On-shell expansion of the nonequilibrium generating functional: Application to superfluid ^{4}He

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The scheme of the on-shell expansion is applied to the nonequilibrium generating functional Γ. It is a systematic way of extracting physical information from Γ; the lowest equation fixes the expectation value of a chosen operator, the first order term is the equation determining the excitation spectrum, and higher orders describe the nonlinear effects among the excited modes. The approximation scheme is fixed at the level of the generating functional, which preserves the symmetry properties of the Hamiltonian. The formalism is illustrated using the model Hamiltonian of the superfluid ^{4}He. [S1063-651X(96)05405-0]

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I. INTRODUCTION

When we discuss a macroscopic system that contains a huge number of degrees of freedom, it is crucial to rewrite the theory in terms of a small number of coordinates. These variables should include experimentally observable ones and we are interested in a theory written using these macroscopic coordinates.

Several methods have been known to accomplish the above task; the method of the projection operator discusses the dynamical evolution of the system only in the space where all the variables are projected onto the space of the variable we are interested in. In this way we get, for example, the equation of motion for the relevant variable. Or, although quite different technically but essentially equivalent in philosophy to the way of the projection operator, we integrate out in path-integral representation over all the variables except for those we need. The resulting theory describes the system in terms of the coordinates that are left fixed.

There is another method to meet the purpose; the method of the Legendre transformation. Here we integrate out over all the variables but do so in the presence of the c-number source term to probe the relevant variable. The probe is set to be zero in the end of the calculation. Consider the equilibrium statistical mechanics and suppose that we are interested in the operator $\hat{O}$. (We use the hat to denote the operator and take a single operator but the generalization to the multiple operator case is straightforward.) The Hamiltonian $\hat{H}$ of the system is changed into $\hat{H}_J \equiv \hat{H} - J\hat{O}$ and trace out by all the coordinates (including $\hat{O}$). Thus we define the generating function, or the Gibbs free energy, $W[J]$ as

$$\exp(-\beta W[J]) = \mathrm{Tr}\, \exp(-\beta \hat{H}_J). \tag{1.1}$$

Here $\beta=(k_B T)^{-1}$; k_B is the Boltzmann constant and T the temperature. The Legendre transformation is done as follows:

$$\Gamma[\phi] \equiv W[J] - J\frac{dW[J]}{dJ}, \quad \phi = -\frac{dW[J]}{dJ} = \langle \hat{O} \rangle. \tag{1.2}$$

In the above expression J is expressed by ϕ through the inversion of the second equation of (1.2) and we insert it into the first one. We call $\Gamma[\phi]$ the Helmholtz free energy. Now we have an identity of the Legendre transformation $d\Gamma[\phi]/d\phi = -J$, and the mathematical expression for removing the probe is the stationary equation

$$\frac{d\Gamma[\phi]}{d\phi} = 0. \tag{1.3}$$

This determines the expectation value of $\hat{O}$ and is in fact an exact self-consistent equation for ϕ. Necessary formulas of the Legendre transformation are summarized in Appendix A.

The method of Legendre transformation deals only with the expectation values so that all the variables that appear in any expressions are c numbers. This is because we have integrated over all the fluctuations. However, since it is done under the presence of the probe coupled to $\hat{O}$, the fluctuations in the channel $\hat{O}$ can be extracted in the form of correlation functions by the appropriate differentiations of $W[J]$ by the probe J. The same is also true for $\Gamma[\phi]$. In this sense $W[J]$ or $\Gamma[\phi]$ has two meanings at the same time: free energy and the generator of correlation functions.

The technique can readily be extended to the dynamical time-dependent case where we introduce the time-dependent probe term and the time-dependent stationary equation determines the time evolution of the expectation value, i.e., equation of motion of $\langle \hat{O} \rangle_t$.

The purpose of this paper is to apply the method of the Legendre transformation, or the generating functional, to the time-dependent nonequilibrium processes and to show how we can get the physical information from the nonequilibrium generating functional. After introducing the definitions of two generating functionals, the method of on-shell expansion is explained and applied to the generating functional. (The method has already been applied to the zero temperature systems [1–5].)

Apart from the obvious hope of elucidating hitherto unnoticed important properties of the nonequilibrium generating functional, which has attracted much attention nowadays, we have other motivations, which are summarized below together with results obtained in this paper. The possible applications of our studies are also suggested.

(i) First of all we have to know how experimentally obtained data are calculable by the generating functional. The on-shell expansion is the formalism invented for this purpose. The process is quite systematic; the stationary equation of the generating functional determines the expectation value and we expand in terms of the small deviation (i.e., small oscillation) from the solution thus fixed. The lowest equation of this expansion takes the form of an eigenvalue equation, which gives us the excitation spectrum above the chosen solution.

(ii) A remarkable fact is that all the higher orders of the on-shell expansion can be summed up and the resulting expression takes the form of the coherent state multiplied by the density matrix. This newly obtained state is a novel state (ground state in the case of zero temperature) which is written as a coherent sum of the modes excited above the old state, thus leading to the connection formula of the two. In the classical mechanical language, the formula relates two minima of the potential by summing up infinite series of the small oscillation around one of the minima.

(iii) In the field theoretical case, one is frequently interested in the condensed ground state and our formula is an exact one, which, in its lowest approximation, coincides with the usual form of the simplest trial state in all known cases. Thus our formula suggests how one takes and improves the trial state in the variational calculations. The statement can be applied to the case where one of the states is unstable. How one can describe the unstable state by the operator referring to the stable ground state is a problem that has a long history. Our formalism may provide a method to this problem.

(iv) When one wants to discuss the gauge theory and when the gauge invariance has to be maintained throughout the calculation, one has to invent somehow a gauge invariant variational approach. But it is not known at present to our knowledge. Since our formulas are exact, they are gauge invariant and they can be a candidate for this trial state. Indeed this was the first motivation for the present investigations.

(v) Take a macroscopic system. Our method can be used to study the problem of how to separate, or how to elucidate the interplay between, the systematic motion and the fluctuation around it. The systematic motion is represented by the expectation value and the fluctuation by the small oscillation. When the small oscillations are added up, the systematic part shows a macroscopic change, which is expressed in our formalism by the shift of the (ground) state.

Below we present the general formalism of the on-shell expansion and then an example is studied taking the superfluid ^{4}He model Hamiltonian. Mathematical manipulations necessary for these topics are mainly contained in Appendixes A–E.

II. NONEQUILIBRIUM GENERATING FUNCTIONALS

A. Definition of $W[J_1,J_2]$ and $\Gamma[\phi_1,\phi_2]$

Let us define the nonequilibrium generating functional. Consider a field theoretical system described by the Hamiltonian operator $\hat{H}$. (Although we take a field theoretical system in this paper, the arguments below apply to any dynamical system.) Since we want to study the dynamical nonequilibrium processes, a time-dependent external force $J(t,\mathbf{x})$ is introduced that couples to some physical quantity $\hat{O}(\mathbf{x})$ of the system. This $J(t,\mathbf{x})$ is a fictitious source to be set to zero in the end. Thus the Hamiltonian of the system changes with time. It is expressed as

$$\hat{H}(t)=\hat{H}-\int d^3\mathbf{x}\, J(t,\mathbf{x})\hat{O}(\mathbf{x}). \tag{2.1}$$

Then the expectation value $\langle \hat{O}(\mathbf{x})\rangle_t$ is given as

$$\langle \hat{O}(\mathbf{x})\rangle_t=\mathrm{Tr}\{\hat{\rho}_I\hat{U}(t,t_I)^{\dagger}\hat{O}(\mathbf{x})\hat{U}(t,t_I)\}, \tag{2.2}$$

$$\hat{U}(t,t_I)=\mathrm{T}\,\exp\left(-\frac{i}{\hbar}\int_{t_I}^{t}ds\;\hat{H}(s)\right), \tag{2.3}$$

where the symbol T implies the time ordering operation and † denotes the adjoint. The matrix $\hat{\rho}_I$ is an arbitrary density operator of the initial time t_I, which need not necessarily be an equilibrium distribution.

Now we try to extend the equilibrium generating functions presented in the Introduction to the nonequilibrium systems. There are two types of nonequilibrium generating functionals, $W[J_1,J_2]$ and $\Gamma[\phi_1,\phi_2]$, which are extensions of Gibb's and Helmholtz's free energy in the equilibrium case, respectively. The definitions of $W[J_1,J_2]$ and $\Gamma[\phi_1,\phi_2]$ are given as follows. The generating functional $W[J_1,J_2]$ is first defined by introducing two kinds of real valued sources $J_1(t)$ and $J_2(t)$:

$$e^{(i/\hbar)W[J_1,J_2]}=\mathrm{Tr}\{\hat{U}_{J_1}\hat{\rho}_I(\hat{U}_{J_2})^{\dagger}\}, \tag{2.4}$$

$$\hat{U}_{J_i}=\mathrm{T}\,\exp\left[-\frac{i}{\hbar}\int_{t_I}^{t_F}dt\left(\hat{H}-\int d^3\mathbf{x}\;J_i(\mathbf{x},t)\hat{O}(\mathbf{x})\right)\right]$$

$$(i=1,2). \tag{2.5}$$

The final time t_F here is taken to be sufficiently large, satisfying $t_I<t<t_F$, where t is the time we look at the system.

The double path formulation of nonequilibrium theory has a long history, starting from Schwinger's work [6–10]. For an extensive investigation, see Refs. [10,11].

Since $J_1\neq J_2$ in (2.4) (otherwise W becomes independent of J_1 and J_2), the time evolution of $\hat{\rho}_I$ is not physical. So $W[J_1,J_2]$ itself is not a physical quantity in contrast to the equilibrium Gibbs free energy $W[J]$ of (1.1), which is a physical one in the sense that it is the free energy of the system with Hamiltonian $\hat{H}-J\hat{O}$. In this sense it is important to note that there is no genuine generating functional of equilibrium type for the nonequilibrium processes. However, this does not invalidate the use of $W[J_1,J_2]$; the functional $W[J_1,J_2]$ does play the role of the generating functional and all the physical quantities (as far as they are related to the channel we are probing) can be extracted from it. These will become clear in the following.

The second nonequilibrium generating functional is defined by the double Legendre transformation,

$$\Gamma[\phi_1,\phi_2]=W[J_1,J_2]-\sum_{i=1}^{2}\int d^4x J_i(x)\frac{\delta W[J_1,J_2]}{\delta J_i(x)}, \tag{2.6}$$

$$\phi_i(x)=(-1)^{i+1}\frac{\delta W[J_1,J_2]}{\delta J_i(x)} \quad (i=1,2), \tag{2.7}$$

where four-dimensional notations have been introduced; $x\equiv(t,\mathbf{x})$ and $\int d^4x\equiv\int_{t_I}^{t_F}dt\int d^3\mathbf{x}$. $\delta/\delta J_i(x)$ signifies the functional derivative defined as

$$\frac{\delta J_i(x)}{\delta J_j(x')}=\delta_{ij}\delta^4(x-x'). \tag{2.8}$$

Here $\delta^4(x)$ is the four-dimensional δ function. Then the physically observed expectation value of $\hat{O}(t,\mathbf{x})$ with $t>t_I$ is given by

$$\phi(x)\equiv\langle\hat{O}(x)\rangle=\frac{\delta W[J_1,J_2]}{\delta J_1(x)}\bigg|_{J_1=J_2=0}$$

$$=-\frac{\delta W[J_1,J_2]}{\delta J_2(x)}\bigg|_{J_1=J_2=0}. \tag{2.9}$$

The equation of motion of $\phi(x)$ is obtained as follows. We note here the inverted relation of (2.7),

$$\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_i(x)}=(-1)^iJ_i(x) \quad (i=1,2), \tag{2.10}$$

which comes from the definitions (2.6) and (2.7) [see (A6)]. In (2.4) we have assumed that $J_{1,2}$ are fictitious sources, which are made to vanish at the end. In case a physical source coupled to $\hat{O}$ is really present, the artificial source term J_i has to be set to a physical source $J(x)$:$J_1(x)=J_2(x)=J(x)$. If the source $J(x)$ is absent, we are considering the case where the nonequilibrium process is realized because the initial density matrix is not equal to the equilibrium distribution. Let us consider the latter case for simplicity. Then we are led to the equation of motion of $\phi(x)$:

$$\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}=\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_2(x)}=0. \tag{2.11}$$

The solution to (2.11) satisfies $\phi_1(x)=\phi_2(x)=\phi(x)$ because of the symmetry under $1\leftrightarrow 2$. Therefore we can use another type of equation of motion,

$$0=\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\bigg|_{\phi_1(x)=\phi_2(x)=\phi(x)}. \tag{2.12}$$

This has a similar form to the equation of motion for the coordinate variable q in classical analytical dynamics, which is obtained by the stationary condition on the action functional $I[q]$; $\delta I[q]/\delta q(t)=0$. Because of this analogy, Γ is also called the effective action.

We recall here the relation between the equation of motion and its solution for the case of a nonvanishing physical source, $J_1=J_2=J\neq 0$. If we set $J_1=J_2=J$ in (2.9) and $\phi_1=\phi_2=\phi$ in (2.10), we get

$$\phi(x)=\frac{\delta W[J_1,J_2]}{\delta J_1(x)}\bigg|_{J_1=J_2=J}, \tag{2.13}$$

$$-J(x)=\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\bigg|_{\phi_1=\phi_2=\phi}, \tag{2.14}$$

which are the solution and the equation of motion under the presence of the physical source $J(x)$, respectively. Actually we get (2.14) by solving (2.13) with respect to $J(x)$, i.e., *inversion* of (2.13). Several important relations involving $W[J_1,J_2]$ and $\Gamma[\phi_1,\phi_2]$ are summarized in Appendix B. When the initial density matrix is of the equilibrium form $\hat{\rho}_I=\exp(-\beta\hat{H})$, it is convenient to introduce another source J_3 in the third imaginary time path. This enables one to study the connection with the equilibrium free energy and is discussed in Appendix C.

B. How to calculate $\Gamma[\phi_1,\phi_2]$

The evaluation of $W[J_1,J_2]$ is based on the definition (2.4). In the case of perturbative expansion, for example, there arises a 2×2 propagator matrix [7] specific to the nonequilibrium processes. When the initial correlation is taken into account and if the initial density matrix is assumed to be the equilibrium one, then the propagator becomes 3×3 [12–14]. The problem is how to calculate $\Gamma[\phi_1,\phi_2]$ by performing the Legendre transformation (2.6). For the zero temperature and equilibrium nonzero temperature cases, the diagrammatical rule has been known [15,16] for several types of operators $\hat{O}$. The results are usually given in the form of the loop expansion.

Up until now there have been three ways of performing the Legendre transformation to get this result: the functional method, the method relying on the combinatorics of the graphs, and the inversion method. Among others, the inversion method [17] consists of taking perturbatively the inverse of the relation $\phi=\phi[J]$ to get $J=J[\phi]$, which is the essential part of the Legendre transformation. This type of manipulation can readily be applied to the nonequilibrium case.

III. ON-SHELL EXPANSION OF $\Gamma[\phi_1,\phi_2]$

Since $\Gamma[\phi_1,\phi_2]$ plays the analogous role of the action functional in classical analytical dynamics, let us consider first a classical mechanical system with the coordinates q_i $(i=1\text{–}N)$. The Lagrangian is written as $L(q_i,\dot{q}_i)$ and in the time interval $t_I\leqslant t\leqslant t_F$, the action is defined to be

$$I[q_i]=\int_{t_I}^{t_F}dt\ L(q_i(t),\dot{q}_i(t)). \tag{3.1}$$

The stationary equation for the action functional is the Euler-Lagrange equation of motion, which is obtained by writing $q_i(t)=q_i^{(0)}(t)+\delta q_i(t)$ and requiring that the action $I[q_i]$ is stationary for $q_i^{(0)}(t)$:

$$0=\frac{\delta I[q_i]}{\delta q_i(t)}=\frac{\partial L}{\partial q_i(t)}-\frac{d}{dt}\frac{\partial L}{\partial\dot{q}_i(t)}. \tag{3.2}$$

Here the derivative $\delta/\delta q_i(t)$ is the functional one defined in (2.8) and the variation is assumed to satisfy the boundary conditions $q_i(t_I)=q_i(t_F)=0$.

