Geometrical Pump in Quantum Transport: Quantum Master Equation Approach

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For an open quantum system, we investigate the pump current that is induced by a slow modulation of control parameters on the bases of the quantum master equation and full counting statistics. We find that the average and the cumulant generating function of the pump are characterized by the geometrical Berry-phase-like quantities in the parameter space, which is associated with the generator of the master equation. By our formulation, we can discuss the geometrical pump under the control of the chemical potentials and temperatures of reservoirs. We demonstrate the formulation by spinless electrons in coupled quantum dots. We show that the geometrical pump is prohibited for the case of non-interacting electrons if we modulate only temperatures and chemical potentials of reservoirs, while the geometrical pump occurs in the presence of an interaction between electrons.

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I. INTRODUCTION

When a quantum system is slowly and periodically modulated by two or more control parameters such as gate voltages, a net number of particles can be transported per period of the modulation even in the absence of dc driving force (e.g., bias voltage). This phenomenon is known as an adiabatic pump. The original idea of the adiabatic pump was proposed by Thouless, where a pump current of a closed quantum system is related to the Berry phase of the ground state of the Hamiltonian. Since then, experimental and theoretical studies of the adiabatic pump have been developed.

Later, the idea of the adiabatic pump has been applied to open quantum systems both in experiments and theories. Theoretically, the average pump current can be expressed by the Berry phase associated with the scattering matrix. The cumulant generating function of pump current can also be described by geometrical quantities. For this reason, the adiabatic pump is referred to as the geometrical pump. The above-mentioned theories are based on the time-dependent scattering theory.

Similar phenomena have been studied in stochastic systems described by classical master equation, which is referred to as the adiabatic stochastic pump. The pump current in the classical stochastic pump has also geometrical properties; the cumulant generating function of the pump current is expressed by a Berry-phase-like quantity that is associated with the generator of the classical master equation. We shall refer to this quantity as the Berry-Sinitsyn-Nemenman (BSN) phase. There have also been several works on the adiabatic pump for quantum open systems described by quantum master equation (QME). However, the geometrical effects in the adiabatic pump described by QME have not been fully understood.

In this paper, we investigate the quantum adiabatic pump on the basis of QME, and derive general formulae of the cumulant generating function and average of the pump. These formulae are geometrical and expressed by a quantum analogous of the BSN phase which is associated with the generator of the QME. Since our theoretical framework is independent of the details of the system, it is useful for analyzing a large variety of applications of the adiabatic pump such as a qubit rotation in quantum dots and a spin pumping. We note that the master equation approach is suitable to analyze systems that include interaction between particles, dissipations, and decoherences.

This paper is organized as follows. In Sec. III A, the QME approach for an open system is discussed. The full counting statistics in the QME approach is discussed in Sec. III B. For the adiabatic pump, the geometrical formulae (BSN phase expressions) for the cumulant generating function and the average of the pumped quantity are derived in Sec. III C. In this formulation, the temperatures and chemical potentials of reservoirs are the control parameters. This is in contrast to most of the conventional studies on the adiabatic pump, where only the parameters in the system Hamiltonian or in the coupling with the reservoirs are considered. In Sec. III D we demonstrate our theory by the spinless electron transport in quantum dot systems. For non-interacting cases with the rotating wave approximation (RWA), we find that no geometrical pump occurs if we control only the temperatures and chemical potentials of reservoirs. In contrast, the geometrical pump occurs for an interacting electron system even when we control only the reservoir parameters. Section IV is devoted to the discussion and conclusion. In Appendix A, we describe the details of the QME in the framework of the full counting statistics. In Appendix B we show the detailed derivation of Eq. (17). In Appendix C, we verify the equivalence between without and within the RWA concerning the unit-time generating function of the cur-
Here the symbol “ˇ” stands for the interaction picture $K$ of the QME depends on several parameters; the system and reservoirs, $\{R_b\}$, where $b$ is an index of reservoirs (see Fig. 1 for a schematic). The total Hamiltonian of the coupled system is $H_{\text{tot}} = H_S + \sum_b (H_b + H_{Sb})$, where $H_S$ is the system Hamiltonian, $H_b$ is the Hamiltonian of the $b$th reservoir $R_b$, and $H_{Sb}$ is the interaction Hamiltonian between $S$ and $R_b$. If the interaction between the system $S$ and the reservoirs is weak, the dynamics of $S$ can be described by a QME for the reduced density matrix of $S$, which is denoted as $\hat{\rho}$. Suppose that the initial state of the system $S$ is decoupled with the reservoirs. Then, up to the second order in the system-reservoir coupling (Born approximation) with the Markov approximation\(^{26}\), the QME for the system $S$ reads

$$\frac{d\hat{\rho}(t)}{dt} = K\hat{\rho}(t),$$

where

$$K \equiv \frac{1}{\hbar}[\hat{H}_S, \hat{\rho}] + \sum_b D_b \hat{\rho},$$

$$D_b \hat{\rho} = -\frac{1}{\hbar^2} \int_0^\infty dt' \text{Tr}_b[\hat{H}_{Sb}, [\hat{H}_{Sb}(-t'), \hat{\rho} \otimes \hat{\rho}_b]].$$

Here the symbol “$\cdots$” stands for the interaction picture with respect to $\hat{H}_S + \sum_b \hat{H}_b$. $\text{Tr}_b$ represents the trace over the $b$th reservoir, and $\hat{\rho}_b = e^{-\beta_b (H_b - \mu_b N_b)} / Z_b$ is the grandcanonical distribution with the inverse temperature $\beta_b$, chemical potential $\mu_b$, and the particle number operator $N_b$ of the $b$th reservoir. The time-evolution generator $K$ of the QME depends on several parameters; the system parameters in $\hat{H}_S$ and $\hat{H}_{Sb}$ such as the energy levels of quantum dots and the tunnel barriers between them, and the reservoir parameters, $\{\beta_b\}$ and $\{\mu_b\}$. We write the set of these parameters as $\alpha$. The right eigenvalue equation for $K$ is written as

$$K \hat{\rho}_n(\alpha) = \lambda_n(\alpha) \hat{\rho}_n(\alpha),$$

where $\lambda_n(\alpha)$ is an eigenvalue of $K$, $n$ is a label of the eigenvalues, and $\hat{\rho}_n(\alpha)$ is the corresponding right eigenvector.

