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Recenzja rozprawy doktorskiej

mgr. Gabrieli Wójtowicz

pt. *Extended Reservoir Approach for Quantum Transport and non-Markovian Dynamics*

It is my pleasure to review and evaluate the doctoral thesis by Ms. Gabriela Wójtowicz, M.Sc. The work has been performed under the supervision of Dr. hab. Marek M. Rams at the Doctoral School of Exact and Natural Sciences of Jagiellonian University in Kraków. It has a form of a cumulative thesis in which the main body consisting of 86 pages is divided into 6 chapters, 2 appendices, and a list of references consisting of 113 items; in the remaining space, 5 publications are attached.

My detailed review below has been made by taking into account the Law on Higher Education and Science (the Act of 20 January 2020, item 85).

I. The Doctoral Student's presence and position in the scientific community, bibliometrics record, and publications related to the doctoral thesis

The work represents the formalism development and numerical simulations in one of the cornerstones of modern Theoretical Solid State Physics—quantum transport theory. The theory of quantum transport began with the pioneering works of Landauer and Büttiker and became a mature field after the works of Meir, Wingreen, and Jauho, who provided a general formula for the time-dependent current through correlated junctions in terms of non-equilibrium Green's functions. Ms. Gabriela Wójtowicz added one more important step to these developments by building on the so-called extended reservoir approach and combining it with the tensor network representation of quantum states. The thesis is based on four published papers and one submitted manuscript in very decent journals (Phys. Rev. A, Phys. Rev. B, and J. Chem.

Phys.) and therefore significantly contributes to the development of the field. Also, Ms. Gabriela Wójtowicz participated in the development of an open-source tensor network library, YASTN. Altogether, it constitutes excellent achievements for a doctoral candidate and establishes Ms. Gabriela Wójtowicz as a recognized member of the quantum transport community.

II. What scientific issue is considered in the thesis, and has it been sufficiently clearly formulated by the author?

The thesis focuses on the problem of quantum transport in the presence of non-Markovian reservoirs. The Markov property expresses the property that the future states of a stochastic process are influenced only by the present, not the past. Thus, non-Markovian means taking memory effects into account. Such conditions are treated by representing the reservoirs as finite systems coupled to the dissipative environment, which maintains a thermal distribution and a steady state. The overall goal of the study, namely, quantum transport in the presence of non-Markovian reservoirs, is clearly formulated in Ch. 1. This chapter lays the foundation of the whole work. Here, basic concepts such as a typical model for quantum transport, the embedding self-energy, the particle current, and the density matrix are introduced. The discussion of the Born and Markov approximations is impressive because a lot of preparatory work is typically required to introduce them. I believe that Ms. Gabriela Wójtowicz found a good compromise between being absolutely rigorous and accessible.

III. Did the dissertation adequately analyze the sources including literature, state of the art, and applications demonstrating sufficient knowledge of the author? Were the conclusions from the review of sources formulated clearly and convincingly?

The thesis is of the cumulative type based on five papers. Each of them contains a very extensive literature review, and, to the best of my knowledge, all relevant publications are mentioned. One can fully appreciate the state-of-the-art of the quantum transport field.

The main body of the thesis is expected to show a broad picture. In my opinion, such a general introduction to the fields of quantum transport, open systems, (non-)equilibrium Green's functions, and tensor network states, which constitute the main theoretical tools that the doctoral candidate is using, is a bit limited. For instance, in Ch. 1 the Lindblad equation is mentioned without

any citations. In Ch. 2 many definitions and properties of the Green functions are simply listed making an impression that these well-known results were obtained in the thesis. Ch. 3 is a bit different in style: it is full of bulk citations, such as [56-59], [62-65], [68-70], [71-75]. Such style might be unavoidable in papers, but for a dissertation individual discussion of each citation is preferable.

IV. Has the author solved the issues posed, with the right method and justified assumptions? What constitutes the author's independent and original work, and what is the position of the dissertation in relation to the state of knowledge? What is the relevance of the dissertation to the physical and technical sciences?

In the dissertation, a whole set of new theoretical tools has been developed, and impressive physical insights have been obtained. Among the main new results are:

1. Detailed analysis of the current anomalies at weak and strong relaxations in the reservoirs and contrasting them with the regime of intermediate relaxation dominated by intrinsic conduction.