If $q_i^{(0)}(t)$ is a solution, i.e., a physically realizable trajectory, then $q_i^{(0)}(t)+\delta q_i(t)$ is not. This is because the variation δq is the one to be taken for the purpose of searching for the physical trajectory. In this sense we call δq the unphysical (or off-shell) variation. (The terminology ''off shell'' will become clear when we discuss the field theory.)

Now consider another physical trajectory that lies near $q_i^{(0)}(t)$ and write it as $q_i(t)=q_i^{(0)}(t)+\Delta q_i(t)$. In this case both $q_i^{(0)}(t)$ and $q_i^{(0)}(t)+\Delta q_i(t)$ satisfy the equation of motion so that $\Delta q_i(t_I)$ and $\Delta q_i(t_F)$ are not zero in general. The variation $\Delta q_i(t)$ is called the physical (or on-shell) variation since it leads to the physically realizable trajectory. The equation satisfied by $\Delta q_i(t)$ is obtained as follows:

$$0=\left(\frac{\delta I[q_i]}{\delta q_i(t)}\right)_{q=q^{(0)}+\Delta q}=\left(\frac{\delta I[q]}{\delta q_i(t)}\right)_{q=q^{(0)}}+\sum_{j=1}^{N}\int_{t_I}^{t_F}dt'\left(\frac{\delta^2 I[q]}{\delta q_i(t)\,\delta q_j(t')}\right)_{q=q^{(0)}}\times\Delta q_j(t')+\cdots. \tag{3.3}$$

Since $q_i^{(0)}(t)$ is a stationary solution and $\Delta q_i(t)$ is assumed to be a small quantity, the equation for the small deviation $\Delta q_j(t)$ is

$$\sum_{j=1}^{N}\int_{t_I}^{t_F}dt'\left(\frac{\delta^2 I[q]}{\delta q_i(t)\,\delta q_j(t')}\right)_{q=q^{(0)}}\Delta q_j(t')=0. \tag{3.4}$$

The solution of the above equation describes a small oscillation around $q_i^{(0)}(t)$. Equation (3.4) can be looked upon as an eigenvalue equation in matrix form with rows and columns specified by (i,t) and (j,t'). Therefore we expect a discrete set of solutions, i.e., the modes of oscillations. Equation (3.4) is therefore called the mode determining equation (on-shell equation in the case of field theory). The higher order equations denoted by dots in Eq. (3.3) determine the scattering among the various modes of small oscillation thus obtained.

In field theoretical systems and for the zero temperature case, we have already shown [1–4] that the complete parallelism between the classical action and the effective action persists and that the formal scheme of on-shell expansion produces the physical quantities such as scattering matrix (S matrix) elements among the excitation modes. These modes themselves are determined by the lowest equation of the on-shell expansion.

The purpose of the present section is to apply the same technique to the nonequilibrium generating functional $\Gamma[\phi_1,\phi_2]$, generalizing the discussions to the field theoretical case. Consider a system described by the Hermitian scalar field $\hat{\phi}(\mathbf{x})$. We have in mind the phonon field, photon field, or the Yukawa meson (Klein-Gordon) field, etc. Let us introduce the canonically conjugate momentum field $\hat{\pi}(\mathbf{x})$. Then the standard Hamiltonian has the structure

$$\hat{H}=\int d^3\mathbf{x}\{\tfrac{1}{2}\hat{\pi}(\mathbf{x})^2+\tfrac{1}{2}\hat{\phi}(\mathbf{x})\omega^2(-\nabla)\hat{\phi}(\mathbf{x})+H_I[\hat{\phi}]\}. \tag{3.5}$$

Here $\omega(-\nabla)$ is the bare dispersion relation of the field ϕ and H_I represents the unharmonic interaction term. The corresponding Lagrangian or the action functional $I[\phi]$ is given as ($\partial_t\equiv\partial/\partial t$)

$$\hat{I}[\phi]=\int d^4x\{\tfrac{1}{2}[\partial_t\hat{\phi}(x)]^2-\tfrac{1}{2}\hat{\phi}(x)\omega^2(-\nabla)\hat{\phi}(x)-H_I[\hat{\phi}]\}. \tag{3.6}$$

In the Heisenberg representation, the following relations hold:

$$\hat{\pi}(t,\mathbf{x})=\partial_t\hat{\phi}(t,\mathbf{x}),\quad [\hat{\pi}(t,\mathbf{x}),\hat{\phi}(t,\mathbf{y})]=\frac{1}{i}\delta^3(\mathbf{x}-\mathbf{y}). \tag{3.7}$$

Now take the operator $\hat{\phi}(\mathbf{x})$ as $\hat{O}$. Then we are going to study the expectation value

$$\langle\hat{\phi}(\mathbf{x})\rangle_t=\mathrm{Tr}\hat{\rho}_I\hat{U}^\dagger(t,t_I)\hat{\phi}(\mathbf{x})\hat{U}(t,t_I). \tag{3.8}$$

The solution to (2.11) is written as $\phi_1(x)=\phi_2(x)\equiv\phi^{(0)}(x)$. Then (2.12) takes the form

$$\left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\right)_{\phi_1=\phi_2=\phi^{(0)}}=0. \tag{3.9}$$

Let us perform our on-shell expansion. For this purpose we expand $\Gamma[\phi_1,\phi_2]$ around $\phi^{(0)}$, writing $\phi_1=\phi_2=\phi^{(0)}+\Delta\phi$:

$$0=\left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\right)_{\phi_1=\phi_2=\phi^{(0)}+\Delta\phi}=\left(\frac{\delta\Gamma}{\delta\phi_1(x)}\right)_0+\sum_{i=1,2}\int_{t_I}^{\infty}d^4y\left(\frac{\delta^2\Gamma}{\delta\phi_1(x)\delta\phi_i(y)}\right)_0\Delta\phi(y)+\frac{1}{2!}\sum_{i_1,i_2=1,2}\int_{t_I}^{\infty}d^4y_1\,d^4y_2\left(\frac{\delta^3\Gamma}{\delta\phi_1(x)\delta\phi_{i_1}(y_1)\delta\phi_{i_2}(y_2)}\right)_0\times\Delta\phi(y_1)\Delta\phi(y_2)+\cdots. \tag{3.10}$$

Here $()_0$ implies that () is evaluated at $\phi=\phi^{(0)}$ and we note the sum over $i=1,2$, which is specific to the nonequilibrium case. We further expand $\Delta\phi$ as

$$\Delta\phi(x)=\Delta\phi^{(1)}(x)+\Delta\phi^{(2)}(x)+\Delta\phi^{(3)}(x)+\cdots, \tag{3.11}$$

assuming that $\Delta\phi^{(n)}$ is of the order $(\Delta\phi^{(1)})^n$. Then we get our on-shell expansion by requiring that (3.10) holds in each power of $\Delta\phi^{(1)}$. The zeroth order vanishes because of (3.9) and for the first order we get the mode determining equation

$$0=\int_{-\infty}^{\infty} d^4y(\Gamma_{11}^{(2)}(x,y)+\Gamma_{12}^{(2)}(x,y))_0\Delta\phi^{(1)}(y),$$
$$\Gamma_{ij}^{(2)}(x,y)\equiv\frac{\delta^2\Gamma}{\delta\phi_i(x)\,\delta\phi_j(y)}. \tag{3.12}$$

Here and in what follows we take $t_I\to-\infty$ for simplicity. Equation (3.12) is the generalization of the mode determining equation of the small oscillation (3.4) to the nonequilibrium system.

Now the following identities are noted, which are functional analogs of (B4) and (B5):

$$\sum_{i_2}\int d^4y\;\Gamma_{i_1i_2}^{(2)}(x,y)(-1)^{i_2+i_3+1}W_{i_2i_3}^{(2)}(y,z)=\delta_{i_1,i_3}\delta^4(x-z), \tag{3.13}$$

$$\sum_{i,j=1,2}(W_{ij}^{(2)}(x,y))_{J_1=J_2}=0, \tag{3.14}$$

$$W_{ij}^{(2)}(x,y)\equiv\frac{\delta^2W}{\delta J_i(x)\,\delta J_j(y)}.$$

By using these relations we can derive

$$-\delta^4(x-z)=\int d^4y(\Gamma_{11}^{(2)}(x,y)+\Gamma_{12}^{(2)}(x,y))(W_{11}^{(2)}(y,z)+W_{12}^{(2)}(y,z))|_{J_1=J_2=J}. \tag{3.15}$$

Indeed this relation follows by choosing $i_1=i_3=1$ in (3.13) and by the repeated use of (3.14). However, $W_{11}^{(2)}+W_{12}^{(2)}$ is the retarded Green's function,

$$(W_{11}^{(2)}(y,z)+W_{12}^{(2)}(y,z))_{J_1=J_2=J}\equiv(W_R^{(2)}(y,z))_J=\frac{i}{\hbar}\theta(y^0-z^0)\langle[\hat{\phi}(y),\hat{\phi}(z)]\rangle_J, \tag{3.16}$$

therefore the relation $(\Gamma_{11}^{(2)}+\Gamma_{12}^{(2)})_0=-(W_R^{(2)})_{J=0}^{-1}$ implies that Eq. (3.12) determines the pole of $W_R^{(2)}$. For constant $\phi^{(0)}$, $(\Gamma_{ij}^{(2)}(x,y))_0$ is a function of $x-y$; therefore in Fourier space (3.12) takes the form

$$(\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p}))_0\Delta\phi^{(1)}(\omega,\mathbf{p})=0. \tag{3.17}$$

The dispersion relation $\omega=\omega(\mathbf{p})$ can be fixed by requiring that we have nonvanishing $\Delta\phi^{(1)}$ and in this case $\Delta\phi^{(1)}$ has the support on the shell defined by $\omega=\omega(\mathbf{p})$ in four-dimensional space of $p=(\omega,\mathbf{p})$. This is the reason we call (3.12) the on-shell equation and our scheme the on-shell expansion. Because the Hamiltonian or the action given in (3.6) is symmetric under $\omega\leftrightarrow-\omega$, $\Gamma^{(2)}(\omega,\mathbf{p})$ is a function of ω^2. Therefore we can write in the vicinity of the shell

$$(\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p}))_0=Z^{-1}(\omega^2-\omega^2(\mathbf{p})), \tag{3.18}$$

where $\sqrt{Z}$ is the wave function renormalization factor, i.e., the inverse of the residue of the pole of $W_R^{(2)}$, of the corresponding mode. In x space, by using the notation $px=\omega t-\mathbf{p}\cdot\mathbf{x}$,

$$\begin{aligned}(\Gamma_{11}^{(2)}(x-y)+\Gamma_{12}^{(2)}(x-y))_0&=\frac{1}{(2\pi)^4}\int d^4p\;\exp(-ip(x-y)](\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p}))_0\\&=-Z^{-1}(\partial_t^2+\omega^2(-\nabla_x))\delta^4(x-y)\equiv-Z^{-1}f(\partial_x)\delta^4(x-y).\end{aligned} \tag{3.19}$$

Here, as indicated, the differentiation applies to the coordinate x. There are two independent solutions to (3.17), each having undetermined constants $C^{(\pm)}$:

$$\Delta\phi^{(1)}(\omega,\mathbf{p})=C(p)\,\delta(\omega^2-\omega^2(\mathbf{p}))=\frac{C(\omega=\omega(\mathbf{p}),\mathbf{p})}{2\omega(\mathbf{p})}\delta(\omega-\omega(\mathbf{p}))+\frac{C(\omega=-\omega(\mathbf{p}),\mathbf{p})}{2\omega(\mathbf{p})}\delta(\omega+\omega(\mathbf{p})). \tag{3.20}$$

Let us define

$$C^{(\pm)}(\mathbf{p})=\frac{C(\omega=\pm\omega(\mathbf{p}),\pm\mathbf{p})}{(2\pi)^4\sqrt{2\omega(\mathbf{p})}}. \tag{3.21}$$

Then, in the coordinate space we have

$$\Delta\phi^{(1)}(x)=\frac{1}{(2\pi)^4}\int d^4p\ \exp(-ipx)\Delta\phi^{(1)}(\omega,\mathbf{p})=\int\frac{d^3\mathbf{p}}{\sqrt{2\omega(\mathbf{p})}}[C^{(+)}(\mathbf{p})\exp(-ip^{(0)}x)+C^{(-)}(\mathbf{p})\exp(ip^{(0)}x)], \tag{3.22}$$

where $\omega(\mathbf{p})=\omega(-\mathbf{p})$ is assumed and $p^{(0)}x=\omega(\mathbf{p})t-\mathbf{p}\cdot\mathbf{x}$. We will see below that $\Delta\phi^{(1)}(x)$ is the wave function of the excited mode. This is shown by deriving another form of $\Delta\phi^{(1)}(x)$ using the technique of formula due to Lehman, Symanzik, and Zimmerman (LSZ) [18,19]. [Here $\Delta\phi^{(1)}(x)$ is a simple plane wave since we have taken $\hat{\phi}(\mathbf{x})$ as $\hat{O}$. If the composite operator $\hat{\phi}(\mathbf{x})\hat{\phi}(\mathbf{y})$, for example, is adopted then $\Delta\phi^{(1)}(x)$ has the dependence on the internal coordinate besides $\exp(ip^{(0)}x)$.]

For the second or higher orders the required relations are

$$\sum_{i=1,2}\int d^4y(\Gamma^{(2)}_{1i}(x,y))_0\Delta\phi^{(2)}(y)+\frac{1}{2!}\sum_{i_1,i_2}\int d^4y_1\ d^4y_2(\Gamma^{(3)}_{1i_1i_2}(x,y_1,y_2))_0\Delta\phi^{(1)}(y_1)\Delta\phi^{(1)}(y_2)=0, \tag{3.23}$$

$$\sum_{i=1,2}\int d^4y(\Gamma^{(2)}_{1i}(x,y))_0\Delta\phi^{(3)}(y)+\frac{1}{2!}\sum_{i_1,i_2}\int d^4y_1\ d^4y_2(\Gamma^{(3)}_{1i_1i_2}(x,y_1,y_2))_0(\Delta\phi^{(1)}(y_1)\Delta\phi^{(2)}(y_2)+\Delta\phi^{(2)}(y_1)\Delta\phi^{(1)}(y_2))$$
$$+\frac{1}{3!}\sum_{i_1,i_2,i_3}\int d^4y_1\ d^4y_2\ d^4y_3(\Gamma^{(4)}_{1i_1i_2i_3}(x,y_1,y_2,y_3))_0\Delta\phi^{(1)}(y_1)\Delta\phi^{(1)}(y_2)\Delta\phi^{(1)}(y_3)=0, \tag{3.24}$$

etc. After some calculations (see Appendix D), $\Delta\phi^{(n)}$ can be expressed by $\Delta\phi^{(1)}$ in a compact multiretarded form:

$$\Delta\phi^{(n)}(x)=\frac{1}{n!}\int d^4y_1\cdots d^4y_n\ d^4z_1\cdots d^4z_n(W_R^{(n+1)})_0(x,y_1,\ldots,y_n)(\overleftarrow{W}_R^{(2)})_0^{-1}(y_1,z_1)(\overleftarrow{W}_R^{(2)})_0^{-1}(y_2,z_2)$$
$$\times\cdots(\overleftarrow{W}_R^{(2)})_0^{-1}(y_n,z_n)\Delta\phi^{(1)}(z_1)\cdots\Delta\phi^{(1)}(z_n), \tag{3.25}$$

$$W_R^{(n+1)}(x,y_1,\ldots,y_n)\equiv\sum_{i_1,\ldots,i_n}\left(\frac{\delta^{n+1}W}{\delta J_1(x)J_{i_1}(y_1)\cdots J_{i_n}(y_n)}\right)_{J_1=J_2}$$
$$=\left(\frac{i}{\hbar}\right)^n\mathrm{Tr}\left(\hat{\rho}_I\sum_{P\{y_1,\ldots,y_n\}}\theta(t_x,t_{y_1},\ldots,t_{y_n})[[\cdots[\hat{\phi}(x),\hat{\phi}(y_1)],\cdots],\hat{\phi}(y_n)]\right.$$
$$\equiv\left(\frac{i}{\hbar}\right)^n\langle R(\hat{\phi}(x)\hat{\phi}(y_1)\cdots\hat{\phi}(y_n))\rangle, \tag{3.26}$$

$$\theta(t_x,t_{y_1},\ldots,t_{y_n})=\theta(t_x-t_{y_1})\theta(t_{y_1}-t_{y_2})\cdots\theta(t_{y_{n-1}}-t_{y_n}).$$

Here we have defined $\langle\rangle=\mathrm{Tr}\hat{\rho}_I()$ and $\Sigma_{P\{y_1,\ldots,y_n\}}$ implies the sum over all possible permutations of $\{y_1,\ldots,y_n\}$. Equation (3.25) expresses the fact that among $n+1$ external lines n lines are amputated by the retarded Green's function. The arrow on $W_R^{(2)}$ implies that it operates to the left, i.e., $(\overleftarrow{W}_R^{(2)})_0^{-1}$ first amputates the pole of $W_R^{(n+1)}$ and then we multiply $\Delta\phi^{(1)}\cdots\Delta\phi^{(1)}$.

