Doctoral Thesis

Variational Theories with Many-Body Correlations for Dilute Bose–Einstein Condensates
（多体相関を含む希薄ボーズ・アインシュタイン凝縮に対する変分理論）

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Contents

Chapter 1 Introduction

In this chapter, we review the previous studies and describe the motivation for our study.

1.1 Bose–Einstein Condensation and Superfluidity

The spin-statistics theorem classifies identical particles into two groups in terms of their spins. One of the groups is associated with particles with half-integer spins called *fermions*, and the other corresponds to particles with integer spins called *bosons*. Fermions and bosons show completely different behaviors at low temperature because they obey different quantum statistics. Fermions obey the statistics with Pauli exclusion principle which forbids two particles from occupying at the same one-particle state. On the other hand, bosons are free from this exclusion principle. Particularly, macroscopic number of bosons condense into the lowest-energy below a certain temperature. This phase transition induced by the quantum statistics of bosons is called *Bose–Einstein condensation* (BEC), which was predicted by Einstein [1] in noninteracting atoms based on the idea in a paper by Bose [2] who gave a new derivation of Planck's formula assuming the radiation is composed of quanta (photons) obeying a particular kind of statistics different from the classical one.

BEC systems are generally dominated over a wave function at the lowest-energy state, called *condensate wave function* $\Psi_0(\boldsymbol{r}, t)$. The wave function corresponds to the order parameter in BEC and describes the behavior of macroscopic number of condensed particles (condensates). One of the striking phenomena associated with BEC is frictionless transport of particles, called "superfluidity". First of all, we introduce some previous theoretical investigations for the relationship between BEC and superfluidity.

1.1.1 History of studies for BEC and superfluidity

The relevance between BEC and superfluidity was pointed out by London [3], who was stimulated by the experiments of liquid ^{4}He below λ point by Kapitza [4] and Allen and Misener [5]. He evaluated the critical temperature of BEC $T_{\rm c}$ using Einstein's theory [1] with material parameters of liquid ^{4}He and compared it with the experimental data of λ-transition temperature T_λ. He obtained $T_{\rm c} \simeq 3.1$, which was qualitatively consistent with $T_\lambda \simeq 2.1$. However, his consideration was not sufficient because the effects of strong interparticle interactions in liquids were neglected completely. Regarding this problem, Landau [6] constructed a theory of interacting quantum liquid. He quantized the Hamiltonian of classical liquid by introducing the density operator $\hat{\rho}(\boldsymbol{r})$ and velocity operator $\hat{\boldsymbol{v}}(\boldsymbol{r})$, and associated the motions of the liquids with their elementary excitations. According to his consideration, quantum liquid possesses the stationary states classified as (1) irrotational potential motion ($\boldsymbol{\nabla} \times \hat{\boldsymbol{v}} = \boldsymbol{0}$) that corresponds to "phonon mode", (2) vortex motions ($\boldsymbol{\nabla} \times \hat{\boldsymbol{v}} \neq \boldsymbol{0}$) that corresponds to "roton mode". Specifically, he considered that the potential motion (1) results in the superfluidity in ^{4}He. Based on his idea with a stability condition for elementary excitations in quantum liquid responsible for motion (1), one can obtain the maximum value of superfluid velocity

v_c as follows [7]:

$$v_c = \min_{\boldsymbol{p}} \frac{\varepsilon_{\boldsymbol{p}}}{|\boldsymbol{p}|}, \tag{1}$$

where $\varepsilon_{\boldsymbol{p}}$ is the elementary excitations of the liquids with momentum $\boldsymbol{p}$ and minimum is calculated over all the value of $\boldsymbol{p}$. Assuming the free-particle dispersion as $\varepsilon_{\boldsymbol{p}} \propto |\boldsymbol{p}|^2$ and substituting it into Eq. (1), we obtain $v_c = 0$, i.e., superfluidity is absent in noninteracting systems. On the other hand, phonon-type dispersion as $\varepsilon_{\boldsymbol{p}} = c|\boldsymbol{p}|$ yields finite superfluid critical velocity. Thus, interaction between particles found to be indispensable for the superfluidity, and the elementary excitation responsible for frictionless motion was concluded to be phonons by his work. Bogoliubov developed a quantum-field-theoretic description of weakly interacting BEC "molecules" and discuss the origin of superfluidity from microscopic viewpoint [8]. He regarded the interaction part in the Hamiltonian as a "mean field" to introduce a quasiparticle operator in BEC and calculated the quasiparticle excitation at $T = 0$. Although his mean-field approximation was limited to the weak-coupling regime, the quasiparticle dispersion was identical with the "phonon excitation" predicted by Landau. Thus, the perturbative small interactions between bosons transformed a free-particle dispersion into a phonon-type dispersion responsible for the frictionless motion in superfluids.

However, one may raise a question here; why does the one-particle excitation by Bogoliubov theory become equivalent to the collective mode by Landau theory ? Regarding this question, Gavoret and Nozierés gave a conclusion that the one-particle excitation is same as the two-particle excitation in BEC systems [9]. They considered the structure of Green's functions in BEC systems based on a perturbation-expansion method developed by Beliaev [10], and showed that one and two-particle Green's function share common poles in the long-wave-length limit. Therefore, low-lying quasiparticle excitations (one-particle excitation) in interacting BEC systems is widely accepted to be identical with collective phonon modes in superfluids.

1.2 Fundamental Theoretical Difficulties and Recent Developments

To understand the relationship between BEC and superfluidity, intensive theoretical studies have been done. However, we encounter fundamental difficulties when we extend the Bogoliubov theory to describe strong-coupling or finite-temperature systems straightforwardly.

Based on Beliaev's formalism, Hugenholtz and Pines proved that there should be no gap in the one-particle-excitation spectrum in BEC in the long-wavelength limit [11]. In this sense, a gapless phonon-like mode predicted by Bogoliubov satisfies the Hugenholtz–Pines theorem. On the other hand, the Bogoliubov theory is not self-consistent and neglects contributions in the Hamiltonian smaller than $O(\sqrt{N_0})$ (N_0: condensed particle number), which is mainly by non-condensed particles (noncondensates). Therefore, Bogoliubov theory or its simple generalization to strong-coupling or finite temperature systems without self-consistency breaks dynamical conservation laws. On the other hand, if we adopt the conventional Wick-decomposition procedure to evaluate the two-body interaction and construct a self-consistent theory satisfying conservation laws [12, 13], we obtain a one-particle excitation with an unphysical gap that contradicts the Hugenholtz–Pines theorem. Because of this "conserving-gapless dilemma", which was pointed out by Hohenberg and Martin

[14], we have difficulty in constructing a reliable microscopic theory of interacting BEC systems even at the mean-field level. To overcome this problem, various theories have been suggested based on perturbation-expansion method [15, 16] and variational method [17]. In the following, we review these recent works.

1.2.1 Perturbation-expansion method

One of the most successful perturbation theories is Φ-derivative approximation, which is known to be applicable to normal systems with satisfying dynamical conservation laws. This method was developed by Baym [18] in order to construct a systematic scheme to describe non-equilibrium phenomena. The conserving-gapless theory, which corresponds to the generalization of the Φ-derivative approximation to BEC systems, satisfies both dynamical conservation laws and the Hugenholtz–Pines theorem simultaneously [15, 16]. This section summarizes the conserving-gapless theory and compares it with a conventional self-consisntent mean-field theory called Hartree–Fock–Bogoliubov (HFB) theory [13].

Here, we consider a system of weakly-interacting bosons with mass m and spin 0, which is described by the following Hamiltonian:

$$\hat{H} = \hat{H}_0 + \hat{H}_{\rm int}, \tag{2}$$

$$\hat{H}_0 = \int d\boldsymbol{r}\hat{\psi}^\dagger(\boldsymbol{r})\Big[-\frac{\hbar^2\nabla^2}{2m} - \mu\Big]\hat{\psi}(\boldsymbol{r}) \equiv \int d\boldsymbol{r}\hat{\psi}^\dagger(\boldsymbol{r})K\hat{\psi}(\boldsymbol{r}), \tag{3}$$

$$H_{\rm int} = \frac{1}{2}\int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2 U(\boldsymbol{r}_1-\boldsymbol{r}_2)\hat{\psi}^\dagger(\boldsymbol{r}_1)\hat{\psi}^\dagger(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_1), \tag{4}$$

where U is the interaction potential and μ is the chemical potential. To construct a perturbation theory, we introduce the Heisenberg equation for $\hat{\psi}(\boldsymbol{r})$ with "imaginary" time τ as follows:

$$\begin{aligned}\frac{\partial\hat{\psi}(\boldsymbol{r}_1;\tau_1)}{\partial\tau_1} \equiv \frac{\partial\hat{\psi}(1)}{\partial\tau_1} &= e^{\tau_1\hat{H}}[\hat{H},\hat{\psi}(\boldsymbol{r}_1)]e^{-\tau_1\hat{H}} \\ &= -K\hat{\psi}(1) + \int d2\bar{U}(1-2)\hat{\psi}^\dagger(2)\hat{\psi}(2)\hat{\psi}(1),\end{aligned} \tag{5}$$

where $(\boldsymbol{r}_1,\tau_1)\equiv 1$ and $\bar{U}(1-2)\equiv U(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\tau_1-\tau_2)$.

In BEC systems, we need to determine the behaviors of condensates Ψ_0 and noncondensates $\delta\hat{\psi} = \hat{\psi}-\Psi_0$ simultaneously. To describe noncondensates, we define a Green's function $-\langle T_\tau\delta\hat{\psi}(1)\delta\hat{\psi}^\dagger(2)\rangle = -[\theta(\tau_1-\tau_2)\langle\delta\hat{\psi}(1)\delta\hat{\psi}^\dagger(2)\rangle + \theta(\tau_2-\tau_1)\langle\delta\hat{\psi}^\dagger(2)\delta\hat{\psi}(1)\rangle] \equiv G(1,2)$, where T_τ represents a time-ordering operator. In addition, anomalous density $\langle\delta\hat{\psi}(\boldsymbol{r}_1)\delta\hat{\psi}(\boldsymbol{r}_2)\rangle$ and anomalous Green's function $\langle T_\tau\delta\hat{\psi}(1)\delta\hat{\psi}(2)\rangle \equiv F(1,2)$ are known to be finite in BEC systems [10]. Noting these facts, we introduce a imaginary-time Green's function in the 2×2 Nambu space defined as

$$\begin{aligned}\hat{G}(1,2) &\equiv -\left\langle T_\tau\begin{pmatrix}\delta\hat{\psi}_1(1)\\ \delta\hat{\psi}_2(1)\end{pmatrix}\Big(\delta\hat{\psi}_2(2)\ \delta\hat{\psi}_1(2)\Big)\right\rangle\hat{\sigma}_3 \\ &= \begin{pmatrix}G(1,2) & F(1,2)\\ -\bar{F}(1,2) & -\bar{G}(1,2)\end{pmatrix} \equiv G_{ij}(1,2),\end{aligned} \tag{6}$$

where $\hat{\sigma}_i$ $(i = 0, 1, 2, 3)$ denotes Pauli matrix and

$$\delta\hat{\psi}_1(1) \equiv e^{\tau_1 \hat{H}} \delta\hat{\psi}(\boldsymbol{r}_1) e^{-\tau_1 \hat{H}}, \ \delta\hat{\psi}_2(1) \equiv e^{\tau_1 \hat{H}} \delta\hat{\psi}^\dagger(\boldsymbol{r}_1) e^{-\tau_1 \hat{H}}. \tag{7}$$

The equations of motion for $\hat{G}$, called Dyson–Beliaev equations, are derived as

$$\int d3[\hat{G}_0^{-1}(1,3) - \hat{\Sigma}(1,3)]\hat{G}(3,2) = \hat{\sigma}_0 \delta(1-2), \tag{8}$$

where $\hat{G}_0^{-1}(1,2) \equiv (-\hat{\sigma}_0 \partial/\partial\tau - \hat{\sigma}_3 K)\delta(1-2)$ and $\delta(1-2) \equiv \delta(\tau_1 - \tau_2)\delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)$. On the other hand, the equation of motion for Ψ_0 is obtained by $\langle \partial\hat{\psi}(\boldsymbol{r};\tau)/\partial\tau \rangle = 0$, which is known as the Gross–Pitaevskii (GP) equation [19, 20] given by

$$\begin{aligned} K\Psi_0(\boldsymbol{r}) + \int d\boldsymbol{r}_1 U(|\boldsymbol{r} - \boldsymbol{r}_1|) \Big\{ \big[|\Psi_0(\boldsymbol{r}_1)|^2 + \langle \delta\hat{\psi}^\dagger(\boldsymbol{r}_1)\delta\hat{\psi}(\boldsymbol{r}_1) \rangle \big] \Psi_0(\boldsymbol{r}) \\ + \langle \delta\hat{\psi}(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}_1) \rangle \Psi_0^*(\bar{\boldsymbol{r}}) + \langle \delta\hat{\psi}^\dagger(\boldsymbol{r})\delta\hat{\psi}(\boldsymbol{r}_1) \rangle \Psi_0(\boldsymbol{r}_1) \Big\} \equiv K\Psi_0(\boldsymbol{r}) + \mathcal{T}(\boldsymbol{r}) = 0, \end{aligned} \tag{9}$$

where we use the approximation $\langle \delta\hat{\psi}^\dagger \delta\hat{\psi}\delta\hat{\psi} \rangle \simeq 0$ within mean-field regime.

Luttinger and Ward introduced the exact equilibrium thermodynamic potential with a functional $\Phi = \Phi[G]$ for a normal Fermi system in terms of the imaginary-time Green's function G [21]. Here, we follow their manner and introduce the generalized form of the thermodynamic potential to an interacting BEC system [15, 16]. The thermodynamic potential is given by

$$\Omega = \int d\boldsymbol{r} \Psi_0^*(\boldsymbol{r}) K \Psi_0(\boldsymbol{r}) + \frac{k_{\rm B}T}{2} {\rm Tr}[\ln(-\underline{\hat{G}}_0^{-1} + \underline{\hat{\Sigma}}) + \underline{\hat{\Sigma}}\ \underline{\hat{G}}] + \Phi, \tag{10}$$

where $\underline{\hat{G}}$ denotes a matrix whose elements are compose of $G_{ij}(1,2)$, its trace is defined as ${\rm Tr}\underline{\hat{G}} = \sum_{i=1,2} \int d1 G_{ii}(1, 1+0_+)$, and Φ generates Σ, Δ, and $\mathcal{T}$ as

$$\frac{\delta\Phi}{\delta\bar{G}(2,1)} = -k_{\rm B}T\Sigma(1,2), \ \frac{\delta\Phi}{\delta\bar{F}(2,1)} = \frac{k_{\rm B}T}{2}\Delta(1,2), \ \frac{\delta\Omega}{\delta\Psi_0^*(\boldsymbol{r})} = k_{\rm B}T\mathcal{T}(\boldsymbol{r}). \tag{11}$$

By these definitions, $\delta\Omega/\delta\hat{G} = \hat{0}$ and $\delta\Omega/\delta\Psi_0$ reproduce Dyson–Beliaev equations and the GP equation simultaneously. We note Eq. (10) reproduces the thermodynamic potential for a normal Bose system by setting $\Psi, F \to 0$.

In the Φ-derivative theory, we need to consider Φ in order to determine what types of diagrams we incorporate in the self-consistent theory. To construct a mean-field theory, we approximate Φ in the lowest order as [15, 16]

$$\begin{aligned} \Phi \simeq \Phi^{(1)} = \frac{k_{\rm B}T}{4} \int d1 \int d1' \int d2 \int d2' \bar{V}(1-2)[\delta(1-1')\delta(2-2') \\ + \delta(1-2')\delta(2-1')]\{2G(1,1')G(2,2') + c_{2b}^{(1)} F(1,2)\bar{F}(1',2') + c_{1a}^{(1)} G(1,1')\Psi_0(2)\bar{\Psi}_0(2') \\ + c_{1b}^{(1)}[F(1,2)\bar{\Psi}_0(1')\bar{\Psi}_0(2') + \bar{F}(1,2)\Psi_0(1')\Psi_0(2')] + c_0^{(1)}\bar{\Psi}_0(1')\bar{\Psi}_0(2')\Psi_0(2)\Psi_0(1)\}, \end{aligned} \tag{12}$$

where $c_{2b}^{(1)}$, $c_{1a}^{(1)}$, $c_{1b}^{(1)}$, $c_0^{(1)}$ numerical weights for respective contributions to Φ. Here, we set all the coefficients unknown and discuss "the gapless condition" the one-particle excitation in homogeneous systems.

