SELF-ENERGY RENORMALIZATION FOR INHOMOGENEOUS NONEQUILIBRIUM SYSTEMS AND FIELD EXPANSION VIA COMPLETE SET OF TIME-DEPENDENT WAVE FUNCTIONS

Y. Kuwahara, Y. Nakamura, and Y. Yamanaka

1Department of Electronic and Physical Systems, Waseda University
Tokyo 169-8555, Japan
a.kuwahara1224@asagi.waseda.jp

2Institute of Condensed-Matter Science, Waseda University
Tokyo 169-8555, Japan
yusuke.n@asagi.waseda.jp

3Department of Electronic and Physical Systems, Waseda University
Tokyo 169-8555, Japan
yamanaka@waseda.jp

Abstract

The way to determine the renormalized energy of inhomogeneous systems of a quantum field under an external potential is established for both equilibrium and nonequilibrium scenarios based on Thermo Field Dynamics. The key step is to find an extension of the on-shell concept valid in homogeneous case. In the nonequilibrium case, we expand the field operator by time-dependent wave functions that are solutions of the appropriately chosen differential equation, synchronizing with temporal change of thermal situation, and the quantum transport equation is derived from the renormalization procedure. Through numerical calculations of a triple-well model with a reservoir, we show that the number distribution and the time-dependent wave functions are relaxed consistently to the correct equilibrium forms at the long-term limit.

a present address: Nagano Prefectural Kiso Seiho High School, Nagano 397-8571, Japan
I. INTRODUCTION

A sound formulation for nonequilibrium systems is desirable in quantum field theory, and will find many applications in wide areas of physics. As regards the testing of such theoretical formulations, systems of trapped, cold atomic gases are particularly ideal as their thermal processes move very slowly and can be observed experimentally. In addition, the experimental results can be compared with theoretical calculations. Another attractive feature is that various nonequilibrium scenarios can be realized in experiments of cold atomic gases.

The two well-known real-time formalisms of nonequilibrium quantum field system are Thermo Field Dynamics (TFD) and the closed time path (CTP) approach. Our arguments in this paper depend entirely on key concepts such as the quasiparticle, the representation space (Fock space), and the renormalization, which are closely related to each other. As TFD that is a canonical formalism is constructed on explicit uses of operator and representation (Fock) space, the above key concepts must be addressed squarely and their implications in TFD have been argued and refined in various ways. On the other hand, CTP, mostly given in the path-integral, is formulated only in terms of Green’s functions, and the roles of operators and representation space are indirect. Thus, TFD is advantageous over CTP for our purpose.

The renormalization performed for nonequilibrium TFD, in which every degree of freedom is doubled and the propagator and self-energy have thermal superscripts \((\mu, \nu = 1, 2)\), determines the renormalized excitation energies from their \((1, 1)\)- and/or \((2, 2)\)-components and derives the quantum transport equation from their \((1, 2)\)-component. The quantum transport equation was first derived from the renormalized condition on the self-energy in the lowest-order perturbation for the homogeneous system. Then, this equation was generalized by Chu and Umezawa as the diagonalization condition on the full propagator for homogeneous systems. Note that application of the diagonalization condition to the full propagator at higher orders is inconsistent with the equilibrium theory, because this application would imply that the Heisenberg and unperturbed number distributions are equal at the equilibrium limit. Thus, to maintain consistency with the equilibrium theory, we seek a new diagonalization condition on the on-shell self-energy. Extension of the method to systems of cold atomic gases that are inhomogeneous because of the trapping potentials is...
not straightforward, because the loss of translational symmetry obscures definitions of the on-shell self-energy on which the renormalization condition is to be imposed. More specifically, the self-energy in the \( k_0 \)-space conjugate to time is, in general, non-diagonal matrices \( \Sigma_{\ell_1,\ell_2}(k_0) \) with indices \( \ell \) of single quasiparticle states, and we are then uncertain as to what is the on-shell, \( k_0 = \omega_{\ell_1}, \omega_{\ell_2} \) or something between them, which is in contrast to homogeneous case in which \( \ell \) is a momentum index \( k \) and we have the diagonal \( \Sigma_{k_1,k_2}(k_0) = \bar{\Sigma}_{k_1}(k_0)\delta_{k_1,k_2} \) owing to the momentum conservation law, and the on-shell is unambiguously achieved by putting \( k_0 = \omega_{k_1} \). We have been attempting several formulations,[21, 22] but they are not entirely satisfactory.

In the meantime, understanding of the nonequilibrium TFD formulation was expanded.[21, 26] By deriving the nonequilibrium TFD formulation from the superoperator formalism presented in Ref. [21], we clarified that this formulation is based on the existence of a quasiparticle picture at each instant of time. In addition, a thermal causality holds, where the macroscopic quantities such as the number distribution should affect the microscopic motions in the future only. The time-dependent unperturbed representation in the interaction picture of nonequilibrium TFD, which is self-consistently selected by the renormalization condition, provides the optimum approximation method. In addition, we demonstrated in Ref. [26] that the thermal causality is an important requirement in deriving the nonequilibrium TFD directly from the classical Hamilton principle for nonconservative systems with doubled degrees of freedom.[27] The thermal causality was also helpful as a guiding principle when we devised a new definition of the on-shell self-energy in Ref. [21].

The two main problems of nonequilibrium TFD to be considered in the present study are (i) the renormalization condition on the self-energy and (ii) the appropriate choice of a complete set of time-dependent eigenfunctions. We present consistent solutions to both the problems. As regards problem (i), we consider the renormalization condition for both equilibrium and nonequilibrium inhomogeneous systems, noting that the nonequilibrium formulation should approach the equilibrium formulation in the long-term limit. The derived quantum transport equations describe the relaxation of the number distribution to the equilibrium form. The problem (ii) arises from the consideration that as the quasiparticle picture should change in time during nonequilibrium processes, particularly when a time-dependent condensate is present, and the field operator should be expanded in an appropriate complete set of time-dependent eigenfunctions.[22, 28] Note that the question as to whether
the time-dependent eigenfunctions converge to the stationary eigenfunctions at equilibrium, following the given differential equation, is not trivial at all. The time-dependent eigenequation is coupled to both of the quantum transport equation and the equation to determine the renormalized energy. In this study, we establish the time-dependent eigenequation that reduces to the usual stationary eigenequation at equilibrium. To confirm the good performance of our formulation, we take a rather simple model of a triple-well with reservoir and perform numerical calculations.

The remainder of this paper is organized as follows. A brief review of the renormalization condition of the stationary homogeneous system is given in Section II. In Section III, we present the renormalization condition of the inhomogeneous system in equilibrium, so as to determine the renormalized excitation energy using the TFD formalism. The main part of this paper is Section IV in which we consider the nonequilibrium inhomogeneous system, establishing the equations for the time-dependent eigenfunctions and giving the renormalization conditions on the $(1, 2)$-component and the $(1, 1)$- and/or $(2, 2)$-components of the on-shell self-energy; hence, the quantum transport equation is derived and the renormalized time-dependent excitation energy is fixed. The formulation obtained in Section IV is applied to a triple-well model with reservoir in Section V. Some analytic expressions of the model are derived in Appendix. Numerical calculations of the model are performed and the results are presented in Section V. Section VI is devoted to a summary.

II. RENORMALIZATION CONDITION OF STATIONARY HOMOGENEOUS SYSTEM

For later comparison, we first outline the well-known renormalization condition of the stationary homogeneous system to determine the energy counter term in the Hamiltonian at zero temperature.

