Reply to the Comment on “General Non-Markovian Dynamics of Open Quantum System”

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This is the reply to the comment by McCutcheon et al. on our paper [1]. In this reply, we show that the comment [2] is incorrect, because: (i) negative frequency modes are physically observable (e.g. [3]); (ii) the single-mode renormalized Hamiltonian with negative frequency, for the open system considered in [1], has a finite lower bound; and (iii) therefore it has no thermodynamic instabilities. Below we provide detailed proofs of the three points listed above. In addition, we also point out many other errors in the comment [2].

The main part of the comment [2] just repeats some calculations already published in [1], regarding the first application studied in [1]. Explicitly,

- The 2nd paragraph in [2] repeats the basic formulas with the master equation that we derived in our previous works and used in [1]. Contrary to the implication in [2], these formulas were not derived in Ref. 2 of the comment.

- The 3rd paragraph presents the main calculation in [2], but it only repeats a very small part of the derivations given in our paper [1].

In our paper [1], we proved in general that: (a) a dissipationless-associated localized mode exists only in the regime with \(J(\omega) = 0\); (b) we applied it to the first application in [1] (with the spectral density \(J(\omega) = 2\pi\eta\omega/\omega_c)^{s-1} \exp(-\omega/\omega_c)\), which is defined for positive frequencies, where \(s < 1\) is sub-Ohmic, \(s = 1\) Ohmic and \(s > 1\) super-Ohmic environments, and \(\omega_c\) is the high frequency cutoff). Therefore, \(J(\omega) = 0\) for \(\omega < 0\), so that a localized mode can exist in the \(\omega < 0\) regime; (c) In [1] we further proved that when \(\eta\omega_c\Gamma(s) > \varepsilon_s\) (the strong coupling regime, where \(\Gamma(s)\) is the gamma function, and \(\varepsilon_s\) is the system’s single-particle energy), a localized mode with negative frequency \(\omega' < 0\) appears.

Following our paper [1], the comment [2] assumed the existence of a localized mode, i.e. the steady-state limit of Eq.(12) in [1], and afterwards they repeated our approach to prove that the localized mode is negative, a result which was already given in our paper, see after Eq. (13) in [1].

The only criticism in this comment [2] (i.e., the 4th paragraph in the comment) is about a very small fraction of the content of [1]: i.e. the physical interpretation of the steady-state limit of Eq.(12) in [1].

- Our interpretation to this steady-state limit is that it leads to a dissipationless dynamics because the steady-state solution keeps oscillating forever, see the discussion after Eq.(13) in [1].

- The comment in [2] argues that the dissipationless regime for strong coupling is unphysical, because it corresponds to a range of parameters where the renormalized Hamiltonian of the system is unbounded from below (i.e. thermodynamically unstable).

It should be obvious to any careful reader that the comment [2] is not relevant to the vast majority of [1], which provides the general non-Markovian dynamics for open systems coupled to the environment via particle-particle exchanges. In fact, three applications (including both fermion and boson systems) are studied on [1] to illustrate the general non-Markovian dynamics given there. The comment does not apply to two of them, but to only one of these three applications, i.e. the example of a nanocavity or a nanomechanical resonator coupled to a reservoir with an Ohmic-type spectral density. For the three applications studied in [1], we present explicitly the analytical solutions, Eq.(12), Eq.(15) and Eq.(17), of the exact non-Markovian dynamics described by the Green function \(u(t)\). The comment [2] focuses only on a subset of a solution [Eq.(12)] of the first application, i.e. the physical interpretation.

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of the steady-state limit of Eq. (12) in [1]. Thus, the scope of the comment [2] is minuscule, compared to many other results in [1], which are not addressed at all by [2].

The authors of [2] do not provide valid justifications to their arguments; namely, how a single-mode renormalized Hamiltonian with negative frequency in an open system is not bounded from below in the steady-state limit, and how this would presumably lead to a “thermodynamically unstable” solution.

