Generalized master equation with nonhermitian operators

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Abstract

By extending the mean-field Hamiltonian to include nonhermitian operators, the master equations for fermions and bosons can be derived. The derived equations reduce to the Markoff master equation in the low-density limit and to the quasiclassical master equation for homogeneuos systems.

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I. INTRODUCTION

An adequate description for low-energy phenomena of fermions is provided by the mean-field approximation in which particles move under the mean-field Hamiltonian; relaxation effects are not taken into account in this approximation [1]. The relaxation effects due to the reservoir, which are important to the irreversibility [2], have been discussed in the literature [1-7]. It was shown that loss and gain should be considered for such effects and that the loss comes from the imaginary part of the self energy[4,8] in the quantum master equation[6].

To include the self energy, it is reasonable to extend the mean-field Hamiltonian to include nonhermitian operators. It will be shown in section II that the master equation for fermions can be derived from such an extension, if we assume that the equation is symmetric with respect to particles and holes. The corresponding equation for bosons is obtained in section III. The nonlinear master equation is obtained in section IV. To compare with other stochastic equations, it is shown in section V that the derived equations reduce to the Markoff master equation [3-5,7] in the low-density limit, and to the quasiclassical master equation[9-11] for homogeneous systems. Conclusions are made in section VI.

II. NONHERMITIAN OPERATORS FOR FERMIONS

In the mean-field approximation, the system of identical particles is described by a one-particle density matrix $\rho_p(t)$ whose trace equals the number of particles.[1] To extend such an approximation, we consider the quantum relaxation effects. For fermions, it will be shown in this section that the equation, including the relaxation term in addition to the Liouville flow, should be of the general form,

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] + \{\rho_p(t), A_p(t)\} - \{I - \rho_p(t), A_{\overline{p}}(t)\}, \tag{1}$$

where $A_p(t)$ and $A_{\overline{p}}(t)$ are hermitian operators arising from the relaxation effect, $H(t)$ is the hermitian operator for the Liouville flow, and I is the identity operator. Here we take $\hbar = 1$, and notations $[A, B]$ and $\{A, B\}$ denote, respectively, the commutator and anticommutator

of operators A and B. As shown in section IV, from Eq. (1) we can intuitively obtain the relaxation term, which is formally derived in Appendix A from the second quantization.

In the mean-field approximation, $\rho_p(t)$ is governed by

$$\rho_p(t) = U(t, t')\rho_p(t')U^\dagger(t, t'), \tag{2}$$

with the time-evolution operator $U(t, t')$ generated by the mean-field Hamiltonian $H(t)$, which is a hermitian operator. To include the self energy with imaginary part, it seems reasonable to extend $H(t)$ to a Hamiltonian $\mathcal{H}(t)$ with a nonhermitian part,

$$\mathcal{H}(t) = H(t) + iA(t) \tag{3}$$

where $A(t)$ is a hermitian operator. Then Eq. (2) is equivalent to

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] + \{\rho_p(t), A(t)\}. \tag{4}$$

The first two terms on the right-hand side of Eq. (1) have been included in Eq. (4) when we set $A(t) = A_p(t)$. However, if we assume the equation for fermions to be symmetric with respect to particles and holes, Eq. (4) must be modified to become Eq. (1), as shown later. The last two terms in Eq. (1) are for the loss and gain factors of particles.

Instead of $\rho_p(t)$, fermions can be described as well by holes, i.e., the vacencies of particle orbitals [10]. First, we diagonalize $\rho_p(t)$ in an orthonormal basis $\{|\psi_\lambda(t)\rangle\}$:

$$\rho_p(t) = \sum_\lambda c_\lambda(t)|\psi_\lambda(t)\rangle\langle\psi_\lambda(t)|, \tag{5}$$

where $c_\lambda(t)$ denotes the number of particles in $|\psi_\lambda(t)\rangle$. Define

$$\rho_{\overline{p}}(t) \equiv I - \rho_p(t) = \sum_\lambda (1 - c_\lambda(t))|\psi_\lambda(t)\rangle\langle\psi_\lambda(t)|. \tag{6}$$

For any normalized state $|\phi\rangle$,

$$\langle\phi|\rho_{\overline{p}}(t)|\phi\rangle = 1 - \langle\phi|\rho_p(t)|\phi\rangle, \tag{7}$$

which is just the number of holes in that state, and therefore it is reasonable to use $\rho_{\overline{p}}(t)$ to represent holes. In fact, we can obtain the density matrix of holes from $\rho_{\overline{p}}(t)$, as shown in Appendix B. In terms of $\rho_{\overline{p}}(t)$, Eq. (4) becomes

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$$\frac{\partial}{\partial t}\rho_{\overline{p}}(t) = \frac{1}{i}[H(t), \rho_{\overline{p}}(t)] - \{I - \rho_{\overline{p}}(t), A(t)\}. \tag{8}$$

However, the form of the equation for $\rho_{\overline{p}}(t)$ is different from that for $\rho_p(t)$ if $A(t) \neq 0$.

