Perturbative method for the derivation of quantum kinetic theory based on closed-time-path formalism

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Within the closed-time-path formalism, a perturbative method is presented, which reduces the microscopic field theory to the quantum kinetic theory. In order to make this reduction, the expectation value of a physical quantity must be calculated under the condition that the Wigner distribution function is fixed, because it is the independent dynamical variable in the quantum kinetic theory. It is shown that when a nonequilibrium Green function in the form of the generalized Kadanoff-Baym ansatz is utilized, this condition appears as a cancellation of a certain part of contributions in the diagrammatic expression of the expectation value. Together with the quantum kinetic equation, which can be derived in the closed-time-path formalism, this method provides a basis for the kinetic-theoretical description.

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I. INTRODUCTION

The nonequilibrium state of a dilute gas system is considered to be described by the one-particle distribution function (1PDF), and such an approach to the nonequilibrium system is called the "kinetic theory" [1]. In the kinetic theory, the 1PDF is the independent dynamical variable of the system, and all the physical quantities in the kinetic theory must be written in terms of the 1PDF. The kinetic equation is an equation of motion of the 1PDF, and the dynamics in the kinetic theory is described by this equation.

A lot of work has been done on the derivation of the quantum kinetic equation (QKE) starting from the level of microscopic field theory. The most popular way may be the one by truncating the BBGKY hierarchy, but here we focus on other ways, which utilize the nonequilibrium Green function technique, such as the generalized Kadanoff-Baym (GKB) formalism [2,3] or the counter-term method [4-6]. Although the QKE can be derived in this Green-function technique, it is not clear how we can treat the Wigner distribution function (WDF), which plays the role of the 1PDF in quantum theory, as the independent variable. In these theories, the WDF appears as a parameter in the nonequilibrium Green function, and hence is fixed from the exterior. So if we are going to calculate some quantity as a functional of the WDF, because the WDF and the microscopic field are not independent, the restriction due to the fixing of the WDF must be taken into account: e.g., in the path-integral formalism, the integrations over the microscopic fields must be carried out under the restriction condition. This restriction has not been considered in the above formalisms, and hence they do not give a complete basis for the kinetic theory.

In this paper, we present a systematic perturbative method to calculate the expectation value of any physical quantity as a functional of the WDF. Our approach is based on the inversion method [7,8], which is somewhat different from the

GKB or the counter-term method. In the inversion method, we introduce an external source J to probe the WDF z, and what is fixed is not the WDF but this source. Hence the calculation can be carried out without the restriction among the microscopic field variable. (The situation is similar to the grand canonical ensemble in the equilibrium theory, where the fixed quantity is the chemical potential coupled to 1PDF, but the source in the inversion method is not a simple time-dependent chemical potential.)

An inversion-method approach to derive the QKE was presented in Refs. [9–12]: The WDF *z* is calculated under the existence of the source, and the relation z=z[J] is inverted into J=J[z]. When we set J=0 in this expression, 0=J[z] gives an equation of motion for WDF, i.e., the QKE.

A way of calculating the physical quantities in terms of the WDF is also given by the inversion method: We first calculate the physical quantity as a functional of the source Q[J], and then substitute J=J[z] into Q[J] to obtain Q[z]=Q[J[z]], which now is a functional of the WDF. The calculation of Q[J] here can be carried out perturbatively with a propagator $-G^{(0)}[J]$, and note that, since no restriction on the microscopic field is there, all the possible diagrams appear.

Our purpose here is to provide a way to calculate directly Q[z] as the functional of WDF. Utilizing the propagator with the same form as the GKB ansatz (expressed as $-G^{(0)}[J^{(0)}[z]]$ in this paper), in which the WDF z is the fixed parameter, the above way of calculating expectation values can be reformulated. Then we show that not all contributions of the diagrams are needed to obtain Q[z], and the contributions that are canceled can be expressed by corresponding time-ordered diagrams: The contributions from a diagram in the nonequilibrium theory can be classified by the temporal order of the vertices in the diagram, and to each temporal ordering of the vertices, a time-ordered diagram (called a configuration in this paper) corresponds. Then if an obtained configuration can be separated into two parts by cutting two propagators at the same instant, the contribution from that configuration is canceled.

In the course of proof, we reformulate the inversion-

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method approach in the framework of the Legendre transformation [8,13,14]. The definition of the nonequilibrium generating functional is slightly modified in a way characteristic to the nonequilibrium theory, and the effective action is defined as the Legendre transformation of it. Then the diagrammatic rule for the effective action discussed in Ref. [15] can be utilized with an extension to the nonequilibrium case. By virtue of this, the QKE can also be expressed in a compact form, which is finally given as Eq. (47).

In the following section, we summarize the inversionmethod approach to the QKE, and reformulate it in the terminology of the Legendre transformation. Then in Sec. III, the diagrammatic rule for the kinetic theory is discussed: The rule to calculate the expectation value as a functional of the WDF is presented in Sec. III B and the rule to derive the QKE is in Sec. III C.

II. INVERSION-METHOD APPROACH TO THE KINETIC EQUATION

In this section, we describe the inversion-method approach to the QKE [9-11].

A. Probing source and the Green function

The system to be considered is the same as in Ref. [11]; a nonrelativistic bosonic field described by the Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_{int}$ with

$$\hat{H}_{0} = \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} \hat{\psi}_{\mathbf{k}}^{\dagger} \hat{\psi}_{\mathbf{k}}, \quad \hat{H}_{\text{int}} = \frac{\lambda}{4} \sum_{\mathbf{k}, \mathbf{k}', \mathbf{q}} \hat{\psi}_{\mathbf{k}+\mathbf{q}}^{\dagger} \hat{\psi}_{\mathbf{k}'-\mathbf{q}}^{\dagger} \hat{\psi}_{\mathbf{k}} \hat{\psi}_{\mathbf{k}'}, \quad (1)$$

and a spatially inhomogeneous initial density matrix $\hat{\rho}$. We consider the case that the interaction \hat{H}_{int} can be treated perturbatively, and for simplicity, the initial correlation is not taken into account. See Ref. [10] for the treatment of the initial correlation. In quantum statistical physics, the natural alternative of the 1PDF will be the WDF defined as

$$f_{\mathbf{K}}(\mathbf{X},t) = \int \frac{d\Delta \mathbf{x}}{V} e^{-i\mathbf{K}\cdot\Delta\mathbf{x}} \left\langle \hat{\psi}^{\dagger} \left(\mathbf{X} - \frac{\Delta \mathbf{x}}{2}, t\right) \hat{\psi} \left(\mathbf{X} + \frac{\Delta \mathbf{x}}{2}, t\right) \right\rangle,$$
(2)

