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DOCTORAL THESIS

Towards understanding of non-ergodic physics in quantum many-body systems

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Oświadczenie

Ja niżej podpisany Adith Sai Aramthottil (nr indeksu: 1180082) doktorant Wydziału Fizyki, Astronomii i Informatyki Stosowanej Uniwersytetu Jagiellońskiego oświadczam, że przedłożona przeze mnie rozprawa doktorska pt. „Towards understanding of non-ergodic physics in quantum many-body systems” jest oryginalna i przedstawia wyniki badań wykonanych przeze mnie osobiście, pod kierunkiem prof. dr. hab. Jakuba Zakrzewskiego. Pracę napisałem samodzielnie.

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JAGIELLONIAN UNIVERSITY

Abstract

Faculty of Physics
Institute of Theoretical Physics

Doctor of Philosophy

Towards understanding of non-ergodic physics in quantum many-body systems

by Adith Sai Aramthottil

A non-equilibrium configuration for an isolated generic quantum many-body system thermalizes, i.e., at long times, to estimate local observables, the density matrix of the non-equilibrium state can be approximated by the associated microcanonical ensemble. Such systems are thus ergodic in the sense of exploring the entire microcanonical shell. The primary interest of this thesis lies in understanding the mechanisms that lead to the breaking of the ergodicity in simplified quantum simulator models.

We make specific explorations of three primary mechanisms that show non-ergodicity. For quantum many-body scars, where specific initial configurations do not thermalize, we contrast their existence with different regimes of lattice gauge theories with well-established non-equilibrium mechanisms. In the case of Hilbert-space fragmentation, we explore how the mechanism is modified in the presence of density-dependent tunneling, which arises naturally for dipolar bosons in optical lattices. For the paradigmatic mechanism for ergodicity breaking, namely many-body localization, we explore its stability on approaching the thermodynamic limit in the presence of a quasi-periodic disorder, the relevant disorder for ultracold atom simulations. We further capture the phenomenology of a bond-disordered model as implemented in Rydberg atom arrays, which hosts a many-body localized regime not characterized by integrals of motion.

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List of Abbreviations

HSC	H eisenberg S pin-1/2 C hain
DOS	D ensity O f S tates
GOE	G aussian O rthogonal E nsemble
GUE	G aussian U nitary E nsemble
GSE	G aussian S ymplectic E nsemble
RD	R andom D isorder
RMT	R andom M atrix T heory
SFF	S pectral F orm F actor
ETH	E igenstate T hermalization H ypothesis
QMBS	Q uantum M any B ody S car
LGT	L attice G auge T heory
RHS	R ight H and- S ide
CC	C harge C onfinement
CD	C harge D econfinement
NN	N earest N eighbor
NNN	N ext- N earest N eighbor
DDT	D ensity- D ependent T unneling
MBL	M any- B ody L ocalization
LIOM	L ocal I ntegrals of M otion
FSS	F inite- S ize S caling
RG	R enormalization G roup
BKT	B erezinskii- K osterlitz- T houless
RSRG-X	R ead- S pace R enormalization G roup for e X cited states

To Achachan, for all the stories.

Chapter 1

Introduction

“The dimmed outlines of phenomenal things all merge into one another unless we put on the focusing-glass of theory, and screw it up sometimes to one pitch of definition and sometimes to another, so as to see down into different depths through the great millstone of the world.”

- James Clerk Maxwell

1.1 To the heart of quantum statistical mechanics

A foundational question on quantum statistical mechanics is how an out-of-equilibrium state attains thermalization, i.e., at long times, local operators are described by the corresponding statistical ensemble (Huang, 2009). *Generic* quantum many-body Hamiltonians that describe isolated systems attain irreversibility, and thermalization as the unitary operators governing the Hamiltonian dynamics lead to high entanglement between different local subsystems. Thus, the isolated system acts as a bath for a local subsystem (Nandkishore & Huse, 2015). These ideas are precisely formulated in the eigenstate thermalization hypothesis (Deutsch, 1991; Srednicki, 1994, 1999), wherein an initial out-of-equilibrium state around a given energy would eventually thermalize around that energy.

A prominent example of a quantum many-body system that breaks away from thermalization is integrable systems, described by a set of conserved operators constructed as a sum of local operators. A simple microcanonical ensemble cannot describe them; instead, one requires a generalized Gibbs ensemble to describe them (Vidmar & Rigol, 2016). These integrable systems, though, in the presence of an arbitrarily small perturbation, might thermalize in the thermodynamic limit (D'Alessio *et al.*, 2016). The questions on the thermalization of such isolated systems, though studied for at least over 4 decades, remained only of abstract theoretical interest until, as condensed matter setups have the phonon problem and are not well isolated, this changed with the advent of ultracold atoms, one could create a well-isolated system that can act as testbeds for integrability and thermalization (Kinoshita *et al.*, 2006).

Over the last two decades, new research has led to other possibilities for systems that avoid thermalization. These include

- **Quantum many-body scars:-** where specific initial non-equilibrium states do not thermalize (Bernien *et al.*, 2017) as they have substantial weights over only an algebraic in system size number of eigenstates (Turner *et al.*, 2018a).
- **Hilbert space fragmentation:-** characterized by exponentially many in system size disconnected dynamical sectors that show up in the presence of a large parameter for specific Hamiltonians, where the effects on dynamics are seen in both the effective kinetically constrained models as well as the original Hamiltonian (Moudgalya *et al.*, 2022; Sala *et al.*, 2020).
- **Many-body localization:-** the most prominent example of a quantum many-body system that breaks thermalization. It was initially developed based on ideas of extending the celebrated ideas of Anderson localization to finite temperature and interaction and later presumed to have a regime where localization persists at arbitrary energy with properties captured by dressed local operators termed as local integrals of motions (Serbyn *et al.*, 2013b).

This thesis attempts to make a small but significant contribution to a theoretical understanding of these non-ergodic phenomenas.

1.2 A confluence of classical and quantum analogue simulations

The dawn of this century was characterized by developments in analogue quantum simulators (Greiner *et al.*, 2002; Jaksch *et al.*, 1998), which are special-purpose simulators restricted to a realizable model in a lab. Different possible platforms have emerged for analogue quantum simulators (Altman *et al.*, 2021), each focusing on a particular property of interest. In this thesis, we consider two of the prominent platforms: ultracold atoms loaded in optical lattices (Gross & Bloch, 2017); optical lattices here are typically formed by interfering with several laser beams in order to realize a fully controllable periodic structure as in a crystal lattice, with a possibility for single-atom detection through the so-called quantum gas microscope (Bakr *et al.*, 2009; Sherson *et al.*, 2010). In optical lattices, one can superimpose the primary optical lattice with a secondary lattice with different wavelength and lattice depth chosen such that for finite systems, they act effectively quasi-periodic onsite potentials (Lüschen *et al.*, 2017; Schreiber *et al.*, 2015). Another platform we consider will be atom arrays with Rydberg interactions, where atoms are held in optical tweezers and thus benefit from single-atom control and arbitrary lattice geometry (Browaeys & Lahaye, 2020). In Rydberg arrays, loading the atoms to specific Rydberg quantum numbers (Franz *et al.*, 2022b) can lead to Ising Hamiltonians with dipolar or van der Waals interactions with the interaction strength and the Rydberg blockade radius governed by the principal quantum number (Whitlock *et al.*, 2017).

Simultaneously, developments were parallelly being made for efficient numerical algorithms for time-evolutions of low-entangled states based on tensor network approaches, namely the time-evolving block decimation (**TEBD**) (Vidal, 2003, 2004). The essential ideas were better formulated in a matrix product state formalism (Verstraete *et al.*, 2008). Consequently, improvements were made to TEBD, leading to an improved algorithm widely considered the best for the time evolution of 1-D systems time-dependent variation principle (**TDVP**) (Goto & Danshita, 2019; Haegeman *et al.*, 2011, 2016; Koffel *et al.*, 2012; Paeckel *et al.*, 2019). Time evolutions that lead to highly entangled states can be simulated using either exact methods or based on the Krylov space method such as the one on expanding the time evolution operator into Chebyshev polynomials of the Hamiltonian matrix (Sierant & Zakrzewski, 2022; Tal-Ezer & Kosloff, 1984). The limit of time going to infinity encoded in the eigenvectors and eigenvalues of the Hamiltonian is relevant for the notion of thermalization, for which more optimized methods than exact diagonalization were developed for high energy eigenstates of quantum many-body systems, in particular, the shift-and-invert method (Luitz *et al.*, 2015; Pietracaprina *et al.*, 2018) and the current state of the art method developed in Kraków, the polynomially filtered exact diagonalization method (Sierant *et al.*, 2020) again based on expanding the Hamiltonian as Chebyshev polynomials.

This thesis will use these numerical methods and theoretical tools to elucidate the nature of the various non-thermalizing phenomena for Hamiltonians in specific analogue quantum simulators. As we will be interested in differentiating thermalizing and non-thermalizing regimes, we will lean more heavily on exact and Chebyshev polynomial-based methods and only use tensor network-based methods in regimes where we are sure that the states never encounter high entanglement.

1.3 Outline

In **Chapter 2**, we introduce the ideas with which the different non-thermalizing regimes will be contrasted. We start with a discussion of statistical mechanics in isolated systems and introduce the notion of thermalization; then, we try to understand the conserved operators in quantum integrable systems through the Heisenberg spin-1/2 chain and find that, as they are characterized by extensive operators constructed with local operators and underlie that due to this local structure integrable systems do not thermalize. Then, we discuss the spectral properties of systems characterized by such conserved operators and contrast with generic systems with no such local structure that thermalizes. Finally, we introduce the eigenstate thermalization ansatz for generic non-integrable Hamiltonians that takes the notion of thermalization to eigenstates.

In **Chapter 3**, we introduce a working definition for quantum-many body scars. Then, we expand on lattice gauge theories and some mechanisms of non-equilibrium behavior in lattice gauge theories. Identifying a model with the presence of charge confinement and charge deconfinement, we present **ARTICLE I** (Aramthottil *et al.*, 2023), where we find the consistent existence of scar states only in the presence of charge deconfinement.

In **Chapter 4**, we elucidate the dipolar bosons in an optical lattice, deriving the extended Bose-Hubbard model, highlighting the presence of a dipole strength dependent density-dependent tunneling term. Then, we introduce the essential ideas for Hilbert space fragmentation and fractionalization. Based on presented ARTICLE II (Aramthottil *et al.*, 2023) then the density-dependent tunneling restricts non-ergodicity even for large dipolar strength and can lead to an exact decoupled ergodic and non-ergodic sector for a particular value of dipolar strength.

In **Chapter 5**, we introduce the paradigmatic model for non-ergodicity, many-body localization, through a historical route. Then, the local integral of the motion framework is introduced to capture the properties of many-body localization. The source of current debates on the stability of many-body localization, the many-body localization crossover, is highlighted. Then, we present ARTICLE III (Aramthottil *et al.*, 2021), which uses the quasi-periodic disorder model relevant to optical lattice experiments. We find in such systems that the crossover is characteristically similar to that of the random disorder case, while with weaker drift for the crossover disorder strength. Finally, we present ARTICLE III (Aramthottil *et al.*, 2024), which introduces a bond-disordered model that is not captured by any integrals of motion, unlike the integrable, stark localizing, or many-body localized systems with the on-site disorder. Instead, we introduce a real-space renormalization scheme to capture this many-body localized regime's nontrivial properties and predict probes for ergodicity breaking.

Finally, we make our concluding remarks in **Chapter 6**.

Chapter 2

Generic quantum many body systems

“We renounce all knowledge of the Hamiltonian.”

- Freeman Dyson

As a precursor to this chapter, we want to point out that most of the results stated here work by placing structure into observations made on various systems (primarily numerical) and that, for generic cases, rigorous proofs are lacking. Exponentially large degrees of freedom of many-body systems are almost always not analytically tractable; thus, *an analytical solution here is the exception and not the norm.*

2.1 Statistical mechanics of isolated systems

In classical isolated systems, the macroscopic behavior arising from microscopic dynamics is constructed with microcanonical ensembles (Huang, 2009), where an equal probability is assumed for all possible configurations in the phase space within the constraints of the system’s conservation laws. While there is no physical sense in taking an ensemble average for real systems, the extension of the Poincaré recurrence theorem (Poincaré, 1890), the ergodic hypothesis, partially resolves this problem. The Poincaré recurrence theorem states that during the time evolution of any finite system, it eventually returns arbitrarily close to its initial state. The **ergodic hypothesis**, in turn, states that during its time evolution, an ergodic system visits every region in the phase space, constrained by the conservation laws in the system and that the time spent in every region in the phase space is proportional to its volume. The ergodic hypothesis thus gives the equal probability requirement of the microcanonical ensemble if one considers observables averaged over very long times. The ergodic hypothesis, though generally presumed to hold for interacting systems, has been proven for relatively few systems, e.g., Sinai billiards (Sinai, 1963), Bunimovich stadium (Bunimovich, 1979).

The notion of the ergodic hypothesis does not give reasonable implications for experimental observations on macroscopic systems as the observables are not averaged, and the time scales required are much smaller in comparison to the time scales required to explore the whole phase space, which is exponentially large in the number of degrees of freedom. To solve this problem, one identifies the notion of “typical” and “atypical” states (D’Alessio *et al.*, 2016). The typical configurations are defined as configurations that give the typical values for macroscopic observables, and the atypical states deviate substantially from the typical states. For example, the number of configurations for a bunch of identical interacting particles whizzing around an elliptical geometry with the average momentum around zero and the average position around the system’s center is much higher than the atypical states. However, if we probe the system externally, forcing all particles to be in a region, this atypical form will quickly evolve into a typical form, as shown in Fig. 2.1. Suppose that the microcanonical ensemble averaging gives values for observables of a system starting from an atypical state (as we already saw, such states are formed on making external probes) after a long time. In that case, we will refer to such a system as thermalizing.

For isolated quantum systems, the definition of **thermalization** can be formulated with the time evolution of a quench state $|\psi\rangle$, which is a state far from the eigenstate of the isolated Hamiltonian $H = H_0 + V$ used to probe far-from-equilibrium behavior; In quantum analogue systems, such states can be prepared, for example, as the ground state for a Hamiltonian H_0 and then make a diabatic change to the Hamiltonian form H before making the time evolution. We shall consider a quantum system to be thermalizing if, for any local observable O , the long-time evolution with the quench state $|\psi\rangle$ gives

$$\lim_{t \rightarrow \infty} \langle \psi(t) | O | \psi(t) \rangle = \text{Tr}[\rho_{\text{ME}} O] \quad (2.1)$$

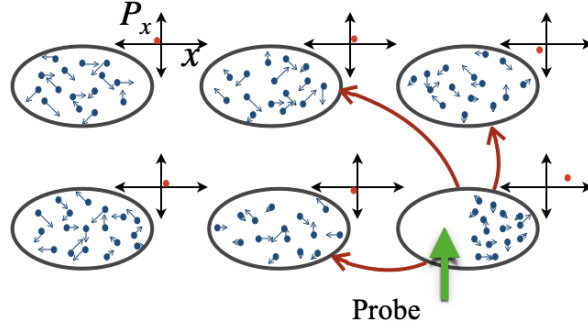


FIGURE 2.1: This illustration shows different configurations of particles whizzing around in a system with elliptical boundaries. The small arrows denote the momentum; we show an atypical configuration as the last one, though not natural, could arise as a non-equilibrium configuration that arises on probing from the outside. We show that this configuration can quickly evolve into different typical configurations.

where ρ_{ME} is the density matrix given by the quantum microcanonical ensemble around the energy $\langle \psi | H | \psi \rangle$.

2.2 Integrable systems

Before we explore the properties of generic Hamiltonians, we explore the special case of **integrable systems**. For classical systems in the sense of Liouville, a Hamiltonian (Arnol'd, 2013) $H(\bar{p}, \bar{q})$ with canonical coordinates $\bar{q} = (q_1, q_2, \dots, q_N)$ and momenta $\bar{p} = (p_1, p_2, \dots, p_N)$ is considered integrable if it has as many functionally independent conserved quantities $\bar{I} = (I_1, I_2, \dots, I_N)$ as the degrees of freedom N ,

$$\{I_j, H\} \quad \forall j \in N, \quad \{I_j, I_k\} \quad \forall j, k \in N \quad (2.2)$$

where $\{f, g\}$ are the Poisson brackets. The meaning of ‘integrable’ here is transparently based on the conserved quantities. The solutions of the equations of motion here are periodic, which translates as regular motion in phase space, leading to the absence of ergodicity, and can easily be probed by looking for regular and toroidal patterns in the Poincaré section (Stöckmann, 1999). Thus, integrability is extremely relevant in classical systems as it explicitly partitions classical models into separate classes of integrable and non-integrable models with manifestly different physical behaviors.

The definition of integrability in quantum mechanical systems is not straightforward (Caux and Mossel, 2011). A straightforward definition of quantum integrability based on modifying the Poisson bracket for commutators and their associated operators is not available, as this definition gives trivial results that all quantum mechanical models are integrable by assuming the associated operators to be built from projectors of the form $\mathcal{P}_\alpha = |\Psi_\alpha\rangle\langle\Psi_\alpha|$. Here, rather than explicitly defining integrability, we will attempt to illustrate integrability using the archetypal model used by Bethe (Bethe, 1931), the Heisenberg spin-1/2 chain (**HSC**). With periodic boundary condition (**PBC**), HSC has the form

$$H_{\text{HSC}} = \sum_{l=1}^{L-1} [s_l^x s_{l+1}^x + s_l^y s_{l+1}^y + s_l^z s_{l+1}^z] \quad (2.3)$$

where, s_l^β are the spin-1/2 operators acting on the l th site with $\beta \in \{x, y, z\}$.

To obtain the possible conserved quantities, we consider Lax operators as a matrix in the auxiliary site a and real site l given as

$$L_{l,a}(u) = u\mathbb{1} + \sum_{\alpha=x,y,z} i s_l^\alpha \otimes \sigma_a^\alpha \quad (2.4)$$

where σ_a^α are the Pauli matrices acting on the auxiliary site a . On defining the permutation matrix $P_{ab} = \frac{1}{2}(\mathbb{1} + \sum_{\alpha=x,y,z} \sigma_a^\alpha \sigma_b^\alpha)$ we find a commutation relation for the Lax operator as

$$R_{ab}(u_1 - u_2)L_{l,a}(u_1)L_{l,b}(u_2) = L_{l,b}(u_2)L_{l,a}(u_1)R_{ab}(u_1 - u_2) \quad (2.5)$$

where $R_{ab} = (u_1 - u_2)\mathbb{1} + iP_{ab}$. Then we can define the monodromy matrix $T_a(u) = L_{N,a}(u) \cdots L_{1,a}(u)$ with repeated use of the commutation relation we are lead to the form

$$R_{ab}(u_1 - u_2)T_a(u_1)T_b(u_2) = T_b(u_2)T_a(u_1)R_{ab}(u_1 - u_2) \quad (2.6)$$

such a relation will directly imply the canonical commutation relation for the transfer matrix $\tau(u) = \text{Tr}_a(T_a(u))$ as

$$[\tau(u_1), \tau(u_2)] = 0. \quad (2.7)$$

Moreover, as the relationship should hold $\forall u_1, u_2 \in \mathbb{C}$, the factors of the formal series expansion must commute with each other. As we will find the first coefficient to be proportional to the Hamiltonian, we can confidently predict the conserved charges in involutions as

$$\mathcal{Q}_\alpha = -i \frac{d^\alpha}{du^\alpha} \ln \tau(u) \Big|_{u=\frac{i}{2}}. \quad (2.8)$$

The first charge from this $\mathcal{Q}_\alpha$ is as stated above $\mathcal{Q}_1 = \sum_l P_{l,l+1} \propto H_{\text{HSC}}$ while higher order terms will also lead to conserved charges that are summed over all sites with operators that act on $\alpha + 1$ sites, for instance, $\mathcal{Q}_2 \propto \sum_l \bar{s}_l \cdot (\bar{s}_l \times \bar{s}_{l+2})$. In addition to these conserved quantities, the H_{HSC} model was found to contain integrals of motion $\mathcal{I}_\alpha$ that act similar to $\mathcal{Q}_\alpha$ on $\alpha + 1$ sites but in addition have longer range operators that decay with distance (Ilievski *et al.*, 2015) compiling these operators one can construct the generalized Gibbs ensemble, ρ_{GGE} (Vidmar & Rigol, 2016). Leading to the long-term evolution of local observables in a quenched state, taking the form

$$\lim_{t \rightarrow \infty} \langle \psi(t) | O | \psi(t) \rangle = \text{Tr}[\rho_{\text{GGE}} O]. \quad (2.9)$$

Although the above example illustrates how integrability arises in quantum many-body systems and is characterized by conserved operators built with local operators and how integrable systems do not satisfy (2.1). Deriving such conserved charges associated with each system is challenging; thus, it cannot be used as a simple diagnostic tool for integrability check like the regular motion in the Poincaré section. In turn, one can use the property that energy levels are uncorrelated and thus follow Poisson statistics as a set of quantum numbers fixes each level. Originally shown for systems with a classical integrable limit by Berry and Tabor (Berry and Tabor, 1977), upon extension to quantum lattice models, the statistics were found to hold for HSC (Poilblanc *et al.*, 1993), XXZ model in the presence of a flux (Rabson *et al.*, 2004), 1-D Hubbard model (Yuzbashyan *et al.*, 2002) and a spin-boson model (Stepanov *et al.*, 2008).

Energy levels in quantum systems do not have a uniform density; the non-uniformity arises from specific physical characteristics of the system. To make universal comparisons for energy levels, one makes an unfolding procedure to separate the global trends of the density of states (**DOS**) from local fluctuations. The unfolding is done by defining a function on the eigenvalues

$$F(E) = \sum_{E_i < E} \Theta(E - E_i) \quad (2.10)$$

where $\{E_i\}$ are the set of eigenvalues of the system, while Θ is a step function. Then, make a fit from $E_{\min}$ to $E_{\max}$ over equidistant points with a polynomial fit. The unfolded eigenvalues are then given as $e_i = f(E_i)$.

Once unfolded, one can predict adjacent energy level gaps, $s_i \equiv e_{i+1} - e_i$. The mean of the level gaps is unity on unfolding, $\langle s_i \rangle = 1$. Once unfolded, the eigenvalues are uncorrelated; thus, the level gap distribution $P(s)$ can be calculated as the probability of finding just an eigenvalue between s and $s + ds$ from a given eigenvalue. To calculate this probability, divide the length s into N intervals and find the probability that there are no levels in each section, $P(s) = (1 - s/N)^N$, and taking the limit $N \rightarrow \infty$ would readily give this as the Poisson distribution $P(s) = e^{-s}$ (Stöckmann, 1999).

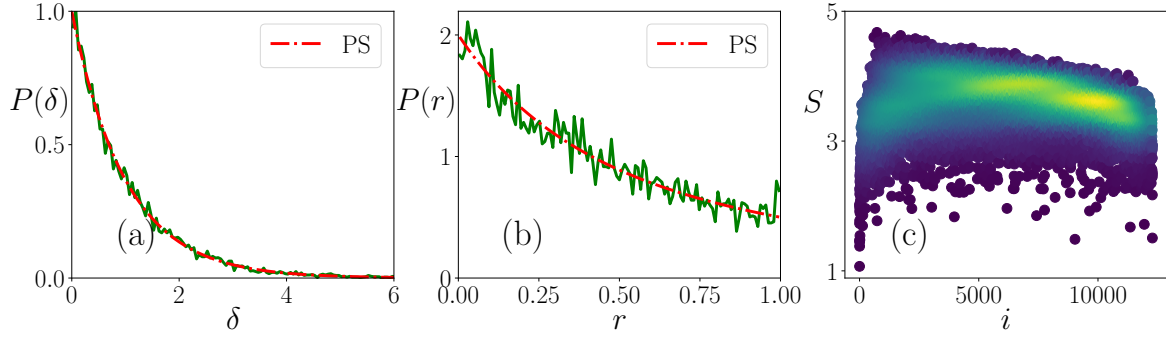


FIGURE 2.2: For HSC (a) a comparison with a Poissonian curve, shown in red dashed-dotted line, with the distribution of level spacing $P(s)$, (b) a comparison with a Poissonian curve, shown in red dashed-dotted line, with the distribution of level spacing ratio $P(r)$. (c) A scatter plot of the entanglement entropy, S , over the eigenindex. All results are considering system size $L = 18$.

A simple way to eliminate the effects of local variations in DOS without unfolding was introduced in (Huse *et al.*, 2014) by defining a level gap ratio

$$r = \frac{\min\{s_i, s_{i+1}\}}{\max\{s_i, s_{i+1}\}} \quad (2.11)$$

The associated distribution is derived with the assumption of uncorrelated energy levels as

$$P(r) = 2/(1+r)^2 \quad (2.12)$$

with typically considered numerical tool being the mean value, $\bar{r} \approx 0.386$ (Atas *et al.*, 2013). In Fig. 2.2 (a,b), we show respectively the comparison with Poisson distribution for the unfolded level statistics and gap ratios for HSC in zero magnetization, $\sum_l^L s_l^z = 0$, parity +1 and spin-inversion +1 sector.

As fixed quantum numbers characterize each eigenvalue and eigenvector, we expect the eigenvector properties to differ substantially from the nearby eigenvectors. We introduce the half-chain entanglement entropy, S , from quantum information theory to explore this (Witten, 2020). The half-chain entanglement entropy captures the entanglement between the two subsystems; it is defined as von Neumann entropy of the reduced density matrix $\rho_{L/2} = \text{Tr}_{1,2,\dots,L/2} |\psi\rangle\langle\psi|$ as

$$S = -\text{Tr}(\rho_{L/2} \ln \rho_{L/2}). \quad (2.13)$$

In Fig. 2.2 (c), we show that S largely fluctuates with the eigen-index i .

2.3 Spectral properties of *generic* quantum many-body systems

Based on the idea that spectral properties for non-analytically solvable problems are way too complex to extract exact information, comparing statistical properties with an ensemble of random matrices was conjectured. Initially used to understand nuclear spectra, the field of random matrix theory (**RMT**) was developed by Wigner, Dyson, Porter, Mehta, and others (Mehta & Normand, 1998). The results were then expanded to semiclassical models with a classical chaotic limit, such as the Sinai billiard problem (Bohigas *et al.*, 1984), where several levels involved in long-time dynamics are substantial. In the case of quantum many-body systems, the exponentially small level spacing would also give broad regimes where universal statistical properties exist. Here, we would presume that the RMT comparisons capture the eigenspectra of systems without any internal structure arising from conserved quantities as in (2.8) rather than assuming these systems to be chaotic. Universal comparisons can be made for systems once unfolded. For systems that has time-reversal symmetry, in which case

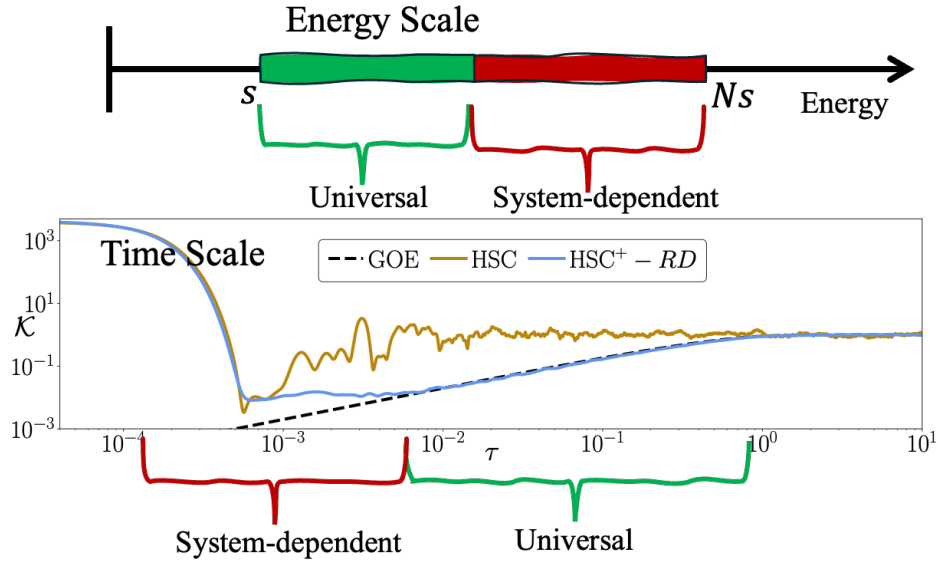


FIGURE 2.3: The top and bottom panels emphasize the regimes where system-dependent properties are shown and regimes of universal character approximated by GOE.

the system is invariant under orthogonal conjugation, the random matrices are approximated by the Gaussian orthogonal ensemble (**GOE**). As we restrict ourselves to autonomous systems in this thesis, we are only concerned with GOE. With the restriction that the joint probability distribution of the matrix elements is invariant under rotation, we are restricted to the form (Stöckmann, 1999)

$$p(H_{11}, H_{12}, \dots, H_{NN}) = \frac{1}{\mathcal{N}} \exp \left(-A \sum_{n,m} H_{nm} \right) \quad (2.14)$$

where, N is the matrix dimension while $\mathcal{N}$ is a normalization constant such that $\int p(H_{11}, H_{12}, \dots, H_{NN}) dH_{11} dH_{12} \dots dH_{NN} = 1$. Making an orthogonal rotation and determining the resultant Jacobi rotation, we find that the joint distribution of eigenvalues are

$$P(e_1, \dots, e_n) \sim \prod_{n>m} (e_n - e_m)^\beta \exp \left(-A \sum_n e_n^2 \right) \quad (2.15)$$

here β gives the Dyson index, which for GOE is $\beta = 1$ while the case $\beta = 0$ corresponds with the uncorrelated case leading to Poisson statistics. For the level spacing distribution, a reasonable estimate can already be made by just considering an ensemble of 2×2 matrices determined by solving the Gaussian integrals

$$\begin{aligned} p(s) &= \int_{-\infty}^{\infty} de_1 \int_{-\infty}^{\infty} de_2 P(e_1, e_2) \delta(s - |e_1 - e_2|) \\ &\propto \int_{-\infty}^{\infty} de_1 \int_{-\infty}^{\infty} de_2 |e_1 - e_2| \exp \left(-A \sum_{n=1,2} e_n^2 \right) \delta(s - |e_1 - e_2|) \end{aligned} \quad (2.16)$$

with the normalization constant and A are determined by the conditions $\int_0^\infty p(s) ds = 1$ and $\int_0^\infty sp(s) ds = 1$ yields

$$p(s) = \frac{\pi}{2} s \exp \left(-\frac{\pi}{4} s^2 \right). \quad (2.17)$$

From this form originally developed by Wigner and referred to as the Wigner surmise, we find that, unlike in the Poisson distribution there is a presence of repulsion, as for small s values it behaves as $p(s) \sim s$. For the level gap ratio, r , which does not need an unfolding procedure, now considering an ensemble of 3×3 GOE matrices one finds the distribution to take the form

$$p(r) = (27/4) \frac{(r + r^2)}{(1 + r + r^2)^{(5/2)}} \quad (2.18)$$

with a mean value estimated as $\bar{r} \approx 0.53590$ (Atas *et al.*, 2013). The correlation between arbitrarily different eigenvalues is estimated by the 2-point correlation function of the form

$$R_2(e_1, e_2) = \frac{N!}{(N-2)!} \int P(e_1, \dots, e_N) de_{2+1} \dots de_N \quad (2.19)$$

An inverse Fourier transform of the two-point correlation function will produce the spectral form factor (**SFF**). The SFF in Hamiltonian systems for numerical purposes is expressed as

$$\mathcal{K}(\tau) = \frac{1}{\eta} \left\langle \left| \sum_{i=1}^N \rho(e_i) e^{-i2\pi e_i \tau} \right|^2 \right\rangle \quad (2.20)$$

where e_i now are the unfolded eigenvalues, ρ is the smooth filter to avoid the influence of spectral edges, and $\langle \rangle$ is the ensemble averaging with normalization factor $\eta = \langle \sum_i |\rho(e_i)|^2 \rangle$. To avoid energy levels at the edges of the spectrum, we use a Gaussian filter $\rho(e_i) = \exp\left(-\frac{(e_i - \bar{e})^2}{2(\mu\sigma)^2}\right)$, where $\bar{e}$ is the average unfolded energy and σ is the standard deviation of the unfolded energy and μ is the parameter that restricts the spectral edges. As the mean level spacing is unity once unfolded, $\tau_H = 1/\langle \delta_k \rangle$. The SFF was used to define timescales in Fig. 2.3 where the system-dependent timescale is until, for the system, the SFF approaches the GOE curve, the Thouless time τ_{Th} , while the universal dynamics is seen from τ_{Th} to the Heisenberg time after which point the system starts resolving the spacing.

$$\mathcal{K}_{\text{GOE}}(\tau) = \begin{cases} 2\tau - \tau \ln(1 + 2\tau), & \text{if } \tau \leq 1, \\ 2 - \tau \ln\left(\frac{2\tau+1}{2\tau-1}\right), & \text{if } \tau > 1. \end{cases} \quad (2.21)$$

As an illustrative example, we consider the HSC Hamiltonian Eq. (2.3) in the presence of random on-site magnetization, denoted as HSC^+ . When the strength of the on-site magnetizations is randomly taken from a box distribution $h_l \in [-W, W]$, we refer to it as random disorder (**RD**) with the disorder strength given by W . The Hamiltonian $\text{HSC}^+ - \text{RD}$ thus takes the form

$$H_{\text{HSC}^+} = \sum_{l=1}^{L-1} [s_l^x s_{l+1}^x + s_l^y s_{l+1}^y + s_l^z s_{l+1}^z] - \sum_l^L h_l s_l^z. \quad (2.22)$$

In the symmetry sector with zero magnetization, on making a similar check to the integrable system for the distribution of level spacing, $P(s)$, and level spacing ratio, $P(r)$ in Fig. 2.4 (a,b), we find the distributions to be well approximated by the GOE results.