By introducing the Hilbert-Schmidt inner product of linear operators $A$ and $B$ on $\mathcal{H}_S$ as $\text{Tr}_S(\hat{A}^\dagger \hat{B})$, we define the adjoint $K^\dagger$ of the QME generator such that $\text{Tr}_S[(K^\dagger \hat{A})^\dagger \hat{B}] = \text{Tr}_S(\hat{A}^\dagger K \hat{B})$ holds for any $\hat{A}$, $\hat{B}$. We then have the left eigenvalue equation for $K$: \(^{31}\)

$$K^\dagger \hat{\ell}_n(\alpha) = \lambda_n^*(\alpha) \hat{\ell}_n(\alpha),$$

where $\hat{\ell}_n(\alpha)$ is the left eigenvector corresponding to the eigenvalue $\lambda_n(\alpha)$. In the following, we assume that $K$ has the zero eigenvalue $\lambda_0 = 0$ without degeneracy, so that $K \hat{\rho}_0 = 0$ and $K^\dagger \hat{\ell}_0 = 0$ hold. This implies that the QME has a unique steady solution $\hat{\rho}_{ss} = \hat{\rho}_0$ for fixed $\alpha$. We note that $\hat{\ell}_0(\alpha) = 1$ (identity operator) holds for any $\alpha$.

### II. GENERAL RESULTS

#### A. Setup

We consider a quantum system $S$ that is weakly coupled to reservoirs $\{R_b\}$, where $b$ is an index of reservoirs (see Fig. 1 for a schematic). The right eigenvalue equation for the system $S$ reads

where

$$\frac{d\hat{\rho}(t)}{dt} = K\hat{\rho}(t),$$

$$K \equiv \frac{1}{\hbar}[\hat{H}_S, \hat{\rho}] + \sum_b D_b \hat{\rho},$$

$$D_b \hat{\rho} = -\frac{1}{\hbar^2} \int_0^\infty dt' \text{Tr}_b[\hat{H}_{Sb}, [\hat{H}_{Sb}(-t'), \hat{\rho} \otimes \hat{\rho}_b]].$$

We consider the statistics of a quantity $\Delta q$ transferred from the reservoirs to the system $S$ during a time interval $\tau$. The measurement scheme of $\Delta q$ is as follows. First, at $t = 0$ we perform a projection measurement of a reservoir variable $Q$ to obtain a measurement outcome $q_0$. We assume $[Q, \hat{N}_b] = 0$ and $[Q, \hat{H}_b] = 0$ for any $b$. For $t > 0$, the system $S$ undergoes the time evolution with interacting with the reservoirs. At $t = \tau$ we again perform a projection measurement of $Q$ to obtain another measurement outcome $q_\tau$. Then $\Delta q$ is defined as $\Delta q = q_\tau - q_0$.

The cumulant generating function of the statistics is given by $S_\tau(\chi) = \ln \int P_\tau(\Delta q) e^{i\chi \Delta q} d\Delta q$, where $P_\tau(\Delta q)$ is the probability of $\Delta q$ during $\tau$. $\chi$ is called the counting field, and the derivatives of $S_\tau(\chi)$ give the cumulants of $P_\tau(\Delta q)$; e.g., $\langle \Delta q \rangle_\tau = \partial S_\tau(\chi) / \partial (i\chi)|_{\chi=0}$. Note that if $Q$ is the $b$th reservoir’s particle number $\hat{N}_b$ (Hamiltonian $\hat{H}_b$), then $\langle \Delta q \rangle_\tau / \tau$ is the average of the particle (energy) current from the $b$th reservoir into the system $S$.

For calculating $S_\tau(\chi)$, we employ a method developed in the context of the full counting statistics\(^{27}\). In this method $S_\tau(\chi)$ is obtained from the solution of the modified equation of motion which is governed by the $\chi$-dependent Hamiltonian. In the QME approach, this reads $S_\tau(\chi) = \ln \text{Tr}_S(\hat{\rho}^\tau(\chi))$, where $\text{Tr}_S$ is the trace over the system $S$ and $\hat{\rho}^\tau(\chi)$ is a solution of the generalized QME (GQME):

$$\frac{d\hat{\rho}^\tau(t)}{dt} = K_\chi \hat{\rho}^\tau(t).$$

Here the modified generator $K_\chi$ is given by

$$K_\chi \hat{\rho}^\tau \equiv \frac{1}{\hbar}[\hat{H}_S, \hat{\rho}^\tau] + \sum_b D_b^\chi \hat{\rho}^\tau,$$

$$D_b^\chi \hat{\rho} \equiv -\frac{1}{\hbar^2} \int_0^\infty dt' \text{Tr}_b[\hat{H}_{Sb}, [\hat{H}_{Sb}(-t'), \hat{\rho} \otimes \hat{\rho}_b]|_\chi],$$

where $\lambda_n(\alpha)$ is an eigenvalue of $K_\chi$.
where $[\hat{O}, \hat{P}]_\chi = \hat{O}^\chi \hat{P} - \hat{P}^\chi \hat{O}$ and $\hat{O}^\chi = e^{-i\chi Q/2} \hat{O} e^{i\chi Q/2}$. See Appendix A for details.

We denote the left and right eigenvectors of $\mathcal{K}_\chi$ (for fixed $\alpha$) corresponding to the eigenvalue $\lambda_0^\chi(\alpha)$ as $\hat{\ell}_0^\chi(\alpha)$ and $\hat{\rho}_0^\chi(\alpha)$, respectively. They are normalized as $\text{Tr}_S(\hat{\ell}_m^\chi(\alpha) \hat{\rho}_0^\chi) = \delta_{mn}$. We assign the label for the eigenvalue with maximum real part to $n = 0$. Then $\hat{\rho}_0^\chi(\alpha)$ is the unit-time cumulant generating function of the steady state for fixed $\alpha$. We assume that the modulation of the parameters $\lambda$ is similar to those in Refs 16, 28. Thus $\lambda_0^\chi(\alpha)$ is the unit-time cumulant generating function for the GQME reduces to the original QME, and $\hat{\ell}_0^\chi$ and $\hat{\rho}_0^\chi$ to $1$ and $\hat{\rho}_\text{ss}$, respectively.

