非平衡母関数

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多自由度系においては、理論を必要な少数自由度に対応する変数で書き直すことが不可欠となるが、この問題は長い間議論されてきた。おもに２つの方法が一般的である。その一つは射影演算子によるものですべての変数の着目する変数への射影成分の運動を考える。他の一つは必要な変数以外で（経路積分表式に於いて）積分してしまうものである。

ここではもう一つ別の方法を紹介する。それはルジャンドル変換によるものであり、どのような系にも適用できる一般的な手法である。まず、見たい変数 O にたいしてプローブ J を挿入する。そして J の存在下ですべての変数で積分して母関数 $W(J)$ を求める。 O に対する情報は $W(J)$ を J で微分すれば O の期待値 $\phi = < O >$ が出てくることからえられる。$W(J)$ をルジャンドル変換して変数を J から ϕ にかえ、新たな母関数 $\Gamma(\phi)$ を定義すればϕ の値は プローブを抜くと言う条件

$$\frac{\partial \Gamma}{\partial \phi} = -J = 0$$

から求めることができる。時間に依存するプローブを用いれば、この式がϕ の運動方程式となる。この方法では c-数である期待値のみを扱うことになる。

以下、この手法を非平衡統計力学に適用する場合に、基礎となる概念や技法を紹介する。最後に場の理論による例題を用いて実際の計算法を説明する。

Non-equilibrium Generating Functional

— Method of On-shell Expansion —

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I Non-equilibrium Generating Functional

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

There have been known several methods to accomplish the above task; the method of 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 equivallent in philosophy to the way of projection operator, we integrate out in path-integral representation all the variables except for those we need. The resulting theory describes the system in terms of the co-ordinates which are left fixed.

There is another method to meet the purpose; the method of Legendre transformation. Here we integrate out over all the variables but it is done 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 calculation. Consider the equilibrium statistical mechanics and suppose that we are interested in the operator $\hat{O}$. (We use the symbol hat to denote the operator and take 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 co-ordinates (including $\hat{O}$). Thus we define the generating function, or the Gibbs free energy, $W[J]$ as

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

$$\Gamma[\phi] \equiv W[J] - J\frac{dW[J]}{dJ}, \qquad \phi = -\frac{dW[J]}{dJ}. \tag{1.2}$$

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.

The method of Legendre transformation deals only with the expectation values and so 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 in 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 $< \hat{O} >_t$.

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

Let us define the non-equilibrium 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 non-equilibrium processes, a time-dependent external force $J(\mathbf{x}, t)$ is introduced which couples to some physical quantity $\hat{O}(\mathbf{x})$ of the system. This $J(\mathbf{x}, t)$ is a fictitious source to be set zero in the end. Thus the Hamiltonian of the system changes with time. It is expressed as

$$\hat{H}(t) = \hat{H} - \int d^3\mathbf{x} J(\mathbf{x}, t)\hat{O}(\mathbf{x}),. \tag{1.4}$$

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

$$\langle\hat{O}(\mathbf{x})\rangle_t = \mathrm{Tr}\{\hat{\rho}_I\hat{U}(t,t_I)^\dagger\hat{O}(\mathbf{x})\hat{U}(t,t_I)\}, \tag{1.5}$$

$$\hat{U}(t,t_I) = \mathrm{T}\exp\left(-\frac{i}{\hbar}\int_{t_I}^{t} ds\hat{H}(s)\right) \tag{1.6}$$

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 non-equilibrium systems. There are two types of the non-equilibrium generating functionals $W[J_1, J_2]$ and $\Gamma[\phi_1,\phi_2]$ which are the extensions of Gibbs' 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 $J_2(t)$;

$$e^{\frac{i}{\hbar}W[J_1,J_2]} = \mathrm{Tr}\{\hat{U}_{J_1}\hat{\rho}_I(\hat{U}_{J_2})^\dagger\}, \tag{1.7}$$

$$\hat{U}_{J_i} = \mathrm{T}\exp\left(-\frac{i}{\hbar}\int_{t_I}^{t_F} dt\{\hat{H} - \int d^3\mathbf{x}J_i(\mathbf{x},t)\hat{O}(\mathbf{x})\}\right) \quad (i=1,2). \tag{1.8}$$

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

The double path formulation of non-equilibrium theory has a long history, starting from Schwinger's work [1, 2, 3, 4, 5]. For an extensive investigation, see the articles [5], [6].

Since $J_1 \neq J_2$ in (1.7) (otherwise W becomes independent of J_1 and J_2), the time evolution of $\hat{\rho}_I$ is not physical. So that $W[J_1,J_2]$ 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 non-equilibrium 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.

Second non-equilibrium generating functional is defined by the double Legendre transformation;

$$\Gamma[\phi_1,\phi_2] = W[J_1,J_2] - \sum_{i=1}^{2}\int d^4x J_i(x)\frac{\delta W[J_1,J_2]}{\delta J_i(x)}, \tag{1.9}$$

$$\phi_i(x) = (-1)^{i+1}\frac{\delta W[J_1,J_2]}{\delta J_i(x)} \quad (i=1,2), \tag{1.10}$$

where the 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

$$\frac{\delta J_i(x)}{\delta J_j(x')} = \delta_{ij}\delta^4(x-x'). \tag{1.11}$$

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

$$\phi(x) \equiv \langle\hat{O}(x)\rangle = \left.\frac{\delta W[J_1,J_2]}{\delta J_1(x)}\right|_{J_1=J_2=0} = -\left.\frac{\delta W[J_1,J_2]}{\delta J_2(x)}\right|_{J_1=J_2=0}. \tag{1.12}$$

The equation of motion of $\phi(x)$ is obtained as follows. We note here the inverted relation of (1.10);

$$\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_i(x)} = (-1)^i J_i(x) \qquad (i=1,2) \tag{1.13}$$

which comes from the definitions (1.9) and (1.10). In (1.7) we have assumed that $J_{1,2}$ are fictitious sources which are made to vanish at the end. In case a phsical source coupled to $\hat{O}$ is really present, the artificial source term J_i has to be set to a physical source $J(t)$: $J_1(t) = J_2(t) = J(x)$. If the source $J(x)$ is absent, we are considering the case where the non-equilibrium 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 $\phi(x)$;

$$\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)} = \frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_2(x)} = 0. \tag{1.14}$$

