Reply to Referee #2

September 20, 2019

We thank the referee for their careful reading and for taking time to communicate many detailed comments, suggestions and questions. This is much appreciated and in the revision, we have taken the referee's points into account.

In the following, we insert our comments (marked by •) into the referee's text *which is in italics.*

1.1 Recommendation explained:

On the one hand, I found the paper convincing of the results presented there. I felt confident that the author performed a careful and thorough proof. On the other hand, I found that the explanation of some very important points is inadequate or completely missing: it relies on familiarity with the author's previous work "M. Konenberg, M. Merkli: Completely positive dynamical semigroups and quantum resonance theory" [1] and does not stand on its own. I came away with too many questions to be able to recommend this paper for publication as it stands. Therefore, I recommend that a major revision is warranted. I explain my concerns in more detail below. I ask that the authors specifically address each of my major comments and overview suggestions in their response.

• The current manuscript has grown out of several years of research and previous papers on the topic, in line with the dynamical resonance theory. Those papers analyze the dynamics of open systems, but it was not realized that the method actually proves the master equation approxiation until the recent paper [1] (Könenberg-Merkli, 2017), which is closest to the present work. We believe that [1] has the disadvantages that (i) it is formulated in a rather technical, curt way, and (ii) it contains a mistake. In the present paper, we give a detailed explanation of the dynamical resonance theory (on which [1] builds) and we de-emphasize some technical aspects. For instance, we limit as much as possible the use of the heavy definitions and notations of the C^* and von Neumann algebra theory in which the method was originally phrased. We have been encouraged to write the present text after presenting the results recently at several conferences. And several researchers in theoretical physics have mentioned to us that they did not know about our results, which they qualified as important in the field. The reason, so we have been told, is partly that [1] is hard to understand for the general theoretical physicist. An important goal of the present paper is to make the methods and results known and accessible to a wider audience. We also present a correction to the mistake in [1] mentioned above.

So yes, the current paper is supposed to stand on its own. This does not mean that we have the space to derive all details. For instance, the result about the spectral analysis of the deformed Liouvillian is a technical theorem which we simply use without derivation (see the text after the figure). Other facts which we find clear, but maybe the uninitiated reader does not, might not have been explained, and we are grateful to the referee to have made the effort to point those out to us.

1.2 Structure of the review:

Major comments that motivated my decision can be found in Sec. 2.1. Overview of the result and further suggestions for revision can be found in Sec. 2.2. Minor comments are in Sec. 2.3, followed by references.

2.1. Major comments

The main concern I have about the paper is that multiple facts are stated without proof or reference. Some of these facts might be known to the reader of [1], as the explanations in that work are clearer. Still, even though [1] does illuminate the meaning of some statements of this manuscript, the statements there were never phrased as Lemmas, therefore I feel that referring them here as common knowledge is inappropriate. Below is the (possibly incomplete) list of statements that suffer from this problem:

a. Page 3: "the reservoir is spatially asymptotically close to equilibrium" - what is the definition of this spatial distance of equilibrium and/or where can it be found?

• We have added definitions explaining the notion of "spatially asymptotically close to equilibrium" in the text after (2.7). We have also included two new references in this regard, the books by O. Bratteli and D.W. Robinson and the book by R. Haag.

b. Page 6: the shorthand notation $e^{i\omega t}g$ *is not explained, if it implies elementwise multiplication* $e^{i\omega(k)t}g(k)$*. Variable* r *is never defined. Variable* Σ *is meant to represent angles in polar coordinates, but it is also stated in an ambiguous way. When* Σ *appears later on Page 14 it is also not clear whether* u *or* Σ *are angles. The footnote on Page 15 finally clarifies it, but it shouldn't be that hard to find! Normally that would be a minor comment but note how this creates a feeling that this manuscript is a second part of some work where this notation was defined in the first part.*

• Right, the variable r should have been $|k|$. We have fixed this and defined the meaning of $e^{i\omega t}g$ as well as the polar coordinates.

c. Page 10: "Liouville operator for the resonance located at the origin." Resonance theory has not been defined at this point, so this phrase is confusing. Even after reading the rest of the paper and [1] this phrase is still confusing.