It is known that in Eqs. (4) and (8), $H(t)$ describes the Liouville flow. To see the physical meaning of $A(t)$ in these two equations, let us consider the special case that $H(t) = 0$ and $A(t) = -\frac{\gamma(t)}{2}|\phi\rangle\langle\phi|$ with $|\phi\rangle$ being a normalized state. Here $\gamma(t)$ is real because $A(t)$ is hermitian. From Eqs. (4) and (8) we obtain for particles and holes, respectively,

$$\frac{\partial}{\partial t}\langle\phi|\rho_p(t)|\phi\rangle = -\gamma(t)\langle\phi|\rho_p(t)|\phi\rangle, \tag{9}$$

$$\frac{\partial}{\partial t}\langle\phi|\rho_{\overline{p}}(t)|\phi\rangle = \gamma(t)(1 - \langle\phi|\rho_{\overline{p}}(t)|\phi\rangle), \tag{10}$$

When $\gamma(t) > 0$, Eq. (9) describes the loss of particles in $|\phi\rangle$. The loss of particles is just the gain of holes, and therefore Eq. (10) should describe the gain of holes in $|\phi\rangle$ if $\gamma(t) > 0$.

It seems natural to set $\gamma(t) < 0$ in Eq. (9) to describe the gain of particles in $|\phi\rangle$. The resulting equation, however, is not of the same form as Eq. (10) with $\gamma(t) > 0$ for the gain of holes. In fact, it seems natural to use

$$\frac{\partial}{\partial t}\langle\phi|\rho_p(t)|\phi\rangle = \gamma'(t)(1 - \langle\phi|\rho_p(t)|\phi\rangle) \tag{11}$$

to describe the gain of particles, just as we describe the gain of holes using Eq. (10), where $\gamma'(t)$ is a positive real number. Similarly, if the loss of holes is described by Eq. (10) with $\gamma(t) < 0$, the loss of particles should also be described by Eq. (11) with $\gamma'(t) < 0$.

To correctly describe loss and gain of particles, we note that the loss rate of particles should be zero when $|\phi\rangle$ has no particle, while from Pauli effect, in fact, the gain rate of particles should be zero when the orbital is filled with particles. Therefore, Eq. (9) is only for the loss of particles with $\gamma(t) > 0$ while the gain of particles is described by Eq. (11) with $\gamma'(t) > 0$. Now the loss and gain rates are proportional to $\langle\phi|\rho_p(t)|\phi\rangle$ and $1 - \langle\phi|\rho_p(t)|\phi\rangle$, respectively. In Appendix C it is shown that Eq. (4) cannot describe the gain of particles in $|\phi\rangle$ no matter what $H(t)$ and $A(t)$ are.

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Because Eqs. (9) and (10) are obtained from the second terms on the right-hand side of Eqs. (4) and (8), respectively, we can see why $\rho_p(t)$ should be governed by Eq. (1), in which $A_p(t)$ and $A_{\overline{p}}(t)$ are for the loss and gain of particles. Eq. (11) may be obtained from Eq. (1) with $H(t) = A_p(t) = 0$ and $A_{\overline{p}}(t) = -\frac{\gamma'(t)}{2}|\phi\rangle\langle\phi|$, while Eq. (9) is obtained with $H(t) = A_{\overline{p}}(t) = 0$ and $A_p(t) = -\frac{\gamma(t)}{2}|\phi\rangle\langle\phi|$. We can see that $A_{\overline{p}}(t)$ is for the loss of holes just as $A_p(t)$ for the loss of particles, by rewriting Eq. (11) with corresponding $\rho_{\overline{p}}(t)$,

$$\frac{\partial}{\partial t}\langle\phi|\rho_{\overline{p}}(t)|\phi\rangle = -\gamma'(t)\langle\phi|\rho_{\overline{p}}(t)|\phi\rangle. \tag{12}$$

Rewriting Eq. (1) with corresponding $\rho_{\overline{p}}(t)$, we arrive at

$$\frac{\partial}{\partial t}\rho_{\overline{p}}(t) = \frac{1}{i}[H(t), \rho_{\overline{p}}(t)] + \{\rho_{\overline{p}}(t), A_{\overline{p}}(t)\} - \{I - \rho_{\overline{p}}(t), A_p(t)\}, \tag{13}$$

which is symmetric to Eq. (1) for $\rho_p(t)$. To include an antihertmitian part in addition to the mean-field Hamiltonian $H(t)$, therefore, we need to include $A_{\overline{p}}(t)$ in addition to $A_p(t)$. In section IV, the quantum master equation for fermions will be derived from Eq. (1). Although all $c_\lambda(t)$ in Eq. (5) are 0 or 1 in the mean-field approximation, they could be fractions in the master equation [1,2].