The solution to (1.14) 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,

$$0 = \frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\Big|_{\phi_1(x)=\phi_2(x)=\phi(x)}. \tag{1.15}$$

This has a similar form of the equation of motion for the co-ordinate 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 remind here the relation between the equation of motion and its solution for the case of non-vanishing physical source, $J_1 = J_2 = J \neq 0$. If we set $J_1 = J_2 = J$ in (1.12) and $\phi_1 = \phi_2 = \varphi$ in (1.13), we get

$$\phi(x) = \left.\frac{\delta W[J_1, J_2]}{\delta J_1(x)}\right|_{J_1=J_2=J}, \tag{1.16}$$

$$-J(x) = \left.\frac{\delta \Gamma[\phi_1, \phi_2]}{\delta \phi_1(x)}\right|_{\phi_1=\phi_2=\phi}, \tag{1.17}$$

which are the solution and the equation of motion under the presence of the physical source $J(x)$ respectively. Actually we get (1.17) by solving (1.16) with respect to $J(x)$; i.e. *inversion* of (1.16). When the initial density matrix is of the equilibrium form $\rho_I = \exp(-\beta \hat{H})$, 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.

1.2 How to calculate $\Gamma[\phi_1, \phi_2]$

The evaluation of $W[J_1, J_2]$ is based on the definition (1.7). In the case of perturbative expansion, for example, there arises 2×2 propagator matrix[2] specific to the non-equilibrium 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[7, 8, 9]. The problem is how to calculte $\Gamma[\phi_1, \phi_2]$ by performing the Legendre transformation (1.9). For the zero temperature and for equilibrium non-zero temperature case, the diagrammatical rule has been known[11, 12] for several types of operators $\hat{O}$. The results are usually given in the form of the loop expansion.

Up to now there are 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[13] 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 non-equilibrium case. In the following, when the superfluid ^{4}He is discussed in Section IV, we need an explicit form of the loop expansion for the non-equilibrium case. For this purpose we generalize the results of loop expansion for the zero temperature or the equilibrium case by introducing the contour time integration.

II On-shell Expansion of $\Gamma[\phi_1, \phi_2]$

On-shell expansion is a technique for extracting physical quantities from the generating functional $\Gamma[\phi_1, \phi_2]$. 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 co-ordinates $q_i, (i = 1 \sim N)$. The Lgrangian is written as $L(q_i, \dot{q}_i)$ and in the time interval $t_I \leq t \leq t_F$, the action is defined to be

$$I[q_i] = \int_{t_I}^{t_F} dt L(q_i(t), \dot{q}_i(t)). \tag{2.1}$$

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 $q_i^{(0)}(t)$.

$$0 = \frac{\delta I[q_i]}{\delta q_j(t)} = \frac{\partial L}{\partial q_i(t)} - \frac{d}{dt}\frac{\partial L}{\partial \dot{q}_i(t)}. \tag{2.2}$$

Here the derivative $\delta/\delta q_j(t)$ is a functional one defined in (1.11) 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 which 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 $\Delta q_j(t)$ 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;

$$0 = \left(\frac{\delta I[q_i]}{\delta q_j(t)}\right)_{q=q^{(0)}+\Delta q}$$

$$= \left(\frac{\delta I[q]}{\delta q_i(t)}\right)_{q=q^{(0)}} + \sum_{j=1}^{N}\int_{t_I}^{t_F} dt' \left(\frac{\delta^2 I[q]}{\delta q_i(t)\delta q_j(t')}\right)_{q=q^{(0)}} \Delta q_j(t') + \cdots \tag{2.3}$$

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

$$\sum_{j=1}^{N}\int_{t_I}^{t_F} dt' \left(\frac{\delta^2 I[q]}{\delta q_i(t)\delta q_j(t')}\right)_{q=q^{(0)}} \cdot \Delta q_j(t') = 0. \tag{2.4}$$

The solution of the above equation describes a small oscillation around $q_i^{(0)}(t)$. Equation (2.4) can be looked upon as an eigenvalue equation in matrix form with rows and columns specified by (j, t'). Therefore we expect discrete set of solutions which are called the modes of oscillations. Equation (2.4) is therefore called the mode determining equation (on-shell equation in the case of field theory). The higher order equations denoted by dots $\cdots$ in eq.(2.3) determine the scattering among the various modes of small oscillation thus obtained.

In field theoretical systems and for zero temperature case, we have already shown[14, 15, 16, 17] that the complete parallelism between the calssical action and the effective action persists and that the formal scheme of on-shell expansion produces the physical quantities such as scattering martix (S-matix) elements among the excitation modes. These modes themselves are determined by the lowest equation of the on-shell expansion.

The purpose of the present Chapter is to apply the same technique to the non-equilibrium genarating 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

$$\hat{H} = \int d^3\mathbf{x}\{\frac{1}{2}\hat{\pi}(\mathbf{x})^2 + \frac{1}{2}\hat{\phi}(\mathbf{x})\omega^2(-\nabla)\hat{\phi}(\mathbf{x}) + H_I[\hat{\phi}]\}. \tag{2.5}$$

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

$$\hat{I}[\phi] = \int d^4x\{\frac{1}{2}\left(\partial_t\hat{\phi}(\mathbf{x})\right)^2 - \frac{1}{2}\hat{\phi}(x)\omega^2(-\nabla)\hat{\phi}(x) - H_I[\hat{\phi}]\}. \tag{2.6}$$

In the Heisenberg representation, the following relations hold:

$$\hat{\pi}(t,\mathbf{x}) = \partial_t\hat{\phi}(t,\mathbf{x}), \qquad [\hat{\pi}(t,\mathbf{x}),\hat{\phi}(t,\mathbf{y})] = \frac{1}{i}\delta^3(\mathbf{x}-\mathbf{y}). \tag{2.7}$$

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

$$\langle\hat{\phi}(\mathbf{x})\rangle_t = \mathrm{Tr}\,\rho_I U^\dagger(t,t_I)\hat{\phi}(\mathbf{x})U(t,t_I). \tag{2.8}$$

The solution to (1.14) always satisfies the relation $\phi_1(x) = \phi_2(x)$ which is written as $\phi^{(0)}(x)$. Then (1.15) takes the form

$$\left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\right)_{\phi_1=\phi_2=\phi^{(0)}} = 0. \tag{2.9}$$