• The phrase in question describes content of papers [16,4] (not what the referee calls [1] in their report (which is [18] in our original manuscript)). Nevertheless, we have rephrased this now.

Also on this page there's a few lines discussing the relationship of this work with [1]. Please say whether this work can be read independently, or the knowledge of the proofs in [1] is necessary to understand the math here. Ideally, please include a list of results that you do not prove but use, and where can they be found. Here under a-g I tried to collect such a list, but I may miss something in the later part of the paper.

• We believe this is now done in the text, thanks to all the modifications inspired by the referee.

d. Page 12: the statement "any vector ... can be approximated arbitrarily well" is given without proof or reference. Thanks for explaining it with an example! Still, I'd like to see one of the following: (1) a proof (2) a reference to a proof (3) state that this is a conjecture that you (and other people in the field) believe to be true but do not include the proof for brevity (4) state that it is a conjecture and the proof is postponed for future work (5) state that it is an obvious/textbook fact and every educated reader should be able to see it for themselves. You see that either of the five possibilities carries a different weight, while the text as written leaves the reader wondering which one of the five is implied. Only on page 23 this fact is explained in more detail, and the reference to [1] is given.

• The statement is a general fact from algebraic quantum theory. We have added a reference now. In the finite dimensional case, the properties in question, cyclicity and separability, are fairly easy to derive, and this is done in the text.

e. Page 13: just a few lines after you say that we're not gonna use the definition of J, and by extension, L_λ, the properties of these objects are immediately used: you state that L_λ annihilates the steady state. This leaves the reader with a sense of unease: which properties of this undefined object are we gonna use later in the paper? I agree that the steady state property may be obvious to some readers, since L_λ is just the total evolution operator. Still, as above in d, you do not state whether this is a trivial fact or it needs a proof.

• This is not a trivial fact (even though it is quite well known). It needs a short proof which is now provided. The proof relies on a couple of properties of the modular conjugation J which we are discussing now as well.

f. Page 14: the self-adjoint property of an undefined operator L_λ is used without a proof or reference.

• We have added the explicit action of J and hence L_λ is defined now. We have introduced a new reference (Fröhlich-Merkli) where it was shown that L_λ is self-adjoint for all λ (Theorem 3.1 in that reference).

Also the way the text about spectral deformation is phrased, it is not the only condition when the following analysis holds. Similarly (A) is not the only assumption under which spectral deformation holds. This foreshadowing however doesn't lead to anything later in the paper. In the results section as well, nothing about the assumption (A) is mentioned. Please state clearly what assumptions have been used to prove your results, and maybe comment on the possibility of a more general proof in the conclusions or introduction (which are both absent from the paper right now).

• We have moved the condition (A) to the front of the paper now and we explain alternative techniques. The upshot is that under (A) we obtain the strongest results but need the biggest regularity of the form factor g, as we explain.

I would also appreciate a comment on how to check for condition (A) for a realistic g(k), see the Overview section. The footnote on Page 15 mentions exponential decay of the correlation function as a physical interpretation of (A), but is it sufficient or only necessary?

• Condition (A) is technical to state and we now give another condition (H) which implies (A), and which is more user friendly (Hardy functions). We give a family of physically relevant form factors which satisfy (A) in the remarks on page 7, and we show how to check that they do satisfy (A). Exponential decay of the correlation function is not necessary for the theory, even though it is assumed in the present paper. Polynomial decay will suffice, but the error estimates in the main results become only polynomially decaying in time as well, as opposed to exponentially decaying. We explain this in the text now and mention, that the detailed analysis for these results are only partially completed so far.

g. Page 18: $\gamma(\lambda)$ appears without definition. Is it γ_{FGR} defined on Page 7? Why is it $< (3/4)\theta_0$? It is again stated without proof or reference.