where $\hat{\psi}(\mathbf{x}) = (1/\sqrt{V}) \Sigma \mathbf{k} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\psi}_{\mathbf{k}}$ and the angular bracket implies the average over initial density matrix $\hat{\rho}$; $\langle \cdots \rangle = \text{Tr} \hat{\rho}$ \cdots . As in Ref. [11], for the sake of perturbative calculation, it is more convenient to work with the Fourier transform of the WDF defined as

$$z_{\mathbf{k},\mathbf{q}}(t) \equiv \langle \hat{\psi}_{\mathbf{q}}^{\dagger}(t) \hat{\psi}_{\mathbf{k}}(t) \rangle = \int d\mathbf{x} e^{-i(\mathbf{k}-\mathbf{q})\cdot\mathbf{x}} f_{(\mathbf{k}+\mathbf{q}/2)}(\mathbf{x},t),$$
(3)

to which we refer simply as the WDF in the following. Note that $z_{\mathbf{q},\mathbf{k}}^* = z_{\mathbf{k},\mathbf{q}}$ holds due to the Hermitian property of $\hat{\rho}$.

Within the closed-time-path (CTP) formalism, Eq. (3) can be represented as

$$z_{\mathbf{k},\mathbf{q}}(t) \propto \int \left[d\psi_1 d\psi_2 \right] \psi_{\mathbf{q}}^*(t) \psi_{\mathbf{k}}(t) \\ \times \exp\left\{ \frac{i}{\hbar} \int_{t_I}^t ds [L(\psi_1) - L(\psi_2)] \right\} \langle \psi_{1,I} | \hat{\rho} | \psi_{2,I} \rangle.$$

$$\tag{4}$$

In the inversion-method approach to the kinetic theory, we introduce a probing source *J* for *z*, and calculate z[J] as a functional of the source. By inverting the relation as J = J[z], the QKE is obtained as an equation of motion for *z* by setting J=0. According to Ref. [9], the proper way to introduce the source $J_{\mathbf{k},\mathbf{q}}$ is that the source is built into the quadratic form of the free part of the Lagrangian in Eq. (4), $L_0(\psi_1) - L_0(\psi_2) = \sum_{ij} \psi_{\mathbf{k},i}^* D_{\mathbf{k}\mathbf{q},ij} \psi_{\mathbf{q},j}$, by

$$\mathcal{D}_{\mathbf{k},\mathbf{q}} = \begin{pmatrix} (i\hbar\partial_t - \boldsymbol{\epsilon}_{\mathbf{k}})\delta_{\mathbf{k},\mathbf{q}} + iJ_{\mathbf{k},\mathbf{q}}(t) & -iJ_{\mathbf{k},\mathbf{q}}(t) \\ -iJ_{\mathbf{k},\mathbf{q}}(t) & -(i\hbar\partial_t - \boldsymbol{\epsilon}_{\mathbf{k}})\delta_{\mathbf{k},\mathbf{q}} + iJ_{\mathbf{k},\mathbf{q}}(t) \end{pmatrix}.$$
(5)

An inverse of this matrix leads to the 2×2 Green function, which is a functional of the source *J*. From the relation $\mathcal{D}G^{(0)} = -i\hbar$, we get

where $z_{\mathbf{k},\mathbf{q}}^{(0)}$ is an unperturbed WDF given by

$$G_{\mathbf{k},\mathbf{q}}^{(0)}[t,s;J] = -\theta(t-s)e^{-i\omega_{\mathbf{k}}(t-s)} \begin{pmatrix} \overline{z}_{\mathbf{k},\mathbf{q}}^{(0)}(s) & z_{\mathbf{k},\mathbf{q}}^{(0)}(s) \\ \overline{z}_{\mathbf{k},\mathbf{q}}^{(0)}(s) & z_{\mathbf{k},\mathbf{q}}^{(0)}(s) \end{pmatrix} \\ -\theta(s-t)e^{i\omega_{\mathbf{q}}(s-t)} \begin{pmatrix} z_{\mathbf{q},\mathbf{k}}^{(0)}(t) & z_{\mathbf{q},\mathbf{k}}^{(0)}(t) \\ \overline{z}_{\mathbf{q},\mathbf{k}}^{(0)}(t) & \overline{z}_{\mathbf{q},\mathbf{k}}^{(0)}(t) \end{pmatrix}, \quad (6)$$

 $z_{\mathbf{k},\mathbf{q}}^{(0)}[t;J] = e^{-i(\omega_{\mathbf{k}} - \omega_{\mathbf{q}})(t-t_{I})} z_{\mathbf{k},\mathbf{q}}^{(0)}(t_{I})$ $+ \frac{1}{\hbar} \int_{t_{I}}^{t} ds \ e^{-i(\omega_{\mathbf{k}} - \omega_{\mathbf{q}})(t-s)} J_{\mathbf{k},\mathbf{q}}(s), \qquad (7)$

and we have used $\bar{z}_{\mathbf{k},\mathbf{q}}^{(0)} = z_{\mathbf{k},\mathbf{q}}^{(0)} + \delta_{\mathbf{k},\mathbf{q}}$ and $\omega_{\mathbf{k}} = \epsilon_{\mathbf{k}}/\hbar$. The unperturbed WDF satisfies an equation of motion

PERTURBATIVE METHOD FOR THE DERIVATION OF ...

$$J_{\mathbf{k},\mathbf{q}}(t) = \{\hbar \partial_t + i(\boldsymbol{\epsilon}_{\mathbf{k}} - \boldsymbol{\epsilon}_{\mathbf{q}})\} z_{\mathbf{k},\mathbf{q}}^{(0)}(t), \qquad (8)$$

and if we replace $z^{(0)}$ by z in Eq. (8), this gives a functional expression of the source J in terms of z in the lowest order of the perturbative inversion. We denote it as $J^{(0)}[z]$. Note that, in this article, whenever the source has an index of the perturbative order as $J^{(i)}$, it should be understood as a functional of z. By the inversion method, we can calculate perturbative correction $\Delta J[z]$ to Eq. (8), and up to the second order of the perturbation, the source is expressed by z as

$$J_{\mathbf{k},\mathbf{q}}(t) = J_{\mathbf{k},\mathbf{q}}^{(0)}[z] + \Delta J_{\mathbf{k},\mathbf{q}}[z] = [\hbar \partial_t + i(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}})] z_{\mathbf{k},\mathbf{q}}(t)$$