We consider the equilibrium state in homogeneous systems where the condensate wave function is expressed by $\Psi_0(\boldsymbol{r}) = \sqrt{n_0}$, where n_0 is condensed-particle-number density. Noting this relation and using the following Fourier transformation of $\hat{G}$ given by

$$\hat{G}(1,2) = \frac{k_{\rm B}T}{\mathcal{V}} \sum_{n=-\infty}^{\infty} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \hat{G}_{\boldsymbol{k},i\varepsilon_n} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_1-\boldsymbol{r}_2)} e^{-i\varepsilon_n(\tau_1-\tau_2)}, \tag{13}$$

with volume $\mathcal{V}$ and Matsubara frequency $\varepsilon_n \equiv 2n\pi k_{\rm B}T$, we obtain the Dyson–Beliaev equations in $(\boldsymbol{k}, \varepsilon_n)$ space as follows:

$$\left(i\varepsilon_n\hat{\sigma}_0 - \hat{H}^{\rm MF}_{\boldsymbol{k}}\right)\hat{G}_{\boldsymbol{k},i\varepsilon_n} = \hat{\sigma}_0, \tag{14a}$$

$$\hat{H}^{\rm MF}_{\boldsymbol{k}} \equiv \begin{pmatrix} \varepsilon_k - \mu + \Sigma^{\rm MF}_{\boldsymbol{k}} & \Delta^{\rm MF}_{\boldsymbol{k}} \\ -\Delta^{\rm MF}_{\boldsymbol{k}} & -\varepsilon_k + \mu - \Sigma^{\rm MF}_{\boldsymbol{k}} \end{pmatrix} \equiv \begin{pmatrix} \xi^{\rm MF}_{\boldsymbol{k}} & \Delta^{\rm MF}_{\boldsymbol{k}} \\ -\Delta^{\rm MF}_{\boldsymbol{k}} & -\xi^{\rm MF}_{\boldsymbol{k}} \end{pmatrix}, \tag{14b}$$

where $\varepsilon_k \equiv \hbar^2|\boldsymbol{k}|^2/2m$ with wave number $\boldsymbol{k}$ and self energies are given as

$$\Sigma^{\rm MF}_{\boldsymbol{k}} = -\frac{N_0(U_{\boldsymbol{0}} + U_{\boldsymbol{k}})}{4\mathcal{V}} c^{(1)}_{1a} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} (U_{\boldsymbol{k}-\boldsymbol{k}'} + U_{\boldsymbol{0}})\rho_{\boldsymbol{k}'}, \tag{15a}$$

$$\Delta^{\rm MF}_{\boldsymbol{k}} = \frac{N_0 U_{\boldsymbol{k}}}{\mathcal{V}} c^{(1)}_{1b} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} U_{\boldsymbol{k}-\boldsymbol{k}'} F_{\boldsymbol{k}'} c^{(1)}_{2b}. \tag{15b}$$

Using $G_{\boldsymbol{k},i\varepsilon_n}$, the one-particle spectral function is defined as

$$A_{\boldsymbol{k},\varepsilon} \equiv -2{\rm Im}G_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+0_+}. \tag{16}$$

Therefore one-particle-excitation spectrum is described by taking the imaginary part of G with replacing $i\varepsilon_n \to \varepsilon + 0_+$. By this procedure, we obtain the spectral function as

$$A_{\boldsymbol{k},\varepsilon} = 2\pi\left[(1+v^2_{\boldsymbol{k}})\delta(\varepsilon - E^{\rm MF}_{\boldsymbol{k}}) - v^2_{\boldsymbol{k}}\delta(\varepsilon + E^{\rm MF}_{\boldsymbol{k}})\right], \tag{17}$$

where $v^2_{\boldsymbol{k}} = [1 - \xi^{\rm MF}_{\boldsymbol{k}}/E^{\rm MF}_{\boldsymbol{k}}]/2$ represents the weight of the spectral function and $E^{\rm MF}_{\boldsymbol{k}}$ is given by

$$E^{\rm MF}_{\boldsymbol{k}} = \sqrt{(\varepsilon_k - \mu + \eta^+_{\boldsymbol{k}})(\varepsilon_k - \mu + \eta^-_{\boldsymbol{k}})},\ \eta^{\pm}_{\boldsymbol{k}} \equiv \Sigma^{\rm MF}_{\boldsymbol{k}} \pm \Delta^{\rm MF}_{\boldsymbol{k}}, \tag{18}$$

which is derived by diagonalizing the effective Hamiltonian $\hat{H}^{\rm eff}_{\boldsymbol{k}}$. Thus, the gapless excitation in a homogeneous system is realized when $-\mu + \eta^-_{\boldsymbol{k}\to\boldsymbol{0}} = -\mu + \Sigma^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}} - \Delta^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}} \to 0$, which corresponds to the Hugenholtz–Pines theorem. Here, we check whether the chemical potential satisfies the relation $\mu = \Sigma^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}} - \Delta^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}}$ or not.

The chemical potential is determined from the GP equation in Eq. (9) by

$$\mu = \frac{N_0 U_{\boldsymbol{0}}}{\mathcal{V}} + \frac{1}{\mathcal{V}}(U_{\boldsymbol{k}} + U_{\boldsymbol{0}}) \sum_{\boldsymbol{k}'\neq\boldsymbol{0}} \rho_{\boldsymbol{k}'} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}'\neq\boldsymbol{0}} F_{\boldsymbol{k}'} U_{\boldsymbol{k}'}. \tag{19a}$$

On the other hand, the stationary condition $\delta\Omega/\delta\Psi^* = 0$, we derive the GP equation as

$$\mu = \frac{c^{(1)}_0 N_0 U_{\boldsymbol{0}}}{\mathcal{V}} - \frac{c^{(1)}_{1a}}{4}\frac{U_{\boldsymbol{k}} + U_{\boldsymbol{0}}}{\mathcal{V}} \sum_{\boldsymbol{k}'\neq\boldsymbol{0}} \rho_{\boldsymbol{k}'} + \frac{c^{(1)}_{1b}}{\mathcal{V}} \sum_{\boldsymbol{k}'\neq\boldsymbol{0}} F_{\boldsymbol{k}'} U_{\boldsymbol{k}'}, \tag{19b}$$

in terms of numerical weights. By comparison between these two expressions, we obtain

$$c_0^{(1)} = 1,\ c_{1a}^{(1)} = -4, c_{1b}^{(1)} = 1. \tag{20}$$

Subtracting Eq. (15b) from (15a) with taking $\boldsymbol{k} \to \boldsymbol{0}$ and using the expression for chemical potential, we obtain

$$\Sigma^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}} - \Delta^{\rm MF}_{\boldsymbol{k}\to\boldsymbol{0}} = \mu - \frac{1 + c_{2b}^{(1)}}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} U_{\boldsymbol{k}} F_{\boldsymbol{k}}. \tag{21}$$

By the conventional procedure for constructing mean-field theory based on the Wick decomposition, we also can obtain self energy and pair potential (HFB theory). In this case, however, the pair potential is derived as

$$\Delta^{\rm HFB}_{\boldsymbol{k}} = \frac{N_0 U_{\boldsymbol{k}}}{\mathcal{V}} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} U_{\boldsymbol{k}-\boldsymbol{k}'} F_{\boldsymbol{k}'}, \tag{22}$$

and thus $c_{2b}^{(1)} = 1$. Therefore, the Hugenholtz-Pines theorem is broken and unphysical gap remains in the excitation spectrum. In the conserving–gapless theory, on the other hand, we construct Φ in order to satisfy this gapless condition. In the present case, we set $c_{2b}^{(1)} = -1$ and thus

$$\Delta^{\rm CG}_{\boldsymbol{k}} = \frac{N_0 U_{\boldsymbol{k}}}{\mathcal{V}} - \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} U_{\boldsymbol{k}-\boldsymbol{k}'} F_{\boldsymbol{k}'}. \tag{23}$$

Note that $\Sigma^{\rm CG}_{\boldsymbol{k}} = \Sigma^{\rm HFB}_{\boldsymbol{k}}$ since $\Sigma^{\rm MF}_{\boldsymbol{k}}$ does not include $c_{2b}^{(1)}$ and all other factors are determined by the GP equation. Because $\Sigma^{\rm MF}_{\boldsymbol{k}}$ and $\Delta^{\rm MF}_{\boldsymbol{k}}$ are determined self-consistently with $\hat{G}$ and Ψ_0, the conserving-gapless theory satisfies conservation laws with realizing the gapless condition.

A systematic construction of $\Phi_n (n > 1)$ is also introduced in Ref. [16] although we have limited the discussion within mean-field approximation here. According to the analysis of one-particle-excitation spectrum based on the conserving-gapless theory up to third order, every excitation for each $\boldsymbol{k}$ should have a finite life time, even in the limit $\boldsymbol{k} \to \boldsymbol{0}$ because of the perturbative contributions beyond mean-field approximation [22]. It implies that one-particle excitation in BEC systems should be distinguished from the collective mode which has infinite lifetime in the long-wave-length limit [23].

From the viewpoint of variational principle in thermodynamics, energetically stable state should be realized by improving a theory. However, the conserving-gapless theory yields higher ground-state energy (free energy) than that by the HFB theory at $T = 0$ ($T \neq 0$), as shown in Fig. 1 in the next section. One of the reasons may be the constraint in the conserving-gapless theory, the Hugenholtz–Pines theorem, which should be satisfied naturally. In other word, it is necessary to find a self-consistent solution which (1) satisfies the Hugenholtz–Pines theorem and (2) yields lower ground-state or free energy.

1.2.2 Variational method

The variational method is a theory that incorporates variational parameters into a certain ground state or density matrix and determine the behaviors of variational parameters from stationary conditions. For instance, in case we consider the ground state described by $|\Phi\rangle = |\Phi[x]\rangle$ with a variational

parameter x, we impose

$$\mathcal{E} = \langle\Phi[x]|\hat{H}|\Phi[x]\rangle \geq \langle\Phi[x_{\rm op}]|\hat{H}|\Phi[x_{\rm op}]\rangle \rightarrow \left.\frac{\delta\mathcal{E}}{\delta x}\right|_{x=x_{\rm op}} = 0, \tag{24}$$

and determine the optimized solution $x_{\rm op}$ from this equation, where $x_{\rm op}$ gives the most "physical" solution over all of x. When the other independent factors in the Hamiltonian also play crucial roles, one may need to increase the number of variational parameters. In this sense, "energetic discussion" is the most important guideline to choose the form of the variational state. Up to the present, intensive studies based on this variational method have been done in various systems. One of the works relating BEC was carried out by Girardeau and Arnowitt [12], who tried to extend the Bogoliuov theory and confirm its applicability to strong coupling systems, such as liquid ^{4}He.

In the Hamiltonian of an interacting BEC system, the interaction term yields various collisional processes because of the presence of condensates. With $\hat{\psi} = \Psi_0 + \delta\hat{\psi}$ ($\Psi_{\mathbf{0}} = O(N_{\mathbf{0}}^{\frac{1}{2}})$), Eq. (4) can be expressed as

$$\begin{aligned}\hat{H}_{\rm int}[\Psi_0, \delta\hat{\psi}] &= O(N_{\mathbf{0}}^2) + O(N_{\mathbf{0}}^{\frac{3}{2}}) + O(N_{\mathbf{0}}) + O(N_{\mathbf{0}}^{\frac{1}{2}}) + O(1) \\ &\equiv \hat{H}_0 + \hat{H}_{\frac{1}{2}} + \hat{H}_1 + \hat{H}_{\frac{3}{2}} + \hat{H}_2.\end{aligned} \tag{25}$$

Explicit forms of $\hat{H}_i$ ($i = 0, 1/2, 1, 3/2, 2$) are given in Eq. (34) in the next chapter. We here point out that Bogoliubov theory extracts contributions only up to $\hat{H}_1$ with a simple perturbation manner. Girardeau and Arnowitt constructed a variational ground state with noncondensates with incorporating the interaction between two noncondensates described by $\hat{H}_2$ within the mean-field approximation. The Girardeau–Arnowitt variational wave function (GA variational wave function) is given by

$$|\Phi_{\rm GA}\rangle = A_{\rm GA}\exp(\hat{\pi}_{\rm GA}^\dagger)\,|N\rangle_0\,,\ \hat{\pi}^\dagger = \frac{1}{2}\sum_{\boldsymbol{k}\neq\mathbf{0}}\phi_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k}}^\dagger\hat{c}_{-\boldsymbol{k}}^\dagger, \tag{26}$$

where $(\hat{c}_{\boldsymbol{k}}^\dagger, \hat{c}_{\boldsymbol{k}})$ are the field operators satisfying the Bose commutation relations, $|N\rangle_0 \equiv (\hat{c}_{\mathbf{0}}^\dagger)^N\,|0\rangle\,/\sqrt{N!}$ with the vacuum $|0\rangle$, $A_{\rm GA}$ is the normalization constant and $\phi_{\boldsymbol{k}}$ corresponds to the variational parameter characterizing pair excitations from condensates. In fact, the GA theory reduces to the HFB theory at $T = 0$, i,e., the one-particle excitation by GA theory also has an unphysical energy gap. Therefore, even in the self-consistent variational theory within mean-field approximation, the fundamental problem remains to be unsolved.

Recently, a better variational wave function beyond the mean-field approximation has been introduced [17]. The improved wave function incorporates $\hat{H}_{\frac{3}{2}}$, called 3/2-*body correlations* in Ref. [17]. To describe $\hat{H}_{\frac{3}{2}}$, the following wave function was introduced:

$$|\Phi\rangle = A_3\exp(\hat{\pi}_{\frac{3}{2}}^\dagger)\,|\Phi_{\rm GA}\rangle\,,\ \hat{\pi}_{\frac{3}{2}}^\dagger = \frac{1}{3!}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3\neq\mathbf{0}} w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\hat{\gamma}_{\boldsymbol{k}_1}^\dagger\hat{\gamma}_{\boldsymbol{k}_2}^\dagger\hat{\gamma}_{\boldsymbol{k}_3}^\dagger, \tag{27}$$

where $\hat{\gamma}_{\boldsymbol{k}}$ is Bogoliubov quasiparticle operator characterized by $\hat{\gamma}_{\boldsymbol{k}}\,|\Phi_{\rm GA}\rangle = 0$ and w is the new variational parameter. In Ref. [17], the ground-state property was investigated with the contact

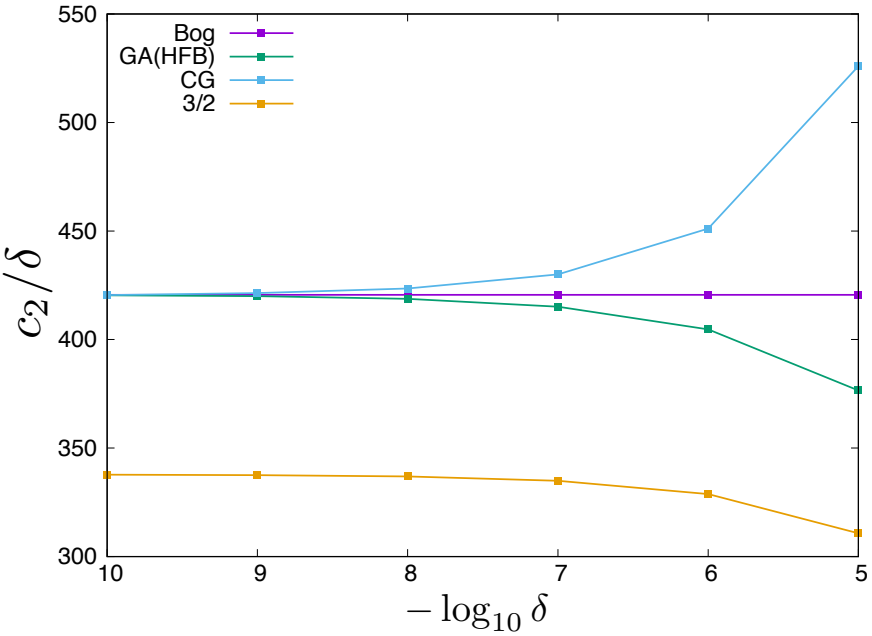

Figure 1: Coupling-constant dependence of c_2 evaluated by the Bogoliubov theory (purple), the GA or HFB theory (green), the conserving-gapless theory (cyan), and the variational theory with 3/2-body correlations (orange).

potential $U = 4\pi\hbar^2 a_U/m$ (a_U: alternative parameter in unit of length, m: mass of bosons) and the ground-state energy per particle was evaluated using the following quantity;

$$\frac{\delta\mathcal{E}}{N} = \frac{\langle\Phi|\hat{H}|\Phi\rangle - \langle\Phi_{\rm Bog}|(\hat{H} - \hat{H}_{3/2} - \hat{H}_2)|\Phi_{\rm Bog}\rangle}{N} \equiv c_2 \times \varepsilon_U a_U^3 \bar{n}, \tag{28}$$

where $|\Phi_{\rm Bog}\rangle$ is the Bogoliubov's ground state, $\bar{n}$ is the total particle-number density, and ε_U is an energy unit given by $\varepsilon_U \equiv \bar{n}U$. Fig. 1 plots the results of c_2 by the Bogoliubov theory, the GA (HFB) theory, the conserving-gapless theory, and the theory with 3/2-body correlations. As seen in the figure, 3/2-body correlations play a role of decreasing the ground-state energy, and their contributions are comparable to the mean-field contributions. Thus, the 3/2-body correlations beyond mean-field approximation should not be omitted in BEC systems, even in the weak-coupling region.

Based on the new wave function, it was shown that the 3/2-body correlations also yield a qualitative change to the one-particle excitation spectrum from the mean-field description. In Ref. [17], the author calculated the first and second moments of the one-particle spectral function, as shown in Fig. 2. The first moment corresponds to the peak value of one-particle spectral function, and the second one corresponds to its width around the peak. Figure 2 shows the respective results by $|\Phi_{\rm Bog}\rangle$, $|\Phi_{\rm GA}\rangle$, and $|\Phi\rangle$. As shown in this figure, 3/2-body correlations have the effect of reducing the peak of the excitation spectrum from the GA spectrum towards the Bogoliubov spectrum and

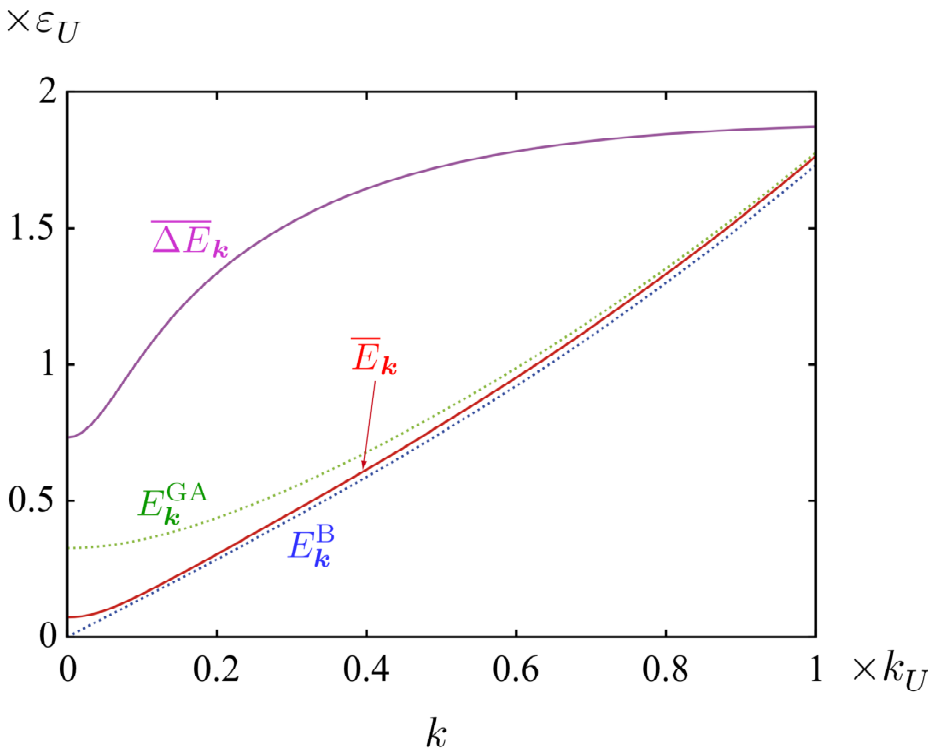

Figure 2: A picture from Ref. [17] : Mean value $\bar{E}_{\boldsymbol{k}}$ and width $\Delta E_{\boldsymbol{k}}$ of the one-particle excitation spectrum, as functions of the wavenumber $k = |\boldsymbol{k}|$ for $\delta = 1.0 \times 10^{-6}$ and $\varepsilon_{k_c}/\varepsilon_U = 100$. The horizontal and vertical axes are normalized by $k_U = \sqrt{2m\varepsilon_U}/\hbar$ and ε_U, respectively. For comparison, the spectra $E_{\boldsymbol{k}}^{\rm GA}$ and $E_{\boldsymbol{k}}^{\rm B}$ obtained by the Girardeau–Arnowitt and Bogoliubov theories, respectively.

the reduction becomes larger for $k \to 0$. Thus, the unphysical energy gap appearing in the self-consistent mean-field theory decreases substantially. In addition, the width of the spectrum was also finite caused by 3/2-body correlations even in the limit $k \to 0$, indicating a finite lifetime of the one-particle excitation. Therefore, the variational theory also predict that the qualitative features of the one-particle excitations differ from that of the collective excitations.