• $\gamma(\lambda)$ was defined in (1.20) (numbering of the first submission). We now recall this definition on and we explain why $\gamma(\lambda) < 3\theta_0/4$. (The answer is that $\gamma(0) = 0$ and so the inequality holds for small λ.)

I'll be happy to provide comments on the remaining pages of the paper, after the requested revisions are implemented.

• We thank the referee for their dedication which we appreciate!

2.2 Overview

Bounding the error of open system evolution approximations is an open problem. The approach taken by the author allows to obtain a powerful theoretical result about those errors. Two approximations to the true open system dynamics are considered: the dynamics driven by the Davies generator, and a renormalized version of it. Davies generator is used widely in the field, while the renormalization is also doable in principle for applications, but has yet to see a use either in theory or numerical experiment. The strengths of the error bounds of this work are as follows:

1. Arbitrarily long time is allowed. Taking advantage of the approach to steady state of the dynamics, the author shows the error becomes bounded by a small number in a long-time limit. This is an intuitive result, but the proof illuminates the relevant system properties affecting it.

2. Arbitrary initial state is allowed. While it is hard in practice to know the initial state of the system and the reservoir, the existence of approximate semigroup dynamics independent of the initial correlations is a surprising result, as many works in the field anticipated non-Markovian description in that case. Note that the evolution of entangled initial states of system and environment is given by Eq. (2.40), that is not presented in the results section, but only referred to. The results section is all about disentangled initial states of the system and environment.

• Yes, the result section is about disentangled initial states – there is not enough space to properly discuss the ramifications and relation to markovianity for disentangled ones. We are planning on analyzing this issue, based on the expansion (3.45), in a separate work.

3. The correct steady state dressed by the interaction with the environment is organically part of the formalism. Few works on open system take that into consideration.

4. Arbitrary spectral density of the bath compared to free space boson spectral density considered in [1]. This is a straightforward generalization.

The weaknesses of the results, where other work or future work would be complementary, are:

1. Generally speaking, the work is aimed at mathematical physicists and not at any practical application for numerical simulation of open systems. And not at theoretical results that seek to give any form of guarantees about practical applications. Specifically, big-O notation used in the presentation of the bounds contains constants C, λ_0 that may depend unfavorably on system parameters. For instance they may contain a power of the system Hilbert space dimension and render the result inapplicable for many-body systems (e.g. for n qubit system the coupling λ_0 would need to be exponentially small with n). A suggestion to the author would be to at least explicitly list which parameters of system and environment do constants C, λ_0 depend on.

• The referee is right in that the error bounds, so far, may depend on system parameters in an unfavourable manner. In particular, it is not known so far how to extend the analysis to a small system with infinitely many levels; this does not seem to be an easy problem. We have added a remark discussing this at the end of Section 2, including a suggestion of how to implement a numerical check.

2. The uniform in time bound on the error is only given for the evolution of the diagonal matrix elements of the density matrix, thus leaving the accuracy of the description of coherences an open question.

• This is not correct. In the results of Sections 2.7 and 2.8, both populations and coherences are controlled. In particular, the Markovian approximation is shown to be valid for all times and for populations and coherences. It is only in the approximation by an asymptotically exact CPT semigroup (Section 2.9) that coherences are not controlled, and this only for a window of intermediate times $\lambda^2 t \approx 1$.

3. The approach is only valid for time-independent Hamiltonians. Any drive of the system, e.g. control pulses, cannot be described by the resonance theory used in the construction.

• This is not true. The resonance theory is applicable also for time-dependent Hamiltonians. We have added relevant references: [Merkli-Starr] and [Abou Salem-Fröhlich], [Bach et al].

