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Date: 26 September 2025

Examiner report on the PhD thesis of Gerardo Suárez:
"Open Quantum Systems Beyond the Markovian Regime"

I have agreed to assess this thesis due to my interest in open quantum systems and strong coupling thermodynamics concepts, such as mean force corrections.

This is an interesting thesis, reporting on theoretical physics work by the PhD candidate, Gerardo Suárez (GS). The thesis investigates accurate and numerically efficient modelling of open quantum systems dynamics. A numerical method to efficiently solve the bath correlation functions is developed, and later used.

The thesis has 4 parts with a total of 17 chapters.
In **Part I** the candidate recaps essential concepts in open quantum systems, including correlation functions and power spectra. The candidate then introduces a number of methods of how correlation functions can be approximated, particularly the decaying exponential method. They also give a helpful table, listing properties of these methods and recommendations of when each is most useful.

In **Part II** the candidate recaps methods of modelling the dynamics of open quantum systems, including the Redfield equation, HEOM and Pseudomodes. Following standard heat current definitions, they give the formal expression for these currents using different open quantum system methods. GS also highlights the impact of a non-commuting Lamb shift. A comment is made about that the existing heat current definitions are not appropriate for the non-Markovian case, but a clear exposition of what is the issue is missing and no answer is given.

Steady state concepts are introduced in **Part III**, particularly the mean force (MF) Hamiltonian, and this section contains results derived by the candidate. In particular, GS here calculates a second-order correction for the MF Hamiltonian. The actual result is hard to decipher, as it still has to be put together from several other equations. A summarising paragraph of what the 2nd order corrected MF Hamiltonian's form is, as well as a discussion of limiting behaviours and comparison to literature are missing.

Somewhat strikingly GS does not refer to highly relevant work of others on the topic of interest. Missing references include a 2021 PRL [10.1103/PhysRevLett.127.250601] by this assessor deriving the general second order correction to the MF state – highly relevant for the student's aim. This PRL is not hard to find, i.e. it is referenced in the review article [91] from which the candidate has reproduced a figure in their thesis as Fig. 13.2. The candidate should have contrasted their 2nd order solution with the 2nd order solution occurring in the literature. Section 13.6 where the connection between MF Hamiltonian and MF state is made would have been a possible place to do so. Comparison to further references is also missing.

In section 13.7 GS develops the MF Hamiltonian to second order for the spin-boson model, and plots the results for a specific spectral density. The results show good agreement of the Redfield & Cumulant method with the reaction coordinate method at low coupling, while at higher coupling discrepancies can be seen (as one may expect when the coupling is no longer "weak"). Again, astonishingly, no comparison is made to the contemporaneous literature, such as the 2nd order MF state calculated by this assessor for the spin-boson model, reported in 2024 NJP [10.1088/1367-2630/ad4818] which was on the arxiv since 2022. It appears that GS and the 2024 NJP perform very similar second order derivations, for the same spectral density. Or perhaps they differ. Either way, a comparison should have been made.

Finally, in **Part IV** the candidate discusses the spin-boson model as an application, and correctly comments on the presence of the localisation-delocalisation phase transition. Fig 14.3 (c) and (d) show that all of the plotted master equation and numerical solutions give reasonable results. Fig 15.3 shows that for a spectral density with a large width, the GKLS approach does not capture the true dynamics while other methods are consistent with each other. In sections 15.1 and 15.2, the candidate discusses special limits of the spin-boson model which occur in the literature, including [47]. Fig 15.7 shows good state fidelity of the cumulant equation, which can be numerically solved much faster than HEOM, for a larger parameter range.

In chapter 16 a heat transport analysis is presented for a two qubit machine. GS finds that the cumulant equation tends to the exact solution even for long times when more parties are involved. Reference to relevant current literature discussing heat transport is missing, for example N. Anto-Sztrikacs, F. Ivander, D. Segal, *J. Chem. Phys.* 156 (21): 214107 (2022), 10.1063/5.0091133. Chapter 17 discusses the damped harmonic oscillator, including Kerr non-linearities. The thesis ends with a short conclusion and outlook.

The thesis is written in reasonable English and includes equations, figures and references. The candidate's results are of some interest, particularly the improvement in speed in calculating some open quantum system properties. However, unfortunately, the layout of the material is not structured very well. Too many sections are introduced just to provide background, and there is limited clarity on what is the students' reproduction of existing literature and what are new scientific results. A clear direction of the thesis is missing. Additionally, figures are often very small, and would not be decipherable in printed form. Figures should also not appear in the footnote section. Some sentences are grammatically incoherent or incomplete (e.g. section title of section 11.1.).

All in all this PhD thesis reaches an acceptable level, correctly discussing a number of existing methods to solve open quantum systems, and making improvements to numerical methods that reduce the computational load while still providing a faithful representation of the dynamics. I highlight here also the candidate's contributions to improving the open source package QuTip for users around the world. **I recommend the work for the award of PhD.**

signed: Janet Anders

Further comments:

- In section 2.2. it is stated that the system-bath interaction generates entanglement. But this seems not necessarily true – could the generated correlations not also be of classical nature?
- There are quite a few typos that should be fixed, eg "We being by" -> We begin by, and "desity".
- In Fig 10.1. the system S is shown to still couple to the bath after a reaction coordinate (RC) has been extracted. This seems inconsistent with the Hamiltonian (10.10) where the system only couples to the RC and the RC couples to the bath.
- Q is defined as the heat current. This is slightly confusing because often the heat is denoted by Q, and its current would then be $\dot{Q}$.
- in Eq. (13.7) the traces should carry a subindex B. Without it the right hand side is a real number and does not define and effective system Hamiltonian.
- Referring to the spectral density (1.65) and (15.3) as "underdamped" is misleading. In contrast to "overdamped" dynamics, "underdamped" dynamics occurs when in the equations of motion the second order derivative cannot be neglected. This occurs independent of the frequency dependence of the spectral density. Similarly, what is called the "overdamped spectral density" (15.2), is usually called "Ohmic".