1.3 Motivation of the Present Study

In the following, we investigate weakly-interacting BEC systems on the basis of the recent variational theory. First, we generalize the variational theory in order to describe various BEC systems. Second, we reconsider the relation between superfluidity and BEC in the context of macroscopic coherence.

1.3.1 Motivation 1 : Construction of the variational theory for various BEC systems

The recent variational theory was constructed for homogeneous single-component BEC systems at $T = 0$. On the other hand, BEC is created in dilute atomic gases by cooling identical bosons in a inhomogeneous magnetic trap. Therefore, when constructing ground states in a realistic BEC

system, a competition between interparticle interaction and inhomogeneity due to the trap potential should be considered [24]. By the recent experimental development, it is possible to realize multi-component BEC systems with internal degrees of freedom, such as Bose–Bose mixture, Bose–Fermi mixture, and spinor BEC. Although such field also have been studied extensively, the collisional processes between different particles tend to be neglected beyond mean-field approximation. Therefore, collisional effects between different particles are also worth investigating. To do this, we also construct a variational wave function of M-component Bose–Bose mixtures with incorporating 2- and 3/2-body correlations between different particles [25]. At zero temperature, condensed particles dominates over weakly-interacting BEC systems, since $N_{\mathbf{0}} \gg 1$. Thus, the GP equation which does not include noncondensates is often used and gives qualitative results. However, at finite temperature, the number of noncondensates is comparable to that of condensates because of the presence of thermally excited particles. Therefore, noncondensates cannot be neglected at finite temperature. In this thesis, we also extend the zero-temperature formalism in order to describe systems at finite temperature [26]. The present variational method is also applicable to the superconducting systems with some modifications, as shown in Ref. [27]. In appendix A, we construct a variational theory of superconductivity at finite temperature based density-matrix formalism in Ref. [26] by incorporating many-body correlations.

1.3.2 Motivation 2 : Reconsideration of the relation between superfluidity and BEC

Phonon excitations responsible for superfluidity have been widely accepted to be identical with low-lying single-particle excitations in interacting BEC systems. It is justified by the work by Gavoret and Nozierés arguing one and two-particle Green's functions share "common poles" in the long-wavelength limit. On the other hand, according to the recent works beyond Bogoliubov theory, low-lying one-particle excitation may be distinguished essentially from the collective excitation. Therefore, it should be worth reconsidering the relation between BEC and superfluidity from microscopic viewpoint.

In 1957, Bardeen, Cooper, and Schrieffer constructed a variational theory of superconductivity [28]. Although the theory is remarkably successful in describing weak-coupling superconductors, the variational state is apparently incompatible with particle-number conservation because it is superposed over different total-particle-number states. This fact is stated by Schrieffer from the beginning [29] and emphasized by Peierls [30] and Leggett [31]. On the other hand, Anderson justified the superposition by considering the exchange of particles between subsystems discussed the emergence of a well-defined macroscopic phase as the key ingredient for superfluidity [32]. However, such fluctuations in the total-particle number never appear in any closed systems. Hence, one may regard the superposition as just a mathematical artifact to exploit features of the grand canonical ensemble in the thermodynamic limit. On the other hand, the recent variational wave functions for BEC systems [17] and superconductors [27] are superposed over *different condensed-particle-number states* within the fixed-number formalism, instead of the total particle number. Fig. 3 shows the squared projection $|\langle N-n|\Phi\rangle|^2$ in Ref. [17], which indicates finite particle-number fluctuation due to the interaction in number-fixed systems. If we assume this mechanism to be correct, a macroscopic phase

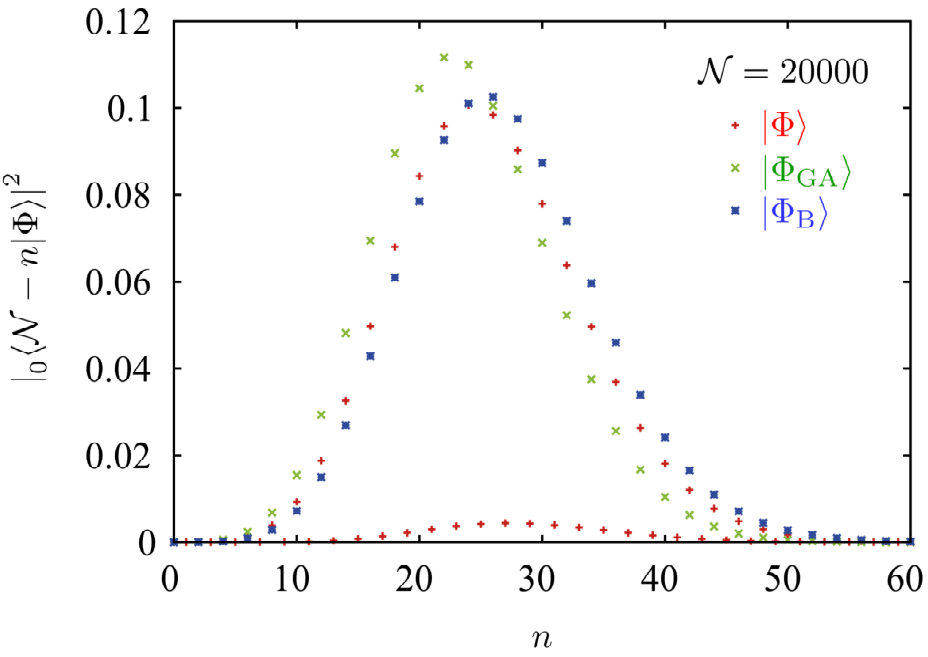

Figure 3: A picture from Ref. [17] : The squared projection $|\langle N-n|\Phi\rangle|^2$ for $\delta = 1.0\times10^{-6}$, $\varepsilon_{k_c}/\varepsilon_U = 100$, and $N = 20000$, where N is the total particle number. For comparison, the corresponding quantities obtained with the Bogoliubov and Girardeau–Arnowitt approximations are also plotted.

emerges in BEC systems naturally and physically due to the interaction even in an isolated system. Indeed, after the realization of BEC systems in experiments on vapors of rubidium [33], evidences for the macroscopic phase coherence in BEC systems, such as macroscopic interference effect [34] and quantum vortices in rotating systems [35], have been observed experimentally. Therefore, we reconsider the relation between BEC and superfluidity based on the idea that the condensed (or noncondensed) particle-number fluctuation due to the interaction induces a macroscopic phase in BEC systems at $T = 0$.

The superfluid particle number is generally different from the number of condensates [36]. Specifically, in strong-coupling systems such as liquid ^{4}He, condensed particle number is only about 10% or less of the total particle number of the liquid even at $T = 0$ [37], while superfluid component approaches the total density [38]. From the viewpoint of macroscopic coherence, these results indicate that all the particles have the same phase at $T = 0$ and it should be maintained dynamically. With this consideration, we observe the relaxation process of the wave function of an interacting BEC system and consider how the macroscopic phase is maintained dynamically. To do this, we generalize the variational method in Ref. [17] so as to describe the dynamics starting from the principle of least action. Specifically, we investigate the role of dynamical 3/2-body correlations beyond mean-field approximations.

It is also possible to apply this method to superconducting systems. In appendix B, we summarize the theory which describes dynamics of superconducting states beyond mean-field approximation.

Chapter 2 Variational Theories for Equilibrium States

Here, we construct a variational wave function that includes 3/2-body correlations with considering the external trap $V(\boldsymbol{r})$. After constructing the variational wave function, we reproduce the solution for single-component homogeneous systems given in Ref. [17]. We also formulate variational methods to (1) inhomogeneous systems (2) M-component Bose–Bose mixtures and (3) finite-temperature systems and show some numerical results based on respective methods.

2.1 Construction of a Variational Wave Function

Here, we consider identical Bose particles with mass m and spin 0 trapped in an external potential $V(\boldsymbol{r})$. The Hamiltonian is given by

$$\begin{aligned}\hat{H} \equiv & \int d\boldsymbol{r}\hat{\psi}^\dagger(\boldsymbol{r})K\hat{\psi}(\boldsymbol{r}) \\ & +\frac{1}{2}\int d\boldsymbol{r}_1\int d\boldsymbol{r}_2\hat{\psi}^\dagger(\boldsymbol{r}_1)\hat{\psi}^\dagger(\boldsymbol{r}_2)U(\boldsymbol{r}_1-\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_2)\hat{\psi}(\boldsymbol{r}_1),\end{aligned} \tag{29}$$

where $\hat{\psi}$ is the boson field operator, K is defined as $K \equiv \hat{\boldsymbol{p}}^2/2m + V(\boldsymbol{r})$ in terms of the momentum operator $\hat{\boldsymbol{p}}$, and $U(\boldsymbol{r}_1-\boldsymbol{r}_2) = U(\boldsymbol{r}_2-\boldsymbol{r}_1)$ is an interaction potential.

We expand $\hat{\psi}(\boldsymbol{r})$ in basis functions $\varphi_q(\boldsymbol{r}) \equiv \langle \boldsymbol{r}|q\rangle$, which are distinguished by a set of quantum numbers q and satisfy orthonormality $\langle q|q'\rangle = \delta_{qq'}$ and completeness $\sum_q |q\rangle\langle q| = 1$, as

$$\hat{\psi}(\boldsymbol{r}) = \sum_q \hat{c}_q\varphi_q(\boldsymbol{r}) \equiv \hat{\psi}_{\rm c}(\boldsymbol{r}) + \hat{\psi}_{\rm nc}(\boldsymbol{r}), \tag{30}$$

where $|q=0\rangle$ ($|q\neq 0\rangle$) denotes the one-particle state of condensates (noncondensates) and $\hat{\psi}_{\rm c}(\boldsymbol{r}) \equiv \hat{c}_0\varphi_0(\boldsymbol{r})$ [$\hat{\psi}_{\rm nc}(\boldsymbol{r}) \equiv \sum_{q\neq 0}\hat{c}_q\varphi_q(\boldsymbol{r})$] denotes the field operator for condensates (noncondensates). Using $(\hat{c}_q, \hat{c}_q^\dagger)$, Eq. (29) is transformed to

$$\hat{H} = \sum_{q_1q_2} K_{q_2q_1}\hat{c}_{q_2}^\dagger\hat{c}_{q_1} + \frac{1}{2}\sum_{q_1q_2q_3q_4} U_{q_4q_3;q_2q_1}\hat{c}_{q_4}^\dagger\hat{c}_{q_3}^\dagger\hat{c}_{q_2}\hat{c}_{q_1} \tag{31}$$

with

$$K_{q_1q_2} = \int d\boldsymbol{r}\varphi_{q_1}^*(\boldsymbol{r})\left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V(\boldsymbol{r})\right]\varphi_{q_2}(\boldsymbol{r}), \tag{32a}$$

$$U_{q_1q_2;q_3q_4} = \int d\boldsymbol{r}_1\int d\boldsymbol{r}_2 U(|\boldsymbol{r}_1-\boldsymbol{r}_2|)\varphi_{q_1}^*(\boldsymbol{r}_1)\varphi_{q_2}^*(\boldsymbol{r}_2)\varphi_{q_3}(\boldsymbol{r}_2)\varphi_{q_4}(\boldsymbol{r}_1). \tag{32b}$$

Our aim is to construct the ground-state wave function of Eq. (31) with Eqs. (32a) and (32b) that describes the weakly interacting inhomogeneous system characterized by an external potential $V(\boldsymbol{r})$. To carry this out, we classify $\hat{H}$ according to the number of noncondensed states involved as

$$\hat{H} = \hat{H}_0 + \hat{H}_{\frac{1}{2}} + \hat{H}_1 + \hat{H}_{\frac{3}{2}} + \hat{H}_2, \tag{33}$$

where

$$\hat{H}_0 = K_{00}\hat{c}_0^\dagger\hat{c}_0 + \frac{1}{2}U_{00;00}\hat{c}_0^\dagger\hat{c}_0^\dagger\hat{c}_0\hat{c}_0, \tag{34a}$$

$$\hat{H}_{\frac{1}{2}} = \sum_{q_1\neq 0}\Big(K_{0q_1}\hat{c}_0^\dagger\hat{c}_{q_1} + \text{H.C.}\Big) + \sum_{q_1\neq 0}\Big(U_{q_1 0;00}\hat{c}_{q_1}^\dagger\hat{c}_0^\dagger\hat{c}_0\hat{c}_0 + \text{H.C.}\Big), \tag{34b}$$

$$\begin{aligned}\hat{H}_1 = &\sum_{q_1,q_2\neq 0} K_{q_2q_1}\hat{c}_{q_2}^\dagger\hat{c}_{q_1} + \sum_{q_1 q_2\neq 0}\Big(U_{q_2 0;q_1 0} + U_{q_2 0;0q_1}\Big)\hat{c}_0^\dagger\hat{c}_0\hat{c}_{q_2}^\dagger\hat{c}_{q_1}\\ &+\frac{1}{2}\sum_{q_1 q_2\neq 0}\Big(U_{00;q_2q_1}\hat{c}_0^\dagger\hat{c}_0^\dagger\hat{c}_{q_2}\hat{c}_{q_1} + \text{H.C.}\Big),\end{aligned} \tag{34c}$$

$$\hat{H}_{\frac{3}{2}} = \sum_{q_1 q_2 q_3\neq 0}\Big(U_{0q_3;q_2q_1}\hat{c}_0^\dagger\hat{c}_{q_3}^\dagger\hat{c}_{q_2}\hat{c}_{q_1} + \text{H.C.}\Big), \tag{34d}$$

$$\hat{H}_2 = \frac{1}{2}\sum_{q_1 q_2 q_3 q_4\neq 0} U_{q_4q_3;q_2q_1}\hat{c}_{q_4}^\dagger\hat{c}_{q_3}^\dagger\hat{c}_{q_2}\hat{c}_{q_1}, \tag{34e}$$

where H.C. denotes the Hermitian conjugate.

Next, we introduce the number-conserving creation-annihilation operators[17, 39]. To carry this out, we give the orthonormal basis function for $q = 0$ as

$$|n\rangle_0 \equiv \frac{(\hat{c}_0^\dagger)^n}{\sqrt{n!}}|0\rangle \ \ (n = 0, 1, 2, \cdots, N). \tag{35}$$

The ground state without correlations is given by $|N\rangle_0$. The number-conserving operators are introduced as $(\hat{\beta}_0^\dagger, \hat{\beta}_0)$ for $n \geq 0$ by $\hat{\beta}_0^\dagger|n\rangle_0 \equiv |n+1\rangle_0$ and $\hat{\beta}_0|n+1\rangle_0 = |n\rangle_0$ with $\hat{\beta}_0|0\rangle \equiv 0$. These operators are expressible in terms of $(\hat{c}_0^\dagger, \hat{c}_0)$ as

$$\hat{\beta}_0^\dagger = \hat{c}_0^\dagger(1 + \hat{c}_0^\dagger\hat{c}_0)^{-\frac{1}{2}}, \tag{36a}$$

$$\hat{\beta}_0 = (1 + \hat{c}_0^\dagger\hat{c}_0)^{-\frac{1}{2}}\hat{c}_0, \tag{36b}$$

and obey $(\hat{\beta}_0^\dagger)^\nu\hat{\beta}_0^\nu|n\rangle_0 = \hat{\beta}_0^\nu(\hat{\beta}_0^\dagger)^\nu|n\rangle_0 = 0$ for integer $\nu \leq n$ and $(\hat{\beta}_0^\dagger)^\nu\hat{\beta}_0^\nu|n\rangle_0 = 0$ for $\nu > n$. Therefore, $(\hat{\beta}_0^\dagger)^\nu\hat{\beta}_0^\nu = 1$ and $\hat{\beta}_0^\nu(\hat{\beta}_0^\dagger)^\nu \simeq 1$ for $\nu = 1, 2, \cdots$. The latter approximation for $\nu \ll N$ is almost exact in the weak-coupling regime where the ground state is composed of the kets $|n\rangle_0$ with $n = O(N)$.

As a first step to construct the ground state, we give an inhomogeneous extension of the GA wave function [12]. First, we define the pair-correlation function as

$$\hat{\pi}^\dagger = \frac{1}{2}\sum_{q_1 q_2\neq 0}\phi_{q_1q_2}\hat{c}_{q_1}^\dagger\hat{c}_{q_2}^\dagger\hat{\beta}_0^2, \tag{37}$$

where $\phi_{qq'} = \phi_{q'q}$ is a variational parameter that characterizes the pair excitation of particles q and q' from condensates. Using $\hat{\pi}^\dagger$, we introduce the ground-state wave function as

$$|\Phi_{\text{GA}}\rangle = A_{\text{GA}}\exp(\hat{\pi}^\dagger)|N\rangle_0 = A_{\text{GA}}\sum_{\nu=0}^{[N/2]}\frac{(\hat{\pi}^\dagger)^\nu}{\nu!}|N - 2\nu\rangle_0, \tag{38}$$

where $[N/2]$ denotes the largest integer that does not exceed $N/2$ and A_{GA} is a normalization constant determined by $\langle\Phi_{\text{GA}}|\Phi_{\text{GA}}\rangle = 1$.