2.4 Eigenstate thermalization hypothesis

Isolated quantum many-body systems are characterized by unitary time evolution; thus, all initial state quantum information must always be preserved within the closed system. As the system retains information of initial times, one can presume that the system never thermalizes. The resolution to this apparent paradox is that, for a long time, the extensive spreading of quantum entanglement will require the measurement of global operators to recover the information of the initial state. This is why in (2.1), we carefully used local observables, relevant probes for experiments. Thus, we can assume that for a subsystem, the rest of the isolated system acts as a thermal bath (Nandkishore & Huse, 2015). These thermalization notions should appear in eigenstates as they characterize $t \rightarrow \infty$. Thus, we would presume that a generic Hamiltonian that thermalizes has highly entangled eigenstates. This claim is substantiated; for example, we show in Fig. 2.4(c) the half-chain entanglement spectrum

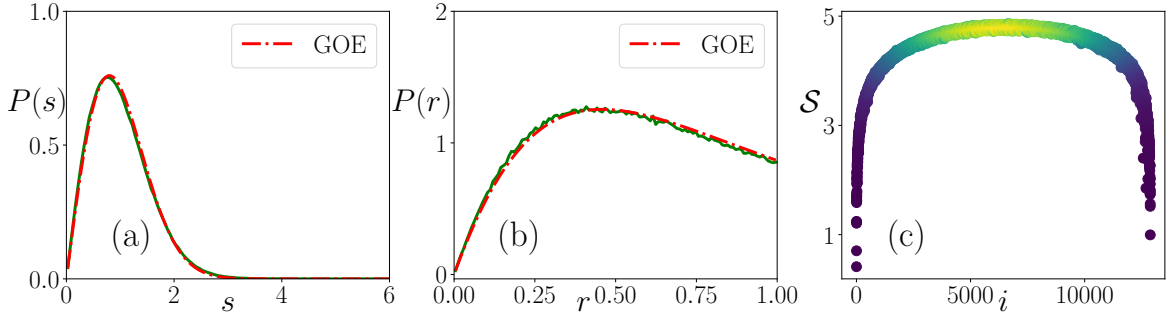


FIGURE 2.4: For $\text{HSC}^+ - \text{RD}$ (a) a comparison with GOE curve, shown in red dashed line, with the distribution of level spacing $P(s)$, (b) a comparison with GOE curve, shown in red dashed line, with the distribution of level spacing ratio $P(r)$. Both (a) and (b) are disorder averaged over 100 realizations. (c) A scatter plot of the entanglement entropy, S , over the eigenindex for a given disorder realization. All results are considering system size $L = 16$ and disorder strength $W = 0.5$.

for the $\text{HSC}^+ - \text{RD}$ model, where in the middle of the spectrum, the entanglement values approach predictions made with a random pure state with normally distributed real coefficients, $S_{\text{RMT}} = (L/2) \ln(2) + [1/2 + \ln(2)]/2 - 1/2$ (Page, 1993; Vidmar & Rigol, 2017), that are motivated by the Gaussian orthogonal ensemble of random matrix theory (D'Alessio *et al.*, 2016).

To characterize thermalization using eigenstates, let us revisit the Gedanken experiment for thermalization starting with the local operator $O = \sum_i O_i |i\rangle \langle i|$, where $O|i\rangle = O_i|i\rangle$ and time evolving with a quenched state $|\psi\rangle$. The average value of O after time τ then reads

$$O(\tau) = \sum_m |c_m|^2 O_{mm} + \sum_{m,n \neq m} e^{-i(E_m - E_n)\tau} c_m^* c_n O_{mn} \quad (2.23)$$

where, $c_m = \langle m|\psi\rangle$ and $O_{mn} = \langle m|O|n\rangle$ with $|m\rangle$ being the eigenvector. The system thermalizes if, after the relaxation time, the average expectation value of the observable $\sum_m |c_m|^2 O_{mm}$ agrees with the microcanonical expectation value and the temporal fluctuation from the average value associated with O_{mn} , for $n \neq m$ is negligible at longer times, so to understand thermalization one needs to take the eigenstates. One would naively assume to approximate the eigenstates with random pure states with normally distributed real coefficients, then the diagonal part of the operator O averaged over the random pure states is given as

$$\overline{O}_{mm} = \frac{1}{\mathcal{D}} \sum_i O_i \equiv \overline{O} \quad (2.24)$$

where $\mathcal{D}$ is the Hilbert space dimension of the Hamiltonian. The off-diagonal part averaged over random pure states is $\overline{O}_{mn} = 0$, $\forall m \neq n$. And finally, the operator elements are given by (D'Alessio *et al.*, 2016)

$$O_{mn} \approx \overline{O} \delta_{mn} + \sqrt{\frac{\overline{O}^2}{\mathcal{D}}} R_{mn}. \quad (2.25)$$

The element R_{mn} here is a random real variable with zero mean and unit variance, $\overline{R}_{mn} = 0$, $|\overline{R}_{mn}|^2 = 1$. As O_{mn} , $m \neq n$ is exponentially smaller as the system size increases, and the O_{mm} values are independent of m , the long time value would reach the saturating value $\overline{O}$ independent of energy. This is expected for RMT, which shows no energy dependence as the microcanonical ensemble.

A more precise mathematical ansatz for eigenstates to capture thermalization based on pioneering work by Deutsch and Srednicki of the eigenstate thermalization hypothesis (**ETH**) (Deutsch, 1991; Srednicki, 1994, 1999)

$$O_{mn} = O(\overline{E}) \delta_{mn} + e^{-S(\overline{E})/2} f_0(\overline{E}, \omega) R_{m,n} \quad (2.26)$$

where $\bar{E} \equiv (E_m + E_n)/2$, $\omega \equiv E_n - E_m$, and $S(E)$ is the thermodynamic entropy at energy E . Both $O(\bar{E})$ and $f_0(\bar{E}, \omega)$ are smooth functions, the value $O(\bar{E})$ is identical to the expectation value of the microcanonical ensemble at energy $\bar{E}$ $O(\bar{E}) = \text{Tr}[\rho_{\text{MC}} O]$, while $f_0(\bar{E}, \omega)$ determines the relaxation time scale.

As a global quench can add a large amount of energy to the system, one needs to make sure that the energy contribution from the quench does not take away from the microcanonical predictions. Again considering the state $|\psi\rangle$ to be an eigenstate of H_0 and then quenching the Hamiltonian to $H = H_0 + V$, where V is a sum of local operators $V = \sum_j h_j$, then the change in energy is (Rigol *et al.*, 2008)

$$\begin{aligned} \delta E &\equiv \sqrt{\langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2} = \sqrt{\langle \psi | V^2 | \psi \rangle - \langle \psi | V | \psi \rangle^2} \\ &= \sqrt{\sum_{i,j} \langle \psi | h_i h_j | \psi \rangle - \langle \psi | h_i | \psi \rangle \langle \psi | h_j | \psi \rangle}. \end{aligned} \quad (2.27)$$

This expression shows us that, in the absence of long-range connected terms in h_j , and if all matrix elements are finite, the width δE scales at most as the square root of the number of lattice sites, i.e., $\delta E \sim \sqrt{V}$ and as energy itself, $\langle \psi | H | \psi \rangle = \langle E \rangle$, is an extensive quantity the relative energy fluctuates as $\delta E / \langle E \rangle \sim 1/\sqrt{V}$. Thus, these quenched processes following ETH should equilibrate easily.

To directly look at how we could also quantify the long-time average of temporal fluctuations of the expectation value of O

$$\begin{aligned} \sigma_o^2 &= \left[\lim_{t_0 \rightarrow \infty} \int_0^{t_0} dt O(t)^2 \right] - \bar{O}^2 \\ &= \left[\lim_{t_0 \rightarrow \infty} \int_0^{t_0} dt \sum_{m,n,p,q} O_{mn} O_{pq} c_m^* c_n c_p^* c_q e^{i(E_m - E_n + E_p - E_q)t} \right] - \bar{O}^2 \\ &= \sum_{m,n \neq m} |c_m|^2 |c_n|^2 |O_{mn}|^2 \leq \max |O_{mn}|^2 \propto \exp[-S(\bar{E})] \end{aligned} \quad (2.28)$$

we get the nice condition thus that the fluctuations with time for an observable is exponentially small in system size. Thus ETH for a Hamiltonian constructed with local operators thus satisfies the thermalization condition (D'Alessio *et al.*, 2016; Rigol *et al.*, 2008; Sierant *et al.*, 2024)

$$\lim_{t \rightarrow \infty} \bar{O}(t) = \text{Tr}[\rho_{\text{MC}} O]. \quad (2.29)$$

As thermalization implies that the local observable at long time is equally spread in the microcanonical ensemble the system is ergodic at the long time limit, hence will use ergodicity and thermalization interchangeably in this thesis.

Chapter 3

Weakly breaking thermalization- Quantum many-body scars

“In all chaos there is a cosmos, in all disorder a secret order.”

- Carl Gustav Jung

3.1 Quantum many-body scars; A brief review and phenomenology

As a starting point, consider the minimal condition for nonthermalization, wherein only very few specific initial states show nonthermalizing behavior as it has a finite overlap with an algebraic number of eigenstates. A situation in which there is a weak or partial violation of ETH by a number of eigenstates that are exponentially smaller than the Hilbert space dimension seems not interesting at first glance, as any such nonergodic eigenstates would not be protected by an energy gap and a local perturbation or induced disorder might lead to hybridization and hence thermalization for large systems. However, surprisingly, a quench experiment done on a Rydberg array with a Neel state (Bernien *et al.*, 2017) showed long time persistent oscillations in the presence of considerable nearest neighbor interaction where the Rydberg array is effectively described by the PXP Hamiltonian, a model generally considered to be nonintegrable; the oscillations were attributed to a small set ($L + 1$), of eigenstates that have significant overlap with the $\mathbb{Z}_2$ state. These nonergodic states were found to be equidistantly embedded in the energy spectrum and termed quantum many-body scar (QMBS) states in (Turner *et al.*, 2018a) in analogy to the phenomenon of scarring in semiclassical single-particle problems like the Bunimovich stadium (Heller, 1984). A follow-up work found that these QMBS states have a very low entanglement entropy (Turner *et al.*, 2018b) compared with generic states and scales in a sub-volume manner $\sim \ln L$.

Nucleated from these results and an independent analytical identification (Moudgalya *et al.*, 2018) in the Affleck-Kennedy-Lieb-Tasaki (AKLT) spin-1 model (Affleck *et al.*, 2004) lead to a flurry of results with attempts to establish QMBS based on numerical results and analytical derivation or embedding of excited states. For a review in comparison with classical periodical orbits (Serbyn *et al.*, 2021), for a review with a focus on embedding matrix product states in a Hamiltonian, refer to (Moudgalya *et al.*, 2022), and for a quasi-particle perspective (Chandran *et al.*, 2023). The definition of scarred states, which has to exist at high energy and when the system is truly nonintegrable, can range from that of just many-body revivals (Chandran *et al.*, 2023) to one that we will use here as the working definition and refer to as true QMBS states (Iadecola and Schecter, 2020)

- (i) concentration of weights on “simple” experimentally relevant quenched initials states
- (ii) embedded in almost equidistant energies in the energy spectrum
- (iii) sub-volume entanglement entropy enabling long-lived coherent oscillations.

3.2 Essential ideas from lattice gauge theory

Space-time lattices with appropriate cutoffs have historically been used to understand field theories in continuous Minkowski space-time (Kogut, 1979). The lattice here is a scaffolding to analyze the difficult nonlinear system with infinite degrees of freedom associated with the field theories. Field

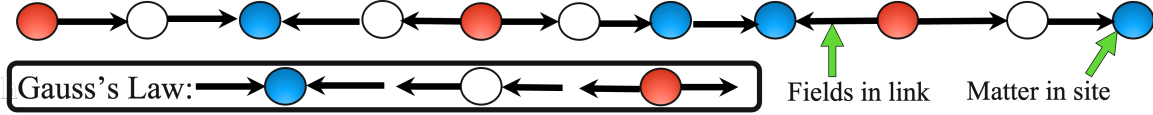


FIGURE 3.1: A sketch showing an LGT in a 1-D lattice with fields in link, matter states in sites, and a Gauss law. For brevity, we do not explicitly consider the strength of fields and quantization of matter.

theories associated with the fundamental fields often contain gauge constraints; for instance, a modern definition of quantum electrodynamics is described by the Lagrangian

$$\mathcal{L}_{\text{QED}} = -\frac{1}{4}F^{\mu\nu}F_{\mu\nu} + \bar{\psi}(i\gamma^\mu\partial_\mu - \gamma^\mu A_\mu - m)\psi \quad (3.1)$$

where ψ represents the fermionic matter, m is the mass and γ are Dirac matrices. The gauge invariant condition here leads to the following transformation

$$A_\mu \rightarrow A_\mu + \partial_\mu f(x), \quad \psi \rightarrow e^{if(x)}\psi, \quad (3.2)$$

that leads to charge conservation, made apparent by Noether's theorem. Thus leading to well-motivated use for lattice gauge theories (**LGTs**).

F. Wegner made the pioneering work on LGTs by introducing an Ising lattice gauge theory (Wegner, 1971) with global up-down symmetry elevated to a local symmetry that showed ideas of a phase transition without spontaneous breaking of magnetization were explored. These ideas on gauge theories were then generalized to continuous abelian groups (Wilson, 1974), and equilibrium quantum field theories were studied by exploiting the Wick rotation of the lattice Lagrangian from real to imaginary time (Wilson, 1974). Our interest here lies squarely on exploiting non-equilibrium phenomena with ideas from LGTs, such as charge confinement, string breaking, and string inversion (Banerjee *et al.*, 2012; Chanda *et al.*, 2020b; Surace *et al.*, 2020) with real-time evolution, the Hamiltonian formalism is best suited for this (Kogut and Susskind, 1975; Kogut, 1979).

As the simplest form to implement the Hamiltonian formalism where non-equilibrium properties from LGTs are present, we consider here the minimal coupling formalism; consider a 1-D chain with discretized matter field on the sites of the chain. A parallel transport for gauge fields between adjacent lattice sites is then defined on the links of the lattice $U_{j+1/2}$. A gauge symmetry is then defined as one that is invariant under a group of local transformations: the gauge transformation acts as

$$\psi_j \rightarrow \Omega_j \psi_j, \quad U_{j+1/2} \rightarrow \Omega_j U_{j+1/2} \Omega_{j+1} \quad (3.3)$$

these local transformations are generated by the generators G_j . The requirement of gauge invariance leads to the properties $[H, G_j] = 0, \forall j$. Moreover, every physical state from Elitzur's theorem (no local gauge symmetry breaking) $|\Psi\rangle$ also needs to be gauge-invariant, meaning that $\Omega_j |\psi\rangle = |\Psi\rangle$, where we will define as physical states that satisfy the condition $G_j |\psi\rangle = 1, \forall j$ in analogy called the *Gauss's law*. Effective ways to simulate such LGTs either in quantum analogue systems or with numerics is to make matter or Gauge integration, which works by explicitly solving *Gauss's law* to eliminate matter or gauge. While the Gauge integration results in long-range constraints, integrating matter fields may just lead to local constraints (Zohar and Cirac, 2019). Local Wilson loops add the kinetic/potential terms for the gauge field, while in 1-D systems, as one cannot make a plaquette, one must fix the gauge constraint in the time domain and take a loop over the same (Kogut, 1979).

QMBS states have been typically observed in the presence of constrained models (Serbyn *et al.*, 2021). As LGTs naturally have local constraints, it is natural to ask whether there is a connection between the non-equilibrium ideas from LGT and QMBS phenomena. Crucially, the weak ergodicity breaking manifested by QMBS states as observed in experiments in spin and bosonic systems (Bernien *et al.*, 2017; Su *et al.*, 2023) can be viewed as LGTs with energy constraints fixed by *Gauss's law*. Parallel to the QMBS results, models were found with confinement leading to deviations from ETH characterized by slow dynamics (Lerose *et al.*, 2020; Surace *et al.*, 2020). Speculations were made

on the relations between confinement and QMBS states. However, this is the antithesis to QMBS, which are translationally invariant quasiparticle states (Chandran *et al.*, 2023) in comparison with nonergodic dynamics from confinement which is quasi-local (Lerose *et al.*, 2020). Thus, the QMBS states in their quasiparticle form are more expected in the deconfined phase; such states have been observed in the absence of a gauge field (Surace *et al.*, 2020) or matter in LGTs (Banerjee and Sen, 2021). Our intention here is to search for the stability of QMBS in a system with both a charge-confined and a charge-deconfined regime in the presence of both matter and gauge fields (Aramthottil *et al.*, 2022).

3.3 Parameter space of the gauged Kitaev chain

The discussions in this section will be heavily based on our interpretation of the work (Borla *et al.*, 2021).

Consider the Kitaev chain which is a tight binding model with a term leading to nearest-neighbor hopping and particle annihilation/creation and a chemical potential controlling the fermion number. The Kitaev chain is thus of the form

$$H_{\text{KC}} = -t \sum_l (c_l^\dagger - c_l)(c_{l+1}^\dagger + c_{l+1}) - \mu \sum_l (c_l^\dagger c_l - 1/2). \quad (3.4)$$

Where $c_l^\dagger$ (c_l) are the spinless fermionic creation (annihilation) operator. The first term on the right-hand side (**RHS**) describes the tunneling and pair production/annihilation processes, and the chemical potential on fermions is controlled by μ . This model exhibits a trivial phase for $\left|\frac{t}{\mu}\right| < \frac{1}{2}$ and a topological phase for $\left|\frac{t}{\mu}\right| > \frac{1}{2}$. One can make a Jordan-Wigner transformation

$$\tau_l^x = (-1)^{\sum_{k<l} n_k} (c_l^\dagger + c_l); \quad \tau_l^z = 2n_l - 1 \quad (3.5)$$

where $n_l = c_l^\dagger c_l$ is the fermion number operator on the model (3.4) giving the transverse-field Ising model

$$H_{\text{TIM}} = -t \sum_i \tau_i^x \tau_{i+1}^x + \frac{\mu}{2} \sum_i \tau_i^z \quad (3.6)$$

Since the Jordan-Wigner transformation is non-local, it drastically alters the physics of the system, with the topological phase now becoming a symmetry-broken phase.

As we already saw, the process of gauging with minimal coupling in the Hamiltonian formalism works by initially enlarging the Hilbert space to include links, which gives the degree of freedom associated with the gauge field, and then shrinking the Hilbert space, thus locking the matter and gauge field together. This process, similar to the Jordan-Wigner transformation, is an invasive non-local procedure that can radically change the associated phase of matter.

The procedure is thus promoting the associated global $U(1)$ symmetry of the system, which is invariant under $\psi(x) \rightarrow e^{i\lambda} \psi(x)$, to a local symmetry, $\psi(x) \rightarrow e^{i\lambda(x)} \psi(x)$, at the cost of introducing a new field $A(x) \rightarrow A(x) + \partial_x \lambda(x)$. These local transformations assumed to be smooth can be discretized by the finite difference method as

$$\psi_j \rightarrow e^{i\lambda_j} \psi_j; \quad A_{j+1/2} \rightarrow A_{j+1/2} + \lambda_{j+1} - \lambda_j \quad (3.7)$$

where $j + 1/2$ are the links between sites j and $j + 1$. If we restrict the degree of freedoms associated with λ_j and $A_{j+1/2}$ to $\{0, \pi\}$ and change the notation to $c_j \equiv \psi_j$, $\sigma_{j+1/2}^z \equiv e^{iA_{j+1/2}}$ and $s_j \equiv e^{i\lambda_j}$ the transformations can be expressed as

$$c_j \rightarrow s_j c_j; \quad \sigma_{j+1/2}^z \rightarrow s_j \sigma_{j+1/2}^z s_{j+1}. \quad (3.8)$$

These transformations can be readily generated by the Gauss operator, defined as

$$G_j \equiv \sigma_{j-1/2}^x (-1)^{n_j} \sigma_{j+1/2}^x \quad (3.9)$$

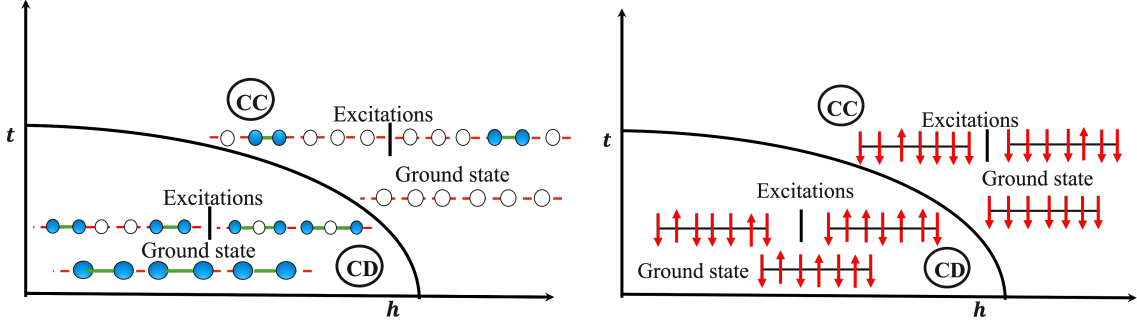


FIGURE 3.2: A sketch showing the confinement and deconfinement regime in the parameter space $t-h$ with $\mu = 1$ for $\mathcal{H}_{\text{GKC}}$ and the matter integrated resultant $\mathcal{H}_{\text{ISC}}$.

and as, $\sigma_{j+1/2}^z \equiv e^{iA_{j+1/2}}$, we can associate $\sigma_{j+1/2}^x \equiv e^{iE_{j+1/2}}$, where $E_{j+1/2}$ is the local electric field. Thus, the gauge-invariance condition can be interpreted as saying that the divergence of the electric field is given by whether or not a site is occupied, mimicking the Gauss law $\nabla \cdot E = \rho$.

The gauging imposes a local constraint, and we will only consider states that are invariant under G_j ; for Gauss law with quantum number $G_j = +1$ the physical states considered are

$$|\psi\rangle \in \mathcal{H}_{\text{sites}} \otimes \mathcal{H}_{\text{links}} \forall j : G_j |\psi\rangle = |\psi\rangle. \quad (3.10)$$

Now that we have the form of basis we need to get the explicit form of the Hamiltonian. In the continuum form coupling with a $\mathbb{Z}_2$ gauge field in the is done by replacing the gauge-dependent operator $\psi(x)$ by the gauge invariant $e^{-i \int_{-\infty}^x A(x') dx'} \psi(x)$. Similarly, the Hamiltonian of the Kitaev chain minimally coupled to a $\mathbb{Z}_2$ gauge field in lattices have the form

$$c_j \rightarrow \cdots \sigma_{j-\frac{3}{2}}^z \sigma_{j-\frac{1}{2}}^z c_j = \left(\prod_{k \leq j} \sigma_{k-\frac{1}{2}}^z \right) c_j. \quad (3.11)$$

The resultant transformation only changes the kinetic term as

$$-t \sum_j (c_j^\dagger + c_j) (c_j^\dagger - c_j) \rightarrow -t \sum_j (c_j^\dagger + c_j) \sigma_{j+\frac{1}{2}} (c_j^\dagger - c_j) \quad (3.12)$$

with a Wilson loop in the Lagrangian space-time lattice and fixing the gauge condition generates an electric field operator $\sigma_{j+\frac{1}{2}}^x$. With the gauge constraint $G_j = +1$, the gauged Kitaev chain (**GKC**) is

$$H_{\text{GKC}} = -t \sum_l (c_l^\dagger - c_l) \sigma_{l+1/2}^z (c_{l+1}^\dagger + c_{l+1}) - \mu \sum_l (c_l^\dagger c_l - 1/2) - h \sum_l \sigma_{l+1/2}^x \quad (3.13)$$

The first term in the RHS describes the tunneling and pair production/annihilation processes mediated by the $\mathbb{Z}_2$ gauge field $\sigma_{j+1/2}^z$ the strength of which is given by the parameter t . Fluctuations in the gauge field are induced by the electric field $\sigma_{j+1/2}^x$ of strength h , and the chemical potential on fermions is controlled by μ . This model is inherently invariant under the local gauge transformation generated by the Gauss operator $G_l = \sigma_{l-1/2}^x (-1)^{n_l} \sigma_{l+1/2}^x$, where $[H_{\text{SKC}}, G_l] = 0$ and $[G_l, G_k] = 0$. Changing the sign of t and making a rotation as $(\sigma^x, \sigma^y, \sigma^z) \rightarrow (\sigma^x, -\sigma^y, -\sigma^z)$ keeps the model invariant, a similar rotation can be made for $h \rightarrow -h$, so it will suffice to explore the $h, t > 0$ parameter space of the model.

In this model, we can do the exact matter integration using the gauge-invariant spin-1/2 variables

$$X_{i+1/2} = \sigma_{i+1/2}^x, \quad Y_{i+1/2} = -i\tilde{\gamma}\sigma_{i+1/2}^y\gamma_{i+1}, \quad Z_{i+1/2} = -i\tilde{\gamma}_i\sigma_{i+1/2}^z\gamma_{i+1}. \quad (3.14)$$

which are confirmed to be bosonic, square to one, commute on different links, and obey the Pauli algebra when on the same link. These variables also commute with the Gauss operator G_j , making them physical. Thus, we can transform to the quantum Ising spin-1/2 chain (**ISC**) in the presence of transverse and longitudinal fields given as

$$H_{\text{ISC}} = \sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1} - t X_i - h Z_i \quad (3.15)$$

to transform the chemical potential, we have made use of the Gauss law, and then a rotation $(X, Y, Z) \rightarrow (Z, Y, -X)$ and from the rotated variable making another rotation $(X, Y, Z) \rightarrow (-X, -Y, Z)$.

We explore the charge confinement and deconfinement regimes in the parameter space for model (3.13) or equivalently (3.15) as shown in the sketch Fig. 3.3. There is a charge confinement (**CC**) regime in this model for large values of h where the ground state is the vacuum state with the absence of gauge fields or fermionic matter; excitation, in this case, are paired fermions which are confined, and separation requires the energy constraint from string tension in this case given by (Alessio20) $E(d) \sim hd$, where d is the length of separation. A symmetry-protected topological Higgs phase for dominant values of t is adiabatically connected to the confined phase (Borla *et al.*, 2021). When $|\mu|$ is the dominant term in the Hamiltonian, i.e., the Ising coupling, for $h = 0$, the ground state spontaneously breaks the translation symmetry, and in 1-dimensional lattices domain wall excitations in symmetry-breaking phases are deconfined. While $\mu < 0$ with $h = 0$ has a ferromagnetic ground state for arbitrarily small values of h , the ground state is paramagnetic. When $\mu > 0$ there is an Ising transition line (Ovchinnikov *et al.*, 2003) (shown as the black curve in Fig. 3.3) within which the antiferromagnetic ground state is preserved and thus we can have a charge deconfined (**CD**) regime; which corresponds with arbitrary distance between fermionic matter or arbitrarily large domains of spins with no energy constraints.

3.4 Summary of ARTICLE I: “Scar states in deconfined $\mathbb{Z}_2$ lattice gauge theories ” (Aramthottil *et al.*, 2022)

Considering the ISC Hamiltonian (3.15), which has a charge deconfined and confined phase, we explore the whole parameter space for possible scar states in ergodic regimes. Global ergodicity is captured using the mean level spacing ratio, $\bar{r}$, as defined in (2.11) and as a possible check for QMBS states, we look the two lowest half-chain entanglement entropy, S as in (2.13) in the middle of the spectrum. We find that the global ergodicity condition with at least two states in the middle of the spectrum with low entanglement is satisfied only in the charge deconfined regime. In the limit $t \ll \mu$, we can make a Schrieffer-Wolff transformation up to $\mathcal{O}(t)$ to obtain the effective Hamiltonian as $H_{\text{eff}} = e^F H e^{-F}$ with F is chosen such that the new terms commute with the unperturbed parts of the Hamiltonian, where

$$F = \frac{-it}{2\mu} \sum_j \left\{ \left(\frac{1+Z_{j-1}}{2} \right) Y_j \left(\frac{1+Z_{j+1}}{2} \right) - \left(\frac{1-Z_{j-1}}{2} \right) Y_j \left(\frac{1-Z_{j+1}}{2} \right) \right\} \quad (3.16)$$

that leads to the derivation of an effective Hamiltonian of the form

$$H_{\text{eff}} = \sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1} - h Z_i - \frac{t}{2} (X_i - Z_{i-1} X_i Z_{i+1}) \quad (3.17)$$

a model with an analytic prediction for the presence of two towers of QMBS states (Iadecola & Schechter, 2020) of the form

$$|S_n^k\rangle = \frac{1}{n! \sqrt{\mathcal{N}(L, n)}} [(\mathcal{Q}^k)^\dagger]^n |\Omega^k\rangle. \quad (3.18)$$

The two towers are built with translational invariant magnon/antimagnon excitations, denoted by $k = 1/2$. A magnon/antimagnon excitation is an up/down spin in a background of spin downs/up; thus, the vacuum state for each case is $|\Omega^{k=1/2}\rangle = |0 \dots 0\rangle / |1 \dots 1\rangle$ with excitations made by with excitations made by $(\mathcal{Q}^k)^\dagger = \sum_{i=1}^L (-1)^i P_{i-1}^k [X_i + (-1)^k Y_i] P_{i+1}^k$, where $P_i^k = (1 + (-1)^k Z_i)/2$. Starting with such a state, $|S_n^k\rangle$, in a regime where the transformation is valid $t, h \ll \mu$, we track these

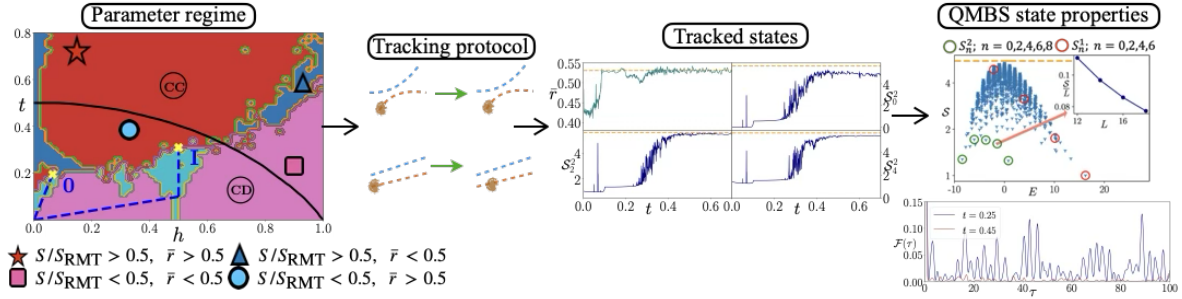


FIGURE 3.3: An outline on ARTICLE I from figures that were taken and modified from (Aramthottil *et al.*, 2022).

states along two paths, “0” and “I”, with changing parameters. The tracking protocol is made by making small parameter changes in the parameter $t + \delta t, h + \delta h$, diagonalizing the Hamiltonian, and finding the new candidate as the eigenstate with the maximum overlap $|\langle E_n(t, h) | S_n^k \rangle|$. The states $|S_n^k\rangle$ are updated with the candidate state if the corresponding energy level is isolated and avoided when coming across narrowly avoided crossings; this process is updated. We find the tracked states satisfy the possible QMBS states at certain parameters (within the charge deconfined regime) with GOE level spacing, and tracked states have low entanglement entropy. We find that path “0” contains both magnon and antimagnon type QMBS states. In contrast, path “I” contains QMBS states just of the antimagnon type, which have almost equidistant energies. At a relevant parameter in path “I”, the antimagnon states are approximately embedded with equidistant energy and have consistently low entanglement entropy compared to other states. In addition, a specific antimagnon state $|S_2^2\rangle$ has a sub-volume growth in entanglement entropy with system size. We also find that the fidelity with a quenched state, $\mathcal{F}(\tau) = |\langle \psi(0) | \psi(t) \rangle|^2$, constructed as a cat state of two excitations of antimagnon states, $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|S_0^2\rangle + |S_2^2\rangle)$, shows consistent revivals in parameters where possible QMBS states can be seen and lead to very small oscillations around $1/L^2$ just as we enter the ergodic regime with the absence of QMBS states. Thus, we conclude that within the finite sizes that we explore, there are true QMBS states that satisfy conditions (i), (ii), and (iii) in the CD regime, while there are no hints of QMBS states in the CC regime.