+ $i\lambda \sum_{\mathbf{q}',\mathbf{m}} \{ z_{\mathbf{q},\mathbf{q}'}^* z_{\mathbf{m}-\mathbf{k},\mathbf{m}-\mathbf{q}'}^* - z_{\mathbf{k},\mathbf{q}'} z_{\mathbf{m}-\mathbf{q},\mathbf{m}-\mathbf{q}'} \}(t)$
- $\frac{\lambda^2}{2\hbar} \sum_{\mathbf{l},\mathbf{m}} \int_{t_I}^s ds \{ e^{i\omega_{\mathbf{q},\mathbf{k},\mathbf{l},\mathbf{m}}^{(1-s)} Z_{\mathbf{q},\mathbf{k},\mathbf{l},\mathbf{m}}^{(2)}(s)$
+ $e^{-i\omega_{\mathbf{k},\mathbf{q},\mathbf{l},\mathbf{m}}^{(1-s)} Z_{\mathbf{k},\mathbf{q},\mathbf{l},\mathbf{m}}^{(2)}(s) \},$ (9)

where $\omega_{\mathbf{q},\mathbf{k},\mathbf{l},\mathbf{m}}^{(2)} = \omega_{\mathbf{q}} + \omega_{\mathbf{m}-\mathbf{k}} - \omega_{\mathbf{l}} - \omega_{\mathbf{m}-\mathbf{l}}$ and

$$Z_{\mathbf{q},\mathbf{k},\mathbf{l},\mathbf{m}}^{(2)} = \sum_{\mathbf{q}',\mathbf{l}',\mathbf{m}'} \{ \overline{z}_{\mathbf{q},\mathbf{q}'}^* \overline{z}_{\mathbf{m}-\mathbf{k},\mathbf{m}'-\mathbf{q}'}^* z_{\mathbf{l},\mathbf{l}'} z_{\mathbf{m}-\mathbf{l},\mathbf{m}'-\mathbf{l}'} - z_{\mathbf{q},\mathbf{q}'}^* z_{\mathbf{m}-\mathbf{k},\mathbf{m}'-\mathbf{q}'}^* \overline{z}_{\mathbf{l},\mathbf{l}'} \overline{z}_{\mathbf{m}-\mathbf{l},\mathbf{m}'-\mathbf{l}'} \}.$$
(10)

The QKE follows from Eq. (9) after the removal of the source in the left-hand side (lhs). This QKE is reduced to the usual Boltzmann equation after the Markovian and local approximations [11].

B. Kinetic-theoretic description in the inversion method

In the kinetic theory, the 1PDF is considered to be an independent dynamical variable and the kinetic equation describes its dynamics. This means a coarse graining from the microscopic field variables to the 1PDF. All other quantities should be expressed in terms of the 1PDF, and their dynamics should follow from the kinetic equation. Since such physical quantities may be defined microscopically by temporary-local functions of the field variables as $\hat{Q}(t) = Q(\hat{\psi}(t))$, in order to obtain a complete framework of kinetic theory, we must express their expectation values as functionals of the 1PDF.

In the inversion-method approach, this can be realized by first calculating perturbatively the expectation value $Q(t) = \langle \hat{Q}(t) \rangle$ with the use of the propagator $-G^{(0)}[J]$ in the preceding section, and then by substituting the source written by the WDF as in Eq. (9) into the obtained functional. The former procedure will provide us with the expectation value as a functional of the source *J*, and the latter reduces it into a functional of the WDF *z*.

From some explicit calculations [12], we can see the following fact: After the substitution of $J = J^{(0)}[z] + \Delta J[z]$ in the second step, if we expand the obtained expression around $J^{(0)}[z]$, the contributions due to the perturbative corrections $\Delta J[z]$ cancel some part of the unperturbed contributions. Such an expansion can be expressed diagrammatically by the usage of a propagator $-G^{(0)}[J=J^{(0)}[z]]$, and the abovementioned cancellation implies that some part of the diagram can be omitted if we want to evaluate the expectation value as a functional of the WDF.

From this observation, it is expected that we can directly calculate the expectation value Q[z] with the use of propagator $-G^{(0)}[J^{(0)}[z]]$ from the first step. Indeed we can do it, and our problem in this paper is to clarify what part of the diagram should be retained in the evaluation of the Q[z]. In fact, the propagator $-G^{(0)}[J^{(0)}[z]]$ has the form of the GKB ansatz with the free particle approximation of the spectral function; it can be obtained by replacing $z^{(0)}[J]$ in Eq. (6) by z. So our consideration here also provides the way to calculate Q[z] in the GKB formalism.

C. Formulation with Legendre transformation

In order to discuss the problem settled in the preceding section, it is convenient to rewrite the inversion method in the framework of the Legendre transformation using the "physical representation" of the CTP formalism [14]. The physical representation of the CTP formalism is introduced by a simple transformation of the variables from ψ_1 and ψ_2 to ψ_C and ψ_{Δ} , which is defined as

$$\psi_C = \frac{\psi_1 + \psi_2}{2}, \quad \psi_\Delta = \psi_1 - \psi_2.$$
 (11)

Then the free part of the Lagrangian is rewritten as

$$L_{0}(\psi_{C},\psi_{\Delta}) = \sum_{\mathbf{k},\mathbf{q}} \begin{pmatrix} \psi_{\mathbf{k},C}^{*} \\ \psi_{\mathbf{k},\Delta}^{*} \end{pmatrix}$$
$$\times \begin{pmatrix} 0 & (i\hbar \partial_{t} - \boldsymbol{\epsilon}_{\mathbf{k}}) \, \delta_{\mathbf{k},\mathbf{q}} \\ (i\hbar \partial_{t} - \boldsymbol{\epsilon}_{\mathbf{k}}) \, \delta_{\mathbf{k},\mathbf{q}} & iJ_{\mathbf{k}\mathbf{q},C}(t) \end{pmatrix}$$
$$\times \begin{pmatrix} \psi_{\mathbf{q},C} \\ \psi_{\mathbf{q},\Delta} \end{pmatrix}, \qquad (12)$$

where we have denoted the source J in Eq. (5) as J_C for convenience. We can see the source J_C is simply coupled to $\psi_{\Delta}^* \psi_{\Delta}$. Correspondingly, the Green function $G^{(0)}[J_C]$ becomes

$$G_{\mathbf{k},\mathbf{q}}^{(0)}[t,s;J_C] = \begin{pmatrix} g_{\mathbf{k},\mathbf{q}}^C[t,s;J_C] & g_{\mathbf{k},\mathbf{q}}^R(t,s) \\ g_{\mathbf{k},\mathbf{q}}^A(t,s) & 0 \end{pmatrix}, \quad (13)$$

where the respective components are defined as

$$g_{\mathbf{k},\mathbf{q}}^{C}[t,s;J_{C}] = -\theta(t-s)e^{-i\omega_{\mathbf{k}}(t-s)} \left(z_{\mathbf{k},\mathbf{q}}^{(0)}[s;J_{C}] + \frac{1}{2}\right) -\theta(s-t)e^{i\omega_{\mathbf{q}}(s-t)} \left(z_{\mathbf{q},\mathbf{k}}^{(0)}[t;J_{C}] + \frac{1}{2}\right), (14)$$

$$g_{\mathbf{k},\mathbf{q}}^{R}(t,s) = -\theta(t-s)e^{-i\omega_{\mathbf{k}}(t-s)}\delta_{\mathbf{k},\mathbf{q}}, \qquad (15)$$

$$g_{\mathbf{k},\mathbf{q}}^{A}(t,s) = \theta(s-t)e^{i\omega\mathbf{q}(s-t)}\delta_{\mathbf{q},\mathbf{k}}.$$
 (16)