C. Geometrical pump

We slowly modulate the parameters $\alpha$ along a curve $\mathcal{C}$ in the parameter space during a time interval $\tau$. If the system is in the instantaneous steady state for the value of $\alpha$, at each time $t$ in the whole of the process, the cumulant generating function for $\Delta q$ for this process is equal to the time integral of the unit-time cumulant generating function $\lambda_0^\chi(\alpha_t)$ of the instantaneous steady state. In general, however, there exists additional (pumped) contribution: $S_\chi(\tau) = \int_0^\tau d\tau \lambda_0^\chi(\alpha_t) + S_\chi^\text{ex}(\alpha)$. We call the latter contribution the excess part. The excess part is intrinsic in the transitions between the steady states, and is of our interest.

We now derive the geometrical expression of the excess part of the generating function by using the method similar to those in Refs 16, 28. First, to solve the GQME for a given curve $\mathcal{C}$ of $\alpha$ in the parameter space, we expand $\hat{\rho}_0^\chi(t)$ as

$$\hat{\rho}_0^\chi(t) = \sum_n c_n(t) e^{\Lambda_0^\chi(t)} \hat{\rho}_0^\chi(\alpha_t),$$

where $\Lambda_0^\chi(t) \equiv \int_0^t dt' \lambda_0^\chi(\alpha_{t'})$. Inserting this equation into Eq. (5) and taking the Hilbert-Schmidt inner product with $\hat{\ell}_0^\chi(\alpha_t)$, we obtain

$$\frac{dc_n(t)}{dt} = - \sum_n c_n(t) e^{\Lambda_0^\chi(t)} \text{Tr}_S \left( \hat{\ell}_0^\chi(\alpha_t) \frac{d\lambda_0^\chi(\alpha_t)}{dt} \right).$$

We assume that the modulation of the parameters $\alpha$ is sufficiently slow. Then we can approximate the sum on the right hand side of Eq. (8) by the contribution only from the term with $n = 0$. By solving this adiabatic approximation equation we obtain

$$c_0(\tau) = c_0(0) \exp \left[ - \int_0^\tau \text{Tr}_S \left( \hat{\ell}_0^\chi(\alpha) \frac{d\lambda_0^\chi(\alpha)}{d\alpha} \right) \right],$$

where $d\hat{\rho}_0(\alpha) \equiv d\alpha \cdot \partial \hat{\rho}_0(\alpha) / \partial \alpha$. If the initial state of the system $S$ is $\hat{\rho}^\chi(0) = \hat{\rho}_\text{ss}(\alpha_0)$, then $c_0(0) = \text{Tr}_S [\hat{\ell}_0^\chi(\alpha_0) \hat{\rho}_\text{ss}(\alpha_0)]$. We again use the adiabatic approximation to obtain

$$\hat{\rho}^\chi(\tau) \simeq c_0(\tau) e^{\lambda_0^\chi(\alpha_t)} \hat{\rho}_0^\chi(\alpha_t) \left[ e^{\lambda_0^\chi(\alpha_t) \tau} \right] .$$

Thus we obtain the excess cumulant generating function $S_\chi^\text{ex}(\tau) = S_\chi(\tau) - \lambda_0^\chi(\tau)$ for the slow modulation:

$$S_\chi^\text{ex}(\tau) = - \int_\mathcal{C} \text{Tr}_S \left( \hat{\ell}_0^\chi(\alpha) \rho_\text{ss}(\alpha) \right) + \lambda_0^\chi(\alpha_t) \rho_\text{ss}(\alpha_t) + \ln \text{Tr}_S \left( \hat{\ell}_0^\chi(\alpha_t) \rho_\text{ss}(\alpha_t) \right) .$$

The right-hand side of Eq. (11) is analogous to the Berry phase, which depends only on the line integral along the curve $\mathcal{C}$ (not on time). We note that $\lambda_0^\chi(\tau)$ corresponds to the dynamical phase.

By differentiating Eq. (11) with respect to $i\chi$, we obtain a geometrical expression of the average excess in the quantity $\Delta q$:

$$\langle \Delta q \rangle^\text{ex} = - \int_\mathcal{C} \text{Tr}_S \left( \hat{\ell}_0^\chi(\alpha) \frac{d\rho_\text{ss}}{d\alpha} (\alpha) \right) \cdot d\alpha,$$

where $\hat{\ell}_0^\chi \equiv \partial \hat{\ell}(\chi)/\partial (i\chi)|_{\chi=0}$. Equations (11) and (12) are regarded as quantum versions of the Berry-Sinitsyn-Nemenman (BSN) phases for the cumulant generating function and the average, respectively, in slow parametric modulation. 16, 21. We refer to $\text{Tr}_S (\hat{\ell}_0^\chi(\alpha_t) \rho_\text{ss}(\alpha_t))$ as the BSN vector potential for average excess quantity.

Equality (12) implies that a finite net quantity of $\Delta q$ can be transferred to the system $S$ for a slow cyclic modulation of the parameters (i.e., for the case where the curve $\mathcal{C}$ is a closed loop) even if there is no dc driving force such as temperature and chemical potential differences. This is an adiabatic pump. By the Stokes theorem, Eq. (12) is rewritten as

$$\langle \Delta q \rangle^\text{ex} = - \int_{\mathcal{S}_C} \sum_{m,n} \frac{1}{2} F_{a_m \alpha_n} d\alpha_m \wedge d\alpha_n,$$

for a cyclic process, where $\wedge$ is the wedge product, $\mathcal{S}_C$ is a surface enclosed by $\mathcal{C}$, and

$$F_{a_m \alpha_n} \equiv \text{Tr}_S \left( \frac{\partial \hat{\ell}_0^\chi(\alpha)}{\partial \alpha_m} \rho_\text{ss}(\alpha_n) - \frac{\partial \hat{\rho}_0^\chi(\alpha)}{\partial \alpha_n} \rho_\text{ss}(\alpha_m) \right).$$

We refer to Eq. (14) as the BSN curvature for average pumped quantity.