III. THE RELAXATION TERM FOR BOSONS

For a boson system described by the one-particle density matrix $\rho_p(t)$, it is reasonable that the decay rate of particles is proportional to $\langle\phi|\rho_p(t)|\phi\rangle$ for any normalized state $|\phi\rangle$. Unlike fermions, however, the gain rate for bosons may not vanish when $\langle\phi|\rho_p(t)|\phi\rangle = 1$, and hence we need to modify the equation for the gain of particles. By using the equation

$$\frac{\partial}{\partial t}\rho_p(t) = -\{I + \rho_p(t), A_{\overline{p}}(t)\}, \tag{14}$$

we have for the gain of particles in any arbitrary normalized ket $|\phi\rangle$

$$\frac{\partial}{\partial t}\langle\phi|\rho_p(t)|\phi\rangle = \gamma(t)(1 + \langle\phi|\rho_p(t)|\phi\rangle), \tag{15}$$

where we set $A_{\overline{p}}(t) = -\frac{\gamma(t)}{2}|\phi\rangle\langle\phi|$ with a real number $\gamma(t) > 0$. Now the rate for bosons to enter $|\phi\rangle$ is proportional to $1 + \langle\phi|\rho_p(t)|\phi\rangle$. The enhancement of the gain rate with increasing $\langle\phi|\rho_p(t)|\phi\rangle$ is consistent with the fact that bosons prefer states filled with many particles.

Therefore, for bosons we shall consider the following equation

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] + \{\rho_p(t), A_p(t)\} - \{I + \rho_p(t), A_{\overline{p}}(t)\} \tag{16}$$

to include the effects due to relaxation if Eq. (14) is suitable for the gain of bosons. As shown in the next section, from Eq. (16) we can intuitively obtain the relaxation term which is formally derived in Appendix A from the second quantization. Hence the modification for the gain of bosons is reasonable.

IV. NONLINEAR QUANTUM MASTER EQUATION

In the last two sections, we obtain Eqs. (1) and (16) so that the loss and gain factors are included in addition to the Liouville flow. To obtain the master equation, first let us consider a two-state system in contact with the reservoir and assume a time-independent Hamiltonian $H(t) = H_0$. Let $|i\rangle$ and $|f\rangle$ be normalized eigenkets of H_0. If the reservoir induces a transition so that particles in $|i\rangle$ tend to jump to $|f\rangle$, there should be a loss factor for $|i\rangle$ and a gain factor for $|f\rangle$. Therefore for $A_{\overline{p}}(t)$ and $A_p(t)$ in Eqs. (1) and (16), respectively, we shall set

$$A_{\overline{p}}^{(fi)}(t) = -\frac{\gamma_1(t)}{2}|f\rangle\langle f|, \tag{17}$$

$$A_p^{(fi)}(t) = -\frac{\gamma_2(t)}{2}|i\rangle\langle i|, \tag{18}$$

where $\gamma_1(t)$ and $\gamma_2(t)$ are positive real numbers. So we have

$$\frac{\partial}{\partial t}\langle f|\rho_p(t)|f\rangle = \gamma_1(t)(1 \pm \langle f|\rho_p(t)|f\rangle), \tag{19}$$

$$\frac{\partial}{\partial t}\langle i|\rho_p(t)|i\rangle = -\gamma_2(t)\langle i|\rho_p(t)|i\rangle. \tag{20}$$

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In the right-hand side of Eq. (19), the " $+$ " and " $-$ " signs are for bosons and fermions, respectively. From the conservation of the number of particles, we have

$$\gamma_1(t)(1 \pm \langle f|\rho_p(t)|f\rangle) = \gamma_2(t)\langle i|\rho_p(t)|i\rangle. \tag{21}$$

We can set a nonnegative number $w_{fi}(t)$ so that $\gamma_1(t) = w_{fi}(t)\langle i|\rho_p(t)|i\rangle$ and $\gamma_2(t) = w_{fi}(t)(1 \pm \langle f|\rho_p(t)|f\rangle)$ in order to satisfy Eq. (21). Then we have

$$A_{\bar{p}}^{(fi)}(t) = -\frac{1}{2}w_{fi}(t)\langle i|\rho_p(t)|i\rangle|f\rangle\langle f|, \tag{22}$$

$$A_{p}^{(fi)}(t) = -\frac{1}{2}w_{fi}(t)(1 \pm \langle f|\rho_p(t)|f\rangle)|i\rangle\langle i|. \tag{23}$$

Taking $A_{\bar{p}}^{(fi)}(t)$ and $A_{p}^{(fi)}(t)$ as $A_p(t)$ and $A_{\bar{p}}(t)$, we can derive the master equation for such a special case after inserting them into Eqs. (1) and (16). Now Eqs. (19) and (20) become

$$\frac{\partial}{\partial t}\langle f|\rho_p(t)|f\rangle = -\frac{\partial}{\partial t}\langle i|\rho_p(t)|i\rangle = w_{fi}(t)\langle i|\rho_p(t)|i\rangle(1 \pm \langle f|\rho_p(t)|f\rangle).$$

In the above equation, the change rates for bosons and fermions are different because of the last factor, which is determined by the number of particles in $|f\rangle$. For bosons the transition becomes faster if there are more particles in $|f\rangle$. On the other hand, for fermions the transition is forbidden when $|f\rangle$ is filled with particles, which is consistent with Pauli effects.