$|\Phi_{\rm GA}\rangle$ is the vacuum state characterized by $\hat{\gamma}_q\,|\Phi_{\rm GA}\rangle = 0$, where $\hat{\gamma}_q$ is the number-conserving quasiparticle operator defined as

$$\hat{\gamma}_q \equiv \sum_{q_1\neq 0}\left(u_{qq_1}\hat{c}_{q_1}\hat{\beta}_0^\dagger - v_{qq_1}\hat{c}_{q_1}^\dagger\hat{\beta}_0\right). \tag{39}$$

Here, we require that $(\hat{\gamma}_q^\dagger, \hat{\gamma}_q)$ obey the Bose commutator relation. In this case, matrices $\underline{u} \equiv (u_{q_1q_2})$ and $\underline{v} \equiv (v_{q_1q_2})$ are given in terms of $\underline{\phi} \equiv (\phi_{q_1q_2})$ and the unit matrix $\underline{1} \equiv (\delta_{q_1q_2})$ by

$$\underline{u} \equiv (\underline{1} - \underline{\phi}\;\underline{\phi}^\dagger)^{-\frac{1}{2}},\;\; \underline{v} \equiv (\underline{1} - \underline{\phi}\;\underline{\phi}^\dagger)^{-\frac{1}{2}}\underline{\phi}. \tag{40}$$

Therefore, they satisfy

$$\underline{u}^\dagger = \underline{u},\;\; \underline{v}^{\rm T} = \underline{v},\;\; \underline{u}\;\underline{u}^\dagger - \underline{v}\;\underline{v}^\dagger = \underline{1},\;\; \underline{u}\;\underline{v} = \underline{v}\;\underline{u}^*, \tag{41}$$

where T denotes the transposition of a matrix. The third and fourth relations are summarized as the following matrix form:

$$\begin{bmatrix} \underline{u} & \underline{v} \\ \underline{v}^* & \underline{u}^* \end{bmatrix}\begin{bmatrix} \underline{u} & -\underline{v} \\ -\underline{v}^* & \underline{u}^* \end{bmatrix} = \begin{bmatrix} \underline{1} & \underline{0} \\ \underline{0} & \underline{1} \end{bmatrix}. \tag{42}$$

Using Eq. (42), $(\hat{c}_q, \hat{c}_q^\dagger)$ are also expressible in terms of $(\hat{\gamma}_q, \hat{\gamma}_q^\dagger)$ as follows:

$$\hat{c}_q\hat{\beta}_0^\dagger = \sum_{q_1\neq 0}\left(u_{qq_1}\hat{\gamma}_{q_1} + v_{qq_1}\hat{\gamma}_{q_1}^\dagger\right), \tag{43a}$$

$$\hat{c}_q^\dagger\hat{\beta}_0 = \sum_{q_1\neq 0}\left(u_{qq_1}^*\hat{\gamma}_{q_1}^\dagger + v_{qq_1}^*\hat{\gamma}_{q_1}\right). \tag{43b}$$

Note that $|\Phi_{\rm GA}\rangle$ only includes pair processes via $\underline{\phi}$, meaning that it has no contributions from $\hat{H}_{\frac{3}{2}}$ and $\hat{H}_{\frac{1}{2}}$, i.e., $\langle\Phi_{\rm GA}|\,\hat{H}_{\frac{3}{2}}\,|\Phi_{\rm GA}\rangle = \langle\Phi_{\rm GA}|\,\hat{H}_{\frac{1}{2}}\,|\Phi_{\rm GA}\rangle = 0$. To incorporate 3/2-body correlations, we need to characterize them by introducing the corresponding variational parameters as outlined below.

Next, we improve $|\Phi_{\rm GA}\rangle$ so that $\hat{H}_{\frac{3}{2}}$ yields finite contributions to lower the variational ground-state energy further. The ground state with a new operator may be introduced as

$$|\Phi\rangle \equiv A_3\exp\left(\hat{\pi}_3^\dagger\right)|\Phi_{\rm GA}\rangle,\;\; \hat{\pi}_3^\dagger \equiv \frac{1}{3!}\sum_{q_1q_2q_3\neq 0} w_{q_1q_2q_3}\hat{\gamma}_{q_1}^\dagger\hat{\gamma}_{q_2}^\dagger\hat{\gamma}_{q_3}^\dagger, \tag{44}$$

where $w_{q_1q_2q_3}$ is a variational parameter characterized by 3/2-body correlations satisfying $\hat{P}_{q_1q_2q_3}w_{q_1q_2q_3} = w_{q_1q_2q_3}$ for any permutation $\hat{P}$ with three elements (q_1, q_2, q_3) and A_3 is the normalization constant expressed as

$$A_3^{-2} = \langle\Phi_{\rm GA}|\exp\left(\hat{\pi}_3\right)\exp\left(\hat{\pi}_3^\dagger\right)|\Phi_{\rm GA}\rangle = \exp\left(\frac{1}{3!}\sum_{q_1q_2q_3\neq 0}|w_{q_1q_2q_3}|^2 + O\Big(|w|^4\Big)\right). \tag{45}$$

Here, we omit the higher-order terms $O\Big(|w|^4\Big)$ in the present weak-coupling consideration. In this case, we obtain

$$\langle\Phi|\,\hat{\gamma}_{q_1}^\dagger\hat{\gamma}_{q_2}^\dagger\hat{\gamma}_{q_3}^\dagger\,|\Phi\rangle = \frac{\delta\ln A_3^{-2}}{\delta w_{q_1q_2q_3}} \simeq w_{q_1q_2q_3}^*. \tag{46}$$

Note that $\langle\Phi|\,\hat{\gamma}^\dagger_{q_1}\hat{\gamma}_{q_2}\hat{\gamma}_{q_3}\,|\Phi\rangle$, $\langle\Phi|\,\hat{\gamma}_{q_1}\hat{\gamma}_{q_2}\,|\Phi\rangle$, and their complex conjugates are neglected since they are all higher-order contributions. In addition, we have $\langle\Phi|\,\hat{H}_{\frac{1}{2}}\,|\Phi\rangle = 0$.

On the basis of $|\Phi\rangle$, we obtain expressions for the ground-state energy and self-consistent equations embodying energy-minimum conditions. To express the ground-state energy explicitly, we define the following quantities:

$$\begin{aligned}
&\rho_{q_1q_2} \equiv \langle\Phi|\,\hat{c}^\dagger_{q_2}\hat{c}_{q_1}\,|\Phi\rangle = \rho^*_{q_2q_1} \\
&= \frac{1}{2}\sum_{q_3\neq 0}\Big(u_{q_1q_3}u^*_{q_2q_3} + v_{q_1q_3}v^*_{q_3q_2}\Big) + \sum_{q_3q_4\neq 0}\Big(u_{q_1q_3}u^*_{q_2q_4} + v_{q_1q_4}v^*_{q_2q_3}\Big)\rho^{\frac{3}{2}}_{q_3q_4} - \frac{1}{2}\delta_{q_1q_2}, \qquad (47a)\\
&F_{q_1q_2} \equiv \langle\Phi|\,\hat{c}_{q_1}\hat{c}_{q_2}(\hat{\beta}^\dagger_0)^2\,|\Phi\rangle = F_{q_2q_1} \\
&= \sum_{q_3\neq 0} u_{q_1q_3}v_{q_3q_2} + \sum_{q_3q_4\neq 0}\Big(u_{q_1q_3}v_{q_2q_4} + v_{q_1q_4}u_{q_2q_3}\Big)\rho^{\frac{3}{2}}_{q_3q_4}, \qquad (47b)\\
&W_{q_1q_2;q_3} \equiv \langle\Phi|\,\hat{c}^\dagger_{q_3}\hat{c}_{q_2}\hat{c}_{q_1}\hat{\beta}^\dagger_0\,|\Phi\rangle \\
&= \sum_{q_4q_5q_6\neq 0}\Big(u_{q_1q_4}u_{q_2q_5}v^*_{q_3q_6}w_{q_4q_5q_6} + v_{q_1q_4}v_{q_2q_5}u^*_{q_3q_6}w^*_{q_4q_5q_6}\Big), \qquad (47c)
\end{aligned}$$

where

$$\rho^{\frac{3}{2}}_{q_1q_2} \equiv \langle\Phi|\,\hat{\gamma}^\dagger_{q_2}\hat{\gamma}_{q_1}\,|\Phi\rangle \simeq \frac{1}{2}\sum_{q_3q_4} w_{q_1q_3q_4}w^*_{q_2q_3q_4} \qquad (48)$$

and we approximate

$$(\hat{c}^\dagger_0)^m(\hat{c}_0)^n \simeq (N_0)^{\frac{m+n}{2}}(\hat{\beta}^\dagger_0)^m(\hat{\beta}_0)^n, \qquad (49)$$

where N_0 denotes the number of condensed particles. Therefore, we obtain an expression for the ground-state energy $\mathcal{E} \equiv \langle\Phi|\,\hat{H}\,|\Phi\rangle$ as

$$\mathcal{E} = \mathcal{E}[\phi_{q_aq_b}, \phi^*_{q_aq_b}, w_{q_aq_bq_c}, w^*_{q_aq_bq_c}] = \mathcal{E}_0 + \mathcal{E}_1 + \mathcal{E}_{\frac{3}{2}} + \mathcal{E}_2, \qquad (50)$$

where

$$\begin{aligned}
\mathcal{E}_0 &= \langle\Phi|\,\hat{H}_0\,|\Phi\rangle = K_{00}N_0 + \frac{1}{2}U_{00;00}N_0^2, \qquad (51a)\\
\mathcal{E}_1 &= \langle\Phi|\,\hat{H}_1\,|\Phi\rangle = \sum_{q_1,q_2\neq 0} K_{q_2q_1}\rho_{q_1q_2} + N_0\sum_{q_1q_2\neq 0}\Big(U_{q_20;q_10} + U_{q_20;0q_1}\Big)\rho_{q_1q_2} \\
&\quad + \frac{N_0}{2}\sum_{q_1q_2\neq 0}\Big(U_{00;q_2q_1}F_{q_1q_2} + \text{C.C.}\Big), \qquad (51b)\\
\mathcal{E}_{\frac{3}{2}} &= \langle\Phi|\,\hat{H}_{\frac{3}{2}}\,|\Phi\rangle = \sqrt{N_0}\sum_{q_1q_2q_3\neq 0}\Big(U_{0q_3;q_2q_1}W_{q_1q_2q_3} + \text{C.C.}\Big), \qquad (51c)\\
\mathcal{E}_2 &= \langle\Phi|\,\hat{H}_2\,|\Phi\rangle \simeq \frac{1}{2}\sum_{q_1q_2q_3q_4\neq 0} U_{q_4q_3;q_2q_1}\Big(F_{q_1q_2}F^*_{q_3q_4} + \rho_{q_2q_4}\rho_{q_1q_3} + \rho_{q_1q_4}\rho_{q_2q_3}\Big), \qquad (51d)
\end{aligned}$$

where C.C. denotes complex conjugate and we use the decomposition as

$$\langle\Phi|\,\hat{c}^\dagger_{q_4}\hat{c}^\dagger_{q_3}\hat{c}_{q_2}\hat{c}_{q_1}\,|\Phi\rangle \simeq F^*_{q_4q_3}F_{q_2q_1} + \rho_{q_2q_4}\rho_{q_1q_3} + \rho_{q_1q_4}\rho_{q_2q_3}. \qquad (52)$$

In principle, the stationary condition $\delta\mathcal{E}=0$ gives self-consistent equations for $\phi_{q_1q_2}$ and $w_{q_1q_2q_3}$. However, the explicit expression for $\delta\mathcal{E}/\delta\phi^*_{q_aq_b}$ is difficult to obtain unlike the case of homogeneous systems. This is because $u_{q_1q_2}$ and $v_{q_1q_2}$ are expressed by $\phi_{q_1q_2}$ as given in Eq. (40), which includes the square root of inverse matrices and is too complicated to perform variational calculations. For this reason, we introduce a potential Ω and consider the conditions equivalent to $\delta\mathcal{E}/\delta\phi^*_{q_aq_b}=\delta\mathcal{E}/\delta w^*_{q_aq_bq_c}=0$ on the basis of Lagrange multipliers. Here, we introduce Ω as

$$\Omega=\mathcal{E}+\mu\left[N-\left(N_0+\sum_{q\neq0}\rho_{qq}\right)\right]+\frac{1}{2}\sum_{q_1q_2\neq0}\left[\delta_{q_1q_2}-\sum_{q_3\neq0}\left(u^*_{q_3q_1}u_{q_3q_2}-v_{q_3q_1}v^*_{q_3q_2}\right)\right]\lambda_{q_2q_1}, \quad (53)$$

where μ and $\lambda_{q_1q_2}$are Lagrange multipliers whose variational conditions give the following constraint conditions:

$$N_0+\sum_{q\neq0}\rho_{qq}=N, \quad (54a)$$

$$\sum_{q_3\neq0}\left(u_{q_1q_3}u^*_{q_2q_3}-v_{q_1q_3}v^*_{q_2q_3}\right)=\delta_{q_1q_2}. \quad (54b)$$

Minimizing Ω instead of $\mathcal{E}$ corresponds to changing the independent variational parameters from $(\phi_{q_1q_2},w_{q_1q_2q_3},\text{C.C.})$ to $(N_0,\mu,u_{q_1q_2},v_{q_1q_2},\lambda_{q_1q_2},w_{q_1q_2q_3},\text{C.C.})$.

Now, we carry out the following variational calculations:

$$\underline{\frac{\delta\Omega}{\delta N_0}=0}\rightarrow\mu=\xi_{00}-\frac{1}{2}(\Delta_{00}+\text{C.C.})+\sum_{q_1q_2\neq0}\left(U_{00;q_1q_2}F_{q_1q_2}+\text{C.C.}\right)$$
$$+\frac{1}{2\sqrt{N_0}}\sum_{q_1q_2q_3\neq0}\left(U_{0q_3;q_2q_1}W_{q_1q_2q_3}+\text{C.C.}\right), \quad (55a)$$

$$\underline{\frac{\delta\Omega}{\delta u^*_{q_aq_b}}=0\ \text{ and }\ \frac{\delta\Omega}{\delta v_{q_aq_b}}=0}$$
$$\rightarrow\sum_{q_1,q_2\neq0}\begin{bmatrix}\xi_{q_aq_1}&\Delta_{q_aq_1}\\-\Delta^*_{q_aq_1}&-\xi^*_{q_aq_1}\end{bmatrix}\begin{bmatrix}u_{q_1q_2}\\v^*_{q_1q_2}\end{bmatrix}(\delta_{q_2q_b}+2\rho^{\frac{3}{2}}_{q_2q_b})+\begin{bmatrix}\chi^{(1)}_{q_aq_b}\\\chi^{(2)}_{q_aq_b}\end{bmatrix}$$
$$=\sum_{q_1\neq0}\begin{bmatrix}u_{q_aq_1}\\v^*_{q_aq_1}\end{bmatrix}\lambda_{q_1q_b}, \quad (55b)$$

$$\underline{\frac{\delta\Omega}{\delta w^*_{q_aq_bq_c}}=0}\rightarrow w_{q_aq_bq_c}=-\frac{b_{q_aq_bq_c}}{a_{q_aq_a}+a_{q_bq_b}+a_{q_cq_c}}, \quad (55c)$$

where we define the following quantities:

$$\xi_{q_a q_b} \equiv K_{q_a q_b} - \mu\delta_{q_a q_b} + N_0(U_{q_a 0;q_b 0} + U_{q_a 0;0 q_b}) + \sum_{q_1 q_2 \neq 0} \Big(U_{q_a q_2;q_b q_1} + U_{q_a q_2;q_1 q_b}\Big)\rho_{q_1 q_2}, \tag{56a}$$

$$\Delta_{q_a q_b} \equiv N_0 U_{q_b q_a;00} + \sum_{q_1 q_2 \neq 0} U_{q_a q_b;q_2 q_1} F_{q_1 q_2}, \tag{56b}$$

$$\chi^{(1)}_{q_a q_b} \equiv 2\sqrt{N_0} \sum_{q_1 q_2 q_3 q_4 \neq 0} \Big[U_{0 q_a;q_2 q_1} v_{q_1 q_3} v_{q_2 q_4} + (U_{q_a q_1;q_2 0} + U_{q_1 q_a;q_2 0}) u^*_{q_1 q_3} v_{q_2 q_4}\Big] w^*_{q_3 q_4 q_b}, \tag{56c}$$

$$\chi^{(2)}_{q_a q_b} \equiv -2\sqrt{N_0} \sum_{q_1 q_2 q_3 q_4 \neq 0} \Big[U_{q_1 q_2;q_a 0} u^*_{q_1 q_3} u^*_{q_2 q_4} + (U_{0 q_2;q_1 q_a} + U_{0 q_2;q_a q_1}) v_{q_1 q_3} u^*_{q_2 q_4}\Big] w^*_{q_3 q_4 q_b}, \tag{56d}$$

$$a_{q_a q_b} \equiv \sum_{q_1 q_2 \neq 0} \xi_{q_1 q_2}(u_{q_2 q_b} u^*_{q_1 q_a} + v_{q_2 q_b} v^*_{q_1 q_a}) + \sum_{q_1 q_2 \neq 0} \Big(\Delta^*_{q_1 q_2} u_{q_2 q_b} v_{q_1 q_a} + \Delta_{q_1 q_2} u^*_{q_2 q_a} v^*_{q_1 q_b}\Big), \tag{56e}$$

$$b_{q_a q_b q_c} \equiv \sqrt{N_0} \sum_{\hat{P}} \hat{P}_{q_a q_b q_c} \sum_{q_1 q_2 q_3 \neq 0} \Big[U_{q_1 q_2;q_3 0} u^*_{q_a q_1} u^*_{q_b q_2} v_{q_c q_3} + U_{0 q_3;q_2 q_1} v_{q_a q_1} v_{q_b q_2} u^*_{q_c q_3}\Big] + \frac{1}{2} \sum_{\hat{P}} \hat{P}_{q_a q_b q_c} \sum_{q_1 \neq q_a \neq 0} a_{q_a q_1} w_{q_1 q_b q_c}. \tag{56f}$$

Within our theory, we can also derive the GP equation [19, 20] including 3/2-body correlations for inhomogeneous systems, which is obtained by $\delta\Omega/\delta\varphi^*_0(\boldsymbol{r}) = 0$:

$$\int d\boldsymbol{r}_1 \Big[\hat{\mathcal{K}}(\boldsymbol{r}, \boldsymbol{r}_1)\varphi_0(\boldsymbol{r}_1) - \Delta(\boldsymbol{r}, \boldsymbol{r}_1)\varphi^*_0(\boldsymbol{r}_1)\Big] = -\int d\boldsymbol{r}_1 U(|\boldsymbol{r} - \boldsymbol{r}_1|)\left[2F(\boldsymbol{r}, \boldsymbol{r}_1)\varphi^*_0(\boldsymbol{r}_1) + \frac{W(\boldsymbol{r}, \boldsymbol{r}_1, \boldsymbol{r}_1)}{\sqrt{N_0}}\right], \tag{57}$$

where we define the following self-consistent conditions:

$$\begin{aligned}\hat{\mathcal{K}}(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv& \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)(\hat{K}_2 - \mu) + \int d\boldsymbol{r}_3 \Big\{U(\boldsymbol{r}_2 - \bar{\boldsymbol{r}}_3)\big[\rho(\bar{\boldsymbol{r}}_3, \bar{\boldsymbol{r}}_3) + N_0|\varphi_0(\bar{\boldsymbol{r}}_3)|^2\big]\Big\} \\ &+ U(\boldsymbol{r}_1 - \boldsymbol{r}_2) \times \big[\rho(\boldsymbol{r}_1, \boldsymbol{r}_2) + N_0\varphi_0(\boldsymbol{r}_1)\varphi^*_0(\boldsymbol{r}_2)\big] \\ \equiv& \delta(\boldsymbol{r}_1 - \boldsymbol{r}_2)(\hat{K}_2 - \mu) + \Sigma(\boldsymbol{r}_1, \boldsymbol{r}_2)\end{aligned} \tag{58a}$$

$$\Delta(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv U(\boldsymbol{r}_1 - \boldsymbol{r}_2)\big[F(\boldsymbol{r}_1, \boldsymbol{r}_2) + N_0\varphi_0(\boldsymbol{r}_1)\varphi_0(\boldsymbol{r}_2)\big], \tag{58b}$$

$$\rho(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv \sum_{q_1 q_2 \neq 0} \rho_{q_1 q_2}\varphi_{q_1}(\boldsymbol{r}_1)\varphi^*_{q_2}(\boldsymbol{r}_2), \tag{58c}$$

$$F(\boldsymbol{r}_1, \boldsymbol{r}_2) \equiv \sum_{q_1 q_2 \neq 0} F_{q_1 q_2}\varphi_{q_1}(\boldsymbol{r}_1)\varphi_{q_2}(\boldsymbol{r}_2), \tag{58d}$$

$$W(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) \equiv \sum_{q_1 q_2 q_3 \neq 0} W_{q_1 q_2 q_3}\varphi_{q_1}(\boldsymbol{r}_1)\varphi_{q_2}(\boldsymbol{r}_2)\varphi^*_{q_3}(\boldsymbol{r}_3). \tag{58e}$$

By solving Eq. (57) with the self-consistent conditions, we obtain the condensate wave function $\varphi_0(\boldsymbol{r})$ deformed by interaction between particles.