For some cyclic processes, the excess pump $\langle \Delta q \rangle^\text{ex}$ vanishes. A sufficient condition for the “no-pumping” is that $F_{a_m \alpha_n} = 0$ holds in $\mathcal{S}_C$ for all $(\alpha_m, \alpha_n)$. We note that if the whole of a curve $\mathcal{C}$ (not necessarily closed) lies in a region of the no-pumping condition, then the average excess pump does not depend on the whole of $\mathcal{C}$ but depends on only the initial and final points of $\mathcal{C}$.
III. APPLICATION TO SPINLESS ELECTRON TRANSPORT IN QUANTUM DOT

In this section, we apply the general framework obtained in the previous section to the transport of spinless electrons in quantum dot systems connected to two electron reservoirs \((b = L, R)\). The spinless electron model can be used for analyzing phenomena in which the spin degrees of freedom are irrelevant. The reservoir Hamiltonian is given by \(H = \sum_k \hbar \omega_k b_k^\dagger b_k\). Here \(\hbar \omega_k\) is the \(k\)th mode energy of the electron in the \(b\)th reservoir, and \(b_k^\dagger (b_k)\) is the corresponding creation (annihilation) operator, which satisfies \(\{b_k^\dagger, b_{k'}\} = \delta_{kk'} \delta_{b'k'}, \{\bar{b}_k^\dagger, \bar{b}_{k'}\} = \{\bar{b}_k, \bar{b}_{k'}\} = 0\). We here take the quantity to be counted as the electron number transferred from the reservoir \(L\) to the system \(S\), i.e., \(\hat{Q} = \sum_k \hat{c}_L^\dagger \hat{c}_L\).

A. Non-interacting electron model with RWA

First we consider a model of non-interacting spinless electrons in a series of \(N\) single-level quantum dots coupled to two reservoirs \((b = L, R)\). The Hamiltonian of the system \(S\) in this model is

\[
\hat{H}_S = \sum_i \varepsilon_i \hat{d}_i^\dagger \hat{d}_i + \sum_{(ii')} v \hat{d}_{i'}^\dagger \hat{d}_{i'} + \text{h.c.,} \tag{15}
\]

where \(\varepsilon_i\) is the level energy of the \(i\)th dot, \(\hat{d}_i^\dagger (\hat{d}_i)\) is the creation (annihilation) operator of the electron in the \(i\)th dot, and \(v\) is the transfer probability amplitude between the dots. This Hamiltonian can be diagonalized by a unitary transformation as \(\hat{H}_S = \sum_j \hbar \omega_j \hat{a}_j^\dagger \hat{a}_j\). Here \(\hbar \omega_j\) is the \(j\)th mode energy of the electron in the system \(S\), and \(\hat{a}_j^\dagger (\hat{a}_j)\) is the corresponding creation (annihilation) operator of the electron, which satisfies the canonical anti-commutation relations of fermion: \(\{\hat{a}_j^\dagger, \hat{a}_{j'}\} = \delta_{jj'}, \{\hat{a}_j^\dagger, \hat{a}_{j'}^\dagger\} = \{\hat{a}_j, \hat{a}_{j'}\} = 0\). The coupling Hamiltonian between the system \(S\) and the \(b\)th reservoir is given by \(\hat{H}_{sb} = \sum_{j,k} V_{bjk} \hat{a}_j^\dagger \hat{c}_k + \text{h.c.}\)

To derive the GQME for this system we use the Born (up to the second order in \(\hat{H}_{sb}\)) and the Markov approximations\(^{28}\). Furthermore, we adopt the RWA, which is a coarse-graining of the time evolution on the time scale longer than that of the system evolution without the coupling with the reservoirs\(^{26,27}\). For \(\chi = 0\) the RWA leads a Lindblad form of the GME and guarantees the complete positivity of the time evolution. We carry out the RWA by averaging over the rapidly oscillating terms in the Born-Markov GQME in the interaction picture (see Appendix A for the detail). Then we obtain the generator \(K_\chi\) of the GQME in the form of \(K_\chi = \sum_j K_{\chi,j}\). Here the GQME generator \(K_{\chi,j}\) for the \(j\)th mode is given by\(^{27}\)

\[
K_{\chi,j} \hat{\rho} = \frac{1}{i \hbar} \left[ \hbar \omega_j \hat{a}_j^\dagger \hat{a}_j + \hat{H}_{\chi}^{\text{Lamb}}, \hat{\rho} \right] - \frac{1}{2 \hbar^2} \sum_{b=L,R} \left( \Phi_{bj}^- (\omega_j) \{ \hat{a}_j, \hat{a}_j^\dagger \hat{\rho} + \hat{\rho} \hat{a}_j^\dagger \hat{a}_j - 2 e^{-i \omega_j} \hat{a}_j^\dagger \hat{\rho} \hat{a}_j \} + \Phi_{bj}^+ (\omega_j) \{ \hat{a}_j^\dagger \hat{\rho} + \hat{\rho} \hat{a}_j - 2 e^{i \omega_j} \hat{a}_j^\dagger \hat{\rho} \hat{a}_j \} \right), \tag{16}
\]

where \(\hat{H}_{\chi}^{\text{Lamb}} = \sum_b \left( \Psi_{bj}^- (\omega_j) \hat{a}_j^\dagger \hat{a}_j - \Psi_{bj}^+ (\omega_j) \hat{a}_j \hat{a}_j^\dagger \right) / 2 \hbar\) is the Lamb shift Hamiltonian, \(\Phi_{bj}^- (\omega) \equiv 2 \pi \sum_k |V_{bjk}|^2 \delta (\omega - \hbar \omega_k) f_b^L (\omega)\) is the power spectrum of the \(b\)th reservoir, \(\Psi_{bj}^\pm (\omega) \equiv P \int_{-\infty}^{\infty} (dw') / \pi \Phi_{bj}^\pm (\omega') / (\omega' - \omega)\), and \(\chi_L = \chi, \chi_R = 0\). Here, \(P\) means the principal value, \(f_b^L (\omega) = 1 / (1 + e^{-\beta_b (\omega - \mu_b)})\) is the fermi distribution function with \(\beta_b, \mu_b\), and \(f_b^L (\omega) = 1 - f_b^L (\omega)\). The control parameters \(\alpha\) in this model can be both the system parameters, the levels \(\{\varepsilon_i\}\), and the transfer \(v\) between the dots, and the reservoir parameters \(\{\mu_b, \beta_b\}\).