4. The bath is required to be free bosonic, coupled linearly to the system and thermal, thus Gaussian for the results presented in the results Section. For the more general result

(2.40), the bath is still free bosonic and coupled linearly to the system, but any initial state is allowed. There are two caveats: in the partial transpose doubled Hilbert space there should be an approximation of the initial state as a rotation of partial transpose of the thermal state. The error of that approximation carries over to the error of the semigroup. Since this error is a norm difference on the combined (and partially transposed doubled) Hilbert space, which is infinite dimensional, one needs to be careful with what it actually means for system observables. Please add a comment about that to a revised text (at the moment it is only briefly discussed deep in the proof, on page 23).

• The initial states we consider are of the form (2.18) (this refers to the numbering of the first submitted manuscript the referee bases his report on). Yes, Ψ_0 is obtained from $\Omega_{\mathrm{SR},\beta,\lambda}$ by application of the operator B', and this operator acts on an infinite dimensional Hilbert space. But B' is a bounded operator. After the 'rotation', B' shows up only in the vector $[(B')^*\Psi_0]_{\bar\theta}$, as *e.g.* in (3.45). Error terms involve the norm of this vector, so those errors depend on θ and Ψ_0 (which also determines B'), but they do not involve the system observable (X in (3.45)).

In the analysis of the asymptotically exact CPT approximation, on p.32, an additional operator D' is introduced in (4.27). This is indeed an unbounded operator, which connects the renormalized vector with the coupled equilibrium $\widetilde\Omega_0 = D'\Omega_{\mathrm{SR},\beta,\lambda}$ *exactly* (as explained after (4.27)). Now the remainder estimates involve an upper bound on the norm of $[(D'B')^*\Psi_0]_{\bar\theta}$, see *e.g.* (4.30). But again, this estimate is entirely decoupled from the observable X and so it does not restrict the choice of X. That $[(D'B')^*\Psi_0]_{\bar\theta}$ has finite norm is shown in Lemma 3.4 of [18], which is referred to in footnote 18 of the present manuscript.

We would like to keep the text as it is here – the referee is right that one has to be careful, technically, but it is not the aim of the current paper to present the details of this particular point. It involves the control of a Dyson series which is not very difficult, but somewhat tedious. This has been done in [18] and is referred to here.

Second caveat is that whatever the initial state is, the majority of the infinite number of bath degrees of freedom should still be thermal at a given temperature. The author comments on that briefly on Page 3, saying about the requirement to be "spatially asymptotically close to equilibrium", but that requirement is never stated explicitly. I would suggest to elaborate on this in the revision.

• This is the same observation as point *a* the referee makes above. We have modified the text to explain in more detail what this condition means, please see the new text in Section 2.2.

5. The interaction $g(k)$ (more carefully, a deformation of it) has to possess an analytic continuation into a strip of finite width in the complex upper half-plane. This condition has a physical interpretation, that is alluded to on Page 6. But it is not completely clear from the text of the paper what physically reasonable functions obey it. For example, does $g(k)$ = const obey it? And would it lead to any divergences elsewhere? Please address these questions, or give other examples you consider relevant.

• We have addressed this in the Referee's question f above. $g(k) = const$ is not admissible – we believe this is now easily understandable with the new text. ($g(k) = const$ would also not be admissible for other reasons than condition (A), as this function must be square integrable.)

6. Possibly related to 5, all the relaxation and decoherence rates in the system have to be of the same order in the coupling as the Fermi Golden rule rate. This is true except for very contrived systems or a strong coupling limit.

• A clarification: For the basic result of the resonance theory, Result 1 (Section 1.7, estimate (2.18)), the relaxation and decoherence rates do *not* have to be of the same order in the coupling. This is actually explained in the text after (2.22). To show our Result 2, (2.27) we do assume that the rates are all of second order in λ. This is natural, since this result says the dynamics is approximated by the Davies generator, which is exactly of second order in λ.

Feel free to use the points of this section as the Introduction. In the current version, I see no reason why the introduction section is missing. I think the paper will benefit greatly from its inclusion.

• Thank you. Yes, we made an introduction and used the points you raise.

