Quantum master equation approach to quantum transport through mesoscopic systems

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For quantum transport through mesoscopic system, a quantum master equation approach is developed in terms of compact expressions for the transport current and the reduced density matrix of the system. The present work is an extension of Gurvitz’s approach for quantum transport and quantum measurement, namely, to finite temperature and arbitrary bias voltage. Our derivation starts from a second-order cumulant expansion of the tunneling Hamiltonian, then follows conditional average over the electrode reservoir states. As a consequence, in the usual weak tunneling regime, the established formalism is applicable for a wide range of transport problems. The validity of the formalism and its convenience in application are well illustrated by a number of examples.

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I. INTRODUCTION

Quantum transport through mesoscopic nanostructures has revealed many impressive features associated with a number of unique natures such as the quantum interferences, discrete levels, and many-body correlations [1]. Depending on the specific systems/problems under study, theoretical formalisms have been developed such as the Landauer-Büttiker theory and the non-equilibrium Green’s function (nGF) approach [1, 2]. However, generally speaking, neither of them implies universal simplicity in practice, for instance, in treating mesoscopic transport in the presence of many-electron Coulomb interaction and inelastic scattering with phonons. In particular, it is even more difficult to describe the transient processes (i.e. time-dependent transport phenomena).

In some particular cases, a relatively simpler method being able to address these issues is the rate equation approach [3, 4, 5, 6, 7]. Originally, the “classical” rate equation is in certain sense of phenomenological form [3]. Our derivation starts from a second-order cumulant expansion of the tunneling Hamiltonian, then follows conditional average over the electrode reservoir states. As a consequence, in the usual weak tunneling regime, the established formalism is applicable for a wide range of transport problems. The validity of the formalism and its convenience in application are well illustrated by a number of examples.

Consider the transport setup schematically shown in Fig. 1 which is described by the following Hamiltonian

\[ H = H_S(a^\dagger_\mu, a_\mu) + \sum_{\alpha=L,R} \sum_{\mu k} \epsilon_{\alpha \mu k} a^\dagger_{\alpha \mu k} d_{\alpha \mu k} + \sum_{\alpha=L,R} \sum_{\mu k} (t_{\alpha \mu k} a^\dagger_\mu d_{\alpha \mu k} + H.c.). \]  

(1)

The remainder of the paper is organized as follows. In Sec. II, starting with the second-order cumulant expansion of the tunneling Hamiltonian, formal expressions for the transport current and the associated master equation are derived. Sec. III is devoted to a number of examples to illustrate the application of the established formalism. Finally, in Sec. IV concluding remarks on the approximations adopted and the connection with nGF approach are presented. In the Appendix, refinement on the cumulant second-order approximation is self-consistently made by including the level broadening effect.
which are also termed as emitter (left electrode) and collector (right electrode), in some places of this paper as usual. The third term describes tunneling between the electrodes and the system. In this paper the electrode reservoir electrons are also attached with the index “μ” to characterize their possible correspondence to the system states. For instance, this will be the typical situation in the spin-dependent transport.

Introducing the reservoir operators $F_{μ} = \sum_{i,k} t_{αi,k} a_{μi,k}^{\dagger}$, we re-express the tunneling Hamiltonian as

$$H' = \sum_{μ} \left( a_{μi}^{\dagger} F_{μ} + \text{H.c.} \right).$$

Then, regarding this tunneling Hamiltonian as perturbation, the second-order cumulant expansion leads us to a formal equation for the reduced density matrix [14]

$$\dot{ρ}(t) = -iLρ(t) - \int_{0}^{t} d\tau \langle L'(t)G(t,\tau)L'(\tau)G^{\dagger}(t,\tau) \rangle ρ(t).$$

Here the Liouvillian superoperators are defined as $L(\cdots) \equiv [H_{S},(\cdots)], L'(\cdots) \equiv [H',(\cdots)]$, and $G(t,\tau)(\cdots) \equiv G(t,\tau)(\cdots)G^{\dagger}(t,\tau)$ with $G(t,\tau)$ the usual propagator (Green’s function) associated with the system Hamiltonian $H_{S}$. The reduced density matrix $ρ(t) = Tr_{B}[ρ(t)],$ and $\langle (\cdots) \rangle = Tr_{B}[\langle \cdots \rangle ρ_{B}]$ with $ρ_{B}$ the density matrix of the electron reservoirs. Notice that Eq. (3) is nothing but an alternative form of the quantum master equation under the second-order Born approximation. The underlining assumption is that the tunneling Hamiltonian is not strong enough, which makes the second-order cumulant expansion reasonable. It is known that this approximation applies well to most dissipative systems in quantum optics. Noticeably, for most transport systems, weak tunneling is also the typical regime where various forms of golden-rule type theories are adopted. In strong tunneling regime, special technique is required, which goes beyond the present second-order Born approximation, and other golden-rule type theories [15].

The trace in Eq. (3) is over all the electrode degrees of freedom, leading thus to the equation of motion of the unconditional reduced density matrix of the system. To describe the transport problem, we should keep track of the record of electron numbers at the collector (emitted from the emitter and passed through the mesoscopic system in between the two electrodes). We therefore classify the Hilbert space of the electrodes as follows. First, we define the subspace in the absence of electron arrived at the collector as “$B^{(0)}$”, which is spanned by the product of all many-particle states of the two isolated reservoirs, formally denoted as $B^{(0)} \equiv \text{span}\{ |Ψ_{L}⟩ \otimes |Ψ_{R}⟩ \}$. Then, we introduce the Hilbert subspace “$B^{(n)}$” ($n = 1, 2, \cdots$), corresponding to $n$-electrons arrived at the collector. The entire Hilbert space of the two electrodes is $B = \oplus_{n} B^{(n)}$.