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

$$\begin{aligned} 0 &= \left(\frac{\delta\Gamma[\phi_1,\phi_2]}{\delta\phi_1(x)}\right)_{\phi_1=\phi_2=\phi^{(0)}+\Delta\phi} \\ &= \left(\frac{\delta\Gamma}{\delta\phi_1(x)}\right)_0 + \sum_{i=1,2}\int_{t_I}^{\infty} d^4y \left(\frac{\delta^2\Gamma}{\delta\phi_1(x)\delta\phi_i(y)}\right)_0 \Delta\phi(y) \\ &+ \frac{1}{2!}\sum_{i_1,i_2}\int_{t_I}^{\infty} d^4y_1 d^4y_2 \left(\frac{\delta^3\Gamma}{\delta\phi_1(x)\delta\phi_{i_1}(y_1)\delta\phi_{i_2}(y_2)}\right)_0 \Delta\phi(y_1)\Delta\phi(y_2) + \cdots. \end{aligned} \tag{2.10}$$

Here $(\cdots)_0$ implies that $(\cdots)$ is evaluated at $\phi = \phi^{(0)}$. We further expand $\Delta\phi$ as

$$\Delta\phi(x) = \Delta\phi^{(1)}(x) + \Delta\phi^{(2)}(x) + \Delta\phi^{(3)}(x) + \cdots, \tag{2.11}$$

assuming that $\Delta\phi^{(n)}$ is of the order $(\Delta\phi^{(1)})^n$. Then we get our on-shell expansion by requiring that (2.10) holds in each power of $\Delta\phi^{(1)}$. The zero-th order vanishes because of (2.9) and for the first order we get the mode determining equation;

$$0 = \int_{-\infty}^{\infty} d^4y \left(\Gamma_{11}^{(2)}(x,y) + \Gamma_{12}^{(2)}(x,y)\right)_0 \Delta\phi^{(1)}(y), \tag{2.12}$$

$$\Gamma_{ij}^{(2)}(x,y) = \frac{\delta^2\Gamma}{\delta\phi_i(x)\delta\phi_j(y)}.$$

Here and in what follows we take $t_I \to -\infty$ for simplicity. Equation (2.12) is the geraralization of the mode determinig equation of the small oscillation (2.4) to the nonequilibrium system.

Now the following identities are noted. The first one is a consequence of the Legendre transformation and the second is a straightforward result of the definition of $W[J_1,J_2]$.

$$\sum_{i_2}\int d^4y\Gamma_{i_1i_2}^{(2)}(x,y)(-1)^{i_2+i_3+1}W_{i_2i_3}^{(2)}(y,z) = \delta_{i_1,i_3}\delta^4(x-z), \tag{2.13}$$

$$\sum_{i,j=1,2}\left(W_{ij}^{(2)}(x,y)\right)_{J_1=J_2}=0, \tag{2.14}$$

$$W_{ij}^{(2)}(x,y)\equiv\frac{\delta^2 W}{\delta J_i(x)\delta J_j(y)} \tag{2.15}$$

By using these relations we can derive

$$-\delta^4(x-z)=\int d^4y\,\left(\Gamma_{11}^{(2)}(x,y)+\Gamma_{12}^{(2)}(x,y)\right)\left(W_{11}^{(2)}(y,z)+W_{12}^{(2)}(y,z)\right)\Big|_{J_1=J_2=J}. \tag{2.16}$$

Indeed this relation follows by choosing $i_1=i_3=1$ in (2.13) and by the repeated use of (2.14). However $W_{11}^{(2)}+W_{12}^{(2)}$ is the retarded Green's function;

$$\left(W_{11}^{(2)}(y,z)+W_{12}^{(2)}(y,z)\right)_{J_1=J_2=J}\equiv\left(W_R^{(2)}(y,z)\right)_J=\frac{i}{\hbar}\theta(y^0-z^0)\langle[\hat\phi(y),\hat\phi(z)]\rangle_J, \tag{2.17}$$

therefore the relation $\left(\Gamma_{11}^{(2)}+\Gamma_{12}^{(2)}\right)_0=-\left(W_R^{(2)}\right)_{J=0}^{-1}$ implies that eq.(2.12) determines the pole of $W_R^{(2)}$. For constant $\phi^{(0)}$, $\left(\Gamma_{ij}^{(2)}(x,y)\right)_0$ is a function of $x-y$, therefore in Fourier space (2.12) takes the form

$$\left(\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p})\right)_0\Delta\phi^{(1)}(\omega,\mathbf{p})=0. \tag{2.18}$$

The dispersion relation $\omega=\omega(\mathbf{p})$ can be fixed by requiring that we have non-vanishing $\Delta\phi^{(1)}$ 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 why we call (2.12) the on-shell equation and our scheme the on-shell expansion. Because the Hamiltonian or the action given in (2.6) 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

$$\left(\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p})\right)_0=Z^{-1}(\omega^2-\omega^2(\mathbf{p})), \tag{2.19}$$

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 $px=\omega t-\mathbf{p}\cdot\mathbf{x}$,

$$\begin{aligned}\left(\Gamma_{11}^{(2)}(x-y)+\Gamma_{12}^{(2)}(x-y)\right)_0&=\frac{1}{(2\pi)^4}\int d^4p\exp(-ip(x-y))\left(\Gamma_{11}^{(2)}(\omega,\mathbf{p})+\Gamma_{12}^{(2)}(\omega,\mathbf{p})\right)_0\\&=-Z^{-1}(\partial_t^2+\omega^2(\nabla_x))\delta^4(x-y)\\&\equiv-Z^{-1}f(\partial_x)\delta^4(x-y).\end{aligned} \tag{2.20}$$

Here, as indicated, the differentiation applies to the coordinate x. There are two independent solutions to (2.18), each having an undetermined constant $C^{(\pm)}$:

$$\begin{aligned}\Delta\phi^{(1)}(\omega,\mathbf{p}) &= C(p)\delta(\omega^2-\omega^2(\mathbf{p}))\\ &= \frac{C(\omega=\omega(\mathbf{p}),\mathbf{p})}{2\omega(\mathbf{p})}\delta(\omega-\omega(\mathbf{p}))+\frac{C(\omega=-\omega(\mathbf{p}),\mathbf{p})}{2\omega(\mathbf{p})}\delta(\omega+\omega(\mathbf{p})).\end{aligned}\tag{2.21}$$