We consider a homogeneous system comprised of a bosonic quantum field $\psi(x)$ having the Hamiltonian

$$H^h = H^h_0 + H_{\text{int}},$$

$$H^h_0 = \int d^3x \, \psi^\dagger(x) \left( -\frac{\nabla^2}{2m} - \mu \right) \psi(x),$$

where $x = (x, t)$ and $m$ and $\mu$ represent the mass and chemical potential, respectively. The
interaction Hamiltonian nonlinear in $\psi(x)$ is not specified, because its explicit form is not essential to our discussion. We set $\hbar = 1$ throughout this paper. The canonical commutation relations are

$$[\psi(x), \psi^\dagger(x')]_{t=t'} = \delta(x-x'), \quad (3)$$
$$[\psi(x), \psi(x')]_{t=t'} = [\psi^\dagger(x), \psi^\dagger(x')]_{t=t'} = 0. \quad (4)$$

It is customary to expand $\psi(x)$ in momentum eigenfunctions, such that

$$\psi(x) = \frac{1}{(2\pi)^{3/2}} \int d^3k e^{ik\cdot x} a_k(t), \quad (5)$$

because the translational symmetry of the homogeneous system implies conservation of the total momentum and the momentum is a good quantum number. Then, $H_0^h$ is diagonalized as

$$H_0^h = \int d^3k \omega_k^0 a_k^\dagger a_k, \quad (6)$$

with the unperturbed bare energy $\omega_k^0 = \frac{k^2}{2m} - \mu$. The interaction shifts the bare energy into a renormalized energy, denoted by $\omega_k$, which is observed. Because of the momentum conservation, both the renormalized unperturbed Hamiltonian $H_u^h$ and the energy counter term $\delta H^h$ are diagonal with respect to the momentum index, such that

$$H_u^h = H_0^h + \delta H^h = \int d^3k \omega_k a_k^\dagger a_k, \quad (7)$$
$$\delta H^h = \int d^3k \delta \omega_k a_k^\dagger a_k. \quad (8)$$

Note that the interaction Hamiltonian is not $H_{\text{int}}$, but $H_I^h$, where

$$H_I^h = H_{\text{int}} - \delta H^h. \quad (9)$$

The renormalization, or the determination of the counter term, is performed as follows. We take the Fourier transform of the self-energy $\Sigma$, which depends on the relative time and coordinate only, with respect to the relative time but with respect to the two coordinates separately, such that

$$\Sigma(x-x', t-t') = \int dk_0 dk d^3k d^3k' e^{-ik_0(t-t')} e^{i(k\cdot x-k'\cdot x')} \tilde{\Sigma}_{kk'}(k_0), \quad (10)$$
$$\tilde{\Sigma}_{kk'}(k_0) = \tilde{\Sigma}_k(k_0) \delta(k-k'). \quad (11)$$
which is the sum of the loop and counter term contributions,

\[ \Sigma_k(k_0) = \Sigma_k^{\text{loop}}(k_0) + \Sigma_k^{\delta H}, \quad \text{with} \quad \Sigma_k^{\delta H} = -\delta \omega_k. \tag{12} \]

We can determine \( \delta \omega_k \) consistently, by imposing the on-shell renormalization condition

\[ \Sigma_k(k_0 = \omega_k) = 0. \tag{13} \]

We also review the renormalization of the homogeneous system in equilibrium, using TFD. In TFD, every degree of freedom is doubled and the thermal Bogoliubov transformation is introduced, such that

\[ a_\mu^\nu k = B^{-1,\mu\nu}[n_k]\xi_\mu^\nu k, \quad \bar{a}_\nu^\mu k = \bar{\xi}_\nu^\mu k B^{\mu\nu}[n_k], \tag{14} \]

where the thermal doublet notations are used:

\[ a_\mu^\nu k = \begin{pmatrix} a_\mu^\nu k \\ \bar{a}_\nu^\mu k \end{pmatrix}, \quad \bar{a}_\nu^\mu k = \begin{pmatrix} a_\mu^\nu k \nonumber \\ -\bar{a}_\nu^\mu k \end{pmatrix}, \]

\[ \xi_\mu^\nu k = \begin{pmatrix} \xi_\mu^\nu k \\ \bar{\xi}_\nu^\mu k \end{pmatrix}, \quad \bar{\xi}_\nu^\mu k = \begin{pmatrix} \xi_\mu^\nu k \nonumber \\ -\bar{\xi}_\nu^\mu k \end{pmatrix}, \]

\[ B^{\mu\nu}[n_k] = \begin{pmatrix} 1 + n_k & -n_k \\ -1 & 1 \end{pmatrix}^{\mu\nu}, \quad B^{-1,\mu\nu}[n_k] = \begin{pmatrix} 1 & n_k \\ 1 & 1 + n_k \end{pmatrix}^{\mu\nu}. \tag{17} \]

The dummy thermal superscripts imply the Einstein summation convention. The matrix \( B^{\mu\nu} \) is called the “thermal Bogoliubov matrix”. The choice of the above form of \( B^{\mu\nu} \) corresponds to the \( \alpha = 1 \) representation of TFD. The canonical commutation relations are

\[ [a_\mu^\nu k, \bar{a}_\nu^\rho k] = [\xi_\mu^\nu k, \bar{\xi}_\rho^\nu k] = \delta_{\mu\nu} \delta_{kk}. \tag{18} \]

Further, the total Hamiltonian for time translation of both the non-tilde and tilde operators is

\[ \hat{H} = H - \hat{H}, \tag{19} \]

which is called the “hat total Hamiltonian”. Here, \( \hat{H} \) is obtained by replacing the non-tilde operators and the c-number coefficients with corresponding tilde operators and their complex conjugates, respectively.

The \( \xi \)-operators annihilate the thermal vacuum \( |0\rangle \), where

\[ \xi_k |0\rangle = \bar{\xi}_k |0\rangle = 0, \quad \langle 0 | \xi_k^\dagger = \langle 0 | \bar{\xi}_k^\dagger = 0. \tag{20} \]
The thermal averages are given by the pure state averages of the thermal vacua. In particular, the number density \( n_k \) is
\[
n_k = \langle 0 | a_k^\dagger a_k | 0 \rangle ,
\]
which is the Bose–Einstein distribution in equilibrium.

The renormalization condition is applied to the self-energy of the \( \xi \)-operators rather than that of the \( a \)-operators, because the \( \xi \)-operators represent the quasiparticles in thermal scenarios. The full and unperturbed propagators of the \( \xi \)-operators, denoted by \( g_{k}^{\mu\nu} \) and \( d_{k}^{\mu\nu} \), respectively, are defined as
\[
\begin{align*}
g_{k}^{\mu\nu}(t_1 - t_2)\delta(k_1 - k_2) &= -i \langle 0 | T [\xi^{\mu}_{k_1}(t_1)\bar{\xi}^{\nu}_{k_2}(t_2)] | 0 \rangle , \\
d_{k}^{\mu\nu}(t_1 - t_2)\delta(k_1 - k_2) &= -i \langle 0 | T [\xi^{\mu}_{k_1}(t_1)\bar{\xi}^{\nu}_{k_2}(t_2)] | 0 \rangle ,
\end{align*}
\]
where \( T \) represents a time-ordered product and the suffix \( H \) implies that the operator is that of the Heisenberg picture. The self-energy \( S_{k}^{\mu\nu}(t_1 - t_2) \) is defined through the Dyson equation, as
\[
\begin{align*}
g_{k}^{\mu\nu}(t_1 - t_2) &= d_{k}^{\mu\nu}(t_1 - t_2) + \int ds_1 ds_2 d_{k}^{\mu\nu}(t_1 - s_1)S_{k}^{\mu\nu'}(s_1 - s_2)g_{k}^{\nu\nu'}(s_2 - t_2) .
\end{align*}
\]
Taking the Fourier transform of \( S_{k}^{\mu\nu}(t_1 - t_2) \) with respect to the relative time \( \tau = t_1 - t_2 \), we obtain
\[
\bar{S}_{k}^{\mu\nu}(k_0) = \int d\tau \bar{S}_{k}^{\mu\nu}(\tau)e^{ik_0\tau} .
\]
We apply the on-shell renormalization condition to the real part of the \((1,1)\)-component, such that
\[
\text{Re} \left[ \bar{S}_{k}^{11}(\omega_k) \right] = 0 .
\]
Here, the counter term contribution is \( \bar{S}_{k}^{\mu\nu,-\delta H}(\omega_k) = -\delta_{\mu\nu}\delta\omega_k \), and \( \delta\omega_k \) is determined. As \( \bar{S}_{k}^{11}(\omega_k) = \bar{S}_{k}^{22\ast}(\omega_k) \), the condition \( \text{Re}[\bar{S}_{k}^{22}(\omega_k)] = 0 \) adds no constraint. The on-shell self-energy \( \bar{S}_{k}^{11}(\omega_k) \) is complex in general, but we do not renormalize its imaginary component, because no sound prescription or renormalizing imaginary component of the energy is known.

III. RENORMALIZATION CONDITION OF INHOMOGENEOUS SYSTEM IN EQUILIBRIUM

In this section, we consider an equilibrium system that is inhomogeneous as a result of an external potential \( V(x) \), along with its renormalization condition, so as to determine the
energy counter term. This renormalization condition is extended to the nonequilibrium case in the next section.