2.2 Equations for Homogeneous Systems

This formulation can be applied to a homogeneous BEC system with $V = 0$ [17] by changing the subscript as $q \to \boldsymbol{k}$ and the basis function as $\varphi_q(\boldsymbol{r}) \to e^{i\boldsymbol{k}\cdot\boldsymbol{r}}/\sqrt{\mathcal{V}}$, where $\boldsymbol{k}$ denotes the wave number of a particle. In this case, the basic matrix elements are given by

$$K_{\boldsymbol{k}\boldsymbol{k}'} = \delta_{\boldsymbol{k},\boldsymbol{k}'}\varepsilon_k,\ U_{\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3\boldsymbol{k}_4} = \frac{\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}}{\mathcal{V}}U_{|\boldsymbol{k}_1-\boldsymbol{k}_3|},\ \phi_{\boldsymbol{k}\boldsymbol{k}'} = \delta_{\boldsymbol{k},-\boldsymbol{k}'}\phi_{\boldsymbol{k}}, \tag{59}$$

with $\phi_{\boldsymbol{k}} = \phi_{-\boldsymbol{k}} = \phi^*_{\boldsymbol{k}}$, $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = w^*_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ and

$$\varepsilon_k = \frac{\hbar^2|\boldsymbol{k}|^2}{2m} = \frac{\hbar^2k^2}{2m},\ U_{|\boldsymbol{k}|} = \int d\boldsymbol{r}U(\boldsymbol{r})e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}. \tag{60}$$

With these relations, we obtain the following variational conditions:

$$\mu = \frac{U_0N_{\boldsymbol{0}}}{\mathcal{V}} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}U_{k'}F_{\boldsymbol{k}'} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}(U_0+U_{k'})\rho_{\boldsymbol{k}'}$$
$$+ \frac{1}{\mathcal{V}\sqrt{N_{\boldsymbol{0}}}}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}U_{k_1}W_{\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3}, \tag{61a}$$

$$(1+2\rho^{\frac{3}{2}}_{\boldsymbol{k}})\begin{bmatrix}\xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}}\\ -\Delta_{\boldsymbol{k}} & -\xi_{\boldsymbol{k}}\end{bmatrix}\begin{bmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{bmatrix} + \begin{bmatrix}\chi^{(1)}_{\boldsymbol{k}}\\ \chi^{(2)}_{\boldsymbol{k}}\end{bmatrix} = \begin{bmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{bmatrix}\lambda_{\boldsymbol{k}}, \tag{61b}$$

$$w_{\boldsymbol{k}_a\boldsymbol{k}_b\boldsymbol{k}_c} = -\frac{b_{\boldsymbol{k}_a\boldsymbol{k}_b\boldsymbol{k}_c}}{a_{\boldsymbol{k}_a}+a_{\boldsymbol{k}_b}+a_{\boldsymbol{k}_c}}, \tag{61c}$$

where

$$\xi_{\boldsymbol{k}} \equiv \xi_{\boldsymbol{k}\boldsymbol{k}} = \varepsilon_k - \mu + \frac{N_{\boldsymbol{0}}}{\mathcal{V}}(U_k+U_0) + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'\neq\boldsymbol{0}}(U_{|\boldsymbol{k}-\boldsymbol{k}'|}+U_{\boldsymbol{0}})\rho_{\boldsymbol{k}'}, \tag{62a}$$

$$\Delta_{\boldsymbol{k}} \equiv \Delta_{\boldsymbol{k},-\boldsymbol{k}} = \frac{N_0U_k}{\mathcal{V}} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'\neq\boldsymbol{0}}U_{|\boldsymbol{k}-\boldsymbol{k}'|}F_{\boldsymbol{k}'}, \tag{62b}$$

$$\chi^{(1)}_{\boldsymbol{k}} \equiv \chi^{(1)}_{\boldsymbol{k}\boldsymbol{k}} = \frac{2\sqrt{N_0}}{\mathcal{V}}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}\delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}\Big[U_{k_2}v_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3} + (U_k+U_{k_2})u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3}\Big]w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}, \tag{62c}$$

$$\chi^{(2)}_{\boldsymbol{k}} \equiv \chi^{(2)}_{\boldsymbol{k}\boldsymbol{k}} = -\frac{2\sqrt{N_0}}{\mathcal{V}}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}\delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}\Big[U_{k_2}u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3} + (U_k+U_{k_2})v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}\Big]w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}, \tag{62d}$$

$$a_{\boldsymbol{k}} = \xi_{\boldsymbol{k}}(u^2_{\boldsymbol{k}}+v^2_{\boldsymbol{k}}) + 2\Delta_{\boldsymbol{k}}u_{\boldsymbol{k}}v_{\boldsymbol{k}}, \tag{62e}$$

$$b_{\boldsymbol{k}_a\boldsymbol{k}_b\boldsymbol{k}_c} \equiv \frac{\sqrt{N_0}}{\mathcal{V}}\delta_{\boldsymbol{k}_a+\boldsymbol{k}_b+\boldsymbol{k}_c}u_{\boldsymbol{k}_a}u_{\boldsymbol{k}_b}u_{\boldsymbol{k}_c}\Big[(U_{k_a}+U_{k_b})(\phi_{\boldsymbol{k}_c}+\phi_{\boldsymbol{k}_a}\phi_{\boldsymbol{k}_b})$$
$$+ (U_{k_b}+U_{k_c})(\phi_{\boldsymbol{k}_a}+\phi_{\boldsymbol{k}_b}\phi_{\boldsymbol{k}_c}) + (U_{k_a}+U_{k_c})(\phi_{\boldsymbol{k}_b}+\phi_{\boldsymbol{k}_a}\phi_{\boldsymbol{k}_c})\Big], \tag{62f}$$

$$\rho^{\frac{3}{2}}_{\boldsymbol{k}} = \frac{1}{2}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2. \tag{62g}$$

Using the relation between $\phi_{\boldsymbol{k}}$ and $(u_{\boldsymbol{k}}, v_{\boldsymbol{k}})$ in Eq. (41) given by

$$u_{\boldsymbol{k}} = \frac{1}{\sqrt{1-\phi_{\boldsymbol{k}}^2}},\ v_{\boldsymbol{k}} = \frac{\phi_{\boldsymbol{k}}}{\sqrt{1-\phi_{\boldsymbol{k}}^2}}, \tag{63}$$

we obtain equation for $\phi_{\boldsymbol{k}}$ as

$$\phi_{\boldsymbol{k}} = \frac{-\xi_{\boldsymbol{k}} + \sqrt{\xi_{\boldsymbol{k}}^2 - \Delta_{\boldsymbol{k}}(\Delta_{\boldsymbol{k}} - \chi_{\boldsymbol{k}})}}{\Delta_{\boldsymbol{k}}}, \tag{64}$$

where $\chi_{\boldsymbol{k}}$ is defined as

$$\begin{aligned}\chi_{\boldsymbol{k}} = \frac{1}{1+2\rho_{\boldsymbol{k}}^{\frac{3}{2}}}\frac{\chi_{\boldsymbol{k}}^{(1)}\phi_{\boldsymbol{k}} - \chi_{\boldsymbol{k}}^{(2)}}{u_{\boldsymbol{k}}} = \frac{2\sqrt{N_0}}{1+2\rho_{\boldsymbol{k}}^{\frac{3}{2}}}\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}\delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}\frac{u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}}{u_{\boldsymbol{k}}} \\ \times\left[U_{k_2}(1+\phi_{\boldsymbol{k}}\phi_{\boldsymbol{k}_2}\phi_{\boldsymbol{k}_3}) + (U_k + U_{k_2})(\phi_{\boldsymbol{k}_2} + \phi_{\boldsymbol{k}}\phi_{\boldsymbol{k}_3})\right].\end{aligned} \tag{65}$$

Conditions for $\phi_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_a\boldsymbol{k}_b\boldsymbol{k}_c}$ set self-consistent equations.

Here, we introduce the model for numerical calculation in the previous study used in Ref. [17]. In this study, numerical calculations were performed for the contact interaction potential $U_k = U$ used widely in the literature to make a direct comparison possible. For convenience, we express this U as

$$U = \frac{4\pi\hbar^2 a_U}{m}. \tag{66}$$

The ultraviolet divergence inherent in the potential were removed by introducing a cutoff wave number $k_{\rm c}$ into every summation over k as

$$\sum_{\boldsymbol{k}}{}' \to \sum_{\boldsymbol{k}}{}'\theta(k_{\rm c} - k). \tag{67}$$

The s-wave scattering length a which originate from U is obtained by

$$\frac{m}{4\pi\hbar^2 a} = \frac{1}{U} + \int\frac{d^3k}{(2\pi)^3}\frac{\theta(k_{\rm c}-k)}{2\varepsilon_k}. \tag{68}$$

which yields

$$a = \frac{a_U}{1 + 2k_{\rm c}a_U/\pi}. \tag{69}$$

If $k_{\rm c}$ is chosen as $k_{\rm c}a_U \ll 1$, we can approximate $a \simeq a_U$. The units of energy and wavenumber were also introduced for performing the numerical calculations. The characteristic energy and wavenumber of this system are defined by

$$\varepsilon_U \equiv \bar{n}U,\ k_U = \sqrt{8\pi a_U\bar{n}}, \tag{70}$$

where $\bar{n} \equiv N/V$. Using these quantities, the dimensionless coupling constants is denoted as $\delta \equiv a_U^3\bar{n}_{\rm all}$. We note that we use this model with some modifications in the second chapter.

2.3 Application (1) : Inhomogeneous Systems in External Traps

As one of the simplest numerical examples, we here consider a 1D system ($\boldsymbol{r} \to z$) trapped by a harmonic oscillator $V(z) = m\omega^2 z^2/2$ with a short-range contact potential written as $U(\boldsymbol{r}_a - \boldsymbol{r}_b) = U(z_a - z_b) = g\delta(z_a - z_b)$. Using the potential, we transform Eq. (57) into

$$\left\{ -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2} + \frac{m\omega^2 z^2}{2} - \mu + \xi(z) \right\} \varphi_0(z) - \Delta(z)\varphi_0^*(z) = -g\left[2F(z)\varphi_0^*(z) + \frac{W(z)}{\sqrt{N_0}} \right], \tag{71}$$

where $X(\boldsymbol{r}) = X(\boldsymbol{r}, \boldsymbol{r})$ ($X = \xi$, Δ, and F) and $W(\boldsymbol{r}) = W(\boldsymbol{r}, \boldsymbol{r}, \boldsymbol{r})$. In the following calculation, we set the units of energy $\varepsilon_\omega = \hbar\omega/2$ and length $l_\omega = (\hbar/m\omega)^{\frac{1}{2}}$.

We point out that it is crucial to choose an appropriate $|q\rangle$ that corresponds to the external potential considered in the present formulation. In the limit $g \to 0$, the condensate wave function $\varphi_0(\boldsymbol{r})$ becomes a Gaussian. On the other hand, $\varphi_0(\boldsymbol{r})$ deforms due to the nonlinear term of the GP equation when we set a larger g, such as in the case of a Thomas–Fermi BEC [40]. With these considerations, we propose two approximations in the weak-coupling region as follows:

(i) : $|q\rangle \simeq |n\rangle$ for all $n \geq 0$,

(ii) : $\langle \boldsymbol{r}|0\rangle = \varphi_0^{\rm GP}(\boldsymbol{r})$ and $|q\rangle \simeq |n\rangle$ for $n > 0$,

where $\varphi_0^{\rm GP}(\boldsymbol{r})$ represents the solution of Eq. (71); integer $n \leq n_{\rm cut}$ is a quantum number that characterizes the energy levels of a harmonic oscillator and $n_{\rm cut}$ is the cutoff energy level. On the basis of the approximation, $\varphi_n(z) = \langle z|n\rangle$ is given as

$$\varphi_n(z) \equiv \left(\frac{1}{2^n n! \sqrt{\pi} l_\omega} \right)^{\frac{1}{2}} H_n\left(\frac{z}{l_\omega} \right) \exp\left(-\frac{z^2}{2l_\omega^2} \right), \tag{72}$$

where H_n denotes the nth Hermite polynomial. Hence, we obtain $K_{n_1 n_2}$ and $U_{n_1 n_2; n_3 n_4}$ as

$$K_{n_1 n_2} = \delta_{n_1 n_2}(2n_1 + 1)\varepsilon_\omega, \tag{73a}$$

$$U_{n_1 n_2; n_3 n_4} = g \int_{-l_{\rm cut}}^{l_{\rm cut}} dz \varphi_{n_1}(z)\varphi_{n_2}(z)\varphi_{n_3}(z)\varphi_{n_4}(z), \tag{73b}$$

where $l_{\rm cut}$ is the cutoff length for numerical calculations.

To carry out the numerical calculations, we introduce the external parameter (coupling constant in a trapped system) as

$$\alpha \equiv \frac{mgl_\omega}{\hbar^2} = \frac{1}{2}\frac{g}{\varepsilon_\omega l_\omega} \ll 1. \tag{74}$$

This parameter denotes the ratio of the scales for the correlation of particles and the harmonic oscillator potential. In this work, we carry out the numerical calculations for $N = 1000$ and $\alpha \sim 1.0 \times 10^{-3}$, where the condensate wave function has an approximately Gaussian profile [41]. In addition, we neglect the $O(|w|^2)$ terms in the self-consistent conditions because they give only a small correction to the ground-state wave function in the weak-coupling regime. We choose $n_{\rm cut} = 40$ ($\varepsilon_{n_{\rm cut}} = 81\varepsilon_\omega$) and $l_{\rm cut} = 10l_\omega$ ($m\omega l_\omega^2/2 = 100\varepsilon_\omega \sim \varepsilon_{n_{\rm cut}}$) for the numerical calculations. We start

the initial self-consistent calculation by substituting the trivial solutions for $g = 0$ and renew the solutions one after another while mixing the old and new solutions with the weight ratio of 80 : 20.

Now, we discuss the numerical results. First, we show the ground-state energy $\mathcal{E}_\sigma$ ($\sigma = 0, 1, 3/2, 2$) to explain the respective energy scales in Tables 5 and 6. From these tables, we see that $|\mathcal{E}_0| \gg |\mathcal{E}_1| \gg |\mathcal{E}_2| > |\mathcal{E}_{\frac{3}{2}}|$. However, $\mathcal{E}_{\frac{3}{2}}$ is comparable to $\mathcal{E}_2$ around $\alpha \sim 1.0 \times 10^{-3}$. In addition, $|\mathcal{E}_{\frac{3}{2}}|/|\mathcal{E}_2|$ seems to increase monotonically as a function of α so that the 3/2-body correlation may be dominant in the relatively strong coupling system, such as the Thomas–Fermi BEC regime. Comparing Tables 5 and 6, we find that approximation (ii) yields lower total ground-state energies than approximation (i) because the deformation of the condensate wave function also lowers the ground-state energy. Hence, one might conclude that (ii) is better than (i). However, (ii) appears to break the orthogonality relation, i.e., $\langle 0|n\rangle \neq \delta_{0n}$ for $n > 0$. To evaluate the ground-state energies more quantitatively, setting appropriate one-particle states with orthogonality relations remains a future task.

Incorporating more variational parameters in the theory is expected to yield a better estimate for the ground-state energy. To see this explicitly, we perform our variational calculations on the basis of the following ground states:

(1) $|\Phi_{\rm GP}\rangle$: We set $\phi_{n_1n_2} = w_{n_1n_2n_3} = 0$.

(2) $|\Phi_{\rm Bog}\rangle$: We obtain $\phi_{n_1n_2}$ while fixing $\rho_{n_1n_2} = F_{n_1n_2} = w_{n_1n_2n_3} = 0$.

(3) $|\Phi_{\rm HFB}\rangle$: We set $\lambda_{n_1n_2} = E_{n_1}\delta_{n_1n_2}$ and $w_{n_1n_2n_3} = 0$. This is equivalent to the problem of diagonalizing the effective Hamiltonian [13].

(4) $|\Phi_{\rm GA}\rangle$: All the variational parameters except $w_{n_1n_2n_3}$ are calculated self-consistently. The ground state is equivalent to the GA wave function.

(5) $|\Phi\rangle$: All the variational parameters are calculated self-consistently.