Let us define

$$C'^{(\pm)}(\mathbf{p})=\frac{C(\omega=\pm\omega(\mathbf{p}),\pm\mathbf{p})}{(2\pi)^4\sqrt{2\omega(\mathbf{p})}}.\tag{2.22}$$

Then, in the coordinate space we have

$$\begin{aligned}\Delta\phi^{(1)}(x) &= \frac{1}{(2\pi)^4}\int d^4p\exp(-ipx)\Delta\phi^{(1)}(\omega,\mathbf{p})\\ &= \int\frac{d^3\mathbf{p}}{\sqrt{2\omega(\mathbf{p})}}[C'^{(+)}(\mathbf{p})\exp(-ip^{(0)}x)+C'^{(-)}(\mathbf{p})\exp(ip^{(0)}x)],\end{aligned}\tag{2.23}$$

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 (plane wave) of the excited mode. This is shown by deriving another form of $\Delta\phi^{(1)}(x)$ using the technique of formula due to 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

$$\sum_{i=1,2}\int d^4y\left(\Gamma^{(2)}_{1i}(x,y)\right)_0\Delta\phi^{(2)}(y)+\frac{1}{2!}\sum_{i1,i_2}\int d^4y_1d^4y_2\left(\Gamma^{(3)}_{1i_1i_2}(x,y_1,y_2)\right)_0\Delta\phi^{(1)}(y_1)\Delta\phi^{(1)}(y_2)=0.\tag{2.24}$$

$$\begin{aligned}&\sum_{i=1,2}\int d^4y\left(\Gamma^{(2)}_{1i}(x,y)\right)_0\Delta\phi^{(3)}(y)\\ &+\frac{1}{2!}\sum_{i1,i_2}\int d^4y_1d^4y_2\left(\Gamma^{(3)}_{1i_1i_2}(x,y_1,y_2)\right)_0(\Delta\phi^{(1)}(y_1)\Delta\phi^{(2)}(y_2)+\Delta\phi^{(2)}(y_1)\Delta\phi^{(1)}(y_2))\\ &+\frac{1}{3!}\sum_{i1,i_2,i_3}\int d^4y_1d^4y_2d^4y_3\left(\Gamma^{(4)}_{1i_1i_2i_3}(x,y_1,y_2,y_3)\right)_0\Delta\phi^{(1)}(y_1)\Delta\phi^{(1)}(y_2)\Delta\phi^{(1)}(y_3)=0,\\ &\text{etc.}\cdots\end{aligned}\tag{2.25}$$

After some calculations, $\Delta\phi^{(n)}$ can be expressed by $\Delta\phi^{(1)}$ in a compact form;

$$\begin{aligned}\Delta\phi^{(n)}(x) &= \frac{1}{n!}\int d^4y_1\cdots d^4y_nd^4z_1\cdots d^4z_n\left(W_R^{(n+1)}\right)_0(x,y_1,\cdots,y_n)\\ &\times\left(\overleftarrow{W}_R^{(2)}\right)_0^{-1}(y_1,z_1)\left(\overleftarrow{W}_R^{(2)}\right)_0^{-1}(y_2,z_2)\cdots\left(\overleftarrow{W}_R^{(2)}\right)_0^{-1}(y_n,z_n)\Delta\phi^{(1)}(z_1)\cdots\Delta\phi^{(1)}(z_n),\end{aligned}\tag{2.26}$$

$$
\begin{aligned}
& W_R^{(n+1)}(x, y_1, \cdots, y_n) \\
\equiv & \sum_{i_1, \cdots i_n} \left(\frac{\delta^{n+1} W}{\delta J_1(x) J_{i_1}(y_1) \cdots J_{i_n}(y_n)} \right)_{J_1=J_2} \\
= & \left(\frac{i}{\hbar}\right)^n \mathrm{Tr} \left(\rho_I \sum_{P\{y_1,\cdots y_n\}} \theta(t_x, t_{y_1}, \cdots, t_{y_n}) [[\cdots[\hat{\phi}(x), \hat{\phi}(y_1)], \cdots], \hat{\phi}(y_n)] \right) \\
\equiv & \left(\frac{i}{\hbar}\right)^n \langle R(\hat{\phi}(x)\hat{\phi}(y_1)\cdots\hat{\phi}(y_n))\rangle. \qquad (2.27)
\end{aligned}
$$

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

Here we have defined $< \cdots >= \mathrm{Tr}\rho_I(\cdots)$ and $\sum_{P\{y_1,\cdots,y_n\}}$ implies the sum over all possible permutations of $\{y_1, \cdots, y_n\}$. Equation (2.26) 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. $\left(\overleftarrow{W}_R^{(2)}\right)_0^{-1}$ 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 purose let us rewrite $\Delta\phi^{(1)}(x)$ using (2.16) and (2.20);

$$
\begin{aligned}
\Delta\phi^{(1)}(x) &= -\int d^4y \int d^4y' \Delta\phi^{(1)}(y) \sum_{i=1,2} \Gamma_{1i}^{(2)}(x-y') \sum_{j=1,2} W_{1j}^{(2)}(y'-y) \qquad (2.28) \\
&= Z^{-1} \int d^4y \Delta\phi^{(1)}(y) f(\overrightarrow{\partial}_x) i < R(\hat{\phi}(x)\hat{\phi}(y)) > . \qquad (2.29)
\end{aligned}
$$

We have used the fact that since the factor $\Delta\phi^{(1)}(y)$ is present we can use the expression (2.20) for $\Gamma^{(2)}$ in (2.28). The arrow indicates that it operates to the right. Since we are assuming the homogeous system, $< R(\hat{\phi}(x)\hat{\phi}(y)) >$ is a function of $x-y$ so that $f(\overrightarrow{\partial}_x) = f(\overrightarrow{\partial}_{-y}) = f(\overrightarrow{\partial}_y)$ (because f is the even function of its argument, see (2.20). Now remembering the fact that eq.(2.12) is equivalent to

$$
f(\overrightarrow{\partial}_y)\Delta\phi^{(1)}(y) = 0, \qquad (2.30)
$$

the partial integration over $\int d^4y$ in (2.29) is performed. The boundary term at spacial 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

$$A\partial_t^2 B = \partial_t(A \overleftrightarrow{\partial_t} B) + (\partial_t^2 A)B, \qquad A \overleftrightarrow{\partial_t} B \equiv A\partial_t B - (\partial_t A)B. \tag{2.31}$$