To use the Legendre transformation formalism, we must introduce another source J_{Δ} coupled to $\psi_C^* \psi_C$, and define the generating functional *W* as

$$\exp\left(\frac{i}{\hbar} W[J_{C}, J_{\Delta}, I_{\Delta}]\right)$$

$$= \int \left[d\psi_{C} d\psi_{\Delta}\right] \langle \psi_{C,I} + \frac{1}{2} \psi_{\Delta,I} | \hat{\rho} | \psi_{C,I} - \frac{1}{2} \psi_{\Delta,I} \rangle$$

$$\times \exp\left[\frac{i}{\hbar} \int_{t_{I}}^{t_{F}} dt \left\{ L_{0}(\psi_{C}, \psi_{\Delta}) - V(\psi_{\Delta}, \psi_{C}) + \sum_{\mathbf{k}, \mathbf{q}} J_{\mathbf{k}\mathbf{q},\Delta} \psi_{\mathbf{k},C}^{*} \psi_{\mathbf{q},C} \right\} \right]$$

$$\times \exp\left[\frac{i}{\hbar} \int_{t_{I}}^{t_{F}} dt I_{\Delta} Q(\psi_{C})\right], \qquad (17)$$

where V is the interaction part of the CTP Lagrangian $H_{int}(\psi_1) - H_{int}(\psi_2)$ written in terms of ψ_C and ψ_{Δ} . The source J_{Δ} is unphysical in the sense that the expectation value of a Hermitian operator is not guaranteed to be real under the existence of this source. It is just introduced so that we can write the WDF z by a derivative of the generating functional, and should be removed after all the calculation. For the same reason, we have introduced the source I_{Δ} , which is coupled to $Q(\psi_C)$ —replacement of $\hat{\psi}$ by ψ_C in the time-local composite operator $Q(\hat{\psi})$ in which we are interested. Note that all the integrands in the exponent of Eq. (17) are local in time.

Here we define two variables

$$z_{\mathbf{kq},C}(t) \equiv \frac{\delta W[J_{\Delta}, J_{C}, I_{\Delta}]}{\delta J_{\mathbf{kq},\Delta}(t)}, \quad z_{\mathbf{kq},\Delta}(t) \equiv \frac{\delta W[J_{\Delta}, J_{C}, I_{\Delta}]}{\delta J_{\mathbf{kq},C}(t)}.$$
(18)

When the sources are removed, z_C is reduced to $\langle T\hat{\psi}^{\dagger}\hat{\psi} + \hat{\psi}\hat{\psi}^{\dagger} + \hat{\psi}^{\dagger}\hat{\psi} + \tilde{T}\hat{\psi}^{\dagger}\hat{\psi}\rangle/4 = z_{\mathbf{k},\mathbf{q}} + \delta_{\mathbf{k},\mathbf{q}}/2$, and z_{Δ} is reduced to $i\langle T\hat{\psi}^{\dagger}\hat{\psi} - \hat{\psi}\hat{\psi}^{\dagger} - \hat{\psi}^{\dagger}\hat{\psi} + \tilde{T}\hat{\psi}^{\dagger}\hat{\psi}\rangle = 0$. Note that we regard $\psi^*\psi$ as $\psi^*(t+0)\psi(t)$ in the course of the path integration. Particularly, $z_{\Delta} = 0$ is realized by removing only the unphysical source J_{Δ} , and in this case, z_C becomes a functional of J_C as

 $z_{\mathbf{k},\mathbf{q}}[J_C] + \delta_{\mathbf{k},\mathbf{q}}/2$. Of course, the nonequilibrium expectation value of symmetrized \hat{Q} is obtained as a functional of the sources J_C by

$$Q[t;J_C] = \frac{\delta W[J_{\Delta}, J_C, I_{\Delta}]}{\delta I_{\Delta}(t)} \bigg|_{J_{\Delta} = I_{\Delta} = 0}.$$
 (19)

To use the variables z_C and z_{Δ} as the independent variables, we define the Legendre transformation of W by

$$\Gamma[z_C, z_\Delta; I_\Delta] \equiv W[J_\Delta, J_C, I_\Delta] - \sum_{\mathbf{k}, \mathbf{q}} \int_{t_I}^{t_F} dt \\ \times (J_{\mathbf{k}\mathbf{q}, \Delta} z_{\mathbf{k}\mathbf{q}, C} + J_{\mathbf{k}\mathbf{q}, C} z_{\mathbf{k}\mathbf{q}, \Delta}), \qquad (20)$$

where J_{Δ} and J_C are functionals of z_C and z_{Δ} , which are obtained by solving Eq. (18). From an identity of the Legendre transformation, we have

$$J_{\mathbf{kq},C}(t) = -\frac{\delta\Gamma[z_C, z_\Delta; I_\Delta]}{\delta z_{\mathbf{kq},\Delta}(t)}, \quad J_{\mathbf{kq},\Delta}(t) = -\frac{\delta\Gamma[z_C, z_\Delta; I_\Delta]}{\delta z_{\mathbf{kq},C}(t)},$$
(21)

and if we remove the unphysical source J_{Δ} , the first equation becomes an equation of motion of $z_{\mathbf{kq},C} = z_{\mathbf{k},\mathbf{q}}[J_C] + \delta_{\mathbf{k},\mathbf{q}}/2$, which corresponds to Eq. (9). In this sense, Γ is referred to as the effective action. Now we can obtain the expectation value of \hat{Q} as a functional of the WDF z_C as follows:

$$Q[t;z_C] = \frac{\delta \Gamma[z_C, z_\Delta; I_\Delta]}{\delta I_\Delta(t)} \Big|_{z_\Delta = I_\Delta = 0}.$$
 (22)

III. DIAGRAMMATIC RULE FOR KINETIC THEORY

Diagrammatic expression of the effective action Γ is well investigated. For an expectation value of nonlocal product $\langle \hat{\psi}^{\dagger}(t) \hat{\psi}(s) \rangle$, the effective action is expressed simply by the two particle irreducible (2PI) diagrams [16]. Here, 2PI diagram is a diagram that cannot be separated by cutting any pair of propagators. For the expectation value of a local product, such as the 1PDF, the situation is more complicated. In this section, we utilize the rules presented in Ref. [15] with a nonequilibrium extension and clarify the meaning of the rule. For notational simplicity, the time arguments and wave-number indices will not explicitly be written if it is not misleading.