Chapter 4

Dipolar bosons from a Hilbert space fragmentation perspective

4.1 Dipolar bosons in an optical lattice

Following the theoretical work in (Jaksch *et al.*, 1998), which showed that ultracold atoms can enter the strongly correlated regime and exhibit a superfluid-Mott insulator quantum phase transition (Greiner *et al.*, 2002), there has been increasing interest in simulating Hubbard models (Gersch and Knollman, 1963; Hubbard, 1963) with cold atoms. However, many of the Hubbard models that are simulated with ultracold atoms do not take the standard form of the Hubbard model and contain terms such as correlated and density-dependent tunneling (Jürgensen *et al.*, 2014; Meinert *et al.*, 2013). One could also consider dipolar bosons that lead to long-range interactions. As these models are experimentally amenable to present cold-atom setups, it is thus worth investigating novel and exotic properties in such systems. The dipolar bosons with deep lattice depth, has already been shown to break the strong ergodicity condition (Li *et al.*, 2021). In this chapter, we explore the lattice at different depths. For ground-state properties of non-standard Hubbard models, check out the review (Dutta *et al.*, 2015) or for more recent results (Chan *da24*).

We consider a weakly interacting dipolar gas on an optical lattice along x and a tight harmonic confinement in the transversal direction. Then using the second quantization formalism describing a gas of N interacting bosons (Dutta *et al.*, 2015) is

$$\begin{aligned} \mathcal{H} = & \int d^3\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[\frac{-\hbar}{2m} \nabla^2 + V_t(\mathbf{r}) \right] \Psi(\mathbf{r}) \\ & + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') V_{int}(\mathbf{r} - \mathbf{r}') \Psi(\mathbf{r}') \Psi(\mathbf{r}) \end{aligned} \quad (4.1)$$

where $\Psi(\mathbf{r})$, $\Psi^\dagger(\mathbf{r})$ are the bosonic field operators that satisfy the commutation relation $[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')] = \delta^3(\mathbf{r} - \mathbf{r}')$. The single-particle trapping potential of the optical lattice is given as

$$V_t(\mathbf{r}) = \frac{m\omega^2}{2}(x^2 + z^2) + V_0 \cos^2(kx) \quad (4.2)$$

here, m is the mass of the cold atom, ω is the transverse harmonic trapping potential, and k is given by the wave vector of the laser used to construct the optical lattice. The interaction between the bosons can be divided into two parts

$$V_{int}(\mathbf{r}) = V_c(\mathbf{r}) + V_d(\mathbf{r}) \quad (4.3)$$

the contact interaction term $V_c(\mathbf{r})$ characterized by the s -wave scattering length, a_s , giving $V_c(\mathbf{r}) = \frac{4\pi\hbar^2 a_s}{m} \delta^3(\mathbf{r})$ (Bloch *et al.*, 2008), denoted as $V_c(\mathbf{r}) = g\delta^3(\mathbf{r})$. For usual bosons, such a term will suffice, giving the usual extended Bose-Hubbard model with nearest-neighbor interaction. In contrast, dipolar bosons contribute to the dipole-dipole interaction $V_d(\mathbf{r})$. If we consider all the dipoles point in the same direction transversal to the lattice, here we assume along the z -direction, we are lead to the dipole-dipole interaction given as

$$V_d(\mathbf{r}) = C \frac{1 - 3\cos^2(\theta)}{r^3} \quad (4.4)$$

here, θ is the angle between the polarization direction of the dipoles and the relative distance $\mathbf{r}$. Here

C represents the dipole-dipole interaction strength giving $C = \mu_0 \mu^2 / 4\pi$ ($C = d^2 / (4\pi\epsilon_0)$) depending on whether the atom has magnetic (electric) dipoles with momentum, $\mu(d)$ where, $\mu_0(\epsilon_0)$ are the permeability(permittivity).

The depth of the potential is quantified by the ratio $s = V_0/E_R$, where $E_R = \hbar^2 k^2 / (2m)$. For the given periodic external potential V_{ext} with sufficiently deep enough lattice ($s > 3$), we need to consider only the lowest Bloch band of the periodic potential, and thus the field operators can be expanded in an orthonormal Wannier basis as

$$\Psi(\mathbf{r}) = \sum_{j=1}^L \mathcal{W}_j(\mathbf{r}) a_j = \sum_{j=1}^L \phi_0(y) \phi_0(z) W_j(x) a_j \quad (4.5)$$

where the j denotes the site indices and $a_j(a_j^\dagger)$ denote the bosonic annihilation and creation operator of a particle localized in the i -th site, which obeys the commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$. The orthogonal basis functions here are products of the ground states of the harmonic oscillators along the transverse directions and the Wannier function of the lowest band along the lattice. Substituting this form in (4.1) we get

$$H = -t \sum_{j=1}^{L-1} (a_j^\dagger a_{j+1} + H.c.) + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} a_i^\dagger a_j^\dagger a_k a_l \quad (4.6)$$

where the single-particle part of the Hamiltonian (4.1) contributes to a uniform chemical potential form (not shown here as we will be dealing with closed systems) and the bare tunneling part, which considers only nearest neighbor contribution as we will assume a deep enough lattice (for shallow lattices $s < 4$ one need to consider next-to-nearest neighbor tunneling (Trotzky *et al.*, 2012)), the tunneling amplitude is given by

$$\begin{aligned} t &= - \int d^3 \mathbf{r} \mathcal{W}_i(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_t(\mathbf{r}) \right] \mathcal{W}_{i+1}(\mathbf{r}) \\ &= \int dx W_i(x) \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V_0 \cos^2(kx) \right] W_{i+1}(x). \end{aligned} \quad (4.7)$$

While the constants arising from the interacting part are given as

$$V_{ijkl} = \int d^3 \mathbf{r} d^3 \mathbf{r}' \mathcal{W}_i(\mathbf{r}) \mathcal{W}_j(\mathbf{r}') V_{\text{int}}(\mathbf{r} - \mathbf{r}') \mathcal{W}_k(\mathbf{r}') \mathcal{W}_l(\mathbf{r}) \quad (4.8)$$

the transverse part of these integrals can be explicitly calculated giving (Bartolo *et al.*, 2013)

$$V_{ijkl} = \int dx dx' W_i(x) W_j(x') V_{1D}(x - x') W_k(x) W_l(x') \quad (4.9)$$

with the potential V_{1D} given as

$$\begin{aligned} V_{1D} &= \left(g_{1D} - \frac{2C}{3\eta^2} \right) \delta(|x - x'|) \\ &+ \frac{C}{\eta^3} \left[\sqrt{\frac{\pi}{8}} e^{(x-x')^2/(2\eta^2)} \left(1 + \frac{(x-x')^2}{\eta^2} \right) \times \text{Erfc} \left(\frac{|x-x'|}{\eta\sqrt{2}} \right) - \frac{|x-x'|}{2\eta} \right] \end{aligned} \quad (4.10)$$

where $\eta = (\hbar/m\omega)^{1/2}$ and $g_{1D} = g/(2\pi\eta)^2$ and Erfc denotes the complementary error function. As the Wannier functions are localized in a site, it is evident that the dominant term here is the on-site interaction strength $U \equiv V_{iiii}$, which will be controlled for convenience by using Feshbach resonances. The most dominant term in our study will be the density-density interaction $((V_{ijij} + V_{jjji})n_i n_j$, where n_i is the number operator in a particular site. As the dipolar potential is slowly varying, one may take out the potential term in the approximation, finding the dipolar interaction from $V_{ijij} = V/(|i-j|^3)$. Another term that comes out of V_{ijkl} and is of the most importance in this study is the term where 3 sites are the same, i.e., V_{iiij} introduced by Hirsch (Hirsch, 1994). This is particularly interesting

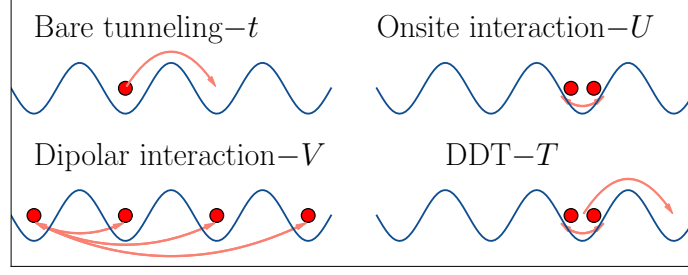


FIGURE 4.1: A sketch showing the characteristics of the different terms in the the extended dipolar boson Hamiltonian (4.11). Here, DDT stands for density-dependent tunneling. This figure was inspire by a figure in (Dutta *et al.*, 2015).

in optical lattices due to the characteristic shape of Wannier functions for sinusoidal potentials. By approximating with just the nearest neighbor, there is the tunneling term $V_{ii(i+1)} a_i^\dagger n_i a_{i+1}$ defined here as the density-dependent tunneling (**DDT**) denoted as $-T$.

Collating all the relevant terms, we finally get the extended Bose-Hubbard (**EBH**) model for dipolar bosons with the complete form

$$\begin{aligned}
 H_{\text{EBH}} = & -t \sum_{j=1}^{L-1} (a_j a_{j+1}^\dagger + \text{H.c.}) + \frac{U}{2} \sum_{j=1}^L n_j (n_j - 1) \\
 & + \frac{V}{2} \sum_{i \neq j} \frac{1}{|i-j|^3} n_i n_j - T \sum_{j=1}^{L-1} [a_j^\dagger (n_j + n_{j+1}) a_{j+1} + \text{H.c}]
 \end{aligned} \quad (4.11)$$

we fix here $U/t = 3$ (which can be fixed using Feshbach resonance). The dipole strength V can be adjusted by changing the dipole orientation θ for a given atomic system. For moderate values of U/T , the magnitude of DDT, T , is approximately linearly proportional to V/t over a broad range of V/t . We will show that this simple result of linear behavior will lead us to interesting results when viewed with the lens of Hilbert space fragmentation, like energy-dependent ergodicity with a considerable amount of ergodic states even at very large V/t , a parameter for quasicancellation of tunneling strengths which leads to dynamically separated sectors of ergodic hard-core bosons and the rest of Fock states (Aramthottil *et al.*, 2023).

4.2 Hilbert space fragmentation with dipolar bosons

A Hamiltonian is considered Hilbert space fragmented if it can be decomposed into dynamically disconnected subspaces, sometimes called the Krylov subspaces (Moudgalya *et al.*, 2022). This decomposition is different from those of conventional symmetries like the global $\mathbb{Z}_2$ or $U(1)$ symmetry in that, in such cases, the number of Krylov subspaces stays a constant or grows as polynomially with system size, whereas, in a fragmented Hilbert space, the subspaces grow exponentially. In addition, one will be able to define product states, which are of experimental relevance, in the dynamically disconnected sectors that continue to be dynamically disconnected.

Such fragmented systems have been seen in cases with dipole-moment (Sala *et al.*, 2020) or center-of-mass conservation (Pai *et al.*, 2019). Another set of examples is in the presence of a large parameter when the effective Hamiltonians could be dynamically disconnected in an emergent way, made more apparent with a Schrieffer-Wolff transformation. Examples of such systems include systems with confinement (Bastianello *et al.*, 2022), as evident in the quasi-local dynamics we discussed in the previous chapter, in the presence of frustration (Lee *et al.*, 2021) or dipolar interactions (Li *et al.*, 2021).

A fragmented Hilbert space could have different dynamical properties within a subspace, ranging from subspaces in which there is just a single state, thus with effectively frozen dynamics, to large subspaces that scale with system size L as α^L , where $0 < \alpha < 2$ for spin-1/2 systems, and satisfies ETH

in this subspace. Fragmented systems where the average subspace dimension tends to 1 effectively fixed with exponentially many (approaching the Hilbert dimension value) of dynamical subsectors emergent from conservation laws are called strongly fragmented or “Hilbert space shattering” (Khemani *et al.*, 2020).

On assuming large on-site interaction in (4.11), thus preventing multiple particles from occupying the same site, effectively making the system hard-core and the density-dependent tunneling term irrelevant even for large values of dipolar interaction, a strong fragmentation of the Hilbert space was found (Li *et al.*, 2021). This strong fragmentation results from the emergence of further nearest terms acting as conserved quantities. As $V \rightarrow \infty$ leads to the conserved quantities (Li, 2021)

$$\mathcal{Q} = \sum_{i \neq j} \frac{\langle n_i n_j \rangle}{|i - j|^3} \quad (4.12)$$

that creates exponentially many sectors. In the study by Li *et al.* (Li *et al.*, 2021), additional consideration of just next-nearest-neighbor (NNN) interaction on top of the nearest neighbor (NN) interaction was found to satisfy the strong fragmentation condition at dipolar interaction strengths $V > 20$, when the NNN interaction starts to be substantial, for small system sizes as verified by the Hamiltonian representation in Fock space and the fractal dimension tending to zero on increasing V/t .

4.3 ARTICLE II: “The role of interaction-induced tunneling in the dynamics of polar lattice bosons” (Aramthottil *et al.*, 2023)

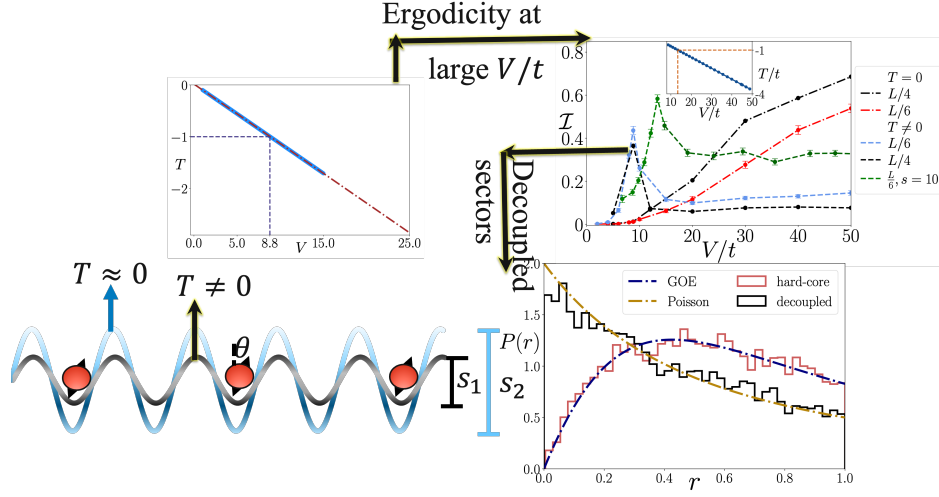
In this article, we look at the effects of dynamics of soft-core dipolar bosons governed by the EBH Hamiltonian (4.11). Initially, by making use of running averages for level spacing ratio, $\bar{r}_\epsilon$, and the DoS, $\mathcal{P}(\epsilon)$, we make a comparison between systems with the presence and absence of DDT at large dipolar potentials $V/t = 50$ and lattice depth $s = 8$. We find that in the absence of DDT, $T = 0$, the system qualitatively behaves as hard-core bosons (Li *et al.*, 2021), as evidenced by the appearance of different sectors showing evidence of Hilbert space fragmentation, and $\bar{r}_\epsilon$ oscillates around the Poisson value indicating Hilbert space shattering. With $T \neq 0$, the dynamical sectors are not strongly formed, and $\bar{r}_\epsilon$ is energy dependent. This energy-dependent effect is also seen with time dynamics. To consider the time dynamics, we consider Fock basis states as the quenched states and define an inhomogeneity $\mathcal{I}(\tau)$ defined as

$$\mathcal{I}(\tau) = \frac{\sum_{i=1}^L [\langle n_i(\tau) \rangle - \rho]^2}{\sum_{i=1}^L [\langle n_i(0) \rangle - \rho]^2} \quad (4.13)$$

with ρ being the density given as $\rho = N/L$ ($= 1/2$ in our case with half-filling). We find that low-energy states saturate to higher values of inhomogeneity while high-energy states saturate to much lower values of inhomogeneity. A naive explanation for the differences in ergodicity between the low-lying and high-lying states is that for the low-lying states at high values of V/t , the number of NN links is very low, resulting in the effective role played by the DDT. In contrast, there is a large number of NN links for high-lying states.

On looking at how the mean gap ratio varies with increasing dipolar potential, we find that in the absence of DDT, the system approaches the Poisson limit of the level gap ratio. In the presence of DDT, there is consistent ergodicity as the system for the maximum dipolar potential we considered $V/t = 50$ just approaches $\bar{r} \approx 0.45$. With time dynamics to make independent of energy state studies on considering a manifold of Fock states with fixed NN chosen such that it falls within the middle of the energy spectrum, we consistently find again that even with increasing dipolar potential, the long time inhomogeneity does not change much, but consistently saturates to a smaller value in comparison in the absence of DDT. We also find that with increasing lattice depths quantified with s , the dependence of the magnitude of T on V becomes weaker. Thus, the long-time inhomogeneity goes to higher values with increasing s .

In addition we find that in case of the presence of DDT there is a certain value of potential which corresponds with $T/t = -1$ at which the level spacing ratio is suppressed and long-time inhomogeneity value peaks. In case of $s = 8$ this corresponds to $V/t = -1$. This is caused due to a quasicancellation of the tunneling part given as $-a_i^\dagger [t + T(n_i + n_{i+1})] a_{i+1} + h.c.$ where in tunneling is suppressed in


 FIGURE 4.2: An outline of ARTICLE II. Taken and modified from (Aramthottil *et al.*, 2023).

cases where a NN pair has value $(n_i + n_{i+1}) = 2$. In addition to quasi-cancellation this restricts the Hamiltonian to two exactly decoupled sectors containing the hard-core bosons and the rest of the soft-core basis. The hard-core decoupled sector leads to shows ergodic behaviour as captured by GOE like level spacing and entanglement entropy that shows concentration around the RMT value and volume-law like growth. In comparison the decoupled sector shows a Poisson like statistics, broadly distributed entanglement entropy and sub-volume growth in entanglement entropy. The effects of an ergodic and non-ergodic subspaces are also seen with time dynamics where the hard-core sector quickly thermalizes while initial states with atleast one double occupancy does not thermalize.

Chapter 5

Many-body localization

5.1 Historical Overview

In his seminal work, Anderson observed that a quantum mechanical particle in a disordered medium inhibits thermalization due to interference effects between multiple-scattering paths (Anderson, 1958). This simple mechanism, referred to as Anderson localization, leads to exponential localization in the position space at any energy and thus provides a natural starting point for strongly breaking ETH in the presence of interaction, as already emphasized by Anderson (Anderson, 1958). Furthermore, Fleishman and Anderson proposed (Fleishman & Anderson, 1980) on the basis of perturbative theory that at low temperatures and weak interaction, localization would be preserved. More than two decades later, (Basko *et al.*, 2006; Gornyi *et al.*, 2005) found that at a fixed interaction strength, there is a critical temperature below which the conductivity vanishes.

Subsequent works driven by numerics gave the current dominant definition of many-body localization (**MBL**) as a *phase* of matter (Nandkishore & Huse, 2015; Oganesyan & Huse, 2007; Pal & Huse, 2010) where at all energies the system avoids thermalization, and thus the long-time local observable on a quenched state is not given by the microcanonical ensemble as defined in (2.29)

$$\lim_{L,t \rightarrow \infty} \bar{O}(t) \neq \text{Tr}[\rho_{\text{MC}} O] \quad (5.1)$$

where to ascertain such a phase, the limit of infinite time, $t \rightarrow \infty$, and the limit of infinite system size (in case of a lattice with uniform lattice spacing), $L \rightarrow \infty$, is important. Restrictions due to Hilbert space growth and predictions on avalanche instability (De Roeck & Huveneers, 2017) in higher dimensions have led to the predominant exploration of MBL in 1-D systems, where it has been proposed to avoid thermalization in a large class of strongly disordered systems that includes spin (Luitz *et al.*, 2015; Oganesyan & Huse, 2007; Santos *et al.*, 2004), bosonic (Hopjan & Heidrich-Meisner, 2020; Orell *et al.*, 2019; Sierant *et al.*, 2017; Sierant & Zakrzewski, 2018) and fermionic (Kozarzewski *et al.*, 2018; Mondaini & Rigol, 2015; Prelovšek *et al.*, 2016; Zakrzewski & Delande, 2018) systems. An initial review with essential ideas can be found in (Altman & Vosk, 2015; Nandkishore & Huse, 2015), more expanded reviews with numerical and experimental results in (Abanin *et al.*, 2019; Alet & Laflorencie, 2018), and a very recent and exhaustive review on MBL with a particular emphasis on the ambiguity of establishing stability of MBL in (Sierant *et al.*, 2024).

5.2 Many-body localization properties

Disordered one-dimensional systems with short-range interaction, e.g., the $\text{HSC}^+ - \text{RD}$ Hamiltonian (2.22), in the presence of strong disorder interpreted to be MBL for systems amenable to numerics has properties that include the area law of entanglement entropy (Bauer & Nayak, 2013), Poissonian level statistics (Oganesyan & Huse, 2007), quasi-conserved local operators (Lüschen *et al.*, 2017; Pal & Huse, 2010; Schreiber *et al.*, 2015), logarithmic growth in entanglement entropy for a quenched state with time that saturates to a value that shows volume growth with system size (Bardarson *et al.*, 2012; Lukin *et al.*, 2019; Serbyn *et al.*, 2013b; Žnidarič *et al.*, 2008) and power-law dephasing dynamics of local observables (Serbyn *et al.*, 2014) for a quenched state. The phenomenology of such properties, analogous to the Fermi liquid theory for interacting fermions, is captured by a simple set of quasilocal conserved operators, the local integrals of motion (Huse *et al.*, 2014; Serbyn *et al.*, 2013a). Contrasted with the integrals of motion of the Yang-Baxter integrable systems (2.8), these local integrals of motion are robust with a weak perturbation.

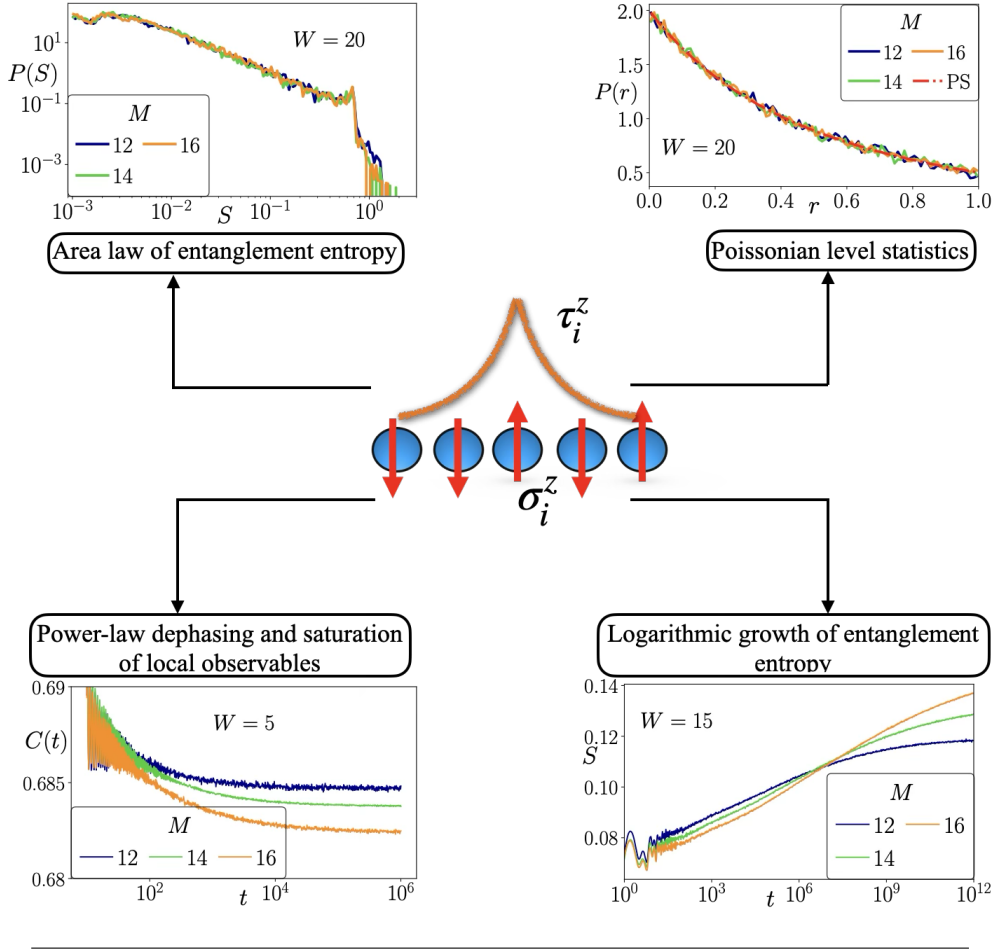


FIGURE 5.1: A sketch showing the LIOMs and a few of the captured phenomenological properties of MBL.

Such local integrals of motion (**LIOMs**) are considered quasilocal as they are built by dressing **local** operators with a quasilocal unitary transformation of the form $U = \prod_i \cdots U_{i,i+1,\dots,i+n-1}^{(n)} \cdots U_{i,i+1,i+2}^{(3)} U_{i,i+1}^{(2)}$, here the n -site unitary operator has at maximum exponentially decreasing with n contributions that differ from unity. In terms of the Frobenius norm, $\|\cdot\|_F$, the weights of contributions can be defined as $\|1 - U_{i,i+1,\dots,i+n-1}^{(n)}\|_F < e^{-n/\zeta}$ where the exponential scale is characterized by the length of the localization ζ .

For the $\text{HSC}^+ - \text{RD}$ Hamiltonian (2.22), often considered the paradigmatic model for MBL. With strong enough disorder, the LIOM operators are given by a simple quasilocal transformation in the s_i^z operator, $\tau_i^z = U s_i^z U^\dagger$. The complete basis of the operators can then be constructed as $\tau_i^{x,y} = U s_i^{x,y} U^\dagger$. By construction we have $[\tau_i^z, H_{\text{HSC}^+}]$ thus, one can expand H_{HSC^+} as

$$H_{\text{MBL}} = \sum_i h_i \tau_i^z + \sum_{i>j} \Gamma_{ij} \tau_i^z \tau_j^z + \sum_{i>j>k} \Gamma_{ijk} \tau_i^z \tau_j^z \tau_k^z + \cdots \quad (5.2)$$

As this representation results from a quasilocal transformation in the s_i^z basis, one can identify the Γ terms for higher-order interaction terms to decay exponentially

$$\Gamma_{ij} \propto \Gamma_0 e^{-|i-j|/\kappa}, \quad \Gamma_{ijk} \propto \Gamma_0 e^{-|i-k|/\kappa} \quad (5.3)$$

where we have defined a new length scale κ .

Based on the above definition of LIOMs, one can attempt to phenomenologically explain a few

of the MBL properties (Abanin *et al.*, 2019); an immediate implication of the quasilocal structure of LIOMs is that the eigenstates thus constructed should have a quasilocal structure in each site; thus, the entanglement entropy that quantifies entanglement between two subsystems must be area law localized; in one-dimensional systems this will imply an entanglement entropy that does not change with system size. The Poisson-level statistics that emerge in the MBL regime can be reasoned as each eigenstate being independent as it is individually fixed by the quantum numbers generated by the τ_i^z operators. The eigenstates thus constructed from τ_i^z could have finite overlaps with eigenstates of local operators, for example, s_i^z , and thus have quasi-conserved simple local operators.

The logarithmic growth in entanglement entropy can be understood by considering a quenched state that has a finite orthogonal part to eigenstates of the LIOM operators, wherein the local orthogonal part is entangled with farther orthogonal parts by second- or higher-order interaction terms in (5.2), leading to generation of entanglement between spins of arbitrary distance. The light cone associated with the entanglement spreading, $X(t)$, then reaches farther sites at longer times at which the interaction energy is significant; thus, $X(t)$ and entanglement entropy can be approximated as

$$X(t) \approx \zeta' \log(\Gamma_0 t), \quad S \propto \zeta' \log(\Gamma_0 t) \quad (5.4)$$

this logarithmic growth of entanglement entropy with time, expected to saturate at values that grow in a volume law fashion with system size, attributed to the interaction part of (5.2) can be used to differentiate MBL from an Anderson localized system where the entanglement entropy saturates to a small value independent of system size (Alet & Laflorencie, 2018; Lukin *et al.*, 2019; Serbyn *et al.*, 2013b).

The spread of entanglements in the light cone $X(t)$ leads to entanglement with an environment of Hilbert space dimension $\mathcal{D}(t) \approx 2^{2X(t)}$, thus on measuring an operator dynamics on an initial quenched state, $|\psi\rangle$ as $\langle\psi|O(t)|\psi\rangle$, overlap of an initial quench state decays as a power-law until it reaches the finite overlap with the τ_i^z eigenstates

$$\langle\psi|O(t)|\psi\rangle \sim \frac{1}{\sqrt{\mathcal{D}(t)}} \approx \frac{1}{(\Gamma_0 t)^a} \quad (5.5)$$

where $a = \zeta' s_0$, here s_0 is the diagonal entropy of the initial quenched state (Abanin *et al.*, 2019; Serbyn *et al.*, 2014).

In the phenomenon of Anderson localization for dimensions $d \geq 3$ with the standard uncorrelated random disorder and nearest-neighbor tunnelings, a localization-delocalization transition is present with a critical disorder strength present dependent upon a single particle mobility edge that separates a localized edge for states at the extremes of the energy spectra from extended states in most of the spectra. A similar many-body mobility edge is found in the many-body localization crossover (Basko *et al.*, 2007; Luitz *et al.*, 2015; Serbyn *et al.*, 2015), also found in a zero-dimensional interacting model (Pawlik *et al.*, 2024). The above LIOM description fails to capture such an energy-dependent presence of extended and localized states and is generally considered a caveat of the LIOM description (Abanin *et al.*, 2019; Alet & Laflorencie, 2018; Nandkishore & Huse, 2015).

Numerical algorithms to identify or characterize LIOMs were proposed from long time averages of local operators (Chandran *et al.*, 2015b), an algorithm based on the application of similarity transformations systematically to eliminate off-diagonal terms (Rademaker & Ortuño, 2016), a numerical algorithm based on stiffness (Mierzejewski *et al.*, 2018) that can be more optimized by data compression (Łydźba *et al.*, 2024). In addition to capturing phenomenological properties of MBL, the derivation of the stability of the MBL phase by Imbrie (Imbrie, 2016a, 2016b) based on Jacobi rotations also makes use of the existence of a LIOM structure.