Using the ground states, we evaluate the energy differences defined by

$$\Delta\mathcal{E}_I \equiv \langle\Phi|\,\hat{H}\,|\Phi\rangle - \langle\Phi_{\rm GP}|\,\hat{H}\,|\Phi_{\rm GP}\rangle\,, \tag{75a}$$

$$\Delta\mathcal{E}_{II} \equiv \langle\Phi_{\rm GA}|\,\hat{H}\,|\Phi_{\rm GA}\rangle - \langle\Phi_{\rm Bog}|\,\hat{H}\,|\Phi_{\rm Bog}\rangle\,, \tag{75b}$$

$$\Delta\mathcal{E}_{III} \equiv \langle\Phi|\,\hat{H}\,|\Phi\rangle - \langle\Phi_{\rm HFB}|\,\hat{H}\,|\Phi_{\rm HFB}\rangle\,, \tag{75c}$$

$$\Delta\mathcal{E}_{IV} \equiv \langle\Phi|\,\hat{H}\,|\Phi\rangle - \langle\Phi_{\rm GA}|\,\hat{H}\,|\Phi_{\rm GA}\rangle\,. \tag{75d}$$

From Tables 3 and 4, we subsequently see the relation $\langle\Phi|\,\hat{H}\,|\Phi\rangle < \langle\Phi_{\rm GA}|\,\hat{H}\,|\Phi_{\rm GA}\rangle < \langle\Phi_{\rm HFB}|\,\hat{H}\,|\Phi_{\rm HFB}\rangle < \langle\Phi_{\rm Bog}|\,\hat{H}\,|\Phi_{\rm Bog}\rangle < \langle\Phi_{\rm GP}|\,\hat{H}\,|\Phi_{\rm GP}\rangle$; thus, $|\Phi\rangle$ seems to be the best solution in terms of constructing the variational wave function. The reason why $|\Phi_{\rm GA}\rangle$ gives lower energy than $|\Phi_{\rm HFB}\rangle$ is traced back to the difference in the manner of setting $\underline{\lambda}$, i.e., the difference between $\underline{u}\ \underline{u}^\dagger - \underline{v}\ \underline{v}^\dagger = \underline{1}$ for $|\Phi_{\rm GA}\rangle$ and ${\rm Tr}[\underline{u}\ \underline{u}^\dagger - \underline{v}\ \underline{v}^\dagger] = 1$ for $|\Phi_{\rm HFB}\rangle$. In the latter case, the quasiparticles do not satisfy the Bose commutator relations because the condition for the off-diagonal parts of $(\underline{u}\ \underline{u}^\dagger - \underline{v}\ \underline{v}^\dagger)$ is not considered to be appropriate. In contrast, $|\Phi_{\rm GA}\rangle$ with $\underline{u}$ and $\underline{v}$ satisfying all the conditions of Eq. (41)

gives a lower ground-state energy than $|\Phi_{\rm HFB}\rangle$. Thus, the appropriate consideration for commutator relations of quasiparticles is indispensable for obtaining the lower ground-state energy.

In addition, $|\Delta\mathcal{E}_{IV}|$ is roughly $100-1000$ times larger than $|\Delta\mathcal{E}_{II}|$. This result indicates that the 3/2-body correlations contribute to the decrease in the ground-state energies more than the 2-body correlations. These results agree with the results of homogeneous systems [17]. Therefore, the mean-field approximation for inhomogeneous BEC systems characterized by the discretized energy levels may not be effective quantitatively even in the weak-coupling region, similarly to the homogeneous systems.

We have constructed the variational wave function for an inhomogeneous system including not only the mean-field 2-body correlations but also the 3/2-body correlations beyond the mean-field approximation. Using the variational wave function, we have carried out a numerical calculation to evaluate the ground-state energy of a 1D system trapped by a harmonic oscillator. Our numerical result shows that 3/2-body correlations decrease the ground-state energies even in a trapped system characterized by the discretized energy level, and their contributions are comparable to those of 2-body correlations, which agree with the results of the homogeneous case [17]. Therefore, when we consider the contributions from noncondensates, self-consistent mean-field approximations may not be valid in BEC systems and 3/2-body correlations should be incorporated. This wave function is expected to give physical pictures beyond mean-field contributions in inhomogeneous systems more microscopically.

Table 1: Ground-state energies based on approximation (i) with $\tilde{\mathcal{E}}_\sigma = \mathcal{E}_\sigma/(N\varepsilon_\omega)$ and $\tilde{\alpha} = \alpha \times 10^3$.

$\tilde{\alpha}$	$\tilde{\mathcal{E}}_0$	$\tilde{\mathcal{E}}_1$	$\tilde{\mathcal{E}}_{\frac{3}{2}}$	$\tilde{\mathcal{E}}_2$	$\tilde{\mathcal{E}}_{\frac{3}{2}}/\tilde{\mathcal{E}}_2$
0.1	1.0399	-5.49×10^{-7}	-6.51×10^{-13}	1.64×10^{-11}	-0.040
0.5	1.20	-1.22×10^{-5}	-3.60×10^{-10}	1.93×10^{-9}	-0.19
1.5	1.60	-7.85×10^{-5}	-2.36×10^{-8}	4.85×10^{-8}	-0.49
2.5	2.00	-1.22×10^{-4}	-1.69×10^{-7}	2.34×10^{-7}	-0.72

Table 2: Ground-state energies based on approximation (ii) with $\tilde{\mathcal{E}}_\sigma = \mathcal{E}_\sigma/(N\varepsilon_\omega)$ and $\tilde{\alpha} = \alpha \times 10^3$.

$\tilde{\alpha}$	$\tilde{\mathcal{E}}_0$	$\tilde{\mathcal{E}}_1$	$\tilde{\mathcal{E}}_{\frac{3}{2}}$	$\tilde{\mathcal{E}}_2$	$\tilde{\mathcal{E}}_{\frac{3}{2}}/\tilde{\mathcal{E}}_2$
0.1	1.0397	-5.47×10^{-7}	-6.57×10^{-13}	1.64×10^{-11}	-0.040
0.5	1.19	-1.19×10^{-5}	-3.72×10^{-10}	1.94×10^{-9}	-0.19
1.5	1.56	-7.71×10^{-5}	-2.43×10^{-8}	4.73×10^{-8}	-0.51
2.5	1.89	-1.55×10^{-4}	-1.57×10^{-7}	2.04×10^{-7}	-0.77

Table 3: Energy differences based on approximation (i) with $\Delta\tilde{\mathcal{E}}_\sigma = \Delta\mathcal{E}_\sigma/(N\varepsilon_\omega)$ and $\tilde{\alpha} = \alpha \times 10^3$.

$\tilde{\alpha}$	$\Delta\tilde{\mathcal{E}}_I$	$\Delta\tilde{\mathcal{E}}_{II}$	$\Delta\tilde{\mathcal{E}}_{III}$	$\Delta\tilde{\mathcal{E}}_{IV}$
0.1	-7.26×10^{-7}	-4.44×10^{-16}	-6.59×10^{-13}	-6.52×10^{-13}
0.5	-1.75×10^{-5}	-2.81×10^{-13}	-4.46×10^{-10}	-3.60×10^{-10}
1.5	-1.46×10^{-4}	-2.83×10^{-11}	-6.23×10^{-8}	-2.36×10^{-8}
2.5	-3.87×10^{-4}	-3.45×10^{-10}	-7.94×10^{-7}	-1.69×10^{-7}

Table 4: Energy differences based on approximation (ii) with $\Delta\tilde{\mathcal{E}}_\sigma = \Delta\mathcal{E}_\sigma/(N\varepsilon_\omega)$ and $\tilde{\alpha} = \alpha \times 10^3$.

$\tilde{\alpha}$	$\Delta\tilde{\mathcal{E}}_I$	$\Delta\tilde{\mathcal{E}}_{II}$	$\Delta\tilde{\mathcal{E}}_{III}$	$\Delta\tilde{\mathcal{E}}_{IV}$
0.1	-7.24×10^{-7}	-1.22×10^{-14}	-6.63×10^{-13}	-6.56×10^{-13}
0.5	-1.72×10^{-5}	-5.61×10^{-12}	-4.61×10^{-10}	-3.72×10^{-10}
1.5	-1.39×10^{-4}	-2.77×10^{-10}	-6.27×10^{-8}	-2.43×10^{-8}
2.5	-3.51×10^{-4}	-1.40×10^{-9}	-6.58×10^{-7}	-1.57×10^{-7}

2.4 Application (2) : M-Component Bose–Bose Mixture

Dilute atomic gases are highly controllable systems for demonstrating various BEC systems experimentally. One of the targets is multi-component BEC systems [42, 43, 44, 45, 46]. In particular, many theoretical studies focusing on its collective features of condensates have been carried out, such as dynamical instabilities and collapsing processes [48, 49, 50, 51, 52, 53, 54]. However, the collisional processes smaller than $O(N_i)$ tend to be neglected, when considering the behavior of condensates of dilute gasses where $N_i \gg 1$ is the number of particle i. In Ref. [25], we have generalized the present variational method to a mixed system and constructed the ground-state wave function

by superposing the variational parameters which characterize 2-body and 3/2-body correlations between different particles. In this section, we summarize the contents of Ref. [25] and show the results of ground-state energies. In addition to the evaluation of ground-state energies, we here derive the correction to the stability condition for 2-component miscible states including 2-body and 3/2-body correlations. While the conventional condition without 2-body and 3/2-body correlations is given by $U_{AB}^2/U_{AA}U_{BB} < 1$ [40] where U_{ij} is the contact potential between particle i and j, many-body effects give finite contributions to this condition as $1 \to 1 + \alpha$.

In the following, we consider a system described by the following Hamiltonian,

$$\hat{H} = \sum_{i=1}^{M} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \varepsilon_{i\boldsymbol{k}} \hat{c}_{i\boldsymbol{k}}^{\dagger} \hat{c}_{i\boldsymbol{k}} + \sum_{i,j=1}^{M} \frac{U_{ij}}{2\mathcal{V}} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}\neq\boldsymbol{0}} \hat{c}_{i\boldsymbol{k}+\boldsymbol{q}}^{\dagger} \hat{c}_{j\boldsymbol{k}'-\boldsymbol{q}}^{\dagger} \hat{c}_{j\boldsymbol{k}'} \hat{c}_{i\boldsymbol{k}}, \tag{76}$$

where $\varepsilon_{i\boldsymbol{k}} \equiv \hbar^2 k^2/2m_i$ denotes the kinetic energy of particle i and $U_{ij} = U_{ji}$ is an effective contact potential for treating scattering effect between particle i and j [40].

How to extend the variational theory is just to include the internal degree of freedom. Therefore, the ground state of of Eq. (76), the miscible state of an interacting M-component system, can be considered by using the following variational wave function:

$$|\Phi_{\rm GA}\rangle = A_{\rm GA} \exp\left(\hat{\Pi}_{\rm GA}^{\dagger}\right) |N_1, N_2, \cdots, N_M\rangle_0 \,, \tag{77a}$$

$$|\Phi\rangle = A_3 \exp\left(\hat{\Pi}_3^{\dagger}\right) |\Phi_{\rm GA}\rangle \,, \tag{77b}$$

where $A_{\rm GA}$ and A_3 are the normalization constant determined by $\langle\Phi_{\rm GA}|\Phi_{\rm GA}\rangle = 1$ and $\langle\Phi|\Phi\rangle = 1$, $|N_1, N_2, \cdots, N_M\rangle_0$ is the ground state of M-component BEC without interaction with $\sum_{i=1}^{M} N_i = N$. $\hat{\Pi}_3^{\dagger}$ and $\hat{\Pi}_{\rm GA}^{\dagger}$ are defined as

$$\hat{\Pi}_3^{\dagger} \equiv \frac{1}{3!} \sum_{i,j,k=1}^{M} \sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}} w_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} \hat{\gamma}_{i\boldsymbol{k}_1}^{\dagger} \hat{\gamma}_{j\boldsymbol{k}_2}^{\dagger} \hat{\gamma}_{k\boldsymbol{k}_3}^{\dagger}, \tag{77c}$$

$$\hat{\Pi}_{\rm GA}^{\dagger} \equiv \sum_{i,j=1}^{M} \hat{\pi}_{ij}^{\dagger} \hat{\beta}_i \hat{\beta}_j = \frac{1}{2} \sum_{i,j=1}^{M} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \phi_{ij\boldsymbol{k}} \hat{c}_{i\boldsymbol{k}}^{\dagger} \hat{c}_{j-\boldsymbol{k}}^{\dagger}, \ \hat{\pi}_{ij}^{\dagger} \equiv \frac{1}{2} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \phi_{ij\boldsymbol{k}} \hat{c}_{i\boldsymbol{k}}^{\dagger} \hat{c}_{j-\boldsymbol{k}}^{\dagger} \tag{77d}$$

where $\hat{\beta}_i$ is a number-conserving operator for multi-component BEC, $\phi_{ij\boldsymbol{k}}$ is a variational parameter which characterizes a pair excitation of particle $(i, \boldsymbol{k})$ and $(j, -\boldsymbol{k})$ from condensates caused by interaction between particles, $w_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ a variational parameter characterizing 3/2-body correlations which satisfies $\hat{P} w_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = w_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ for any permutation $\hat{P}$ with three elements $(i, \boldsymbol{k}_1)$, $(j, \boldsymbol{k}_2)$, and $(k, \boldsymbol{k}_3)$, and $(\hat{\gamma}, \hat{\gamma}^{\dagger})$ a set of Bogoliuobov operators introduced by

$$\hat{\gamma}_{i\boldsymbol{k}} \equiv \sum_{j=1}^{M} [u_{ij\boldsymbol{k}} \hat{c}_{j\boldsymbol{k}} - v_{ij\boldsymbol{k}} \hat{c}_{j-\boldsymbol{k}}^{\dagger}], \tag{77e}$$

$$\hat{\gamma}_{i-\boldsymbol{k}}^{\dagger} \equiv \sum_{j=1}^{M} [-v_{ij-\boldsymbol{k}}^{*} \hat{c}_{j\boldsymbol{k}} + u_{ij-\boldsymbol{k}}^{*} \hat{c}_{j-\boldsymbol{k}}^{\dagger}]. \tag{77f}$$

with

$$u_{ij\boldsymbol{k}} = (\underline{u}_{\boldsymbol{k}})_{ij} = (\underline{1} - \underline{\phi}_{\boldsymbol{k}} \underline{\phi}_{\boldsymbol{k}}^{\dagger})_{ij}^{-\frac{1}{2}}, \ v_{ij\boldsymbol{k}} = (\underline{v}_{\boldsymbol{k}})_{ij} = (\underline{u}_{\boldsymbol{k}} \underline{\phi}_{\boldsymbol{k}})_{ij} \tag{77g}$$

where underlined functions represent $M \times M$ matrices and $(\underline{1})_{ij} = \delta_{ij}$. Here, we define the following quantities for later convenience,

$$\rho_{ij\boldsymbol{k}} \equiv \langle \Phi | \, \hat{c}^{\dagger}_{i\boldsymbol{k}} \hat{c}_{j\boldsymbol{k}} \, | \Phi \rangle \,, \tag{78a}$$

$$F_{ij\boldsymbol{k}} \equiv \langle \Phi | \, \hat{c}_{i\boldsymbol{k}} \hat{c}_{j-\boldsymbol{k}} \, | \Phi \rangle \,, \tag{78b}$$

$$W_{ij;j\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3} \equiv \langle \Phi | \, \hat{c}^{\dagger}_{j-\boldsymbol{k}_3} \hat{c}_{j\boldsymbol{k}_2} \hat{c}_{i\boldsymbol{k}_1} \, | \Phi \rangle \,. \tag{78c}$$

The definition in Eqs. (77e) and (77f) is a natural extension of Bogoliubov operators in one-component systems to M-component systems. The minimization of the energy functional expressed by variational parameters can be performed most easily in terms of $\Omega \equiv \mathcal{E} - \sum_i \mu_i N_i$, where μ_i denotes the Lagrange multipliers. Specifically, we determine $\psi_i \equiv \langle \hat{c}_{\boldsymbol{0}i} \hat{\beta}^{\dagger}_i \rangle \simeq \sqrt{N_{i\boldsymbol{0}}} e^{i\varphi_i}$, $\phi_{ij\boldsymbol{k}}$ and $w_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ from the stationarity conditions,

$$\frac{\delta \Omega}{\delta \psi^*_i} = 0, \ \frac{\delta \Omega}{\delta \phi^*_{ij\boldsymbol{k}}} = 0, \ \frac{\delta \Omega}{\delta w^*_{ijk\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}} = 0. \tag{79}$$

In considering the system composed of $M \geq 3$ types of bosons, we need to solve Eq. (79) simultaneously with $M + M^2 + M^3$ types of variational functions in principle. We note all the variational parameters turned out to be real numbers from our numerical calculations for $M = 2$ systems in miscible state.

In a homogeneous 2-component system, it is known that the system becomes unstable by (i) forming denser states containing both components called droplets [53] when $U_{ij} \ll -\sqrt{U_{AA}U_{BB}}$, or (ii) causing a phase separation into two components [54] when $U_{ij} \gg \sqrt{U_{AA}U_{BB}}$. The stability condition for a homogeneous system is given by $U_{ij}^2 < U_{ii}U_{jj}$ [40], which is derived neglecting 3/2-body and 2-body correlations. In this section, we reconsider the stability condition for a 2-component system composed of particles A and B on the basis of the ground-state wave function including 3/2-body and 2-body correlations. Here, we assume that all the variational parameters are real numbers. Under such assumption, the functional Ω is given in terms of variational parameters by

$$\Omega = \Omega[\psi_A, \psi_B, \phi_{AA}, \phi_{AB} = \phi_{BA}, \phi_{BB}, w_{AAA}, w_{ABA}, w_{BAB}, w_{BBB}]. \tag{80}$$

For the homogeneous solution to be stable, Ω must have a minimum value with respect to all the variational parameters and the second-order variation of Ω be always positive. Therefore,

$$\delta^2 \Omega = \boldsymbol{\eta}^T A \boldsymbol{\eta} > 0 \tag{81}$$

where $\boldsymbol{\eta}$ is a column vector composed of small variations in all the variational parameters in all the $\boldsymbol{k}$ space and A is the corresponding Hessian matrix [47].