Now the above formulas are rewritten by the operator form through the reverse use of the LSZ reduction technique [18,19] and we get another physical interpretation of our expansion scheme. In particular infinite series of on-shell expansion can be summed up into a coherent state of the excitation mode. Consider first $\Delta\phi^{(1)}(x)$. We show that it is related to the wave function of the excited mode. For this purpose let us rewrite $\Delta\phi^{(1)}(x)$ using (3.15) and (3.19);

$$\Delta\phi^{(1)}(x)=-\int d^4y\int d^4y'\ \Delta\phi^{(1)}(y)\sum_{i=1,2}\Gamma^{(2)}_{1i}(x-y')\sum_{j=1,2}W^{(2)}_{1j}(y'-y) \tag{3.27}$$

$$=Z^{-1}\int d^4y\ \Delta\phi^{(1)}(y)f(\vec{\partial}_x)i\langle R(\hat{\phi}(x)\hat{\phi}(y))\rangle. \tag{3.28}$$

We have used the fact that since the factor $\Delta\phi^{(1)}(y)$ is present we can use the expression (3.19) for $\Gamma^{(2)}$ in (3.27). The arrow indicates that it operates to the right. Since we are assuming the homogeneous system, $\langle R(\hat{\phi}(x)\hat{\phi}(y))\rangle$ is a function of $x-y$ so that $f(\vec{\partial}_x)=f(\vec{\partial}_{-y})=f(\vec{\partial}_y)$ [because f is the even function of its argument, see (3.19)]. Now remembering the fact that Eq. (3.12) is equivalent to

$$f(\vec{\partial}_y)\Delta\phi^{(1)}(y)=0, \tag{3.29}$$

the partial integration over $\int d^4y$ in (3.28) is performed. The boundary term at spatial infinity is assumed to vanish by utilizing the wave packet regularization for the plane wave. We keep the boundary term at $t=\pm\infty$ by using the identity

$$A\partial_t^2 B=\partial_t(A\overleftrightarrow{\partial}_t B)+(\partial_t^2 A)B, \quad A\overleftrightarrow{\partial}_t B\equiv A\partial_t B-(\partial_t A)B. \tag{3.30}$$

By (3.29) we get, using the notation $y=(y^0,\mathbf{y})$, the following expression. Note that we have taken $t_I=-\infty$:

$$\Delta\phi^{(1)}(x)=Z^{-1}\int d^4y\ \partial_{y^0}(\Delta\phi^{(1)}(y)\overleftrightarrow{\partial}_{y^0}i\langle R(\hat{\phi}(x)\hat{\phi}(y))\rangle)=iZ^{-1}\left(\lim_{y^0\to\infty}-\lim_{y^0\to t_I}\right)\int d^3\mathbf{y}\ \Delta\phi^{(1)}(y)\overleftrightarrow{\partial}_{y^0}\langle R(\hat{\phi}(x)\hat{\phi}(y))\rangle. \tag{3.31}$$

We recall here that $\lim_{y^0\to\infty}$ makes a vanishing contribution because of the presence of the θ function in $W_R^{(2)}$ and also that at equal time the fields $\hat{\phi}(t,\mathbf{x})$ commute among themselves. Thus we arrive at

$$\Delta\phi^{(1)}(x)=\langle[\hat{\phi}(x),\hat{A}]\rangle, \tag{3.32}$$

$$\hat{A}=-iZ^{-1}\int d^3\mathbf{y}\{\Delta\phi^{(1)}(y)\hat{\pi}(y)-(\partial_{y^0}\Delta\phi^{(1)}(y))\hat{\phi}(y)\}_{y^0=t_I}. \tag{3.33}$$

In momentum representation $\hat{A}$ takes a simple form. Let us expand $\hat{\phi}$ and $\hat{\pi}$ in terms of the creation and annihilation operators:

$$\hat{\phi}(t_I,\mathbf{x})=\frac{1}{(2\pi)^{3/2}}\int\frac{d^3\mathbf{p}}{\sqrt{2\omega(\mathbf{p})}}[\hat{a}(\mathbf{p})e^{-ip^{(0)}x_I}+\hat{a}(\mathbf{p})^\dagger e^{ip^{(0)}x_I}], \tag{3.34}$$

$$\hat{\pi}(t_I,\mathbf{x})=\frac{-i}{(2\pi)^{3/2}}\int d^3\mathbf{p}\sqrt{\frac{\omega(\mathbf{p})}{2}}[\hat{a}(\mathbf{p})e^{-ip^{(0)}x_I}-\hat{a}(\mathbf{p})^\dagger e^{ip^{(0)}x_I}], \tag{3.35}$$

where $p^{(0)}x_I=\omega(\mathbf{p})t_I-\mathbf{p}\cdot\mathbf{x}$ and

$$[\hat{a}(\mathbf{p}),\hat{a}(\mathbf{k})^\dagger]=\delta^3(\mathbf{p}-\mathbf{k}), \tag{3.36}$$

while other commutators are zero. Now inserting (3.22), (3.34), and (3.35) into the definition (3.33), we get

$$\hat{A}=a^\dagger-a, \tag{3.37}$$

$$a^{(\dagger)}\equiv Z^{-1}(2\pi)^{3/2}\int d^3\mathbf{p}\ C^{(\mp)}(\mathbf{p})\hat{a}(\mathbf{p})^{(\dagger)}. \tag{3.38}$$

At this point we assume the initial density matrix to be the equilibrium one: $\hat{\rho}_I=\exp(-\beta\hat{H})$. Then $\hat{\rho}_I$ does not change the number of particles corresponding to a or $a^\dagger$. This is seen as follows. Since $t_I=-\infty$, $\hat{\phi}(t_I,\mathbf{x})$ corresponds to in-field of the LSZ formalism and $\hat{a}^{(\dagger)}$ annihilates or creates the mode, which is an eigenstate of the total Hamiltonian. Recall here that it is defined by the pole of $W_R^{(2)}$.

Now $\Delta\phi^{(1)}(x)$ can be looked upon as a linear combination of the wave function of the state (which is not normalized) containing one excited mode annihilated or created by a or $a^\dagger$. In order to see this, let us write (3.32) explicitly in the number representation using (3.37):

$$\begin{aligned}\Delta\phi^{(1)}(x)&=\sum_n\rho_{I_{nn}}\langle n|[\hat{\phi}(x),a^\dagger-a]|n\rangle\\&=\sum_n\rho_{I_{nn}}\{-\sqrt{n}\langle n|\hat{\phi}(x)|n-1\rangle\\&\quad+\sqrt{n+1}\langle n|\hat{\phi}(x)|n+1\rangle+\sqrt{n+1}\langle n+1|\hat{\phi}(x)|n\rangle\\&\quad-\sqrt{n}\langle n-1|\hat{\phi}(x)|n\rangle\}.\end{aligned} \tag{3.39}$$

Here the summation over the indices other than n is suppressed and the following notations have been used:

$$a|n\rangle=\sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle.$$

The above result is the generalization of the zero temperature case to finite temperature where the excited modes and the thermal background are present at the same time. Indeed we can show that (3.39) reduces to the known expression if we keep only the ground state $|0\rangle$ in the sum. Using $a|0\rangle=\langle 0|a^\dagger=0$, we see that $\Delta\phi^{(1)}(x)$ is written as

$$\Delta\phi^{(1)}(x)=\langle 0|\hat{\phi}(x)|1\rangle+\text{c.c.},$$

where c.c. implies the complex conjugate. The above expression is precisely the wave function of the mode for the case of Hermite field.

Consider next $\Delta\phi^{(2)}(x)$, which can be handled in a similar manner:

$$\Delta\phi^{(2)}(x)=\int d^4y_1\int d^4y_2\ iZ^{-1}\Delta\phi^{(1)}(y_1)f(\vec{\partial}_{y_1})iZ^{-1}\Delta\phi^{(1)}(y_2)f(\vec{\partial}_{y_2})\langle R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2))\rangle. \tag{3.40}$$

The integration over y_2 is done first. Following the same process as we have done above, the partial integration leads to

$$\begin{aligned}\int d^4y_2 iZ^{-1}\Delta\phi^{(1)}(y_2)f(\vec{\partial}_{y_2})\langle R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2))\rangle &= iZ^{-1}\int d^4y_2\ \partial_{y_2^0}(\Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0}\langle R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2))\rangle)\\ &= iZ^{-1}\int d^3\mathbf{y}_2\left(\lim_{y_2^0\to\infty}-\lim_{y_2^0\to t_I}\right)\Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0}\langle R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2))\rangle\\ &= -iZ^{-1}\int d^3\mathbf{y}_2\ \Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0}\langle[R(\hat{\phi}(x)\hat{\phi}(y_1)),\hat{\phi}(y_2)]\rangle|_{y_2^0=t_I}\\ &= \langle[R(\hat{\phi}(x)\hat{\phi}(y_1)),\hat{A}]\rangle. \end{aligned} \tag{3.41}$$

The remaining integration of y_1 can be done similarly with the result

$$\Delta\phi^{(2)}(x)=\frac{1}{2!}\langle[[\hat{\phi}(x),\hat{A}],A]\rangle. \tag{3.42}$$

Looking at the above expressions, it is an easy task to guess the results for general $\Delta\phi^{(n)}(x)$. In fact by using the mathematical induction technique, we can show the following form:

$$\Delta\phi^{(n)}(x)=\frac{1}{n!}\langle[[\cdots[[\hat{\phi}(x),\hat{A}],\hat{A}],\cdots],\hat{A}]\rangle. \tag{3.43}$$

Now it is a simple matter to sum up over n and we get

$$\begin{aligned}\Delta\phi(x)&=\sum_{n=1}^{\infty}\Delta\phi^{(n)}(x)\\ &=\mathrm{Tr}[\hat{\rho}_I\exp(-\hat{A})\hat{\phi}(x)\exp(\hat{A})]\\ &=\mathrm{Tr}[\exp(\hat{A})\hat{\rho}_I\exp(-\hat{A})\hat{\phi}(x)].\end{aligned} \tag{3.44}$$

Usually the initial density matrix is written with $\hat{\pi}(\mathbf{x})$ and $\hat{\phi}(\mathbf{x})$ so that, by noting the definition of (3.33) of $\hat{A}$, we get the c-number shift of the initial variables:

$$\exp(\hat{A})\hat{\rho}_I(\hat{\pi}(\mathbf{x}),\hat{\phi}(\mathbf{x}))\exp(-\hat{A}) =\hat{\rho}_I(\hat{\pi}(\mathbf{x})-\pi_c(\mathbf{x}),\hat{\phi}(\mathbf{x})-\phi_c(\mathbf{x})), \tag{3.45}$$

$$\pi_c(\mathbf{x})=Z^{-1}(\partial_{x^0}\Delta\phi^{(1)}(x))_{t_I}, \tag{3.46}$$

$$\phi_c(\mathbf{x})=Z^{-1}(\Delta\phi^{(1)}(x))_{t_I}. \tag{3.47}$$

The initial coordinate is shifted as it should:

$$\begin{aligned}\Delta\phi(t_I,\mathbf{x})&=\mathrm{Tr}(\hat{\rho}_I\{\hat{\phi}(t_I,\mathbf{x})+[\hat{\phi}(t_I,\mathbf{x}),-iZ^{-1}\hat{A}]\}),\\ &=\mathrm{Tr}(\hat{\rho}_I\{\hat{\phi}(t_I,\mathbf{x})+(-iZ^{-1})i\Delta\phi^{(1)}(t_I,\mathbf{x})\}),\end{aligned} \tag{3.48}$$

$$=\mathrm{Tr}(\hat{\rho}_I\hat{\phi}(t_I,\mathbf{x}))+Z^{-1}\Delta\phi^{(1)}(t_I,\mathbf{x}). \tag{3.49}$$

In the momentum representation,

$$\exp(\hat{A})\hat{\rho}_I(\hat{a}(\mathbf{p}),\hat{a}^\dagger(\mathbf{p}))\exp(-\hat{A}) =\hat{\rho}_I(\hat{a}(\mathbf{p})-\tilde{C}^{(+)}(\mathbf{p}),\hat{a}^\dagger(\mathbf{p})-\tilde{C}^{(-)}(\mathbf{p})), \tag{3.50}$$

$$\tilde{C}^{(\pm)}(\mathbf{p})\equiv Z^{-1}(2\pi)^{3/2}C^{(\pm)}(\mathbf{p}).$$

Note that $\exp(-\hat{A})$ coincides with the familiar operator, which brings about the coherent state.

Now we have at hand a way of searching for the correct condensed state; vary $\tilde{C}^{(\pm)}(\mathbf{p})$ in such a way that $\Delta\phi(x)$ becomes constant in time. Then $\tilde{C}^{(\pm)}(\mathbf{p})$ is determined and we get the density matrix corresponding to the condensed state. This is illustrated for superfluid ^{4}He in the next section. (Application of this technique to other real physical systems is under way.)

IV. SUPERFLUID ^{4}He: AN EXAMPLE

Let us exemplify the formulas obtained above taking the system of ^{4}He. Here the complex (i.e., non-Hermite) field operator $\hat{\psi}(\mathbf{x})$ of ^{4}He has a nonvanishing expectation value below the temperature T_c corresponding to the onset of the Bose condensation. The model Hamiltonian is the usual one [20]:

$$\hat{H}=\int d^3\mathbf{x}\ \hat{\psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2-\mu\right)\hat{\psi}(\mathbf{x}) +\frac{1}{2}\int d^3\mathbf{x}\ d^3\mathbf{y}\ \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})U_0(\mathbf{x}-\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}),$$

$$U_0(\mathbf{x}-\mathbf{y})=U_0(\mathbf{y}-\mathbf{x}),\quad [\hat{\psi}(t,\mathbf{x}),\hat{\psi}^\dagger(t,\mathbf{y})]=\delta^3(\mathbf{x}-\mathbf{y}). \tag{4.1}$$

Here $U_0(\mathbf{x}-\mathbf{y})$ is the assumed repulsive potential of the helium atom and μ the chemical potential. In the following we take, for simplicity, the local form of the potential; $U_0(\mathbf{x}-\mathbf{y})=U_0\delta^3(\mathbf{x}-\mathbf{y})$. Below we set $\phi^{(\dagger)}(x)\equiv\langle\hat{\psi}^{(\dagger)}(x)\rangle$ and introduce the notations

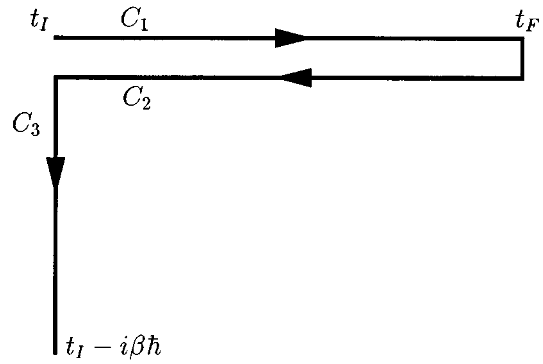


FIG. 1. Contour paths C_1, C_2, C_3.

$$\hat{\psi}^\alpha \equiv (\hat{\psi}^\dagger, \hat{\psi}), \quad \hat{\psi}^{\dagger\alpha} \equiv (\hat{\psi}, \hat{\psi}^\dagger), \quad \phi^\alpha = (\phi^\dagger, \phi),$$
$$\phi^{\dagger\alpha} = (\phi, \phi^\dagger) \quad (\alpha = 1,2). \tag{4.2}$$

(The superscript α has nothing to do with the subscript i or j, which discriminates the branch of the two real time paths.) We need two kinds of sources J_i, $\overline{J_i}$ and define

$$\hat{H}_{J_i}(t) = \hat{H} - \int d^3\mathbf{x}\{J_i(x)\hat{\psi}^\dagger(\mathbf{x}) + \overline{J_i}(x)\hat{\psi}(\mathbf{x})\}. \tag{4.3}$$

In the above definition, $i=1,2,3$. If $i=3$, we are assuming the equilibrium initial distribution $\hat{\rho}_I = \exp(-\beta\hat{H})$ and the time variable takes the imaginary value; $t = t_I - i\tau$, with $0 \leq \tau \leq \hbar\beta$.

