## Reply to the Comment on "General Non-Markovian Dynamics of Open Quantum System"

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The letter [1] presents three examples. For the steady-state solution of the first example, i.e., the dissipationless part of Eq.(12) in [1], the 2nd version of the Comment [2] claimed that "this [dissipationless] regime exists if and only if the total Hamiltonian is unbounded from below, casting serious doubts on the usefulness of this result." In the following, we shall show that this Comment is again incorrect.

The total Hamiltonian used in the first example in [1] is  $H_{\text{tot}} = \omega_s a^{\dagger} a + \sum_k \omega_k b_k^{\dagger} b_k + \sum_k V_k (a^{\dagger} b_k + b_k^{\dagger} a)$ . Diagonalizing  $H_{\text{tot}}$  leads to  $H_{\text{tot}} = \omega_b C^{\dagger} C + \sum_k \omega_k' D_k^{\dagger} D_k$ , where  $\omega_b = \omega_s - \int_0^{\infty} \! d\omega \frac{J(\omega)}{\omega - \omega_b}$  is the renormalized mode of the system, and  $\omega_k < \omega_k' < \omega_{k+1}$ . The operators  $\{C^{\dagger}, D_k^{\dagger}\}$  are all normal modes of the total system after a Bogoliubov transformation from the basis  $\{a^{\dagger}, b_k^{\dagger}\}$  [3], and  $C^{\dagger}$  is just the single-excitation given in [2]. In the continuous limit,  $\omega_k' = \omega_k$ . Thus, the first mistake made in [2] is that at operator level,  $H_{\text{tot}}$  is not given only by  $C^{\dagger}$ .

Secondly, Arai and Hirokawa proved [4] that the spectrum of the above Hamiltonian in the strong-coupling regime is unbound from below when the particle number in the renormalized mode  $\omega_b$  is unbound. However, due to the conservation of the total particle number,  $[H_{\text{tot}}, N_{\text{tot}}] = 0$ , where  $N_{\text{tot}} = a^{\dagger}a + \sum_{k} b_{k}^{\dagger}b_{k}$ , the total Hamiltonian can be written as a direct sum of decomposed Hamiltonians. Each decomposed Hamiltonian with fixed total particle number always has a lower bound for arbitrary coupling  $V_k$  [5]. A similar "unbound" ground state energy also exists for the total Hamiltonian of a Dirac particle in QED, where the possible trouble from the unbound ground-state energy in QED is avoided due to the total momentum conservation, i.e., the decomposed Hamiltonian with fixed total momenta has a lower bound for arbitrary QED coupling [6]. Thus, the second mistake made in [2] was not to consider the important role of the particle number conservation.

Furthermore, because  $H_{\text{tot}}$  is not simply given by the single-excitation  $C^{\dagger}$ , the third mistake made in [2] is that the possible energy divergence claimed in [2] is not applicable to the non-Markovian dynamics studied in [1]. Non-Markovian dynamics relies on the initial states of the total system. The exact master equation formalism given in [1] requires that the initial states of the total system must be a direct product state between the system and its environment. These states always carry a positive-definite total energy. This decoupling condition must be obeyed for any exact master equation derived from the Feynman-Vernon influence functional [7]. Otherwise one cannot carry out the influence functional and thereby would be unable to derive the exact master equation. Thus, due to the total energy conservation, the total

To be more specific, let us begin with the valid initial state:  $|\psi(t_0)\rangle = a^{\dagger}|0,\{0_k\}\rangle$ , in which the system initially contains one particle, and the environment is in its vacuum, i.e., the system and the environment are initially decoupled [7]. The corresponding energy of the total system is just the energy carried by the particle in the initial state, i.e.,  $E_{\rm tot} = \omega_s > 0$ . Solving exactly the Schrödinger equation with this initial state, the steady state of the total system is  $|\psi(t \to \infty)\rangle = \left[e^{-i\omega_b t} \mathcal{Z}\left(a^{\dagger} + \sum_k \frac{V_k}{\omega_b - \omega_k} b_k^{\dagger}\right) + \right]$  $\sum_k e^{-i\omega_k t} [\omega_k - \omega_s - \Delta(k) + i\gamma(k)]^{-1} b_k^{\dagger} |0, \{0_k\}\rangle$  which is a superposition of the renormalized mode  $\omega_b$  of the system plus all other possible modes  $\omega_k$  of the environment, where the first term gives the dissipationless part of the system in [1]. The derivation of this result is given in [3]. In the strong-coupling regime,  $\omega_b$  is negative, as shown in [1], but the energy of the total Hamiltonian is positive,  $E_{\rm tot} = \omega_s > 0$ , because the total Hamiltonian and the total particle number are conserved during the time evolution. Let us now extend the above solution to the initial states  $|\psi_n(t_0)\rangle \propto (a^{\dagger})^n |0,\{0_k\}\rangle$ , where  $n=1,2,3,\cdots$ , can be any arbitrary integer. The corresponding steady state of the total system is  $|\psi_n(t)\rangle$  $(\infty) \propto \left[ e^{-i\omega_b t} \mathcal{Z} \left( a^{\dagger} + \sum_k \frac{V_k}{\omega_b - \omega_k} b_k^{\dagger} \right) + \sum_k e^{-i\omega_k t} [\omega_k - \omega_s - \Delta(k) + i\gamma(k)]^{-1} b_k^{\dagger} \right]^n |0, \{0_k\}\rangle.$  The total energies of all these states  $E_{\text{tot,n}} = n\omega_s > 0$  (positive-definite). In fact, for all valid initial states and the corresponding exact solutions of the master equation given in [1], the total Hamiltonian is always positive-definite. This is consistent with the fact that the total Hamiltonian with fixed total particle numbers has a lower bound, due to the total particle number conservation. Thus, the above-quoted criticism in [2] is obviously incorrect. The Comment [2] ignored the validity of the exact master equation derived from the Feynman-Vernon influence functional to reach an incorrect conclusion.

The only correct part in the Comment is the last part of [2], where they pointed out that the problem exists in their own works, i.e., Refs. 3 and 4 in [2] for the quantum Brownian motion (QBM). This is because the QBM used a system-environment coupling  $H_{\text{int}} = \sum_{k} c_k x q_k =$  $\sum_{k} c'_{k} (a^{\dagger}b_{k} + ab_{k}^{\dagger} + a^{\dagger}b_{k}^{\dagger} + ab_{k})$ , which breaks the conservation of the total particle number,  $[H_{\rm int}, N_{\rm tot}] \neq 0$ . Because of this, the QBM will cause both dynamical and thermodynamic instabilities in the strong-coupling regime, as claimed in their Comment [2]. The authors of [2] did not realize that the instabilities of the QBM in the strong-coupling regime come from the breakdown of the total particle number conservation. Our studies focus on systems preserving the total particle number conservation and therefore do not have such problem (see more discussions in [8]). They mistakenly believe that the instability

other Hamiltonians.

- [1] W. M. Zhang, et al., Phys. Rev. Lett. 109, 170402 (2012). [2] D. P. S. McCutcheon, et al., Comment (unpublished). [3] See derivations given in the derivations given Supplemental Materials [URL].
- [4] A. Arai and M. Hirokawa, Rev. Math. Phys. 12, 10851135 (2000), see Theorem 6.3.
- [5] See Proposition 2.5 in the Report by M. Hirokawa [URL].
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