2. Estimation of the optimal relaxation that approximates the continuum limit of the reservoirs.

3. Generalization of the extended reservoir approach to periodically driven systems via the Floquet approach.

The main achievement of the thesis is, in my opinion, method development and benchmarking. Each of the five papers is illustrated with numerous physical examples (single-site noninteracting and two-site interacting impurities, as well as periodically driven 8-site lattice), discussions of different physical limits (underdamped, intermediate and overdamped, different reservoir discretizations), and connections to complementary theories (for instance Landauer's formula with finite-time relaxation by Gruss, Vlizhanin and Zwolak, steady-state DMFT with an auxiliary quantum master equation approach by Arrigoni, Knap and von der Linden).

This work is, thus, very valuable as it sets the foundation for the exploration of new technologically-relevant scenarios, e.g., large many-body transport calculations with tensor networks. It can probe time-dependent states within interacting, driven, dissipative quantum systems. Treatment of challenging

many-body systems where larger and more complex impurity physics gives rise to intricate phenomena represents interesting prospects for the application of the method.

V. Has the author demonstrated the ability to present correctly and convincingly obtained results in a concise, clear, and editorially correct manner?

Ms. Gabriela Wójtowicz demonstrated excellent scientific results in the attached papers. For this reason, there was no need to repeat all the technical details in the main part of the thesis. Rather, Ch.1-6 can be used for more general discussions, such as motivation and justification of the methods, their historical development, and their place in the big picture. Because the thesis is based on three complicated fields of theoretical physics—open systems, non-equilibrium Green's functions, and Tensor Networks—finding a balance between being consistent and, therefore, extensive and being pedagogical was not an easy task. Ms. Gabriela Wójtowicz nicely used this opportunity, and offered a very clear and concise presentation, albeit technical in some places.

While I am overly satisfied with the presented scope of the material, in some places the discussion could have been more accurate. Below is a short list:

1. The material is not equally distributed among the six chapters. Ch. 5 is very short.

2. In full generality, charge currents are lead- and time-dependent. The main definition in Eq.(1.6) does not take these aspects into account nor it is stated that this is a definition for the steady-state current.

3. The Born and Markov approximations are conceptually very different. The former represents a way to approximately take interactions into account, whereas the latter is a statement about the time-evolution. These two aspects are not clearly distinguished in Ch.1.

4. It is stated that Green's function methods may not be efficacious for interacting models. Recently, there has been great progress in this direction, in particular, due to the development of linear-scaling methods based on the Generalized Kadanoff-Baym Ansatz.

5. Time-evolution is mentioned twice: Eq.(1.8) and Eq.(2.1). The latter is generally not correct. This can be appreciated by comparing with definitions (2.3-2.6). All non-equilibrium Green's functions are defined as averages

over some suitably chosen state and depend only on the single-particle indices. It is also easy to verify that G from Eq.(2.2) does not fulfill Eq. (2.1), and retarded G from Eq.(2.9) upon the Fourier transform (2.8) does not fulfill Eq.(2.5).

6. The definition of the Schmidt decomposition given by Eq.(6.2) in Ch. 6 is inconsistent with other equations in the same chapter, Eq.(6.1) in particular. This can be appreciated by comparing the sum indices in both cases. In the case of Eq.(6.2), the right-hand side depends on sigma indices, whereas the left-hand side according to Eq.(6.1) does not depend on them.

7. In Sec. 6.4 it is written, "In Sec.6.3 we study the entanglement structure and compute the OSEE for vectorization." However, Operator–space entanglement entropy (OSEE) is introduced for the first time in Sec.6.4.

I emphasize that these are minor points that by no means lower listed above numerous merits of the dissertation.

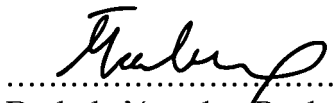
VI. Formal style

The thesis is written in good technical English and obeys all scientific requirements concerning the text, bibliography, and graphical material. The basic ideas, analytical treatments, and results of numerical simulations are described appropriately.

VII. Conclusions

The thesis is of high scientific quality concerning the content and the presentation. It confirms the deep understanding of the related physical formalisms and numerical methods by Ms. Gabriela Wójtowicz. Moreover, the thesis will serve as a durable publication in the field of quantum transport and as a basis for further investigations of interacting, driven, dissipative open quantum systems.

The scientific quality of the thesis is excellent. I recommend admission for Ms. Gabriela Wójtowicz to the subsequent stages of the Ph.D. procedure and the public defense.



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