By (2.30) we get, using the notation $y = (y^0, \mathbf{y})$, the following expression. Note that we have taken $t_I = -\infty$.

$$\begin{aligned}\Delta\phi^{(1)}(x) &= Z^{-1}\int d^4y\partial_{y^0}\left(\Delta\phi^{(1)}(y)\overleftrightarrow{\partial}_{y^0}\, i < R(\hat{\phi}(x)\hat{\phi}(y)) >\right) \\ &= iZ^{-1}(\lim_{y^0\to\infty} - \lim_{y^0\to t_I})\int d^3\mathbf{y}\Delta\phi^{(1)}(y)\overleftrightarrow{\partial}_{y^0} < R(\hat{\phi}(x)\hat{\phi}(y)) > .\end{aligned}$$

We note here that $\lim_{y^0\to\infty}$ makes vanishing contribution because of the presence of 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

$$\Delta\phi^{(1)}(x) = < [\hat{\varphi}(x), \hat{A}] >, \tag{2.32}$$

$$\hat{A} = -iZ^{-1}\int d^3\mathbf{y}\left(\Delta\phi^{(1)}(y)\hat{\pi}(y) - (\partial_{y^0}\Delta\phi^{(1)}(y))\hat{\phi}(y)\right)_{y^0=t_I}. \tag{2.33}$$

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;

$$\hat{\phi}(t_I, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\int \frac{d^3\mathbf{p}}{\sqrt{2\omega(\mathbf{p})}}\left(\hat{a}(\mathbf{p})e^{-ip^{(0)}x_I} + \hat{a}(\mathbf{p})^\dagger e^{ip^{(0)}x_I}\right). \tag{2.34}$$

$$\hat{\pi}(t_I, \mathbf{x}) = \frac{-i}{(2\pi)^{3/2}}\int d^3\mathbf{p}\sqrt{\frac{\omega(\mathbf{p})}{2}}\left(\hat{a}(\mathbf{p})e^{-ip^{(0)}x_I} - \hat{a}(\mathbf{p})^\dagger e^{ip^{(0)}x_I}\right), \tag{2.35}$$

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

$$[\hat{a}(\mathbf{p}), \hat{a}(\mathbf{k})^\dagger] = \delta^3(\mathbf{p} - \mathbf{k}), \tag{2.36}$$

while other commutators are zero. Now inserting (2.23), (2.34) and (2.35) into the definition (2.33), we get

$$\hat{A} = a^\dagger - a+, \tag{2.37}$$

$$a^{(\dagger)} \equiv Z^{-1}(2\pi)^{3/2}\int d^3\mathbf{p}C^{(\mp)}(\mathbf{p})\hat{a}(\mathbf{p})^{(\dagger)}, \tag{2.38}$$

At this point we assume that the initial density matrix to be the equilibrium one: $\rho_I = \exp(-\beta\hat{H})$. 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 LSZ formalism and $\hat{a}^{(\dagger)}$ annihilates or creates the mode which is an eigen-state 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 (2.32) explicitly in the number representation using (2.37);

$$\begin{aligned}\Delta\phi^{(1)}(x) &= \sum_n \rho_{Inn} < n|[\hat{\phi}(x), a^\dagger - a]|n > \\ &= \sum_n \rho_{Inn}\{- < n|\hat{\phi}(x)|n-1> + < n|\hat{\phi}(x)|n+1> \\ &\quad + < n+1|\hat{\phi}(x)|n> - < n-1|\hat{\phi}(x)|n>\}. \end{aligned} \tag{2.39}$$

Here the summation over the indices other than n is supressed and the following notations have been used,

$$a|n>=|n-1>, \qquad a^\dagger|n>=|n+1> .$$

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 same time. Indeed we can show that (2.39) reduces to the known expression if we keep only the ground state $|0>$ in the sum. Using $a|0>=<0|a^\dagger=0$, we see that $\Delta\varphi^{(1)}(x)$ is written as

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

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 $\Delta\varphi^{(2)}(x)$ which can be handled in a similar manner:

$$\Delta\phi^{(2)}(x) = \int d^4y_1 \int d^4y_2 iZ^{-1}\Delta\phi^{(1)}(y_1)f(\overrightarrow{\partial}_{y_1})iZ^{-1}\Delta\phi^{(1)}(y_2)f(\overrightarrow{\partial}_{y_2}) < R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2)) > . \tag{2.40}$$

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

$$\begin{aligned}&\int d^4y_2 iZ^{-1}\Delta\phi^{(1)}(y_2)f(\overrightarrow{\partial}_{y_2}) < R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2)) > \\ &= iZ^{-1}\int d^4y_2\partial_{y_2^0}[\Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0} < R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2)) >] \\ &= iZ^{-1}\int d^3\mathbf{y}_2(\lim_{y_2^0\to\infty} - \lim_{y_2^0\to t_I})\Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0} < R(\hat{\phi}(x)\hat{\phi}(y_1)\hat{\phi}(y_2)) > \\ &= -iZ^{-1}\int d^3\mathbf{y}_2\Delta\phi^{(1)}(y_2)\overleftrightarrow{\partial}_{y_2^0} < [R(\hat{\phi}(x)\hat{\phi}(y_1)), \hat{\phi}(y_2)] > |_{y_2^0=t_I} \\ &= < [R(\hat{\phi}(x)\hat{\phi}(y_1)), \hat{A}] > . \end{aligned} \tag{2.41}$$

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

$$\Delta\phi^{(2)}(x) = \frac{1}{2!} < [[\hat{\phi}(x), \hat{A}], \hat{A}] > . \tag{2.42}$$

Looking at 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:

$$\Delta\phi^{(n)}(x) = \frac{1}{n!} < [[\cdots[\hat{\phi}(x), \hat{A}], \hat{A}], \cdots], \hat{A}] > . \tag{2.43}$$

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

$$\begin{aligned} \Delta\phi(x) &= \sum_{n=1}^{\infty} \Delta\phi^{(n)}(x) \\ &= \mathrm{Tr}\left(\rho_I \exp(-\hat{A})\hat{\phi}(x)\exp(\hat{A})\right) = \mathrm{Tr}\left(\exp(\hat{A})\rho_I \exp(-\hat{A})\hat{\phi}(x)\right). \end{aligned} \tag{2.44}$$