In this case, the free Hamiltonian is given by

\[
H_0 = \int \! d^3x \, \psi^\dagger(x) h_0(x) \psi(x), \quad \text{with} \quad h_0(x) = -\frac{\nabla^2}{2m} + V(x) - \mu . \tag{27}
\]

Contrary to the homogeneous case, the expansion of \( \psi(x) \) into the momentum eigenfunctions is not useful. We may expand \( \psi(x) \) in a complete set of the eigenfunctions for \( h_0(x) \) so that \( H_0 \) is diagonalized, but the renormalized unperturbed Hamiltonian for the inhomogeneous system with the counter term \( \delta H \), the general form of which is

\[
H_u = H_0 + \delta H , \tag{28}
\]

\[\delta H(t) = \int \! d^3x d^3x' \, \psi^\dagger(x, t) \delta \omega(x, x') \psi(x', t) , \tag{29}\]

is non-diagonal. The diagonal form of \( H_u \) is essential, but the diagonal forms of \( H_0 \) and \( \delta H \) are not required. Therefore, we adopt the complete orthonormal set of eigenfunctions \( \{u_\ell(x)\} \), where

\[
\int \! d^3x' \, h_u(x, x') u_\ell(x') = \omega_\ell u_\ell(x) , \quad h_u(x, x') = \delta(x - x') h_0(x) + \delta \omega(x, x') , \tag{30}\]

with \( \delta \omega(x, x') = \delta \omega^*(x', x) \), so as to expand \( \psi(x) \) as

\[
\psi(x) = \sum_\ell u_\ell(x) a_\ell(t) . \tag{31}\]

In fact, \( H_u \) has a diagonal form, where

\[
H_u = \sum_\ell \omega_\ell a_\ell^\dagger a_\ell . \tag{32}\]

The counter term is written as

\[
\delta H(t) = \sum_{\ell_1, \ell_2} \delta \omega_{\ell_1, \ell_2} a_{\ell_1}^\dagger(t) a_{\ell_2}(t) , \tag{33}\]

with \( \delta \omega_{\ell_1, \ell_2} = \int \! d^3x d^3x' \, u_{\ell_1}^\dagger(x) \delta \omega(x, x') u_{\ell_2}(x') . \tag{34}\]

We provide a TFD formulation of the inhomogeneous system above in thermal scenarios (both equilibrium and nonequilibrium), doubling every degree of freedom and introducing the thermal Bogoliubov transformation with the number distribution \( n_\ell \) and the thermal
vacuum, in parallel with that for the homogeneous system given in the previous section. For the equilibrium case, the parameter \( n_\ell \) is the stationary Bose-Einstein distribution, i.e.,

\[
n_\ell = \frac{1}{e^{\beta \omega_\ell} - 1}.
\]  

(35)

However, for the nonequilibrium case, this parameter is a unknown function of \( t \), denoted by \( n_\ell(t) \). The full and unperturbed propagators of the \( \xi \)-operators are, in general, defined as

\[
g^{\mu\nu}_{\ell_1\ell_2}(t_1, t_2) = -i \left\langle 0 \mid T \left[ \xi^{\mu}_{\ell_1}(t_1) \bar{\xi}^{\nu}_{\ell_2}(t_2) \right] \mid 0 \right\rangle,  
\]

(36)

\[
d^{\mu\nu}_{\ell_1\ell_2}(t_1, t_2) = -i \left\langle 0 \mid T \left[ \xi^{\mu}_{\ell_1}(t_1) \bar{\xi}^{\nu}_{\ell_2}(t_2) \right] \mid 0 \right\rangle,  
\]

(37)

respectively. The self-energy \( S^{\mu\nu}_{\ell_1\ell_2}(t_1, t_2) \) is defined in the Dyson equation,

\[
g^{\mu\nu}_{\ell_1\ell_2}(t_1, t_2) = d^{\mu\nu}_{\ell_1\ell_2}(t_1, t_2)
+ \sum_{m_1 m_2} \int ds_1 ds_2 \, d^{\mu\nu}_{\ell_1 m_1}(t_1, s_1) S^{\mu\nu}_{m_1 m_2}(s_1, s_2) g^{\nu\nu}_{m_2 \ell_2}(s_2, t_2),
\]

(38)

and has the following properties:

\[
S^{11}_{\ell_1\ell_2}(t_1, t_2) = \begin{pmatrix} S^{11}_{\ell_1\ell_2}(t_1, t_2) & S^{12}_{\ell_1\ell_2}(t_1, t_2) \\ 0 & S^{22}_{\ell_1\ell_2}(t_1, t_2) \end{pmatrix},
\]

(39)

\[
S^{11}_{\ell_1\ell_2}(t_1, t_2) \propto \theta(t_1 - t_2), \quad S^{22}_{\ell_1\ell_2}(t_1, t_2) \propto \theta(t_2 - t_1),
\]

(40)

\[
S^{11}_{\ell_1\ell_2}(t_1, t_2) = S^{22*}_{\ell_2\ell_1}(t_2, t_1), \quad S^{12}_{\ell_1\ell_2}(t_1, t_2) = -S^{12*}_{\ell_2\ell_1}(t_2, t_1).
\]

(41)

Note that \( S^{21}_{\ell_1\ell_2} = 0 \), which is inherent to the \( \alpha = 1 \) representation. Further, the phase symmetry is assumed to be unbroken.

In this section, we restrict ourselves to equilibrium cases in which the propagators and self-energy are functions of the relative time \( \tau = t_1 - t_2 \). Then, the Fourier transformation of \( S^{\mu\nu}_{\ell_1\ell_2}(\tau) \) with respect to \( \tau \) is defined by

\[
S^{\mu\nu}_{\ell_1\ell_2}(k_0) = \int d\tau \, S^{\mu\nu}_{\ell_1\ell_2}(\tau) e^{i k_0 \tau},
\]

(42)

which is the sum of the loop contribution (denoted by \( \tilde{S}^{\mu\nu, \text{loop}}_{\ell_1\ell_2}(k_0) \)) and the contribution from \( -\delta H \), where

\[
\tilde{S}^{\mu\nu, -\delta H}_{\ell_1\ell_2}(k_0) = -\delta \omega_{\ell_1\ell_2} \begin{pmatrix} 1 & n_{\ell_2} - n_{\ell_1} \\ 0 & 1 \end{pmatrix}^{\mu\nu}.
\]

(43)
The loop contribution is expressed in spectral form \cite{13, 23}, such that

\[
\begin{align*}
\bar{S}_{\ell_1 \ell_2}^{11, \text{loop}}(k_0) &= \bar{\sigma}_{\ell_1 \ell_2}(k_0) - i\pi \sigma_{\ell_1 \ell_2}(k_0), \\
\bar{S}_{\ell_1 \ell_2}^{22, \text{loop}}(k_0) &= \bar{\sigma}_{\ell_1 \ell_2}(k_0) + i\pi \sigma_{\ell_1 \ell_2}(k_0), \\
\bar{S}_{\ell_1 \ell_2}^{12, \text{loop}}(k_0) &= (n_{\ell_2} - n_{\ell_1})\sigma_{\ell_1 \ell_2}(k_0) - i\pi \{n_{\ell_1} + n_{\ell_2} - 2n(k_0)\}\sigma_{\ell_1 \ell_2}(k_0),
\end{align*}
\]

where $\sigma_{\ell_1 \ell_2}(\kappa)$ is the spectral function with the Hermitian property $\sigma_{\ell_1 \ell_2}(\kappa) = \sigma_{\ell_2 \ell_1}^*(\kappa)$, and

\[
\bar{\sigma}_{\ell_1 \ell_2}(k_0) = \int_{-\infty}^{\infty} d\kappa \mathcal{P} \frac{\sigma_{\ell_1 \ell_2}(\kappa)}{k_0 - \kappa}.
\]

No definite renormalization condition for the inhomogeneous system in thermal scenarios (both equilibrium and nonequilibrium) has been established. The difficulty lies in the fact that the self-energy and the counter term are first non-diagonal in the index of the quantum number $\ell$. Our previous attempt was to apply the "on-shell" renormalization condition only to the elements, which are diagonal in both the index $\ell$ and the thermal index, i.e., $\text{Re} \bar{S}_{\ell \ell}^{11}(\omega_k) = \text{Re} \bar{S}_{\ell \ell}^{22}(\omega_k) = 0$, following the homogeneous case. However, it must be mentioned that $\delta\omega_{\ell_1 \ell_2}$ ($\ell_1 \neq \ell_2$) are then left undetermined. Furthermore, the element $\bar{S}_{\ell_1 \ell_2}^{12}(\omega_k)$ is non-vanishing in general. This is undesirable, as the condition $S^{12}[\omega_k : t] = 0$ (this notation will be defined in Eq. (68)) is used to derive the quantum transport equation in the nonequilibrium case, and the equilibrium theory should be a stationary limit of the nonequilibrium case.