In order to consider the complete condition that Ω has a minimum value, all the eigenvalues of A must be positive, i.e., $\det A > 0$. However, It is difficult to show it completely both analytically and computationally because A is quite a large matrix. Here, we consider some necessary conditions that Ω has a minimum value,

$$\frac{\partial^2 \Omega}{\partial \psi_i^2} > 0, \quad \det A_{\psi_A \psi_B} > 0, \tag{82}$$

where $A_{\psi_A\psi_B}$ is a sub-matrix of A defined by

$$A_{\psi_A\psi_B} \equiv \begin{pmatrix} \dfrac{\partial^2\Omega}{\partial\psi_A^2} & \dfrac{\partial^2\Omega}{\partial\psi_A\partial\psi_B} \\ \dfrac{\partial^2\Omega}{\partial\psi_B\partial\psi_A} & \dfrac{\partial^2\Omega}{\partial\psi_B^2} \end{pmatrix}. \tag{83}$$

$\partial^2\Omega/\partial\psi_i\partial\psi_j$ is calculated by

$$\frac{\partial^2\Omega}{\partial\psi_i\partial\psi_j} = \frac{4\sqrt{N_{i\mathbf{0}}N_j^{\mathbf{0}}}}{\mathcal{V}}U_{ij}(1+c_{ij}), \tag{84}$$

where

$$\begin{aligned} c_{ii} =& \frac{-N}{2U_{ii}N_{i\mathbf{0}}}\Bigg[\sum_{i'=A,B}(1-\delta_{i,i'})\sqrt{\frac{N_{i'\mathbf{0}}}{N_{i\mathbf{0}}}}\frac{U_{AB}}{N}\sum_{\boldsymbol{k}\neq\mathbf{0}}(F_{AB\boldsymbol{k}}+\rho_{AB\boldsymbol{k}}) \\ &+ \frac{N}{\sqrt{N_{i\mathbf{0}}}}\sum_{i'=A,B}\frac{U_{ii'}}{N_{\rm all}^2}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\mathbf{0}}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3\mathbf{0}}W_{ii';i'\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3}\Bigg] \end{aligned} \tag{85a}$$

$$c_{AB} = \frac{N}{2\sqrt{N_{A\mathbf{0}}N_{B\mathbf{0}}}}\frac{1}{N}\sum_{\boldsymbol{k}\neq\mathbf{0}}\Big[F_{AB\boldsymbol{k}}+\rho_{AB\boldsymbol{k}}\Big] = c_{BA} \tag{85b}$$

The first condition of (82) with (84), (85a) and (85b) demands the relation $U_{ii} > 0$ since $1+c_{ii}$ with $|c_{ii}| \ll 1$ is always positive. On the other hand, the second condition of (82) with (84), (85a) and (85b) gives the following stability condition

$$\begin{aligned} & U_{AA}U_{BB}\Big(1+c_{AA}\Big)\Big(1+c_{BB}\Big) - U_{AB}^2\Big(1+c_{AB}\Big)^2 > 0 \\ \rightarrow & \frac{U_{AB}^2}{U_{AA}U_{BB}} < \frac{1+(c_{AA}+c_{BB})+c_{AA}c_{BB}}{1+2c_{AB}+c_{AB}^2} \equiv 1+\alpha, \end{aligned} \tag{86}$$

where α is the correction value which is determined after solving Eq. (79) self-consistently and obtaining $|\Phi\rangle$. The conventional relation $U_{AB}^2/U_{AA}U_{BB} < 1$ is obtained by putting $\alpha = 0$ ($c_{AA} = c_{AB} = c_{BB} = 0$), which corresponds to the calculation with w_{AAA}, w_{BBB}, w_{ABA}, $w_{BAB} \to 0$ and $N_{i\mathbf{0}} \to N_i$. In the following, we show $\alpha \neq 0$ numerically.

We show that the ground state incorporating terms of Hamiltonian smaller than $O(\sqrt{N_i})$ gives lower energy than the one given by the eigenstate of the approximated Hamiltonian $\hat{H}_{\rm Bog} \equiv \hat{H}_0 + \hat{H}_1$. In order to see this clearly, we diagonalize $\hat{H}_{\rm Bog}$ and obtain the ground-state energy as follows,

$$\mathcal{E}_{\rm eff} = \mathcal{E}_{\rm eff}^{(0)} + \mathcal{E}_{\rm eff}^{(1)} \tag{87}$$

where we define the following quantities,

$$\mathcal{E}_{\rm eff}^{(0)} \equiv \sum_{i=A,B}\sum_{j=A,B}\frac{U_{ij}}{2\mathcal{V}}N_iN_j, \tag{88a}$$

$$\mathcal{E}_{\rm eff}^{(1)} \equiv -\frac{1}{2}{\sum_{\boldsymbol{k}}}'\Big[\sum_{i=A,B}E_i(k)-\sum_{\sigma=+,-}E_\sigma(k)\Big], \tag{88b}$$

$$E_i(k) \equiv \varepsilon_k^i + \bar{n}_iU_{ii}, \tag{88c}$$

$$E_\pm(k) \equiv \frac{1}{\sqrt{2}}\Bigg[\big(E_A^{\rm Bog}(k)\big)^2+\big(E_B^{\rm Bog}(k)\big)^2 \pm\sqrt{\Big\{\big(E_A^{\rm Bog}(k)\big)^2-\big(E_B^{\rm Bog}(k)\big)^2\Big\}^2+16\bar{n}_A\bar{n}_B\varepsilon_k^A\varepsilon_k^BU_{AB}^2}\Bigg]^{\frac{1}{2}}, \tag{88d}$$

$$E_i^{\rm Bog}(k) \equiv \sqrt{\varepsilon_k^i(\varepsilon_k^i+2\bar{n}_iU_{ii})}, \tag{88e}$$

with $\bar{n}_i \equiv N_i/\mathcal{V}$. We have confirmed that $\langle\Phi|\,\hat{H}_{\rm Bog}\,|\Phi\rangle$ estimated by our variational calculations with w_{AAA}, w_{BBB}, w_{ABA}, $w_{BAB} \to 0$ and $N_{i\boldsymbol{0}} \to N_i$ coincides with $\mathcal{E}_{\rm eff}$ numerically.

Table 5: $\tilde{\mathcal{E}}_{\rm eff}^{(0)}$, $\tilde{\mathcal{E}}_{\rm eff}^{(1)}$ and $\Delta\tilde{\mathcal{E}}$ in various cases and conditions with $\varepsilon_{k_{\rm c}} = 25\varepsilon_{U_{AA}}$ and $|U_{AB}|/\sqrt{U_{AA}U_{BB}} = 0.95$.

Case	$\tilde{\mathcal{E}}_{\rm eff}^{(0)}$	$\tilde{\mathcal{E}}_{\rm eff}^{(1)}$	$\Delta\tilde{\mathcal{E}}_{(I)}$	$\Delta\tilde{\mathcal{E}}_{(II)}$	$\Delta\tilde{\mathcal{E}}_{(III)}$	$\Delta\tilde{\mathcal{E}}_{(IV)}$	$\Delta\tilde{\mathcal{E}}_{(V)}$
(A_+)	0.488	−5.62	2730	80.9	79.0	62.4	22.8
(B_+)	0.492	−5.72	1530	82.9	81.0	49.3	24.2
(C_+)	1.10	−11.9	3800	162	158	109	52.7
(A_-)	0.0125	−5.62	2730	18.2	16.9	1.29	−3.69
(B_-)	0.188	−5.72	1530	42.7	41.2	10.2	7.01
(C_-)	0.150	−11.9	3800	81.9	79.0	31.3	18.5

Table 6: $\tilde{\mathcal{E}}_{\rm eff}^{(0)}$, $\tilde{\mathcal{E}}_{\rm eff}^{(1)}$ and $\Delta\tilde{\mathcal{E}}$ in various cases and conditions with $\varepsilon_{k_{\rm c}} = 100\varepsilon_{U_{AA}}$ and $|U_{AB}|/\sqrt{U_{AA}U_{BB}} = 0.95$.

Case	$\tilde{\mathcal{E}}_{\rm eff}^{(0)}$	$\tilde{\mathcal{E}}_{\rm eff}^{(1)}$	$\Delta\tilde{\mathcal{E}}_{(I)}$	$\Delta\tilde{\mathcal{E}}_{(II)}$	$\Delta\tilde{\mathcal{E}}_{(III)}$	$\Delta\tilde{\mathcal{E}}_{(IV)}$	$\Delta\tilde{\mathcal{E}}_{(V)}$
(A_+)	0.488	−13.0	6120	392	377	335	230
(B_+)	0.492	−13.3	4080	402	387	304	237
(C_+)	1.10	−27.4	9990	770	743	623	472
(A_-)	0.0125	−13.0	6120	62.6	50.5	10.3	−5.24
(B_-)	0.188	−13.3	4080	191	178	96.3	86.1
(C_-)	0.150	−27.4	9990	350	326	208	171

Table 7: $\tilde{\mathcal{E}}^{(0)}_{\rm eff}$, $\tilde{\mathcal{E}}^{(1)}_{\rm eff}$ and $\Delta\tilde{\mathcal{E}}$ in various cases and conditions with $\varepsilon_{k_{\rm c}} = 25\varepsilon_{U_{AA}}$ and $|U_{AB}|/\sqrt{U_{AA}U_{BB}} = 0.98$.

Case	$\tilde{\mathcal{E}}^{(0)}_{\rm eff}$	$\tilde{\mathcal{E}}^{(1)}_{\rm eff}$	$\Delta\tilde{\mathcal{E}}_{(I)}$	$\Delta\tilde{\mathcal{E}}_{(II)}$	$\Delta\tilde{\mathcal{E}}_{(III)}$	$\Delta\tilde{\mathcal{E}}_{(IV)}$	$\Delta\tilde{\mathcal{E}}_{(V)}$
(A_+)	0.495	−5.78	2610	84.2	82.2	66.2	23.3
(B_+)	0.497	−5.82	1710	85.0	83.1	51.8	24.5
(C_+)	1.12	−12.1	4210	166	162	114	53.0
(A_-)	0.00500	−5.78	2610	15.2	13.8	−1.19	−5.87
(B_-)	0.183	−5.82	1710	40.8	39.3	8.72	5.62
(C_-)	0.135	−12.1	4210	77.9	75.0	28.2	15.3

Since our interest is to estimate the ground-state energies including $\hat{H}_{3/2}$ and $\hat{H}_2$, we calculate the quantity defined by

$$\tilde{\mathcal{E}}^{(0)}_{\rm eff} \equiv \mathcal{E}^{(0)}_{\rm eff}/(N\varepsilon_{U_{AA}}) = \frac{1}{2}\sum_{i=A,B}\sum_{j=A,B}\frac{N_iN_j}{N^2_{\rm all}}\frac{U_{ij}}{U_{AA}} \tag{89a}$$

$$\tilde{\mathcal{E}}^{(1)}_{\rm eff} \equiv \mathcal{E}^{(1)}_{\rm eff}/(N\varepsilon_{U_{AA}}) \times \delta_A^{-\frac{1}{2}}, \tag{89b}$$

$$\Delta\tilde{\mathcal{E}} \equiv (\mathcal{E} - \mathcal{E}_{\rm eff})/(N\varepsilon_{U_{AA}}) \times \delta_A^{-1}, \tag{89c}$$

and evaluate their values for the six cases,

$(A_\pm)$ $m_A : m_B = \bar{n}_A : \bar{n}_B = 1 : 1$

$(B_\pm)$ $m_A : m_B = 1 : 1$, $\bar{n}_A : \bar{n}_B = 1 : 4$

$(C_\pm)$ $m_A : m_B = 4 : 1$, $\bar{n}_A : \bar{n}_B = 1 : 1$

where $\pm$ denotes the sign of U_{AB}. When we carry out numerical calculations, we set external coupling constants as $\delta_A = \delta_B = 1.0 \times 10^{-6}$, where $\delta_i \equiv a^3_{U_{ii}}\bar{n}$.

Incorporating more variational parameters in the theory is expected to yield a better estimate for the ground-state energy. To see this explicitly, we have performed our variational calculations for the five cases.

- (I) $N_{i\mathbf{0}} \to N_i$ and $\phi_{AB} = w_{AAA} = w_{BBB} = w_{ABA} = w_{BAB} = 0$. This case corresponds to the Bogoliubov theory with no correlations between different species.
- (II) $N_{i\mathbf{0}} \to N_i$ and $w_{AAA} = w_{BBB} = w_{ABA} = w_{BAB} = 0$. This case corresponds to the eigenstate of $\hat{H}_{\rm Bog}$ or standard multi-component GP theory [**?**].
- (III) $w_{AAA} = w_{BBB} = w_{ABA} = w_{BAB} = 0$. This case corresponds to $|\Phi_{\rm GA}\rangle$.
- (IV) $w_{ABA} = w_{BAB} = 0$.
- (V) All the variational parameters are calculated self-consistently.

The corresponding energies are denoted by $\Delta\tilde{\mathcal{E}}_{(I)}$, $\Delta\tilde{\mathcal{E}}_{(II)}$, $\Delta\tilde{\mathcal{E}}_{(III)}$, $\Delta\tilde{\mathcal{E}}_{(IV)}$ and $\Delta\tilde{\mathcal{E}}_{(V)}$. As shown in Table. 5 - 7, we can confirm the relation $\Delta\tilde{\mathcal{E}}_{(I)} \gg \Delta\tilde{\mathcal{E}}_{(II)} > \Delta\tilde{\mathcal{E}}_{(III)} > \Delta\tilde{\mathcal{E}}_{(IV)} > \Delta\tilde{\mathcal{E}}_{(V)}$ for all the cases of $(A_\pm)$, $(B_\pm)$ and $(C_\pm)$. Therefore, the ground state of 2-component miscible state with the contributions from 2-body and 3/2-body correlations is constructed through this self-consistent calculations. In addition, as we see the tables, $|\Delta\tilde{\mathcal{E}}_{(II)} - \Delta\tilde{\mathcal{E}}_{(III)}| < |\Delta\tilde{\mathcal{E}}_{(III)} - \Delta\tilde{\mathcal{E}}_{(V)}|$ in all the cases. This result indicates that 3/2-body correlations contribute to lower the ground-state energies more than 2-body correlations. In this sense, the mean-field approximation for mixture BEC systems is not effective quantitatively even in the weak-coupling region, as well as the one-component systems[17].

Table 8: c_{ij} and α with various cases.

$\frac{\lvert U_{AB}\rvert}{\sqrt{U_{AA}U_{BB}}}$	Cut off	Case	$\frac{c_{AA}}{\sqrt{\delta_A}}$	$\frac{c_{AB}}{\sqrt{\delta_A}}$	$\frac{c_{BB}}{\sqrt{\delta_A}}$	$\frac{\alpha}{\sqrt{\delta_A}}$
0.95	$\varepsilon_{k_c} = 25\varepsilon_{U_{AA}}$	(A_+)	4.88	−5.09	4.88	20.2
		(B_+)	19.5	−5.10	1.24	31.3
		(C_+)	7.79	−4.08	1.97	18.1
		(A_-)	4.97	5.21	4.97	−0.486
		(B_-)	19.9	5.22	1.26	10.6
		(C_-)	7.90	4.15	1.99	1.58
0.95	$\varepsilon_{k_c} = 100\varepsilon_{U_{AA}}$	(A_+)	11.7	−12.2	11.7	49.1
		(B_+)	46.7	−12.2	2.98	76.0
		(C_+)	18.8	−9.82	4.74	44.0
		(A_-)	12.3	12.9	12.3	−1.18
		(B_-)	49.0	12.9	3.11	25.7
		(C_-)	19.5	10.2	4.91	3.84
0.98	$\varepsilon_{k_c} = 25\varepsilon_{U_{AA}}$	(A_+)	5.21	−5.27	5.21	21.2
		(B_+)	20.8	−5.27	1.32	33.0
		(C_+)	8.31	−4.21	2.10	19.0
		(A_-)	5.30	5.40	5.30	−0.183
		(B_-)	21.2	5.40	1.34	11.6
		(C_-)	8.43	4.30	2.12	1.95

Next, we discuss the correction to the stability condition given by inequality (86). Table. 8 shows c_{AA}, c_{AB}, c_{BB} and α obtained by numerical calculation based on the ground state with condition (V). As shown in the table, all the corrections are of order $\sqrt{\delta_A}$, which mainly originate from the terms related to $\rho_{AB}(k)$ and $F_{AB}(k)$ in Eq. (85a) and (85b). 3/2-body correlations also give $O(\delta_A)$ contributions. In case with $U_{AB} > 0$, we see from the table that α becomes always positive so that the stable regions of miscible state seem to be extended. Indeed, we checked our numerical

calculation showed convergence even when $U_{AB} = \sqrt{U_{AA}U_{BB}}$. On the other hand, in case with $U_{AB} < 0$, α may become negative, especially when $\bar{n}_A : \bar{n}_B = m_A : m_B = 1 : 1$. Under such condition, we have numerically found that the ground-state energies increased towards divergence as iterative calculations proceeded and the self-consistent calculations became unstable in the range of $U_{AB} \lesssim -0.985\sqrt{U_{AA}U_{BB}}$. It is difficult to determine the critical point in detail numerically because it is not until we succeed in the self-consistent calculation that we can calculate α. However, these results indicate that many-body effects may change the stable regions of miscible states.

2.5 Application (3) Extension to Finite-Temperature Systems

By introducing a *variational density matrix* $\hat{\rho}_{\rm v}$ instead of the ground state in previous sections, our variational approach has been extended to the finite-temperature systems. In this section, we summarize how to construct the theory for finite-temperature systems and introduce some results briefly shown in [26]. This work has mainly been carried out by my collaborator A. Kirikoshi.

At finite temperature, we minimize the grand potential Ω following the variational principle

$$\Omega_{\rm v} = {\rm Tr}\hat{\rho}_{\rm v}[\hat{H} - \mu\hat{N} + \beta^{-1}\ln\hat{\rho}_{\rm v}] \geq \Omega, \tag{90}$$

where $\beta \equiv (k_{\rm B}T)^{-1}$ and Ω is the exact grand potential. Therefore, the choice of $\hat{\rho}_{\rm v}$ that yields lower value of $\Omega_{\rm v}$ is crucial and the form of $\hat{\rho}_{\rm v}$ is determined by the energy-minimum condition $\delta\Omega_{\rm v} = 0$. Here, we incorporate 3/2-body correlations based on the idea in the theories at $T = 0$ by choosing the following form of $\hat{\rho}_{\rm v}$:

$$\hat{\rho}_{\rm v} = \exp[\beta(\Omega_{\rm vLW} - \hat{H}_{\rm v})],\ \Omega_{\rm vLW} \equiv -\beta^{-1}\ln{\rm Tr}e^{-\beta\hat{H}_{\rm v}}, \tag{91}$$

with

$$\hat{H}_{\rm v} = \hat{H}_{\rm v}^{\rm MF} + \hat{H}_{\rm v}^{3} \equiv \sum_{\boldsymbol{k}\neq\boldsymbol{0}} E_{\boldsymbol{k}}\hat{\gamma}_{\boldsymbol{k}}^{\dagger}\hat{\gamma}_{\boldsymbol{k}} + \frac{1}{3!}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}} (b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\hat{\gamma}_{\boldsymbol{k}_1}^{\dagger}\hat{\gamma}_{\boldsymbol{k}_2}^{\dagger}\hat{\gamma}_{\boldsymbol{k}_3}^{\dagger} + b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}^{*}\hat{\gamma}_{\boldsymbol{k}_1}\hat{\gamma}_{\boldsymbol{k}_2}\hat{\gamma}_{\boldsymbol{k}_3}), \tag{92}$$

where $E_{\boldsymbol{k}}$ and $b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ represent variational parameters. Note that quasiparticle operators described by $(u_{\boldsymbol{k}}, v_{\boldsymbol{k}})$ also include another variational parameter $\phi_{\boldsymbol{k}}$. Therefore, we optimize $\Omega_{\rm v}$ with three variational parameters $(\phi_{\boldsymbol{k}}, E_{\boldsymbol{k}}, b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3})$. If we set $b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = 0$, we obtain the solution by HFB theory [13].