A. Diagrammatic expression of the effective action

First we consider a diagrammatic expansion of the generating functional W. The building blocks of the diagram constitute a 2×2 propagator $-\tilde{G}^{(0)}$ given below, an interaction vertex $V(\psi_{\Delta}, \psi_C)$ given in Eq. (17) and an external leg $Q(\psi_C)$ coupled to I_{Δ} . In the diagram, an arrow expresses the contraction operator

$$-\sum_{\mathbf{k},\mathbf{q}} \int dt ds \left(\frac{\delta}{\delta \psi_{\mathbf{k},C}(t)} \right) \\ \times \tilde{G}^{(0)}_{\mathbf{k},\mathbf{q}}(t,s) \left(\frac{\delta}{\delta \psi^*_{\mathbf{q},C}(s)} \right) \right).$$
(23)

The 2×2 Green function $\tilde{G}^{(0)}$ is defined as an inverse of the matrix in the bilinear form of the exponent in Eq. (17),

$$\tilde{G}^{(0)}[J_C, J_\Delta] \equiv \frac{i}{\hbar} \begin{pmatrix} J_\Delta & i\hbar\partial_t - \epsilon \\ i\hbar\partial_t - \epsilon & iJ_C \end{pmatrix}^{-1} = \begin{pmatrix} \tilde{g}^C & \tilde{g}^R \\ \tilde{g}^A & \tilde{g}^\Delta \end{pmatrix},$$
(24)

where the tilde implies the unphysical case $J_{\Delta} \neq 0$. Using the physical case $J_{\Delta} = 0$ given in Eqs. (14)–(16), the components of Eq. (24) can be written as

$$\tilde{g}^{C}[J_{\Delta}, J_{C}] \equiv \left(1 - g^{C}[J_{C}]\frac{J_{\Delta}}{i\hbar}\right)^{-1} g^{C}[J_{C}], \qquad (25)$$

$$\tilde{g}^{R}[J_{\Delta}, J_{C}] \equiv \left(1 + \tilde{g}^{C}[J_{C}, J_{\Delta}]\frac{J_{\Delta}}{i\hbar}\right)g^{R},$$
(26)

$$\tilde{g}^{A}[J_{\Delta}, J_{C}] \equiv g^{A} \left(1 + \frac{J_{\Delta}}{i\hbar} \tilde{g}^{C}[J_{C}, J_{\Delta}] \right),$$
(27)

$$\widetilde{g}^{\Delta}[J_{\Delta}, J_{C}] \equiv g^{A} \left(\frac{J_{\Delta}}{i\hbar} - \frac{J_{\Delta}}{i\hbar} \widetilde{g}^{C}[J_{C}, J_{\Delta}] \frac{J_{\Delta}}{i\hbar} \right) g^{R}$$
(28)

with a shorthand notation. Of course $\tilde{G}^{(0)}$ is reduced to $G^{(0)}$ in Eq. (13) by setting $J_{\Delta}=0$. Note that retarded or advanced nature of g^R or g^A , respectively, is recovered only in the physical case $J_{\Delta}=0$.

Then the generating functional W can be expressed as

$$\frac{i}{\hbar} W[J, I_{\Delta}] = \operatorname{Tr} \ln \widetilde{G}^{(0)}[J] + \kappa[J, I_{\Delta}], \qquad (29)$$

where J expresses the set of J_{Δ} and J_{C} , and κ is the sum of all the connected diagrams constructed by the propagator $-\tilde{G}^{(0)}[J]$, the vertex V, and the external leg I_{Δ} . For simplicity, we suppress the argument I_{Δ} in this section.



FIG. 1. Examples of time-ordered configurations. The open circle expresses the external point Q. The diagram (a) can be arranged into eight configurations shown in (b) and (c). The difference between groups (b) and (c) will be clarified at the end of Sec. III B.

Next we evaluate Eq. (29) at $J=J^{(0)}[z]+\Delta J[z]$ [cf. (9)], and substitute it into the definition (20) of the effective action Γ . Expanding Γ around $J=J^{(0)}[z]$ in terms of $\Delta J[z]$, the terms linear in ΔJ are canceled, and we obtain

$$\frac{i}{\hbar}\Gamma[z] = \operatorname{Tr}\ln\widetilde{G}^{(0)}[J^{(0)} + \Delta J] + \kappa[J[z]] - \frac{i}{\hbar}\{(J_{\Delta}^{(0)} + \Delta J_{\Delta})z_{C} + (J_{C}^{(0)} + \Delta J_{C})z_{\Delta}\}$$
(30)

$$=\frac{i}{\hbar}\Gamma^{(0)}[z] - \frac{1}{2\hbar^2} \begin{pmatrix} \Delta J_{\Delta} \\ \Delta J_{C} \end{pmatrix} \Delta_2 \begin{pmatrix} \Delta J_{\Delta} \\ \Delta J_{C} \end{pmatrix} + \tilde{\kappa}[z],$$
(31)

where $\Gamma^{(0)}$, Δ_2 , and $\tilde{\kappa}$ are defined, respectively, by

$$\frac{i}{\hbar}\Gamma^{(0)}[z] = \operatorname{Tr}\ln\tilde{G}^{(0)}[J^{(0)}] - \frac{i}{\hbar}\{J_{\Delta}^{(0)}z_{C} + J_{C}^{(0)}z_{\Delta}\}, \quad (32)$$

$$\Delta_2(t,s) \equiv - \begin{pmatrix} \tilde{g}^C(t,s)\tilde{g}^C(s,t) & i\tilde{g}^R(t,s)\tilde{g}^A(s,t) \\ i\tilde{g}^A(t,s)\tilde{g}^R(s,t) & -\tilde{g}^\Delta(t,s)\tilde{g}^\Delta(s,t) \end{pmatrix},$$
(33)

$$\widetilde{\kappa}[z] \equiv \kappa[J[z]] + \operatorname{Tr} \sum_{k \ge 3} \frac{1}{k} \left\{ \frac{1}{i\hbar} \widetilde{G}^{(0)}[J^{(0)}] \begin{pmatrix} \Delta J_{\Delta} & 0\\ 0 & i\Delta J_C \end{pmatrix} \right\}^k.$$
(34)

Equation (31) corresponds to Eq. (3.21) in Ref. [15], and then, as it is proved in Ref. [15], the effective action can be expressed as

$$\frac{i}{\hbar} \Gamma[z] = \mathcal{R}_2 \left(\frac{i}{\hbar} W[J^{(0)}[z]] \right) - \frac{i}{\hbar} \sum_{\mathbf{k},\mathbf{q}} \int_{t_I}^{t_F} dt \\ \times (J^{(0)}_{\mathbf{kq},\Delta}[z] z_{\mathbf{kq},C} + J^{(0)}_{\mathbf{kq},C}[z] z_{\mathbf{kq},\Delta}).$$
(35)

Here, \mathcal{R}_2 is a diagrammatic operation defined by the following process.