We here propose a new renormalization condition for an inhomogeneous equilibrium system that determines all the elements of $\delta\omega_{\ell_1 \ell_2}$, and that simultaneously induces vanishing of the on-shell $\bar{S}_{\ell_1 \ell_2}^{12}$. The concept of the on-shell energy becomes vague in an inhomogeneous system, because the self-energy $\bar{S}_{\ell_1 \ell_2}^{12}(k_0)$ is not diagonal with respect to the index $\ell$ and no well-grounded definition of the on-shell $(k_0 = \omega_{\ell_1}, \omega_{\ell_1}$ or something between them) is known. In order to define the on-shell energy in the present case, we recall that the full propagator of the $\alpha = 1$ representation is rewritten in the interaction picture as

\[
g^{\mu\nu}_{\ell_1 \ell_2}(t_1, t_2) = -i\theta(t_1 - t_2) \langle 0 | \xi_{\ell_1}^\mu(t_1) \bar{U}(t_1, t_2) \xi_{\ell_2}^\nu(t_2) \bar{U}(t_2, -\infty) | 0 \rangle \\
- i\theta(t_2 - t_1) \langle 0 | \xi_{\ell_2}^\nu(t_2) \bar{U}(t_2, t_1) \xi_{\ell_1}^\mu(t_1) \bar{U}(t_1, -\infty) | 0 \rangle,
\]

because $\langle 0 | \bar{U}(\infty, t) = \langle 0 | \bar{U}(t, t') \rangle | 0 \rangle$. Here $\bar{U}(t, t')$ is the time-translation operator and is given explicitly by

\[
\bar{U}(t, t') = T \left[ \exp \left[ -i \int_{t'}^{t} ds \bar{H}(s) \right] \right],
\]

10
with the hat interaction Hamiltonian \( \hat{H}_f(t) = \hat{H}(t) - \hat{H}_u(t) \). Its form in nonequilibrium case is seen in Eq. (67) below. Note that \( \langle 0 | \hat{H}_f(t) | 0 \rangle = 0 \) in the \( \alpha = 1 \) representation of TFD\([13]\). Equation (48) indicates that the retarded and advanced parts of the full propagator exclusively describe the transitions into the fixed final states of the quasiparticle \( \langle 0 | \xi_\mu \rangle \) with \( \mu = 1 \), and \( \langle 0 | \bar{\xi}_\nu \rangle \) with \( \nu = 2 \), respectively. Therefore, we define the on-shell self-energy in the stationary case, setting \( k_0 = \omega_{\ell_1} \) and \( \omega_{\ell_2} \) for its retarded and advanced parts, respectively. Explicitly, the on-shell self-energies in equilibrium are \( \bar{S}_{\ell_1 \ell_2}^{11}(\omega_{\ell_1}), \bar{S}_{\ell_1 \ell_2}^{22}(\omega_{\ell_2}), \bar{S}_{\ell_1 \ell_2}^{12,+}(\omega_{\ell_1}), \) and \( \bar{S}_{\ell_1 \ell_2}^{12,-}(\omega_{\ell_2}), \) where

\[
\bar{S}_{\ell_1 \ell_2}^{12}(k_0) = \bar{S}_{\ell_1 \ell_2}^{12,+}(k_0) + \bar{S}_{\ell_1 \ell_2}^{12,-}(k_0),
\]

and \( \bar{S}_{\ell_1 \ell_2}^{12,+}(k_0) \) and \( \bar{S}_{\ell_1 \ell_2}^{12,-}(k_0) \) are retarded and advanced parts, respectively. In this scenario, the renormalization conditions such as \( \bar{S}_{\ell_1 \ell_2}^{11}(\omega_{\ell_1}) = 0 \) or \( \bar{S}_{\ell_1 \ell_2}^{22}(\omega_{\ell_2}) = 0 \) would be inconsistent, as \( \bar{S}_{\ell_1 \ell_2}^{11,\text{loop}}(\omega_{\ell_1}) \) and \( \bar{S}_{\ell_1 \ell_2}^{22,\text{loop}}(\omega_{\ell_2}) \) are non-Hermitian matrices and cannot cancel the Hermitian counter term. Thus, we devise a renormalization condition on the following combination of on-shell self-energies:

\[
0 = \bar{S}_{\ell_1 \ell_2}^{11}(\omega_{\ell_1}) + \bar{S}_{\ell_1 \ell_2}^{22}(\omega_{\ell_2}),
\]

\[
= -2\delta\omega_{\ell_1 \ell_2} + i\sigma_{\ell_1 \ell_2}(\omega_{\ell_1}) + i\sigma_{\ell_1 \ell_2}(\omega_{\ell_2}) - i\pi\sigma_{\ell_1 \ell_2}(\omega_{\ell_1}) + i\pi\sigma_{\ell_1 \ell_2}(\omega_{\ell_2}) .
\]

(51)

As this matrix equation is Hermitian, all the elements \( \delta\omega_{\ell_1 \ell_2} \) are obtained consistently. Equation (51) implies that no imaginary part of the diagonalized energy is renormalized. Taking the combination, or the Hermitian part of the on-shell \( \bar{S}_{\ell_1 \ell_2}^{11,\mu} \), corresponds to taking the real part of the on-shell self-energy of the homogeneous system as in (26), which is rewritten equivalently as \( \bar{S}_{\ell_1 \ell_2}^{11}(\omega_{\ell_1}) + \bar{S}_{\ell_1 \ell_2}^{22}(\omega_{\ell_2}) = 0 \).

Next, we consider the on-shell self-energy with superscript \((1, 2)\), i.e., \( \bar{S}_{\ell_1 \ell_2}^{12,+}(\omega_{\ell_1}) + \bar{S}_{\ell_1 \ell_2}^{12,-}(\omega_{\ell_2}) \), which can be manipulated as

\[
\bar{S}_{\ell_1 \ell_2}^{12,+}(\omega_{\ell_1}) + \bar{S}_{\ell_1 \ell_2}^{12,-}(\omega_{\ell_2}) = (n_{\ell_2} - n_{\ell_1}) \left\{ \bar{S}_{\ell_1 \ell_2}^{11}(\omega_{\ell_1}) + \bar{S}_{\ell_1 \ell_2}^{22}(\omega_{\ell_2}) \right\} = 0 ,
\]

(52)

from

\[
\bar{S}_{\ell_1 \ell_2}^{12,+}(\omega_{\ell_1}) = (n_{\ell_2} - n_{\ell_1}) \left\{ -\delta\omega_{\ell_1 \ell_2} + i\sigma_{\ell_1 \ell_2}(\omega_{\ell_1}) \right\} ,
\]

(53)

\[
\bar{S}_{\ell_1 \ell_2}^{12,-}(\omega_{\ell_2}) = (n_{\ell_2} - n_{\ell_1}) \left\{ -\delta\omega_{\ell_1 \ell_2} + i\sigma_{\ell_1 \ell_2}(\omega_{\ell_2}) \right\} .
\]

(54)
Thus, the renormalization condition (51) yields vanishing on-shell self-energy with superscript $(1, 2)$ simultaneously.

This way we have obtained the one-shell renormalization conditions Eqs. (51) and (52) successfully in a sense that all the matrix elements (both $\mu, \nu$ and $\ell_1, \ell_2$ simultaneously) of the on-shell self-energy vanish.

IV. RENORMALIZATION CONDITION OF INHOMOGENEOUS SYSTEM IN NONEQUILIBRIUM

In this section, the renormalization method to determine the counter term for inhomogeneous systems in equilibrium is extended to nonequilibrium scenarios. Now, the counter term depends on time, as $\delta \omega(x, x', t)$. In addition, $h_u$ in Eq. (30) also depends on time, i.e.,

$$h_u(x, x', t) = \delta(x - x')h_0(x) + \delta \omega(x, x', t).$$

We begin with the equation for the unperturbed field

$$i \frac{\partial}{\partial t} \psi(x) = \int d^3x' h_u(x, x', t)\psi(x)|_{t=t'},$$

and the equation for the quasiparticle

$$i \frac{d}{dt} a_\ell(t) = \omega_\ell(t)a_\ell(t),$$

both of which are expected to be generated by the unperturbed Hamiltonian

$$H_u = \int d^3x d^3x' \psi(x)h_u(x, x', t)\psi(x)|_{t=t'},$$

$$= \sum_\ell \omega_\ell(t)a_\ell(t)a_\ell(t).$$

Then, $\psi(x)$ is expanded in terms of the time-dependent functions $\{v_\ell(x)\}$, such that

$$\psi(x) = \sum_\ell v_\ell(x)a_\ell(t),$$

with $v_\ell(t)$ satisfying

$$i \frac{\partial}{\partial t} v_\ell(x) = \int d^3x' h_u(x, x', t)v_\ell(x')|_{t=t'} - \omega_\ell(t)v_\ell(x),$$

with $\omega_\ell(t) = \int d^3x d^3x' v_\ell(x)h_u(x, x', t)v_\ell(x')|_{t=t'}$. 