In the following, we shall show that the comment [2] is incorrect.

1. **Negative frequency modes are physical.**
   - It is well-known that in free-field theory, the negative-frequency part of light is directly related to its positive counterpart (the photon is also its own antiparticle), and photons with negative frequencies correspond to backward photon propagations in time. Thus, one only needs to consider the positive-frequency part. However, when photons propagate in a medium, generating negative-frequency modes that are distinct from the positive-frequency mode is physically possible.
   - Such a negative-frequency radiation phenomenon was indeed recently observed experimentally, see Ref. [3].
   - The negative-frequency localized mode induced via system-reservoir couplings in [1] is physically interesting, and it may provide another nontrivial system for negative-frequency radiation, which could be experimentally observed in the future.

2. **The renormalized Hamiltonian of our open system is bounded from below, so the comment [2] is incorrect.**
   - First of all, one can easily show that the total Hamiltonian in [1,2], $H_{\text{tot}} = H_S + H_E + H_{\text{int}} = \omega_0 a^\dagger a + \sum_k \omega_k b_k^\dagger b_k + \sum_k V_k (a^\dagger b_k + b_k^\dagger a)$, commutes with the total particle number of the total system $N_{\text{tot}} = n_s + \sum_k n_k = a^\dagger a + \sum_k b_k^\dagger b_k$. Thus, the total energy and the total particle number are conserved. An initial state of the total system, $\rho_{\text{tot}}(t_0) = \rho_S(t_0) \otimes \rho_E(t_0)$, is used in deriving our master equation, where the system’s initial state $\rho_S(t_0)$ is arbitrary, and the environmental initial state is a thermal state $\rho_E(t_0) = \frac{1}{Z} e^{-\beta E}$. The average total energy and the average total particle number for this initial state are given by $\langle H_{\text{tot}} \rangle = \omega_0 (n_s) + \sum_k \omega_k \langle n_k \rangle = E_{\text{tot}} \geq 0$, and $N_{\text{tot}} = \langle n_s \rangle + \sum_k \langle n_k \rangle$, and both are indeed independent of the coupling $V_k$. Thus, the system is physically well-defined for an arbitrary system-environment coupling strength, because this does not violate any physical law.
   - Now we can prove that the renormalized Hamiltonian in our system has a finite lower bound. The steady-state renormalized Hamiltonian $H_S = -\omega' a^\dagger a$, where $|\omega'|$ is a finite real number (which is indeed very small $< 0.05$, as shown in the insert of the second graph of Fig. 1 in [2]). Since the average total particle number $N_{\text{tot}}$ is conserved, the lowest bounded energy for the renormalized Hamiltonian is $E_{\text{lowest}} = -\omega' |N_{\text{tot}}|$, if all particles dissipate into the system. This cannot happen for an open system, and it also breaks the total energy conservation. Consequently, the particle number in the system must be smaller than $N_{\text{tot}}$. Thus in the steady-state limit, the steady-state renormalized energy of the system always obeys the inequality $\tilde{E}_S \equiv \langle H_S \rangle > E_{\text{lowest}}$. Namely, the steady-state renormalized Hamiltonian is bounded from below.
   - The renormalized Hamiltonian of the above system in the steady-state limit can become unbounded from below only if the square of the renormalized frequency is negative, i.e. $\omega'^2 < 0$, or the renormalized frequency is an infinitely-large negative number, i.e. $\omega' \rightarrow -\infty$. In our system, the first case cannot occur because $\omega'$ is always a real number by the definition of the renormalized frequency given by Eq. (3a) in [1]. The second case also does not occur because it has been demonstrated that the renormalized frequency is a negative but finite real number, see Fig. 1 in the comment [2]. This further proves that the steady-state renormalized Hamiltonian is bounded from below in our system.
   - In general, the physics of open systems is not governed by the renormalized Hamiltonian. Its dynamics is described by dissipation and fluctuations in a non-unitary way, through the master equation of the reduced density matrix. For open systems, only talking about the renormalized Hamiltonian of the system is not physically meaningful.
   - Mathematically, in the steady-state limit, the whole dynamical problem of the open system has already been solved; namely, one can obtain the steady-state solution of the reduced density matrix without using the steady-state renormalized Hamiltonian. In fact, the solution of the reduced density matrix is explicitly determined by the Green function $u(t)$, as it was shown recently in [5]. Deriving the solution of $u(t)$, as done in [1], has fully solved the dynamics of the system, as emphasized in [1]. Thus, the renormalized Hamiltonian in the steady-state limit is irrelevant to the physics of the system.
3. Since the steady-state renormalized Hamiltonian is bounded from below, there are no issues regarding thermodynamic instabilities.