In this model within the RWA, we analytically obtain the BSN vector potential (see Appendix B for the derivation):

\[
\text{Tr}_S \left( \frac{\rho^{|\alpha\beta\alpha^c\beta^c|}}{\partial \alpha} \right) = \sum_j \frac{\Gamma_{Lj}(\omega_j) \partial}{\Gamma_{Lj}(\omega_j)} \left( \frac{\sum_b \Gamma_{bj}(\omega_j) f_b^L(\omega_j)}{\Gamma_{Lj}(\omega_j)} \right) \tag{17}
\]

where \(\Gamma_{Lj}(\omega_j) \equiv \sum_b \Gamma_{bj}(\omega_j)\), and \(\Gamma_{bj}(\omega_j) \equiv \Phi_{bj}^+(\omega_j) + \Phi_{bj}^-(\omega_j)\) is the spectral function of the \(b\)th reservoir. Also we can calculate the BSN curvature as

\[
F_{\alpha_m \alpha_n} = \sum_j \frac{\partial}{\partial \alpha_m} \left( \frac{\Gamma_{Lj}(\omega_j)}{\Gamma_{Lj}(\omega_j)} \right) \frac{\partial}{\partial \alpha_n} \left( \frac{\sum_b \Gamma_{bj}(\omega_j) f_b^L(\omega_j)}{\Gamma_{Lj}(\omega_j)} \right). \tag{18}
\]

From Eq. (13), we find that no net excess number of electrons flow per cycle if only the reservoir parameters \(\{\beta_L, \mu_L, \beta_R, \mu_R\}\) are modulated with the system parameters fixed. This is because the spectral function is written as \(\Gamma_{bj}(\omega_j) = 2 \pi \sum_k |V_{bjk}|^2 \delta (\omega_j - \hbar \omega_k)\), so that \(\Gamma_{Lj}/\Gamma_j\) in Eq. (13) is independent of \(\{\beta_L, \mu_L, \beta_R, \mu_R\}\). We note that this result is characteristic of fermion systems. Indeed, in a model of single two-level system connected to two bosonic heat reservoirs, there exists heat pump by cyclic modulations of the temperatures of the two reservoirs\(^{21}\). This difference between the results for the fermion and boson reservoirs comes from the particle statistics, which leads that \(<c^\dagger c + cc^\dagger>\) is independent of (depending on) the reservoir parameters for fermion (boson) reservoir. Because \(\Phi_{bj}^+ \) and \(\Phi_{bj}^-\) are respectively proportional to \(<c^\dagger c>_b\) and \(<cc^\dagger>_b\), the particle statistics determines whether \(\Gamma_{bj} = \Phi_{bj}^+ + \Phi_{bj}^-\) depends on the reservoir parameters.

Before closing this subsection, we make a remark on the validity of the RWA on the transport systems. The
GQME gives the same result either with or without the RWA, as far as the transport between the system and the reservoirs is studied, whereas it is known that the internal current in the system vanishes in nonequilibrium steady states under the RWA. In Appendix C, we analytically show that the unit-time cumulant generating function $\lambda_0(\alpha)$ of the quantity transferred from the reservoirs to the system in the steady state for fixed $\alpha$ is equivalent between the GQMEs within and without the RWA. We also confirm numerically that the results of the adiabatic pump within the RWA quantitatively agree with those without the RWA in the next subsection.

B. Non-interacting electron in double quantum dot without RWA

Next we consider a non-interacting double quantum dot system coupled to two reservoirs, as illustrated in Fig. 2 (a). We assume the wide band limit: $\Gamma_{bj}(\omega) = \Gamma_{bj}^{0} = \text{const}$. In this subsection we use three different methods for calculating $\langle \Delta q \rangle_j^R$ in modulations of the control parameters of the model. In the first method (denoted by RWA), we apply our results within the RWA [Eqs. (17) and (18)]. In the second one (denoted by NonRWA1), we numerically solve the eigenvalue problem of the GQME generator $K_q$ without RWA, and use Eq. (12). In the third method (denoted by NonRWA2), we numerically solve the time evolution differential equation of the GQME without RWA, and use $S_\tau(\chi) = \text{Tr}_S \rho^N(\tau)$.

In Fig. 2 (b), we plot the excess electron number $\langle \Delta q \rangle_j^R$ transferred from the reservoir L to the system for non-cyclic modulations of $\beta_L$, $\mu_L$, and $\mu_R$ along the curves illustrated in the inset of Fig. 2 (b). We plot the dependence of $\langle \Delta q \rangle_j^R$ on the final value of the right reservoir chemical potential $\mu_R$ of the modulations. We see that all the results agree within the numerical precision. This implies that the no-pumping condition described below Eq. (13) within the RWA still holds without the RWA. We have also confirmed that the absolute value of the BSN curvature computed without the RWA is less than $10^{-6}$ in the space of the reservoir parameters, which is zero within the numerical precision.

In Fig. 2 (c), we plot the BSN curvature $F_{\varepsilon_1,\varepsilon_2}$ calculated by the method of NonRWA1 as a function of $\varepsilon_1$ and $\varepsilon_2$. We see that the curvature takes the non-zero values in this case. Therefore we have a finite geometrical pump for the slow periodic modulation of the dot levels (system parameters). We note that this result of the BSN curvature also agrees with the RWA result given by Eq. (13), although not shown in the figure.

We also calculate $\langle \Delta q \rangle_j^R$ for the cyclic process depicted in Fig. 2 (c). In Fig. 2 (d), we plot $\langle \Delta q \rangle_j^R$ calculated by NonRWA2 as a function of the cycle period $\tau_c$ for various values of the amplitude $\Gamma_b^{0}$ of the spectral function. We see that for large $\tau_c$, the asymptotic results by NonRWA2 agree with the results by RWA and NonRWA1. This supports the validity of the adiabatic approximation used in deriving Eq. (12) for slow modulations. The characteristic time for the validity of the adiabatic approximation becomes shorter as $\Gamma_b^{0}$ increases, which implies that $\tau_c \gg \hbar/\Gamma_{bj}$ is an adiabatic condition.