(1) The first process of \mathcal{R}_2 can be expressed schematically as



(36)

to which we refer as the "cut-and-patch" operation: If there is a two particle reducible (2PR) part in the diagram, separate the graph into two pieces by cutting the corresponding pair of propagators. In each of the separated diagrams, make the resultant two external lines contract $\psi_C^*(t)\psi_C(t)$ or $i\psi_{\Delta}^*(t)\psi_{\Delta}(t)$, which we call the z_C or z_{Δ} leg, respectively. Then reconnect the two diagrams by contracting their z-legs with Δ_2^{-1} .

(2) Carry out the procedure (1) in all possible ways, and sum up all the resulting diagrams including the original one. For example,



(37)

where Δ_2^{-1} is expressed by thick lines.

As it was discussed in Ref. [15], the operation \mathcal{R}_2 cancels some part of the 2PR diagrams, and in this sense, Γ has a modified 2PI property. It is reduced to the usual 2PI when we discuss an effective action of the nonlocal operator $\hat{\psi}^{\dagger}(t)\psi(s)$. In the following, we will clarify what are the contents of this modified 2PI property.

B. Meaning of the diagrammatic rule

Recovering the argument I_{Δ} in Eq. (35), the expectation value Q as a functional of the 1PDF is obtained from Eq. (22) as

$$Q[t;z_C] = \mathcal{R}_2 \left(\frac{\delta W[J^{(0)}[z], I_\Delta]}{\delta I_\Delta(t)} \right) \Big|_{z_\Delta = I_\Delta = 0}.$$
 (38)

Note that $J^{(0)}[z]$ in Eq. (35) does not depend on I_{Δ} . Diagrammatically, inside the operation \mathcal{R}_2 is a sum of all the connected diagrams with one external point expressing $Q(\psi_C)$. For definiteness, we consider a case \hat{Q} $= \hat{\psi}^{\dagger}_{\mathbf{q}} \hat{\psi}^{\dagger}_{\mathbf{q}'} \hat{\psi}_{\mathbf{k}'} \hat{\psi}_{\mathbf{k}}$ as an example. In the following, since we have set $z_{\Delta} = I_{\Delta} = 0$ in Eq. (38), the Green function $\tilde{G}^{(0)}[J^{(0)}[z]]$ is reduced to Eq. (13) in which $z^{(0)}[J_C]$ is replaced by z.

1. Time-ordered configuration and causality

Before considering the operation \mathcal{R}_2 , we define the terminologies "time-ordered configuration" and "causality."

In the nonequilibrium Green function technique, because the propagator depends explicitly on time, the evaluation of a diagram may be carried out as a function of time as follows. For all possible ways of time ordering of the vertices, the diagram is arranged in such a way that the vertices are put on the time axis from right to left. Then assigning the factors of propagators and vertices, each time ordering gives different contribution. In the following, we refer to the diagram with a fixed time ordering of the vertices as the "time-ordered configuration" or simply the configuration. For example, the diagram in Fig. 1(a) can be arranged as the eight configurations shown in Figs. 1(b) and 1(c). Other possible configurations can be eliminated by the following mechanism.

The vertices in the diagram expresses $V(\psi_1) - V(\psi_2)$ rewritten as ψ_{Δ} and ψ_{C} , which is odd in ψ_{Δ} for generic V, and contains at least one ψ_Δ or ψ_Δ^* . Then, we can conclude that the time-ordered configuration like Fig. 2, where a vertex is on the latest time, vanishes: Assuming the vertex of Fig. 2 is on time t, $\psi_{\Delta}(t)$ or $\psi_{\Delta}^{*}(t)$ therein must be contracted by $g^{A}(t,s)$ or $g^{\overline{R}}(s,t)$ (t > s), respectively (recall that we are working in the physical case $J_{\Delta}=0$), and their advanced or retarded character leads to the vanishing. This implies that when we calculate an expectation value of a physical quantity at time t, the interaction at time later than t does not contribute since the configuration like Fig. 2 cannot be avoided. In other word, the time-ordered configuration of the diagram for Q must have the external point Q on the latest time within the diagram. In this paper, we call such a fact the "causality."

2. Meaning of the operation \mathcal{R}_2

Now we consider the meaning of the operation \mathcal{R}_2 in Eq. (38). For this purpose, we first examine the cut-and-patch operation. Since we are considering the physical case $z_{\Delta} = 0$, the $\Delta\Delta$ component of $\tilde{G}^{(0)}$ as well as the $\Delta\Delta$ component of Δ_2 vanish. Then, because Δ_2^{-1} can be written as

$$\Delta_{2}^{-1} = -\begin{pmatrix} g^{C}g^{C} & ig^{R}g^{A} \\ ig^{A}g^{R} & 0 \end{pmatrix}^{-1} \\ = \begin{pmatrix} 0 & i\{g^{A}g^{R}\}^{-1} \\ i\{g^{R}g^{A}\}^{-1} & -\{g^{R}g^{A}\}^{-1}g^{C}g^{C}\{g^{A}g^{R}\}^{-1} \end{pmatrix},$$
(39)

the *CC* component of Δ_2^{-1} disappears. Thus, in Eq. (36), the connection of two z_C legs is absent.

Moreover, in Eq. (38), the connection of two z_{Δ} legs is forbidden by the following reason. Since there is only one external point Q in each diagram for Eq. (38), the external point belongs to only one of the two subdiagrams connected by Δ_2^{-1} . Then, if both of the two subdiagrams are connected with their z_{Δ} legs, the one that does not contain the external point Q must vanish due to causality: The z_{Δ} leg at time t is



FIG. 2. Vanishing configuration due to causality. [For definiteness, the four-point interaction in Eq. (1) is considered.]

produced by a pair of Green functions $g^{R}(s,t)$ and $g^{A}(t,s')$, which implies they must be connected to vertices at time *s* and *s'* later than *t*. So, if the subdiagram does not have an external point, any time-ordered configuration of the subdiagram must have a vertex that is possessed at the latest time as shown in Fig. 3, and this gives a vanishing contribution due to the causality discussed in the preceding section.