12
This corresponds to Eq. (30) at the stationary limit. It follows from Eq. (61) and the assumption of Hermiticity of \( \delta \omega(x, x', t) \) that

\[
\frac{d}{dt} \int d^3 x \, v_\ell^*(x) v_\ell(x) = 0 , \tag{63}
\]

\[
\frac{\partial}{\partial t} \left[ \sum_\ell v_\ell(x, t) v_\ell^*(x', t) \right] = 0 . \tag{64}
\]

Consequently, \( \{v_\ell(x)\} \) remains a complete orthonormal set at any time \( t \), if it is taken to be a complete orthonormal set at the initial time. This is necessary for consistency of the above formulation, given in Eqs. (65) – (62).

We now turn to the nonequilibrium TFD formalism by doubling every degree of freedom and introducing the unknown time-dependent number distribution \( n_\ell(t) \). As \( \delta \omega_{\ell_1 \ell_2}(t) \) is determined by the renormalization condition, the quantum transport equation for \( n_\ell(t) \) is similarly derived from the renormalization condition in TFD.

The hat unperturbed Hamiltonian of the system under consideration is

\[
\hat{H}_u(t) = \hat{H}_0(t) + \delta \hat{H}(t) - \hat{Q}(t) , \tag{65}
\]

where \( \hat{H}_0(t) = H_0(t) - \bar{H}_0(t) \), \( \delta \hat{H}(t) = \delta H(t) - \delta \bar{H}(t) \), and the thermal counter term, which mixes non-tilde and tilda operators and drives the nonequilibrium thermal changes, is

\[
\hat{Q}(t) = -i \sum_\ell \bar{n}_\ell(t) \bar{\xi}^\dagger_\ell(t) \bar{\xi}^\dagger_\ell(t) . \tag{66}
\]

As the hat total Hamiltonian is given in Eq. (19), the hat interaction Hamiltonian is

\[
\hat{H}_I(t) = \hat{H}_{\text{int}}(t) - \delta \hat{H}(t) + \hat{Q}(t) . \tag{67}
\]

The on-shell self-energy in equilibrium, on which the renormalization condition is imposed, can be defined with regard to the Fourier component with respect to the relative time. However, the same approach cannot be employed in the nonequilibrium case, where the time-translation symmetry is lost. Instead, we consider the following quantity, which is a functional of an arbitrary function \( \omega(t) \) as well as a function of \( t \):

\[
\bar{S}^{\mu \nu}_{\ell_1 \ell_2} [\omega; t] = \bar{S}^{\mu \nu+}_{\ell_1 \ell_2} [\omega; t] + \bar{S}^{\mu \nu-}_{\ell_1 \ell_2} [\omega; t] , \tag{68}
\]

\[
\bar{S}^{\mu \nu+}_{\ell_1 \ell_2} [\omega; t] = \int d\tau \, \theta(\tau) S^{\mu \nu}_{\ell_1 \ell_2} (t, t - \tau) e^{i \int_{t-}^{t_1} ds \omega(s)} , \tag{69}
\]

\[
\bar{S}^{\mu \nu-}_{\ell_1 \ell_2} [\omega; t] = \int d\tau \, \theta(-\tau) S^{\mu \nu}_{\ell_1 \ell_2} (t + \tau, t) e^{i \int_{t+}^{t_1} ds \omega(s)} . \tag{70}
\]
Although this is certainly a generalization of the Fourier components for stationary systems, infinitely many possible generalizations exist. However, as discussed in Ref. [21], the thermal causality that the macroscopic time-dependent quantities such as \( n_\ell(t) \) affect the microscopic motions in the future only yields the above expression uniquely. As for the index \( \ell \), repeating the argument in the equilibrium case that yields the renormalization conditions given in Eqs. (51) and (52), we define the on-shell self-energy components by setting \( \omega(t) = \omega_1(t) \) and \( \omega_2(t) \) for the retarded part \( \bar{S}^{\mu\nu,+}_{\ell_1\ell_2} \) and the advanced part \( \bar{S}^{\mu\nu,-}_{\ell_1\ell_2} \), respectively. First, we impose the renormalization condition

\[
0 = \bar{S}^{11}_{\ell_1\ell_2} [\omega_{\ell_1}; t] + \bar{S}^{22}_{\ell_1\ell_2} [\omega_{\ell_2}; t],
\]

\[
= -2\delta \omega_{\ell_1\ell_2}(t) + \bar{S}^{11,\text{loop}}_{\ell_1\ell_2} [\omega_{\ell_1}; t] + \bar{S}^{22,\text{loop}}_{\ell_1\ell_2} [\omega_{\ell_2}; t],
\]

which fixes \( \delta \omega_{\ell_1\ell_2}(t) \). As seen for Eq. (52), all the elements of the on-shell self-energy with superscript \((1,2)\) vanish as a result of the condition given in (51) in the equilibrium case, and the on-shell self-energy with superscript \((1,2)\) adds no additional restriction. We note that \( \delta \omega_{\ell_1\ell_2}(t) \) that are elements of the Hermitian matrix generally have non-zero imaginary parts in off-diagonal elements \( (\ell_1 \neq \ell_2) \). While both the completeness and orthonormality of \( \{v_\ell(x)\} \) are retained, the temporal evolution of each \( v_\ell(x) \) is not represented simply by a time-dependent phase factor. In fact, the non-vanishing imaginary part of \( \delta \omega_{\ell_1\ell_2}(t) (\ell_1 \neq \ell_2) \) plays a crucial role in relaxation of \( \{v_\ell(x)\} \), which will be confirmed numerically in Section V. On the other hand, the quantum transport equation follows from the renormalization condition on the on-shell self-energy with superscript \((1,2)\). Considering the fact that the number distribution parameter \( n_\ell(t) \) is labeled by a single \( \ell \), unlike \( \delta \omega_{\ell_1\ell_2}(t) \), we require application of the renormalization condition on the diagonal elements of the on-shell self-energy \( S^{12} \) only, such that

\[
0 = \bar{S}^{12+}_{\ell\ell} [\omega_\ell; t] + \bar{S}^{12-}_{\ell\ell} [\omega_\ell; t],
\]

\[
= -i\dot{n}_\ell(t) + S^{12,\text{loop}}_{\ell\ell} [\omega_\ell; t].
\]

This is the quantum transport equation for a nonequilibrium inhomogeneous system.

In this section, we summarized the TFD formulation for the nonequilibrium inhomogeneous system, using the time-dependent complete orthonormal set of wave functions. Note that, on deriving the thermal matrix self-energy according to the Feynman method, we can solve the set of simultaneous equations, (61), (71), and (72), self-consistently.
V. TRIPLE-WELL MODEL WITH RESERVOIR AND RESULTS OF NUMERICAL CALCULATIONS

Solving the set of simultaneous equations, in particular the quantum transport equation (72), requires a large number of numerical calculations, which generates a heavy computational load. To show that the formulation in the previous section gives consistent results and to specifically demonstrate the manner in which the equations are solved, we consider an open triple-well model coupled with a reservoir, in which the positions of the three wells are \( x = 1, 0, -1 \). The model Hamiltonian is

\[
H = H_0 + H_{\text{int}} ,
\]

\[
H_0(t) = \psi^\dagger(t) h_0 \psi(t) + \sum_{k=1}^N (\Omega_k - \mu) R_k^\dagger(t) R_k(t),
\]

\[
H_{\text{int}}(t) = g \sum_{x=-1}^1 \sum_{k=1}^N \left[ R_k^\dagger(t) \psi_x(t) + \psi_k^\dagger(t) R_k(t) \right] ,
\]

where we use column vector notation for the three-component \( \psi_x(t) \) of the triple-well system \((x = 1, 0, -1)\). Then,

\[
\psi(t) = \begin{pmatrix} \psi_1(t) \\ \psi_0(t) \\ \psi_{-1}(t) \end{pmatrix} , \quad h_0 = \begin{pmatrix} -\mu & -J & 0 \\ -J & -\mu & -J \\ 0 & -J & -\mu \end{pmatrix} ,
\]

with chemical potential \( \mu \) and inter-well hopping \( J \). The operators \( R_k \) represent the degrees of freedom of the reservoir. The canonical commutation relations are

\[
[\psi_x(t), \psi_{x'}^\dagger(t')] = \delta_{xx'} , \quad [R_k(t), R_{k'}^\dagger(t')] = \delta_{kk'} , \quad \text{others} = 0.
\]