- The comment [2] argued that since the steady-state renormalized Hamiltonian is unbounded from below, it has no ground state, so it is “thermodynamically unstable”. This is certainly not a question now, because, as we have shown in point (2.) above, the steady-state renormalized Hamiltonian has a finite lower bound. To be more specific, there exists only one localized mode for the system studied, as we have shown in [1], and its frequency $\omega'$ is negative but finite in the steady-state limit. Meanwhile, the total particle number is conserved. Thus, the steady-state renormalized Hamiltonian $\tilde{H}_S = -|\omega'|a^\dagger a$ could lead to the lowest (or ground state) energy of the system given by $E_0 > -|\omega'|N_{\text{tot}}$, where $N_{\text{tot}}$ is the total particle number. This leads to the thermodynamic stability condition (i.e., the H-stability$^1$), discussed in the literature [3]. Thus we prove that the main claim of [2] (that the renormalized Hamiltonian with a negative frequency has no ground state, so it is “thermodynamically unstable”) is incorrect.

- Moreover, the first application studied in [1] is a single-mode nanocavity (photons) or nanomechanical resonator (phonons). Talking, as in [2], about thermodynamic instability (which is about instability of matter [3]) for such a system is not physical, because matter is made of atoms, not photons and phonons.

The above three points (1,2,3) provide detailed proofs that the comment in [2] is totally incorrect. But the comment [2] contains additional errors:

4. The 5th paragraph in [2] is also erroneous.

- In the 5th paragraph in [2], the authors first comment that the existence of localized modes for a spectral density with band gaps, in other two applications in [1], is a natural result. But for the first application, the Ohmic-type spectral density of the environment is $J(\omega) = 0$ for the regime $\omega < 0$. This means that the regime $\omega < 0$ can be regarded as a generalized band-gap regime for a free bosonic environment. The existence of localized modes for the first application and for the other two applications in [1] originates indeed from the same reason, i.e., $J(\omega) = 0$ for a frequency range in which the localized mode locates, see after Eq. (10) in [3]. Thus the comments in [2] on the first application and on the other two applications contradict each other.

- The comment [2] also claims that the oscillatory behavior for the super-Ohmic environment in the Ref. 2 of the comment [2], due to the suppression of the low frequency part of $J(\omega)$, is analogous to the result obtained for environments with band gaps in [1]. This is again incorrect. As we have proven rigorously in [1], localized-modes only exist in the regime $J(\omega) = 0$, see after Eq. (10) in [1]. If $J(\omega) \to 0$, but not strictly equals to zero, it is not possible to have a localized mode, and thus cannot have a dissipationless oscillation in the steady-state limit. This becomes clear for all the three spectral densities of Super-ohmic ($s > 1$), sub-Ohmic ($s < 1$) and Ohmic ($s = 1$) environments, $J(\omega) = 2\pi\eta\omega(\omega/\omega_c)^{s-1}e^{-\omega/\omega_c}$, where the high-frequency part ($\omega \gg \omega_c$) of the spectra is also suppressed (depleted), but no localized mode (no long-time oscillation) exits over that regime, contradicting their claim. Furthermore, in the supplemental material of [1], we presented a detailed calculation of the localized modes for a sharply-cut-off Lorentz spectral density, and showed that when the cut-off is removed, so that both the low- and high-frequency sides of the spectral density approach zero, then the localized modes and the corresponding dissipationless oscillations just vanish.

