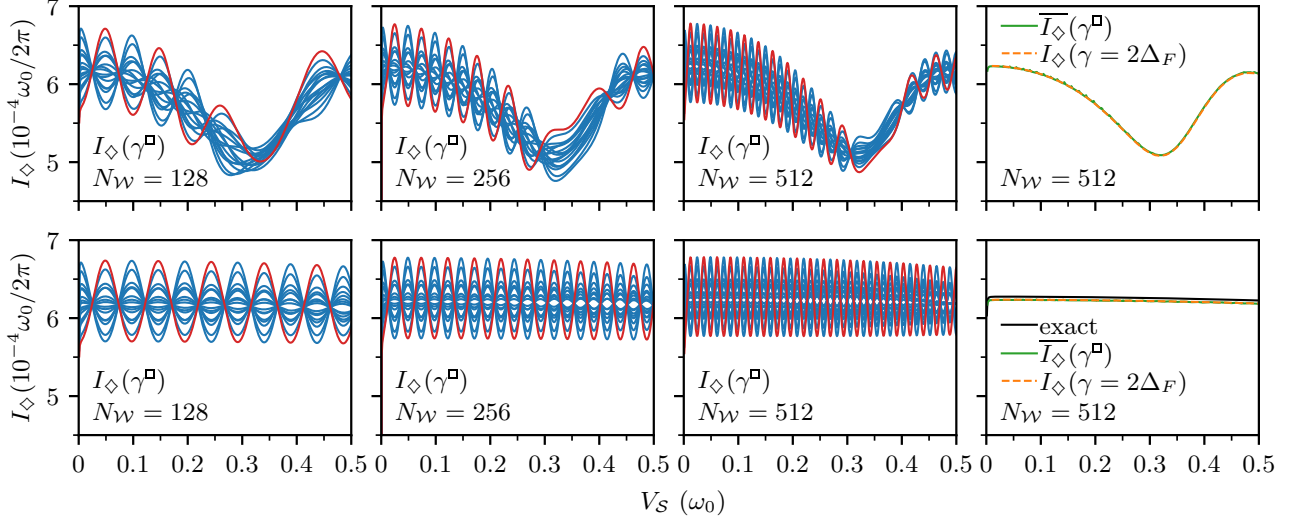


FIG. A1. **Failure of the standard relaxation choice.** Setup is the same as in Fig. 2, but we scan the coupling amplitude V_S in $\mathcal{S}$. Top row represents time-dependent simulations, and the bottom row shows the results within RWA. In the first three columns, the red line is a result of an often used $\gamma^\square = \Delta_F$ (without the shift, $s_m = s_r = 0$), with blue lines showing deviation on small discretization perturbation with $s_m, s_r \in \{0, \frac{1}{3}, \frac{2}{3}, 1\}$ for the same $\gamma^\square$, calculated for growing number of reservoir modes N_W . In the last column, we show the median current over those shifts (green lines), and a current at a stable $\gamma = 2\Delta_F$ (orange lines). Those two results closely overlap each other. The proper convergence is further corroborated in RWA by comparing with the thermodynamic limit results (Landauer formula; black line). The instability of the results for standard $\gamma^\square$ without shifts is of a similar order to actual physical features in the sufficiently converged $I_\Diamond(V_S)$ in the last column, and does not appreciably decrease with growing N_W .

gives Eq. (23) up to corrections of order $\omega_i/\mathcal{W}$. Note that, in reality, the system may have many frequencies but these all influence the relevant parameters in higher orders. The effective depletion rate $\gamma_{\mathcal{R}}^-$ follows similarly.

Appendix C: Landauer formula

For a time-independent, non-interacting model, we can calculate the current flowing through the system directly in the continuum limit using non-equilibrium Green's functions [89, 90]. We employ it for our approximate time-independent reference models, further corroborating proper convergence of ERA results to the continuum limit. We collect the relevant equations here.

The retarded (advanced) Green's function for $\mathcal{S}$ is

$$\mathbf{G}^{r(a)}(\omega) = \frac{1}{\omega - \bar{\mathbf{H}}_S - \Sigma_{\mathcal{L}}^{r(a)}(\omega) - \Sigma_{\mathcal{R}}^{r(a)}(\omega)}, \quad (\text{C1})$$

where the single-particle system Hamiltonian is

$$H_S = \sum_{i,j \in \mathcal{S}} [\bar{\mathbf{H}}_S]_{ij} c_i^\dagger c_j. \quad (\text{C2})$$

The retarded (advanced) self-energies follow as

$$\Sigma_\alpha^{r(a)}(\omega) = \int \frac{d\omega'}{2\pi} \frac{\mathbf{J}_\alpha(\omega')}{\omega - \omega' \pm i\eta}, \quad (\text{C3})$$

where $\mathbf{J}_\alpha(\omega)$ is the spectral function defining reservoir α and the limit of $\eta \rightarrow 0^+$ is taken at the end of the calculation. These quantities give the spectral densities $\mathbf{\Gamma}^\alpha(\omega) = i(\Sigma_\alpha^r(\omega) - \Sigma_\alpha^a(\omega)) = -2\text{Im} \Sigma_\alpha^r(\omega)$ (note that these are the spectral functions, but we retain both sets of terminology to correspond to other literature). With this, the current is given by the Landauer formula,

$$I = \int \frac{d\omega}{2\pi} (f^{\mathcal{L}}(\omega) - f^{\mathcal{R}}(\omega)) \text{tr} [\mathbf{\Gamma}^{\mathcal{L}} \mathbf{G}^r \mathbf{\Gamma}^{\mathcal{R}} \mathbf{G}^a], \quad (\text{C4})$$

where $f^\alpha(\omega)$ is the Fermi-Dirac distribution in Eq. (18).

Note that, in the RWA we employ in Sec. IV B, the reservoir spectral functions in Eq. (11) get shifted, and the single non-zero element of Eq. (11) now reads

$$J_\alpha(\omega) = \frac{8v_0^2}{\mathcal{W}^2} \sqrt{\mathcal{W}^2 - 4(\omega - \bar{\omega}_\alpha)^2}, \quad (\text{C5})$$

with $\bar{\omega}_\alpha = \pm \omega W_S / 2\Delta_S$ for $\alpha = \mathcal{L}(\mathcal{R})$, respectively. The self-energies follow from Eq. (C3) as

$$\Sigma_\alpha^{r(a)}(\omega) = \frac{2}{\omega - \bar{\omega}_\alpha \pm iJ_\alpha(\omega)}, \quad (\text{C6})$$

where again we only write the non-zero matrix element. The integration interval in Eq. (C4) is reduced to overlapping parts of shifted reservoir bandwidths where $|\omega - \bar{\omega}_\alpha| < \mathcal{W}/2$.

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