Usually the initial density matrix is written by $\hat{\pi}(\mathbf{x})$ and $\hat{\phi}(\mathbf{x})$ so that. by noting the definition of (2.33) of $\hat{A}$, we get the c-number shift of the initial variables:

$$\exp(\hat{A})\rho_I\left(\hat{\pi}(\mathbf{x}), \hat{\phi}(\mathbf{x})\right)\exp(-\hat{A}) = \rho_I\left(\hat{\pi}(\mathbf{x}) - \pi_c(\mathbf{x}), \hat{\phi}(\mathbf{x}) - \phi_c(\mathbf{x})\right), \tag{2.45}$$

$$\pi_c(\mathbf{x}) = Z^{-1}\left(\partial_{x^0}\Delta\phi^{(1)}(x)\right)_{t_I}, \tag{2.46}$$

$$\phi_c(\mathbf{x}) = Z^{-1}\left(\Delta\phi^{(1)}(x)\right)_{t_I}. \tag{2.47}$$

The initial coordinate is shifted as it should:

$$\begin{aligned} \Delta\phi(t_I, \mathbf{x}) &= \mathrm{Tr}\left(\rho_I\{\hat{\phi}(t_I, \mathbf{x}) + [\hat{\phi}(t_I, \mathbf{x}), -iZ^{-1}\hat{A}]\}\right) \\ &= \mathrm{Tr}\left(\rho_I\{\hat{\phi}(t_I, \mathbf{x}) + (-iZ^{-1})i\Delta\phi^{(1)}(t_I, \mathbf{x})\}\right) \qquad (2.48) \\ &= \mathrm{Tr}\left(\rho_I\hat{\phi}(t_I, \mathbf{x})\right) + Z^{-1}\Delta\phi^{(1)}(t_I, \mathbf{x}). \qquad (2.49) \end{aligned}$$

In the momentum representation

$$\begin{aligned} \exp(\hat{A})\rho_I\left(\hat{a}(\mathbf{p}), \hat{a}^\dagger(\mathbf{p})\right)\exp(-\hat{A}) &= \rho_I\left(\hat{a}(\mathbf{p}) - \tilde{C}^{(+)}(\mathbf{p}), \hat{a}^\dagger(\mathbf{p}) - \tilde{C}^{(+)}(\mathbf{p})\right), \qquad (2.50) \\ \tilde{C}^{(\pm)}(\mathbf{p}) &\equiv Z^{-1}(2\pi)^{3/2}C^{(\pm)}(\mathbf{p}). \end{aligned}$$

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

Now we have at hand a novel way of searching for the correct condensed state; vary $\tilde{C}^{(\pm)}(\mathbf{p})$ in such a way that $\Delta\phi(x)$ becomes stationary 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.)

III 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 non-vanishing expectation value below the temperature T_c corresponding to the onset of Bose condensation. The model Hamiltonian is the usual one[20]

$$\hat{H} = \int d^3\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int d^3\mathbf{x}d^3\mathbf{y}\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})U_0(\mathbf{x}-\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x}),$$
$$U_0(\mathbf{x}-\mathbf{y}) = U_0(\mathbf{y}-\mathbf{x}), \qquad [\hat{\psi}(t,\mathbf{x}), \hat{\psi}^\dagger(t,\mathbf{y})] = \delta^3(\mathbf{x}-\mathbf{y}). \tag{3.1}$$

Here $U_0(\mathbf{x}-\mathbf{y})$ is the assumed repulsive potential of the Herlium atom and μ the chemical potential. Below we set $\phi^{(\dagger)}(x) \equiv \langle\hat{\psi}^{(\dagger)}(x)\rangle$ and introduce the notations,

$$\hat{\psi}^\alpha \equiv (\hat{\psi}^\dagger, \hat{\psi}),, \quad \hat{\psi}^{\dagger\alpha} \equiv (\hat{\psi}, \hat{\psi}^\dagger),, \qquad \phi^\alpha = (\phi^\dagger, \phi), \quad \phi^{\dagger\alpha} = ((\phi, \phi^\dagger), \qquad (\alpha = 1,2). \tag{3.2}$$

(Don't mix the superfix α with the suffix i or j which discriminates the branch of the two real time paths.) We need two kinds of sources J_i, $\bar{J}_i$ and define

$$\hat{H}_{J_i}(t) = \hat{H} - \int d\mathbf{x}\{J_i(x)\hat{\psi}^\dagger(\mathbf{x}) + \bar{J}_i(x)\hat{\psi}(\mathbf{x})\} \tag{3.3}$$

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 $0 \le \tau \le \hbar\beta$.

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 formalisn due to Schwinger[1], Keldysh[2], Hao et.al. [5], to the three time path including the imaginary time path. See for this purpose Niemi and Semenoff[4], Wagner[8], Fukuda[9]. The contour time integral $\int_C dt$ extends over the contour C which runs as $C_1 \to C_2 \to C_3$. 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;

$$J(t) = J_i(t) \quad \text{if t is on} \quad C_i (i = 1,2,3). \tag{3.4}$$

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

$$\exp \frac{i}{\hbar} W[J_1, J_2, J_3] \equiv \exp \frac{i}{\hbar} W[J] = \mathrm{Tr} T_C \exp\left(-\frac{i}{\hbar}\int_C dt \hat{H}_J(t)\right), \tag{3.5}$$

where $\hat{H}_J(t)$ is equal to $\hat{H}_{J_i}(t)$ given in (3.3) if t is on C_i with $i = 1,2,3$ respectively. The contour δ function is introduced as

$$\int_C dt \delta_C(t-t') f(t) = f(t'). \tag{3.6}$$

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

$$\theta_C(t-t') = \int_C^t dt'' \delta_C(t''-t'). \tag{3.7}$$

$$\frac{\delta f(t)}{\delta f(t')} = \delta_C(t-t'). \tag{3.8}$$

As for the Legendre transformed Γ, the formula of the loop expansion has been established by several authors[11, 12] but these works are limited to the zero temperature case or to the equilibrium systems. The non-equilibrium case where the imaginary time path is absent has been discussed by Hao et.al.[5] . We use in the following the contour time path defined above in case where the imaginary time path is needed. It turs out that the use of contour integral makes it easy to generalize the known results to the non-equilibrium case.