With the above classification of the reservoir states, the average over states in the entire Hilbert space “$B$” in Eq. (3) is replaced with states in the subspace “$B^{(n)}$”, leading to a conditional master equation

$$\dot{ρ}^{(n)}(t) = -iLρ^{(n)}(t) - \int_{0}^{t} d\tau Tr_{B^{(n)}}[L'(t)G(t,\tau)L'(τ)G^{\dagger}(t,τ)ρ_{T}(t)].$$

Here $ρ^{(n)}(t) = Tr_{B^{(n)}}[ρ_{T}(t)],$ which is the reduced density matrix of the system conditioned by the number of electrons arrived at the collector until time $t$. Now we transform the Liouvillian operator product in Eq. (3) into the conventional Hilbert form:

$$L'(t)G(t,τ)L'(τ)G^{\dagger}(t,τ)ρ_{T}(t) = [H'(t)G(t,τ)H'(τ)G^{\dagger}(t,τ)ρ_{T}(t) - G(t,τ)H'(τ)G^{\dagger}(t,τ)ρ_{T}(t)H'(t)] + \text{H.c.} \equiv [I - II] + \text{H.c.}.$$
over the subspace “$B^{(n)}$ yields

$$\text{Tr}_{B^{(n)}}[I] = \sum_{\mu, \nu} \left\{ \text{Tr}_B[F^\dagger_\mu(t)F_\nu(\tau)] \rho_B^{(n)} \right\} \times \{ a_\mu G(t, \tau) a_\nu G^\dagger(t, \tau) \rho_B^{(n)} \} + \text{Tr}_B[F_\mu(t)F_\nu(\tau)] \rho_B^{(n)} \times \{ a_\mu G(t, \tau) a_\nu G^\dagger(t, \tau) \rho_B^{(n)} \} \}

(6a)$$

$$\text{Tr}_{B^{(n)}}[II] = \sum_{\mu, \nu} \left\{ \text{Tr}_B[f^\dagger L_\nu(\tau) \rho_B^{(n)} f L_\mu(t)] \times \{ G(t, \tau) a_\nu G^\dagger(t, \tau) \rho_B^{(n)} a_\mu \} + \text{Tr}_B[f_\nu(\tau) \rho_B^{(n)} f^\dagger L_\mu(t)] \times \{ G(t, \tau) a_\nu G^\dagger(t, \tau) \rho_B^{(n)} a_\mu \} + \text{Tr}_B[f_\nu(\tau) \rho_B^{(n)} f L_\mu(t)] \times \{ G(t, \tau) a_\nu G^\dagger(t, \tau) \rho_B^{(n)} a_\mu \} \}

(6b)$$

Here we have utilized the orthogonality between states in different subspaces, which in fact leads to the term selection from the entire density operator $\rho_T$. (ii) Due to the closed nature of the transport circuit, the extra electrons arrived at the collector (right reservoir) will flow back into the emitter (left reservoir) via the external circuit. Also, the rapid relaxation processes in the reservoirs will quickly bring the reservoirs to the local thermal equilibrium state determined by the chemical potentials. As a consequence, after the procedure (i.e. the state selection) done in Eq. (6), the electron reservoir density matrices $\rho_B^{(n)}$ and $\rho_B^{(n+1)}$ should be replaced by $\rho_B^{(0)}$, i.e., the local thermal equilibrium reservoir state, which leads the reservoir correlation functions in Eq. (6) to be, respectively, $\langle f^\dagger_\alpha(t) f_\nu(\tau) \rangle = C_\alpha^{(+)}(t - \tau)$, and $\langle f_\alpha(t) f^\dagger_\nu(\tau) \rangle = C_\alpha^{(-)}(t - \tau)$. Here $\langle \cdots \rangle$ stands for $\text{Tr}_B[(\cdots)\rho_B^{(0)}]$, with the usual meaning of thermal average. Obviously, $\langle F^\dagger_\alpha(t) F_\nu(\tau) \rangle = C_\alpha^{(+))(t - \tau)} = \sum_{n=L, R} C_{\alpha \nu}^{(+)}(t - \tau)$, and $\langle F_\alpha(t) F^\dagger_\nu(\tau) \rangle = C_\alpha^{(-)}(t - \tau) = \sum_{n=L, R} C_{\alpha \nu}^{(-)}(t - \tau)$.

Under the Markovian approximation, the time integral in Eq. (4a) is replaced by $\frac{1}{2} \int_{-\infty}^{\infty} dt$. This approximation considerably simplifies the result. For instance, substituting the first term of Eq. (4a) into the time integral of Eq. (4), we have $\int_{-\infty}^{\infty} d\tau C_{\alpha \nu}^{(+)\dagger}(t - \tau) a_\alpha [e^{-i\epsilon(t-\tau)} a^\dagger_\nu] \rho_B^{(n)}(t) = a_\alpha [C_{\alpha \nu}^{(+)\dagger}(-\epsilon)] a^\dagger_\nu \rho_B^{(n)}(t)$. Other terms can be similarly integrated out, leading to

$$\dot{\rho}_B^{(n)} = -i \mathcal{L} \rho_B^{(n)} - \frac{1}{2} \sum_{\alpha} \left\{ [a_\alpha^\dagger A_\alpha^{(-)}(t) + \rho_B^{(n)} A_\alpha^{(+)} a_\alpha^\dagger] \right\} - A_{L \mu}^{(-)} a_\mu \rho_B^{(n)} A_{L \mu}^{(+)} - A_{R \mu}^{(-)} \rho_B^{(n+1)} a_\mu - A_{R \mu}^{(+)} a_\mu \rho_B^{(n+1)} A_{R \mu}^{(-)} + \text{H.C.} \}