Here we introduce the notion of the complex contour of the time integration in order to write various formulas in a compact way. We are going to generalize the double path formalism due to Schwinger [6], Keldysh [7], Chou *et al.* [10], to the three time paths including the imaginary time path. See for this purpose Niemi and Semenoff [9], Wagner [13], and Fukuda and co-workers [14]. The contour time integral $\int_C dt$ extends over the contour C, which runs as $C_1 \to C_2 \to C_3$ (see Fig. 1). Each path is defined to be $C_1: t_I \to t_F$ and $C_2: t_F \to t_I$ (return path) $C_3: t_I \to t_I - i\beta\hbar$ (imaginary time path). The contour time ordering operator T_C orders the time sequence according to its location on the contour. Furthermore the following notation is used:

$$J(t) = J_i(t) \quad \text{if } t \text{ is on } C_i \quad (i=1,2,3). \tag{4.4}$$

With these notations and assuming the equilibrium initial distribution, we can write

$$\exp\frac{i}{\hbar}W[J_1,J_2,J_3] \equiv \exp\frac{i}{\hbar}W[J]$$
$$= \mathrm{Tr}\,\mathrm{T}_C \exp\left(-\frac{i}{\hbar}\int_C dt\, \hat{H}_J(t)\right), \tag{4.5}$$

where $\hat{H}_J(t)$ is equal to $\hat{H}_{J_i}(t)$ given in (4.3) if t is on C_i with $i=1,2,3$, respectively. The contour δ function is introduced as

$$\int_C dt\,\delta_C(t-t')f(t) = f(t'). \tag{4.6}$$

Similarly the contour θ function and the contour functional differentiation are defined:

$$\theta_C(t-t') = \int_C^t dt''\,\delta_C(t''-t'), \tag{4.7}$$

$$\frac{\delta f(t)}{\delta f(t')} = \delta_C(t-t'). \tag{4.8}$$

As for the Legendre transformed Γ, the formula of the loop expansion has been established by several authors [15,16] but these works are limited to the zero temperature case or to the equilibrium systems. The nonequilibrium case where the imaginary time path is absent has been discussed by Chou *et al.* [10]. We use in the following the contour time path defined above in the case where the imaginary time path is needed. It turns out that the use of the contour integral makes it easy to generalize the known results to the nonequilibrium case.

A. On-shell expansion

1. The case $\hat{O} = \hat{\psi}^\alpha$

Let us take a stationary homogeneous solution $\phi^\alpha \equiv \langle \hat{\psi}^\alpha(x)\rangle$. (For $T \leq T_c$, there are two solutions.) For the moment we consider only J_1 and J_2 assuming $J_3 = 0$. Then the on-shell condition takes the form

$$(i\hbar\partial_t + \Omega(-\nabla))\Delta\phi^{(1)}(x) = 0,$$
$$(-i\hbar\partial_t + \Omega(-\nabla))\Delta\phi^{\dagger(1)}(x) = 0. \tag{4.9}$$

Here $\Omega(-\nabla)$ is the complete dispersion relation including the corrections due to the interaction. The solution in Fourier space is written as

$$\Delta\phi^{(\dagger)(1)} = \int d^3\mathbf{p}\; C^{(\pm)}(\mathbf{p})e^{(\mp ip^{(0)}x)}, \tag{4.10}$$

where $p^{(0)}x = \Omega(\mathbf{p})t - \mathbf{p}\cdot\mathbf{x}$. In the formula (3.25), owing to the presence of the on-shell projection $\Delta\phi^{(1)}$, $(W_R^{(2)})^{-1}$ can be replaced by its pole part:

$$(W_R^{(2)})^{-1}_{\psi^\dagger\psi}(x,y) = -Z^{-1}(i\hbar\partial_{t_x} + \Omega(-\nabla_x))\delta^4(x-y), \tag{4.11}$$
$$(W_R^{(2)})^{-1}_{\psi\psi^\dagger}(x,y) = -Z^{-1}(-i\hbar\partial_{t_x} + \Omega(-\nabla_x))\delta^4(x-y).$$

Here $\sqrt{Z}$ is the wave function renormalization factor of the ^{4}He field.

Inserting (4.9) and (4.11) into (3.25), the reverse use of the LSZ reduction formula, as was done in the previous section, leads to the following expression, which has the n-fold commutator:

$$\Delta\phi^{\alpha,(n)}(x) = \frac{1}{n!}\langle[[\cdots[\hat{\psi}^\alpha(x),\hat{A}],\cdots],\hat{A}]\rangle,$$

$$\hat{A} \equiv Z^{-1}\int d^3\mathbf{y}(\Delta\phi^{(1)}(y)\hat{\psi}^\dagger(y) - \Delta\phi^{\dagger(1)}(y)\hat{\psi}(y))_{y^0=t_I}. \tag{4.12}$$

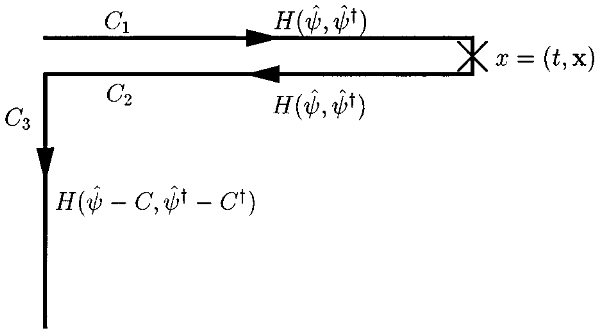


FIG. 2. Contour paths C_1,C_2,C_3 corresponding to (4.20).

Let us rewrite $\hat{A}$ by expanding $\hat{\psi}^{(\dagger)}$ in terms of the creation or annihilation operator:

$$\hat{\psi}^{(\dagger)}(t_I,\mathbf{x})=\frac{1}{(2\pi)^{3/2}}\int d^3\mathbf{p}\ \hat{a}(\mathbf{p})^{(\dagger)}e^{\mp ip^{(0)}x_I}, \quad (4.13)$$

where $p^{(0)}x_I=\Omega(\mathbf{p})t_I-\mathbf{p}\cdot\mathbf{x}$. Now inserting (4.10) and (4.13) into the definition (4.12), we get

$$\hat{A}=a^\dagger-a, \quad (4.14)$$

$$a^{(\dagger)}\equiv Z^{-1}(2\pi)^{3/2}\int d^3\mathbf{p}\ C^{(\pm)}(\mathbf{p})\hat{a}(\mathbf{p})^{(\dagger)}. \quad (4.15)$$

Assuming the equilibrium initial density matrix, we have the following expression for the wave function analogous to (3.39):

$$\begin{aligned}\Delta\phi^{(\dagger)(1)}(x)&=\sum_n \rho_{I_{nn}}\langle n|[\hat{\phi}^{(\dagger)}(x),a^\dagger-a]|n\rangle\\&=\sum_n \rho_{I_{nn}}\{-\sqrt{n}\langle n|\hat{\phi}^{(\dagger)}(x)|n-1\rangle\\&\quad+\sqrt{n+1}\langle n|\hat{\phi}^{(\dagger)}(x)|n+1\rangle\\&\quad+\sqrt{n+1}\langle n+1|\hat{\phi}^{(\dagger)}(x)|n\rangle\\&\quad-\sqrt{n}\langle n-1|\hat{\phi}^{(\dagger)}(x)|n\rangle\}. \quad (4.16)\end{aligned}$$

We can sum up $\Delta\phi^{\alpha,(n)}(x)$ into an exponential form to get $\Delta\phi^\alpha(x)$ as follows:

$$\Delta\phi^\alpha(x)=\sum_{n=1}^{\infty}\Delta\phi^{\alpha,(n)}(x)=\mathrm{Tr}(\hat{\rho}_I[\hat{\psi},\hat{\psi}^\dagger]e^{-\hat{A}}\hat{\psi}^\alpha(x)e^{\hat{A}}) \quad (4.17)$$

$$=\mathrm{Tr}(\hat{\rho}_I[\hat{\psi}',\hat{\psi}'^\dagger]\hat{\psi}^\alpha(x)). \quad (4.18)$$

$$\hat{\psi}'=\hat{\psi}-Z^{-1}\Delta\phi^{(1)}(t_I),\qquad \hat{\psi}'^\dagger=\hat{\psi}^\dagger-Z^{-1}\Delta\phi^{\dagger(1)}(t_I).$$

Equation (4.18) tells us that $\Delta\phi^\alpha(x)$ is the same as $\langle\hat{\psi}^\alpha(x)\rangle$ but with the initial operator inside $\hat{\rho}_I$ shifted by the amount $-Z^{-1}\Delta\phi^{\alpha,(1)}(t_I,\mathbf{x})$, which is a c number. This is reminiscent of the shift of boundary conditions under the on-shell variation in classical analytical dynamics; see the discussion preceding (3.3). However, only the shift of the initial value comes in the formula here compared with the

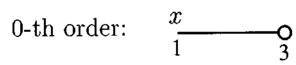


FIG. 3. The zeroth-order diagram of $\Delta\phi(x)$.

case of the classical mechanics where the change of $q(t)$ at both $t=t_I$ and $t=t_F$ appear. The reason is that we have a closed time path for the case of finite temperature while the time flows straight from $t=-\infty$ to $+\infty$ in the zero temperature case.

2. Identity involving $\Delta\phi$

Below we consider the relation of the constant solution of the nonequilibrium equation of motion and the stationary solution of the equilibrium free energy by deriving a functional identity. For this purpose it is convenient to introduce the probe J_3 into the imaginary time axis and define $W[J_1,J_2,J_3]$. (See Appendix C for the general discussion of W or Γ of three variables.) In the following we do not perform the Legendre transformation in J_3, therefore $\Gamma[\phi_1,\phi_2]$ is the Legendre transformation of $W[J_1,J_2,J_3]$ in J_1 and J_2 only and J_3 is assumed to be a parameter in this transformation. Furthermore J_3 is taken to be a constant; J_3 does not contain x. For notational simplicity J_3 is not written explicitly below for $\Gamma[\phi_1,\phi_2]$. With this notation, we have the relation, by (A13),

$$\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}=\frac{\delta\Gamma[\phi_1,\phi_2,\phi_3]}{\delta\phi_1(x)}. \quad (4.19)$$

Now take the uncondensed solution $\phi^{\alpha(0)}=0$ and assume that $Z^{-1}\Delta\phi^{(\dagger)}(t_I,\mathbf{x})\equiv C^{(\dagger)}=\text{const}$. By this choice we are expanding around the normal solution and summing up the unstable modes excited above the uncondensed solution. Then the naive diagrammatical consideration can be applied to (4.18) using the Feynman rule given in Appendix E. We write (4.18) as

$$\Delta\phi^\alpha(x)=\mathrm{Tr}(\hat{\rho}_I(\hat{\psi}-C,\hat{\psi}^\dagger-C^\dagger)\hat{\psi}^\alpha(x)). \quad (4.20)$$

In Fig. 2, Eq. (4.20) is illustrated. The diagram giving a nonvanishing contribution to $\Delta\phi^{(\dagger)}(x)$ contains at least one $C^{(\dagger)}$ and several lower-order diagrams are shown in Figs. 3, 4, and 5 for $\Delta\phi(x)$. The point x is denoted by 1 in the figure but it can be 2 or + since $\langle\hat{\psi}_1(x)\rangle=\langle\hat{\psi}_2(x)\rangle$ so that $\langle\hat{\psi}^{(+)}(x)\rangle=\langle\hat{\psi}_1(x)\rangle=\langle\hat{\psi}_2(x)\rangle$. [See (C5) for the definition.] At each vertex the number 1 or 2 or 3 is assigned to indicate the path to which it belongs. The line represents one

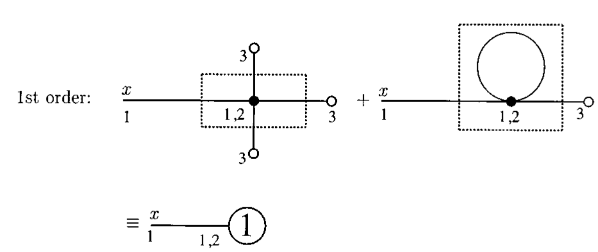


FIG. 4. The first-order diagrams of $\Delta\phi(x)$.

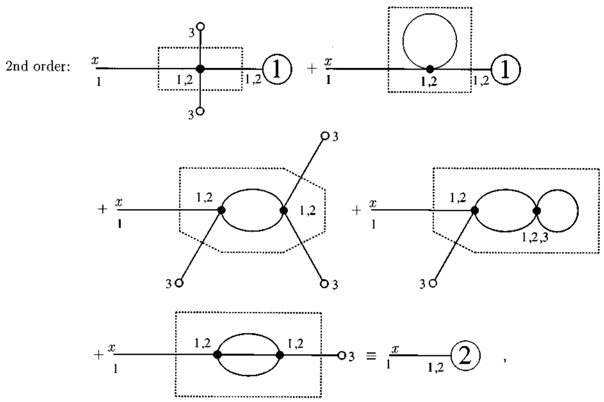


FIG. 5. The second-order diagrams of $\Delta\phi(x)$.