5.3 Many body localization crossover

Disorder and eigenstate averaged quantities $\bar{X}$, such as the mean gap ratio or the entanglement entropy rescaled with RMT values $\mathcal{S} = \bar{S}/S_{\text{RMT}}$, can be assumed to go to a specific point in the ergodic regime $(\bar{r}, \mathcal{S}) \rightarrow (0.536, 1)$ and the MBL regime $(\bar{r}, \mathcal{S}) \rightarrow (0.386, 0)$, leading to a possible crossover between the two regimes. Initial exact diagonalization studies (Kjäll *et al.*, 2014; Luitz *et al.*, 2015; Pal & Huse, 2010), considered MBL as a stable phase in the thermodynamic limit, thus presuming that the crossover is a phase transition, were interested in understanding this transition. This presumed

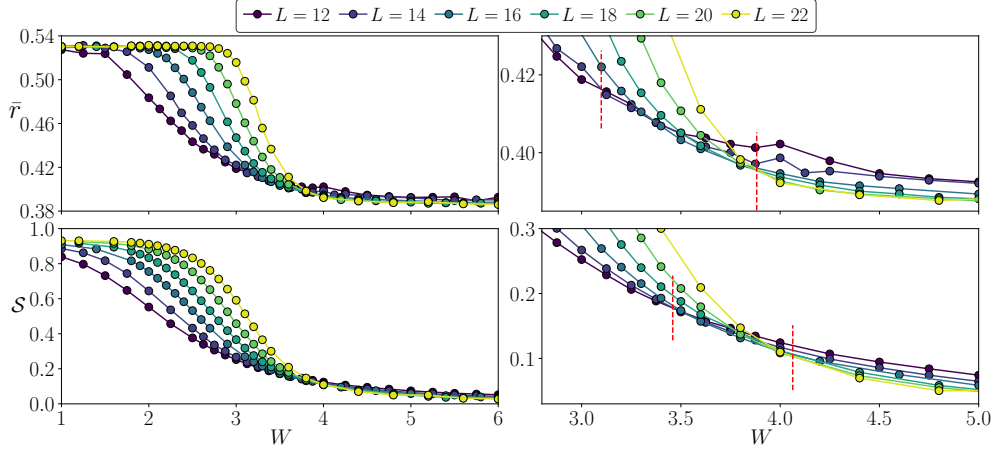


FIGURE 5.2: A sketch showing mean gap ratio $\bar{r}$ and the rescaled average entanglement entropy going to a specific value for the ergodic, small W , and MBL regime large W . The right panel is a zoomed image emphasizing the drift of the crossing disorder strength; the dashed red lines denote the crossing disorder strengths associated with the largest and smallest system sizes considered.

transition was characterized as a ‘usual’ phase transition in analogy with the 3-d Anderson model (Abrahams *et al.*, 1979). A phase transition with a single-parameter scaling hypothesis is characterized by the correlation length ξ that diverges near the critical disorder strength and acts as the dominant length scale (Cardy, 1996); thus a normalized quantity $\bar{X}$ can be expressed as

$$\bar{X} = \mathcal{G}(L/\xi) \quad (5.6)$$

where $\mathcal{G}(\cdot)$ is a continuous function. In the ‘usual’ transition case, the correlation diverges as a power-law

$$\xi_0 = \frac{1}{|W - W^*|^\nu} \quad (5.7)$$

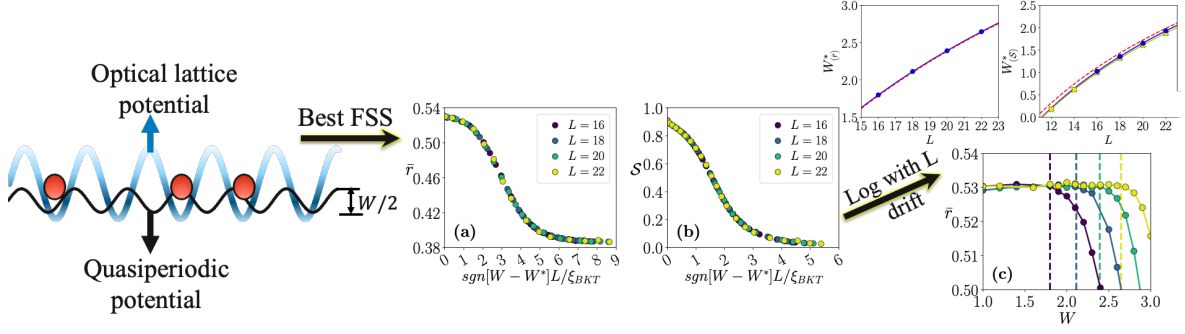
near the critical disorder strength W^* . This transition was corroborated by initial studies in the real-space renormalization group (RG) studies (Potter *et al.*, 2015; Vosk *et al.*, 2015). However, numerical exact diagonalization studies on making a finite-size scaling analysis found it to violate the Harris-Chayes criterion that restricts the exponent to be $\nu \geq 2/d$ (Chandran *et al.*, 2015a; Chayes *et al.*, 1986; Harris, 1974; Khemani *et al.*, 2017), while numerical studies predominantly found values $\nu \sim 1$ (Kjäll *et al.*, 2014; Luitz *et al.*, 2015; Pal & Huse, 2010).

More recent phenomenological approaches (Dumitrescu *et al.*, 2019; Goremykina *et al.*, 2019; Morningstar & Huse, 2019; Morningstar *et al.*, 2020) that take into account the avalanche mechanism (De Roeck & Huveneers, 2017) as the leading scenario for the possible transition based on the growth of Griffith’s region and works by dividing the disordered spin chain into “thermalizing” and “MBL” regions of spins, where the ergodic regions can thermalize the nearby MBL regions provided that the relevant matrix elements are big enough compared to the level spacing of the block. These RG studies found a Berezinskii–Kosterlitz–Thouless (BKT) like transition with correlation length given as

$$\xi_{\text{BKT}} = \exp \left(\frac{b_{\pm}}{\sqrt{|W - W^*|}} \right) \quad (5.8)$$

where $b_{\pm}$ are non-universal constants that might be different on the two sides of the transition. A better finite-size scaling for $\bar{X}(W, L)$ was found with ξ_{BKT} in comparison to ξ_0 (Hopjan *et al.*, 2021; Laflorencie *et al.*, 2020; Šuntajs *et al.*, 2020a, 2020b).

These simple forms of correlation lengths run into a problem when considering the crossing point between two curves with different system sizes $\bar{X}(L_1, W), \bar{X}(L_2, W)$, the crossing point W_c defined as


 FIGURE 5.3: An outline of ARTICLE IV as taken and modified from (Aramthottil *et al.*, 2024).

when $\bar{X}(L_1, W_c) = \bar{X}(L_2, W_c)$ for $L_1 \neq L_2$ corresponds with the critical disorder strength $W^* = W_c$ as evident from (5.6) (Sierant *et al.*, 2024). However, W_c increases with increasing L for values of L amenable to numerics, as already seen in (Oganesyan & Huse, 2007) but was not given much importance as it was found to slow down with increasing system size. This motivated unbiased finite-size scaling studies with L dependent functional forms for critical disorder strengths $W^*(L)$, which surprisingly found the critical disorder strength to increase linearly with system size $W^*(L) \propto \alpha L$, and a correlation function of the BKT-like form to best approximates $\bar{X}(W, L)$ (Šuntajs *et al.*, 2020a, 2020b). A simple extrapolation of this result implies that the MBL regime does not exist in the thermodynamic limit. At the same time, it is also possible that such scaling slows down in higher system sizes and is consistent with an MBL phase in the thermodynamic limit; at the least, it takes into question the existence of MBL from previous finite-size numerics.

Similar ambiguous results are seen from the time evolution of autocorrelation functions, defined as $C(t) = \sum_i \langle s_j^z(t) s_j^z \rangle$ where the average is taken over Fock states and disorder realizations, the autocorrelation values seem to decay in a power-law fashion $C(t) \propto t^{-\beta}$ upto the thouless time (found to grow exponentially with system size from exact diagonalization studies) with increasing disorder strength the exponent β seems to be decreasing exponentially $\beta \propto e^{-cW}$ as collated from (Chanda *et al.*, 2020b; Doggen *et al.*, 2018; Luitz *et al.*, 2017; Sierant & Zakrzewski, 2022) in (Sierant *et al.*, 2024). If the algebraic decay does not slow down at higher system sizes for longer times, we will find $C(t) \rightarrow 0$, and thus the system thermalizes in the thermodynamic limit. Other quantities like entanglement entropy growth also show unresolved critical disorder strengths as with disorder strength around W_c , entanglement entropy increases as a power-law with a small exponent that increases with system size rather than as logarithmic on time (Chanda *et al.*, 2020a; Evers *et al.*, 2023), in addition, if one resolves the entanglement entropy to a number entropy part, that captures the entropy of a subsystem over different particle number/magnetization sectors and thus is directly linked to transport, for Hamiltonians with a $U(1)$ symmetry and seems to show a consistent $\log(\log(t))$ growth (Ghosh, 2022; Kiefer-Emmanouilidis *et al.*, 2020).

5.4 ARTICLE III: “Finite-size scaling analysis of the many-body localization transition in quasiperiodic spin chains” (Aramthottil *et al.*, 2021)

In ARTICLE III (Aramthottil *et al.*, 2021), we consider the HSC^+ Hamiltonian (2.22), with a quasiperiodic disorder (QPD) where the on-site potentials h_l are given as

$$h_l = \frac{W}{2} \cos(2\pi kl + \phi) \quad (5.9)$$

here k is an incommensurability factor, which we take to be the inverse golden ratio $k = (\sqrt{5} - 1)/2$, and ϕ is a random phase taken from a uniform distribution $\phi \in [0, 2\pi)$ with each ϕ giving a “disorder

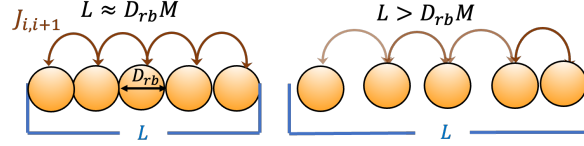


FIGURE 5.4: A sketch for disorder strength generated with decreasing density as caused by fluctuations in $J_{i,i+1}$ values. The strength of the curved arrows corresponds with the magnitude of $J_{i,i+1}$

realization” characterized by the disorder strength W . In practical optical lattice setups, such a model is extremely relevant as the disorder is added as an additional laser with ratios of laser wavelengths taken such that, there are no repetition for finite lattices. In this work, we focus on the finite-size scaling (**FSS**) analysis based on the cost-function mechanism as developed in (Šuntajs *et al.*, 2020a, 2020b) for H_{HSC}^+ -RD. We consider the two prominent functional forms for the correlation length ξ_0, ξ_{BKT} and assume size-dependent functional forms for the critical disorder strength, $W^*(L)$, and make unbiased FSS analysis going upto system sizes $L = 22$. We find that assuming no finite-size drifts the power-law functional form ξ_0 best approximates the correlation length with the critical exponent approaching unity $\nu = 0.87$ for $\mathcal{S}$; this is roughly consistent with the Harris-Luck criterion (Luck, 1993) for QPD systems ($\nu \geq 1/D$), while for $\bar{r}$ the critical exponent is substantially farther from unity $\nu = 0.54$. On assuming different functional forms for $W^*(L)$, we find that the best approximation is found with a BKT-like correlation length ξ_{BKT} and the parameters $b_- \neq b_+$ with the functional form for critical disorder strength $W^* = W_0 + W_1 \ln(L)$. We find that with an almost fixed value of (W_0, W_1, b_+) , there are a lot of b_- values that minimize the cost function. While, if we just make the FSS analysis on the localized regime we find the minimized quantities for $\bar{r}$ $(W_0, W_1, b_+) \rightarrow (-5.59, 2.66, 1.61)$, while $\mathcal{S}$ has minimized values $(W_0, W_1, b_+) \rightarrow (-6.62, 2.78, 2.83)$. Taking a generic functional form $W^* = W^*(L)$, also shows consistent results with the logarithmic drift. The logarithmic drift gives disorder strengths corresponding to disorder strengths where $\bar{r}$ deviates from RMT values. On extrapolating the logarithmic functional form to $L = 50$, with $\bar{r}$, $W^*(50) \simeq 4.83$ while for $\mathcal{S}$, $W^*(50) \simeq 4.25$, values consistent with a time evolution study with $L = 50$ that predicts $W^* \simeq 4.8$ (Doggen & Mirlin, 2019). Interestingly, these values also where the imbalance showed phase oscillations for a wide interval of system sizes $L \in [12, 200]$ (Sierant & Zakrzewski, 2022).

5.5 Summary of ARTICLE IV: “Phenomenology of many-body localization in bond-disordered spin chains” (Aramthottil *et al.*, 2024)

In this work, we focus on a bond-disordered spin-1/2 XXZ chain relevant for a Rydberg array setup (Franz *et al.*, 2022a, 2022b; Signoles *et al.*, 2021)

$$H_{\text{BD}} = \sum_{i=1}^{M-1} J_{i,i+1} (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y + \Delta s_i^z s_{i+1}^z) \quad (5.10)$$

here, M is the number of spins; the couplings are fixed with a power-law $J_{i,i+1} = |x_i - x_{i+1}|^{-6}$ where x_i denotes the spin position within the length L , the parameter $\Delta = -0.73$ relevant for a Rydberg state of rubidium 87. Fixing the Rydberg blockade (Lukin *et al.*, 2001) diameter as D_{rb} , defines an excluded density $\rho = D_{rb}M/L$. With decreasing density, the spins can explore more possible configurations, increasing effective disorder strength, $W = 1/\rho - 1$. Typical studies on MBL consider the presence of on-site disorder; the phenomenological properties in the MBL regime can be described within the LIOM framework as described above. We try to extract the description of this system using an extension of the strong disorder renormalization group (Dasgupta & Ma, 1980; Fisher *et al.*, 1989) to excited states, referred to as the real space renormalization group for excited states (RSRG-X). The RSRG-X decimation scheme works by deconstructing the Hamiltonian into

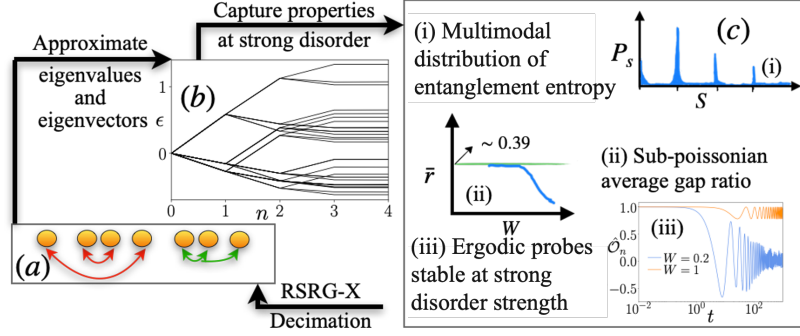


FIGURE 5.5: An outline of ARTICLE IV as taken and modified from (Aramthottil *et al.*, 2024).

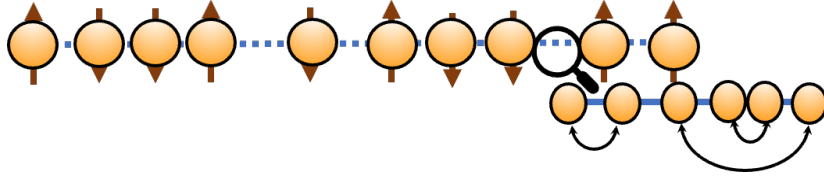


FIGURE 5.6: A sketch of the eigenstate.

a sum of local operators, finding the local operator with the largest energy gap, setting the spins associated with the local operator to an eigenstate of the local operator, and modifying the nearby operators. This decimation procedure is repeatedly followed. The energy gaps are progressively smaller and thus approximate the eigenstate at higher times, eventually approximating the entire eigenstate. The initial Hamiltonian is constructed out of two site operators which have eigenstates of the form $|Z_{+/-}\rangle \equiv |\uparrow\uparrow\rangle / |\downarrow\downarrow\rangle$, $|\pm\rangle \equiv (1/\sqrt{2})(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$. In cases where the spins are fixed with $|Z_{\pm}\rangle$ the effective nearby bonds are modified to have a chemical potential form with first-order perturbation theory, which can lead to a generation of a domain of spins while fixing an operator with the states $|\pm\rangle$ leads to the effective nearby bonds joined together to form a similar two site operator as the one that constructs the Hamiltonian with modified parameters which can lead to the formation of correlated spins at an arbitrary distance. The RSRG-X procedure hints at the structure of a generic eigenstate, which contains domains of spins and regions with arbitrarily long correlations made by the $|\pm\rangle$ states. One can immediately reason about a few peculiar properties of this system, such as a multimodal distribution in entanglement entropy, where each peak corresponds to the triplet/singlet state that can pass through the bond. A sub-Poisson value for $\bar{r}$ at strong disorder happens partially due to the clustering of eigenvalues and the presence of quasi-degeneracies captured by the RSRG-X procedure. In standard on-site disordered systems, one can use the average value of long-time spin site operators, s_i^z , as a probe for ergodicity breaking. In the strong disorder regime, they are expected to be exponentially close to the LIOM operator. In the bond-disordered XXZ model, though, there is a memory effect depending on the choice of state fixed in the decimation scheme, i.e., either leading to long-range correlation with $|\pm\rangle$ or domains of nearby spins with $|Z_{\pm}\rangle$ thus one cannot define a set of LIOM operators for the bond-disordered Hamiltonian. Instead, one can define a set of operators associated with each eigenstate. These operators are verified to act as ergodicity-breaking indicators, with the emergence of ergodicity as captured by $\bar{r}$ approaching the GOE value corresponding with the long-time averages of the ergodicity probes going to zero. Finally, we also hint at how this procedure can be generalized for generic systems based on the RSRG-X mechanism for obtaining phenomenological properties of non-paradigmatic models of MBL.

Chapter 6

Conclusion

This thesis attempted to make specific contributions to the three prominent non-ergodic phenomena hosted in isolated quantum many-body systems.

For the minimal example of ergodicity breaking, the quantum many-body-scarring phenomena. Motivated by initial perceptions of connections with essential ideas for non-equilibrium dynamics from lattice gauge theory like charge confinement, string breaking, and string inversion, (Banerjee *et al.*, 2012; Chanda *et al.*, 2020b; Surace *et al.*, 2020) we explore an LGT model that hosts a charge confined and a charge deconfined regime. With standard numerical tools, we found this model to host stable quantum many-body scar states in the charge deconfined regime. This result has to be contrasted with that of slow dynamics seen in the presence of charge confinement in a large number of models (for exhaustive references (Lerose *et al.*, 2020)); essentially, these systems have quasilocal dynamics and are more closely related to Hilbert space fragmentation (Yang *et al.*, 2020), unlike quantum many-body scar states which are quasi-particle states with translational invariance. The implications of our results are that there is a possibility of having “simple” non-equilibrium configurations that do not thermalize in the charge-deconfined phase for high energy physics where the charge-deconfined phases like the quark-gluon plasma is expected to thermalize requires further exploration.

In the case of dipolar bosons in an optical lattice where the dynamics are characterized by Hilbert space fragmentation with fragmentation arising with emergent conserved nearest-neighbor and further nearest terms (Li *et al.*, 2021), we explored the implications of density-dependent tunneling (Hirsch, 1994) term, which is of practical importance in ultracold atoms. The strong Hilbert space fragmentation for large dipolar strengths is modified to host a mobility edge with ergodicity increasing with increasing energy and a consistent residual amount of ergodic states independent of dipolar strength. In addition, we find for a relatively weak dipolar strength a regime where ergodicity is suppressed due to the quasicancellation of tunneling terms, leading to an exact decoupling of the Hamiltonian into an ergodic and non-ergodic sector. That leads to an interesting Gedanken experiment wherein, in the same setup, if one starts with a Fock state in the hard-core boson sector, the system thermalizes whereas, on starting with a Fock state with at least one site doubly site does not thermalize.

Next, we dealt with the paradigmatic model of systems that avoid thermalization, namely, the phenomenon of many-body localization in the presence of a disorder. We studied the many-body localization crossover for a quasiperiodic system, the relevant model for ultracold atoms in optical lattices (Lüschen *et al.*, 2017; Schreiber *et al.*, 2015). In making an unbiased finite-size scaling analysis, we found that a power-law correlation length with a fixed critical disorder strength characterized the critical behavior. However, assuming a drift for the critical disorder strength, we find that the correlation function is BKT-like, with the critical disorder strength showing a logarithmic drift. By extrapolating the logarithmic functional form to $L = 50$, the disorder strength values found are consistent stability of local operators with time evolution (Doggen & Mirlin, 2019); these values also correspond to where the imbalance showed phase oscillations for a wide interval of system sizes $L \in [12, 200]$ (Sierant & Zakrzewski, 2022). In contrast to the quasi-periodic disorder a random disorder, a BKT-like correlation function is found with a linear drift. Although both systems will become ergodic in the thermodynamic limit, the sublinear disorder strength in the quasiperiodic system might indicate a slowdown with higher system sizes.

Further, we look at a bond-disordered model implemented in Rydberg arrays that hosts a many-body localized regime with strong disorder. Using a real-space renormalization group scheme (Pekker *et al.*, 2014), we extract the eigenstate structure of this model in the presence of strong disorder. The scheme thus makes predictions for properties of the model, such as the multi-modal distribution of entanglement entropy and sub-Poissonian mean gap ratio, which are numerically verified. We also construct ergodicity probes for Rydberg atom experiments (Franz *et al.*, 2022a, 2022b; Signoles *et*

et al., 2021) using the scheme. Most importantly, we find that this model, unlike other cases of strong ergodicity breaking like integrable systems, strong Hilbert space fragmentation, or typical many-body localized systems with on-site disorder, is not characterized by a simple set of integrals of motion (Ilievski *et al.*, 2015; Łydźba *et al.*, 2024; Serbyn *et al.*, 2013a), opening up a new mechanism for ergodicity breaking and localization.

Chapter 7

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7.1 ARTICLE I

Scar states in deconfined $\mathbb{Z}_2$ lattice gauge theories

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The weak ergodicity breaking induced by quantum many-body scars (QMBSs) represents an intriguing concept that has received great attention in recent years due to its relation to unusual nonequilibrium behavior. Here, we reveal that this phenomenon can occur in a particular regime of a lattice gauge theory, where QMBSs emerge due to the presence of an extensive number of local constraints. In particular, by analyzing the gauged Kitaev model, we provide an example where QMBSs appear in a regime where charges are deconfined. By means of both numerical and analytical approaches, we find a variety of scarred states far away from the regime where the model is integrable. The presence of these states is revealed both by tracing them directly from the analytically reachable limit, as well as by quantum quenches showing persistent oscillations for specific initial states.

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Introduction. The thermalization properties of isolated quantum systems are currently under intensive investigation in different areas of modern quantum physics [1–4]. In this context, huge attention has been recently devoted towards the study of a large variety of Hamiltonians where the ergodicity is weakly broken [5–24]. In particular, in such models quenches from carefully designed initial states reveal persistent many-body revivals that apparently contradict ergodicity [5,25]. The reason for such an absence of thermalization turns out to be the presence of specific eigenstates called quantum many-body scars (QMBSs) characterized, in particular, by a subvolume entanglement law [6–14,21,24,26]. It is worth noting that similar regular states have been previously identified [27] for chaotic quantum billiards in relation to semiclassical periodic orbit quantization [28,29]. Moreover, the concept of scarred symmetry, closely related to QMBSs, has been introduced in studies of a hydrogen atom in a strong magnetic field [30].

With the advent of a new generation of cold-atom quantum simulators [31–35], the weak ergodicity breaking manifested by QMBSs has been experimentally detected in constrained spin [5] and bosonic [36] models. Crucially, both realizations can be viewed as lattice gauge theories (LGTs) where the energy constraints are induced by the Gauss law fixing the relation between gauge and charge variables. Motivated by the recent progress achieved in the last years in implementing LGTs in quantum simulators [37–42], an impressive theoretical effort has been devoted towards a better understanding

of simple gauge-invariant theories [17,18,43–57]. In this direction, the connection between Gauss law and QMBSs has recently gained attention both in $U(1)$ [16,58] and $\mathbb{Z}_2$ [13] LGTs. Here, indeed, the weak ergodicity breaking associated with the slow oscillatory dynamics can be interpreted as a *string inversion* phenomenon. Crucially, it has to be underlined that all LGTs, where QMBSs have been identified, are characterized by charge confinement. This regime implies that only particle-antiparticle bound states exist and therefore charges can be observed in composite structures only. These effective pairs, together with an emergent new symmetry, generate the slowdown of quantum dynamics and have been shown to be intricately connected to the presence of QMBSs [59].

Thus it seems natural to wonder whether confinement is a prerequisite to observe QMBSs in LGTs. In this Letter, we tackle this question by investigating the recently introduced gauged one-dimensional (1D) Kitaev model [16,60,61], whose ground state displays a confined phase as well as a regime where charges are not bounded in pairs, thus describing a deconfined phase. We study its low-entanglement states and show that QMBSs are present in the ergodic deconfined phase and are absent in the ergodic confined regime of the model. Importantly, we are able to continuously track QMBSs down from the analytic prediction valid in the quasi-integrable regime and therefore provide their partial classification.

Model and observables. The Hamiltonian of the p -wave superconducting Kitaev chain minimally coupled to a $\mathbb{Z}_2$ gauge

field introduced in Refs. [16,60,61] reads

$$H = -t \sum_j (c_j^\dagger - c_j) \sigma_{j+1/2}^z (c_{j+1}^\dagger + c_{j+1}) - \mu \sum_j \left(c_j^\dagger c_j - \frac{1}{2} \right) - h \sum_j \sigma_{j+1/2}^x. \quad (1)$$

Here, $c_j^\dagger$ (c_j) denotes the fermionic creation (annihilation) operator and t describes the tunneling and pair production/annihilation processes mediated by the $\mathbb{Z}_2$ gauge field $\sigma_{j+1/2}^z$ defined on the links between the nearest-neighbor sites. Fluctuations in the gauge field are induced by the electric field $\sigma_{j+1/2}^x$ of strength h and the number of fermions is fixed by the chemical potential μ . Here, $\sigma_{j+1/2}^i$ stands for standard Pauli matrices.

As required in LGTs, the model (1) is invariant under the local gauge transformation generated by the Gauss operator $G_j = \sigma_{j-1/2}^x (-1)^{n_j} \sigma_{j+1/2}^x$, where $[H, G_j] = 0$ and $[G_i, G_j] = 0$. Therefore, the physical states are those that satisfy the Gauss law, $G_j |\psi\rangle = \pm |\psi\rangle$, for all j sites [62].

The Hamiltonian (1) can be written in terms of gauge-invariant transformed Pauli operators:

$$X_{i+\frac{1}{2}} = \sigma_{i+\frac{1}{2}}^x, \quad (2)$$

$$Y_{i+\frac{1}{2}} = (c_i^\dagger - c_i) \sigma_{i+\frac{1}{2}}^y (c_{i+1}^\dagger + c_{i+1}), \quad (3)$$

$$Z_{i+\frac{1}{2}} = (c_i^\dagger - c_i) \sigma_{i+\frac{1}{2}}^z (c_{i+1}^\dagger + c_{i+1}). \quad (4)$$

Upon this transformation and with periodic boundary conditions, the gauged Kitaev model corresponds to the quantum Ising model with both transverse and longitudinal fields,

$$H = \sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1} - t X_i - h Z_i. \quad (5)$$

Notice that the model is now defined on a dual lattice, where the index i corresponds to the links of the original model (1).

For $\mu > 0$, the phase diagram of the model (5), as shown in Fig. 1, is characterized by the presence of both an anti-ferromagnetic (AFM) order and a paramagnetic (PM) phase depending on parameters t and h [63]. The AFM phase turns out to be of great interest, since it supports domain-wall excitations associated with the antiferromagnetic order caused by the spontaneous breaking of the $\mathbb{Z}_2$ Ising and translational symmetries. In 1D these last two features imply domain-wall deconfinement. Therefore, in the gauged Kitaev Hamiltonian, (1), such an AFM order corresponds to charge deconfinement (CD), where fermions are free to expand without any string tension. On the other hand, the PM regime corresponds to a phase characterized by charge confinement (CC), where fermions appear only as bound pairs.

In the limit $t \ll \mu$ it is possible to perform a Schrieffer-Wolff transformation (in agreement with Ref. [60]; for a higher-order expansion, see Ref. [64]), with

$$S = \frac{-it}{2\mu} \sum_j \left\{ \left(\frac{1+Z_{j-1}}{2} \right) Y_j \left(\frac{1+Z_{j+1}}{2} \right) - \left(\frac{1-Z_{j-1}}{2} \right) Y_j \left(\frac{1-Z_{j+1}}{2} \right) \right\}, \quad (6)$$

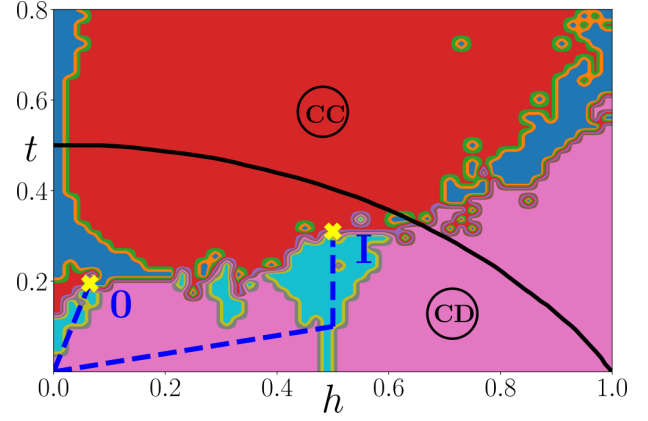


FIG. 1. Properties of the Ising model (5) in $t-h$ parameter space for $L = 16$ and $\mu = 1$. QMBs may exist in chaotic regions with a mean gap ratio $r > 0.5$ and low-entanglement entropy $S < 0.5$ with respect to the GOE value. The corresponding disconnected blue region lies entirely in the charge deconfined (CD) regime. The charge confinement (CC) region lies mainly within the regime of chaotic, $r > 0.5$, but with lowest entropy states, $S > 0.5$, thus with no chance for QMBs. The pink color marks the mixed dynamics regime, $r < 0.5$, $S < 0.5$; in the dark blue region, $r < 0.5$, $S > 0.5$. “0” and “I” denote paths along which QMBs states are followed using level dynamics.

to obtain an effective Hamiltonian $H_{\text{eff}} = e^S H e^{-S} = H + [S, H] + \mathcal{O}(t^2)$. Notice that S is chosen in such a way that the new terms commute with the unperturbed part of the Hamiltonian $\sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1}$ to the leading order in the expansion, thus preserving its block-diagonal structure while also including all virtual processes within each sector. The derived effective Hamiltonian,

$$H_{\text{eff}} = \sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1} - h Z_i - \frac{t}{2} (X_i - Z_{i-1} X_i Z_{i+1}), \quad (7)$$

turns out to be the well-known model discussed in detail in Ref. [13], where two towers of QMBs have been identified. The latter are of the form

$$|S_n^k\rangle = \frac{1}{n! \sqrt{\mathcal{N}(L, n)}} [(\mathcal{Q}^k)^\dagger]^n |\Omega^k\rangle, \quad (8)$$

with $k = 1, 2$, $|\Omega^1\rangle = |0 \cdots 0\rangle$, $|\Omega^2\rangle = |1 \cdots 1\rangle$, and $(\mathcal{Q}^k)^\dagger = \sum_{i=i_1}^L (-1)^i P_{i-1}^k [X_i + (-1)^k Y_i] P_{i+1}^k$, with projection operators $P_i^k = [1 + (-1)^k Z_i]/2$. Such QMBs describe n -magnon and n -antimagnons excitations for $k = 1$ and $k = 2$, respectively [13].

As already pointed out, the Schrieffer-Wolff transformation described above links the models (5) and (1) with the effective spin model (7) only for $t \ll \mu$. In this limit, the states given by Eq. (8) become true QMBs of Hamiltonian (7), as it was studied in Ref. [13]. It appears natural to wonder whether, following the states (8) in the parameter space, it is possible to also find scarred states in the gauged Kitaev chain beyond the $t \ll \mu$ limit.

Level dynamics. In order to investigate this point, we first determine in which regime of parameters the model (5) can be considered as ergodic, and thus where the regular states may

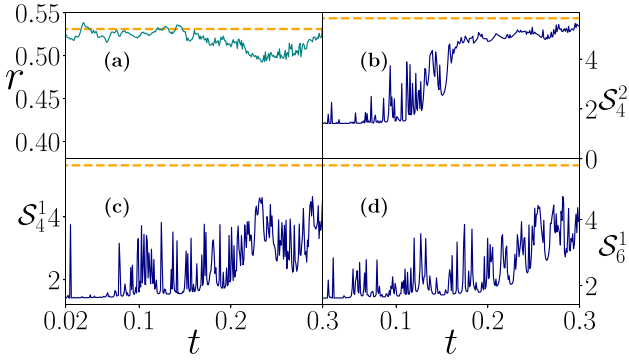


FIG. 2. (a) The gap ratio r and (b) half-chain entanglement entropy (S) along path 0 for the S_4^2 state from the antimagnon family; (c) S_4^1 and (d) S_6^1 from the magnon family, all for $L = 18$. States may be followed despite narrow avoided crossings indicated by spikes of the entanglement entropy. The antimagnon state loses its low EE feature around $t = 0.14$ while magnonlike QMBs may be followed up to $t \approx 0.2$.

be called QMBs. Ergodicity may be revealed by the adjacent mean gap ratio r [65] between subsequent level spacings Δ_i ,

$$r_i = \frac{\min\{\Delta_i, \Delta_{i+1}\}}{\max\{\Delta_i, \Delta_{i+1}\}}, \quad (9)$$

where $r \simeq 0.531$ corresponds to the fully ergodic regime [as described by the Gaussian orthogonal ensemble (GOE) [66]] and $r \simeq 0.386$ indicates the quasi-integrable regime [65,67]. As shown in Fig. 1, our model shows strong indications of near-integrable behavior for $h \ll \mu$ or $t \ll \mu$. Outside this region, the model is expected to be nonintegrable. The next step is then to identify the region where the entanglement entropy (EE) of some eigenstates is well below the GOE estimate, as QMBs should have low, subvolume entropy. The half-chain EE is defined in a standard way as $S = -\text{Tr}[\rho_{L/2} \ln \rho_{L/2}]$ [68]. We compare it to the typical GOE value for a given system size. Once the two lowest EE states have a relative EE sufficiently low (say half of the GOE value), there is the chance that those states are indeed scarred. Figure 1 shows by a light blue color the domains where both $r > 0.5$ and states with a sufficiently low EE exist.