In Eqs. (74) and (75), \( \Omega_k \) and \( g \) are the energy spectrum of the reservoir system and the coupling constant between the triple-well and the reservoir system, respectively. The total number of \( R_k \), denoted by \( N \), is taken to be \( \infty \) at the final calculation stage. At the limit \( N \to \infty \), we replace \( N \delta_{kk'} \to \delta(k - k') \) and \( 1/N \sum_{k=1}^N \to \int_0^\Delta dk \) with \( \Omega_k = \Delta \), where \( \Delta \) represents the bandwidth of the reservoir energy spectrum. The coupling constant \( g \) is small and of order \( 1/\sqrt{N} \), and the finite coupling constant is defined by

\[
\bar{g} = \sqrt{Ng}.
\]
The energy counter term is a $3 \times 3$ matrix, and $\delta H$ is

$$\delta H = \psi^\dagger(t) \delta \omega^x(t) \psi(t),$$  \hspace{1cm} (79)

$$\delta \omega^x(t) = \begin{pmatrix}
\delta \omega_{11}(t) & \delta \omega_{10}(t) & \delta \omega_{1-1}(t) \\
\delta \omega_{01}(t) & \delta \omega_{00}(t) & \delta \omega_{0-1}(t) \\
\delta \omega_{-11}(t) & \delta \omega_{-10}(t) & \delta \omega_{-1-1}(t)
\end{pmatrix}. \hspace{1cm} (80)$$

The matrix $\delta \omega^x(t)$ is assumed to be Hermitian, so that $\delta H$ is a Hermitian operator.

The field is expanded as

$$\psi(t) = \sum_\ell a_\ell(t) v_\ell(t).$$  \hspace{1cm} (81)

Here, the wave function $v_\ell(t)$, represented by the column vector

$$v_\ell(t) = \begin{pmatrix} v_{1\ell}(t) \\
v_{0\ell}(t) \\
v_{-1\ell}(t)
\end{pmatrix}, \hspace{1cm} (82)$$

is a solution of

$$i \frac{d}{dt} v_\ell(t) = h_u(t) v_\ell(t) - \omega_\ell(t) v_\ell(t),$$  \hspace{1cm} (83)

with

$$h_u(t) = h_0 + \delta \omega^x(t), \hspace{0.5cm} \omega_\ell(t) = v_\ell^\dagger(t) h_u(t) v_\ell(t).$$  \hspace{1cm} (84)

Note the property $h_u^\dagger(t) = h_u(t)$, and that $\{v_\ell(t)\}$ is a complete orthonormal set according to the general discussion around Eqs. (63) and (64). The three eigenstates are labeled by $\ell = g, o, e$, as in Appendix A. Some analytic expressions, necessary for concrete numerical calculations but not important for our general formulation, are skipped here and are given in Appendix.

We move to nonequilibrium TFD, as explained in the previous section, by doubling every degree of freedom and introducing the time-dependent number distribution $n_\ell(t)$. The number distribution of the reservoir $N_k$ is the Bose-Einstein distribution, such that

$$N_k = \frac{1}{e^{\beta(\Omega_k - \mu)} - 1},$$  \hspace{1cm} (85)

at temperature $1/\beta$. The thermal counter term $\hat{Q}$ is in the unperturbed Hamiltonian, as in Eqs. (65) and (66). Following the Feynman diagram method of nonequilibrium TFD, we
obtain the expression of the full propagator of $\psi_\mu^\ell(t)$, $-i\langle 0 | T \left[ \psi_\mu^\ell(t_1) \bar{\psi}_\mu^\ell(t_2) \right] | 0 \rangle$, from which the corresponding self-energy is extracted, i.e.,

$$
\Sigma_{x_1x_2}^{\mu\nu}(t_1, t_2) = \left\{ -\delta_{\omega_{x_1x_2}(t_1)}\delta_{\mu\nu} + i \sum_\ell \tilde{n}_\ell(t_1)v_{x_1\ell}(t_1)v_{x_2\ell}(t_2)T_0^{\mu\nu} \right\} \delta(t_1 - t_2) + g^2 \int_0^{k_c} dk \ D_k^{\mu\nu}(t_1 - t_2),
$$

(86)

$$
T_0 = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix},
$$

(87)

where $D_k^{\mu\nu}$ is the unperturbed propagator of $R_\mu^\ell(t)$

$$
D_k^{\mu\nu}(t_1 - t_2) = \left[ B^{-1}[N_k] \begin{pmatrix} -i\theta(t_1 - t_2) & 0 \\ 0 & i\theta(t_2 - t_1) \end{pmatrix} B[N_k] \right]^{\mu\nu} e^{-\Omega_k(t_1-t_2)}.
$$

(88)

Next, from Eq. (86), we can derive the self-energy of $\xi_\mu^\ell(t)$, such that

$$
S_{\ell_1\ell_2}^{\mu\nu}(t_1, t_2) = \left\{ -\delta_{\omega_{\ell_1\ell_2}(t_1)} \begin{pmatrix} n_{\ell_2}(t_2) - n_{\ell_1}(t_1) & 0 \\ 0 & 1 \end{pmatrix}^{\mu\nu} - i\tilde{n}_{\ell_1}(t_1)\delta_{\ell_1\ell_2} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}^{\mu\nu} \right\} \delta(t_1 - t_2)
$$

$$
+ g^2 I_{\ell_1}(t_1) I_{\ell_2}(t_2) \int_0^{k_c} dk \ e^{-i\Omega_k(t_1-t_2)} \times \begin{pmatrix} -i\theta(t_1 - t_2) & -i\theta(t_1 - t_2)n_{\ell_2}(t_2) - i\theta(t_2 - t_1)n_{\ell_1}(t_1) + iN_k \\ 0 & i\theta(t_2 - t_1) \end{pmatrix}^{\mu\nu},
$$

(89)

where

$$
I_\ell(t) = \sum_x v_{xt}(t).
$$

(90)

We substitute (89) into Eqs. (68) – (70), and for the renormalization conditions of Eqs. (71) and (72), we explicitly obtain

$$
\delta_{\omega_{\ell_1\ell_2}(t)} = -\frac{g^2}{2} \int_0^{k_c} dk \int_{-\infty}^{t} ds \ \left\{ I_{\ell_1}^*(t)I_{\ell_2}(s)e^{-i\eta_{\ell_1}(t,s)} - I_{\ell_1}^*(s)I_{\ell_2}(t)e^{-i\eta_{\ell_2}(t,s)} \right\},
$$

(91)

$$
\tilde{n}_{\ell}(t) = -2g^2\text{Re} \left[ \int_0^{k_c} dk \int_{-\infty}^{t} ds I_{\ell}^*(t)I_{\ell}(s)e^{-i\eta_{\ell}(t,s)} \{ n_{\ell}(s) - N_k \} \right],
$$

(92)

$$
\eta_{\ell}(t, s) = \Omega_{\ell}(t - s) - \int_s^{t} d\tau \ \omega_{\ell}(\tau).
$$

(93)

These expressions are non-Markovian in general. We here consider the Markovian limit; that is, the system changes so slowly that $I_\ell(s)$, $n_\ell(s)$, and $\omega_\ell(\tau)$ in the integrands above
can be replaced with $I_\ell(t), n_\ell(t),$ and $\omega_\ell(t)$. Then, Eqs. (91) and (92) are simplified as

$$\delta \omega_{\ell_1, \ell_2}(t) = -\frac{\bar{g}^2}{2} I^*_{\ell_1}(t) I_{\ell_2}(t) \int_0^{k_c} dk \left[ \mathcal{P} \left\{ \frac{1}{\Omega_k - \omega_{\ell_1}(t)} + \frac{1}{\Omega_k - \omega_{\ell_2}(t)} \right\} 
+ i \pi \{ \delta(\Omega_k - \omega_{\ell_1}(t)) - \delta(\Omega_k - \omega_{\ell_2}(t)) \} \right],$$

(94)

$$\dot{n}_\ell(t) = -2\pi \bar{g}^2 |I_\ell(t)|^2 \int_0^{k_c} dk \delta(\Omega_k - \omega_\ell(t)) \{ n_\ell(t) - N(\omega_\ell(t)) \}. \quad (95)$$

Finally, to proceed to numerical calculations, it is necessary to fix the $k$-dependence of $\Omega_k$.