In general, the reservoir may induce many transitions when the system contains many orbitals. Assume that the transitions are within an orthonormal complete set S in which each orbital n corresponds to a normalized ket $|n\rangle$. The transition $n \to n'$ should induce the loss and gain in n and n' without changing the number of particles; we shall set $A_{\bar{p}}^{(n'n)}(t) = -\frac{1}{2}w_{n'n}(t)\langle n|\rho_p(t)|n\rangle|n'\rangle\langle n'|$ and $A_{p}^{(n'n)}(t) = -\frac{1}{2}w_{n'n}(t)(1 \pm \langle n'|\rho_p(t)|n'\rangle)|n\rangle\langle n|$ for such a transition. To include all transitions, we shall set $A_{\bar{p}}(t) = \sum_{(n'n)} A_{\bar{p}}^{(n'n)}(t)$ and $A_p(t) = \sum_{(n'n)} A_p^{(n'n)}(t)$: Eqs. (1) and (16) become

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] + \sum_{(n'n)}\{\rho_p(t), A_p^{(n'n)}(t)\} - \sum_{(n'n)}\{I \pm \rho_p(t), A_{\bar{p}}^{(n'n)}(t)\}, \tag{24}$$

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$$= \frac{1}{i}[H(t), \rho_p(t)] - \frac{1}{2}\sum_{(n'n)} w_{n'n}(t)(1 \pm \langle n'|\rho_p(t)|n'\rangle)\{\rho_p(t), |n\rangle\langle n|\}$$

$$+ \frac{1}{2}\sum_{(n'n)} w_{n'n}(t)\langle n|\rho_p(t)|n\rangle\{I \pm \rho_p(t), |n'\rangle\langle n'|\},$$

which is a nonlinear equation. Comparing the above equation to Eq. (A16) derived in Appendix A, we can see that the relaxation term can also be obtained formally from the second quantization, by considering a system composed of noninteracting particles in contact with the reservoir.

V. DISCUSSIONS

For stochastic processes, several equations are used under different conditions [1-11]. It will be shown in this section that we can derive the Markoff master equation [3-5,7] and quasiclassical master equation [9-11] from Eq. (24). An extension of Eq. (24) is also obtained after comparing Eq. (24) with the quantum master equation [6].

Consider the homogeneous case first. That is, the Hamiltonian and the density matrix commute with the momentum operators $\mathbf{P}$, and S is composed of the eigenlevels of $\mathbf{P}$. Let $|\mathbf{p}\rangle$ be the plane wave with the momentum $\mathbf{p}$. By setting $f(\mathbf{p}, t) \equiv \langle \mathbf{p}|\rho_p(t)|\mathbf{p}\rangle$, we obtain from Eq. (24)

$$\frac{\partial}{\partial t}f(\mathbf{p}, t) = \sum_{\mathbf{p}'} w_{\mathbf{p}\mathbf{p}'}(t)[1 \pm f(\mathbf{p}, t)]f(\mathbf{p}', t) \tag{25}$$

$$- \sum_{\mathbf{p}'} w_{\mathbf{p}'\mathbf{p}}(t)[1 \pm f(\mathbf{p}', t)]f(\mathbf{p}, t),$$

which is just the quasiclassical master equation.[2,10]

Next we consider the low-density limit. If we diagonalize $\rho_p(t)$ as

$$\rho_p(t) = \sum_{\lambda} c_\lambda |\psi_\lambda(t)\rangle\langle\psi_\lambda(t)|,$$

then all $c_\lambda(t)$ are small, such that $I \pm \rho_p(t) = \sum_\lambda [1 \pm c_\lambda(t)]|\psi_\lambda(t)\rangle\langle\psi_\lambda(t)| \simeq I$. In addition, $A_p^{(n'n)}(t)$ in Eq. (24) can be reduced to $-\frac{1}{2}\sum_{(n'n)} w_{n'n}(t)|n\rangle\langle n|$. If coeffecients $w_{n'n}(t)$ are independent of t, Eq. (24) is reduced to

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] - \frac{1}{2}\sum_{(n'n)} w_{n'n}\{\rho_p(t), |n\rangle\langle n|\} \tag{26}$$

$$+ \sum_{(n'n)} w_{n'n}\langle n|\rho_p(t)|n\rangle|n'\rangle\langle n'|.$$

The above equation is just the so-called Markoff master equation [3-5,7]:

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] - \frac{1}{2}\sum_{(n'n)} w_{n'n}\{\rho_p(t), |n\rangle\langle n|\} \tag{27}$$

$$+ \sum_{n'n} w_{n'n}\langle n|\rho_p(t)|n\rangle|n'\rangle\langle n'| - \sum_{n\neq n'} \Gamma_{n'n}\langle n|\rho_p(t)|n'\rangle|n\rangle\langle n'|,$$

with all $\Gamma_{n'n} = 0$. The last term of Eq. (27) is the so-called pure-dephasing term. In the Markoff master equation, $\{\Gamma_{n'n}\}$ is a set of nonnegative numbers with $\Gamma_{n'n} = \Gamma_{nn'}$. It is easy to see that for fermions the pure-dephasing term is symmetric with respect to particles and holes, and hence it seems that we can add such term into Eq. (1). The positivity of $\rho_p(t)$, however, can be broken under a pure-dephasing term, as shown in Appendix D.