Thus it is enough to consider the connection of the z_{Δ} leg and z_C leg, where the external point belongs to the subdiagram with the z_{Δ} leg. In contrast to the z_{Δ} leg, the z_C leg must be possessed on the latest time within the subdiagram: Otherwise, some vertex must be possessed on the latest time because the subdiagram with the z_C leg does not have the external point, and the configuration in Fig. 2 cannot be avoided. As the result, the time-ordered configurations for Qhave a generic form shown in Fig. 4: In the subdiagram with the z_{Δ} leg, the external point Q is on the latest time, and the z_{Δ} leg is connected to the vertices on the later time (it need not be on the earliest time of the subdiagram). On the other hand, the subdiagram with z_C leg has the leg on the latest time.

Let us see the joint of the $z_{\mathbf{k'k},\Delta}$ leg at *t* and $z_{\mathbf{qq'},C}$ leg at *s* by $i\{g^Rg^A\}_{\mathbf{kk'},\mathbf{qq'}}^{-1}(t,s)$. The $z_{\mathbf{k'k},\Delta}$ leg at time *t* is produced by a pair of propagators which can be written as

$$ig_{\tilde{\mathbf{k}},\mathbf{k}}^{R}(t',t)g_{\mathbf{k}',\tilde{\mathbf{k}}'}^{A}(t,t'') = i\theta(t'-t'')e^{-i\omega_{\tilde{\mathbf{k}}}(t'-t'')}g_{\tilde{\mathbf{k}},\mathbf{k}}^{R}$$

$$\times(t'',t)g_{\mathbf{k}',\tilde{\mathbf{k}}'}^{A}(t,t'') + i\theta(t''-t')$$

$$\times e^{i\omega_{\tilde{\mathbf{k}}'}(t''-t')}g_{\tilde{\mathbf{k}},\mathbf{k}}^{R}(t'',t)g_{\mathbf{k}',\tilde{\mathbf{k}}'}^{A}(t,t'').$$
(40)

On the other hand, the $z_{\mathbf{qq'},C}$ leg at time *s* is produced by a pair of propagators, one of which is $-g_{\mathbf{q},\tilde{\mathbf{q}}}^{R}(s,s')$ or $-g_{\mathbf{q},\tilde{\mathbf{q}}}^{C}(s,s')$ and the other is $-g_{\tilde{\mathbf{q}'},\mathbf{q'}}^{A}(s'',s)$ or



FIG. 3. The time-ordered configuration of subdiagram with a z_{Δ} leg but without the external point. (For convenience, the time *s* is chosen to be later than s'.)



FIG. 4. The generic structure of the diagram for Q[z].

 $-g_{\tilde{\mathbf{q}}',\mathbf{q}'}^{C}(s'',s)$. As discussed above, the z_{C} leg is nonzero only when s > s', s'', and the following relations hold in this case:

$$\theta(t'-s)e^{-i\omega_{\mathbf{q}}(t'-s)}g_{\mathbf{q},\tilde{\mathbf{q}}}^{R/C}(s,s') = g_{\mathbf{q},\tilde{\mathbf{q}}}^{R/C}(t',s'),$$

$$\theta(t''-s)e^{i\omega_{\mathbf{q}'}(t''-s)}g_{\tilde{\mathbf{q}}',\mathbf{q}'}^{A/C}(s'',s) = g_{\tilde{\mathbf{q}},\mathbf{q}'}^{A/C}(s'',t'').$$
(41)

With the aid of Eqs. (40) and (41), we have

$$\sum_{\mathbf{k},\mathbf{k}',\mathbf{q},\mathbf{q}'} \int dt ds \, i g_{\mathbf{\tilde{k}},\mathbf{k}}^{R}(t',t) g_{\mathbf{k}',\mathbf{\tilde{k}}'}^{A}(t,t'') i$$

$$\{-g^{R}g^{A}\}_{\mathbf{k}\mathbf{k}',\mathbf{q}\mathbf{q}'}^{-1}(t,s) g_{\mathbf{q},\mathbf{\tilde{q}}}^{R/C}(s,s') g_{\mathbf{\tilde{q}}',\mathbf{q}'}^{A/C}(s'',s)$$

$$= -g_{\mathbf{\tilde{k}},\mathbf{\tilde{q}}}^{R/C}(t',s') g_{\mathbf{\tilde{q}}',\mathbf{\tilde{k}}'}^{A/C}(s'',t''), \qquad (42)$$

where t', t'' > s', s'' holds. This implies that the joint of z_{Δ} and z_C legs can simply be expressed as



Note that, on the rhs of Eq. (43), the time order of the vertices is restricted unlike usual diagrams: The vertices originally connected to the z_{Δ} leg are on later time than those originally connected to z_C leg. This implies that the diagram on the rhs of Eq. (43) contains only the configurations that can be separated into two parts by cutting the pair of propagators at the same instant. In this sense, we call such a timeordered configuration "instantaneous 2PR configuration." For instance, the configurations shown in Fig. 1(b) are instantaneous 2PR, and those in (c) are instantaneous 2PI. Summarizing, the cut-and-patch operation (36) extracts an instantaneous 2PR configuration from the original diagram with the opposite signature.

The second process of \mathcal{R}_2 is to cut and patch in all possible ways and to sum up the resultant diagrams. This process ensures that the instantaneous 2PR configuration is precisely canceled out after \mathcal{R}_2 is carried out. As it was shown above, the cut-and-patch process just restricts the time ordering of the vertices, and except the signature, the contribution produced by the cut-and-patch process is included in the original diagram. Then we should count how many times the same contribution appears throughout \mathcal{R}_2 . Considering a configuration that is instantaneous 2PR with respect to N pairs of propagators, such a configuration appears in a diagram where k of the corresponding N pairs of the propagators are cut and patched. There are $_NC_k$ ways of choosing k pairs

and the signature $(-1)^k$ is assigned. Thus through the total process of \mathcal{R}_2 , the instantaneous 2PR configuration appears $\sum_k (-1)^k {}_N C_k = 0$ times.