(7)$$

Here $A_{\alpha \mu}^{(\pm)} = \sum_{\nu} C_{\alpha \nu}^{(\pm)}(\pm \mathcal{L}) a_\nu$, and $A_{\alpha \mu}^{(\pm)} = \sum_{n=L, R} A_{\alpha \mu}^{(\pm)}$. The spectral functions $C_{\alpha \nu}^{(\pm)}(\pm \mathcal{L})$ are defined in terms of the Fourier transform of the reservoir correlation functions, i.e., $C_{\alpha \nu}^{(\pm)}(\pm \mathcal{L}) = \int_{-\infty}^{\infty} dt C_{\alpha \nu}^{(\pm)}(t) e^{\pm i \mathcal{L} t}$. We want to remark here that this time integral leads to “exact” energy conservation for electron transfer between the electrodes and the central system. This “conservation law” would cause errors in the near-resonance bias. For instance, at zero temperature and for electrode Fermi level(s) lower than but very close to certain system level, the present “energy conservation law” does not permit any electron occupation on the concerned system level. Nevertheless, the nGF-based quantum kinetic theory allows occupation under the same condition. The underlying reason is the neglect of level broadening in present treatment, whose inclusion is referred to the Appendix.

The “$n$”-dependence of Eq. (7) is analogous to the usual rate equation, despite its formal matrix/operator feature. Each term of Eq. (7) can be similarly interpreted as for the conventional “$c$-number” rate equation. Compared with the Bloch equation derived by Gurvitz et al. in Ref. 7, in Eq. (7), $\rho^{(n)}$ is also coupled to $\rho^{(n+1)}$ which is absence from Ref. 7. This feature originates from the general nature that Eq. (7) is established under non-zero transport current and noise spectrum [13]. Remarkably, with the knowledge of $\rho^{(n)}(t)$, one is readily able to compute the various transport properties, such as the transport current and noise spectrum [13]. Based on Eq. (7) straightforwardly leads to

$$I(t) = e \sum_n n \text{Tr} \left[ \dot{\rho}_B^{(n)}(t) \right]

(8)$$

Here the unconditional density matrix $\rho = \sum_n \rho^{(n)}$ satisfies an even simpler equation, which can be easily derived
by summing up Eq. (7) over “n”

\[ \dot{\rho} = -i\mathcal{L}\rho - \frac{1}{2} \sum_{\mu} \left\{ [a^{(-)}_{\mu}, A^{(-)}_{\mu}\rho + \rho A^{(+)}_{\mu}] + \text{H.c.} \right\}. \]  

(9)

Eqs. (8) and (9) together with (7) constitute the principal result of this work, which can serve as a convenient starting point to compute transport current under wide range of conditions, such as in the presence of many-body Coulomb interaction, at finite temperatures and for arbitrary voltages. Moreover, the current expression and the associated master equation are free from state representation and the specific system Hamiltonian, which therefore holds the merit of unification in its applications. For instance, for quantum transport through an interacting system, which is usually a challenging problem, one can first diagonalize the isolated system Hamiltonian, then do the Liouvillian operation easily in the eigen-state representation. In the following, as application of this approach we only illustrate a number of simple examples, and remain the systematic applications to more interesting problems to be the subject of forthcoming works.

III. ILLUSTRATIVE APPLICATIONS

A. Single Level System

As a preliminary application of Eq. (4), let us consider the resonant transport through a single level system. Under wide-band approximation for the electrodes, the reservoir electron correlation functions read \( C^{(\pm)}_{\alpha}(t-\tau) = |t_{\alpha}|^2 \sum_k e^{\pm i\epsilon_k(t-\tau)} n^{(\pm)}_{\alpha}(\epsilon_k) \), where \( n^{(\pm)}_{\alpha}(\epsilon_k) = n_{\alpha}(\epsilon_k) \) is the Fermi distribution function, and \( n^{(\pm)}_{\alpha}(\epsilon_k) = 1 - n_{\alpha}(\epsilon_k) \). Then the spectral function can be easily carried out as

\[ A^{(\pm)}_{\alpha} = C^{(\pm)}_{\alpha}(\pm \mathcal{L})a = \Gamma_{\alpha} n^{(\pm)}_{\alpha}(E_0)a. \]  

(10)

Here, \( \Gamma_{\alpha} = 2\pi g_{\alpha}|t_{\alpha}|^2 \), with \( g_{\alpha} \) the density of states of the “\( \alpha \)” electrode. In the special case of zero temperature and large bias voltage \( \mu_L \gg E_0 \gg \mu_R \), which is in fact the applicable condition of Gurvitz’s approach 7, we simply have \( A^{(+)}_{L} = \Gamma_{L}a \), \( A^{(-)}_{L} = 0 \), \( A^{(+)}_{R} = \Gamma_{R}a \), and \( A^{(-)}_{R} = 0 \). Substituting these into Eq. (4) yields

\[ \dot{\rho}^{(n)} = -i\mathcal{L}\rho^{(n)} - \frac{1}{2} \left\{ [\Gamma_{L}a^{\dagger}a\rho^{(n)} + \Gamma_{L}\rho^{(n)}a^{\dagger}a^{\dagger} - \Gamma_{L}a^{\dagger}a^{\dagger}\rho^{(n-1)}a^{\dagger} - \Gamma_{R}a^{\dagger}a^{\dagger}\rho^{(n-1)}a^{\dagger}] + \text{H.c.} \right\}. \]  