With the suspected regions identified, we start the analysis with $|S_n^k(t, h)\rangle$ states for the Hamiltonian (5) with parameters $t, h \ll \mu$, e.g., for $t_0 = h_0 = 0.001$ (we set $\mu = 1$ in the following), with the aim of tracking such initial states $|S_n^k(t_0, h_0)\rangle$ following their possible deformations induced by making small changes in the parameters, $t = t_0 + \delta t$ and $h = h_0 + \delta h$. As examples we consider paths indicated by “0” and “I” in Fig. 1.

Every time we update the parameters, we diagonalize the Hamiltonian in the symmetry sector with momentum $p = 0$ and parity $+1$ (we consider n even only) and find the new candidate $|E_n(t, h)\rangle$ by maximizing the overlap $O = |\langle E_n(t, h) | S_n^k(t_0, h_0) \rangle|$. For an isolated level, the new state is accepted, $|S_n^k\rangle$ is updated, and we repeat the procedure. Special care is taken to diabatically cross narrow avoided crossings [68].

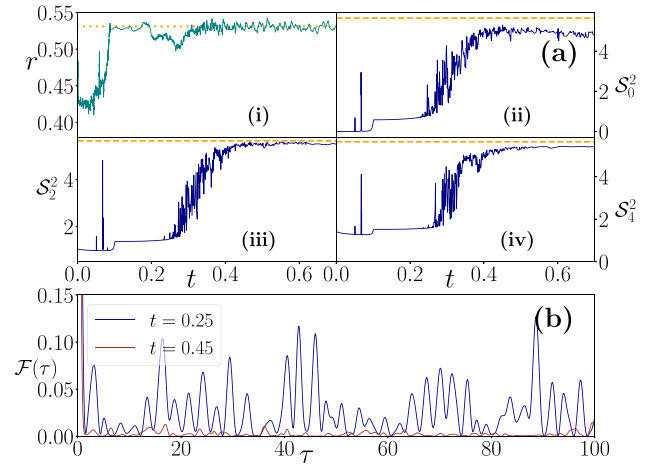


FIG. 3. (a) is as Fig. 2 but for path I and $L = 18$. Along this path only antimagnon excitations may be followed while magnons appear at the edges of the energy spectrum only. (b) Time dependence of the fidelity relative to an initial state $|\psi(0)\rangle$ and evolved with (5) at $h = 0.5$ and different values of t for $L = 16$ ($\mu = 1$).

Figure 2 shows tracking the QMBs states identified as $|S_n^k(t, h)\rangle$ along path 0. Both magnon and antimagnon excitations, as given by (8), may be followed. This path lies almost fully in the chaotic regime as revealed by r statistics, so the observed low EE states may be truly considered as QMBs, observed, let us stress, deep in the deconfined region.

The path indicated as I also remains in the deconfined phase, extending to large values of h (cf. Fig. 1). Levels are followed through a regular, weakly perturbed region, along the straight line $t = 0.2h$ up to $h = 0.5$. Then path I turns upwards, staying in the chaotic region up to the point $(t, h) = (0.3, 0.5)$. Along this vertical part, the tracked low EE states, shown in Fig. 3(a), are truly the QMBs embedded in the chaotic spectrum. As seen from the EE values, the scarred character of the followed states is slowly lost due to, as verified [68], various avoided crossings.

As discussed in the Introduction, the presence of QMBs can be further revealed by the persistent time oscillations of an out-of-equilibrium configuration. To reveal this aspect, we prepare an initial state given by the equal superposition of two states of the form (8) for small t, h values, $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|S_0^2\rangle + |S_2^2\rangle)$. After this initialization, we let this state evolve with Hamiltonian (5) and we calculate the fidelity $\mathcal{F}(\tau) = |\langle \psi(0) | \psi(\tau) \rangle|^2$, where τ is the time (in units of inverse μ). At $t = 0.25$, we observe for other choices of finite persistent oscillations of $\mathcal{F}(\tau)$ as expected for QMBs states, and this behavior persists until the end of path I [compare Fig. 3(b)]. Beyond this limit ($t > 0.3$), low-entanglement states disappear and $\mathcal{F}(\tau)$ shows irregular oscillations around the mean value of about $1/L^2$, as expected for thermal states.

Figure 4 visualizes the presence of QMBs by showing the value of S for all eigenstates at $t = 0.2$ and $h = 0.5$, where the system is in the weak ergodic regime. The entropy still reveals a fingerlike structure that indicates the existence of hidden, unidentified symmetries. The states enclosed in circles are those tracked up from the near-integrable limit. The

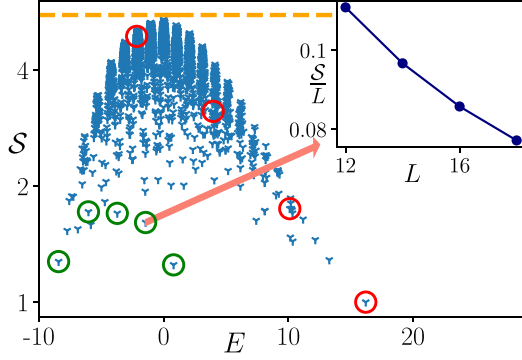


FIG. 4. The half-chain entanglement entropy (S) of all the eigenstates at $t = 0.2$, $h = 0.5$ for $L = 16$. The orange dashed line gives the S_{RMT} value. Circles denote different QMBs obtained via our tracking procedure. Green circles denote the antimagnonlike family S_n^2 for $n = 0, 2, 4, 6, 8$ while red circles the magnonlike states S_n^1 with $n = 0, \dots, 6$ counting from the right-hand side. Inset: The half-chain entanglement entropy divided by system size ($\frac{S}{L}$) for the S_2^2 state showing its subvolume property as expected for QMBs.

members of the antimagnonlike family S_k^2 , denoted by green circles, have very low-entanglement entropies as compared to other states of similar energy. They are thus truly QMBs. The inset reveals a subvolume scaling of the entanglement entropy of the S_2^2 state. The magnon excitations, on the other hand, dissolve among other states (in the high density of states region).

In summary, motivated by recent predictions of finding QMB states in a confined regime [59,69] of LGTs, we investigated the thermalization properties of the gauged Kitaev chain. We observe that deep in the confined phase even states with the smallest entanglement entropy have relatively large, volume-law values indicating a lack of QMBs. On the other hand, for relatively large values of the electric field, some states reveal low-entanglement entropy. We can identify these states by following them from the very small t, h values for which analytic predictions are available [13]. Such states result to be true QMBs and are found uniquely in the deconfined phase, which turns out to be a weakly ergodic regime characterized by the GOE-like mean gap ratio. The

presence of QMBs has been further verified by studying their time dynamics. By building an initial state given by the superposition of two QMBs, the fidelity of the state shows pronounced oscillations with no sign of thermalization. The adiabatic following of the states breaks down at the end points of our chosen paths due to energy-level mixing, where interestingly QMBs also disappear. In conclusion, our results unambiguously reveal that QMBs occur even in deconfined regimes of LGTs, thus paving the way toward a deeper understanding of the connection between the lack of thermalization and local symmetries.

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Supplementary material to “Scar States in Deconfined $\mathbb{Z}_2$ Lattice Gauge Theories”

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ENTANGLEMENT ENTROPY

We use the half-chain entanglement entropy, $\mathcal{S}$, as a useful measure of eigenstates properties. The half-chain entanglement entropy is defined as the von Neumann entropy of the reduced density matrix $\rho_{L/2}$

$$\mathcal{S} = -\text{Tr}[\rho_{L/2} \ln \rho_{L/2}]. \quad (\text{S.1})$$

where $\rho_{L/2} = \text{Tr}_{1,\dots,L/2} |\psi\rangle\langle\psi|$ is obtained by tracing out half of the system for eigenstate $|\psi\rangle$. The typical state in the ergodic regime obeys RMT prediction given by $\mathcal{S}_{RMT} = (L/2) \ln(2) + (1/2 + \ln(1/2))/2 - 1/2$ [1–3]. A substantial difference from $\mathcal{S}_{RMT}$ for states in the middle of the spectrum can be taken as a signature of nonergodic states, although to really observe a sub-volume property of the entanglement entropy for a given state one has to study the entropy dependence on the system size (see the inset in Fig. 4 in the main text).

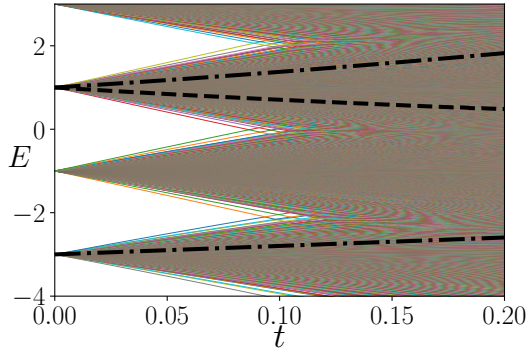


FIG. S1. The energy levels along the path “0”. The regularly spaced multiply degenerate levels at $h = t = 0$ split when parameters increase along $t = 3h$ line. The dashed line as well as two dash-dotted lines denote the position of antimagnon and two magnon excitations whose entanglement entropy is presented in Fig. 2 of the main text. As seen all three states lie in the middle, high density of states, regime of the spectrum.

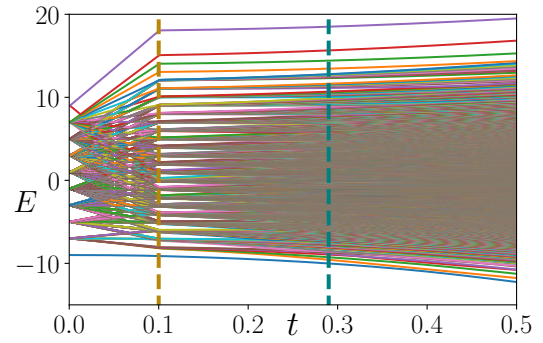


FIG. S2. The energy levels along the path-I. The regularly spaced levels split following the line $t = 0.2h$ up to $t = 0.1$. From there h remains constant, $h = 0.5$ while t increases up to $t \approx 0.3$ which is the point where all the high density states have high entanglement entropy($\mathcal{S}$).

Breaking of Adiabaticity on path ‘I’ example

The initial state $|S_n^k(t_0, h_0)\rangle$ is identified from the mapping between the Hamiltonian of quantum Ising chain in both transverse and longitudinal fields (5) and the effective Hamiltonian (7) at $t_0, h_0 = 0.001$. The Hamiltonian, H , (5) is then diagonalized with the `smaeq:kitll` parameter change of $\delta h = 0.001$ and $\delta t = 0.0002$ and a state $|E_n(t, h)\rangle$ is identified as the state which has a maximum overlap with $|S_n^k(t_0, h_0)\rangle$ among all the eigenstates of $H(t_0 + \delta t, h_0 + \delta t)$.

Figure S3 shows the exemplary overlaps along path I.

To adiabatically follow the suspected QMBS state $|S_n^k(t, h)\rangle$ is updated along the paths. But this is only done so, if for the next 10 diagonalizations (for a parameter change of $\Delta h = 0.01$ and $\Delta t = 0.002$) the eigenindex of the state $|E_n(t + \Delta t, h + \Delta h)\rangle$ does not change from its value at $|E_n(t, h)\rangle$. This procedure allows us to overcome problems encountered while passing the avoided crossings (see also below). The following protocol is continued until the final value of h along a given path is reached.

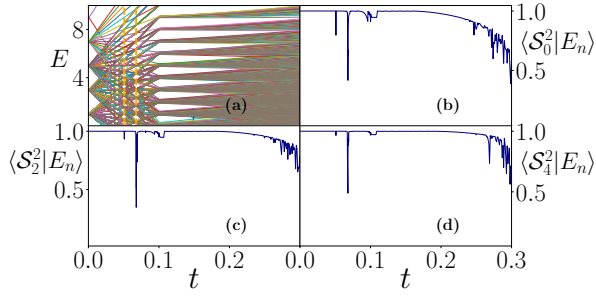


FIG. S3. The overlaps along the path I of three antimagnon states. The sharp overlap drops at the beginning of the path, in almost integrable regions is due to multiple avoided crossings indicated by vertical dashed lines in the level diagram (top, left)

Later we continue updating t only with $\delta t = 0.001$ while keeping h constant.

This procedure runs into difficulties when avoided crossings are met. In the regime corresponding to mixed regular and chaotic dynamics (as revealed statistically by the gap ratio, r , being between Poissonian and GOE values) the avoided crossings are isolated. Such avoided crossings may be crossed diabatically with care. Once we reach the irregular regime multiple avoided crossings typically arise and only those states can be traced that are almost decoupled in the process of changing the parameters. Such a situation is well known from chaotic, single particle, strongly scarred systems such as quantum billiards or hydrogen atom in a strong magnetic field (see e.g. [4]). While in generalized time reversal invariant systems small avoided crossings are highly probable [5, 6] overlapping avoided crossings dissolve the scar character of the state unless a periodic orbit [7] or symmetry [8] reinforces this character after the crossing. While this intuition is based on a single particle systems, we expect the similar qualitative behavior for the possible preservation of QMBS.

Figure S1 presents the level dynamics along the path “0”, i.e $t = 3h$ line. eq:kit Fig. S2 shows the level dynamics for PATH I. At $t \in [0.0, 0.1]$ the r value is nearly Poissonian and all the identified QMBS states can be tracked. In fact, a simple structure of the tilted transverse Ising Hamiltonian (5) reproduced here for clarity

$$H = \sum_{i=1}^L \frac{\mu}{2} Z_i Z_{i+1} - t X_i - h Z_i. \quad (\text{S.2})$$

identifies that for $t, h \ll 1$ the states are ordered by number of dimers as given by the operator $D = \sum_{i=1}^L Z_i Z_{i+1}$. Once $h > 0$ those states form a manifold split by $\sum Z_i$ operator eigenvalues. Only at the crossings of the manifolds the term $t \sum_i X_i$ mixes eigenstates of Z_i leading to nontrivial avoided crossings, compare Fig. S4. It is at these avoided crossings that sharp spikes visible in the

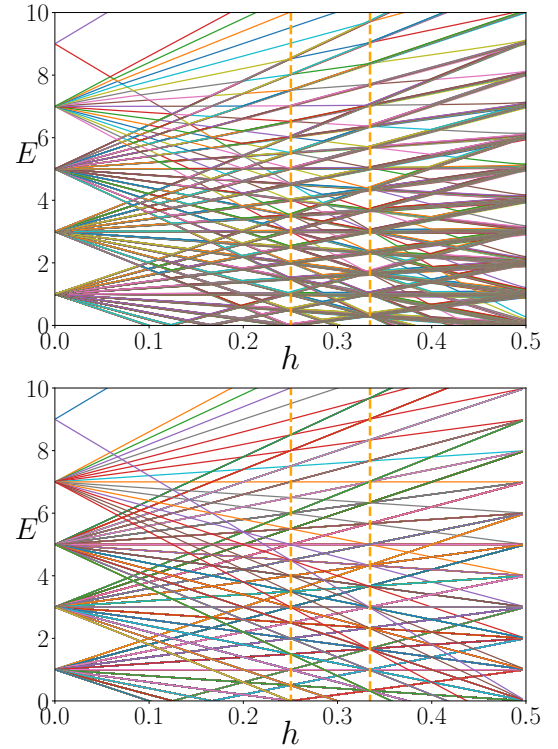


FIG. S4. An enlarged image of Fig. S2 – top – restricted to the parameters where the peaks in entanglement entropy of the followed state and in r value for the spectrum appear - compare Fig. 3(a) of the main text. Note that the range of h corresponds via $t = 0.2h$ relation defining path I to $t \in [0, 0.1]$. The orange dashed lines represents the location of t values for the peaks. The bottom plot shows the integrable system states energies obtained by putting $t = 0$ in the Hamiltonian, (S.2).

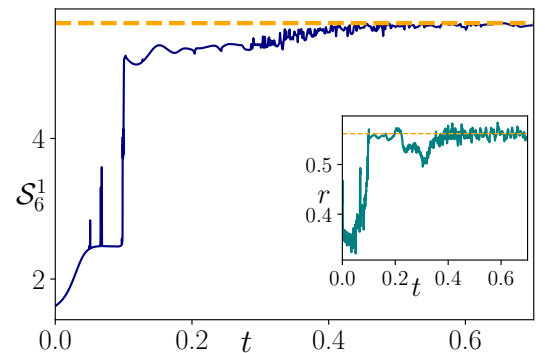


FIG. S5. Attempt to follow the magnon type state $\mathcal{S}_6^1$ along path I. Once gap ratio reaches values close to GOE limit the entropy of the followed state rapidly and significantly increases indicating that the scarred character is lost.

entropy t scans along the path I appear. Here also the mean gap ratio shows the unusual peaks.

For larger $t \in [0.1, 0.3]$ the r value is GOE-like indicating an ergodic character, in this region only the QMBS states built out of antimagnons are sustained indicating these states to be characteristically different from the other states. At $t > 0.3$ the levels become strongly mixed and the Hilbert space splitting into characteristic bands disappears. Then all the tracked states lose their QMBS characteristics.

Magnon States

The scar states built out of magnon states which were located at the middle of the spectrum (in the region of a high density of states) tracked along path I were lost on entering the ergodic regime. This is in contrary to path “0” when both magnon and antimagnon excitations could be followed. For the path I, only antimagnon states may be followed and linked to QMBS in the ergodic regime. The example of our attempt to track a magnon state

along path I is summarized in Fig. S5.

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7.2 ARTICLE II

Role of interaction-induced tunneling in the dynamics of polar lattice bosons

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Intersite dipolar interactions induce, even in absence of disorder, an intriguing nonergodic dynamics for dipolar bosons in an optical lattice. We show that the inherent dipole-induced density-dependent tunneling, typically neglected, plays a crucial role in this dynamics. For shallow-enough lattices, the delocalization stemming from the interaction-induced hopping overcomes the localization induced by intersite interactions. As a result, in stark contrast to the more studied case of hard-core bosons, delocalization is counterintuitively strengthened when the dipolar strength increases. Furthermore, the quasicancellation between bare and interaction-induced tunneling may lead, near a lattice-depth-dependent value of the dipole strength, to an exact decoupling of the Hilbert space between ergodic hard-core states and strongly nonergodic soft-core ones. Our results show that interaction-induced hopping should play a crucial role in future experiments on the dynamics of polar lattice gases.

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I. INTRODUCTION

Many-body localization (MBL) has attracted in recent years a major attention as a paradigmatic manifestation of nonergodic dynamics in the presence of disorder [1–3]. While the very existence of MBL in the thermodynamic limit remains a controversial and extensively discussed topic [4–14], experimental signatures of nonergodic dynamics in finite systems on a timescale of several hundreds of tunneling times have been clearly observed [15–20]. Recent years have brought also a number of examples of nonergodic dynamics in disorder-free systems, ranging from implementations of lattice gauge theories [21–23], to tilted lattices and smooth potentials [24–29]. A prominent example, related to an approximate global constraint and an appropriate choice of the initial state, is given by the so-called quantum scars [22,30–32]. Approximate global constraints result often in Hilbert-space fragmentation [33].

A particularly interesting example of Hilbert-space fragmentation and disorder-free nonergodic dynamics is provided by polar gases in optical lattices [34]. A sufficiently large dipole strength results in an emerging dynamical constraint given by the approximate conservation of the number of pairs of nearest-neighbor (NN) particles. This, combined with the eventual conservation of the number of next-to-NN pairs, results in Hilbert space shattering [34] and strongly nonergodic dynamics in hard-core systems. In those systems, on-site interactions are assumed large-enough to prevent more than one particle per lattice site.

In this work we show that the dynamics of soft-core dipolar bosons, with possibly multiply occupied sites, may be drastically different than their hard-core counterparts. This marked

difference results from the crucial role played by interaction-induced density-dependent tunneling (DDT). Although DDT may be generally relevant in Hubbard models with strong-enough on-site interactions [35,36], it is particularly relevant in polar lattice gases due to the long-range dipole-dipole interactions, as shown by recent studies of their ground-state properties [37–40]. Our results show that due to DDT, a growing dipole strength results in enhanced particle delocalization, in a stark contrast to the hard-core case. Moreover, DDT induces, for a particular, lattice-depth-dependent dipolar strength, a quasicancellation between kinetic tunneling and DDT leading to a peculiar exact decoupling of the Hilbert space into ergodic and strongly nonergodic states.

The structure of the paper is as follows. Section II introduces the lattice model under consideration. Section III is devoted to the spectral properties of soft-core bosons. Section IV discusses how the effect of DDT on the spectral properties translates into a markedly modified particle dynamics. In Sec. V we study the case in which the bare hopping and the DDT quasicancel. Finally, in Sec. VI, we summarize our conclusions.

II. MODEL

We consider externally oriented dipolar bosons in a deep one-dimensional (1D) optical lattice. The system is well described by the extended Bose-Hubbard (EBH) model:

$$\hat{\mathcal{H}}_{EBH} = -t \sum_{j=1}^{L-1} (\hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.c.}) + \frac{U}{2} \sum_{j=1}^L \hat{n}_j (\hat{n}_j - 1)$$

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$$\begin{aligned}
& + \frac{V}{2} \sum_{i \neq j} \frac{1}{|i-j|^3} \hat{n}_i \hat{n}_j \\
& - T \sum_{j=1}^{L-1} [\hat{a}_j^\dagger (\hat{n}_j + \hat{n}_{j+1}) \hat{a}_{j+1} + \text{H.c.}], \quad (1)
\end{aligned}$$

where $a_j^\dagger$ (a_j) denotes the bosonic creation (annihilation) operator, and t is the bare tunneling amplitude. The first line of Eq. (1) is the standard Bose-Hubbard model, in which the on-site interaction strength U results from both contactlike and dipole-dipole interactions. We fix $U/t = 3$ below. The second line describes the intersite dipolar interactions characterized by the dipolar strength V , which may be tuned by changing the dipole orientation with respect to the lattice axis. We note in passing that keeping U fixed while changing V requires tuning the contact interaction, via, e.g., a Feshbach resonance. We assume a strong confinement transversal to the lattice axis, since otherwise the $1/r^3$ decay of the dipolar interaction should be generally modified [41,42].

The last line in Eq. (1) corresponds to the DDT, with amplitude T , which, interestingly, is negative. For a given lattice depth V_0 (which we characterize below by $s = V_0/E_R$, with E_R the recoil energy), and employing the appropriate form of the on-site functions (see the Appendix A), one finds that, for the moderate value of U/t considered, T is linearly proportional to V over a broad range of V/t values (Fig. 1). Particularly relevant, as discussed below, is the case in which $T/t = -1$, which occurs for an s -dependent critical V/t .

We consider in the following a half-filled lattice, with $N = L/2$ bosons in L sites, with open boundary conditions. This choice facilitates the comparison with previous studies on hard-core bosons [34]. Since the maximal site occupation equals the total particle number, we are limited in our exact diagonalization analysis to system sizes up to $L = 16$ (which corresponds to a large Hilbert space dimension of 490 314 states). Although this precludes a reliable extrapolation to the thermodynamic limit, it provides already a clear qualitative picture, and it is quantitatively relevant for site-resolved experiments on ultracold gases in optical lattices, also typically limited to a small number of sites [19,20].

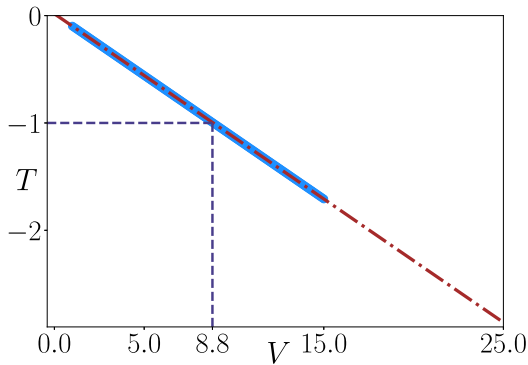


FIG. 1. Relation between the DDT rate T and V for $U/t = 3$ and $s = 8$. The dash-dotted line shows the almost perfect correspondence with a linear function. The dashed lines emphasize that $T/t = -1$ at $V/t = 8.8$.

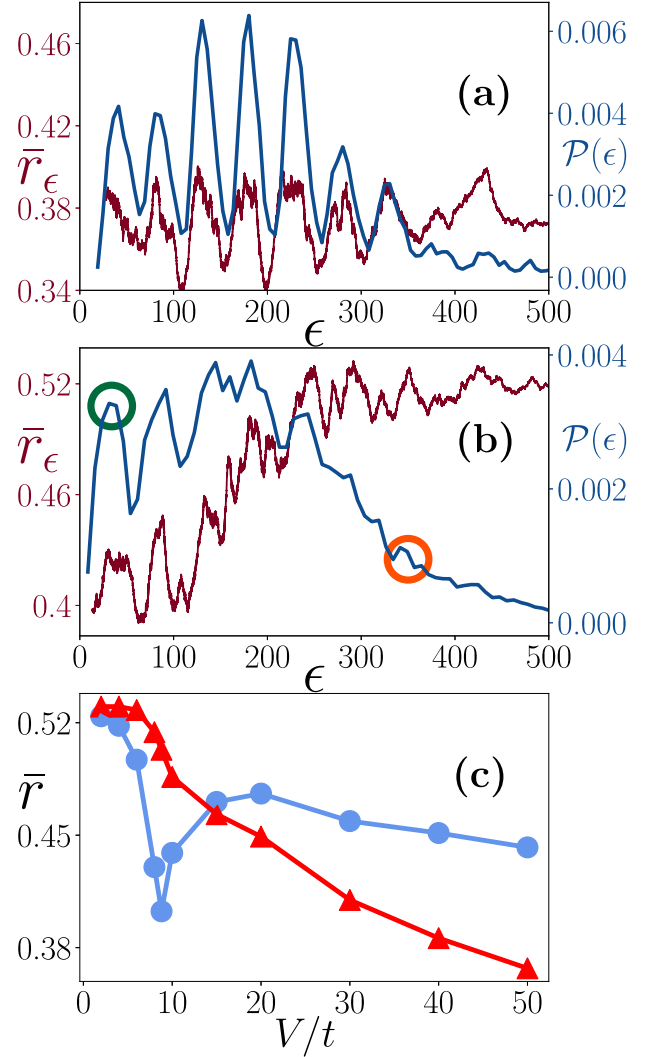


FIG. 2. Energy dependence of the DoS, $\mathcal{P}(\epsilon)$, and the gap ratio, $\bar{r}_\epsilon$, for $T = 0$ (a) and in the presence of DDT (b) for $L = 16$ with $V/t = 50$. The circles indicate the initial states employed in Fig. 4(b). (c) The mean gap ratio, $\bar{r}$, for $s = 8$ and $L = 14$ as a function of V/t with (circles) and without (triangles) DDT.

III. SPECTRAL PROPERTIES

In this section, we discuss how DDT radically modifies the spectral properties of soft-core polar lattice gases.

A. Density of states

Hard-core dipolar bosons undergo Hilbert-space shattering for large-enough V/t due to the emergent constraint induced by the approximate conservation of the number of NN and next-to-NN pairs [34]. A similar behavior is shared by soft-core bosons in the absence of DDT. Figure 2(a) shows the density of states (DoS), $\mathcal{P}(\epsilon)$, for $L = 16$ with $V/t = 50$ and $s = 8$. The DoS presents pronounced peaks corresponding to different number of occupied NN links, $N_{NN} = \sum_{j=1}^{L-1} \langle n_j n_{j+1} \rangle$. In contrast, in the presence of DDT,

Hilbert-space fragmentation is largely washed out [Fig. 2(b)], even for large V/t , indicating the lack of conservation of N_{NN} .

B. Mean gap ratio

The DDT also strongly modifies the level-spacing statistics. This is best observed in the behavior of the gap ratio, defined as $r_n = \min(\delta_n, \delta_{n+1})$ where $\delta_n = E_n - E_{n-1}$ with $\{E_n\}$ being the ordered set of eigen-energies [43]. The mean gap ratio $\bar{r}$ is evaluated as the average value over the whole spectrum. In Fig. 2(c), we depict $\bar{r}$ for $L = 14$, $s = 8$ and different ratios V/t . Integrable systems, with Poissonian level statistics, are characterized by $\bar{r} \approx 0.386$, whereas for ergodic time-reversal invariant systems one expects $\bar{r} \approx 0.53$, corresponding to the Gaussian orthogonal ensemble (GOE) of random matrices. We observe the latter behavior only for low V/t . For increasing V/t , a general decrease of $\bar{r}$ is observed. Whereas for $T = 0$ the gap ratio reaches a Poissonian value for large V/t , signaling quasi-integrability, the presence of DDT results in a mixed dynamics, with the value of $\bar{r}$ lying in between Poissonian and GOE statistics. Note as well the pronounced sharp minimum at $V/t = 8.8$, which is related to the condition $T/t = -1$, discussed in detail in Sec. V.

C. Energy dependence of the gap ratio

The r_n values present a marked energy dependence, which plays a crucial role in the dynamics (see Sec. IV). In order to monitor this dependence, we introduce the scaled energy $\tilde{\epsilon} \in [0, 1]$, defined as $\tilde{\epsilon} = (\epsilon - \epsilon_{\min})/(\epsilon_{\max} - \epsilon_{\min})$, where $\epsilon_{\min}$ ($\epsilon_{\max}$) is the minimum (maximum) eigenenergy for a given V/t . We determine the gap ratio $\bar{r}_{\tilde{\epsilon}}$ as the rolling average of 4000 energy gaps in the scaled energy interval around a given $\tilde{\epsilon}$.

In the absence of DDT [see Fig. 3(a)], the whole spectrum is ergodic at low V/t . At $V/t \approx 10$, a strong energy dependence appears in the form of approximately ergodic fingers separated by approximately regular regions. This structure correlates with the modulation of the density of states [see Fig. 2(a)].

The situation is markedly different in the presence of DDT [see Figs. 2(b) and 3(b)]. High-lying eigenstates remain ergodic even for very large V/t ratios. Only low-lying states are significantly nonergodic, with a gap ratio close to the Poissonian value, since these states are characterized by a small number of NN links, reducing the effective role played by the DDT. At the largest V/t values, approximately one half of the states belongs to the ergodic sector, explaining the fact that $\bar{r}$ saturates around 0.45 [Fig. 2(c)]. This strongly suggests that the dynamics of polar lattice gases initially built from low-energy eigenstates must be markedly different from that of systems prepared in high-energy ones. Whereas the former should reveal localization features, the latter should present ergodic dynamics. Note as well, that the spectrum becomes to a large extent Poissonian at $V/t = 8.8$ (for $s = 8$), corresponding with the dip in $\bar{r}$ observed in Fig. 2(c).

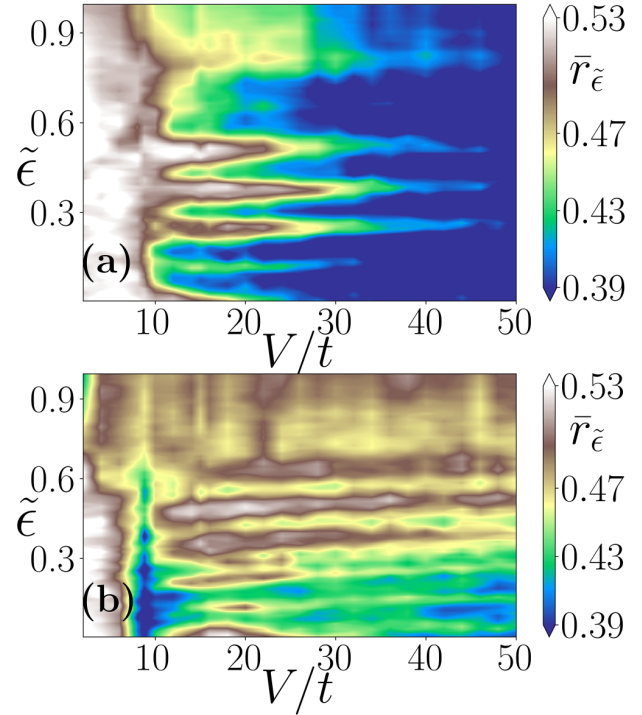


FIG. 3. Energy dependent gap ratio, $\bar{r}_{\tilde{\epsilon}}$, as a function of the dipolar interaction strength, V/t , and the scaled energy, $\tilde{\epsilon}$, for $L = 14$ sites and $s = 8$ with $T = 0$ (a) and with DDT (b).

IV. PARTICLE DYNAMICS

In this section, we show how the modified spectral properties translate into a radically altered dynamics in the presence of DDT.

A. Homogeneity

We consider the time evolution of the system when starting with an initial Fock state, $|\varphi\rangle$. In view of the expected energy-dependence of the dynamics, we choose carefully the initial state such that its energy lies at the center of an energy window with a large DoS, avoiding regions of low density of states occurring due to a possible Hilbert-space fragmentation. Whereas recent MBL experiments have employed an initial density wave [15,16], this is not a good choice for a polar lattice gas with large V/t , since it lies at the extremes of the spectrum. Instead, we consider a manifold of initial Fock states, with a given number of NN pairs, N_{NN} .