3.1 On-shell expansion

3.1.1 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

$$(i\hbar\partial_t + \Omega(-\nabla))\, \Delta\phi^{(1)}(x) = 0, \qquad (-i\hbar\partial_t + \Omega(-\nabla))\, \Delta\phi^{\dagger(1)}(x) = 0. \tag{3.9}$$

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

$$\Delta\phi^{(\dagger)(1)} = \int d^3\mathbf{p} C^{(\pm)}(\mathbf{p}) e^{(\mp i p^{(0)} x)}, \tag{3.10}$$

where $p^{(0)}x = \Omega(\mathbf{p})t - \mathbf{p}\cdot\mathbf{x}$. In the formula (2.26), owing to the presence of the on-shell projection $\Delta\phi^{(1)}$, ${W_R^{(2)}}^{-1}$ can be replaced by its pole part;

$$\begin{cases} W^{(2)}_{R\ \psi^\dagger\psi}{}^{-1}(x,y) = -Z^{-1}(i\hbar\partial_{t_x} + \Omega(-\nabla_x))\delta^4(x-y), \\ W^{(2)}_{R\ \psi\psi^\dagger}{}^{-1}(x,y) = -Z^{-1}(-i\hbar\partial_{t_x} + \Omega(-\nabla_x))\delta^4(x-y). \end{cases} \tag{3.11}$$

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

Inserting (3.9), (3.11) into (2.26), the reverse use of the LSZ reduction formula, as was done in the previous Chapter, leads to the following expression which has the n-fold commutator:

$$\begin{aligned} &\Delta\phi^{\alpha,(n)}(x) = \frac{1}{n!}\langle[[\cdots[\hat{\psi}^\alpha(x), \hat{A}], \cdots], \hat{A}]\rangle, \\ &\hat{A} \equiv Z^{-1}\int d^3\mathbf{y}\left(\Delta\phi^{(1)}(y)\hat{\psi}^\dagger(y) - \Delta\phi^{\dagger(1)}(y)\hat{\psi}(y)\right)_{y^0=t_I}. \end{aligned} \tag{3.12}$$

Let us rewrite $\hat{A}$ by expanding $\hat{\psi}^{(\dagger)}$ in terms of the creation and annihilation operators;

$$\hat{\psi}^{(\dagger)}(t_I, \mathbf{x}) = \frac{1}{(2\pi)^{3/2}}\int d^3\mathbf{p}\hat{a}(\mathbf{p})^{(\dagger)}e^{\mp ip^{(0)}x_I} \tag{3.13}$$

where $p^{(0)}x_I = \Omega(\mathbf{p})t_I - \mathbf{p}\cdot\mathbf{x}$. Now inserting (3.10) and (3.13) into the definition (3.12), we get

$$\hat{A} \ = \ a^\dagger - a \tag{3.14}$$

$$a^{(\dagger)} \ \equiv \ Z^{-1}(2\pi)^{3/2}\int d^3\mathbf{p}C^{(\pm)}(\mathbf{p})\hat{a}(\mathbf{p})^{(\dagger)}, \tag{3.15}$$

Assuming the equilibrium initial density matrix, we have the following expression for the wave function analogous to (2.39);

$$\begin{aligned} \Delta\phi^{(\dagger)(1)}(x) &= \sum_n \rho_{I nn} < n|[\hat{\phi}^{(\dagger)}(x), a^\dagger - a]|n > \\ = \ &\sum_n \rho_{I nn}\{- < n|\hat{\phi}^{(\dagger)}(x)|n-1> + < n|\hat{\phi}^{(\dagger)}(x)|n+1> \\ &\qquad + < n+1|\hat{\phi}^{(\dagger)}(x)|n > - < n-1|\hat{\phi}^{(\dagger)}(x)|n >\}. \end{aligned} \tag{3.16}$$

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

$$\begin{aligned} \Delta\phi^\alpha(x) \ &= \ \sum_{n=1}^{\infty}\Delta\phi^{\alpha,(n)}(x) \\ &= \ \mathrm{Tr}\left(\rho_I[\hat{\psi}, \hat{\psi}^\dagger]e^{-\hat{A}}\hat{\psi}^\alpha(x)e^{\hat{A}}\right) \qquad (3.17) \\ &= \ \mathrm{Tr}\left(\rho_I[\hat{\psi}', \hat{\psi}'^\dagger]\hat{\psi}^\alpha(x)\right). \qquad (3.18) \\ \hat{\psi}' \ &= \ \hat{\psi} - Z^{-1}\Delta\phi^{(1)}(t_I), \qquad \hat{\psi}'^\dagger = \hat{\psi}^\dagger - Z^{-1}\Delta\phi^{\dagger(1)}(t_I). \end{aligned}$$

Equation (3.18) tells us that $\Delta\phi^\alpha(x)$ is the same as $\langle\hat{\psi}^\alpha(x)\rangle$ but with the initial operator inside ρ_I shifted by the amount $-Z^{-1}\Delta\phi_i^{(1)}(t_I, \mathbf{x})$ 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 preceeding (2.3). However only the shift of the initial value comes in the formula here compared with the 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 straightly from $t = -\infty$ to $+\infty$ in zero temperature case.

It can be shown that if we choose $C^{\pm}(\mathbf{p})$ in such a way that $\Delta\phi(x)$ be independent of x, then $\phi^{(0)} + \Delta\phi$ represents another stationary value of the equilibrium free energy.

3.1.2 the case $\hat{O} = \hat{\psi}^\alpha\hat{\psi}^\alpha$

Next the pairing condensation is discussed. In super-fluid ^{4}He, many people pointed out that not only ψ^α but also $\psi^\alpha\psi^\alpha$ may condense. There has been controversy concerning the existence or the absence of the gap in the excitation spectrum. But the gap can be sown to be absent in full order using the symmetry transformation property of $\Gamma[\phi_1, \phi_2]$.