(11)

To obtain the matrix form of this equation, let us choose the empty (level) state \( |0\rangle \) and the occupied state \( |1\rangle \) as representation basis. Straightforwardly, by computing the matrix elements of the terms of Eq. (11) one by one, we obtain

\[ \dot{\rho}^{(n)}_{00} = -\Gamma_{L}\rho^{(n)}_{00} + \Gamma_{R}\rho^{(n-1)}_{11}, \]

\[ \dot{\rho}^{(n)}_{11} = -\Gamma_{R}\rho^{(n)}_{11} + \Gamma_{L}\rho^{(n)}_{00}. \]  

(12)

This is the result derived by Gurvitz et al under the limits mentioned above 7.

B. Multi-Level System

Now we consider the transport through a multi-level system as shown in Fig. 1, under arbitrary voltage and at finite temperature. The system Hamiltonian simply reads \( H_S = \sum_{\mu=1}^{N} E_\mu \hat{a}_\mu \hat{a}_\mu^\dagger \). Also, let us assume that the level separation is much larger than the characteristic level widths, i.e., \( |E_\mu - E_{\mu-1}| \gg \Gamma_L, \Gamma_R \), which leads to the correlation function \( C^{(\pm)}_{\alpha\mu}(t) \approx \delta_{\mu_1\mu} C^{(\pm)}_{\alpha\mu_1}(t) \). This assumption neglects the interference effect of electron tunneling through different levels, which is significant only in the case \( |E_\mu - E_{\mu-1}| < \Gamma_L, \Gamma_R \). Similar to single level system, we have \( A^{(\pm)}_{R\mu} = \Gamma_{R}(E_\mu)n^{(\pm)}_{\mu}(E_\mu)a_\mu \). For this simplified model, the reduced system density matrix is the direct product of the individual single level density matrix, i.e., \( \rho = \otimes_{\mu=1}^{N} \rho_{\mu} \), and the steady-state solution of the single level density matrix in unoccupied state of the \( \mu \)th level from the occupied (unoccupied) state of the \( \mu \)th level, and the occupation probability \( p_{\mu} \) reads

\[ p_{\mu} = \frac{n_{L}(E_\mu)\Gamma_{L}(E_\mu) + n_{R}(E_\mu)\Gamma_{R}(E_\mu)}{\Gamma_{L}(E_\mu) + \Gamma_{R}(E_\mu)}. \]  

(13)

Substituting the obtained \( A^{(\pm)}_{R\mu} \) and \( \rho \) into the current expression Eq. (5), we arrive at an expression for the steady-state current as

\[ I = e \sum_{\mu} \frac{\Gamma_{L}(E_{\mu})\Gamma_{R}(E_{\mu})}{\Gamma_{L}(E_{\mu}) + \Gamma_{R}(E_{\mu})} [n_{L}(E_{\mu}) - n_{R}(E_{\mu})]. \]  

(14)

This result clearly manifests the typical step-like I-V characteristics, where each step corresponds to involving a new level into the conduction by increasing the bias voltage, with the standard resonant current \( e\Gamma_{L}\Gamma_{R}/(\Gamma_{L} + \Gamma_{R}) \).

C. Non-interacting Coupled Quantum Dots

In the above multi-level system the quantum coherence or nature of quantum superposition of system states is not manifested, and the result can be obtained via classical rate equations. To reveal more clearly the quantum nature of the developed formalism, in this subsection we consider transport through system of a coupled quantum dots 7. In this case, the non-diagonal elements of density matrix, which have no classical counterparts, will appear in the equations of motion and play essential role.

The Hamiltonian of the coupled quantum dots reads

\[ H_S = E_1 a_1^{\dagger}a_1 + E_2 a_2^{\dagger}a_2 + \Omega(a_1^{\dagger}a_2 + a_2^{\dagger}a_1), \]

where each dot contains a single resonant level \( E_1 \) \( E_2 \), and the two dots are coupled by \( \Omega \). In principle, for any system the master equation 7 or 9 can be expressed and solved in the
system eigenstate representation. Here, for the coupled quantum dots, we would like to present a more elegant method in terms of the language of Bogoliubov transformation, to explicitly carry out the superoperators $A_{\alpha \mu}^{(\pm)}$. To diagonalize $H_S$, the standard Bogoliubov transformation defines a pair of new electron operators as follows: $b_1 = u a_1 + v a_2$, and $b_2 = v a_2 - u a_1$. The desired diagonalized Hamiltonian reads $H_S = E_1 b_1^\dagger b_1 + E_2 b_2^\dagger b_2$. The diagonalization condition $(E_2 - E_1)u v + \Omega (u^2 - v^2) = 0$, together with the normalization condition $u^2 + v^2 = 1$, uniquely determine the transformation coefficients $u$ and $v$, and the eigen-energies read accordingly, $E_1 = E_1 u^2 + E_2 v^2 + 2 \Omega u v$, and $E_2 = E_1 v^2 + E_2 u^2 - 2 \Omega u v$. Simple algebra leads to $\mathcal{L} a_1 = (-\tilde{E}_1)^n b_1 - (-\tilde{E}_2)^n b_2$, and $\mathcal{L} a_2 = (-\tilde{E}_1)^n b_1 - (-\tilde{E}_2)^n b_2$. Notice that in the wide-band approximation for the electrode reservoirs, $C_{\alpha \mu}^{(\pm)}(\pm L) = \Gamma_n a_{\alpha \mu}^{(\pm)} (\pm L)$. We thus have

\begin{align}
A_{L}^{(\pm)} &= \Gamma_L \left[ u n_L(E_1) b_1 - v n_L(E_2) b_2 \right], \\
A_{R}^{(\pm)} &= \Gamma_R \left[ u n_R(E_1) b_1 + v n_R(E_2) b_2 \right].
\end{align}