Eq. (26) is, in fact, a particular case of the quantum master equation [6,12],

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] - \frac{1}{2}\sum_{l}\{\rho_p(t), \mathcal{W}_l\mathcal{W}_l^\dagger\} + \sum_{l}\mathcal{W}_l^\dagger\rho_p(t)\mathcal{W}_l \tag{28}$$

if we set

$$\mathcal{W}_l = \sqrt{w_{n'n}}|n\rangle\langle n'|, \tag{29}$$

where $\{w_{n'n}\}$ is a set of positive constants and $l \equiv (n', n)$. Therefore, Eq. (28) can be taken as a generalization of Eq. (26). Similarly, we can generalize Eq. (24) to

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] - \frac{1}{2}\sum_{l}\{\rho_p(t), \mathcal{W}_l(t)(I \pm \rho_p(t))\mathcal{W}_l^\dagger(t)\} \tag{30}$$

$$+ \frac{1}{2}\sum_{l}\{I \pm \rho_p(t), \mathcal{W}_l^\dagger(t)\rho_p(t)\mathcal{W}_l(t)\}$$

with an arbitrary set of operators $\{\mathcal{W}_l(t)\}$. Eq. (30) can be obtained from Eqs. (1) and (16) by setting $A_p(t) = -\frac{1}{2}\sum_l \mathcal{W}_l(t)(I \pm \rho_p(t))\mathcal{W}_l^\dagger(t)$ and $A_{\bar{p}}(t) = -\frac{1}{2}\sum_l \mathcal{W}_l^\dagger(t)\rho_p(t)\mathcal{W}_l(t)$, and it

can be reduced to Eq. (28) in the low-density limit (under which $I \pm \rho_p(t) \simeq I$). Therefore, Eqs. (1) and (16) are general equations for quantum stochastic processes. It is shown in Ref. 13 that under suitable assumptions the positivity of $\rho_p(t)$ is preserved under Eqs. (24) and (30). In addition, for fermions we have $\langle \alpha | \rho_p(t) | \alpha \rangle \leq 1$ for all normalized ket $|\alpha\rangle$, if such a relation holds initially.

As mentioned in section II, we shall include the second term of Eq. (1) if the time-evolution operator $U(t, t')$ in Eq. (2) is generated by a nonhermitian Hamiltonian $\mathcal{H}(t)$. For fermions we can operate such a time-evolution operator on the matrix $\rho_{\overline{p}}(t)$, which is defined in Eq. (6) for holes, and obtain the following equation

$$\frac{\partial}{\partial t} \rho_{\overline{p}}(t) = \frac{1}{i}[H(t), \rho_{\overline{p}}(t)] + \{\rho_{\overline{p}}(t), A(t)\}. \tag{31}$$

Replacing $A(t)$ by $A_{\overline{p}}(t)$, we can see that the last term of Eq. (1) corresponds to the last term of the above equation, after rewriting Eq. (1) as Eq. (13). Therefore, by considering the nonhermitian Hamiltonian, Eq. (1) can also be derived by including the last terms in both Eqs. (4) and (31), while in section II it is derived from Pauli effects. Setting $A'(t) = A_p(t) \mp A_{\overline{p}}(t)$ with the signs " $-$ " and " $+$ " for bosons and fermions, actually we can rewrite Eqs. (1) and (16) as

$$\frac{\partial}{\partial t} \rho_p(t) = \frac{1}{i}[H(t), \rho_p(t)] + \{\rho_p(t), A'(t)\} - 2A_{\overline{p}}(t). \tag{32}$$

But it is easy to see that for fermions, Eq. (1) is of a symmetric form with respect to particles and holes, after rewriting Eq. (1) as Eq. (13). To compare the equations for bosons and fermions, we shall use Eq. (16) for bosons, rather than the above one, when Eq. (1) is used for fermions.

In the quasiparticle theory [14-16], which is a good approximation for many-electron systems, with suitable assumptions the wavefunction $\Psi(t)$ of a quasiparticle (or a quasihole) is governed by [16]

$$i\frac{\partial}{\partial t}|\Psi(t)\rangle = \mathcal{H}(t)|\Psi(t)\rangle. \tag{33}$$

Here the nonhermitian Hamiltonian $\mathcal{H}(t)$ is defined in Eq. (3), and its nonhermitian part is due to the finite lifetimes of the quasiparticles (quasiholes). The above equation can correspond to Eq. (4) or Eq. (31) by rewriting it as

$$\frac{\partial}{\partial t}\rho'(t) = \frac{1}{i}[H(t), \rho'(t)] + \{\rho'(t), A(t)\}, \tag{34}$$

with $\rho'(t) \equiv |\Psi(t)\rangle\langle\Psi(t)|$. From the quasiparticle theory, therefore, we can see why the nonhermitian part of the Hamiltonian should correspond to the decay of particles or that of holes. Since in an orbital the decay of particles (holes) is equivalent to the increase of holes (particles), it is natural to consider both the last terms of Eqs. (4) and (31) to obtain Eq. (1), as mentioned above. But it should be emphasized that in this paper particles and holes are, respectively, the filled and empty parts of any orbitals, while in the quasiparticle theory they are the filled and empty parts above and below the Fermi energy. While Eq. (1) can be applied to a nonequilibrium Fermi system with no well-defined Fermi energy, in the quasiparticle theory the system is not far away from the equilibrium and we shall still consider Fermi energy. In addition, Eq. (1) describes the time evolution of a whole system, but in the above equation we are only interested in the energy and lifetime of a quasiparticle or quasihole, and do not consider the third term of Eq. (1) or Eq. (13).