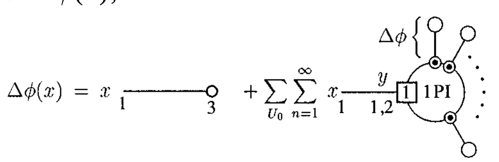
of the six propagators shown in Appendix E. Let us evaluate the first order diagram Fig. 3; the vertex at the end of the line is $-\mu C$ and the line is the zero momentum limit of $G^{(-)}(x;\tau,\mathbf{y})$; see (E5). We integrate this quantity by applying $\int_0^{\hbar\beta} d\tau$ and the result of this process is

$$e^{-i\omega_{\mathbf{k}=0}(t-t_I)}/(-\mu)=1+\int_{t_I}^{\infty} d^4y \frac{1}{i\hbar}\Delta_R(x-y).$$

Thus the value of Fig. 3 is

$$C+\int_{t_I}^{\infty} d^4y \frac{1}{i\hbar}\Delta_R(x-y)(-\mu C).$$

In Figs. 4 and 5, the one-particle irreducible part is enclosed by dotted lines. By one-particle irreducible part, we mean a part of a graph that is not separated into two parts if we cut any one of the propagators contained in it. It is easy to convince oneself that the one-particle reducible parts sum up to $\Delta\phi$ itself but it is now x independent. Thus, summing up all the diagrams of higher order, we arrive at the following form of $\Delta\phi(x)$;



$$= (-\mu C)\frac{e^{-i\omega_{\mathbf{k}=0}(t-t_I)}}{-\mu} - \int_{t_I}^{\infty} d^4y \frac{1}{i\hbar}\Delta_R(x-y)\left(\frac{\delta\Gamma_{\text{int}}}{\delta\phi_1^\dagger(y)}\right)_{\phi_1=\phi_2=\Delta\phi}$$
$$= C - \int_{t_I}^{\infty} d^4y \frac{i}{\hbar}\Delta_R(x-y)\left[\mu C + \left(\frac{\delta\Gamma_{\text{int}}}{\delta\phi_1^\dagger(y)}\right)_{\phi_1=\phi_2=\Delta\phi}\right]. \tag{4.21}$$

Here $\Delta_R(x-y)$ is given in Appendix E. In (4.21) Σ_{U_0} implies the sum over the graphs that contain at least one U_0 and we notice that

$$\mu C=\left(\frac{\delta\Gamma_{\text{tree}}}{\delta\phi_1^\dagger(x)}\right)_{\phi_1=\phi_2=C}.$$

In the above expressions we have separated Γ as the sum of the free part and the part due to interactions $\Gamma=\Gamma_{\text{free}}+\Gamma_{\text{int}}$. In this way we can write

$$\Delta\phi(x)=C-\int d^4y \frac{1}{i\hbar}\Delta_R(x-y)\left[\left(\frac{\delta\Gamma_{\text{free}}}{\delta\phi_1^\dagger(y)}\right)_{\phi_1=\phi_2=C}+\left(\frac{\delta\Gamma_{\text{int}}}{\delta\phi_1^\dagger(y)}\right)_{\phi_1=\phi_2=\Delta\phi}\right]. \tag{4.22}$$

Up until now we did not write the J_3 dependence explicitly but J_3 has to be set to zero to get back to the original theory. Now we write (4.22) in terms of $\Gamma[\phi_1,\phi_2,\phi_3]$. Since $J_3=0$ implies $\delta\Gamma/\delta\phi_3=0$ and since the formula (4.19) holds for the free part and the interacting part separately, Eq. (4.22) is transformed into

$$\Delta\phi(x)=C-\int d^4y \frac{1}{i\hbar}\Delta_R(x-y)\left[\left(\frac{\delta\Gamma_{\text{free}}}{\delta\phi_1^\dagger(y)}\right)_{(*)}+\left(\frac{\delta\Gamma_{\text{int}}}{\delta\phi_1^\dagger(y)}\right)_{(**)}\right], \tag{4.23}$$

where Γ represents $\Gamma[\phi_1,\phi_2,\phi_3]$ and $(*)$ and $(**)$ imply

$$(*): \phi_1=\phi_2=C, \quad \frac{\delta\Gamma}{\delta\phi_3}=0,$$

$$(**): \phi_1=\phi_2=\Delta\phi, \quad \frac{\delta\Gamma}{\delta\phi_3}=0,$$

respectively. Now suppose that $\phi_1=\phi_2=\phi_3=C$ is a solution to

$$\frac{\delta\Gamma}{\delta\phi_1}=\frac{\delta\Gamma}{\delta\phi_2}=\frac{\delta\Gamma}{\delta\phi_3}=0,$$

then by the property (C13), $\phi=C$ coincides with the stationary solution to the equilibrium free energy; $\delta\Gamma_\beta/\delta\phi|_{\phi=C}=0$. If we put this solution into (4.23), then the term inside [ ] vanishes and $\Delta\phi(x)$ becomes C consistently. Thus we have shown that the true value of the condensation C is calculable by requiring $\Delta\phi(x)$ to be time independent.

3. The case $\hat{O}=\hat{\psi}^\alpha\hat{\psi}^\alpha$

Next the pairing condensation is discussed. In superfluid ^{4}He, it has been pointed out that not only ψ^α but also $\psi^\alpha\psi^\alpha$ may condense [21]. There has been controversy in this case concerning the existence or the absence of the gap in the excitation spectrum. But the gap can be shown to be absent by our formalism; see the arguments at the end of Sec. IV B.

Here the result of the application of the on-shell expansion to the pairing theory is briefly summarized below. We will see that in our formalism the Bogoliubov angle naturally comes in. For this purpose the pairing is taken up in momentum representation $\langle\hat{\psi}(-\mathbf{p})\hat{\psi}(\mathbf{p})\rangle$, $\langle\hat{\psi}^\dagger(\mathbf{p})\hat{\psi}^\dagger(-\mathbf{p})\rangle$ by adding the source term to the Hamiltonian separately for two time paths as follows:

$$\hat{H}_{J_i}=\hat{H}-\int d^3\mathbf{p}(J_{i\psi^\dagger\psi^\dagger}(t,\mathbf{p})\hat{\psi}^\dagger(\mathbf{p})\hat{\psi}^\dagger(-\mathbf{p})$$
$$+J_{i\psi\psi}(t,\mathbf{p})\hat{\psi}(-\mathbf{p})\hat{\psi}(\mathbf{p})).$$

We do not write the J_3 dependence and the argument goes through in a similar way as in the case of $\langle\hat{\psi}^\alpha\rangle$. We first define the generating functional W as before and introduce the notations for $\alpha=1,2$:

$$J_i^\alpha(t,\mathbf{p})=(J_{i\psi^\dagger\psi^\dagger}(t,\mathbf{p}),J_{i\psi\psi}(t,\mathbf{p})),$$
$$\Phi_i^\alpha(t,\mathbf{p})=(\Phi_i^\dagger(t,\mathbf{p}),\Phi_i(t,\mathbf{p}))=\frac{\delta W}{\delta J_i^\alpha(t,\mathbf{p})}. \tag{4.24}$$

Then Γ is introduced as

$$\Gamma[\Phi_1^\alpha,\Phi_2^\alpha]=W[J_1^\alpha,J_2^\alpha]-\sum_{i,\alpha}\int dt\int d^3\mathbf{p}\; J_i^\alpha(t,\mathbf{p})\Phi_i^\alpha(t,\mathbf{p}). \tag{4.25}$$

The equation that governs the time development of the order parameter is written as

$$\left(\frac{\delta\Gamma}{\delta\Phi_1^\alpha(t,\mathbf{p})}\right)_{\Phi_1=\Phi_2=\Phi}=0. \tag{4.26}$$

On-shell expansion around the uncondensed solution $\Phi^{(\dagger)(0)}=0$ is obtained by writing

$$\Phi^\alpha(t,\mathbf{p})=\Phi^{\alpha(0)}+\Delta\Phi^\alpha(t,\mathbf{p}),$$

where the variables without the subscript i are the physical quantities that take the same value for $i=1$ and 2:

$$\Phi^\alpha=(\Phi^\dagger,\Phi),\quad \Phi(t,\mathbf{p})=\langle\hat{\psi}(t,-\mathbf{p})\hat{\psi}(t,\mathbf{p})\rangle,$$
$$\Phi^\dagger(t,\mathbf{p})=\langle\hat{\psi}^\dagger(t,\mathbf{p})\hat{\psi}^\dagger(t,-\mathbf{p})\rangle.$$

Then $\Delta\Phi^\alpha(t,\mathbf{p})$ is obtained, after some algebra, as follows:

$$\Delta\Phi^\alpha(t,\mathbf{p})=\Delta\Phi^{\alpha,(1)}(t,\mathbf{p})+\Delta\Phi^{\alpha,(2)}(t,\mathbf{p})+\cdots$$
$$=\mathrm{Tr}\Big\{e\int d^3\mathbf{q}\hat{A}_2(t_I,\mathbf{q})\hat{\rho}_I(\hat{\psi},\hat{\psi}^\dagger)$$
$$\times e^{-\int d^3\mathbf{q}\hat{A}_2(t_I,\mathbf{q})}\hat{\Phi}^\alpha(t,\mathbf{p})\Big\},$$
$$=\mathrm{Tr}\{\hat{\rho}_I(\hat{\psi}',\hat{\psi}'^\dagger)\hat{\Phi}^\alpha(t,\mathbf{p})\}.$$

Here the following notations are employed:

$$\hat{\psi}'=\cosh\theta_\mathbf{k}\hat{\psi}(\mathbf{k})-\exp(i\,\arg\varphi_\mathbf{k})\sinh\theta_\mathbf{k}\hat{\psi}^\dagger(-\mathbf{k}),$$
$$\hat{\psi}'^\dagger=\cosh\theta_\mathbf{k}\hat{\psi}^\dagger(\mathbf{k})-\exp(i\,\arg\varphi_\mathbf{k}^\dagger)\sinh\theta_\mathbf{k}\hat{\psi}(-\mathbf{k}),$$
$$\hat{A}_2(t_I,\mathbf{q})=Z^{-1}[\Delta\Phi^{(1)}(t_I,\mathbf{q})\hat{\psi}^\dagger(t_I,\mathbf{q})\hat{\psi}^\dagger(t_I,-\mathbf{q})$$
$$-\Delta\Phi^{\dagger(1)}(t_I,\mathbf{q})\hat{\psi}(t_I,-\mathbf{q})\hat{\psi}(t_I,\mathbf{q})],$$
$$\varphi_\mathbf{k}=Z^{-1}[\Delta\Phi^{(1)}(t_I,\mathbf{k})+\Delta\Phi^{(1)}(t_I,-\mathbf{k})],\theta_\mathbf{k}=|\varphi_\mathbf{k}|.$$

The angle $\theta_\mathbf{k}$ is nothing but the Bogoliubov angle, which is determined by requiring that $\Delta\Phi_i(t,\mathbf{p})$ is independent of t. As in the case of $\langle\hat{\psi}^\alpha\rangle$, this coincides with the condition of minimizing equilibrium free energy.

We summarize our findings of this section. On-shell expansion naturally changes the initial density matrix into

$$e^{C\hat{\psi}^\dagger-C^\dagger\hat{\psi}}\hat{\rho}_I e^{-C\hat{\psi}^\dagger+C^\dagger\hat{\psi}},\quad e^{\theta(\hat{\psi}^\dagger\hat{\psi}^\dagger-\hat{\psi}\hat{\psi})}\hat{\rho}_I e^{\theta(-\hat{\psi}^\dagger\hat{\psi}^\dagger+\hat{\psi}\hat{\psi})},$$

which causes the shift of the operator $\hat{\psi}$ of the initial state by c number $C^{(\dagger)}$ or the rotation of the pair field by the amount θ. It is our claim that $C^{(\dagger)}$ or θ can be obtained by the requirement that $\langle\hat{\psi}\rangle_t$ or $\langle\hat{\psi}\hat{\psi}\rangle_t$ be independent of t, which coincides with the value fixed by minimizing the equilibrium free energy. The above form of the transformed density matrix implies that the new state is constructed by adding an infinite number of the unstable modes present in the uncondensed state in a coherent way.

B. Symmetry breaking and Goldstone mode

When the symmetry of the Hamiltonian or the Lagrangian is broken by the ground state, the on-shell equation tells us about the existence of the Goldstone mode as an excited state and its explicit form of wave function. Since we are working in finite temperature, the symmetry breaking nature is characterized by the nonzero thermal expectation value of the symmetry breaking order parameter. We first discuss the problem in general terms. (For the special case, the problem has been discussed in Ref. [10].)

Let us assume that the field operator has several components denoted by $\hat{\phi}_n(x)$, $n=1,2,\ldots,N$, and suppose that the Hamiltonian or the Lagrangian density $L(\hat{\phi})\equiv L(\hat{\phi}_n(x),\partial_\mu\hat{\phi}_n(x))$, where $\partial_\mu=(\partial_0,\nabla)$, be invariant under a continuous global transformation of the field whose infinitesimal version is given as

$$\hat{\phi}_n(x)\rightarrow\hat{\phi}_n(x)+\sum_m a_{n,m}\hat{\phi}_m(x), \tag{4.27}$$

where $a_{n,m}$ is an infinitesimal transformation parameter independent of x. Consider the generating functional $W[J_1,J_2]$ defined by (2.4) and (2.5) with the operator $\hat{O}$ replaced by $\hat{\phi}_n(x)$ (with $t_I=-\infty$):

$$e^{(i/\hbar)W[J_1,J_2]}=\mathrm{Tr}\,\hat{K}^{J_1}\hat{\rho}_I(\hat{K}^{J_2})^\dagger \tag{4.28}$$

$$\hat{K}^{J_i}=\mathrm{T}\,\exp\left[-\frac{i}{\hbar}\int_{-\infty}^{\infty}dt\left(\hat{H}-\sum_n\int d^3\mathbf{x}\,J_{in}(x)\hat{\phi}_n(\mathbf{x})\right)\right]$$
$$(i=1,2). \tag{4.29}$$

Then $W[J_1,J_2]$ is invariant under

$$J_{in}(x)\rightarrow J_{in}(x)-\sum_m J_{im}(x)a_{m,n}\quad(i=1,2). \tag{4.30}$$

Therefore we have the relation

$$0=\sum_{i=1}^{2}\sum_{nm}\int d^4x\frac{\delta W}{\delta J_{in}(x)}J_{im}(x)a_{m,n}$$
$$=\sum_{i}\sum_{nm}\int d^4x(-1)^{i+1}\phi_{in}(x)J_{im}(x)a_{m,n}$$
$$=-\sum_{i}\sum_{nm}\int d^4x\frac{\delta\Gamma}{\delta\phi_{im}(x)}\phi_{in}(x)a_{m,n}. \tag{4.31}$$

We have used the relations (2.7) and (2.10). This expresses the symmetry of the Hamiltonian in terms of Γ. Now differentiate (4.31) with respect to $\phi_{1k}(y)$ and set $\phi_{1n}(x)=\phi_{2n}(x)$ to a symmetry breaking solution $\phi_n^{(0)}$, satisfying

$$\left.\frac{\delta\Gamma[\phi]}{\delta\phi_{1n}(x)}\right|_{\phi_{1n}(x)=\phi_{2n}(x)=\phi_n^{(0)}}=0. \tag{4.32}$$

We assume that $\phi_n^{(0)}$ is space-time independent. After making the substitution $x\leftrightarrow y$, we get

$$\int d^4y\sum_{m,l}[\Gamma^0_{1n,1m}(x,y)+\Gamma^0_{1n,2m}(x,y)]a_{m,l}\phi_l^{(0)}=0, \tag{4.33}$$

$$\Gamma^0_{in,jm}(x,y)\equiv\left(\frac{\delta^2\Gamma}{\delta\phi_{in}(x)\delta\phi_{jm}(y)}\right)_{\phi_1=\phi_2\equiv\phi^{(0)}}. \tag{4.34}$$

The equation (4.33) just takes the form of the on-shell equation (3.12). Since the integration $\int d^4y$ projects out $(\omega,\mathbf{k})=(0,\mathbf{0})$, it says that there is an excitation mode satisfying the dispersion relation $\omega(\mathbf{k}=0)=0$, as long as $\phi_n^{(0)}\neq 0$. This is the Goldstone mode $|G\rangle$ appearing as a consequence of the symmetry breaking with the wave function $\Delta\phi^{(1)}(x)=a_{n,m}\phi_m^{(0)}$ at four momentum $(\omega,\mathbf{k})=(0,\mathbf{0})$. See (3.39). Recall here that the above arguments are full order ones.

Let us study an example by taking the system of superfluid ^{4}He. The Hamiltonian (4.1) is invariant under the phase transformation

$$\hat{\psi}(x)\equiv(\hat{\psi}(x)^\dagger,\hat{\psi}(x))\rightarrow(\exp(-i\theta)\hat{\psi}(x)^\dagger,\exp(i\theta)\hat{\psi}(x))$$
$$\sim((1-i\theta)\hat{\psi}(x)^\dagger,(1+i\theta)\hat{\psi}(x)). \tag{4.35}$$

Therefore $a_{1,1}=-i\theta$, $a_{2,2}=i\theta$, $a_{1,2}=a_{2,1}=0$, and we see that the wave function of the Goldstone mode at four momentum in the space of $\phi^\alpha=(\phi^1,\phi^2)=(\hat{\psi}^\dagger,\hat{\psi})$ is proportional to $(-\phi^{(0)\dagger},\phi^{(0)})$. This is the wave function of the Goldstone mode corresponding to the symmetry (4.35). By putting $\mathbf{k}=0$ in the mode determining equation we can show, after some algebra, that $(\Delta\phi^\dagger(-k),\Delta\phi(k))=(-\phi^{(0)\dagger},\phi^{(0)})$ satisfies it if we set $k_0=0$ there. This is of course in accord with the Hugenholtz-Pines theorem [22].