(15)

With this result, the explicit form of the master equation can be easily obtained for arbitrary offset of the dot levels ($E_1$ and $E_2$). To compare with the Bloch equations derived by Gurvitz et al. [7], consider the special configuration of the two dot levels in resonance, i.e., $E_1 = E_2 = E_0$. For this setup, $u = -v = 1/\sqrt{2}$, and $E_{1,2} = E_0 \mp \Omega$. Moreover, in the large bias voltage limit $\mu_L \gg \tilde{E}_2, \tilde{E}_1 \gg \mu_R$, we simply have $A_{L}^{(\pm)} = \Gamma_L a_1$, $A_{R}^{-} = 0$, $A_{R}^{+} = 0$, and $A_{R}^{(\pm)} = \Gamma_R a_2$. Substituting them into Eq. (17), an explicit form of conditional master equation is obtained as

\begin{align}
\dot{\rho}^{(n)} &= -i \mathcal{L} \rho^{(n)} - \frac{1}{2} \left\{ [\rho^{(n)} \Gamma_L a_1 a_1^\dagger + a_2^\dagger \Gamma_R a_2 \rho^{(n)} - a_1^\dagger \rho^{(n)} \Gamma_L a_1 - \Gamma_R a_2 \rho^{(n-1)} a_1^\dagger] + \text{H.c.} \right\}.
\end{align}

(16)

In the electron number representation $\{ |1\rangle, |2\rangle, |3\rangle, |4\rangle \}$, which correspond to, respectively, the states of no electron in the two dots, one electron in the left (right) dot, and two electrons in each dot, Eq. (16) can be precisely recast to the result derived in Ref. [8] where the quantum coherence nature beyond the classical rate equation was particularly emphasized.

**D. Single Level System in the Presence of Charging Effect**

The above examples do not involve many-electron Coulomb interaction. In this subsection, we consider the simplest example of transport through single level system in the presence of Coulomb charging effect. The system Hamiltonian reads $H_S = \sum_{\mu} (E_0 + \frac{2}{4} \mu) n_\mu$. Here the index $\mu$ labels the spin up ($\uparrow$) and spin down ($\downarrow$) states, and $\mu$ stands for the opposite spin orientation. The electron number operator $n_\mu = a_\mu^\dagger a_\mu$, and the Hubbard term $U n_{\uparrow} n_{\downarrow}$ describe the charging effect. Obviously, the reservoir correlation function is diagonal with respect to the spin indices, i.e., $C_{\alpha \mu \nu}(t) = \delta_{\mu \nu} C_{\alpha \mu \nu}(t)$. We thus have

\begin{align}
A_{\alpha \mu}^{(\pm)} &= C_{\alpha \mu \nu}^{(\pm)}(\pm L) a_\mu = C_{\alpha \mu \nu}^{(\pm)}(\mp \mu U) a_\mu.
\end{align}

(17)

Moreover, for either spin-up or spin-down electrons, the spectral functions $C_{\alpha \mu \nu}^{(\pm)}(E)$ are identical to Eq. (10). For present system, the four basis states can be chosen as $|1\rangle = |00\rangle_{\uparrow \downarrow}$, $|2\rangle = |10\rangle_{\uparrow \downarrow}$, $|3\rangle = |01\rangle_{\uparrow \downarrow}$, and $|4\rangle = |11\rangle_{\uparrow \downarrow}$. Also in the limiting case of zero temperature and large bias voltage ($\mu_L \gg E_0 + U > E_0 \gg \mu_R$), inserting Eq. (17) into Eq. (17) and carrying out the matrix elements associated with the above four basis states, we obtain

\begin{align}
\rho_1^{(n)} &= -2 \Gamma_L \rho_{11}^{(n-1)} + \Gamma_R \rho_{22}^{(n-1)} + \Gamma_R \rho_{33}^{(n-1)}, \\
\rho_2^{(n)} &= -2 \Gamma_R \rho_{22}^{(n-1)}, \\
\rho_3^{(n)} &= -2 \Gamma_R \rho_{22}^{(n)} + \Gamma_L \rho_{11}^{(n)} + \Gamma_R \rho_{44}^{(n-1)}, \\
\rho_4^{(n)} &= -2 \Gamma_R \rho_{44}^{(n)} + \Gamma_L \rho_{33}^{(n)},
\end{align}

(18a)

(18b)

(18c)

(18d)

where $\Gamma' = (2 \pi g_0 |\alpha|^2) e^{-E_0 + U}$. Satisfactorily, Eq. (18) is nothing but the result obtained in Ref. [9] under the same limiting conditions.