VI. CONCLUSION

It is shown in this paper that the master equation for fermions is of a symmetric form with respect to particles and holes, and hence can be derived by extending the mean-field Hamiltonian to include an antihermitian part. The equation for bosons is also obtained. The derived equations reduce to the Markoff master equation in the low density limit and to the quasiclassical master equation for homogeneous systems.

APPENDIX A: MARKOFF MASTER EQUATION

Consider a system $\mathcal{S}$ coupled to a reservoir R. The total Hamiltonian $H = H_\mathcal{S} + H_R + \mathcal{V}$, where $H_\mathcal{S}$, H_R, and $\mathcal{V}$ are the operators for the system, the reservoir, and the interaction between $\mathcal{S}$ and R, repectively. In addition, $[H_\mathcal{S}, H_R] = 0$. If the system is composed of noninteracting identical particles, we can write

$$H_\mathcal{S} = \sum_n \varepsilon_n c_n^\dagger c_n, \qquad (A1)$$

with $\{c_n, c_{n'}^\dagger\} = \delta_{n,n'}$ and $\{c_n, c_{n'}\} = 0$ for femions and $[c_n, c_{n'}^\dagger] = \delta_{n,n'}$ and $[c_n, c_{n'}] = 0$ for bosons.

Assume $\mathcal{V} = \sum_{n \neq n'} f_{n,n'} c_n^\dagger c_{n'}$, where $f_{n,n'}$ contain the operators for R and satisfy $f_{n,n'} = f_{n',n}^\dagger$. Under suitable assumptions [3,4,7] the density matrix ρ_R of the reservoir can be expanded by the eigenlevels $|r\rangle$ of H_R:

$$\rho_R = \sum_r F(E_r) |r\rangle\langle r|. \qquad (A2)$$

Here E_r is the eigenvalue corresponding to $|r\rangle$ and $F(E_r)$ is the thermal equilibrium distribution. Let $\rho_\mathcal{S}(t)$ be the density matrix of the system and $\rho_C(t)$ be the total density matrix, then

$$\rho_\mathcal{S}(t) = \sum_r \langle r|\rho_C(t)|r\rangle. \qquad (A3)$$

In addition, at $t = 0$ we assume that

$$\rho_C(0) = \rho_\mathcal{S}(0) \otimes \rho_R \qquad (A4)$$

with positive $\rho_\mathcal{S}(0)$ satisfying the normalization condition $tr\rho_\mathcal{S}(0) = 1$.

Choose $\mathcal{H}_0 = H_\mathcal{S} + H_R$ as the unperturbed Hamiltonian, the time-evolution operator, $\mathcal{U}^{(I)}(t, t')$, in the interaction picture satisfies

$$\frac{\partial}{\partial t}\mathcal{U}^{(I)}(t, t') = \mathcal{V}^{(I)}(t)\mathcal{U}^{(I)}(t, t'), \qquad (A5)$$

where $\mathcal{V}^{(I)}(t) = \sum_{n\neq n'} f_{n,n'}^{(I)}(t)e^{i(\varepsilon_n - \varepsilon_{n'})t}c_n^\dagger c_{n'}$ with $f_{n,n'}^{(I)}(t) = e^{iH_R t}f_{n,n'}e^{-iH_R t}$. At $t > 0$, we have

$$\rho_C^{(I)}(t) = \mathcal{U}^{(I)}(t)\rho_C(0)\mathcal{U}^{(I)\dagger}(t). \qquad (A6)$$

in the interaction picture. After expanding $\rho_{\mathcal{S}}^{(I)}(t)$ to the second order with respect to $\mathcal{V}$ and assume that $Tr\rho_R f_{n,n'} = 0$ [3,4] we have

$$\rho_{\mathcal{S}}^{(I)}(t) - \rho_{\mathcal{S}}(0) = it[\rho_{\mathcal{S}}(0), \Sigma_R] - t\{\rho_{\mathcal{S}}(0), \Sigma_I\} + \sum_{r,r'} F(E_r) \int_0^t \int_0^t \times \qquad (A7)$$

$$\sum_{m\neq m', n\neq n'} dt_1 dt_2 e^{i[(\varepsilon_n - \varepsilon_{n'})t_1 + (\varepsilon_m - \varepsilon_{m'})t_2]} \langle r|f_{n,n'}^{(I)}(t_1)|r'\rangle\langle r'|f_{m,m'}^{(I)}(t_2)|r\rangle c_n^\dagger c_{n'}\rho_{\mathcal{S}}(0)c_m^\dagger c_{m'},$$

where Σ_R and Σ_I are the real and imaginary parts of

$$\Sigma \equiv \frac{i}{t}\sum_{r,r'} F(E_r) \int_0^t dt_1 \int_0^{t_1} dt_2 \langle r|\mathcal{V}^{(I)}(t_1)|r'\rangle\langle r'|\mathcal{V}^{(I)}(t_2)|r\rangle. \qquad (A8)$$

If t is much longer than the correlation time of the reservoir, Σ is just the self energy [4,8].