We want to stress here again that we have started from the generating functional Γ, which preserves the symmetry of the Hamiltonian under (4.35) and we have done no further approximations. This leads automatically to the correct Goldstone spectrum in contrast to the literature [23], where some adjustments in the course of the calculation are needed.

Another example is the excitation spectrum in the case where the pairing occurs. As has been stated, there has been controversy [21] about the presence or the absence of the gap in the case of pairing condensation. But it is clear from our discussions that there is no gap in all orders of perturbation if the expansion parameter is invariant under the transformation (4.35). Here it is crucial that both $\langle\hat{\psi}^{(\dagger)}\rangle$ and $\langle\hat{\psi}^{(\dagger)}\hat{\psi}^{(\dagger)}\rangle$ have nonvanishing values as stationary solutions. This is in contrast with the case of the superconductor where $\langle\hat{\psi}^{(\dagger)}\rangle=0$ and the gap is present. See Ref. [24] for details.

ACKNOWLEDGMENT

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APPENDIX A: FORMULAS OF LEGENDRE TRANSFORMATION

Here several formulas of Legendre transformation are collected that are sufficient for the discussions in this paper. In the formulas below conjugate variables of Legendre transformation are denoted by J_i and ϕ_i. The index i represents all the attributes characterizing the variable including space-time coordinate x: $\phi_i=\phi_a(x)$, where the index a represents discrete degrees of freedom other than x. Therefore Σ_i implies actually $\int d^4x\Sigma_a$. Kronecker δ_{ij} signifies $\delta_{ab}\delta^4(x-y)$, where $\delta^4(x-y)$ is the four-dimensional Dirac δ function. For example, $\partial\phi_i/\partial\phi_j=\delta_{ij}$ implies the functional derivative $\delta\phi_a(x)/\delta\phi_b(y)=\delta_{ab}\delta^4(x-y)$. The summation convention is employed where the repeated index is summed or integrated over.

Legendre transformation between $W[J]$ and $\Gamma[\phi]$ is defined as follows:

$$\Gamma[\phi]=W[J]-J_i\frac{\partial W[J]}{\partial J_i}, \tag{A1}$$

where ϕ is defined by

$$\phi_i=\frac{\partial W[J]}{\partial J_i}. \tag{A2}$$

This is inverted to get

$$J_i=J_i[\phi], \tag{A3}$$

which is inserted into (A1). In this sense, Eq. (A1) is written more explicitly as

$$\Gamma[\phi]=W[J[\phi]]-J_i[\phi]\phi_i. \tag{A4}$$

1. Conjugate relation

Differentiating (A4) by ϕ_j,

$$\frac{\partial\Gamma[\phi]}{\partial\phi_j}=\frac{\partial W[J]}{\partial J_i}\frac{\partial J_i}{\partial\phi_j}-\frac{\partial J_i}{\partial\phi_j}\phi_i-J_j. \tag{A5}$$

By (A2), we get

$$\frac{\partial\Gamma[\phi]}{\partial\phi_i}=-J_i \quad \text{or} \quad \Gamma_i^{(1)}[\phi]=-J_i . \tag{A6}$$

2. Inverse matrix relation

Differentiating (A2) with respect to ϕ_j we have, using (A6),

$$\delta_{ij}=\frac{\partial\phi_i}{\partial\phi_j}=\frac{\partial^2 W[J]}{\partial J_i\partial J_k}\frac{\partial J_k}{\partial\phi_j}=-\frac{\partial^2 W[J]}{\partial J_i\partial J_k}\frac{\partial^2\Gamma[\phi]}{\partial\phi_k\partial\phi_j}. \tag{A7}$$

We write this relation briefly as

$$W_{ik}^{(2)}\Gamma_{kj}^{(2)}=\Gamma_{ik}^{(2)}W_{kj}^{(2)}=-\delta_{ij} . \tag{A8}$$

The first equality is obtained by either noting that $\Gamma^{(2)}$ and $W^{(2)}$ are a symmetric matrix or by differentiating (A6) by J_j .

3. Differentiation by spectator parameter

Let α_a be some parameter that is regarded as a constant (a spectator) when we make the Legendre transformation. Then the inverse process (A2) through (A3) is written more explicitly as

$$\phi_i=\frac{\partial W[J,\alpha]}{\partial J_i}=\phi_i[J,\alpha] \tag{A9}$$

$$\rightarrow J_i=J_i[\phi,\alpha]. \tag{A10}$$

Now we take the derivative of $\Gamma[\phi,\alpha]$ by α_a with ϕ fixed. This is easily done as follows:

$$\Gamma[\phi,\alpha]=W[J[\phi,\alpha],\alpha]-J_i[\phi,\alpha]\phi_i , \tag{A11}$$

$$\frac{\partial\Gamma[\phi,\alpha]}{\partial\alpha_a}=\frac{\partial W[J,\alpha]}{\partial\alpha_a}+\frac{\partial W[J,\alpha]}{\partial J_i}\frac{\partial J_i[\phi,\alpha]}{\partial\alpha_a} -\frac{\partial J_i[\phi,\alpha]}{\partial\alpha_a}\phi_i . \tag{A12}$$

Thus we get

$$\frac{\partial\Gamma[\phi,\alpha]}{\partial\alpha_a}=\frac{\partial W[J,\alpha]}{\partial\alpha_a}. \tag{A13}$$

Higher derivatives are obtained straightforwardly by (A13).

APPENDIX B: IDENTITIES OF THE SECOND DERIVATIVES OF $W[J_1,J_2]$ AND $\Gamma[\phi_1,\phi_2]$

We take a field theoretical system and use the notation $x=(t,\mathbf{x})$. In order to make the formulas explicit, we write the x dependence separately in this appendix. In the following the repeated Roman index is summed over 1 and 2, while the repeated space-time variable is integrated as $\int_{-\infty}^{\infty}d^4x$. The following ways of writing are adopted below:

$$W_{i_1 i_2\cdots i_n}^{(n)}(x_1,x_2,\ldots,x_n)\equiv\frac{\delta^n W}{\delta J_{i_1}(x_1)\,\delta J_{i_2}(x_2)\cdots\delta J_{i_n}(x_n)}, \tag{B1}$$

and similarly for Γ. For $J_1=J_2$ we introduce a special notation defined by the superscript J as follows:

$$W_{i_1 i_2\cdots i_n}^{(n)J}(x_1,x_2,\ldots,x_n) \equiv(W_{i_1 i_2\cdots i_n}^{(n)}(x_1,x_2,\ldots,x_n))_{J_1(x)=J_2(x)=J(x)} . \tag{B2}$$

For Γ we use also superscript J but it implies that it is evaluated at the value of $\phi_i(x)$ satisfying (2.14). The superscript 0 then implies the stationary value $\phi_i^{(0)}(x)$ $\phi_i(x)$ corresponding to $J_1=J_2=0$, for example,

$$\Gamma_{i_1 i_2\cdots i_n}^{(n)0}(x_1,x_2,\ldots,x_n) \equiv(\Gamma_{i_1 i_2\cdots i_n}^{(n)}(x_1,x_2,\ldots,x_n))_{\phi_1(x)=\phi_2(x)=\phi^{(0)}(x)} . \tag{B3}$$

We first note two important identities:

$$\Gamma_{ij}^{(2)}(x,y)(-1)^{i+j}W_{j,k}^{(2)}(y,z)=W_{i,j}^{(2)}(x,y)(-1)^{i+j}\Gamma_{j,k}^{(2)}(y,z) =-\delta_{ik}\delta^4(x-z), \tag{B4}$$

$$\sum_{i,j=1,2} W_{i,j}^{(2)J}(x,y)=0. \tag{B5}$$

The first identity is obtained by differentiating (2.10) by $\phi_j(z)$ and is an example of the formula (A7). The second one is a consequence of the definition of $W[J_1,J_2]$ given in (2.4). In order to see this, let us take the derivative of (2.7) with respect to J, keeping in mind the form (2.4):

$$W_{11}^{(2)J}(x,y)=\frac{i}{\hbar}\langle \mathrm{T}\hat{O}(x)\hat{O}(y)\rangle,$$

$$W_{12}^{(2)J}(x,y)=-\frac{i}{\hbar}\langle \hat{O}(y)\hat{O}(x)\rangle, \tag{B6}$$

$$W_{21}^{(2)J}(x,y)=-\frac{i}{\hbar}\langle \hat{O}(x)\hat{O}(y)\rangle,$$

$$W_{22}^{(2)J}(x,y)=\frac{i}{\hbar}\langle \tilde{\mathrm{T}}\hat{O}(x)\hat{O}(y)\rangle. \tag{B7}$$

Here $\tilde{\mathrm{T}}$ denotes the antitime ordering and $\hat{O}(x)$ is the Heisenberg operator defined by

$$\hat{O}(x)=\hat{U}^{\dagger}(t,t_I)\hat{O}(t=0,\mathbf{x})\hat{U}(t,t_I),$$

where $\hat{U}(t,t_I)$ is given in (2.3) and the expectation value is defined by $\langle\rangle\equiv\mathrm{Tr}\hat{\rho}_I\cdots$. Because the sum of the above four equations is identically zero owing to the definition of T and $\tilde{T}$, Eq. (B5) follows.

We consider next the relations for the retarded Green's function. Take $i=k=1$ in (B4), then

$$\Gamma_{1,j}^{(2)}(x,y)(-1)^j W_{j,1}^{(2)}(y,z)=W_{1,j}^{(2)}(x,y)(-1)^j\Gamma_{j,1}^{(2)}(y,z) =\delta^4(x-z). \tag{B8}$$

Here we use (B4) and (B5) to rewrite (B8) in the form

$$(\Gamma_{1,1}^{(2)J}(x,y)+\Gamma_{1,2}^{(2)J}(x,y))(W_{1,1}^{(2)J}(y,z)+W_{1,2}^{(2)J}(y,z)) = -\delta^4(x-z). \tag{B9}$$

But we note the relation

$$W_{1,1}^{(2)J}(y,z)+W_{1,2}^{(2)J}(y,z)=\frac{i}{\hbar}\{\langle \mathrm{T}\hat{O}(y)\hat{O}(z)\rangle-\langle\hat{O}(z)\hat{O}(y)\rangle\} = \frac{i}{\hbar}\theta(y^0-z^0)\langle[\hat{O}(y),\hat{O}(z)]\rangle. \tag{B10}$$

Therefore $\Sigma_j\Gamma_{1,j}^{(2)J}(x,y)$ is the inverse of the retarded Green's function.

A more general proof of the identity (B5) is as follows. By this technique we can derive various identities. For this purpose let us put $J_1(x)=J_2(x)\equiv J(x)$ in (2.7). Since $\phi_1(x)=\phi_2(x)\equiv\phi(x)$ in this case, we have the identity

$$\left(\frac{\delta W[J_1,J_2]}{\delta J_1(x)}\right)_{J_1(x)=J_2(x)\equiv J(x)}+\left(\frac{\delta W[J_1,J_2]}{\delta J_2(x)}\right)_{J_1(x)=J_2(x)\equiv J(x)}=0. \tag{B11}$$

Differentiating (B11) by $J(y)$ we get (B5). Further differentiation leads to various correlation equalities.

Now the same process is applied to Γ. Setting $\phi_1(x)=\phi_2(x)=\phi(x)$ in (2.10), we have the following identity:

$$\left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\right)_{\phi_1(x)=\phi_2(x)\equiv\phi(x)} +\left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_2(x)}\right)_{\phi_1(x)=\phi_2(x)\equiv\phi(x)}=0. \tag{B12}$$

Let us differentiate (B12) by $\phi(y)$, then we obtain an analog of (B5):

$$\sum_{i,j=1,2}\Gamma_{i,j}^{(2)J}(x,y)=0. \tag{B13}$$

Using (B4), (B8), and (B13), another identity analogous to (B9) is obtained:

$$(W_{1,1}^{(2)J}(x,y)+W_{1,2}^{(2)J}(x,y))(\Gamma_{1,1}^{(2)J}(y,z)+\Gamma_{1,2}^{(2)J}(y,z)) = -\delta^4(x-z). \tag{B14}$$

APPENDIX C: EXPANSION OF W OR Γ IN POWERS OF $J^{(-)}$ OR $\phi^{(-)}$—RELATION WITH EQUILIBRIUM FREE ENERGY

Let us define $W[J_1,J_2,J_3]$ by introducing another source J_3 in the imaginary time path:

$$e^{(i/\hbar)W[J_1,J_2,J_3]}=\mathrm{Tr}\{\hat{U}_{J_1}\hat{\rho}_I^{J_3}\hat{U}_{J_2}^{\dagger}\}, \tag{C1}$$

$$\hat{\rho}_I^{J_3}=\mathrm{T}_\tau\exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\{\hat{H}-J_3(\tau)\hat{O}\}\right), \tag{C2}$$

where T_τ implies the τ ordering and we suppress the space coordinate that is defined in (2.5). The corresponding Γ is also defined as follows:

$$\Gamma[\phi_1,\phi_2,\phi_3]=W[J_1,J_2,J_3]-\int_{t_I}^{\infty}dtJ_1(t)\phi_1(t) +\int_{t_I}^{\infty}dtJ_2(t)\phi_2(t)-\frac{1}{i}\int_0^{\hbar\beta}d\tau J_3(\tau)\phi_3(\tau). \tag{C3}$$

Here we have introduced

$$\frac{\delta W}{\delta J_i(t)}=(-)^{i+1}\phi_i\quad(i=1,2),\qquad\frac{\delta W}{\delta J_3(\tau)}=\frac{1}{i}\phi_3(\tau). \tag{C4}$$

The following change of variables is performed at this point:

$$J^{(+)}=\tfrac{1}{2}(J_1+J_2),\qquad J^{(-)}=J_1-J_2 \tag{C5}$$

or equivalently

$$J_1=J^{(+)}+\tfrac{1}{2}J^{(-)},\qquad J_2=J^{(+)}-\tfrac{1}{2}J^{(-)}. \tag{C6}$$

We have the same relations for $\phi^{(+)}$ and $\phi^{(-)}$. In the following we consider $W[J^{(+)},J^{(-)},J_3]$ and $\Gamma[\phi^{(+)},\phi^{(-)},\phi_3]$. It is easy to get the following relations:

$$\frac{\delta W}{\delta J^{(-)}(t)}=\phi^{(+)}(t),\qquad\frac{\delta W}{\delta J^{(+)}(t)}=\phi^{(-)}(t), \tag{C7}$$

$$J_1\phi_1-J_2\phi_2=J^{(+)}\phi^{(-)}+J^{(-)}\phi^{(+)}.$$

Thus we can write

$$\Gamma[\phi^{(+)},\phi^{(-)},\phi_3]=W-\int_{t_I}^{\infty}dtJ^{(+)}(t)\frac{\delta W}{\delta J^{(+)}(t)} -\int_{t_I}^{\infty}dtJ^{(-)}(t)\frac{\delta W}{\delta J^{(-)}(t)} -\int_0^{\hbar\beta}d\tau J_3(\tau)\frac{\delta W}{\delta J_3(\tau)}.$$