**E. Interacting Quantum Dot with Zeeman Splitting**

In this subsection, we revisit the model studied in Sec. III-D, but slightly modify it by allowing for a finite spin splitting, i.e., $H_S = \sum_{\alpha \mu} (E_\mu a_\mu^\dagger a_\mu + \frac{2}{4} C_{\alpha \mu} a_\mu n_\mu)$, where the non-zero Zeeman splitting is characterized by $E_1 - E_2 = \Delta$. The transport properties of this system has been studied recently by Thielmann et al. [10], by applying the real-time diagrammatic technique [11]. Here we show our master equation approach can solve this non-trivial model in a more transparent way.

As done previously, we first carry out the commutator $\mathcal{L} a_\mu = [H_S, a_\mu] = -W_\mu a_\mu$, where $W_\mu = E_\mu \delta_{\mu \mu} + E_2 \delta_{\mu 1} + U (n_\uparrow \delta_{\mu 1} + n_\downarrow \delta_{\mu 2})$. Noting that $[H_S, W_\mu] = 0$, we have $\mathcal{L} a_\mu = - (W_\mu) a_\mu$. Accordingly, $A_{\alpha \mu}^{(\pm)} = C_{\alpha \mu \nu}^{(\pm)}(\mp W_\mu) a_\mu$. In the wide-band approximation and assuming an energy-independent coupling strength $\Gamma_L (\Gamma_R)$ with the left (right) electrode, explicit expressions for $A_{\alpha \mu}^{(\pm)}$ are obtained as $A_{\alpha \mu}^{(\pm)}(\pm L/R) = \Gamma_L/R S_L/R (W_\mu) a_\mu$. In the occupation number representation, i.e., $|1\rangle = |00\rangle_{\uparrow \downarrow}$, $|2\rangle = |10\rangle_{\uparrow \downarrow}$, $|3\rangle = |01\rangle_{\uparrow \downarrow}$, and $|4\rangle = |11\rangle_{\uparrow \downarrow}$, the master equation Eq. (19) can be easily solved, and via Eq. (8), the current can be computed quite straightforwardly. In the following, we explicitly carry out the result in different voltage regimes. For the sake of being able to obtain analytic result, we focus on the limiting case of zero temperature. Moreover, without loss of generality, we assume that the bias voltage makes the Fermi level of the right
electrode be always lower than the quantum dot energy levels during transport. Therefore, all \( n_R^{(+)} \) at the four energies, say, \( E_\uparrow, E_\downarrow, E_\uparrow + U, \) and \( E_\downarrow + U \), are zero.

Regime (i): \( \mu_L > E_\uparrow + U, E_\downarrow + U, E_\uparrow, E_\downarrow > \mu_R \). In this high bias regime, the corresponding Fermi functions are 
\[
n_L^{(+)}(E_\uparrow) = n_L^{(+)}(E_\downarrow) = n_L^{(+)}(E_\uparrow + U) = 1, \]
and the master equation Eq. \( \ref{eq:master} \) reads
\[
\begin{align*}
\dot{\rho}_{11} &= -2\Gamma_L \rho_{11} + \Gamma_R \rho_{22} + \Gamma_R \rho_{33}, \\
\dot{\rho}_{22} &= -\Gamma_R + \Gamma_L \rho_{22} + \Gamma_L \rho_{11} + \Gamma_R \rho_{44}, \\
\dot{\rho}_{33} &= -\Gamma_L \rho_{33} + \Gamma_R \rho_{22} + \Gamma_R \rho_{44}, \\
\dot{\rho}_{44} &= -2\Gamma_R \rho_{44} + \Gamma_L \rho_{22} + \Gamma_L \rho_{33}.
\end{align*}
\]

(19)

To evaluate the stationary current, only stationary solution is required, which are easily obtained as, respectively, \( \rho_{22} = \rho_{33} = \Gamma_L \Gamma_R / (\Gamma_L + \Gamma_R)^2 \), \( \rho_{11} = (\Gamma_L / \Gamma_R) \rho_{22} \), and \( \rho_{44} = (\Gamma_L / \Gamma_R) \rho_{22} \). Then, from Eq. \( \ref{eq:master} \) the current is simply carried out as
\[
I(t \to \infty) = e \Gamma_R (\rho_{22} + \rho_{33} + 2\rho_{44}) = \frac{2e \Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}. \tag{20}
\]

Regime (ii): \( E_\uparrow + U > \mu_L > E_\downarrow + U, E_\uparrow, E_\downarrow > \mu_R \).
The Fermi functions in this case read \( n_L^{(+)}(E_\uparrow + U) = 0 \), \( n_L^{(+)}(E_\downarrow) = n_L^{(+)}(E_\uparrow + U) = 1 \), and the resulting master equation is
\[
\begin{align*}
\dot{\rho}_{11} &= -2\Gamma_L \rho_{11} + \Gamma_R \rho_{22} + \Gamma_R \rho_{33}, \\
\dot{\rho}_{22} &= -\Gamma_R + \Gamma_L \rho_{22} + \Gamma_L \rho_{11} + \Gamma_R \rho_{44}, \\
\dot{\rho}_{33} &= -\Gamma_R \rho_{33} + \Gamma_L \rho_{11} + \Gamma_R \rho_{44}, \\
\dot{\rho}_{44} &= -2\Gamma_R \rho_{44} + \Gamma_L \rho_{22} + \Gamma_L \rho_{33}.
\end{align*}
\]

(21)