To calculate the third term on the right hand side of Eq. (A7), let $\langle r|f_{n,n'}|r'\rangle = |\langle r|f_{n,n'}|r'\rangle|e^{i\theta_{n,n'}(r,r')}$. Since $f_{n,n'} = f_{n',n}^\dagger$, $\theta_{n,n'}(r,r') = -\theta_{n',n}(r',r)$. Assume that $\theta_{n,n'}(r,r')$ is random with respect to r' while $|\langle r|f_{n,n'}|r'\rangle|$ varies slowly with respect to r'. In addition, when $(n, n') \neq (m', m)$, $\phi_{n,n',m,m'}(r,r') \equiv \theta_{n,n'}(r,r') - \theta_{m,m'}(r,r')$ is still random. That is, the change of $\theta_{n,n'}(r,r')$ due to the reservoir is random, and there is no correlation between different transitions. Under these assumptions, only those terms with $(n, n') = (m', m)$ in the summation do not vanish.

After some calculations, we can set $w_{n'n} = \sum_{r,r'} F(E_r)|\langle r|f_{n,n'}|r'\rangle|^2\delta_{E_n+E_r,E_{n'}+E_{r'}}$ as the transition rate for particles to jump from n to n' so that

$$\Sigma_I = \frac{1}{2}\sum_{n\neq n'} w_{n'n}c_n^\dagger c_{n'}c_{n'}^\dagger c_n. \qquad (A9)$$

Ignoring Σ_R [3,4], Eq. (41) in the Schrödinger picture becomes

$$\frac{\partial}{\partial t}\rho_{\mathcal{S}}(t)|_{t=0} = i[\rho_{\mathcal{S}}(t), H_{\mathcal{S}}] - \frac{1}{2}\sum_{n\neq n'} w_{n'n}\{c_n^\dagger c_{n'}c_{n'}^\dagger c_n, \rho_{\mathcal{S}}(t)\} \qquad (A10)$$

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$$+ \sum_{n \neq n'} w_{n'n} c_{n'}^\dagger c_n \rho_\mathcal{S}(t) c_n^\dagger c_{n'}.$$

Assuming that the above equation holes at any time [3,4] and setting $\mathcal{A}_{n'n} = \sqrt{w_{n'n}} c_{n'}^\dagger c_n$, we can reduce the above equation to be

$$\frac{\partial}{\partial t} \rho_\mathcal{S}(t) = \frac{1}{i}[H_\mathcal{S}, \rho_\mathcal{S}(t)] - \frac{1}{2} \sum_{n \neq n'} \{\mathcal{A}_{n'n}^\dagger \mathcal{A}_{n'n}, \rho_\mathcal{S}(t)\} + \sum_{n \neq n'} \mathcal{A}_{n'n} \rho_\mathcal{S}(t) \mathcal{A}_{n'n}^\dagger, \qquad (A11)$$

which is just the quantum master equation [6] with the second and third terms as the loss and gain factors.

Let $|n\rangle$ be the orbital corresponding to c_n, and $\rho_p(t)$ be the one-particle density matrix satisfying $\langle n|\rho_p(t)|n'\rangle = Tr c_n^\dagger c_{n'} \rho_\mathcal{S}(t)$. From Eq. (A10), the diagonal terms satisfy

$$\frac{\partial}{\partial t} \langle n|\rho_p(t)|n\rangle = \sum_{n' \neq n} [-w_{n'n} Tr(c_n^\dagger c_n c_{n'} c_{n'}^\dagger \rho_\mathcal{S}(t)) + w_{nn'} Tr(c_{n'}^\dagger c_{n'} c_n c_n^\dagger \rho_\mathcal{S}(t))], \qquad (A12)$$

and phases are governed by

$$\frac{\partial}{\partial t} \langle n|\rho_p(t)|n''\rangle = i(\varepsilon_{n''} - \varepsilon_n)\langle n|\rho_p|n''\rangle \qquad (A13)$$

$$- \frac{1}{2} \sum_{n' \neq n} w_{n'n} Tr(c_{n'} c_{n'}^\dagger c_n^\dagger c_{n''} \rho_\mathcal{S}(t)) + \frac{1}{2} \sum_{n' \neq n} w_{nn'} Tr(c_{n'}^\dagger c_{n'} c_{n''} c_n^\dagger \rho_\mathcal{S}(t))$$

$$+ \frac{1}{2} \sum_{n' \neq n''} w_{n''n'} Tr(c_{n''} c_n^\dagger c_{n'}^\dagger c_{n'} \rho_\mathcal{S}(t)) - \frac{1}{2} \sum_{n' \neq n''} w_{n'n''} Tr(c_n^\dagger c_{n''} c_{n'} c_{n'}^\dagger \rho_\mathcal{S}(t)),$$

where $n \neq n''$.