We are interested in how the initial inhomogeneous population in the lattice redistributes at time $\tau > 0$ amongst the sites, and in particular whether it becomes eventually homogeneous, washing out any information about the initial distribution. Density homogenization is best analyzed using the inhomogeneity parameter:

$$\mathcal{I}(\tau) = \frac{\sum_{i=1}^L [\langle \hat{n}_i(\tau) \rangle - \rho]^2}{\sum_{i=1}^L [\langle \hat{n}_i(0) \rangle - \rho]^2}, \quad (2)$$

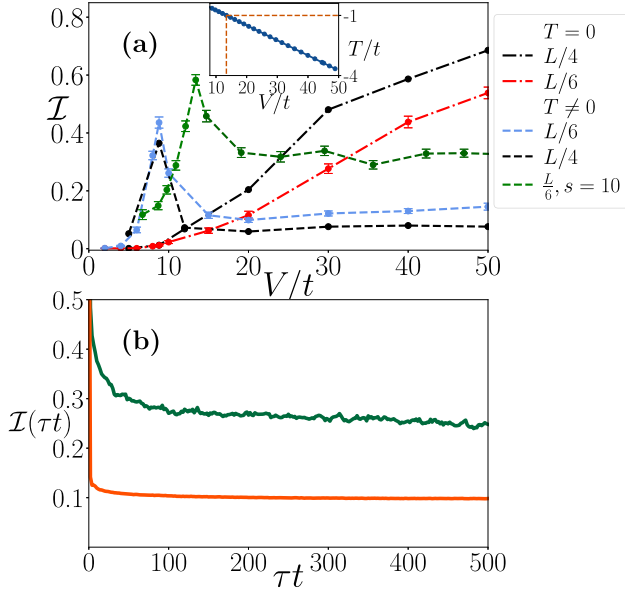


FIG. 4. (a) Inhomogeneity $\mathcal{I}(\tau_f = 500/t)$ as a function of V/t , for $L = 12$ and $s = 8$. The curves (see legend) depict different cases without ($T = 0$) and with DDT ($T \neq 0$), for initial states with $N_{NN} = L/6$ and $L/4$. We depict as well the case with $s = 10$ and $N_{NN} = L/6$. Observe that the peak of enhanced inhomogeneity is at $V/t = 8.8$ for $s = 8$ but at $V/t \approx 13$ for $s = 10$, corresponding to the different value of V/t at which $T/t = -1$ (see inset for the dependence of T/t on V/t for $s = 10$). Error bars indicate the result from the bootstrap estimate based on data for about 200 initial conditions in each sector. (b) Inhomogeneity $\mathcal{I}(\tau)$ for $L = 16$ with $V/t = 50$, for initial states with two different energies corresponding to the cases indicated by circles in Fig. 2(b).

with $\rho = N/L$ ($= 1/2$ in our case). Note that $0 < \mathcal{I} < 1$, with 0 (1) indicating a fully homogeneous (inhomogeneous) distribution.

Figure 4 shows $\mathcal{I}(\tau_f)$ for different V/t ratios, after an experimentally accessible time $\tau_f = 500/t$ [24]. We obtain $\mathcal{I}(\tau_f)$ after averaging over initial Fock states with $N_{NN} = L/4$, which is the most populated sector in the possibly fragmented Hilbert space [34]. In Fig. 4, we depict as well our results for $N_{NN} = L/6$ for comparative purposes. As for the case of hard-core bosons, in the absence of DDT, when V/t grows the inhomogeneity at a fixed time increases, indicating the strongly nonergodic character of the dynamics. In contrast, the presence of DDT results even for large V/t in a low (but non zero) inhomogeneity, reflecting the delocalizing role played by the DDT, in agreement with the markedly different spectral properties.

The above-mentioned energy dependence of the level statistics is reflected in the different dynamics observed for initial conditions belonging to different spectral regions. We illustrate this point in Fig. 4(b), where we depict the evolution of the inhomogeneity for $L = 16$ with $V/t = 50$, and two different initial conditions indicated in Fig. 2(b). For initial Fock states with $N_{NN} = 0$ (corresponding to low energies) $\mathcal{I}(t)$ remains very significant even at $\tau_f = 500$, the largest time considered. This is in agreement with the fact that the corresponding eigenstates present an approximately

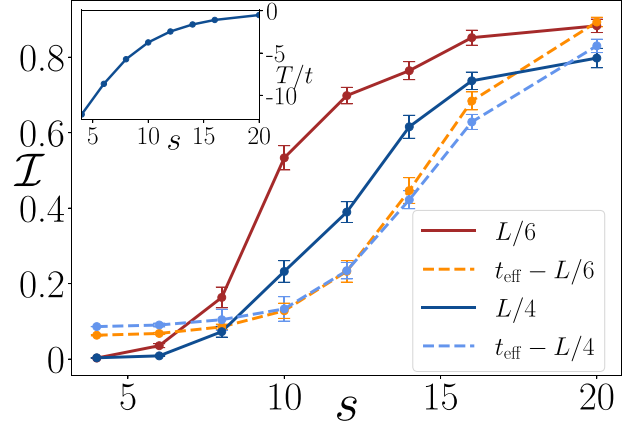


FIG. 5. Inhomogeneity $\mathcal{I}(\tau_f = 500/t)$ as a function of the lattice depth, s , for $L = 12$ with $V/t = 50$, for initial states with $N_{NN} = L/4$ (blue solid curve) and $N_{NN} = L/6$ (red solid curve). The dashed lines show the corresponding results in the mean field approximation when DDT is replaced by an effective hopping rate t_{eff} . The inset shows T/t as a function of s for the case under consideration.

Poissonian level statistics [Fig. 3(b)]. In contrast, the inhomogeneity reaches much lower values for initial states with $N_{NN} = L/4$, which lie at high energies, and are characterized by an approximately GOE level spacing [Fig. 3(b)]. Whether the nonzero saturation value of $\mathcal{I}$ is due to the small system size (resembling the behavior observed in the disordered XXZ model [14]) or to a not fully chaotic behavior cannot be determined with the system sizes studied here.

B. Dependence on the lattice depth

In the absence of DDT, the static and dynamic properties of the EBH model are given by the value of V/t and U/t , irrespective of the actual lattice depth s (which is just relevant for fixing the overall time scale $1/t$). The situation changes when considering the effect of the DDT. The value of T is an s -dependent function of V/t . For a fixed V/t ratio, T/t decreases when s increases, and hence the effect of DDT is reduced. The dynamics is hence markedly dependent on the lattice depth.

This dependence is illustrated in Fig. 5, where we plot as a function of s the inhomogeneity $\mathcal{I}(\tau_f = 500/t)$ for $L = 12$ with $V/t = 50$, and different initial sectors. For low-enough s , the DDT is relevant, and the system reaches homogeneity despite the large V/t value. In contrast, for deeper lattices, the delocalizing effect of the DDT becomes less relevant compared to the localizing role of intersite interactions. As a result, $\mathcal{I}(\tau_f)$ reaches large values indicating strongly nonergodic dynamics.

C. Mean-field analysis

A qualitative understanding of the effect of the DDT is provided by applying mean-field decoupling [39]:

$$-\hat{a}_i^\dagger[t + T(\hat{n}_i + \hat{n}_j)]\hat{a}_j \simeq -(t + 2\rho T)\hat{a}_i^\dagger\hat{a}_j. \quad (3)$$

Since in our case $\rho = 1/2$, DDT results in an effective mean-field hopping rate $t_{\text{eff}} = t + T$. It becomes evident that $T/t = -1$ is a special case, which we discuss in Sec. V. The dynamics is hence not regulated by the ratio V/t , as in the absence of DDT, but rather by $V/t_{\text{eff}} = \frac{V/t}{1+T/t}$. Since $T(V) = \alpha(s) + \beta(s)V$, with $\beta(s) < 0$, the ratio approaches $V/t_{\text{eff}} \simeq -\frac{1}{\beta(s)}$ for a sufficiently large V/t . Hence, increasing the dipolar strength does not result (as in the absence of DDT) in a diverging ratio between inter-site interactions and hopping, which leads necessarily to localization, but rather in a saturated ratio, $|V/t_{\text{eff}}|_{\text{max}}$. This maximal ratio depends on the lattice depth, increasing with growing s . This explains two relevant qualitative features in Figs. 4 and 5: The independence of $\mathcal{I}$ of V/t for large-enough V/t , and the very low inhomogeneity observed even for low s . The latter results from the low value of $|V/t_{\text{eff}}|_{\text{max}}$.

In Fig. 5 we compare our results using the full EBH in Eq. (1) with those obtained in the mean-field-inspired model in which the DDT is replaced by modifying the kinetic tunneling t into t_{eff} . As expected, the effective mean-field model reproduces well the qualitative features, although there are marked quantitative differences due to the significant density fluctuations in the system.

V. CRITICAL DIPOLE STRENGTH

Interestingly, in contrast to what happens for large V/t , the presence of DDT may result in a strongly non-ergodic dynamics for relatively modest values of V/t , for which the model without DDT would predict ergodicity. As already hinted in previous sections this occurs when $T/t \simeq -1$, for which the bare hopping and the DDT quasicancel each other [40]. This is reflected in the marked minimum observed in the average gap ratio $\bar{r}$ in Fig. 2 and the corresponding maximum in the inhomogeneity in Fig. 4.

For $T/t = -1$, the hard-core Hilbert subspace, with maximally one particle per site, exactly decouples from those states with at least one site with double or higher occupation. These two subspaces present markedly different spectral properties. Whereas the hard-core boson subspace presents GOE-like statistics ($\bar{r} \approx 0.527$), matching the behavior observed in Ref. [34], the rest of the Hilbert space (the soft-core subspace) shows an approximately Poissonian statistics ($\bar{r} \approx 0.4$) as the states in this subspace are strongly affected by the destructive interplay between kinetic and interaction-induced tunneling occurring for $T/t = -1$. This behavior is, as other properties, energy dependent.

A. Eigenstate properties

Let us consider first the eigenstate properties in both the hard- and soft-core sectors for $T/t = -1$. We focus in particular on the half-chain entanglement entropy, $\mathcal{S} = -\text{Tr}[\rho_{L/2} \ln \rho_{L/2}]$, where the reduced density matrix $\rho_{L/2} = \text{Tr}_{1,\dots,L/2} |\psi\rangle\langle\psi|$ is obtained after tracing out half of the system for a given eigenstate $|\psi\rangle$. Figure 6(a) shows $\mathcal{S}$ for the hard-core sector for $L = 18$ with $V/t = 8.8$ and $s = 8$, corresponding with $T/t = -1$. It displays a fingerlike structure due to partial Hilbert-space fragmentation. Thus, for the evaluation of the average entropy we consider only eigenstates

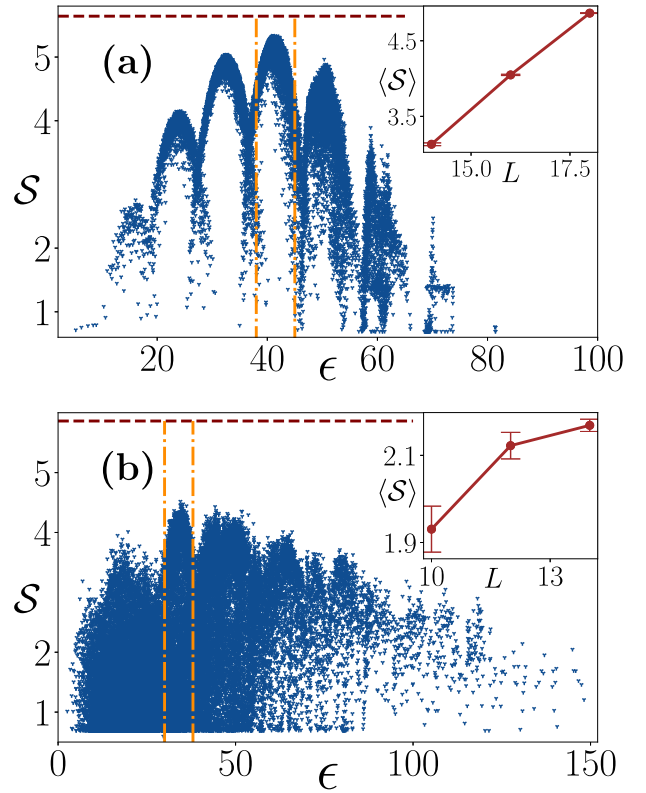


FIG. 6. (a) Entanglement entropy $\mathcal{S}$ for the hard-core sector at $T/t = -1$ ($V/t = 8.8$ for $s = 8$) for $L = 18$. The dashed horizontal line corresponds to the random-matrix theory value. Vertical lines indicate a single sector taken to calculate the average entropy (shown in the inset for different system sizes). Panel (b) shows the entanglement entropy for the remaining decoupled sector for $L = 14$. The average entropy does not depend significantly on the system size for this nonergodic sector.

corresponding to a single finger, as denoted by vertical dotted-dashed lines in Fig. 6(a). The hard-core sector is characterized by large entropies, with the average growing linearly with the system size, indicating volume-law scaling, characteristic of delocalized states and nonintegrable dynamics. A similar analysis for the soft-core sector reveals a much broader distribution of $\mathcal{S}$ with many low entanglement states, and a much weaker entropy growth with the system size [Fig. 6(b)]. This characterisation of the eigenstates nicely matches with the gap ratio histograms shown in Fig. 7. The dashed-dotted theoretical predictions drawn in Fig. 7 are $P(r) = 2/(1+r)^2$ for the Poissonian case and $P(r) = 27(r+r^2)/8(1+r+r^2)^{5/2}$, a good approximation for the GOE case [44].

B. Time dynamics

The spectral properties at $T/t = -1$ translate into a markedly different dynamics for the hard-core and the soft-core sectors. Figure 8(a) shows (for $L = 12$, $s = 8$, and $V/t = 8.8$) the long-time evolution of the inhomogeneity for different initial states within the $N_{NN} = L/6$ sector. The hard-core sector (family I) behaves ergodically, with $\mathcal{I}$ practically vanishing for times $\tau > 200/t$.

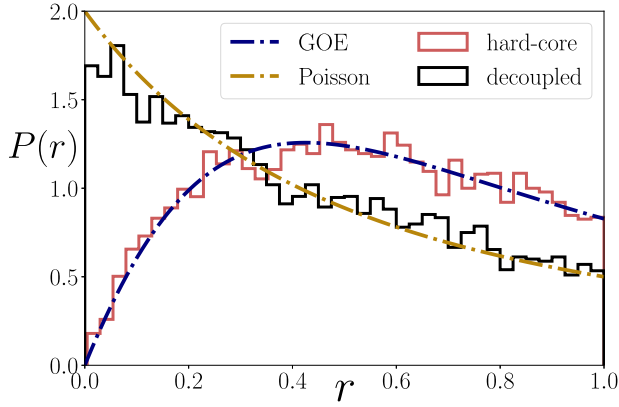


FIG. 7. Histogram $P(r)$ of the gap ratio, r , for $s = 8$ and $V/t = 8.8$ (corresponding to $T/t = -1$). The dashed-dotted lines correspond to the GOE and Poisson predictions. The histograms are presented separately for the two decoupled sectors of hard-core bosons (with GOE statistics) and the remaining soft-core subspace (showing close to Poissonian behavior). The values for r are chosen from within the orange dashed-dotted lines indicated in Fig. 6. In the hard-core sector we consider $L = 18$, whereas for the soft-core one (richer in eigenstates) we are restricted to $L = 14$.

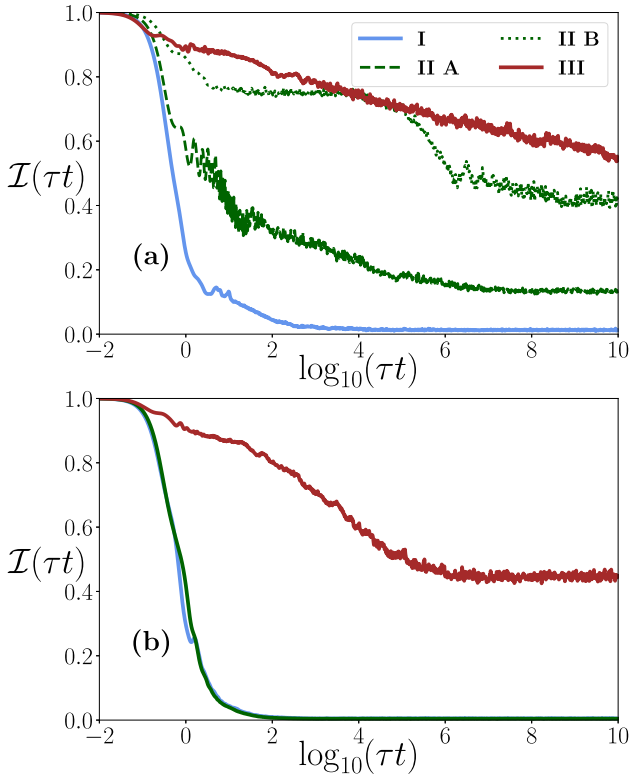


FIG. 8. (a) Inhomogeneity $\mathcal{I}$ as a function of time, τ for $T/t = -1$ ($V/t = 8.8$ for $s = 8$), for initial Fock states in the $N_{NN} = L/6$ sector. Family **I** corresponds to hard-core states; family **II** consists of initial states with a single doubly occupied states, and family **III** is formed by the remaining initial Fock states with higher fillings per site. The family **II** is further split into subfamily **A**, which contains states with a single $|\dots 12\dots\rangle$ or $|\dots 21\dots\rangle$ arrangement, and subfamily **B** which does not consist of such Fock states. Panel (b) shows the results without DDT for the same initial states. In all cases, $L = 12$.

In the soft-core sector, states with a single double-occupancy (family **II**) decay much slower. Those with a single pair $|\dots 12\dots\rangle$ (subfamily **II A**) present a rapid initial decay of $\mathcal{I}$ corresponding to the spreading of the remaining three bosons over the available space, resembling family **I**. After a short time (of the order of $1/t$), a slower decay of $\mathcal{I}$ takes place determined by the highly nonresonant mixing of the occupied pair with the rest. The rest of family **II**, with a single double-occupancy surrounded by empty sites, decays much slower already at short times and then presents a pronounced plateau (at this stage a single occupancy still survives the dynamics) finally reaching a nonzero value. The rest of the soft-core states (family **III**) is characterized by a single large occupancy, and presents a very slow dynamics.

In absence of DDT [Fig. 8(b)] initial states belonging to families **I** or **II** undergo a rapid homogenization. Interestingly, only a partial homogenization occurs for a single high-occupancy initial states. This is due to the energy penalty induced by the on-site interaction [45].

Finally, we note that the splitting of the Hilbert space into decoupled sectors results solely from the $T/t = -1$ condition, being independent of the character of interactions. Since it is independent of the considered $1/r^3$ tail, we expect a similar effect for any long-range potential.

VI. CONCLUSIONS

Our results show that interaction-induced hopping should play a crucial role in future experiments on the dynamics of polar lattice gases. Density-dependent tunneling strongly modifies the dynamics of soft-core dipolar bosons in one-dimensional lattices. For shallow-enough lattices, the delocalizing effect resulting from the interaction-induced hopping overcomes the localization effect induced by the intersite interactions. As a result, counterintuitively and in stark contrast to the hard-core case, delocalization is strengthened when the dipolar strength increases. Interestingly, although this is generally the case, at a critical dipole strength the density-dependent hopping quasiscals the bare hopping resulting in a separation of the Hilbert space in ergodic hard-core states and strongly nonergodic soft-core ones.

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APPENDIX: PARAMETERS OF THE EXTENDED BOSE-HUBBARD MODEL

The calculation of the parameters of the extended Bose-Hubbard model closely parallels the technique described in detail in Ref. [40]. We assume a quasi-one-dimensional model with an optical lattice along x , and a tight harmonic confinement in the transversal directions, leading to the single-particle trapping potential

$$V_t(\mathbf{r}) = \frac{m\omega^2}{2}(y^2 + z^2) + V_0 \cos^2(kx), \quad (\text{A1})$$

where m is the particle mass, ω is the harmonic trapping frequency along y and z , and k is the wave vector of the laser that forms the optical lattice.

The Hamiltonian of the system may be expressed as (see, e.g., [36]):

$$\begin{aligned} \hat{H} = & \int d^3\mathbf{r} \hat{\Psi}^\dagger(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_t(\mathbf{r}) \right] \hat{\Psi}(\mathbf{r}) \\ & + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\Psi}^\dagger(\mathbf{r}) \hat{\Psi}^\dagger(\mathbf{r}') V_{\text{int}}(\mathbf{r} - \mathbf{r}') \hat{\Psi}(\mathbf{r}') \hat{\Psi}(\mathbf{r}) \end{aligned} \quad (\text{A2})$$

with the bosonic field operators $\hat{\Psi}(\mathbf{r})$ and $\hat{\Psi}^\dagger(\mathbf{r})$ that obey the commutation relation $[\hat{\Psi}(\mathbf{r}), \hat{\Psi}^\dagger(\mathbf{r}')] = \delta^3(\mathbf{r} - \mathbf{r}')$. $V_{\text{int}}(\mathbf{r} - \mathbf{r}')$ describes interactions between bosons that is conveniently split into the contact and dipole-dipole terms:

$$V_{\text{int}}(\mathbf{r}) = V_c(\mathbf{r}) + V_d(\mathbf{r}). \quad (\text{A4})$$

The contact term is characterized by the s -wave scattering length, a_s . Using the customary notation, $V_c(\mathbf{r}) = g\delta^{(3)}(\mathbf{r})$, with $g = 4\pi\hbar^2 a_s/m$. Dipole-dipole interactions give a second interaction term, $V_d(\mathbf{r})$. We consider dipoles polarized by an external field along the z axis (perpendicular to the axis of the optical lattice) with

$$V_d(\mathbf{r}) = C \frac{1 - 3\cos^2(\theta)}{r^3}, \quad (\text{A5})$$

where θ is the angle between the dipole and $\mathbf{r}$. The dipole-dipole interaction is anisotropic in space since the force depends on the dipole orientation. The strength of the dipole-dipole interactions $C = \mu_0\mu^2/4\pi$ ($C = d^2/(4\pi\epsilon_0)$) for magnetic (electric) dipoles with moment μ (d) where μ_0 (ϵ_0) are the magnetic (electric) permeability, respectively.

For sufficiently deep optical lattice ($s = V_0/E_R > 3$, where $E_R = \hbar^2 k^2/(2m)$) we may expand the field operator as

$$\hat{\Psi}(\mathbf{r}) = \sum_{j=1}^L \mathcal{W}_j(\mathbf{r}) \hat{a}_j = \sum_{j=1}^L \phi_0(y)\phi_0(z)W_j(x) \hat{a}_j, \quad (\text{A6})$$

where $j = 1, \dots, L$ denotes the site index, and the operator $\hat{a}_j$ annihilates boson at site j . The corresponding basis function $\mathcal{W}_j(\mathbf{r})$ is the product of the ground states of the harmonic oscillators along y, z , and the Wannier function (of the lowest band) along the lattice (shallower lattices may implicate the necessity of taking higher bands into account). Plugging Eq. (A6) into Eq. (A3), one expresses the Hamiltonian in as a polynomial of the annihilation and creation operators.

Employing the orthogonality of the Wannier functions, one arrives at the form

$$\hat{H} = -t \sum_{j=1}^{L-1} (\hat{a}_j^\dagger \hat{a}_{j+1} + \text{H.c.}) + \frac{1}{2} \sum_{i,j,k,l} V_{ijkl} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l, \quad (\text{A7})$$

where the integrals V_{ijkl} are explicitly given as

$$V_{ijkl} = \int d^3\mathbf{r} d^3\mathbf{r}' \mathcal{W}_i(\mathbf{r}) \mathcal{W}_j(\mathbf{r}') V_{\text{int}}(\mathbf{r} - \mathbf{r}') \mathcal{W}_k(\mathbf{r}') \mathcal{W}_l(\mathbf{r}). \quad (\text{A8})$$

The single-particle tunneling amplitude is obtained from the single-particle part of the Hamiltonian

$$\begin{aligned} t = & - \int d^3\mathbf{r} \mathcal{W}_i(\mathbf{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V_t(\mathbf{r}) \right] \mathcal{W}_{i+1}(\mathbf{r}) \\ = & \int dx W_i(x) \left[\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} - V_0 \cos^2(kx) \right] W_{i+1}(x), \end{aligned} \quad (\text{A9})$$

where we limit ourselves to NN tunneling only, assuming a sufficiently deep optical lattice (for shallow lattices, with $s = V_0/E_R < 4$, one might need to include next-to-NN tunnelings into the picture; see, e.g., Ref. [46].)

As it turns out the integrals over perpendicular directions can be explicitly carried out [47–50], yielding

$$V_{ijkl} = \int dx dx' W_i(x) W_j(x') V_{1D}(x - x') W_k(x) W_l(x'), \quad (\text{A10})$$

where the effective quasi-one-dimensional potential is given by

$$\begin{aligned} V_{1D} = & \left(g_{1D} - \frac{2C}{3l^2} \right) \delta(|x - x'|) \\ & + \frac{C}{l^3} \left[\sqrt{\frac{\pi}{8}} e^{(x-x')^2/(2l^2)} \left(1 + \frac{(x-x')^2}{l^2} \right) \right. \\ & \times \text{Erfc} \left(\frac{|x-x'|}{l\sqrt{2}} \right) - \frac{|x-x'|}{2l} \left. \right], \end{aligned} \quad (\text{A11})$$

in terms of the harmonic oscillator length in the perpendicular direction, $l = (\hbar/m\omega)^{1/2}$ and the effective 1D contact interaction strength $g_{1D} = g/(2\pi l^2)$. In Eq. (A11) δ stands for Dirac delta function and Erfc for the complementary error function. Note that the term proportional to the delta function contains contributions from both the contact and dipole-dipole interactions.

The largest contribution is given by the on-site interaction term (diagonal in $ijkl$ indices), traditionally denoted as $U \equiv V_{iiii}$. For contact interactions this is the dominant term. For long-range dipolar interactions the next important term has the form of a density-density interaction ($V_{ijij} + V_{ijji}$) $\hat{n}_i \hat{n}_j$ (for $i \neq j$) where often only the NN term for $j = i \pm 1$ is taken into account. We mention parenthetically that while for contact interactions V_{ijij} and V_{ijji} are identical, for a dipolar potential one finds that $|V_{ijij}| \ll |V_{ijji}|$. Since Wannier functions are well localized on sites, for tight perpendicular binding and $1/r^3$ potential one may approximate $V_{ijij} = V/|i-j|^3$ recovering the typical dipolar tail; here $V = V_{0110}$ is the value of the integral for the NNs. A standard extended Bose-Hubbard model (see, e.g., [51]) considers just terms

involving U and V coefficients and neglects the dipolar tail. The latter may play an important role in the dynamics of the system [34,42], and may differ from the standard $1/r^3$ decay if the transversal confinement is not sufficiently strong [42].

Other important terms, introduced by Hirsch [35] for strongly correlated spinful fermions, are density-dependent tunnelings (DDT), also called correlated hoppings, coming

from V_{ijkl} terms with three equal indices. The most important corresponds to NN correlated tunneling, e.g. $V_{iii(i+1)}\hat{a}_i^\dagger\hat{n}_i\hat{a}_{i+1}$. For shortness of notation the corresponding amplitude is denoted by T (or rather, due to some historical reasons $-T$ [36]). Taking together contributions containing U , V , and T terms, one arrives at the extended Bose-Hubbard Hamiltonian of Eq. (1).

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7.3 ARTICLE III

Finite-size scaling analysis of the many-body localization transition in quasiperiodic spin chains

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We analyze the finite-size scaling of the average gap ratio and the entanglement entropy across the many-body localization (MBL) transition in one dimensional Heisenberg spin chain with quasiperiodic (QP) potential. By using the recently introduced cost-function approach, we compare different scenarios for the transition using exact diagonalization of systems up to 22 lattice sites. Our findings suggest that the MBL transition in the QP Heisenberg chain belongs to the class of the Berezinskii-Kosterlitz-Thouless transition, the same as in the case of uniformly disordered systems as advocated in recent studies. Moreover, we observe that the critical disorder strength shows a clear sublinear drift with the system size as compared to the linear drift seen in random disordered models, suggesting that the finite-size effects in the MBL transition for the QP systems are less severe than that in the random disordered scenario. Moreover, deep in the ergodic regime, we find an unexpected double-peak structure of distribution of on-site magnetizations that can be traced back to the strong correlations present in the QP potential.

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I. INTRODUCTION

Generic isolated quantum many-body systems are expected, according to the eigenstate thermalization hypothesis [1–3], to approach equilibrium described by an appropriate statistical ensemble determined by a few global integrals of motion such as energy or total momentum—see [4,5]. One exception to this hypothesis is provided by the phenomenon of many-body localization (MBL) [6,7], which occurs in the presence of strong disorder and interactions. In this dynamical phase the approach to equilibrium is inhibited and the system indefinitely preserves detailed information about its initial state due to the presence of local integrals of motion [8–11]. In consequence, the transport is slowed down and eventually suppressed [12–15], and the entanglement spreads slowly [16–18].

The combination of strong disorder and interactions makes the phenomenon of MBL tractable only in exact numerical calculations for relatively small lattice systems [19,20]. This makes understanding of ergodic to MBL transition a formidable undertaking, especially in conjunction with nonperturbative mechanisms of delocalization of the MBL phase [21–23]. Despite intensive research [20,24–36] the status of the MBL phase is not fully understood as shown by the recent debate about the stability of MBL [37–45]. On the other hand, the existence of MBL is essentially certified

in sufficiently strongly disordered spin chains as shown in [46,47].

Two primary hypotheses proposed to describe the MBL transition assume that the correlation length ξ in the system (A) diverges at the transition in a power-law fashion $\xi_0 = \frac{1}{|W-W^*|^\nu}$, where ν is a critical exponent and W^* is the critical disorder strength, and (B) assumes a Berezinskii-Kosterlitz-Thouless (BKT) scaling: $\xi_{\text{BKT}} = \exp\{\frac{b_\pm}{\sqrt{|W-W^*|}}\}$, where $b_\pm$ are nonuniversal parameters on the two sides of the transition.

The hypothesis I of power-law divergence of ξ was supported by the early real-space renormalization group approaches [48,49]. However, the majority of numerical studies typically found the critical exponent $\nu \sim 1$ [27,50] violating the Harris bound $\nu > 2$ [51–53]. An exception is provided by the system size scaling of the Schmidt gap [54]. The hypothesis of BKT scaling I is supported by real-space renormalization group approaches [55–58] based on the avalanche scenario of delocalization of the MBL phase [22,59] and advocated by the recent numerical studies [60–62].

The phenomenon of MBL may also occur when the random disorder (RD) in the system is replaced by a quasiperiodic (QP) potential [63–71]. MBL in QP systems was studied in a number of experimental settings [72–75] (we note that the RD could, in principle, be introduced in such systems via a speckle potential [76]). QP potential has a period incommensurate with the lattice constant; hence it breaks the translational invariance effectively acting as a disorder. However, the strong long-range correlations present in the QP potential may severely affect the properties of the MBL transition [77,78], and lead to significantly smaller variations in

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system properties from one disorder realization to another one as compared to the RD scenario [77,79]. Furthermore, due to lack of local fluctuations in the QP potential, a mechanism giving rise to the ergodic seeds that could initialize the avalanches delocalizing the MBL phase remains to be identified [80]. So far, studies of MBL in QP systems concentrated mainly on the scenario I for the MBL transition, finding a critical exponent $\nu \sim 1$ [77,81,82] apparently satisfying the Harris-Luck criterion ($\nu > 1$) [83]. This value of the critical exponent was not confirmed by the real-space renormalization group calculation of [78], which finds $\nu \sim 2.4$. Moreover, the recent examination of local integrals of motion in the QP systems [84] suggest that $\nu \gtrsim 2$ and that the critical disorder strength for the transition to MBL is much larger than previously expected.

Motivated by these results we decided to perform a quantitative comparison of the scalings I and I in QP systems. To that end we follow the cost-function approach proposed in [60], which allows also for a direct comparison with the RD case. Contrary to the expectations [80], we find that the BKT scaling leads to better finite-size collapses of the data for the QP model than the hypothesis of power-law divergence of correlation length. In either of the cases we find that the drift of the critical disorder strength with system size L is weaker than in systems with RD and slows down with increase of L . Moreover, we find an unexpected behavior of spin correlation functions in the ergodic phase of the model that we trace back to strong correlations in the QP potential.

The rest of this work is structured as follows. In Sec. II, we give a brief introduction to the QP system considered in this work and to the corresponding physical quantities used for the analysis of the ergodic-MBL transition. We discuss the appearance of an exotic double-peak structure in the distribution of on-site spin expectation values deep in the ergodic phase in Sec. III. Section IV is devoted to the core of our results, where we present the detailed analysis of the finite-size scaling across the MBL transition in the QP system. Finally, we draw our conclusions in Sec. V.