Now we expand W or Γ in powers of $J^{(-)}$ or $\phi^{(-)}$. Since these variables are unphysical ones being set to zero in the end, we need an expansion coefficient that is linear in $J^{(-)}$ or $\phi^{(-)}$ in practical problems. Then the following equation is obtained easily:

$$W[J^{(+)},J^{(-)}=0,\,J_3]=W_\beta[J_3]. \tag{C8}$$

Here $W_\beta[J_3]$ is related to the imaginary time free energy as

$$W_\beta[J_3]=\frac{\hbar}{i}\ln\mathrm{Tr}\hat{\rho}_I^{J_3}.$$

But together with (C8), the second equation of (C7) tells us that

$$\phi^{(-)}\to 0 \quad \text{as} \quad J^{(-)}\to 0.$$

On the other hand, the identity of the Legendre transformation

$$\frac{\delta\Gamma}{\delta\phi^{(+)}(t)}=-J^{(-)}(t)$$

implies that in the above limit Γ loses the dependence on $\phi^{(+)}$. Thus when $J^{(-)}\to 0$, we have a second imaginary time free energy;

$$\Gamma[\phi^{(+)},\phi^{(-)}=0,\phi_3] = W_\beta[J_3]-\int_0^{\hbar\beta}d\tau J_3(\tau)\frac{\delta W_\beta[J_3]}{\delta J_3(\tau)} = \Gamma_\beta[\phi_3]. \tag{C9}$$

Consider next the linear term in $J^{(-)}$ or $\phi^{(-)}$. By definition

$$\frac{\delta W}{\delta J^{(-)}(t)}\bigg|_{J^{(-)}=0}=\phi^{(+)}(t)\bigg|_{J^{(-)}=0},$$

$$\frac{\delta \Gamma}{\delta \phi^{(-)}(t)}\bigg|_{\phi^{(-)}=0}=-J^{(+)}(t)\bigg|_{\phi^{(-)}=0},$$

so that the following dual forms are obtained:

$$W[J^{(+)},J^{(-)},J_3]=W_\beta[J_3]+\int_{t_I}^{\infty}dt J^{(-)}(t)\phi^{(+)}(t) +O[(J^{(-)})^2], \tag{C10}$$

$$\Gamma[\phi^{(+)},\phi^{(-)},\phi_3]=\Gamma_\beta[\phi_3]-\int_{t_I}^{\infty}dt \phi^{(-)}(t)J^{(+)}(t) +O[(\phi^{(-)})^2], \tag{C11}$$

where on the right-hand side of these equations, $\phi^{(+)}(t)$ or $J^{(+)}(t)$ is actually

$$\phi^{(+)}(t)=\phi^{(+)}(J^{(-)}=0,J^{(+)},J_3;t),$$

$$J^{(+)}(t)=J^{(+)}(\phi^{(-)}=0,\phi^{(+)},\phi_3;t).$$

It can be shown that the expansion coefficients of higher orders are expressed by the multiple retarded anticommutators of the operator $\hat{O}$. On the other hand, the Tailor expansion in terms of $\phi^{(+)}$ brings about the multiple retarded commutator, which has a real physical meaning and will be reproduced in Sec. III and Sec. IV A. See also Ref. [10].

We have seen that in the limit when $J^{(-)}$ or $\phi^{(-)}$ goes to zero the imaginary time free energy is reproduced. But another important limit exists where the equilibrium free energy is recovered. This is the case when

$$\phi_1(t)=\phi_2(t)=\phi_3(\tau)=\text{const},$$

i.e.,

$$\phi^{(+)}(t)=\phi_3(\tau)\equiv\phi=\text{const}\times\phi^{(-)}(t)=0.$$

Obviously the above relation is transformed to that of J variables as follows;

$$J_1(t)=J_2(t)=J_3(\tau)=\text{const}',$$

i.e.,

$$J^{(+)}(t)=J_3(\tau)\equiv J=\text{const}'\times J^{(-)}(t)=0.$$

Thus we get

$$J^{(+)}(\phi^{(-)}=0,\phi^{(+)}=\phi_3\equiv\phi)=J_3(\phi^{(-)}=0,\phi^{(+)}=\phi_3\equiv\phi) =-i\frac{\delta\Gamma_\beta[\phi]}{\delta\phi}. \tag{C12}$$

In this way we arrive at

$$\frac{\delta\Gamma}{\delta\phi^{(-)}(t)}\bigg|_{\phi^{(-)}=0,\phi^{(+)}=\phi_3=\phi}=i\frac{\delta\Gamma_\beta[\phi]}{\delta\phi}. \tag{C13}$$

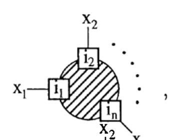
The corresponding obvious equation for W is

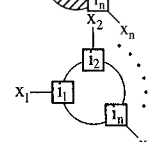
$$\frac{\delta W}{\delta J^{(-)}(t)}\bigg|_{J^{(-)}=0,J^{(+)}=J_3=J}=i\frac{\delta W_\beta}{\delta J}. \tag{C14}$$

In Sec. III, we discuss the on-shell expansion of Γ, which is the expansion of $[\delta\Gamma/\delta\phi^{(-)}(t)]|_{\phi^{(-)}=0}$ in powers of $\phi^{(+)}$. We will see that the multiple retarded commutator emerges and the expansion relates two different density matrices corresponding to condensed or uncondensed ground state.

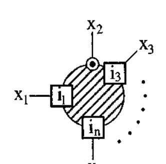
APPENDIX D: SOLUTION OF ON-SHELL EXPANSION

Here the solutions of higher orders of the on-shell expansion (3.23), etc. are studied and (3.25) is derived. For this purpose the graphical notations are introduced.

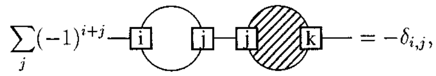
$W^{(n)J}_{i_1 i_2\cdots i_n}(x_1,x_2,\ldots,x_n) =$  , (D1)

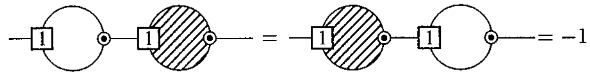
$\Gamma^{(n)J}_{i_1 i_2\cdots i_n}(x_1,x_2,\ldots,x_n) =$  . (D2)

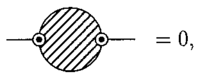
If the vertex is summed over $i_2=1,2$, then we denote it as, for example,

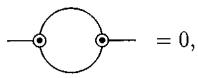
$\sum_{i_2=1,2} W^{(n)J}_{i_1 i_2\cdots i_n}(x_1,x_2,\ldots,x_n) =$  . (D3)

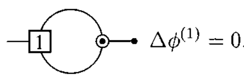
With this notation, (B4), (B9), (B5), (B13), (B14), and (3.12) are represented as

(B.4) 

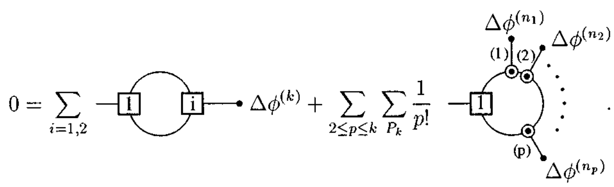
(B.9), (B.14) 

(B.5) 

(B.13) 

(3.12) 

Looking at (3.24), we can write $\Delta\phi^{(k)}(x)$ for general k as follows:



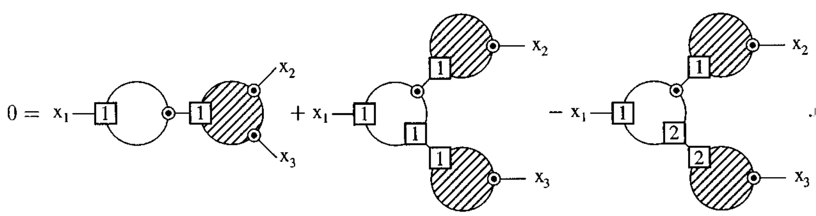
(D4)

In the above equation, the summation is taken in the following way. First we divide k points into p groups with n_α (with $\alpha=1,2,\ldots,p$) points contained in αth group $(n_\alpha \geqslant 1)$. Thus $\Sigma_{\alpha=1\sim p} n_\alpha = k$. Σ_{P_k} implies the sum over all possible grouping of k points into p groups and the sum over all possible n_α satisfying $\Sigma_{\alpha=1\sim p} n_\alpha = k$. Finally we sum over p of course.

Now apply $\delta/\delta J_1(x) + \delta/\delta J_2(x)$ to (B9). When it operates on the functional of ϕ, we have to use the chain differentiation rule:

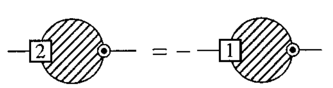
$$\frac{\delta}{\delta J_i(x)} = \frac{\delta\phi_j(y)}{\delta J_i(x)} \frac{\delta}{\delta\phi_j(y)} = (-1)^{j+1} \frac{\delta^2 W}{\delta J_i(x)\,\delta J_j(y)} \frac{\delta}{\delta\phi_j(y)}.$$

Thus we get, after renaming of the space-time points,



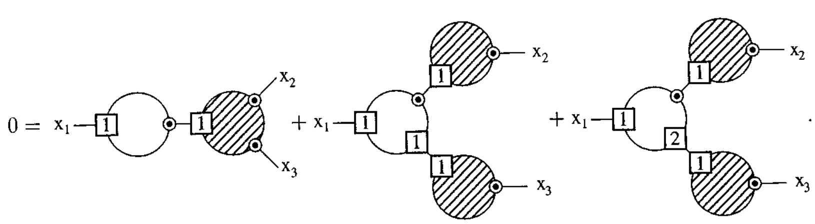
(D5)

Here we insert into (D5) the following relation obtained by rewriting (B5):



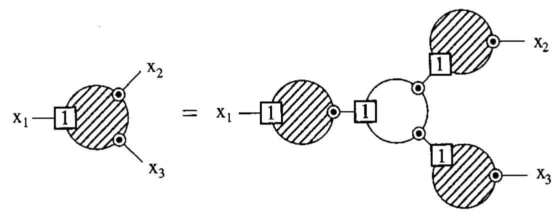
(D6)

In this way (D5) is further transformed as

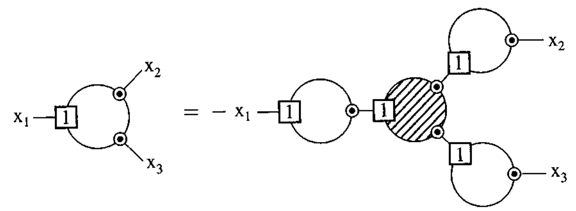


(D7)

From (D7) and (B14), the following two equations are obtained:

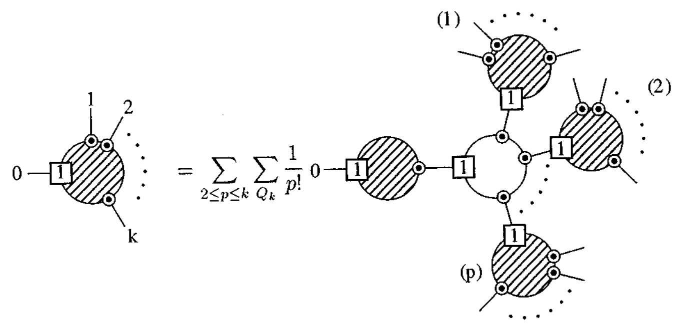


(D8)



(D9)

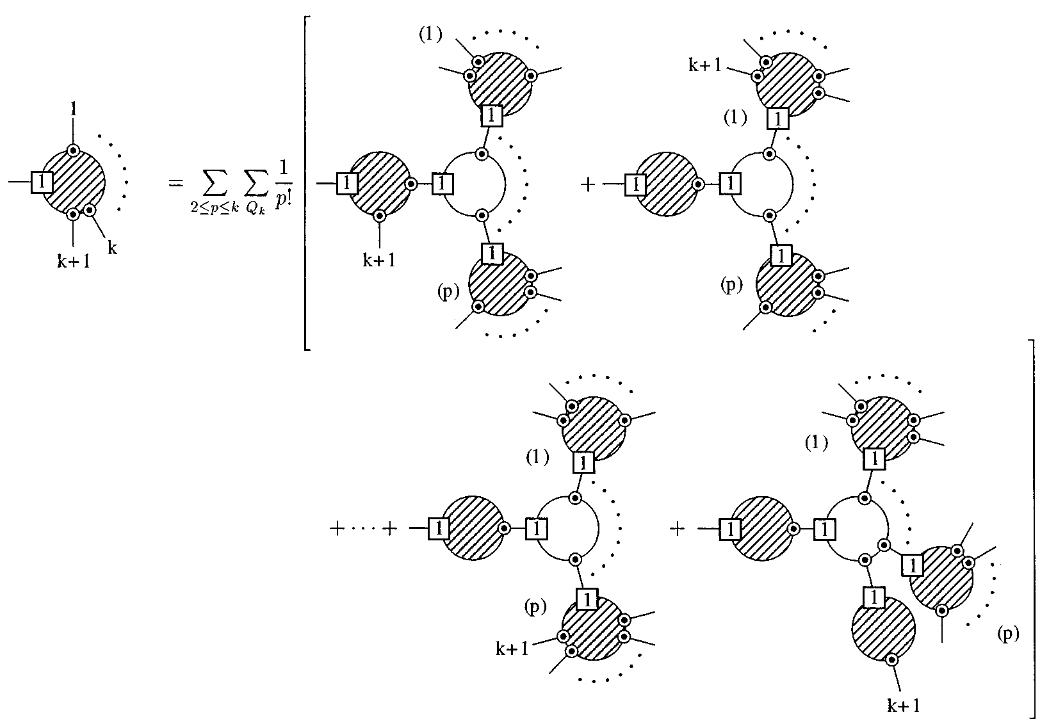
The relation (D8) suggests the general formula for $k \geqslant 2$ as represented in the following equation:



(D10)

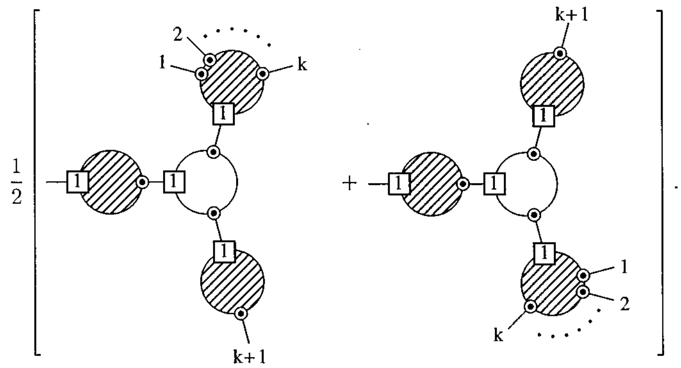
Here Σ_{Q_k} implies the following process. k points are divided into p groups with n_α points satisfying $\Sigma_{\alpha=1\sim p} n_\alpha = k$, and $1 \sim k$ external legs are distributed to these groups. Finally we sum over all possible ways in these processes. It should be remarked that $1\sim k$ legs are assumed to be distinguishable in these processes. This is different from the summation Σ_{P_k}.

The proof of (D10) can be done by a mathematical induction. Outline of the proof runs as follows: Assume (D10) is correct for k and apply again $\delta/\delta J_1(x) + \delta/\delta J_2(x)$ on both sides of (D10). Then we get



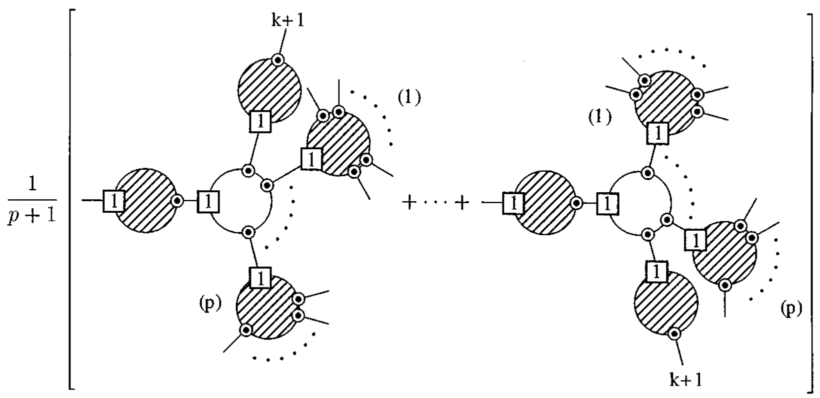
(D11)

Let us rewrite the first term of (D11) by applying (D8) to the part involving index $(k+1)$. After that we can use the assumption of the induction. As a result the first term is transformed into



(D12)

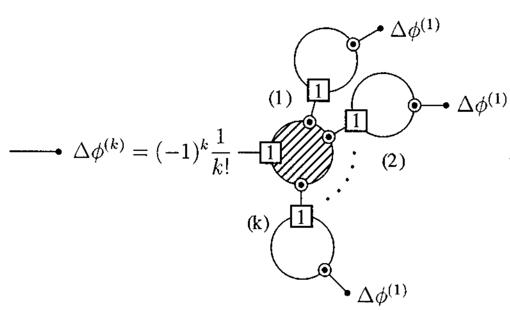
Here we have used the obvious symmetry character of $\Gamma^{(3)}$. Also by the symmetry of $\Gamma^{(p)}$ the last term of (D11) is rewritten as



(D13)

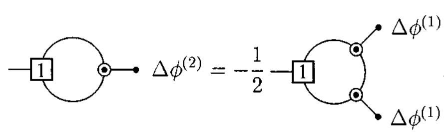
Collecting these observations, we see that (D10) holds for $k+1$.