As a result, the operation \mathcal{R}_2 on a diagram implies that we can eliminate the instantaneous-2PR configurations, which will be produced from the original diagram. For example, considering Eq. (38) in the fourth order of the perturbation, when we evaluate the diagram shown in Fig. 1(a), we only need to calculate the contributions of the instantaneous 2PI configurations shown in Fig. 1(b), and can eliminate the instantaneous 2PR ones in (b). A simpler example can be seen in Ref. [11] (explicit calculations are shown in Ref. [12]), where the four-point function is calculated up to the first order of the perturbation. There appear tadpole diagrams, but their contributions are canceled when the four-point function is expressed in terms of the WDF. From the view point of our rule, the contribution from the tadpole diagrams in Ref. [11] can be eliminated by the \mathcal{R}_2 operation in Eq. (38) because all of the time-ordered configurations produced from those diagrams are instantaneous 2PR.

C. Quantum kinetic equation

Finally, we summarize the rule for deriving the QKE. The physical source J_C as a functional of z_{Δ} is obtained by setting $z_{\Delta}=0$ in the first equation of Eq. (21) since this condition is equivalent to $J_{\Delta}=0$. With the use of Eq. (35), it can be expressed as

$$J_{C}[t;z_{C}] = J_{C}^{(0)}[t;z_{C}] - \int ds \left. \frac{\delta J_{\Delta}^{(0)}(s)}{\delta z_{\Delta}(t)} \right|_{z_{\Delta}=0} \\ \times \left\{ \left. \mathcal{R}_{2} \left(\frac{\delta W}{\delta J_{\Delta}(s)} \right)_{J=J^{(0)}[z_{\Delta}=0]} - z_{C}(s) \right\}, \quad (44) \right\}$$

and the QKE for the WDF z_C is obtained by setting $J_C[t;z_C]=0$.

To obtain the explicit expression of $\delta J_{\Delta}/\delta z_{\Delta}$ in Eq. (44), we differentiate the identity $z = z^{(0)}[J^{(0)}[z]]$ with respect to z, and obtain

$$\begin{pmatrix} \frac{\delta J_{\Delta}^{(0)}}{\delta z_C} & \frac{\delta J_{\Delta}^{(0)}}{\delta z_{\Delta}} \\ \frac{\delta J_C^{(0)}}{\delta z_C} & \frac{\delta J_C^{(0)}}{\delta z_{\Delta}} \end{pmatrix}_{z_{\Delta}=0} = \begin{pmatrix} \frac{\delta z_C^{(0)}}{\delta J_{\Delta}} & \frac{\delta z_C^{(0)}}{\delta J_{\Delta}} \\ \frac{\delta z_{\Delta}^{(0)}}{\delta J_{\Delta}} & \frac{\delta z_{\Delta}^{(0)}}{\delta J_C} \end{pmatrix}_{J=J^{(0)}[z_{\Delta}=0]}^{-1} .$$
(45)

Because $z_C^{(0)}[t; J_{\Delta}, J_C]$ and $z_{\Delta}^{(0)}[t; J_{\Delta}, J_C]$ are given by $-\tilde{g}^C(t,t)$ and $-i\tilde{g}^{\Delta}(t,t)$, respectively, their derivatives can be calculated using the definitions (25) and (28). Then we can see that the rhs of Eq. (45) is nothing but Δ_2^{-1} (multiplied by $i\hbar$) given in Eq. (39), and $\delta J_{\Delta}^{(0)}/\delta z_{\Delta}$ is reduced to

$$\frac{\delta J_{\mathbf{q'k'},\Delta}^{(0)}(s)}{\delta z_{\mathbf{kq},\Delta}(t)}\bigg|_{z_{\Delta}=0} = -\hbar \{g^{A}g^{R}\}_{\mathbf{kq},\mathbf{k'q'}}^{-1}(t,s)$$
$$= -\{\hbar \partial_{t} + i(\boldsymbol{\epsilon}_{\mathbf{k}} - \boldsymbol{\epsilon}_{\mathbf{q}})\}$$
$$\times \delta_{\mathbf{k},\mathbf{k'}} \delta_{\mathbf{q},\mathbf{q'}} \delta(t-s). \tag{46}$$

Thus, in the rhs of Eq. (44), the last term in the braces compensates for the first term [cf. (8)], and the QKE can simply be written as

$$\{\hbar \partial_t + i(\boldsymbol{\epsilon}_{\mathbf{k}} - \boldsymbol{\epsilon}_{\mathbf{q}})\}\{\mathcal{R}_2(\boldsymbol{z}_{\mathbf{k}\mathbf{q},C}[t; \boldsymbol{J}_C = \boldsymbol{J}_C^{(0)}[\boldsymbol{z}_C]])\} = 0.$$
(47)

The QKE can be derived by calculating the instantaneous 2PI configurations of the diagrams for $z_{\mathbf{kq},C}$, and by operating $\{\hbar \partial_t + i(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{q}})\}$. This rule can be confirmed by the example in Ref. [11] (details are in Ref. [12]). There, it is explicitly shown that the tadpole diagrams for z_C are canceled through the process of inversion. According to our rule, the tadpole diagrams in Ref. [11] must vanish because they necessarily lead to instantaneous 2PR configurations.

IV. DISCUSSION

We have presented a systematic method by which to calculate an expectation value Q(t) of some physical quantity \hat{Q} as a functional of the WDF z. Using the propagator $G^{(0)}[J^{(0)}[z]]$, which has a form of the GKB ansatz, the precise expression of Q[z] is obtained by eliminating the instantaneous 2PR configurations from the calculations. This is due to a restriction that must be taken into account in the course of the perturbative calculation: the integration over

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the microscopic field variable must be carried out in a way so that the value of the WDF is fixed.

As pointed out in Sec. II B, the method presented here can straightforwardly be used in the GKB formalism. What we have used for the propagator is a GKB ansatz with the freeparticle approximation of the spectral function a(t,s) $=g^{R}(t,s)-g^{A}(t,s)$. The GKB ansatz is defined for a more general form of the spectral function, which implies a corresponding renormalization of the free part of the Lagrangian. Even using a more generic form of the spectral function, our method is applicable if conditions (40) and (41) are held with the replacement of the free-particle spectral function $e^{-i\omega(t-s)}$ by the renormalized one a(t,s). (These conditions are nothing but the semigroup property discussed in Ref. [17].) Other parts of the proof are based on the retarded or advanced character of the propagators, which is not affected by the use of a generic spectral function. Thus, even in the generic GKB formalism, where the diagrammatic rule may be different due to the renormalization, the instantaneous 2PR configuration can be eliminated if the semigroup property is held for the GKB ansatz.

Note that our method is not valid for the time correlation function of \hat{Q} such as $\langle \hat{Q}(t)\hat{Q}(s)\rangle$ because we have used the condition that the external point expressing $Q(\psi_C)$ appears only once in the diagram. For the calculation of the time correlation function of the composite operator, some of the instantaneous 2PR configuration may not be canceled.

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