2.2. Minor comments:

Page 2: "to describe irreversible effects it is necessary to pass to a limit..." depending on one's definition of irreversibility and its description, a reader may disagree with this statement. E.g. chaotic classical systems may be reversible formally, but irreversible in practice as the numerical precision needed to revert their dynamics is required to be exponentially more precise with time.

• Right. We do not want to enter into the details of a precise definition of irreversibility. We simply mean that the small system is driven to some final state showing, for instance, thermalization and decoherence. We have slightly changed this sentence now.

Also a note on grammar: single quotation marks like 'continuous set' are used in many places in the paper, and I feel they can be dropped in many of those places.

• Ok, done.

The equation 1.6 for the Fock space is using conventions that I am unfamiliar with. The definition of the Fock space in [1] was much more reader-friendly for physics community.

• Ok, we have adopted that notation now.

Page 4: it might be common knowledge, but maybe mentioning how do we know that eigenvalues and eigenvectors of $\mathcal{L}$ exist (as opposed to the general Jordan form) would be nice.

• This property is *assumed* here, as stated in the text. It is commonly satisfied (we have added footnote 4) but there are natural situations where the property is not satisfied. This has dynamical consequences which are under investigation (deviation from exponential decay). We do not feel we should discuss this in more detail, as results are pending.

Page 6: Repeating what was said in the overview, please say more clearly if the current status of the proof necessitates the exponential decay of correlations, and the proof may be extended to power law decay in the future.

• The current status is that we assume condition (A) (or (H)), which implies exponential decay of correlations. We are working on extending the theory to include the case of power law decay of correlations. This is stated in the points after condition (H) now.

A factor of i appeared in 1.16 compared to 1.11, which implies a different definition of ϵ_j *was used for those two formulas.*

• Right. We have introduced an i in (2.11) now to make the notation homogeneous.

Page 9: It was confusing to me that you follow the diagonal of the density matrix in the eigenbasis of H_S*, while the steady state is diagonal in the eigenbasis of* $\tilde{H}_S$*. I even thought it is a misprint, but then looking at the proof I see that this is indeed what's proven. Please comment why the unperturbed Hamiltonian eigenstate populations can be known with better accuracy than other matrix elements. Will the bound 1.32 persist for eigenstate populations of* $\tilde{H}_S$*?*

• The phases due to the free system dynamics are not compatible with the those of the approximate dynamics. This is the reason why populations better approximated than coherences (in the populations, those free system dynamics phases do not appear). We have added formula (1.32) explaining this in a precise way. We do not believe that (1.32) (as in the referee's question) will hold for eigenstate populations of the renormalized Hamiltonian, again, since different phases are generated by $H_{\rm S}$ and $\widetilde{H}_{\rm S}$.

Page 10: Sentence "An approximate system dynamics valid for all times was..." maybe needs a new paragraph. I didn't realize you're talking about a different result after in-depth discussion of [1].

• Ok, done.

Title: the motivation for stating that your method 'overcomes the weak coupling limit' is found in the abstract. You say "time must not exceed an upper bound depending on the system- environment interaction strength (weak coupling regime). Here, we show that the Markov approximation is valid for fixed coupling strength and for all times." It implies the definition of WCL as a property of the evolution. I feel a more intuitive definition of WCL is that the coupling strength is smaller than all other energy scales in the system, including 1/evolution time. If you phrase it that way, I feel like less people will have an issue with the title. I personally am fine with the title and abstract as they are.

• Point taken. We have modified the title and abstract. A change in title is not usually advisable, we believe (for instance, the paper is already on the arXiv and now it will have two titles...) However, one of our goals is to reach a wider readership within the physics community (not only mathematical physicists) and so we are happy to follow and value this input from the referee. We would be open for a further change here, if the referee gave their opinion.

References: while there are no strict requirements on reference formatting at submission, I would suggest putting references in the order of appearance in the text, as opposed to current alphabetical order.

• We will go through this exercise if the manuscript gets accepted for publication in the AOP.