Here the result of the applicaton of the on-shell expansion to the paring 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 the case of $\langle\hat{\psi}^\alpha\rangle$. We first define the generating functional W as before and introduce the notations for $\alpha = 1, 2$;

$$J_i^\alpha(t,\mathbf{p}) = (J_{i\ \psi^\dagger\psi^\dagger}(t,\mathbf{p}), J_{i\ \psi\psi}(t,\mathbf{p})), \quad \Phi_i^\alpha(t,\mathbf{p}) = (\Phi_i^\dagger(t,\mathbf{p}), \Phi_i(t,\mathbf{p})) = \frac{\delta W}{\delta J_i^\alpha(t,\mathbf{p}}. \tag{3.19}$$

Then Γ is introduced as

$$\Gamma[\Phi_1^\alpha, \Phi_2^\alpha] = W[J_1^\alpha, J_2^\alpha] - \sum_{i,\alpha}\int dt\int d^3\mathbf{p} J_i^\alpha(t,\mathbf{p})\Phi_i^\alpha(t,\mathbf{p}). \tag{3.20}$$

Then the equation which governs the time development of the order parameter is written as

$$\left(\frac{\delta\Gamma}{\delta\Phi_1^{\alpha}(t,\mathbf{p})}\right)_{\Phi_1=\Phi_2=\Phi}=0. \tag{3.21}$$

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

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

where the varibles without the suffix i is the physical quantities;

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

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

$$\begin{aligned}\Delta\Phi^{\alpha}(t,\mathbf{p}) &= \Delta\Phi^{\alpha,(1)}(t,\mathbf{p})+\Delta\Phi^{\alpha,(2)}(t,\mathbf{p})\cdots\\ &= \mathrm{Tr}\left(e^{\int d^3\mathbf{q}\hat{A}_2(t_I,\mathbf{q})}\rho_I[\hat{\psi},\hat{\psi}^{\dagger}]e^{-\int d^3\mathbf{q}\hat{A}_2(t_I,\mathbf{q})}\hat{\Phi}^{\alpha}(t,\mathbf{p})\right)\\ &= \mathrm{Tr}\left(\rho_I[\hat{\psi}',\hat{\psi}'^{\dagger}]\hat{\Phi}^{\alpha}(t,\mathbf{p}).\right).\end{aligned}$$

Here the following notations are employed;

$$\begin{aligned}&\hat{\psi}'=\cosh\theta_{\mathbf{k}}\hat{\psi}(\mathbf{k})-\exp(i\arg\varphi_{\mathbf{k}})\sinh\theta_{\mathbf{k}}\hat{\psi}^{\dagger}(-\mathbf{k}),\\ &\hat{\psi}'^{\dagger}=\cosh\theta_{\mathbf{k}}\hat{\psi}^{\dagger}(\mathbf{k})-\exp(i\arg\varphi_{\mathbf{k}}^{\dagger})\sinh\theta_{\mathbf{k}}\hat{\psi}(-\mathbf{k}),\\ &\hat{A}_2(t_I,\mathbf{q})=Z^{-1}(\Delta\Phi^{(1)}(t_I,\mathbf{q})\hat{\psi}^{\dagger}(t_I,\mathbf{q})\hat{\psi}^{\dagger}(t_I,-\mathbf{q})-\Delta\Phi^{\dagger(1)}(t_I,\mathbf{q})\hat{\psi}(t_I,-\mathbf{q})\hat{\psi}(t_I,\mathbf{q})),\\ &\varphi_{\mathbf{k}}=Z^{-1}\left(\Delta\Phi^{(1)}(t_I,\mathbf{k})+\Delta\Phi^{(1)}(t_I,-\mathbf{k})\right),\quad \theta_{\mathbf{k}}=|\varphi_{\mathbf{k}}|.\end{aligned}$$

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 $\langle\psi^{\alpha}\rangle$, this will coincide 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

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

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 tranformed 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.

References

[1] J. Schwinger, J. Math. Phys. **2** 407 (1961).

[2] L. V. Keldysh: Zh. Eksp. Teor. Fiz., **39** 167 (1960). [Sov. Phys. JETP, **12** (1961), 142].

[3] R.P. Feynman and F.L. Vernon, Ann. Phys. **24** 118 (1963).

[4] A.J. Niemi and G.W. Semenoff, Ann. Phys. **152** 105 (1984). Nucl. Phys. B **230** [FS 10] 181 (1984).

[5] K. Chou, Z. Su, B. Hao and L. Yu, Phs. Rep. **118** 1 (1985).

[6] N. P. Landsman and Ch. G. van Weert, Phys. Rep. **145** 141 (1987).

[7] L. P. Kadanoff and G. Baym; "*Quantum Statistical Mechanics*", W. A. Benjamin Publishing Company Inc., New York, 1962.

[8] M. Wagner, Phys. Rev. B **44** (1991), 6104.

[9] R. Fukuda, M. Sumino and K. Nomoto, Phys. Rev. A **45** (1992), 3559;

[10] R. Fukuda and M. Sumino, Phys. Rev. A **44** (1991), 6252.

[11] C. De Dominicis and P. C. Martin, J. Math. Phys. **5** (1964), 14; **5** (1964), 31.

[12] G. Jona-Lasinio, Nuovo Cimento **34** 1790 (1995);
R. Jackiw, Phys. Rev. D **9** (1974), 1686; M. Cornwall, R. Jackiw and E. Tomboulis, Phys. Rev. D **10** (1974), 2428;
R. Fukuda and E. Kyriakopoulos, Nucl. Phys. **B 85** (1975), 345.

[13] R. Fukuda, Phys. Rev. Lett. **61** (1988), 1549;
M. Ukita, M. Komachiya and R. Fukuda, Int. J. Mod. Phys. A **5** (1990), 1789;
T. Inagaki and R. Fukuda, Phys. Rev. B **46** (1992), 10931.
K. Okumura, Prog. Theor. Phys. **87** (1992), 703; "Effective Action of local composite operators —-case of ϕ^4 theory, itintrant electron model and QED", Keio Univ. preprint, 1994. to appear in Int. J. Mod. Phys. A.
S. Yokojima, Phys. Rev. D **51** (1995), 2996.

[14] R. Fukuda, Prog. Theor. Phys. **78** 1487 (1978).

[15] R. Fukuda, M. Komachiya and M. Ukita, Phys. Rev. D**38** 3747 (1988).

[16] M. Komachiya, M. Ukita and R. Fukuda, Phus. Rev. D**42** 2792 (1990).

[17] R. Fukuda, in *Proceedings of 1991 Nagoya Spring School on Dynamical Symmetry Breaking* p 223, ed. by K. Yamawaki.

[18] H. Lehmann, K. Symanzik and W. Zimmermann, Nuovo Cimento **1** 205 (1955).

[19] As a text book, see for example, C. Izykson and J. B. Zuber, *Quantum Field Theory*, MacGraw-Hill, 1980.

[20] See, for example, A. L. Fetter and J. D. Walecka, *Quantumm Theory of Many-Particle System*, McGraw-Hill, New York 1971.