Solution of the stationary state reads, respectively, \( \rho_{22} = \Gamma_L \Gamma_R (\Gamma_L + 2\Gamma_R) / (\Gamma_L + \Gamma_R)^3 \), \( \rho_{33} = \rho_{11} + 2\Gamma_L \Gamma_R (\Gamma_L + \Gamma_R)^2 / (\Gamma_L + \Gamma_R)^3 \), and \( \rho_{44} = \Gamma_L \Gamma_R (\Gamma_L + \Gamma_R)^2 / (\Gamma_L + \Gamma_R)^3 \). Note that \( \rho_{11} = 1 - \rho_{22} - \rho_{33} - \rho_{44} \), which is irrelevant to the current. Straightforwardly, we obtain the current
\[
I(t \to \infty) = e \Gamma_R (\rho_{22} + \rho_{33} + 2\rho_{44}) = \frac{2e \Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}. \tag{22}
\]

Regime (iii): \( E_\uparrow + U, E_\downarrow + U > \mu_L > E_\uparrow, E_\downarrow > \mu_R \).
The Fermi functions \( n_L^{(+)}(E_\downarrow) = n_L^{(+)}(E_\uparrow) = 1 \), and \( n_L^{(+)}(E_\downarrow + U) = n_L^{(+)}(E_\uparrow + U) = 0 \). The corresponding master equation reads
\[
\begin{align*}
\dot{\rho}_{11} &= -2\Gamma_L \rho_{11} + \Gamma_R \rho_{22} + \Gamma_R \rho_{33}, \\
\dot{\rho}_{22} &= -\Gamma_R \rho_{22} + \Gamma_L \rho_{11} + (\Gamma_L + \Gamma_R) \rho_{44}, \\
\dot{\rho}_{33} &= -\Gamma_R \rho_{33} + \Gamma_L \rho_{11} + (\Gamma_L + \Gamma_R) \rho_{44}, \\
\dot{\rho}_{44} &= -2(\Gamma_L + \Gamma_R) \rho_{44}.
\end{align*}
\]

(23)

The stationary-state solution of the reduced density matrix leads to the transport current as
\[
I(t \to \infty) = e \Gamma_R (\rho_{22} + \rho_{33} + \rho_{44}) = \frac{2e \Gamma_L \Gamma_R}{2\Gamma_L + \Gamma_R}. \tag{24}
\]

Regime (iv): \( E_\uparrow + U, E_\downarrow + U, E_\uparrow > \mu_L > E_\downarrow > \mu_R \). In this setup, only \( n_L^{(+)}(E_\downarrow) = 1 \), and all other Fermi functions are zero. Similarly, we first carry out the master equation
\[
\begin{align*}
\dot{\rho}_{11} &= -\Gamma_L \rho_{11} + \Gamma_R \rho_{22} + \Gamma_R \rho_{33}, \\
\dot{\rho}_{22} &= -\Gamma_L \rho_{22} + (\Gamma_L + \Gamma_R) \rho_{44}, \\
\dot{\rho}_{33} &= -\Gamma_R \rho_{33} + (\Gamma_L + \Gamma_R) \rho_{44}, \\
\dot{\rho}_{44} &= -2(\Gamma_L + \Gamma_R) \rho_{44}.
\end{align*}
\]

(25)

Then, the stationary transport current is calculated via the stationary-state solution of the density matrix as
\[
I(t \to \infty) = e \Gamma_R (\rho_{22} + \rho_{33}) = \frac{e \Gamma_L \Gamma_R}{\Gamma_L + \Gamma_R}. \tag{26}
\]

Remarkably, we have precisely recovered all the Coulomb plateaus presented in Ref. [10] which go beyond simple intuition and are obtained there by a not easily accessible real-time diagrammatic technique. This example may shine light on the convenience of our approach in applications.

IV. CONCLUDING REMARKS

In summary, we have developed an efficient master equation approach for quantum transport through mesoscopic systems, and demonstrated its application by a number of examples. Compared with the previous work by Gurvitz [3], the present study not only generalizes the applicable conditions to finite temperature and arbitrary voltage, but also identifies the adopted approximation which appears not very clear in Ref. [3]. That is, by treating the electrodes as (Fermi) thermal baths, the major approximation adopted in our derivation is the standard second-order Born approximation for the coupling (tunneling) Hamiltonian. It is known that this well-justified approximation makes the resultant quantum master equation applicable in a large number of dissipative systems (e.g. in quantum optics), provided the system-bath coupling is not so strong. Favorably, the illustrated examples in this paper also show its applicability in quantum transport. Moreover, the developed master equation approach holds the obvious advantages of application convenience and straightforwardness, as well as the ability to address many-body correlation, inelastic scattering, and transient behavior, which are usually difficult issues in mesoscopic transport.

In comparison with the nGF approach, we found that the structure of Eq. \( \ref{eq:nGF} \) is in fact identical to the formal expression of current in terms of non-equilibrium correlation functions \( \mathbb{F} \). The nGF approach remains the relatively hard task to searching for particular techniques (e.g. the Feynman diagram or equation of motion) to carry out those correlation functions. In this sense, the obtained Eq. \( \ref{eq:nGF} \) is nothing but the explicit Markovian result under the second-order Born approximation for the
tunneling Hamiltonian. In principle, further systematic corrections are possible along the line of going beyond the Born approximation, to include higher order contribution of tunneling. Finally, we mention that Eq. 8 can be derived from the formal nGF expression of current, however, the present derivation along the line of Ref. 7 is interesting, and the particular result Eq. 7 from this unique method is of great value, which contains rich information and can be conveniently employed, for instance, to calculate the noise spectrum 2 13 15.