For definiteness, we take the quadratic form

$$\Omega_k = k^2. \quad (96)$$

The substitution of Eq. (96) into Eqs. (94) and (95) yields

$$\delta \omega_{\ell_1, \ell_2}(t) \nonumber \quad = -\frac{\bar{g}^2}{2} I^*_{\ell_1}(t) I_{\ell_2}(t) \left\{ \bar{C}(\omega_{\ell_1}(t)) + \bar{C}(\omega_{\ell_2}(t)) - i\pi C(\omega_{\ell_1}(t)) + i\pi C(\omega_{\ell_2}(t)) \right\},$$

(97)

$$\dot{n}_\ell(t) = -2\pi \bar{g}^2 |I_\ell(t)|^2 C(\omega_\ell(t)) \{ n_\ell(t) - N(\omega_\ell(t)) \}, \quad (98)$$

with

$$C(\omega) = \frac{1}{2\sqrt{\omega\Delta}}, \quad C(\omega) = \frac{1}{2\sqrt{\omega\Delta}} \log \frac{\sqrt{\Delta} - \sqrt{\omega}}{\sqrt{\Delta} + \sqrt{\omega}}. \quad (99)$$

We present the results of numerical calculations for the set of simultaneous equations, Eqs. (83), (97), and (98). The latter two equations are derived under the Markovian approximation.

We simulate the following nonequilibrium situation: The triple-well system and the reservoir are in equilibrium with temperature $1/\beta$ for $t < 0$, and at $t = 0$ the coupling constant changes suddenly. For $t > 0$, while the reservoir retains the equilibrium distributions with the same temperature ($1/\beta$), the triple-well system follows a nonequilibrium process. We set the parameters as follows: total particle number of triple-well system at initial time (and for $t < 0$) $\sum_\ell n_\ell = 10$; $\beta = 1/J$; and $\Delta = 10J$. The coupling constant is primarily fixed to $\bar{g} = 0.2J$ for $t < 0$ and $\bar{g} = 0.1J$ for $t \geq 0$, but $\bar{g}$ for $t < 0$ is varied for comparison.

First, we prepare the parameters in the initial equilibrium stage, $v_{x\ell}(0) = u_{x\ell}, \omega_\ell(0),$ and $n_\ell(0)$, following the method given in Section III. The $\bar{g}$-dependence of the eigenfunctions $u_{x\ell}$
FIG. 1. $\bar{g}$-dependence of the components $|u_{\pm 1g}|$ of the initial wave function that is affected by the energy renormalization at equilibrium. This plot shows that $|u_{\pm 1g}|$ deviates only slightly from 0.5 (the value in noninteracting case) for finite $\bar{g}$.

FIG. 2. Temporal behavior of $|v_{\pm 1g}(t)|$

that originates solely from the counter term $\delta \omega_{\xi_1,\xi_2}$ is weak, as is depicted in Fig. 1. Then, self-consistent numerical calculations are performed to solve Eqs. (83), (97), and (98).

As regards the results of $\{v_{x\ell}(t)\}$, Fig. 2 shows $|v_{\pm 1g}(t)|$. The most significant point to note is that $|v_{x\ell}(t)|$ relax to the stationary forms of equilibrium. The numerical calcula-
tions indicate that the non-vanishing imaginary components of the off-diagonal $\delta \omega_{\ell_1,\ell_2}(t)$ in Eq. (97) are crucial for the relaxation of $|v_{x\ell}(t)|$. Whereas the counter term $\delta \omega_{\ell_1,\ell_2}$ affects $v_{x\ell}(0) = u_{x\ell}$ slightly, as mentioned above, it causes a qualitative change of the temporal behavior of $v_{x\ell}(t)$ through the imaginary components of its off-diagonal elements. If we renormalized only the diagonal counter terms $\delta \omega_{\ell\ell}(t)$, putting $\delta \omega_{\ell_1,\ell_2}(t) = 0$ ($\ell_1 \neq \ell_2$), the solution of Eq. (83) with the initial condition $v_{\ell}(0) = u_{\ell}$ would be a time-dependent phase factor $\times u_{\ell}$, where

$$u_{\ell} = \begin{pmatrix} u_{1\ell} \\ u_{0\ell} \\ u_{-1\ell} \end{pmatrix},$$  \hspace{1cm} (100)$$

and never approaches the final stationary form.

Figure 3 (a) shows the variation of each number distribution $n_{\ell}(t)$ ($\ell = g, o, e$) in time. Although the changes in $n_o(t)$ and $n_e(t)$ are not clearly visible, which is due to the selection of a rather low temperature and the weak dependence of the eigenfunctions on $\bar{g}$, as shown in Fig. 1, $n_g(t)$ approaches a certain value and the final distributions are the equilibrium distributions with $1/\beta$. In order to see it clearly, we plot $|n_g(t) - n_g(\infty)|$ in Fig. 3 (b).

It is remarkable that both the number distributions and the time-dependent eigenfunctions, following the respective equations, are relaxed naturally to the respective equilibrium forms at the long-term limit.

VI. SUMMARY

In this paper, we studied the renormalization conditions for inhomogeneous systems of a quantum field due to a trapping potential for both equilibrium and nonequilibrium cases, using the TFD formalism. Unlike a homogeneous system in which the full propagator, self-energy, and counter term are diagonal in the momentum index because of the total momentum conservation, the inhomogeneous system inevitably provides their non-diagonal matrix forms in terms of the quantum number $\ell$. Here, it was shown that the $\alpha = 1$ representation of TFD allows the unique definition of the on-shell self-energy in the equilibrium case. Further, the renormalization condition on the on-shell self-energy with thermal superscripts $(1, 1)$ and $(2, 2)$ determines all the elements of the Hermitian part of the matrix
counter term. Simultaneously, all the elements of the on-shell self-energy with superscript $(1, 2)$ vanish automatically, which is necessary for extension to nonequilibrium systems.

Next, we discussed the renormalization condition for nonequilibrium inhomogeneous systems. The core concept was that the nonequilibrium theory should approach the above equilibrium theory smoothly at the long-term limit. The on-shell self-energy in equilibrium was defined uniquely from a combination of the thermal causality and the treatment of the matrix structure in the equilibrium case. Further, the temporally changing quasiparticle picture naturally generates expansion of the unperturbed field in terms of the time-dependent
wave functions $\{v_\ell(x)\}$. Finally, we imposed the renormalization condition on the on-shell self-energy with thermal superscripts $(1, 1)$ and $(2, 2)$, which specifies all the matrix elements of the time-dependent energy counter term, and the other condition on the diagonal part of that with thermal superscript $(1, 2)$, which gives the quantum transport equation for $n_\ell(t)$. Thus, we obtained a set of three coupled equations, i.e., the equations for $v_\ell(x)$ and $n_\ell(t)$, and the equation to determine the renormalized energy $\omega_\ell(t)$. It is crucial that the solutions of these equations relax to the corresponding equilibrium forms. For the latter, the imaginary components of the off-diagonal elements of the counter term $\delta\omega_{\ell_1\ell_2}(t)$ are crucial.

In order to determine the efficacy of our theory, we performed numerical calculations of a triple-well model attached to a reservoir. The numerical results show that not only $n_\ell(t)$, but also $v_\ell(x)$ (following their respective equations), approaches the correct stationary forms at the long-term limit.

There are several research questions related to the formulation presented in this paper that can be explored in future work. First, we should study more realistic models of cold atomic systems, performing numerical calculations that may have heavy computational loads. In particular, the extension of the present formulation to a cold atomic system with a Bose-Einstein condensate would be very intriguing\cite{1, 2}, because the nonequilibrium phase transition could then be described. The Bose-Einstein condensation is interpreted as a spontaneous breakdown of the $U(1)$ global gauge symmetry, and the zero (Nambu-Goldstone) mode always appears\cite{12, 13, 29}. As was previously discussed in Ref.\cite{30, 31}, the quantum fluctuations of the zero mode cannot be suppressed in a trapped system, but should be properly incorporated in any analysis. The problem of the renormalization condition including the zero mode remains open. Further, the extension to relativistic field systems such as the Klein-Gordon field and Dirac field\cite{32} will find many applications.