II. MODEL AND OBSERVABLES

We consider the paradigmatic model for MBL studies, namely the 1D Heisenberg spin-1/2 chain of length L with the following Hamiltonian:

$$\hat{H} = \sum_{l=1}^{L-1} [\hat{S}_l^x \hat{S}_{l+1}^x + \hat{S}_l^y \hat{S}_{l+1}^y + \hat{S}_l^z \hat{S}_{l+1}^z] + \sum_{l=1}^L h_l \hat{S}_l^z, \quad (1)$$

where $\hat{S}_l^\alpha$ ($\alpha = x, y, z$) are the spin-1/2 operators and h_l denote the on-site potentials. In this work, we consider the QP Heisenberg chain where the on-site potentials h_l are given as

$$h_l = (W/2) \cos(2\pi kl + \phi). \quad (2)$$

We fix k as the inverse golden ratio $k = (\sqrt{5} - 1)/2$ and ϕ is a random phase taken from the uniform distribution between $[0, 2\pi)$. The amplitude W of the QP field plays a role of the “disorder strength” in the considered system. Hence we sometimes refer to the QP potential (2) for a given value of ϕ as a “disorder realization” and refer to the average over ϕ as

the “disorder average.” We note that the QP disorder calls for the enforcement of an open boundary condition.

To investigate a crossover between the ergodic and the MBL regimes, we consider two widely used observables, namely the half-chain entanglement entropy (EE) $\mathcal{S}$ of the eigenstates [27,85] and the average gap ratio $\bar{r}$ [24,86]. For a given disorder realization, the energy-level gap ratios are defined as

$$r_n \equiv \frac{\min\{\Delta_n, \Delta_{n+1}\}}{\max\{\Delta_n, \Delta_{n+1}\}}, \quad (3)$$

where $\Delta_n = E_n - E_{n+1}$ are the spacings between subsequent eigenenergies. The average gap ratio $\bar{r}$ is then obtained by first averaging r_n within a given disorder realization and, subsequently, over different disorder realizations. The average gap ratio is equal to the random matrix theory (RMT) prediction $\bar{r} \approx 0.531$ in the fully delocalized regime of models preserving the generalized time reversal symmetry (the case we consider here), while for fully localized systems it takes the value characteristic for Poisson distribution $\bar{r} \approx 0.386$ [86].

The half-chain EE is defined as the von Neumann entropy of the reduced density matrix $\rho_{L/2}$ as follows:

$$\mathcal{S}_{L/2} = -\text{Tr}[\rho_{L/2} \ln \rho_{L/2}], \quad (4)$$

where $\rho_{L/2} = \text{Tr}_{1,2,\dots,L/2} |\psi\rangle \langle \psi|$ is obtained by tracing out half of the system. To minimize the system-size dependence of the EE, we rescale it by the corresponding RMT value $\mathcal{S}_{\text{RMT}} = (L/2) \ln(2) + [1/2 + \ln(1/2)]/2 - 1/2$ as $\mathcal{S} = \mathcal{S}_{L/2}/\mathcal{S}_{\text{RMT}}$ [87–89]. Finally, as in the case for $\bar{r}$, we average the rescaled EE over eigenstates corresponding to a particular disorder realization, and then over different disorder realizations.

In this work, we consider the system (1) of size $L \in [10, 22]$ and vary the disorder strength W within the range $[0.4, 6]$. The variations of the average gap ratio and the half-chain EE with increasing W , as the system undergoes a crossover between the ergodic to the MBL regimes, are shown in Fig. 1 for $L \in [12, 22]$. At each particular W and system size L , the observables are calculated by averaging over eigenstates near the rescaled energy

$$\epsilon = \frac{E - E_{\min}}{E_{\max} - E_{\min}} = 0.5 \quad (5)$$

for a given disorder realization, and subsequently over different realizations demarcated by different random phases ϕ . The numbers of eigenvalues and disorder realizations used in this study for each length L are enumerated in Table I. For system size $L \leq 14$ we use the standard exact diagonalization (ED) method for dense matrices, while for $L \geq 16$ the recently developed *polynomially filtered exact diagonalization* (POLFED) method [20] is used. The results of both algorithms were compared between each other for $L = 16$ and also verified with the standard “shift-and-invert” diagonalization scheme [19]. No difference up to machine precision has been detected.

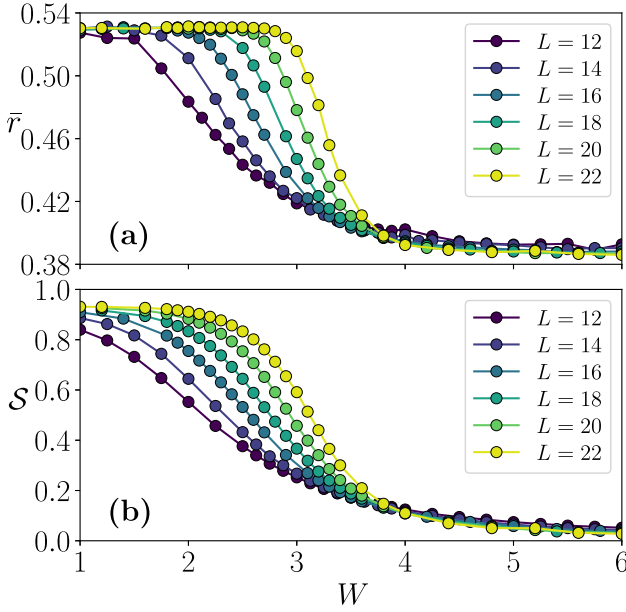


FIG. 1. Dependence of (a) the average gap ratio $\bar{r}$ and (b) the half-chain EE S on the amplitude W of the QP disorder for different system sizes $L \in [12, 22]$.

III. NON-GAUSSIAN BEHAVIOR OF $\langle \hat{s}_i^z \rangle$ IN THE ERGODIC REGIME

In the QP system considered here, the site dependent potential h_i is fully correlated and its values on all lattice sites are determined by the value of the phase ϕ . In this section we demonstrate that this property of the QP potential affects the system properties profoundly even deep in the ergodic regime.

For the standard Heisenberg model with RD, the probability distribution $\mathcal{P}(s^z)$ for site-resolved spin expectation values $s_i^z = \langle \hat{s}_i^z \rangle$ for midenergy eigenstates ($\epsilon \approx 0.5$) has a U shape with peaks at $s^z \simeq \pm 0.5$ in the MBL phase due to the presence of local integrals of motion that have substantial overlaps with $\hat{S}_i^z$ operators [61,90–93]. According to the eigenstate thermalization hypothesis, $\mathcal{P}(s^z)$ has a Gaussian distribution with a peak at $s^z = 0$ and variance that quickly decreases with L deep in the ergodic regime. In the intermediate regime between ergodic and MBL phases, the distribution of s^z acquires long tails, with the bulk of the distribution concentrated in the

TABLE I. Number of eigenstates and the number of realizations used in this work.

L	No. eigenstates	No. realizations
10	252	30000
12	300	2000
14	340	5000
16	720	2000
18	900	2000
20	1000	1000
22	1000	1000

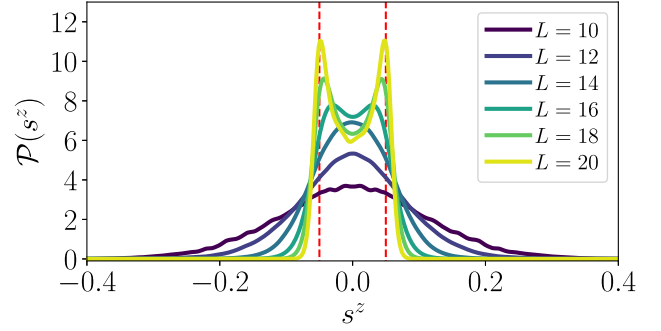


FIG. 2. Probability distribution $\mathcal{P}(s^z)$ for site-resolved spin expectation values s^z with field strength $W = 1$. We find for $L \geq 16$ double peaks start to appear. The red dashed lines are drawn at $s_z = \pm 0.05$ to give an estimate of the location of peaks for $L = 20$.

peak at $s^z = 0$. Both types of behavior were observed for the Heisenberg model in, e.g., Refs. [35,61,94,95].

Figure 2 shows the probability distribution $\mathcal{P}(s^z)$ of s^z for system sizes $L \in [10, 20]$ and disorder strength $W = 1$ that lies deep inside the ergodic regime (for $W = 1$ the average gap ratio is $\bar{r} \approx 0.531$ and $S \approx 1$; see Fig. 1). Strikingly, for larger system sizes, $\mathcal{P}(s^z)$ is not Gaussian anymore. Rather, $\mathcal{P}(s^z)$ develops characteristic peaks that appear at nonzero s^z (e.g., $s^z \simeq \pm 0.05$ for $L = 20$).

On closer inspection, the double-peak structure in $\mathcal{P}(s^z)$ appears deep in the ergodic regime for sufficiently large system size—it is apparent already for $W = 0.4$ for $L = 18$, as shown in Fig. 3(a). With the increase of the QP potential amplitude W , the distance between peaks increases. At the same time, the central minimum gets shallower and, upon further increase of W , the double peak structure slowly vanishes while the system is still in the ergodic regime. For example, for $L = 18$, the double peak disappears at around $W \simeq 2$ [while the gap ratio is still approximately given by RMT value $\bar{r} \approx 0.531$; see Fig. 3(a)]. For larger W , the probability distribution $\mathcal{P}(s^z)$ starts to resemble the expected Gaussian curve (e.g., at $W = 2.1$ and 2.3). The $\mathcal{P}(s^z)$ distribution starts to admit the U-shape characteristic for the MBL regime only at much larger amplitudes of the QP potential; for instance, $W \approx 3.6$ for the system size $L = 18$.

Moreover, the probability distribution $\mathcal{P}(|s_i^z - s_{i+1}^z|)$ for the nearest-neighbor spin differences $|s_i^z - s_{i+1}^z|$ also shows a peak at nonzero $|s_i^z - s_{i+1}^z|$ deep in the ergodic regime, where $\mathcal{P}(s^z)$ shows the characteristic double-peaked structure [compare Fig. 3(b)]. This shows that the nearest-neighbor spins are more likely to be in opposite orientations even in the ergodic phase of the Heisenberg model with QP potential. This behavior is particularly exotic since the ordering of adjacent spins arises for states in the middle of the spectrum of a system with average gap ratio $\bar{r}$ in agreement with RMT.

The distribution of $\mathcal{P}(s^z)$ is qualitatively similar to a distribution of field differences $h_i - h_{i+1} \equiv \epsilon$ at neighboring sites, which for the QP potential (2) is given by $P(\epsilon) = [2\pi \sin(\pi k)]^{-1} \{1 - [\epsilon/2\pi \sin(\pi k)^2]\}^{-1/2}$. The distribution $P(\epsilon)$ has characteristic peaks at $\epsilon = \pm 2\pi \sin(\pi k)$. The value of ϵ determines how resonant the local tunneling is, strongly affecting system properties both for noninteracting models

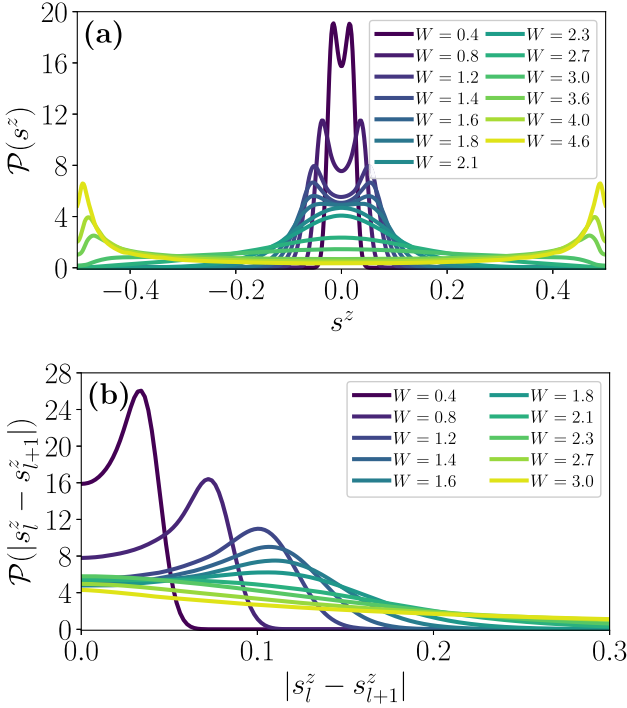


FIG. 3. (a) Probability distribution $\mathcal{P}(s^z)$ for site-resolved spin expectation values s^z with varying field strength W for the system size $L = 18$. For this system size, the characteristic double-peak nature of the probability distribution disappears at $W \simeq 2$ and the U-shaped pattern corresponding to the MBL phase starts to appear for $W \gtrsim 3.5$. (b) The probability distribution $\mathcal{P}(|s_l^z - s_{l+1}^z|)$ for the nearest-neighbor spin differences $|s_l^z - s_{l+1}^z|$ with varying field strength W for the system size $L = 18$. Interestingly, $\mathcal{P}(|s_l^z - s_{l+1}^z|)$ attains its maximum value at nonzero $|s_l^z - s_{l+1}^z|$ deep in the ergodic regime for $W \lesssim 2$ for this particular system size.

[96] as well as for the MBL transition [69]. It seems reasonable to us that the characteristic shape of $\mathcal{P}(\varepsilon)$ for the QP potential determines the double peak structure of $\mathcal{P}(s^z)$. However, we are not able to pinpoint a precise mechanism leading to the characteristic shape of $\mathcal{P}(s^z)$ deep in the ergodic regime of the QP system.

The conclusions relevant for the finite-size scaling analysis in the rest of this work are as follows: (i) the behavior of $\mathcal{P}(s^z)$ in the QP system is much different than in the random case preventing us from analyzing the ergodic-MBL transition with the chain breaking mechanism of [61]; (ii) the characteristic for the QP potential structure of $\mathcal{P}(s^z)$ appears only if the system is sufficiently large; hence we consider mostly $L \geq 16$ in our finite size scaling analysis. This choice is also motivated by the fact that the average gap ratio $\bar{r}$ does not vary smoothly with W for $L \leq 14$.

IV. FINITE-SIZE SCALING ANALYSIS

We now present the results of the finite-size scaling of the average gap ratio and the half-chain EE in the QP Heisenberg chain. First, we analyze the system by considering a fixed critical point W^* independent of the system size. Then, we

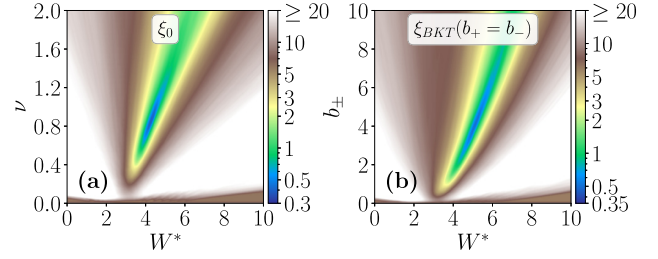


FIG. 4. Pattern of the cost function $\mathcal{C}_S$ for the rescaled EE $\mathcal{S}$ as a function of the minimizing parameters W^* and (a) ν for the correlation length ξ_0 or (b) $b_{\pm} = b_+ = b_-$ for the correlation length ξ_{BKT} .

consider more general scenarios with different size-dependent functional forms of the critical disorder strength.

The basic principle for finite-size scaling is that near the critical point W^* the correlation length ξ diverges [97] either according to I for a standard second-order phase transition or according to I for a BKT transition. As a result, the normalized observable, X , takes a functional form

$$X = \mathcal{G}(L/\xi), \quad (6)$$

where $\mathcal{G}(\cdot)$ is a continuous function.

For the finite-size scaling analysis, we follow the recently proposed method of minimizing a cost function introduced by Łuntajs *et al.* [60]. Unlike other scaling methods it does not assume the observables to take a particular functional form of L/ξ but rather that the observables are simply monotonic functions of L/ξ . The cost function for a quantity $X = \{X_j\}$ that consists of N values at different W and L is defined as

$$\mathcal{C}_X = \frac{\sum_{j=1}^{N-1} |X_{j+1} - X_j|}{\max\{X_j\} - \min\{X_j\}} - 1, \quad (7)$$

where X_j 's are sorted according to nondecreasing values of $\text{sgn}[W - W^*]L/\xi$. For an ideal collapse with X being a monotonic function of $\text{sgn}[W - W^*]L/\xi$, we must have $\sum_j |X_{j+1} - X_j| = \max\{X_j\} - \min\{X_j\}$, and thus $\mathcal{C}_X = 0$. However, in our case it will suffice that the best collapse corresponds to the global minima of $\mathcal{C}_X$ for different correlation lengths and functional forms of $W^*(L)$. In Appendix A, we provide details about the numerical optimization of the cost function performed in this work.

A. Comparisons of finite-size scaling for system-size independent critical disorder strength

Let us first consider the scenario when the critical disorder strength W^* is independent of the system size L . We make a comparison between different types of finite-size scaling, where the correlation lengths are given by power law (ξ_0) and that of a BKT transition (ξ_{BKT}). For the BKT scaling, we consider both the constrained symmetric condition $b_+ = b_-$ and the free asymmetric condition $b_+ \neq b_-$. For a visualization of the cost function for the rescaled EE, $\mathcal{S}$, we plot $\mathcal{C}_S$ in both cases of the power-law correlation and the BKT one with $b_+ = b_-$ in Fig. 4. In this scenario, definite minima of the cost function in the landscapes of the minimizing parameters can be seen. The resulting residual values of the cost

TABLE II. Cost function $\mathcal{C}_X$ comparison for finite-size scaling with fixed critical disorder strength.

	ξ_0	$\xi_{\text{BKT}}(b_+ = b_-)$	$\xi_{\text{BKT}}(b_+ \neq b_-)$
$\mathcal{C}_r$	0.635	0.808	0.769
$\mathcal{C}_S$	0.326	0.419	0.402

function $\mathcal{C}_r$ ($\mathcal{C}_S$) obtained in the minimization procedure for the considered scenarios of the transition and for the average gap ratio (half-chain EE) are shown in Table II. The finite-size scaling with power-law correlation length ξ_0 provides better data collapse in comparison to that with ξ_{BKT} as seen by the values of the cost function.

The best data collapses, i.e., with the power-law correlation length ξ_0 , for each observable are presented in Fig. 5. The critical disorder strength turns out to be $W_{(\bar{r})}^* = 3.97$ and $W_{(S)}^* = 4.27$ respectively for the average gap ratio $\bar{r}$ and the half-chain EE $\mathcal{S}$. However, the critical exponent ν that we extract from the data collapse is 0.54 and 0.87 for $\bar{r}$ and $\mathcal{S}$, respectively. While $\nu_{(S)} \sim 1$ matches pretty well with the recent results for a similar QP chain (with added next-neighbor tunnelings) [77], the exponent for $\bar{r}$ ($\nu_{(\bar{r})} \sim 0.5$) contradicts those results. Therefore, while $\nu_{(S)}$ is close to obeying the Harris-Luck criteria of $\nu > 1$ [83], $\nu_{(\bar{r})}$ strongly violates it.

For second-order phase transitions the finite size scalings are usually best represented by a fixed critical disorder strength, while for BKT scaling even for system sizes of $O(1000)$ we expect a drift of the form $\sim 1/\ln(L)^2$ [98]. The phenomenological renormalization group studies find more exotic finite-size scaling for MBL in RD systems [55–58], and the proper mechanism for the MBL transition in QP systems is yet to be put forth. Thus we assume W^* to take different functional forms with the system size L , and continue our analysis on the finite-size scaling assuming W^* now to be dependent on the system size L in the following subsection. This is also motivated by similar studies on quenched disordered systems that found a linear drift in critical disorder strength with increasing length [20,37,60]. While few previous studies have commented on this behavior being relatively weak for QP systems (thus emphasizing that QP systems are relatively stable) [69,77,81], to the best of our knowledge these have not been based on substantial quantitative arguments.

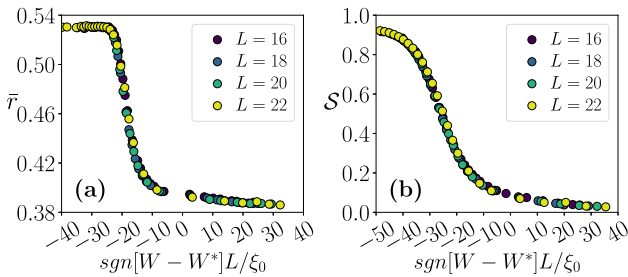


FIG. 5. Finite-size scaling for fixed critical disorder strength W^* assuming the power-law divergence of the correlation length ξ_0 for (a) the average gap ratio $\bar{r}$ and (b) the half-chain EE $\mathcal{S}$. For $\bar{r}$ we find $W^* = 3.97$ and $\nu = 0.54$ and for $\mathcal{S}$ we get $W^* = 4.27$ and $\nu = 0.87$.

TABLE III. Cost-function $\mathcal{C}_X$ comparison for finite-size scaling with system-size dependent drifts in the critical disorder strength.

	$W^0 + W^1 L$	$W^0 + W^1 \ln L$	$W^*(L)$
$\mathcal{C}_r[\xi_0]$	0.200	0.192	0.192
$\mathcal{C}_r[\xi_{\text{BKT}}(b_+ = b_-)]$	0.221	0.147	0.144
$\mathcal{C}_r[\xi_{\text{BKT}}(b_+ \neq b_-)]$	0.206	0.143	0.139
$\mathcal{C}_S[\xi_0]$	0.076	0.076	0.076
$\mathcal{C}_S[\xi_{\text{BKT}}(b_+ = b_-)]$	0.151	0.039	0.035
$\mathcal{C}_S[\xi_{\text{BKT}}(b_+ \neq b_-)]$	0.117	0.034	0.026

B. Finite-size scaling for system-size dependent critical disorder strength

We now move to the finite-size scaling analysis of the relevant quantities where we assume that the critical disorder strength has drifts with the system size L . Specifically, we consider the following functional forms for the critical point W^* (we refer to Appendix B for a comparison with alternative system-size dependencies that asymptotically lead to fixed critical points in the thermodynamic limit): (1) a linear drift with respect to L , $W^* = W^0 + W^1 L$, as in for the uniformly distributed random Heisenberg chain considered in [37,60], (2) a logarithmic drift $W^* = W^0 + W^1 \ln L$, and (3) the most generic $W^* = W^*(L)$, where $W^*(L)$ are chosen individually for each L .

As before, we consider both power-law I and (both symmetric and asymmetric) BKT I scenarios for the ergodic-MBL transition.

The corresponding values for the cost function for the mentioned scenarios are presented in Table III for comparison. Importantly, by comparing the values of the cost function with those presented in Table II, we find that the finite-size scaling with system-size dependent critical disorder strength produces much better results than that with a fixed critical point. We note that the scaling with power-law type correlation length still works better for the linear drift in critical point ($W^* = W^0 + W^1 L$) compared to the BKT ones. Interestingly, the performance of scaling with the linear drift is significantly worse than the scalings with the logarithmic drift ($W^* = W^0 + W^1 \ln L$) and for generic system-size dependence $W^* = W^*(L)$. This is especially relevant for the BKT scenario of the transition (compare the data in Table III). These observations unravel significant differences between the ergodic-MBL transitions in the Heisenberg model with QP potential and in the model with RD, where the scaling with a linear drift having BKT type divergence in correlation length performs the best [60].

In Fig. 6, we show the finite-size scaling with the correlation length $\xi_{\text{BKT}}(b_- = b_+)$ with the logarithmic drift for $\bar{r}$ and $\mathcal{S}$. However, for symmetric BKT scaling ($b_- = b_+$), we find that the values of (W^0, W^1) , as presented in the caption of Fig. 6, are not similar for $\bar{r}$ and $\mathcal{S}$. On the other hand, while the condition $b_- \neq b_+$ only results in marginal improvements in the cost function (see Table III), the extracted values of (W^0, W^1) are similar for $\bar{r} \rightarrow (-6.57, 2.92)$ and for $\mathcal{S} \rightarrow (-6.28, 2.70)$. The nonuniversal constants (b_-, b_+) obtained with the logarithmic drift are found to be $(23.72, 1.82)_{(\bar{r})}$ and $(0.14, 2.75)_{(\mathcal{S})}$ respectively for $\bar{r}$ and $\mathcal{S}$ [similar values

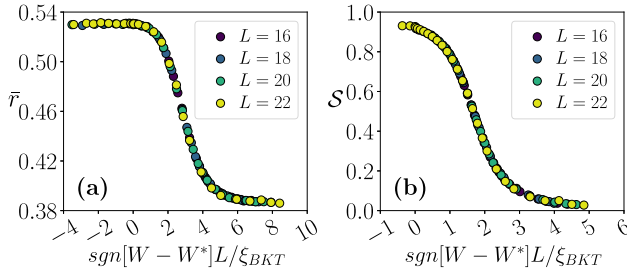


FIG. 6. Finite-size scaling with the logarithmic drift in the critical disorder strength having (symmetric) BKT correlation length $\xi_{\text{BKT}}(b_- = b_+)$ for (a) $\bar{r}$ and (b) $\mathcal{S}$. For $\bar{r}$ we find $W^0 = -6.05$, $W^1 = 2.77$, and $b_{\pm} = 1.79$, while for $\mathcal{S}$ we get $W^0 = -8.19$, $W^1 = 3.17$, and $b_{\pm} = 3.17$.

are also obtained for generic $W^* = W^*(L)$. Note here that, while the values of b_+ , for both $\bar{r}$ and $\mathcal{S}$, are quite similar to those of the constant $b_{\pm}$ extracted for the symmetric BKT scaling, the values of b_- are markedly different, which seems to be unusual. Nevertheless, these observations suggest that the finite-size scaling in two sides of the critical point is very much asymmetrical. Such an asymmetric scaling at the ergodic-MBL transition has also been hinted at for the Heisenberg system with RD [61] (see also [99]).

However, the minimization of the cost function for the BKT scaling with the asymmetric free condition $b_- \neq b_+$ relies on a number of technical subtleties, and the corresponding results must be taken with caution. Specifically, we find that there are multitudes of degeneracies in the values of the minimized cost function that appear for different sets of the values of the parameters (W^0, W^1, b_-, b_+) . The numbers quoted for the BKT scaling with the free condition ($b_- \neq b_+$) in the preceding paragraph are just one example of (W^0, W^1, b_-, b_+) that minimizes $\mathcal{C}_X[\xi_{\text{BKT}}(b_- \neq b_+)]$. However, we also notice that (W^0, W^1, b_+) remains similar in values between different minimizing sets, but b_- fluctuates a lot in values between these sets. For these reasons, we now continue the finite-size scaling having BKT correlation length ξ_{BKT} with the data taken only from the localized side, i.e., only with the constant b_+ . Such analysis is also motivated by the results of [61] that show that the BKT type finite-size scaling performs best when looking from the localized side in the random disordered Heisenberg chain, while a volumic scaling is revealed in the ergodic side where the scaling variable is a ratio between the corresponding Hilbert space dimension and a disorder-dependent nonergodicity volume that diverges exponentially at the critical point.

For the finite-size scaling only from the localized side, we keep the definition of the cost function [Eq. (7)] unchanged but only include the data points $\{X_j\}$, $X \in \{\bar{r}, \mathcal{S}\}$, that satisfy $\text{sgn}[W - W^*]L/\xi > 0$. In Table IV we display the corresponding values of the cost function for system-size dependent critical disorder strengths as in Table III. As before, we again find that the logarithmic drift as well as generic $W^* = W^*(L)$ outperforms the scaling with the linear drift. Figure 7 shows the data collapse for the finite-size scaling with the logarithmic drift for both $\bar{r}$ and $\mathcal{S}$. Corresponding minimizing parameters (W^0, W^1, b_+) are given in the figure

TABLE IV. Cost function $\mathcal{C}_X$ for the finite-size scaling performed on the localized side.

	$W^0 + W^1 L$	$W^0 + W^1 \ln L$	$W^*(L)$
$\mathcal{C}_{\bar{r}}[\xi_{\text{BKT}}]$	0.074	0.07	0.07
$\mathcal{C}_{\mathcal{S}}[\xi_{\text{BKT}}]$	0.066	0.033	0.026
$\mathcal{C}_{\mathcal{S}}[\xi_{\text{BKT}}]_{[L \in \{12, 22\}]}$	0.4	0.26	0.25

caption. In Fig. 8 we show the different W^* values obtained by minimizing the cost function for generic $W^* = W^*(L)$ for finite-size scaling on the localized side with BKT correlation length. Moreover, we find that these values fit perfectly with a logarithmic functional form, again indicating a logarithmic drift in the given system sizes. The fit parameters obtained are also very similar to the ones obtained by minimizing with the logarithmic drift, especially for $\bar{r}$ where both are effectively identical. To understand better the drift of the critical point with the system size, we perform the same analysis with the inclusion of the data for $L = 12$ and 14 for the half-chain EE $\mathcal{S}$ [see Fig. 8(b)]. In this case also, we find that the scaling is best described by the critical point having a logarithmic drift or the generic $W^* = W^*(L)$ (see Table IV). In fact, both scenarios perfectly fit to the functional form $W^0 + W^1 \ln L$, as shown by the bold lines in Fig. 8. For $\bar{r}$ we find $W^0 = -5.58$ and $W^1 = 2.66$, while for $\mathcal{S}$ we get $W^0 = -6.86$ and $W^1 = 2.84$ from the fit. In (b), we also perform the same analysis including the data for $L = 12$ and 14 , and the extracted values of $W^*(L)$ are presented by the yellow crosses. In this also, $W^*(L)$ fits to logarithmic functional form with $W^0 = -6.78$ and $W^1 = 2.8$, which are very close in values to the previous case.

To further illustrate the system size behavior of the critical point we compare, in Fig. 9, the critical disorder strengths for the BKT type scaling of $\bar{r}$ in the localized regime considering different functional forms of the critical point. Interestingly, we get that for the logarithmic drift and for the generic $W^* = W^*(L)$ the critical points are located at values for which the average gap ratio $\bar{r}$ just starts to deviate from the RMT value (~ 0.531).

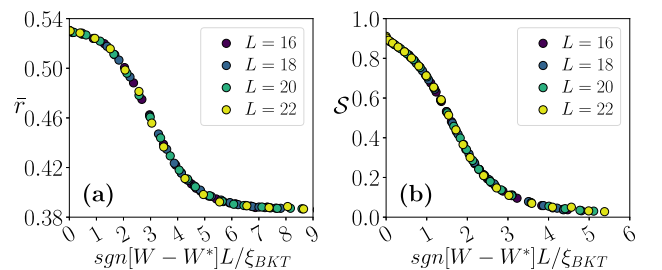


FIG. 7. Finite-size scaling in the localized regime with the logarithmic drift in the critical disorder strength having BKT correlation length $\xi_{\text{BKT}}(b_+)$ for (a) $\bar{r}$ and (b) $\mathcal{S}$. For $\bar{r}$ we find $W^0 = -5.59$, $W^1 = 2.66$, and $b_+ = 1.61$, while for $\mathcal{S}$ we get $W^0 = -6.62$, $W^1 = 2.78$, and $b_+ = 2.83$.

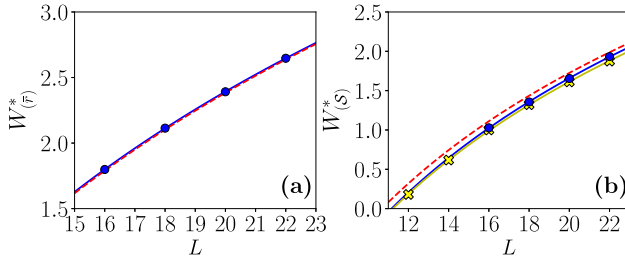


FIG. 8. Critical points W^* obtained for different values of L (shown by the solid blue circles) extracted from the finite-size scaling in the localized regime having BKT correlation length $\xi_{\text{BKT}}(b_+)$ assuming generic system-size dependence $W^* = W^*(L)$ for (a) average gap ratio $\bar{r}$ and (b) half-chain EE S . In (b), we also perform the same analysis including the data for $L = 12$ and 14 , and the extracted values of $W^*(L)$ are presented by the yellow crosses. Solid lines represent the fit of the W^* to the functional form $W^0 + W^1 \ln L$ (see the text), and the red dashed lines correspond to the values obtained by minimizing the cost function for the logarithmic drift $W^* = W^0 + W^1 \ln L$ (see Fig. 7).