Disjointing from Eq. (A12), so that $c_{n'}$ and $c_{n'}^\dagger$ are paired, we have

$$\frac{\partial}{\partial t} \langle n|\rho_p(t)|n\rangle = -\frac{1}{2} \sum_{n'} w_{n'n}(1 \pm \langle n'|\rho_p(t)|n'\rangle)\langle n|\rho_p(t)|n\rangle \qquad (A14)$$

$$+ \frac{1}{2} \sum_{n'} w_{nn'}(1 \pm \langle n|\rho_p(t)|n\rangle)\langle n'|\rho_p(t)|n'\rangle,$$

while from Eq. (A13) we have

$$\frac{\partial}{\partial t} \langle n|\rho_p(t)|n''\rangle|_{n \neq n''} = i\langle n|[\rho_p(t), H_0]|n''\rangle \qquad (A15)$$

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$$-\frac{1}{2}\sum_{n'}(w_{n'n''}+w_{n'n})(1\pm\langle n'|\rho_p(t)|n'\rangle)\langle n|\rho_p(t)|n''\rangle$$

$$\pm\frac{1}{2}\sum_{n'}(w_{nn'}+w_{n''n'})\langle n|\rho_p(t)|n''\rangle\langle n'|\rho_p(t)|n'\rangle.$$

Here the signs "$+$" and "$-$" in the symbol "$\pm$" are for bosons and fermions, respectively. Although in Eq. (A13) the disjointness is not allowed for $n' = n$ or $n'' = n$, it is suitable to ignore such a problem if the summation is over many terms.

It has been shown that Eq. (A14) corresponds to a semiclassical master euqation. Although Eq. (A15) looks complicated, with some calculations we can see that $\rho_p(t)$ is governed by the following equation,

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H_0, \rho_p(t)] - \frac{1}{2}\sum_{(n'n)}w_{n'n}(1\pm\langle n'|\rho_p(t)|n'\rangle)\{\rho_p(t), |n\rangle\langle n|\} \qquad (A16)$$

$$+\frac{1}{2}\sum_{(n'n)}w_{n'n}\langle n|\rho_p(t)|n\rangle\{I\pm\rho_p(t), |n'\rangle\langle n'|\},$$

when Eq. (A15) is considered together with Eq. (A14). The last two terms in the above equation just correspond to the relaxation term derived in section IV.

APPENDIX B

Consider a partially filled band in a crystal. Because holes are vacencies of any orbitals in this paper, the reference energy for holes is different from that for particles. In a specific orbital, different wavefunctions are used for particles and holes to obtain the correct crystal momentum, charge, and the transition energy [10]. We diagonalize $\rho_p(t)$ as in Eq. (5), the number of holes in λ is $1 - c_\lambda(t)$, so the density matrix of holes is

$$\rho_h(t) = \sum_\lambda [1 - c_\lambda(t)]|\psi_\lambda^c(t)\rangle\langle\psi_\lambda^c(t)|, \qquad (B1)$$

where ψ_λ^c is the wavefunction for holes in orbital λ. It is easy to see that we can obtain $\rho_h(t)$ from $\rho_{\bar{p}}(t)$ after transforming the wavefunctions.

APPENDIX C

To see that we cannot describe the gain of particles in orbital $|\phi\rangle$ by Eq. (4), we just need to consider the special case when no particle occupies $|\phi\rangle$ at $t = 0$, i.e. $\langle\phi|\rho_p(0)|\phi\rangle = 0$. For any $|\phi'\rangle$ orthogonal to $|\phi\rangle$, we have

$$|\langle\phi|\rho_p(0)|\phi'\rangle| \leq \langle\phi|\rho_p(0)|\phi\rangle^{1/2}\langle\phi'|\rho_p(0)|\phi'\rangle^{1/2} = 0, \qquad (C1)$$

from Cauchy's inequality, because $\rho_p(0)$ must be positive. Expanding $H(0)$, $A(0)$, and $\rho_p(0)$ in Eq. (4) by using any orthonormal completet set containing $|\phi\rangle$, it is easy to see that $\frac{\partial}{\partial t}\langle\phi|\rho_p(0)|\phi\rangle = 0$ for any $H(0)$ and $A(0)$. However, the gain rate should be the largest at $t = 0$.

The change of the number of particles due to the loss and gain factors should be proportional to t. If we take those terms of the order t^2, of course, the Liouville flow described by $H(t)$ can also induce the increase of particles in $|\phi\rangle$.

APPENDIX D

To see that the positivity of $\rho_p(t)$ can be broken by including the pure-dephasing terms, consider a system in which only three orbitals $|1\rangle$, $|2\rangle$, and $|3\rangle$ are allowed, and assume that the Hamiltonian H_0 is diagonalized by these three orbitals. Let the equation for the time evolution of $\rho_p(t)$ be

$$\frac{\partial}{\partial t}\rho_p(t) = \frac{1}{i}[H_0, \rho_p(t)] - \Gamma|2\rangle\langle 2|\rho_p(t)|3\rangle\langle 3| - \Gamma|3\rangle\langle 3|\rho_p(t)|2\rangle\langle 2|. \qquad (D1)$$

Assume, for example, that initially,

$$\rho_p(0) = \frac{1}{3}(|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|) \qquad (D2)$$

$$+\frac{10}{27}(|1\rangle\langle 2| + |2\rangle\langle 1| + |1\rangle\langle 3| + |3\rangle\langle 1|) + \frac{2}{9}(|2\rangle\langle 3| + |3\rangle\langle 2|).$$

After calculations, it is easy to see that $\rho_p(0)$ is positive, but one of the eigenvalue of ρ_p becomes negative as $t \to \infty$.

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