**ACKNOWLEDGMENTS**

This work is supported in part by JSPS KAKENHI Grant No. 16K05488. The authors thank RIKEN iTHES for offering us the opportunity to discuss this work during the workshop on “Thermal Quantum Field Theories and Their Applications” (2016).
Appendix A: Manipulations of Triple-well model with reservoir

We summarize some analytic expressions of the model in Section V, necessary for numerical calculations.

The system symmetry under the reflection $x = 1 \leftrightarrow -1$ restricts the parameters in the matrix $\delta \omega^x(t)$ in Eq. (80), such that

$$
\begin{align*}
\delta \omega_{11}(t) &= \delta \omega_{-1-1}(t), \quad \delta \omega_{1-1}(t) = \delta \omega_{-11}(t), \\
\delta \omega_{10}(t) &= \delta \omega_{-10}(t), \quad \delta \omega_{01}(t) = \delta \omega_{0-1}(t).
\end{align*}
$$

Eventually, the matrix $\delta \omega^x(t)$ is parameterized by three real functions $\delta \omega_{11}(t), \delta \omega_{00}(t), \delta \omega_{1-1}(t)$ and one complex function $\delta \omega_{10}(t)$, where

$$
\delta \omega^x(t) = \begin{pmatrix}
\delta \omega_{11}(t) & \delta \omega_{10}(t) & \delta \omega_{1-1}(t) \\
\delta \omega_{10}^*(t) & \delta \omega_{00}(t) & \delta \omega_{10}^*(t) \\
\delta \omega_{1-1}(t) & \delta \omega_{10}(t) & \delta \omega_{11}(t)
\end{pmatrix}.
$$

We find a constant normalized solution for Eq. (83) with Eq. (A2), i.e.,

$$
v_o(t) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix},
$$

for it can be confirmed that $h_0(t)v_o = \omega_o(t)v_o$, with $\omega_o(t) = \delta \omega_{11}(t) - \delta \omega_{1-1}(t)$, or that $h_0 v_o = 0$ and $\delta \omega(t)v_o = \omega_o(t)v_o$. This is a single allowed eigenstate with odd parity, and the remaining two normalized states, having even parities and being orthogonal to $v_o(t)$, are generally expressed as

$$
v_g(t) = \frac{e^{i\beta_g(t)}}{\sqrt{2(a^2(t) + b^2(t))}} \begin{pmatrix} a(t) \\ \sqrt{2}b(t)e^{i\theta(t)} \\ a(t) \end{pmatrix},
$$

$$
v_e(t) = \frac{e^{i\beta_e(t)}}{\sqrt{2(a^2(t) + b^2(t))}} \begin{pmatrix} b(t) \\ -\sqrt{2}a(t)e^{i\theta(t)} \\ b(t) \end{pmatrix},
$$

where the five real functions $a(t), b(t), \theta(t), \beta_g(t)$, and $\beta_e(t)$ are determined by solving Eq. (83). In the stationary (equilibrium) limit, $v_g(t), v_o(t)$, and $v_e(t)$ become the ground,
first excited, and second excited states, respectively. For later discussions, we introduce the unitary matrix

\[ V(t) = \begin{pmatrix} v_g(t) & v_o(t) & v_e(t) \end{pmatrix}, \quad V^\dagger(t)V(t) = V(t)V^\dagger(t) = I, \quad (A6) \]

and the Hermitian matrix

\[ \delta \omega^\ell(t) = V^\dagger(t)\delta \omega^\ell(t)V(t) = \begin{pmatrix} \delta \omega_{gg}(t) & \delta \omega_{go}(t) & \delta \omega_{ge}(t) \\ \delta \omega_{go}^*(t) & \delta \omega_{oo}(t) & \delta \omega_{oe}(t) \\ \delta \omega_{ge}^*(t) & \delta \omega_{oe}^*(t) & \delta \omega_{ee}(t) \end{pmatrix}. \quad (A7) \]

Each element of this matrix, \( \delta \omega_{\ell_1\ell_2}(t) \) (\( \ell_1, \ell_2 = g, o, e \)), is determined in the renormalization condition Eq. (71). Substituting Eqs. (A2), (A4), and (A5) into (A7), we obtain

\[ \delta \omega_{go}(t) = \delta \omega_{oe}(t) = 0, \quad (A8) \]
\[ \delta \omega_{oo}(t) = \delta \omega_{11}(t) - \delta \omega_{1-1}(t). \quad (A9) \]

As regards \( I_\ell(t) \) in Eq. (90), we note that the explicit form of \( v_o(t) \) in Eq. (A3) gives

\[ I_o(t) = 0. \quad (A10) \]

REFERENCES

[1] C.J. Pethick and H. Smith, *Bose–Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, 2008).

[2] A. Griffin, T. Nikuni, and E. Zaremba., it Bose–Condensed Gases at Finite Temperatures, (Cambridge University Press, Cambridge, 2009)

[3] K.B. Davis and et al, *Phys. Rev. Lett.* 75, 3969 (1995).

[4] H.-J. Miesner et al, *Science* 279, 1005 (1998).

[5] A. Sommer, M. Ku, and G. Roati, and M.W. Zwierlein, *nature* 472, 201 (2011).

[6] T. Giamarchi et al (Eds.), *Strongly Interacting Quantum Systems out of Equilibrium, Lecture Notes of the Les Houches Summer School: Volume 99, August 2012*, (Oxford University Press, Oxford, 2016).
[7] D.S. Jin et al, Phys. Rev. Lett. 78, 764 (1997).
[8] M. Yamashita, M. Koashi, and N. Imoto, Phys. Rev. A 59, 2243 (1999).
[9] S.A. Morgan, M. Rusch, D.A.W. Hutchinson, and K. Burnett, Phys. Rev. Lett. 91, 250403 (2003).
[10] S.A. Morgan, Phys. Rev. A 72, 043609 (2005).
[11] A. Bezett and P.B. Blakie, Phys. Rev. A 79, 023602 (2009).
[12] H. Umezawa, H. Matsumoto, and M. Tachiki, Thermo Field Dynamics and Condensed States (North-Holland, Amsterdam, 1982).
[13] H. Umezawa, Advanced Field Theory — Micro, Macro, and Thermal Physics (AIP, New York, 1993).
[14] J. Schwinger, J. Math. Phys. 2, 407 (1961).
[15] L.V. Keldysh, Sov. Phys. JETP 20, 1018 (1965).
[16] L.P. Kadanoff and G. Baym, Quantum Statistical Mechanics (Benjamin, New York, 1962).
[17] P. Danielewicz, Ann. Phys. 152, 239 (1984).
[18] K. Chou, Z. Su, B. Hao and L. Yu, Phys. Rep. 118, 1 (1985).
[19] Y. Yamanaka, H. Umezawa, K. Nakamura, and T. Arimitsu, Int. J. Mod. Phys. A 9, 1153 (1994).
[20] H. Chu and H. Umezawa, Int. J. Mod. Phys. A 10, 1693 (1995).
[21] Y. Nakamura and Y. Yamanaka, Ann. Phys. 331, 51 (2013).
[22] T. Sunaga, M. Mine, M. Okumura, and Y. Yamanaka, Ann. Phys. 325, 426 (2010).
[23] Y. Nakamura and Y. Yamanaka, Ann. Phys. 326, 1070-1083 (2011).
[24] Y. Kuwahara, Y. Nakamura, and Y. Yamanaka, JPS Conf. Proc. 1, 012101 (2014).
[25] Y. Nakamura, Y. Kuwahara, and Y. Yamanaka, JPS Conf. Proc. 1, 012098 (2014).
[26] Y. Kuwahara, Y. Nakamura, and Y. Yamanaka, Phys. Lett. A 377, 3102 (2013).
[27] C.R. Galley, Phys. Rev. Lett. 110, 174301 (2013).
[28] H. Matsumoto and S. Sakamoto, Prog. Theor. Phys. 105, 573 (2001).
[29] M. Blasone, G. Vitiello, and P. Jizba, Quantum Field Theory and its macroscopic manifestations: Boson Condensation, Ordered Patterns and Topological Defects (Imperial College Press, London, 2011).
[30] Y. Nakamura, J. Takahashi, and Y. Yamanaka, Phys. Rev. A 89, 013613 (2014).
[31] Y. Nakamura, T. Kawaguchi Y. Torii, and Y. Yamanaka, Ann. Phys. 376, 484 (2017).
[32] Y. Mizutani, T. Inagaki, Y. Nakamura, and Y. Yamanaka, *Prog. Theor. Phys.* **126**, 681 (2011).