APPENDIX: LEVEL-BROADENING EFFECT

To make the derived formulas Eqs. (7)-(9) more accurately applicable to arbitrary voltage, additional care is needed as any of the individual system levels is approaching to the Fermi surface of the electrode. For the sake of description clarity, let us take the single-level resonance system as an example to highlight the key point. As mentioned previously, the treatment in Sec. II under the second-order Born approximation has neglected level broadening effect, which would cause certain errors in some particular cases. For instance, current flowing through the resonance system would be strictly forbidden under the near-resonance condition, i.e., as the resonance level $E_0$ is a little bit higher than $\mu_L$ ($\mu_L > \mu_R$). However, it is well known that a full quantum treatment will give nonzero current in this situation 2 3. For bias voltage such that the resonance level (together with its broadening) is within the range of the two Fermi levels (i.e. $\mu_L > E_0 > \mu_R$), common result of resonance current will be predicted by our master equation approach and the nGF-based quantum transport theory. In spite of this, it would be desirable to remove the drawback of inaccuracy of our approach in the near-resonance situation.

To account for the level-broadening effect, we return to the evaluation of $A_{\alpha\mu}^{(\pm)} = \sum_{\nu} C_{\alpha\nu\mu}^{(\pm)}(\pm L)a_{\nu\mu}$. Without loss of generality, we restrict our description in the diagonal case $C_{\alpha\mu\mu}^{(\pm)}(t) = 0$. More general description is straightforward provided one has clarified the correlation between “$f_\mu$” and “$f_\nu$”. Using the free-electron-gas model for the electrodes, $A_{\alpha\mu}^{(\pm)}$ can be expressed as

$$A_{\alpha\mu}^{(\pm)} = 2 \sum_k \tau_{\alpha\mu\mu}^{(\pm)}(\epsilon_k) \int_0^\infty dt e^{\pm i\epsilon_k t} e^{\pm i\epsilon_L t} a_{\alpha\mu}. \quad (A.1)$$

In our previous treatment, we have replaced the time integral $\int_0^\infty dt$ by $\int_{-\infty}^\infty dt$, under the spirit of Markovian approximation. As a result, the time integration gives rise to a $\delta$-function, $2\pi\delta(\epsilon_k + \mathcal{L})$, which characterizes energy conservation for electron transfer between the central system and the electrodes. Mathematically, this procedure is equivalent to dropping the imaginary (principal) part of integral, and keeping only the real part. Now, notice that $e^{\pm i\epsilon_L t} a_{\mu}$ describes the quantum evolution of the $E_\mu$ state (level) associated with the isolated system Hamiltonian. As a standard procedure, the system level broadening effect due to coupling with the electrodes can be implemented by inserting a damping factor $e^{-\Gamma e t} = e^{-i(\Gamma_L + \Gamma_R) t}$ into the integrand of the time integral 15. After this, by keeping only the real part of the integral and adopting the typical wide-band approximation for the electrodes, we have

$$A_{\alpha\mu}^{(\pm)} = \Gamma_{\alpha\mu} \int \frac{d\epsilon_k}{2\pi} \tilde{a}_{\alpha\mu}(\epsilon_k + \mathcal{L}) n_{\alpha}(\epsilon_k)a_{\mu}. \quad (A.2)$$

Here the standard Lorentzian spectral density function reads $\tilde{a}_{\alpha\mu}(\omega + \mathcal{L}) = 2\Gamma_{\alpha\mu}/[(\omega + \mathcal{L})^2 + \Gamma_{\alpha\mu}^2]$. Formally introducing $N_{\alpha\mu}^{(\pm)}(-\mathcal{L}) \equiv \int \frac{d\epsilon_k}{2\pi} \tilde{a}_{\alpha\mu}(\epsilon_k - \mathcal{L}) n_{\alpha}(\epsilon_k)$, we re-express (A.2) in a very compact form as

$$A_{\alpha\mu}^{(\pm)} = \Gamma_{\alpha\mu} N_{\alpha\mu}^{(\pm)}(-\mathcal{L})a_{\mu}. \quad (A.3)$$

Elegantly, $N_{\alpha\mu}^{(\pm)}(-\mathcal{L})$ can be regarded as the counterpart of the Fermi function $n_{\alpha}(\mathcal{L})$ after accounting for the level broadening. Combining (A.3) with Eqs. (7)-(9), we complete the generalization of the formalism.

As an illustrative application of the generalized formalism, we re-consider the transport through the (free) multi-level system. Straightforwardly, the current expression of Eq. (13) becomes

$$I = e \sum_{\mu} \frac{\Gamma_L(E_{\mu}) \Gamma_R(E_{\mu})}{\Gamma_L(E_{\mu}) + \Gamma_R(E_{\mu})} \times \int \frac{d\epsilon_k}{2\pi} \tilde{a}_{\alpha\mu}(\epsilon_k - E_{\mu})[n_{\alpha}(\epsilon_k) - n_R(\epsilon_k)]. \quad (A.4)$$

This is the well-known formula for resonant tunneling current, which is valid for arbitrary voltage including the near-resonance situation.

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[18] A more formal and rigorous treatment is possible by improving the second-order Born approximation. Namely, by self-consistently including higher order contribution of the tunneling Hamiltonian $H'$, the operator $\tilde{a}_\mu(t) \equiv e^{\pm i\mathcal{L}_\mu t}a_\mu$ would satisfy a master-type equation, $\dot{\tilde{a}}_\mu = i\mathcal{L}\tilde{a}_\mu - \mathcal{R}\tilde{a}_\mu$, and the second (damping) term coincides precisely with the one of Eq. (9). This treatment can be termed as a self-consistent Born approximation. However, the simple implementation of a damping factor as done in present Appendix will be more convenient in practice.