Now we are in a position to prove the following general formula for $\Delta\phi^{(k)}$ as shown in (D14);



(D14)

Consider first the case $k=2$. The relation (3.23) is written graphically as follows:

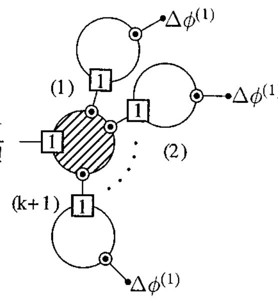


(D15)

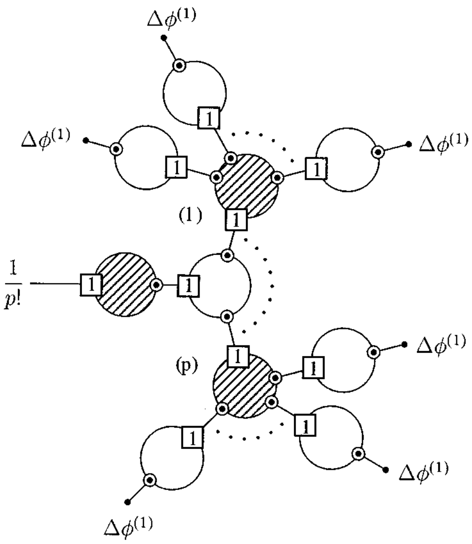
Therefore, by using (D9) and (B14), we first get the $k=2$ version of (D14) plus a term proportional to $\Delta\phi^{(1)}$, which satisfies a homogeneous equation (3.12). However, we are finally interested in the sum $\Delta\phi^{(1)}+\Delta\phi^{(2)}+\cdots+\Delta\phi^{(n)}+\cdots$ and for the sum it can be absorbed by the redefinition of the scale of $\Delta\phi^{(1)}$. Therefore we neglect such a term in the solution of $\Delta\phi^{(k)}$.

The general proof is again due to the mathematical induction; assume (D14) is correct for k. Then using (D10), the right-hand side of (D14) for $k+1$ is transformed as follows:

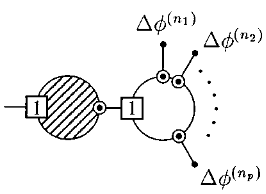
$$(\text{right-hand side})_{k+1} = \frac{(-1)^{k+1}}{(k+1)!}$$



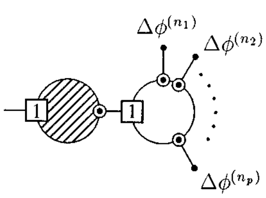
$$= \frac{(-1)^{k+1}}{(k+1)!} \sum_{2\le p\le k+1} \sum_{Q_{k+1}} \frac{1}{p!}$$



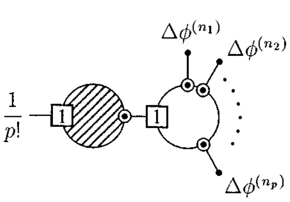
$$= \frac{(-1)^{k+1}}{(k+1)!} \sum_{2\le p\le k+1} \sum_{Q_{k+1}} \frac{1}{p!}(-1)^{n_1+n_2+\cdots+n_p} n_1!n_2!\cdots n_p!$$



$$= \frac{(-1)^{k+1}}{(k+1)!} \sum_{2\le p\le k+1} \sum_{P_{k+1}} \frac{(-1)^{k+1}(k+1)!}{n_1!n_2!\cdots n_p!}\frac{1}{p!} n_1!n_2!\cdots n_n!$$



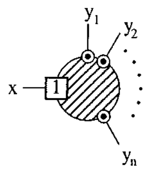
$$= \sum_{2\le p\le k+1} \sum_{P_{k+1}} \frac{1}{p!}$$



$= \longrightarrow\!\bullet\ \Delta\phi^{(k+1)}$.

Here in the last equality we have used (D4).

Finally the following formula is proved, which expresses $W^{(n+1)0}_{1,i_1 i_2\cdots i_n}(x,y_1,y_2,\ldots,y_n)$ in the operator form. It is given by the multiple retarded Green's function,



$$= \left(\frac{i}{\hbar}\right)^n \sum_{P\{y_1,y_2,\cdots,y_n\}} \theta(t_x, t_{y_1}, t_{y_2}, \ldots, t_{y_n}) \times \langle [\cdots[[\hat{\phi}(x), \hat{\phi}(y_1)], \hat{\phi}(y_2)], \ldots, \hat{\phi}(y_n)] \rangle, \tag{D16}$$

where we have defined

$$\theta(t_x, t_{y_1}, t_{y_2}, \ldots, t_{y_n}) = \theta(t_x - t_{y_1})(t_{y_1} - t_{y_2}) \cdots \theta(t_{y_{n-1}} - t_{y_n}), \tag{D17}$$

and $\Sigma_{P_{\{y_1,y_2,\ldots,y_n\}}}$ signifies the sum over all possible permutations of $\{y_1, y_2, \ldots, y_n\}$. We will write in the following

$$\sum_{P_{\{y_1,y_2,\ldots,y_n\}}} \theta(t_x, t_{y_1}, t_{y_2}, \ldots, t_{y_n}) \times [\cdots[[\hat{\phi}(x), \hat{\phi}(y_1)], \hat{\phi}(y_2)], \cdots \hat{\phi}(y_n)] \equiv R(\hat{\phi}(x), \hat{\phi}(y_1), \hat{\phi}(y_2), \ldots, \hat{\phi}(y_n)). \tag{D18}$$

The proof of (D16) is rather trivial. [For $n=1$ it has already been derived in (B10).] As for general n, consider the equation

$$(W_1^{(1)}(x))_{J_1=J_2=J} = \langle (\hat{U}_J)^\dagger \hat{\phi}(x) \hat{U}_J \rangle. \tag{D19}$$

$W^{(n+1)0}_{1,i_1 i_2 \cdots i_n}(x, y_1, y_2, \ldots, y_n)$ is obtained by differentiating (D19) through $J(y_1), J(y_2), \ldots, J(y_n)$ and taking $J=0$. Assume $t_1 \geqslant t_2 \geqslant \cdots \geqslant t_n$ (every t_i is smaller than $x^0 = t$ of course) and operator $\delta/\delta J(y_1)$. It operates on both $\hat{U}_J$ and $(\hat{U}_J)^\dagger$, producing the commutator $[\hat{\phi}(x), \hat{\phi}(y_1)]$. Because of the assumed time ordering, further application of $\delta/\delta J(y_2)$ brings about the commutator of the above commutator and $\hat{\phi}(y_2)$, etc. For general time ordering, we have only to supply the factor $\theta(t_x, t_{y_1}, t_{y_2}, \ldots, t_{y_n})$ and sum over all possible combinations of the ordering. This proves (D16).

APPENDIX E: FEYNMAN RULE OF NON-HERMITE FIELD—PERTURBATIVE RULE FOR W IN NORMAL CASE

The nonequilibrium Feynman rule of $W[J]$ in the normal case has been derived in [14] using the path-integral technique. Since for the normal case the Feynman rule is compactly given, we present it here. It is used in Sec. IV A 2. In Ref. [14] the initial density matrix is assumed to be of the equilibrium canonical form. The rule is slightly different for the Hermite and the non-Hermite field and we have to use the results of the latter for the ^{4}He Hamiltonian (4.1). The source term is inserted as in (4.3) and using (4.5), the expectation value is given, for example, by

$$\phi(x) = \langle \hat{\psi}(x) \rangle = \left.\frac{\delta W[J]}{\delta J_1(x)}\right|_{J_1=J_2=0, \bar{J}_1=\bar{J}_2=0} = -\left.\frac{\delta W[J]}{\delta J_2(x)}\right|_{J_1=J_2=0, \bar{J}_1=\bar{J}_2=0}. \tag{E1}$$

Let us introduce $(\pm)$ variables as in (C5) and the same for ψ and ϕ. Since the dependence on $J^{(-)}$ is essential, we assume $J^{(+)}=0$ but the recovery of nonvanishing $J^{(+)}$ is easy. Then, writing $\hbar\omega_{\mathbf{k}} = (\hbar^2\mathbf{k}^2/2m) - \mu$ and understanding that all the $\phi^{(\dagger)}$'s are set to zero in the end (normal case), the formula is expressed as [14]

$$\exp\frac{i}{\hbar}W[J] = \prod_{\mathbf{k}} f_\beta(\omega_{\mathbf{k}}) e^{\beta\hbar\omega_{\mathbf{k}}} \exp S_0 \times \exp\left(-\frac{i}{\hbar}\int_C dt V(\psi(t), \psi^\dagger(t))\right)\Bigg|_{\psi=\psi^\dagger=0}. \tag{E2}$$

Here V is given by the interaction part of the Hamiltonian (4.1):

$$V(\hat{\psi}(t), \hat{\psi}^\dagger(t)) \equiv \frac{1}{2}\int d^3\mathbf{x}\, d^3\mathbf{y}\, \hat{\psi}^\dagger(t,\mathbf{x}) \hat{\psi}^\dagger(t,\mathbf{y}) \times U_0(\mathbf{x}-\mathbf{y}) \hat{\psi}(t,\mathbf{y}) \hat{\psi}(t,\mathbf{x}). \tag{E3}$$

If we write explicitly

$$\frac{i}{\hbar}\int_C dt V(\psi(t), \psi^\dagger(t)) = \frac{i}{\hbar}\int_{t_I}^\infty dt V(\psi_1(t), \psi_1^\dagger(t)) - \frac{i}{\hbar}\int_{t_I}^\infty dt V(\psi_2(t), \psi_2^\dagger(t)) + \frac{1}{\hbar}\int_0^{\hbar\beta} d\tau V(\psi_3(\tau), \psi_3^\dagger(\tau)). \tag{E4}$$

S_0 is the differential operator, which is written by the variables $\psi^{(\dagger)(\pm)}$ and $\psi_3 \equiv \psi$ as follows:

$$S_0=\int\int dt\,ds\,d^3\mathbf{x}\,d^3\mathbf{y}\left(\frac{\delta}{\delta\psi^{(+)}(x)}+\frac{i}{\hbar}\overline{J^{(-)}}(x)\right)\Delta_R(x-y)\frac{\delta}{\delta\psi^{(-)\dagger}(x)}$$
$$+\int\int dt\,ds\,d^3\mathbf{x}\,d^3\mathbf{y}\frac{\delta}{\delta\psi^{(-)}(x)}\Delta_A(x-y)\left(\frac{\delta}{\delta\psi^{(+)\dagger}(y)}+\frac{i}{\hbar}J^{(-)}(y)\right)$$
$$+\int\int dt\,ds\,d^3\mathbf{x}\,d^3\mathbf{y}\left(\frac{\delta}{\delta\psi^{(+)}(x)}+\frac{i}{\hbar}\overline{J^{(-)}}(x)\right)\overline{\Delta}(x-y)\left(\frac{\delta}{\delta\psi^{(+)\dagger}(y)}+\frac{i}{\hbar}J^{(-)}(y)\right)$$
$$+\int\int ds\,d\tau\,d^3\mathbf{x}\,d^3\mathbf{y}\frac{\delta}{\delta\psi(\tau,\mathbf{x})}\overline{G^{(+)}}(\tau,\mathbf{x};y)\left(\frac{\delta}{\delta\psi^{(+)\dagger}(y)}+\frac{i}{\hbar}J^{(-)}(y)\right)$$
$$+\int\int dt\,d\tau\,d^3\mathbf{x}\,d^3\mathbf{y}\left(\frac{\delta}{\delta\psi^{(+)}(x)}+\frac{i}{\hbar}\overline{J^{(-)}}(x)\right)\overline{G^{(-)}}(x;\tau,\mathbf{y})\frac{\delta}{\delta\psi^{\dagger}(\tau,\mathbf{y})}$$
$$+\int\int d\tau\,d\tau'\,d^3\mathbf{x}\,d^3\mathbf{y}\frac{\delta}{\delta\psi(\tau,\mathbf{x})}\overline{D(}\tau,\mathbf{x};\tau',\mathbf{y})\frac{\delta}{\delta\psi^{\dagger}(\tau',\mathbf{y})}. \qquad \text{(E5)}$$

Here the notation $x=(t,\mathbf{x}),y=(s,\mathbf{y})$ is used. There are six kinds of propagators and it should be noticed that $\phi^{(-)}$ is connected only to $\phi^{(+)}$ and not to $\phi^{(-)}$ or ϕ_3. The propagators are given by

$$\Delta_R(x-y)=\theta(t-s)\int\frac{d^3\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-i\omega_{\mathbf{k}}(t-s)},$$

$$\Delta_A(x-y)=-\theta(s-t)\int\frac{d^3\mathbf{k}}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-i\omega_{\mathbf{k}}(t-s)},$$

$$\overline{\Delta}(x-y)=\int\frac{d^3\mathbf{k}}{(2\pi)^3}\left(f_\beta(\omega_k)+\frac{1}{2}\right)e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-i\omega_{\mathbf{k}}(t-s)},$$

$$\overline{G^{(+)}}(\tau,\mathbf{x};t,\mathbf{y})=\int\frac{d^3\mathbf{k}}{(2\pi)^3}[f_\beta(\omega_{\mathbf{k}})+1]\times e^{-\omega_{\mathbf{k}}\tau}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})+i\omega_{\mathbf{k}}(t-t_I)},$$

$$\overline{G^{(-)}}(x;\tau,\mathbf{y})=\int\frac{d^3\mathbf{k}}{(2\pi)^3}f_\beta(\omega_{\mathbf{k}})e^{\omega_{\mathbf{k}}\tau}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-i\omega_{\mathbf{k}}(t-t_I)},$$

$$D(\tau,\mathbf{x};\tau',\mathbf{y})=\int\frac{d^3\mathbf{k}}{(2\pi)^3}f_\beta(\omega_{\mathbf{k}})e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}e^{-\omega_{\mathbf{k}}(\tau-\tau'-\beta\hbar/2)}\times\{\theta(\tau-\tau')e^{\omega_{\mathbf{k}}\beta\hbar/2}+\theta(\tau'-\tau)e^{-\omega_{\mathbf{k}}\beta\hbar/2}\}.$$

The expectation value of any operator of normal ordered form $\hat{O}(\hat{\psi}^\dagger,\hat{\psi})$ can be calculated by an appropriate differentiation of (E2) with respect to $J^{(-)}$ and $\overline{J^{(-)}}$. Or it can be alternatively obtained by using the formula $\langle\hat{O}\rangle=\mathrm{Tr}\hat{\rho}_I\hat{U}^\dagger\hat{O}\hat{U}/\mathrm{Tr}\hat{\rho}_I$. This is calculable by inserting the factor $O(\psi^\dagger(x),\psi(x))$ at the end of (E2) and discarding the diagrams that are not connected with the inserted operator $\hat{O}$. Taking only the connected graphs is equivalent to the division by $\mathrm{Tr}\hat{\rho}_I$.

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