5. The last paragraph of the comment [2] makes another obvious error. In order to support their argument, [2] considers a different model, not studied in [1]: quantum Brownian motion, which has the system-environment coupling $H_{\text{int}} = \sum_k c_k x_k \dot{q}_k$. They argued that such a coupling is not only thermodynamically but also dynamically unstable (i.e., the square of the renormalized frequency $\omega'^2 < 0$). This part of the Comment is irrelevant to our work [1] because we did not study that model. Moreover, [2] provides an incorrect comment to their own previous works. Specifically,

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1 The so-called H-stability is a condition for the existence of the thermodynamic limit of the Helmholtz free energy for homogeneous macroscopic systems containing large particle numbers (about $10^{20} \sim 10^{30}$), for a Hamiltonian $H$ with an interaction potential for massive particles. For more discussions see [4].
• The comment [2] is not aware that this system-environment coupling is fundamentally different from the system-environment coupling considered in [1]. The former, in [2], breaks the conservation of the total particle number at the quantum level, but the later, in [1], does not. To see this very easily, we rewrite their Hamiltonian in second-quantized form: 
\[ H_{\text{int}} = \sum_k \epsilon_k (a^\dagger b_k + a b^\dagger_k + a^\dagger b^\dagger_k + b_k) \]. It is obvious that the last two terms in the Hamiltonian represent particle-pair production and annihilation, and thus these terms break the conservation of the total particle number of the total system. Physically, it is the breakdown of the total particle number conservation that could induce the dynamical instability in the strong-coupling regime in their model, but not in our systems. Because of the violation of particle number conservation law, we did not study this model in our theory.

• Although it is irrelevant to our work in [1], it may still be worth pointing out that even for the above coupling with a dynamical instability, one cannot say that the corresponding dynamics is unphysical. Whether or not such a dynamical instability is physically meaningful or meaningless depends on the problem one wants to study. For example, in the pioneering and original study of quantum Brownian motion by Caldeira and Leggett [6], they explored the quantum tunneling of a dissipative system through a harmonic oscillator coupled to a thermal bath, to see whether its quasiclassical dynamics is given by the classical damping equation of motion with the same potential. Thus, using the above system-environment coupling, they suggested to add a counterterm into the total Hamiltonian to remove the dynamical instability induced by the renormalized-frequency effect. However, as Caldeira and Leggett also pointed out in their original paper, when one tries to study the physical nature of the system coupled with its environment, the frequency-renormalized effect (although it could lead to a dynamic instability) has a real physical significance and must be taken into account. More information on this can be found in the detailed discussion on pages 388-390 in [6]. This proves that the naive claim given in [2] (that the solution is unphysical when it has an unstable dynamics) is incorrect.

• Indeed, dynamical instabilities naturally occur in a variety of physical phenomena, such as various chemical reactions, avalanches, chain reactions, nuclear fission, shock waves, implosions, explosions, phase transitions, among many other examples. There is no physical principle stating that dynamical or thermodynamic instabilities are unphysical. Indeed, the occurrence of a new-type of instability often implies a phase transition in the physical system that leads to the discovery of new physical phenomena.

In conclusion, we have shown that due to the conservation of the total energy and total particle number of the example under consideration, the steady-state renormalized Hamiltonian with a single-mode negative frequency is bounded from below. This directly proves that the comment [2] is incorrect. The comment [2] also contains many other errors and misunderstandings of fundamental physics. All the mathematical calculations in [2] just repeat some of the calculations in [1] and reproduce a minuscule fraction of the results in [1].

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