C. Summary of the finite-size scaling analysis

Our analysis shows that, when the critical disorder strength is considered to be system-size independent, the power-law scaling provides better results compared to the BKT scaling. However, the critical exponents that we obtain from the scaling of the average gap ratio $\bar{r}$ and half-chain entanglement entropy S are found to be $\nu_{(\bar{r})} \sim 0.5$ and $\nu_{(S)} \sim 1$, respectively. While the latter is roughly consistent with the Harris-Luck criterion for the QP systems [83], the former clearly breaks the criterion. This suggests that the transition in

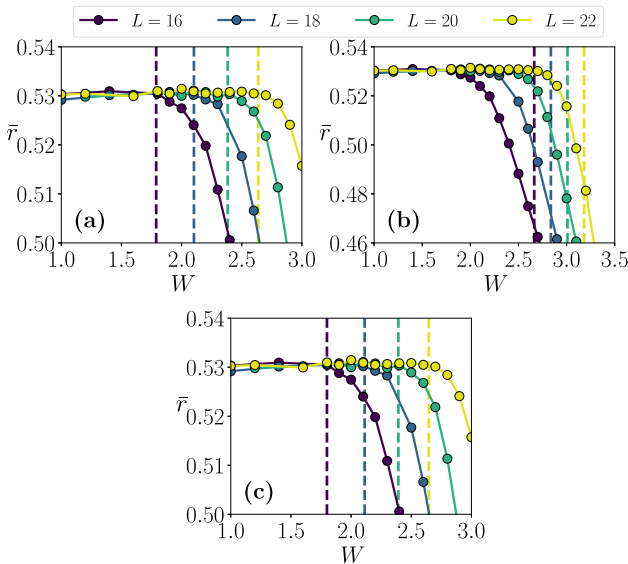


FIG. 9. Critical disorder strengths for different system sizes, as shown by the vertical dashed lines, obtained from the BKT scaling of $\bar{r}$ in the localized regime by assuming (a) a logarithmic drift and (b) a linear drift of the critical point with respect to the system size, as well as by considering (c) generic $W^* = W^*(L)$.

this QP system is not stable within the system sizes considered here, in contradiction with the predictions of [77,81].

On the other hand, by assuming that the critical point drifts with increasing system size, we find that the finite-size scaling performs best for the BKT scenario with a logarithmic drift (within available system sizes) of the critical disorder strength. The system-size dependent critical disorder strengths that we extract from the scaling of $\bar{r}$ and S are respectively $W_{(\bar{r})}^* = -5.58 + 2.66 \ln L$ and $W_{(S)}^* = -6.86 + 2.84 \ln L$ (see Fig. 8 and the corresponding discussions in the text), which results in $W_{(\bar{r})}^* \simeq 2.64$ and $W_{(S)}^* \simeq 1.97$ for a system of size $L = 22$, with both being very close to the ergodic regime. On the other hand, since our study is performed for a very narrow window in the system sizes (specifically, $L \in [16, 22]$), we cannot be sure that the drift is indeed logarithmic. By analyzing the data of the entanglement entropy in the range $L \in [12, 22]$, we see that the logarithmic drift still persists in this wider range. This shows clearly that the critical disorder strength is certainly *sublinear* with respect to the system size in contrast to the situation for the Heisenberg chain with RD. Interestingly, a previous study done on the same model has predicted $W^* \simeq 4.8 \pm 0.5$ using time evolution of large systems ($L = 50$) [69] that closely matches our prediction ($W_{(\bar{r})}^* \simeq 4.83$ and $W_{(S)}^* \simeq 4.25$ for $L = 50$) when the logarithmic drift of W^* is extrapolated to $L = 50$. This is also consistent with the value of critical disorder strength reported recently in [84].

V. CONCLUDING REMARKS

In this work, we have performed a detailed analysis of the ergodic-MBL transition in a finite-size quasiperiodic Heisenberg model. In the ergodic regime, instead of the expected Gaussian probability distribution of on-site magnetization $\mathcal{P}(s_z)$, we found an exotic double-peak structure of $\mathcal{P}(s_z)$. This highlights the importance of correlations in the QP potential showing differences between QP and RD models even in the ergodic regime.

A detailed analysis of the power-law I and the BKT I scenarios suggests that the latter is better suited to describe the system size scaling at the transition to the MBL phase. The similar approach points towards the BKT scaling at the transition in RD systems [60]. Taken literally, this suggests that MBL transitions belong to the same BKT universality class, in contradiction with [77]. However, this result must be interpreted with caution due to the narrow interval of system sizes available both for QP and RD systems.

Our analysis of system size drifts of the critical disorder strength W^* in the QP model shows that W^* increases sublinearly with L and that the finite size effects are less severe than in the RD case. The increased stability of the MBL regime of QP systems in comparison to the RD case is further supported by results for time evolution [100]. This suggests that QP systems may be better suited to understanding the asymptotic behavior of the MBL phase [44].

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APPENDIX A: MINIMIZATION OF THE COST FUNCTION

For minimizing the cost function, we employ a combination of the differential evolution method and the Nelder-Mead simplex algorithm implemented in SciPy [101] respectively for global and local optimizations. For each minimization procedure, we run a series of independent differential evolution algorithms each having different random seed followed by a Nelder-Mead simplex method. We employ ~ 100 such independent realizations to find the optimal solution. At each differential evolution method we allow up to 10^4 iterations with a relative tolerance of convergence 10^{-4} and with a population size of 10^3 .

However, one crucial point in our analysis is about the stability of results obtained in the minimization of the cost function keeping in mind that the data X_i used [either $\bar{r}(L, W)$ or the rescaled entropies] are obtained with some statistical error due to disorder averaging. To test that, we consider the rescaled EE example and assume that $\mathcal{S}$ values for each L and W are Gaussian distributed with centers at the obtained mean values and the standard deviations given by errors of these means. Probing the data over 1000 such Gaussian distributed realizations and performing the cost-function analysis, we

TABLE V. Cost-function $\mathcal{C}_X$ comparison for finite-size scaling with asymptotic functional forms of critical disorder strength.

	ξ_0	ξ_{BKT}
$\mathcal{C}_{\bar{r}}: W_0$	0.635	0.808
$\mathcal{C}_{\bar{r}}: W_0 + W_1/L$	0.633	0.788
$\mathcal{C}_{\bar{r}}: W_0 + W_1/[\ln(L)]$	0.554	0.737
$\mathcal{C}_{\mathcal{S}}: W_0$	0.326	0.419
$\mathcal{C}_{\mathcal{S}}: W_0 + W_1/L$	0.307	0.402
$\mathcal{C}_{\mathcal{S}}: W_0 + W_1/[\ln(L)]$	0.286	0.419

obtain for the symmetric BKT case, i.e., the one depicted in Fig. 6(b), the value $\mathcal{C}_{\mathcal{S}}[\xi_{\text{BKT}}(b_+ = b_-)] = 0.040 \pm 0.004$, which matches the 0.039 value in Table III. Similarly, taking the localized regime only, i.e., corresponding to Fig. 7(b), we obtain $\mathcal{C}_{\mathcal{S}}[\xi_{\text{BKT}}] = 0.034 \pm 0.003$ as compared to the corresponding value in Table IV of 0.033. Moreover, in these cases, the minimizing parameters remain virtually unchanged up to two decimal places. These agreements in values as well as such small errors in the cost function that occur in the third decimal place confirm that the cost-function analysis is very stable with respect to the statistical errors that come with disorder averaging.

APPENDIX B: ASYMPTOTIC FUNCTIONAL FORMS FOR CRITICAL DISORDER STRENGTH

On making a cost-function analysis with functional forms that asymptotically leads to a finite value, we find the cost-function improvements over the fixed critical point to be marginal in comparison with linear or logarithmic drift. This is shown in Table V.

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7.4 ARTICLE IV

Phenomenology of Many-Body Localization in Bond-Disordered Spin Chains

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Many-body localization (MBL) hinders the thermalization of quantum many-body systems in the presence of strong disorder. In this Letter, we study the MBL regime in bond-disordered spin-1/2 XXZ spin chain, finding the multimodal distribution of entanglement entropy in eigenstates, sub-Poissonian level statistics, and revealing a relation between operators and initial states required for examining the breakdown of thermalization in the time evolution of the system. We employ a real space renormalization group scheme to identify these phenomenological features of the MBL regime that extend beyond the standard picture of local integrals of motion relevant for systems with disorder coupled to on-site operators. Our results pave the way for experimental probing of MBL in bond-disordered spin chains.

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Introduction—The eigenstate thermalization hypothesis (ETH) [1–4] conjectures that quantum many-body systems thermalize and reach equilibrium state determined solely by a few macroscopic quantities, irrespective of the details of the initial state. Many-body localization (MBL) [5–11] has been proposed as a mechanism to avoid thermalization for a large class of strongly disordered systems, including spin [12–14], bosonic [15–18], fermionic [19–22], and Floquet systems [23–32]. Explorations of MBL have been primarily driven by numerical studies restricted by the computationally accessible system sizes [33,34] and timescales [35–37]. Consequently, it is unclear whether the observed MBL regime remains stable in the asymptotic limit of infinite system size and infinite time [38–41], motivating studies of persistent slow dynamics and prevalent system size drifts of ergodicity breaking indicators in strongly disordered interacting systems [42–50], as reviewed in [11].

The MBL regime is characterized, on experimentally relevant timescales and system sizes, by the slow growth of entanglement in dynamics [51–54], power-law decay of local correlation functions [55,56], Poissonian level statistics [57–61], and area-law entanglement of eigenstates [62,63]. Local integrals of motions (LIOMs) [64,65] provide a unifying framework that captures the phenomenology of MBL [10,62,64] in the vast class of systems [12–32]. The LIOMs in the MBL regime can be constructed as long-time averages of local operators [66], with perturbative approaches [67], with flow equation methods [68–71] or direct numerical optimization [72–75]. In the paradigmatic disordered XXZ spin chain, LIOMs, $\hat{\tau}_i^z$, are

the z component of the spin operator $\hat{s}_i^z$ transformed by a quasilocal unitary [10,67,76]. This paradigm applies whenever the disorder is coupled to on-site operators, which become exact LIOMs in the strong disorder limit.

This Letter focuses on many-body systems in which the disorder is *not* coupled to on-site operators. We argue that the standard picture of LIOMs does not capture the phenomenology of MBL in such systems. Instead, the real space renormalization group for excited states (RSRG-X) [77], relevant for Hamiltonians constructed out of local operators with a broad distribution of energy gaps, provides a phenomenological description of the system's behavior at large disorder strengths. Instead, the real space renormalization group for excited states (RSRG-X) [77] provides a phenomenological description of the system's behavior at large disorder strengths. As a concrete example, we consider a random-bond XXZ spin-1/2 chain relevant for experiments with ultracold Rydberg atoms [78–81]. For the considered model, the RSRG-X predicts sub-Poissonian level statistics, multimodal structure of the entanglement entropy distribution in eigenstates at large disorder strengths, and allows for identification of operators that may be conserved in the time evolution of experimentally relevant initial states and hence serve as order parameters for the MBL regime, see Fig. 1. We show that the nontrivial memory effects of the RSRG-X procedure prevent us from finding a global set of LIOMs for the considered system even in the infinite disorder limit. We discuss how to extend our procedure to obtain experimentally verifiable predictions for other types of many-body systems.

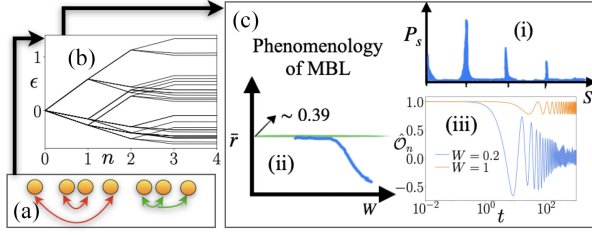


FIG. 1. The RSRG-X scheme approximates the eigenstates and eigenvalues of the bond-disorder XXZ spin chain, capturing the phenomenology of the MBL regime at large disorder strength W . (a) RSRG-X identifies and decimates the bonds between spins approximating eigenvalues (ϵ) for a single realization of Hamiltonian (1) with $M = 8$ spins, see panel (b). (c) Properties captured by the RSRG-X procedure: (i) nontrivial entanglement entropy distribution, (ii) sub-Poissonian mean gap ratio, (iii) lack of thermalization of $\hat{C}_n$ at large W .

The model—We consider the random-bond XXZ spin chain

$$\hat{\mathcal{H}} = \sum_{i=1}^{M-1} J_{i,i+1} (\hat{s}_i^x \hat{s}_{i+1}^x + \hat{s}_i^y \hat{s}_{i+1}^y + \Delta \hat{s}_i^z \hat{s}_{i+1}^z) \quad (1)$$

with open boundary conditions, where, $\hat{s}_i^\beta$ are the spin-1/2 operators acting on the i site with $\beta \in \{x, y, z\}$, $J_{i,i+1}$ are couplings and M is the number of spins. We focus exclusively on the zero-magnetization sector and avoid the special case of the non-abelian SU(2) symmetry by imposing $|\Delta| \neq 1$ [82]. The remaining symmetry of the model is $\mathbb{Z}_2$ spin inversion symmetry $\mathcal{C}$. The Hamiltonian (1) is relevant for experiments with Rydberg atoms confined in an array of microtraps [83,84]. Investigations of these models have demonstrated a weak breaking of the ETH in the presence of interactions [81] and glassy dynamics of selected operators [79,80]. With that motivation in mind, we assume that the couplings in (1) take values according to a power-law $J_{i,i+1} = |x_i - x_{i+1}|^{-\alpha}$, where x_i denotes the position of the i th spin within the length L occupied by the system, and $\Delta = -0.73$, $\alpha = 6$ relevant for a Rydberg state of rubidium 87. Fixing the Rydberg blockade [85] diameter as D_{rb} results in an excluded density $\rho = D_{rb}M/L$. With decreasing density ρ , spins can explore more positional configurations within L there are more possible configurations present, leading to an increase of the effective disorder strength $W = 1/\rho - 1$, associated with the random distribution of $J_{i,i+1}$, in the model [86] and thus to the MBL regime. In [87], we describe our algorithm to generate particle configurations $\{x_i\}$ avoiding the issue of the Rényi parking constant [107].

Decimation scheme—To understand the MBL phenomenology of (1), we employ the RSRG-X scheme [77]. The scheme proceeds iteratively by identifying the largest energy gap, diagonalizing the corresponding local operator,

setting the state of the relevant spins into one of the obtained eigenstates, and perturbatively modifying the nearby effective local operators and the associated energy gaps [77,108]. The energy gaps encountered at each step of this procedure, which we refer to as a decimation, are progressively smaller. Hence, the chosen eigenstates fix the time dynamics at longer times, eventually producing an approximation of the eigenstate of (1) when the last spin is fixed. If the distribution of energy gaps is steadily broadening in the subsequent decimation steps, the scheme is increasingly well controlled and may become asymptotically exact [109–112]. Here, relying on the broadness of the initial gap distribution, the RSRG-X is employed to obtain insights about relatively small systems relevant for numerical and experimental studies.

The RSRG-X proceeds as follows. The Hamiltonian (1) can be written as a sum of two-site local operators of the form

$$\hat{\mathcal{H}}_{i,i+1} = J_{i,i+1} \left(\frac{(\hat{s}_i^+ \hat{s}_{i+1}^- + h.c.)}{2} + \Delta_{i,i+1} \hat{s}_i^z \hat{s}_{i+1}^z \right), \quad (2)$$

with eigenbasis $|Z_\pm\rangle, |\pm\rangle$ where, $|Z_{+/-}\rangle \equiv |\uparrow\uparrow\rangle/|\downarrow\downarrow\rangle$, and $|\pm\rangle \equiv (1/\sqrt{2})(|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$ and the parameter $\Delta_{i,i+1} = \Delta$. The relevant energy gap associated with each local operator is taken as the maximum of its energy gaps, so that any of the eigenstates can be chosen freely. This is a valid approximation if the energy scales are controlled by the couplings $J_{i,i+1}$. Let us assume that the largest relevant energy gap is associated with the local operator $\hat{\mathcal{H}}_{4,5}$. In that case, we select the bond between spins $i = 3, i = 4$ and fix the state of the two spins as $|Z_\pm\rangle, |\pm\rangle$. We now describe how the neighboring operators, i.e., $\hat{\mathcal{H}}_{2,3}$ and $\hat{\mathcal{H}}_{4,5}$ are perturbatively modified for each of the choices.

For states $|\pm\rangle$, there are no contributions to the nearest operators within the first-order perturbation. The second-order perturbation results in the formation of a bond between spins $i = 2, i = 5$, described by $\hat{\mathcal{H}}_{2,5}$ of the form as in (2) with couplings modified to $\tilde{J}_{2,5} = [J_{2,3}J_{4,5}/(1 \mp \Delta_{3,4})J_{3,4}]$, $\tilde{\Delta}_{2,5} = [\mp \Delta_{2,3}\Delta_{4,5}(1 \mp \Delta_{3,4})/2]$. The choice $|Z_\pm\rangle$, within the first-order perturbation modifies the operators $\hat{\mathcal{H}}_{2,3}$ and $\hat{\mathcal{H}}_{4,5}$ to take a chemical potential form [113]

$$\hat{\mathcal{H}}'_{2,3} = \pm \frac{1}{2}(\Delta_{2,3}J_{2,3}\hat{s}_2^z), \quad \hat{\mathcal{H}}'_{4,5} = \pm \frac{1}{2}(\Delta_{4,5}J_{4,5}\hat{s}_5^z), \quad (3)$$

while the second order term leads to a bond between $i = 2, 5$ with $\tilde{J}_{2,5} = -(J_{2,3}J_{4,5}/2J_{3,4})\{[1/(1 - \Delta_{3,4})] + [1/(1 + \Delta_{3,4})]\}$ and $\tilde{\Delta}_{2,5} = 0$. The first-order modification of $\hat{\mathcal{H}}'$ is typically much stronger than the second-order bond and the neighboring operators admit the chemical potential form in the following steps of the scheme. For instance, a decimation of the bond between sites $i = 4, i = 5$, would

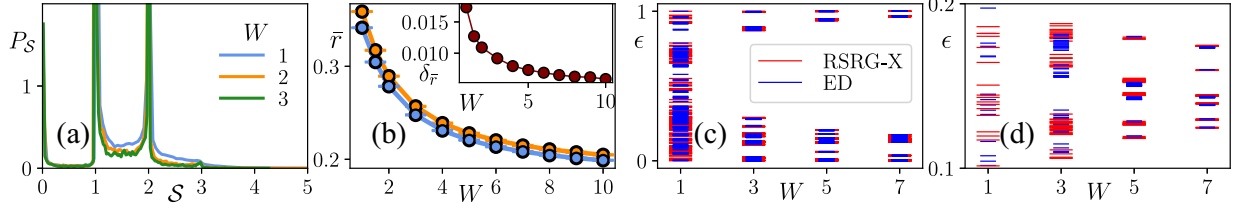


FIG. 2. (a) Distribution P_S of half-chain entanglement entropy S for $M = 20$ and varying disorder strength W . (b) The mean gap ratio obtained by RSRG-X ($\bar{r}_{\text{RG}}$, blue) is compared with ED results ($\bar{r}_{\text{ED}}$, orange). The inset shows $\delta\bar{r} = \bar{r}_{\text{ED}} - \bar{r}_{\text{RG}}$. The system size is $M = 10$, with 25 000 disorder realizations and all the eigenvalues are considered. (c) The rescaled energies ϵ obtained with ED are compared with RSRG-X result for a single disorder realization; (d) enlarged image of the same. All the results for the $\mathcal{C} = +1$ symmetry sector.

result in fixing the eigenstate at site 5 to $|\uparrow\rangle/|\downarrow\rangle$ and modifying the next operator as $\hat{\mathcal{H}}'_{5,6} = \frac{1}{2}(\Delta_{5,6}J_{5,6}\hat{\sigma}_6^z) - \frac{1}{2}(\Delta_{5,6}J_{5,6}\hat{\sigma}_6^z)$. This may lead to a process of growth of domains of spins fixed in states $|\uparrow\rangle/|\downarrow\rangle$ which stops if the next operator to be modified already has the form $\hat{\mathcal{H}}'$. The spin polarized domains $|\uparrow\rangle/|\downarrow\rangle$ may extend over already decimated pair of sites with states fixed as $|\pm\rangle$. The generation of $\hat{\mathcal{H}}'$ operators through the first order perturbation suffices in all scenarios except when degenerate states $|K_+\rangle \equiv |\uparrow\rangle|Z_-\rangle|\uparrow\rangle$, $|K_-\rangle \equiv |\downarrow\rangle|Z_+\rangle|\downarrow\rangle$ are formed. Then, the second order perturbation needs to be taken into account leading to operators of the form $\hat{\mathcal{H}}$ with modified parameters, see Ref. [87].

A generic approximation of an eigenstate stemming from RSRG-X is associated with arbitrary choices of $|Z_\pm\rangle$, and $|\pm\rangle$ throughout the decimation scheme. To qualitatively understand the properties of these eigenstates, we start by assuming that only states $|\pm\rangle$ have been chosen in the decimation scheme. This leads to formation of bonds $\hat{\mathcal{H}}_{l_i, r_i}$ between arbitrarily distant spins, resulting in states $|\pm\rangle_{l_i, r_i}$. The spatial distribution of the correlations of states within this subsystem is analogous to a random singlet phase found for the ground state of (1) [108,109], or for the excited states in the absence of interactions ($\Delta = 0$) [114,115]. In contrast, fixing of the eigenstate as $|Z_\pm\rangle$ in the decimation procedure leads to growth of a domain which breaks the spin inversion symmetry $|\uparrow/\downarrow\rangle_{l_m} \cdots |\uparrow/\downarrow\rangle_{l_2} |Z_{+/-}\rangle_{l_1, r_1} |\uparrow/\downarrow\rangle_{r_2} \cdots |\uparrow/\downarrow\rangle_{r_m}$ (except for the configurations involving $|K_+\rangle$ and $|K_-\rangle$). When the energy scales are not controlled by the couplings J , i.e., when $\Delta \gg 1$, such spin inversion symmetry breaking domains extend through the entire system [113]. In contrast, in our case, a generic eigenstate is formed by domains with spins polarized along the z direction and subsystems in which the state is a product of triplet/singlet states $|\pm\rangle$ [116].

Eigenstates and eigenvalues—To demonstrate that the eigenstates of the random-bond XXZ spin chain (1) at large W indeed feature the structure predicted by the RSRG-X, we analyze the half-chain entanglement entropy $S = -\text{tr}(\rho \log_2(\rho))$, where $\rho = \text{tr}_B(|\psi\rangle\langle\psi|)$ is the reduced

density obtained by tracing out the spins in half of the system and $|\psi\rangle$ is the considered eigenstate. The distribution of S , calculated by exact diagonalization (ED) and shown in Fig. 2(a), exhibits peaks at integer values. The peaks correspond to different numbers of the bonds in triplet/singlet states $|\pm\rangle$ cut by the bipartition of the system, confirming the intuitive picture predicted by the RSRG-X. The peaks get broadened at smaller disorder strengths W due to the contribution of the higher order terms not taken into the account by our decimation scheme. The observed distribution of S is starkly different from the XXZ spin-1/2 chain which, in the large W limit, collapses to a single peak at $S = 0$ [117].

The RSRG-X also approximates the eigenvalues ϵ_k of (1). We compare the RSRG-X prediction with the ED results by calculating the gap ratio $r_k \equiv (\min\{\delta_k, \delta_{k+1}\}) / \max\{\delta_k, \delta_{k+1}\}$ (here $\delta_k \equiv \epsilon_{k+1} - \epsilon_k$) averaged over the entire spectrum of the system and disorder realizations, shown in Fig. 2(b). The RSRG-X qualitatively reproduces the behavior of $\bar{r}$, and, in particular, predicts the sub-Poissonian value $\bar{r} < 0.386 = \bar{r}_{PS}$ at larger W , where $\bar{r}_{PS} \approx 0.386$ [118] is the value for Poissonian level statistics found in the MBL regime of models with a complete set of LIOMs [10]. The sub-Poissonian level statistics arises due to multiple quasidegeneracies in the spectrum, qualitatively captured by the RSRG-X procedure. A closer inspection reveals that the $\bar{r}$ from the RSRG-X is systematically underestimating the ED value, which we attribute to higher order processes neglected by the RSRG-X. In [87], we show that this discrepancy is smaller when the distribution of J 's is wider, i.e., given by a power law with $\alpha > 6$.

Memory effects along the RSRG-X branch—Each step n of the RSRG-X is associated with choice of the states $|Z_\pm\rangle$, $|\pm\rangle$ or, in case of the single-site decimations, with $|\uparrow/\downarrow\rangle$. While fixing $|\pm\rangle$ results only in decimation of the involved spins and renormalization of the parameters of the bond linking their neighbors, the selection of $|Z_\pm\rangle$ affects non-trivially the subsequent steps of the scheme. Each choice of $|Z_\pm\rangle$ introduces a possibility of the growth of the domain of spins polarized along the z direction. This may arise whenever the interactions are present in the system, i.e.,

when $|\Delta_{i,i+1}| > 0$. The triplet or singlet states $|\pm\rangle$ cannot extend over the already fixed spin polarized domains. Consequently, various branches of RSRG-X lead to eigenstates corresponding to different partitions of the system into spin polarized and triplet or singlet domains. Therefore, in contrast to the models in which the disorder is coupled to the on-site operators, we cannot find a complete set of (quasi-)local operators that would commute with the Hamiltonian (1).

Probing the MBL regime with time dynamics—Time evolution of the average value $s(t)$ of $\hat{s}_i^z$ operator is an experimentally realizable way of studying the breakdown of thermalization in the standard disordered XXZ spin chain. For an initial state taken as the eigenstate $|\psi_Z\rangle$ of $\hat{s}_i^z$ operators, $s(t)$ decays to zero in the ergodic regime, while, deep in the MBL regime, for large W , $s(t)$ remains close to unity even at long times [50,55,56]. This procedure, however, would not work for the bond-disordered XXZ spin chain. Because of the nontrivial relations between decimations along various branches of RSRG-X and the presence of eigenstates at any energy density with triplet or singlet domains, the average $s(t)$ may dephase to zero irrespective of the disorder strength W .

To circumvent this issue, we propose to set as an initial state, $|\psi_{\text{in}}\rangle$, the approximation of eigenstate obtained with RSRG-X and to measure average values of operators $\hat{O}_n$ related to the RSRG-X branch leading to $|\psi_{\text{in}}\rangle$. For decimations involving $|\pm\rangle$ we choose $\hat{O}_n = \hat{T}_{i,j} \equiv (\hat{s}_i^+ \hat{s}_j^- + \text{H.c.})$, while for $|Z_{\pm}\rangle$, we select $\hat{O}_n = \hat{P}_{i,j} \equiv 4\hat{s}_i^z \hat{s}_j^z$ [119]. For single-site decimations, we consider the operator $\hat{O}_n = 2\hat{s}_i^z$. The obtained average values $\mathcal{O}_n$ decay to zero in the ergodic regime, while remain close to their starting value as presented in Fig. 1(c)(iii). In Fig. 3(a), we show a particular position configuration and decimation scheme along a selected RSRG-X branch.

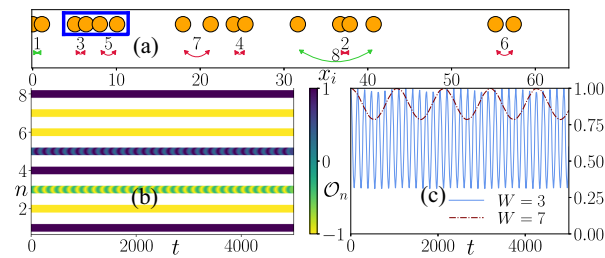


FIG. 3. (a) The decimation scheme for one configuration of spins at $W = 3$ and $M = 16$; connected spins represent decimation steps with $|\pm\rangle$ (in red) or $|Z_{\pm}\rangle$ (in green) fixed, and the numbers denote the number n of the step; the blue box denotes an ergodic bubble. (b) Time evolution of the average values $\mathcal{O}_n$ of operators corresponding to the RSRG-X branch shown in (a). (c) Time evolution of $\mathcal{O}_n(t)$ for the step $n = 5$; the bold (dashed) line corresponds to $W = 3$ ($W = 7$).

The initial state has a simple tensor product structure $|\psi_{\text{in}}\rangle = |Z_+\rangle^1 \otimes |-\rangle^2 \otimes |-\rangle^3 \otimes |+\rangle^4 \otimes |+\rangle^5 \otimes |-\rangle^6 \otimes |-\rangle^7 \otimes |Z_-\rangle^8$, where the superscripts represent the decimation step n . In Fig. 3(b), we present the time evolution of the operators $\hat{O}_n$ and find that the expectation values are preserved except for $\hat{O}_3$ and $\hat{O}_5$ which reveal oscillations. The oscillations are due to a local narrow distribution of J_s , represented by a box in Fig. 3(a). This is an example of an ergodic bubble [120–122] where local disorder is weaker than its average over the whole system. Figure 3(c) details the time oscillations at the ergodic bubble, whose amplitude and frequency decrease with increase of W .

To further demonstrate the validity of the procedure to probe the breakdown of ergodicity in time dynamics, we consider a long-time averaged expectation value $|\bar{\mathcal{O}}| = |\int_0^T \mathcal{O}_n(t) dt|$. Disorder averaged $\langle |\bar{\mathcal{O}}| \rangle$ serves as an ergodicity breaking indicator. As shown in Fig. 4(a), $\langle |\bar{\mathcal{O}}| \rangle$ decays to zero in the ergodic regime, where the mean gap ratio $\bar{r}$ (for detailed finit-size scaling analysis, see Ref. [87]) admits the GOE value $\bar{r}_{\text{GOE}} \approx 0.53$ characteristic for ergodic systems. In contrast, in the MBL regime, where $\bar{r}$ approaches (or is smaller than) the Poissonian value $\bar{r}_{\text{PS}}$, the $\langle |\bar{\mathcal{O}}| \rangle$ is close to unity, showing clearly the lack of thermalization in the system.

Generalization—Let us now consider a generic Hamiltonian of the form $H = \sum_{[\mu]} h_{[\mu]} \otimes_i \hat{s}^{\mu_i}$, where each $h_{[\mu]}$ is drawn from a certain, sufficiently broad, distribution [123], and $\otimes_i \hat{s}^{\mu_i}$ is a local operator. In general, the disorder is not coupled to the on-site operators, hence the standard LIOMs are insufficient to grasp the phenomenological properties of the system at large W . Instead, in the absence of any special symmetry that would lead to resonances, see e.g. [82], the RSRG-X scheme would suffice to identify the properties of the MBL regime in the system. Decimating the largest energy gap, a second-order perturbation theory would lead to virtual connections between the neighboring subsystems, giving rise to non-local operators conserved at large W . The first-order perturbation theory would fix the states of the nearby subsystems and could suppress the long-range correlations.

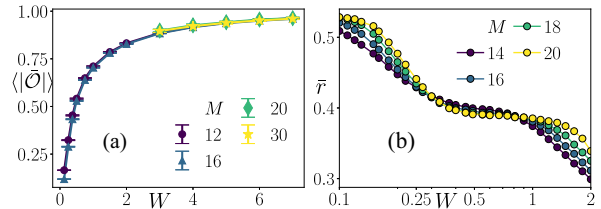


FIG. 4. (a) Long-time (up to $t = 5000$) averages $\langle |\bar{\mathcal{O}}| \rangle$ of operators found in the RSRG-X procedure (see text), averaged over 10 random RSRG-X branches and over 50 disorder realizations. (b) Mean gap ratio $\bar{r}$ as a function of disorder strength W for number of spins M with $\mathcal{C} = +1$.

Conclusion—We studied the MBL regime arising at large disorder strengths in the bond-disordered spin-1/2 XXZ chain. The phenomenology of the MBL regime in the considered system differs significantly from models with disorder coupled to on-site operators, widely studied in the context of MBL [10,11]. Consequently, the standard picture of LIOMs does not describe the MBL regime in the bond-disordered XXZ spin chain, which is characterized by multimodal distribution of entanglement entropy in eigenstates, sub-Poissonian level statistics, nontrivial interplay of operators and the initial state, which has to be accounted for when probing the breakdown of ergodicity with time dynamics. The RSRG-X scheme provides a qualitative understanding of the MBL regime by approximating the highly excited eigenstates as products of domains of spins polarized along the z direction and regions in which spins are paired into triplet or singlet states. The interplay between the two types of domains leads to nontrivial memory effects in the RSRG-X scheme, disallowing the identification of a global set of LIOMs for the model. We argued that the predictions of RSRG-X become quantitatively valid at strong disorder for system sizes accessible to exact diagonalization, provided that the initial distribution of couplings in the model is sufficiently broad.

The bond-disordered XXZ spin-1/2 chain is relevant for Rydberg atoms platforms, which provide a setting to experimentally test our results. The idea of applying the RSRG-X scheme to extract phenomenological properties of MBL regime can be straightforwardly extended to other systems in which the disorder is not coupled to on-site operators. Another question involves examination of the other phenomenological features of the MBL regime in bond-disordered spin chains. For instance, the participation entropies that characterize the spread of eigenstates in the eigenbasis $\hat{s}_i^z$, see, e.g., [124], would not be vanishing even in the $W \rightarrow \infty$ limit due to the presence of triplet or singlet domains in the eigenstates. These questions are left for further studies.

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