We note that all the results by RWA and NonRWA1 agree with each other not only qualitatively but also quantitatively. This implies that the rotating wave approximation is valid in discussing transport between the system and the reservoirs under slow modulations of the parameters.

C. Interacting electron model

We next consider an interacting spinless electron system in a double quantum dot. We take the system Hamil-
In this model, an electron in one dot interacts with an electron in the other dot. We investigate the excess electron transfer as a function of the interaction strength $U$ for various values of the interaction strength $U$ obtained from the numerical diagonalization method without the RWA. We observe the two positive and two negative peaks. In Fig. 3 (d), we plot the position of one of the positive peaks and that of one of the negative peaks. We see that the positions of the negative peaks move as $U$ increases, whereas those of the positive ones do not. Moreover we find that these peak positions are located around at the energies necessary to add one electron; the approximate position of the positive peaks are $(\mu_1, \mu_R) = (\hbar \omega_1, \hbar \omega_2)$ and $(\hbar \omega_2, \hbar \omega_1)$, and those of the negative ones are $(\mu_L, \mu_R) = (\hbar \omega_2 + U, \hbar \omega_1 + U)$. This implies that the positive and negative peaks merge for non-interacting system ($U = 0$), and thus the curvature $F_{\mu_L, \mu_R}$ becomes zero in $(\mu_L, \mu_R)$-space to achieve the no-pumping condition mentioned below Eq. (18). This result also implies that, for $U > 0$, an adiabatic pump can occur even if only the reservoir parameters are modulated.

Indeed, Fig. 3 (e) shows the $U$-dependence of the excess electron transfer $(\langle \Delta q \rangle_{\tau_c})_{ex}$ for cyclic processes [cycle 1 and 2 depicted in Fig. 3 (e)], where $(\langle \Delta q \rangle_{\tau_c})_{non}$ is non-zero for $U > 0$. Note that the direction of the cycle 2 is opposite to that of the cycle 1. We also note that $(\langle \Delta q \rangle_{\tau_c})_{ex}$ for the cycle 1 becomes a constant for $U \lesssim 1[\text{meV}]$, because the positive peak positions of $F_{\mu_L, \mu_R}$ do not move as $U$ increases. In contrast, $(\langle \Delta q \rangle_{\tau_c})_{ex}$ for the cycle 2 has a peak at $U \approx 0.5[\text{meV}]$ and becomes nearly zero for $U \gtrsim 1[\text{meV}]$. This results from the fact that the negative peak positions of $F_{\mu_L, \mu_R}$ move away from the cycle 2 as $U$ increases.

### IV. DISCUSSION AND CONCLUSION

By using a QME approach, we have derived a geometrical expressions of the cumulant generating function and the average of the pumped (excess) quantity transferred from a reservoir to the system under slow modulation of control parameters, where the BSNS phases and the BSNS curvature of the QME play crucial roles.

For non-interacting electrons in quantum dot systems, there is no pump current when only the temperatures and chemical potentials of the reservoirs are modulated. In contrast, for an interacting system, the pump current can be observed even in this situation. We note that the modulations of only the chemical potentials of the reservoirs are required for the pump. This has an advantage for the control of the pump in experiments, since the modulation of chemical potential is easier than that of the temperatures. As shown in Fig. 3 (e), for a cyclic modulation of the chemical potentials, the pump current depends not only on the difference of the chemical potentials but also on their average. This implies that the average number of electrons in the system $S$ is important for the pump. For example, when we modulate the chemical potentials as $\mu_L(t) = \mu_c + \mu_+ \sin(2\pi t/\tau_c)$ and $\mu_R(t) = \mu_c + \mu_+ \sin(2\pi t/\tau_c)$, $\mu_c$ affects the quantity of the pump. This fact may be applicable for switching the pump by the change of $\mu_c$ or the electron density, which can be controlled by a gate voltage.

Since we applied the method of the full counting statistics, we can calculate the fluctuation of the pump variable. It is a future issue to analyse the detailed properties of the fluctuation in the adiabatic pump. It is also interesting to investigate the relation between the present geometrical expression of the adiabatic pump based on the QME and the conventional geometrical expressions based on the scattering theory. The investigations of non-adiabatic pump, non-Markovian situation, and spin...
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Appendix A: Generalized quantum master equation without and within the RWA

We here derive the concrete form of the GQME (5)-(6) without and within the RWA.

We start from the total Hamiltonian (system plus reservoirs) given as

$$\hat{H}_{tot} = \hat{H}_S + \sum_b \hat{H}_b + u \sum_b \hat{H}_{Sb},$$

(A1)

Here, for simplicity, we assume that the reservoir Hamiltonian $\hat{H}_b$ and the coupling Hamiltonian $\hat{H}_{Sb}$ between the system and the reservoir are respectively written as

$$\hat{H}_b = \sum_k \hbar \Omega_{bk} \hat{c}^+_b \hat{c}_b,$$

(A2)

$$\hat{H}_{Sb} = \sum_k \left( V_{bk} \hat{a}^+_b \hat{c}_b + V^*_{bk} \hat{a}_b \hat{c}^+_b \right),$$

(A3)

where $\hat{a}_i$ is a single-particle mode annihilation operator in the system $S$, $i_b$ is the index of the system mode that couples to the $b$th reservoir, and $\hat{c}_b$ is the $k$th mode annihilation operator in the $b$th reservoir. We denote the eigenenergy of the system Hamiltonian $\hat{H}_S$ as $E_x$, and the corresponding energy eigenstate as $| E_x \rangle$. We also assume that all the eigenenergies of $\hat{H}_S$ are non-degenerate.

We consider the quantity $\hat{Q} = \sum_b \sum_k q_{jk} \hat{c}_j^\dagger \hat{c}_k$ to be counted, and define the current of $\hat{Q}$ from the reservoirs to the system $S$ as positive.

For the derivation of the GQME, it is convenient to introduce the eigenoperators$^{20}$ from $\hat{a}_b$:

$$\hat{a}_b^{(\omega_s)} = \sum_{E_x} | E_x - \hbar \omega_S \rangle \langle E_x - \hbar \omega_S | \hat{a}_b | E_x \rangle \langle E_x |, \quad (A4)$$

$$\hat{a}_b^{\dagger (\omega_s)} = \sum_{E_x} | E_x + \hbar \omega_S \rangle \langle E_x + \hbar \omega_S | \hat{a}_b^{\dagger} | E_x \rangle \langle E_x |. \quad (A5)$$

Then the modified coupling Hamiltonian in the interaction picture is written as

$$\hat{H}_{Sb}(t) = e^{-ix\hat{Q}/2} e^{-(\hat{H}_S + \hat{H}_b) t / i \hbar} \hat{H}_{Sb} e^{(\hat{H}_S + \hat{H}_b) t / i \hbar} e^{ix\hat{Q}/2} = \sum_k \sum_{\omega_i} \left( V_{bk} \hat{a}_b^{\dagger (\omega_i)} \hat{c}_b e^{i \omega_{bk}/2} e^{-i(\omega_{bk} - \Omega_{bk}) t} + V^*_{bk} \hat{a}_b^{\dagger (\omega_i)} \hat{c}^+_b e^{-i \omega_{bk}/2} e^{-i(\omega_{bk} - \Omega_{bk}) t} \right). \quad (A6)$$

We assume that the initial state of the total system is written as $\rho_{tot}(0) = \rho_0 \otimes \rho_{res}$, where $\rho_0$ is an initial state of the system $S$, $\rho_{res} = \bigotimes_b \rho^{G}_b$, and $\rho^{G}_b = e^{-\beta_b (\hat{H}_b - \mu_b N_b) / \beta}$ is the grand-canonical state of the $b$th reservoir. Then substituting Eq. (A6) into Eq. (5), we obtain the GQME

\begin{align}
\frac{d}{dt} \hat{\rho}^{x}(t) &= \frac{1}{i \hbar} \left[ \hat{H}_S, \hat{\rho}^{x}(t) \right] \\
- \frac{\hbar^2}{2 \hbar^2} \sum_{\omega,\omega'_s} \sum_{\omega,\omega'_b} \left\{ \hat{\Phi}_b^{\pm}(\omega'_s) \left\{ \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) + \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} - e^{-i \chi(\omega'_s)} \left( \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} + \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \right) \right\} \right. \\
&+ \hat{\Phi}_b^{\pm}(\omega'_s) \left\{ \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) + \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} - e^{-i \chi(\omega'_s)} \left( \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} + \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \right) \right\} \\
&+ \hat{\Phi}_b^{\pm}(\omega'_s) \left\{ \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) + \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} - e^{-i \chi(\omega'_s)} \left( \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} + \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \right) \right\} \\
&+ \hat{\Phi}_b^{\pm}(\omega'_s) \left\{ \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) + \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \hat{a}^{(\omega'_b)} - e^{-i \chi(\omega'_s)} \left( \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} + \hat{a}^{(\omega'_b)} \hat{\rho}^{x}(t) \hat{a}^{(\omega'_b)} \right) \right\}, \\
\end{align}

where we used

\begin{align}
\int_0^\infty dt' e^{i x t'} &= \pi \delta(x) + i \frac{P}{\omega}.
\end{align}

Here, $q(\Omega_{bk}) \equiv q_{bk}$, and

$$\hat{\Phi}_b^{\pm}(\omega) = \sum_k 2 \pi \delta(\Omega_{bk} - \omega) | V_{bk} \rangle \langle f_{bk} |, \quad (A9)$$

$$\hat{\Psi}_b^{\pm}(\omega) = 2 \sum_k P | V_{bk} |^2 \frac{f_{bk}^{\pm}}{\Omega_{bk} - \omega}. \quad (A10)$$
\[
\hat{\Psi}_b^\pm (\omega; \chi) = 2 \sum_k P \frac{|V_{bk}|^2 f_{bk}^\pm e^{i\chi \nu_b^L(\Omega_{bk})}}{\Omega_{bk} - \omega}, \tag{A11}
\]

\[
f_{bk}^+ = \text{Tr}_b \{ \hat{\rho} \hat{\epsilon}_{bk} \hat{\epsilon}_{bk}^\dagger \} = \frac{1}{1 + e^{\beta_b (\Omega_{bk} - \mu_b)}}, \tag{A12}
\]

\[
f_{bk}^- = \text{Tr}_b \{ \hat{\rho} \hat{\epsilon}_{bk} \hat{\epsilon}_{bk} \} = 1 - f_{bk}^+. \tag{A13}
\]

Equation (A7) is the concrete form of the GQME without the RWA.

When we transform Eq. (A7) in the interaction picture, we see that rapidly oscillating terms proportional to \( e^{\pm i(\omega_z - \omega_y)t} \) appear. In the RWA we neglect these terms. Thus we obtain the GQME with the RWA by leaving only the terms with \( \omega_z = \omega_y \) in Eq. (A7).

For the non-interacting models in Secs. III A and B, because the eigenoperators are the mode operators themselves, the GQMEs for these models, in particular Eq. (10) for the RWA case, are derived.

### Appendix B: Derivation of Eq. (17)

In the model in Sec. III A within the RWA, the eigenvalues and the eigenvectors of \( K_\chi \) can be decomposed into those of \( K_{\chi, J} \). That is, \( \lambda^\chi_{0,j} = \sum_j \lambda^\chi_{0,j} \hat{\epsilon}^\chi_{0,j} \), and \( \hat{\epsilon}^\chi_{0,j} = \otimes_j \hat{\epsilon}^\chi_{0,j} \), where \( \lambda^\chi_{0,j} \) is the eigenvalue of \( K_{\chi, J} \) with maximum real part, and \( \hat{\epsilon}^\chi_{0,j} \) and \( \hat{\rho}^\chi_{0,j} \) are respectively the corresponding left and right eigenvectors, which are operators on the \( j \)th mode Hilbert space.

When we represent the left and right eigenvectors in the basis of the number states (denoted by \( |0_j\rangle \) and \( |1_j\rangle \)) of the \( \hat{a}_j \) such that \( \hat{a}_j |0_j\rangle = 0 \) and \( |1_j\rangle = \hat{a}_j^\dagger |0_j\rangle \), we can show that \( \langle m_j | \hat{\epsilon}^\chi_{0,j}(1 - m_j) | n_j \rangle = \langle m_j | \hat{\rho}^\chi_{0,j}(1 - m_j) | n_j \rangle = 0 \) (\( m = 0, 1 \)), and

\[
\begin{pmatrix}
\langle 0_j | \hat{\epsilon}^\chi_{0,j} | 0_j \rangle \\
\langle 1_j | \hat{\epsilon}^\chi_{0,j} | 1_j \rangle
\end{pmatrix}
= \begin{pmatrix}
1 \\
\chi
\end{pmatrix}, \tag{B1}
\]

\[
\begin{pmatrix}
\langle 0_j | \hat{\rho}^\chi_{0,j} | 0_j \rangle \\
\langle 1_j | \hat{\rho}^\chi_{0,j} | 1_j \rangle
\end{pmatrix}
= C_j(\chi) \begin{pmatrix}
1 \\
\chi
\end{pmatrix}, \tag{B2}
\]

where

\[
v_j(\chi) = \frac{\sum_b (\Phi^+_{b,j}(\omega_j) - \Phi^-_{b,j}(\omega_j)) + \sqrt{D_j}}{2(\Phi^+_{b,j}(\omega_j) e^{i\chi} + \Phi^-_{b,j}(\omega_j))},
\]

\[
w_j(\chi) = \frac{\sum_b (\Phi^+_{b,j}(\omega_j) - \Phi^-_{b,j}(\omega_j)) + \sqrt{D_j}}{2(\Phi^+_{b,j}(\omega_j) e^{-i\chi} + \Phi^-_{b,j}(\omega_j))},
\]

\[
D_j \equiv \Gamma_j^2 - 4(1 - e^{i\chi})\Phi^+_{L,j}(\omega_j)\Phi^-_{R,j}(\omega_j)
- 4(1 - e^{-i\chi})\Phi^+_{L,j}(\omega_j)\Phi^-_{R,j}(\omega_j),
\]

\[
\Gamma_j = \sum_b \Gamma_{b,j}, \text{ and } \Gamma_{b,j} = \Phi^+_{b,j}(\omega_j) + \Phi^-_{b,j}(\omega_j). \]

From the normalization condition for \( \chi = 0 \), \( \text{Tr}_S \Phi^+_{b,j}(\omega_j) = 1 \), we have \( C_j(0) = \sum_b \Phi^-_{b,j}(\omega_j) / \Gamma_j \). Thus we obtain the BSN vector potential:

\[
\text{Tr}_S \left( \hat{\rho}^0_{b,j} \frac{\partial \hat{\rho}^0_{b,j}}{\partial \alpha} \right) = \left. \frac{\partial v_j(\chi)}{\partial (i\chi)} \right|_{\chi = 0} \frac{\partial (C_j(0)w_j(0))}{\partial \alpha}, \tag{B3}
\]

which becomes the desired result after straightforward calculation.

### Appendix C: Equivalence of the unit-time cumulant generating functions with and without the RWA

#### 1. Matrix representation of GQME generator

To show the equivalence, we introduce the matrix representation of \( K_\chi \) by using the eigenstates \( |E_x\rangle \) of \( H_\Sigma \): the \( (y', x') \) matrix element is given as \( (K_\chi \chi, y', x') = \text{Tr}_S \left[ (|E_y\rangle \langle E_y|)^\dagger (K_\chi |E_x\rangle \langle E_x|) \right] \), where \( x'x' \) (\( yy' \)) is the index for the column (row) of the matrix.

In this representation, we can show that within the RWA \( (K_\chi^{\text{RWA}} \chi, y', x') = (K_\chi^{\text{RWA}} \chi, y, x') = 0 \) if \( x' \neq x \) and \( y' \neq y \). This implies that \( K_\chi^{\text{RWA}} \) is a block diagonal matrix that is composed of \( (K_\chi^{\text{RWA}} \chi, yy, xx) \) and \( (K_\chi^{\text{RWA}} \chi, y', x') \) with \( x' \neq x \) and \( y' \neq y \). We also note that a relation holds between the matrices of the generators without and with the RWA: \( (K_\chi^{\text{RWA}} \chi, yy, xx) = (K_\chi^{\text{RWA}} \chi, yy, xx) \).

#### 2. Equivalence of \( \lambda^\chi \) with and without RWA

As is mentioned in Sec. III B, the unit-time cumulant generating function in a steady state is given by the eigenvalue \( \lambda^\chi \) of the generator \( K_\chi \) with maximum real part.

Within the RWA, \( \lambda^\chi \) is determined by the eigenvalue of \( (K_\chi^{\text{RWA}} \chi, yy, xx) \), one of the blocks of \( (K_\chi^{\text{RWA}} \chi, yy', xx') \).

Without the RWA, the eigenvalues of \( K_\chi \) is determined by a perturbation theory with respect to \( \nu = u^2 \). From Eq. (A7), we see that the unperturbed part of \( K_\chi \) is \( -((E_x - E_x')/\hbar) \delta_{E_x, E_x'} \), and is diagonal. Therefore, the unperturbed eigenvalue is \( -(E_x - E_x')/\hbar \). This implies that the eigenvalue of zero has d-fold degeneracy, where \( d = \dim H_\Sigma \). Thus by the perturbation theory for degenerate case, the first order eigenvalue is determined by the eigenvalue equation for the matrix in the degenerate subspace, i.e., \( (K_\chi |yy, xx\rangle \chi, yy, xx) \). Furthermore, since \( (K_\chi^{\text{RWA}} \chi, yy, xx) = (K_\chi^{\text{RWA}} \chi, yy, xx) \), the first order eigenvalues are equivalent to those of \( (K_\chi^{\text{RWA}} \chi, yy, xx) \). Therefore \( \lambda^\chi \) without the RWA is equivalent to \( \lambda^\chi \) within the RWA in \( O(\nu) \). This verification of the equivalence is sufficient since the master equation is valid up to \( O(\nu) \).
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