Based on $\hat{\rho}_{\rm v}$, we obtain the following expression for $\Omega_{\rm v}$:

$$\begin{aligned}
\Omega_{\rm v} &= {\rm Tr}\hat{\rho}_{\rm v}\hat{H} - {\rm Tr}\hat{\rho}_{\rm v}\hat{H}_{\rm v} + \Omega_{\rm vLW} \\
&= \frac{U_{\boldsymbol{0}}N_{\boldsymbol{0}}^2}{2\mathcal{V}} - \mu N_{\boldsymbol{0}} + \sum_{\boldsymbol{k}\neq\boldsymbol{0}}[\varepsilon_k - \mu]\rho_{\boldsymbol{k}} + \frac{N_{\boldsymbol{0}}}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}[(U_0 + U_k)\rho_{\boldsymbol{k}} + U_k F_{\boldsymbol{k}}] \\
&+ \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}U_{k_1}(\psi_{\boldsymbol{0}}^{*}W_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} + \psi_{\boldsymbol{0}}W_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}^{*}) \\
&+ \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'\neq\boldsymbol{0}}[(U_0 + U_{|\boldsymbol{k}-\boldsymbol{k}'|})]\rho_{\boldsymbol{k}}\rho_{\boldsymbol{k}'} + U_{|\boldsymbol{k}-\boldsymbol{k}'|}F_{\boldsymbol{k}}F_{\boldsymbol{k}'}] - \sum_{\boldsymbol{k}\neq\boldsymbol{0}} E_{\boldsymbol{k}}\rho_{\boldsymbol{k}}^{\rm qp} \\
&- \frac{1}{3!}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}} (b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}^{*}w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} + b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}^{*}) + \Omega_{\rm vLW},
\end{aligned} \tag{93a}$$

where we define the following quantities

$$\psi_{\mathbf{0}} \equiv \mathrm{Tr}\hat{c}_{\mathbf{0}} \tag{93b}$$

$$N_{\mathbf{0}} \equiv \mathrm{Tr}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}_{\mathbf{0}}, \tag{93c}$$

$$\rho_{\boldsymbol{k}} \equiv \mathrm{Tr}\hat{c}^{\dagger}_{\boldsymbol{k}}\hat{c}_{\boldsymbol{k}}, \tag{93d}$$

$$F_{\boldsymbol{k}} \equiv \mathrm{Tr}\hat{c}_{\boldsymbol{k}}\hat{c}_{-\boldsymbol{k}}, \tag{93e}$$

$$W_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} \equiv \mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{-\boldsymbol{k}_3}\hat{c}_{\boldsymbol{k}_2}\hat{c}_{\boldsymbol{k}_1}, \tag{93f}$$

$$\rho^{\mathrm{qp}}_{\boldsymbol{k}} \equiv \mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{\gamma}^{\dagger}_{\boldsymbol{k}}\hat{\gamma}_{\boldsymbol{k}} = \frac{\delta\Omega_{\mathrm{vLW}}}{\delta E_{\boldsymbol{k}}}, \tag{93g}$$

$$w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} \equiv \mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{\gamma}_{\boldsymbol{k}_1}\hat{\gamma}_{\boldsymbol{k}_2}\hat{\gamma}_{\boldsymbol{k}_3} = \frac{\delta\Omega_{\mathrm{vLW}}}{\delta b^{*}_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}}, \tag{93h}$$

and the following approximations are used:

$$\mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}_{\mathbf{0}}\hat{c}_{\mathbf{0}} \simeq N^2_{\mathbf{0}}, \tag{93i}$$

$$\mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}^{\dagger}_{\boldsymbol{k}}\hat{c}_{\mathbf{0}}\hat{c}_{\boldsymbol{k}} \simeq N_{\mathbf{0}}\rho_{\boldsymbol{k}}, \tag{93j}$$

$$\mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}_{\boldsymbol{k}}\hat{c}_{-\boldsymbol{k}} \simeq \psi^{*2}_{\mathbf{0}}F_{\boldsymbol{k}}, \tag{93k}$$

$$\mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{\mathbf{0}}\hat{c}^{\dagger}_{-\boldsymbol{k}_3}\hat{c}_{\boldsymbol{k}_2}\hat{c}_{\boldsymbol{k}_1} \simeq \psi^{*2}_{\mathbf{0}}W_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}, \tag{93l}$$

$$\begin{aligned}\mathrm{Tr}\hat{\rho}_{\mathrm{v}}\hat{c}^{\dagger}_{\boldsymbol{k}_1}\hat{c}^{\dagger}_{\boldsymbol{k}_2}\hat{c}_{\boldsymbol{k}_3}\hat{c}_{\boldsymbol{k}_4} \simeq{}& (\delta_{\boldsymbol{k}_1,\boldsymbol{k}_4}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_3} + \delta_{\boldsymbol{k}_1,\boldsymbol{k}_3}\delta_{\boldsymbol{k}_2,\boldsymbol{k}_4})\rho_{\boldsymbol{k}_3}\rho_{\boldsymbol{k}_4} \\ &+ \delta_{\boldsymbol{k}_1,-\boldsymbol{k}_2}\delta_{\boldsymbol{k}_3,-\boldsymbol{k}_4}F_{\boldsymbol{k}_1}F_{\boldsymbol{k}_4}.\end{aligned} \tag{93m}$$

In the theories at $T = 0$, we have obtained ρ^{qp} perturbation in terms of one of the variational parameters w. On the other hand, it is necessary to determine the form of ρ^{qp} and w at finite temperature. To obtain the explicit expressions of $\rho^{\mathrm{qp}}_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$, we introduce a Luttinger–Ward method based on a Green's function for quasiparticle operators and derive self-consistent equations for the Green's function in the following.

The quasiparticle Green's function is introduced as follows:

$$\mathcal{G}_{\boldsymbol{k}}(\tau_1,\tau_2) = -\mathrm{Tr}\rho_{\mathrm{v}}\hat{T}_{\tau}\hat{\gamma}^1_{\boldsymbol{k}}(\tau_1)\hat{\gamma}^2_{\boldsymbol{k}}(\tau_2) = -\mathrm{Tr}\rho_{\mathrm{v}}\hat{T}_{\tau}\hat{\gamma}^1_{\boldsymbol{k}}(\tau_1-\tau_2)\hat{\gamma}^2_{\boldsymbol{k}} \equiv \mathcal{G}_{\boldsymbol{k}}(\tau_1-\tau_2), \tag{94}$$

where $\hat{T}_{\tau}$ is a time-ordered operator for imaginary time τ and $\hat{\gamma}^1_{\boldsymbol{k}}(\tau) \equiv e^{\tau\hat{H}_{\mathrm{v}}}\hat{\gamma}_{\boldsymbol{k}}e^{-\tau\hat{H}_{\mathrm{v}}}$ and $\hat{\gamma}^2_{\boldsymbol{k}}(\tau) \equiv e^{\tau\hat{H}_{\mathrm{v}}}\hat{\gamma}^{\dagger}_{\boldsymbol{k}}e^{-\tau\hat{H}_{\mathrm{v}}}$ are the Heisenberg representation for quasiparticle operators. This imaginary-time Green's function has a boundary condition given by $\mathcal{G}_{\boldsymbol{k}}(\tau+\beta) = \mathcal{G}_{\boldsymbol{k}}(\tau)$. Thus, we can express the Green's function in the energy domain in terms of the Fourier coefficient of $\mathcal{G}_{\boldsymbol{k}}(\tau)$ as

$$\mathcal{G}_{\boldsymbol{k}}(\tau) = \frac{1}{\beta}\sum_{n=-\infty}^{\infty} e^{-i\varepsilon_n\tau}\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}, \tag{95}$$

where $\varepsilon_n \equiv 2n\pi/\beta$ (n: integer) is called the Matsubara energy for bosons. Because the basis functions $\{e^{i\varepsilon_n\tau}/\sqrt{\beta}\}$ with $\tau \in [0,\beta]$ form a complete orthonormal set for $\mathcal{G}_{\boldsymbol{k}}(\tau)$, we obtain $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$ by integrating $\mathcal{G}_{\boldsymbol{k}}(\tau)e^{i\varepsilon_n\tau}$ over $\tau \in [0,\beta]$.

To construct the self-consistent equations for $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$, we define a self energy $\mathcal{S}$ expressed by $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$, we use the method introduced by Luttinger and Ward [21]. As shown by Luttinger and Ward, $\Omega_{\rm vLW} = \Omega_{\rm vLW}[\mathcal{G}]$ can be expressed in terms of $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$ as

$$\Omega_{\rm vLW}[\mathcal{G}] = \frac{1}{\beta}\sum_{n\neq 0}\sum_{\boldsymbol{k}\neq\boldsymbol{0}}\left[e^{i\varepsilon_n 0_+}\ln[-{\mathcal{G}^{(0)}}^{-1}_{\boldsymbol{k},i\varepsilon_n} + \mathcal{S}_{\boldsymbol{k},i\varepsilon_n}] + \mathcal{S}_{\boldsymbol{k},i\varepsilon_n}\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}\right] + \Phi_{\rm vLW}[\mathcal{G}] \tag{96}$$

where $\Phi_{\rm vLW}$ consists of all the skeleton diagrams in the simple perturbation expansion with respect to $\hat{H}^3_{\rm v}$ for $\Omega_{\rm vLW}$ with replacement of free quasiparticle's propagator $\mathcal{G}^{(0)}$ with $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$. Here, $\mathcal{G}^{(0)}$ is defined by

$$\mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n} = \frac{1}{i\varepsilon_n - E_{\boldsymbol{k}}}. \tag{97}$$

The equation for $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$ is determined by the stationary condition for $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$ as $\delta\Omega_{\rm vLW}/\delta\mathcal{G}_{\boldsymbol{k},i\varepsilon_n} = 0$. Therefore, we obtain "Dyson equation for $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$" as follows:

$$\mathcal{G}_{\boldsymbol{k},i\varepsilon_n} = \frac{1}{i\varepsilon_n - E_{\boldsymbol{k}} - \mathcal{S}_{\boldsymbol{k},i\varepsilon_n}}, \tag{98}$$

where we define the self-energy$\mathcal{S}$ in terms of the functional derivative of $\Phi_{\rm vLW}$ as

$$\mathcal{S}_{\boldsymbol{k},i\varepsilon_n} = -\beta\frac{\delta\Phi_{\rm vLW}}{\delta\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}}. \tag{99}$$

Therefore, Eq. (98) is solved self-consistently with the condition (99). The self-energy $\mathcal{S}_{\boldsymbol{k},i\varepsilon_n}$ given by Eq. (99) is determined by $\Phi_{\rm vLW}$. Therefore, we need to determine the form of $\Phi_{\rm vLW}$ with introducing some kind of approximations. Here, we incorporate a scheme based on the skeleton expansion, i.e., the Φ-derivative approximation into our variational method. In the following, we summarize how to construct $\Phi_{\rm vLW}$ briefly.

Following the manner of Φ-derivative approximation, we introduce $\Phi_{\rm vLW}$ as follows:

$$\Phi_{\rm vLW} = -\frac{1}{\beta}[\langle\hat{S}(\beta)\rangle_{\rm HFB,connect} - 1]_{\rm skeleton,\mathcal{G}^{(0)}\to\mathcal{G}}, \tag{100}$$

where $\langle\cdots\rangle_{\rm HFB}$ denotes the average by $\hat{\rho}_{\rm v}[b = b^* = 0]$, $\langle\cdots\rangle_{\rm HFB,connected}$ represents the "connected contributions" included in $\langle\cdots\rangle_{\rm HFB}$, the subscript "skeleton" represents "skeleton diagrams without self-energy corrections", the subscript $\mathcal{G}_0 \to \mathcal{G}$ represents "replacement of $\mathcal{G}_0$ in $\Phi_{\rm vLW}$ by $\mathcal{G}$", and $\hat{S}(\beta)$ is an operator to carry out the perturbation expansion defined by

$$\hat{S}(\beta) \equiv e^{\beta\hat{H}^{\rm MF}_{\rm v}}e^{-\beta\hat{H}_{\rm v}} = 1 + \sum_{m=1}^{\infty}\frac{1}{n!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\int_0^\beta d\tau_m\hat{T}_\tau\hat{H}^3_{\rm v}(\tau_1)\cdots\hat{H}^3_{\rm v}(\tau_m). \tag{101}$$

Thus, $\Phi_{\rm vLW} = \sum_{n=1}^{\infty}\Phi^n_{\rm vLW}$ formally consists of infinite closed skeleton diagrams with $\mathcal{G}_0$ replaced by $\mathcal{G}$. We note $\Phi^{n=2p+1}_{\rm vLW} = 0$ (p: integer), i.e., only even-order contributions remain. In the following, we proceed our calculation with approximating $\Phi_{\rm vLW}$ as $\Phi_{\rm vLW} \simeq \Phi^{(2)}_{\rm vLW}$, where $\Phi^{(2)}_{\rm vLW}$ is expressed by

$$\begin{aligned}\Phi^{(2)}_{\rm vLW} =& \frac{1}{3!\beta}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}|b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}|^2\int_0^\beta d\tau_1\int_0^\beta d\tau_2\mathcal{G}_{\boldsymbol{k}_1}(\tau_1-\tau_2)\mathcal{G}_{\boldsymbol{k}_2}(\tau_1-\tau_2)\mathcal{G}_{\boldsymbol{k}_3}(\tau_1-\tau_2)\\ =& \frac{1}{3!\beta^2}\sum_{n_1n_2n_3\neq 0}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}|^2\delta_{n_1+n_2+n_3,0}\mathcal{G}_{\boldsymbol{k}_1,i\varepsilon_{n_1}}\mathcal{G}_{\boldsymbol{k}_2,i\varepsilon_{n_2}}\mathcal{G}_{\boldsymbol{k}_3,i\varepsilon_{n_3}}.\end{aligned} \tag{102}$$

Therefore, the self energy is

$$\mathcal{S}_{\boldsymbol{k},i\varepsilon_n} \simeq -\frac{1}{2\beta}\sum_{n_2n_3\neq 0}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}} |b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2\delta_{n+n_2+n_3,0}\mathcal{G}_{\boldsymbol{k}_2,i\varepsilon_{n_2}}\mathcal{G}_{\boldsymbol{k}_3,i\varepsilon_{n_3}}. \tag{103}$$

Therefore, we here solve Eq. (98) with (103), instead of Eq. (99).

Using $\mathcal{G}_{\boldsymbol{k},i\varepsilon_n}$, we can evaluate $\rho^{\rm qp}_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ as follows:

$$\rho^{\rm qp}_{\boldsymbol{k}} = -\frac{1}{\beta}\sum_{n\neq 0}\mathcal{G}_{\boldsymbol{k},i\varepsilon_n} \tag{104a}$$

$$w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\frac{1}{\beta^2}\sum_{n_1n_2n_3\neq 0}\delta_{n_1+n_2+n_3,0}\mathcal{G}_{\boldsymbol{k}_1,i\varepsilon_{n_1}}\mathcal{G}_{\boldsymbol{k}_2,i\varepsilon_{n_2}}\mathcal{G}_{\boldsymbol{k}_3,i\varepsilon_{n_3}}. \tag{104b}$$

Therefore, by solving variational conditions for $(\phi_{\boldsymbol{k}}, E_{\boldsymbol{k}}, b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3})$ with $(\rho^{\rm qp}_{\boldsymbol{k}}[\mathcal{G}], w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}[\mathcal{G}])$ described by Eq. (98) and (103), we obtain the equilibrium state at finite temperature. The variational conditions for $(\phi_{\boldsymbol{k}}, E_{\boldsymbol{k}}, b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3})$ can be obtained by the same procedures as the theory at zero temperature. The variational conditions are calculated as follows:

$$\phi_{\boldsymbol{k}} = \frac{-\xi_{\boldsymbol{k}} + \sqrt{\xi^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}}(\Delta_{\boldsymbol{k}} - \chi_{\boldsymbol{k}})}}{\Delta_{\boldsymbol{k}}}, \tag{105}$$

$$E_{\boldsymbol{k}} = (u^2_{\boldsymbol{k}} + v^2_{\boldsymbol{k}})\xi_{\boldsymbol{k}} + 2\Delta_{\boldsymbol{k}}u_{\boldsymbol{k}}v_{\boldsymbol{k}}, \tag{106}$$

$$\begin{aligned} b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = {}& \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}}\frac{\sqrt{N_{\boldsymbol{0}}}}{\mathcal{V}}u_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}[(U_{k_1}+U_{k_2})(\phi_{\boldsymbol{k}_3}+\phi_{\boldsymbol{k}_1}\phi_{\boldsymbol{k}_2}) \\ & + (U_{k_1}+U_{k_3})(\phi_{\boldsymbol{k}_2}+\phi_{\boldsymbol{k}_1}\phi_{\boldsymbol{k}_3}) + (U_{k_2}+U_{k_3})(\phi_{\boldsymbol{k}_1}+\phi_{\boldsymbol{k}_2}\phi_{\boldsymbol{k}_3})], \end{aligned} \tag{107}$$

with self-consistent conditions for $\xi_{\boldsymbol{k}} = \delta\Omega_{\rm v}/\delta\rho_{\boldsymbol{k}}$, $\Delta_{\boldsymbol{k}} = \delta\Omega_{\rm v}/\delta F_{\boldsymbol{k}}$, and $\chi_{\boldsymbol{k}}$ whose forms are the same as those by zero-temperature formalism.

Here, we confirm the connection between this theory and the zero-temperature formalism by taking the zero-temperature limit. To do this, we introduce the following Lehmann representation for Green's function:

$$\mathcal{G}_{\boldsymbol{k},i\varepsilon_n} = \int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\frac{\mathcal{A}_{\boldsymbol{k},\varepsilon}}{i\varepsilon_n - \varepsilon}, \tag{108}$$

where $\mathcal{A}$ is the spectral function for $\mathcal{G}$ satisfying

$$\int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\mathcal{A}_{\boldsymbol{k},\varepsilon} = 1. \tag{109}$$

Using the spectral function, we obtain the expressions of $\rho^{\rm qp}_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ as follows:

$$\rho^{\rm qp}_{\boldsymbol{k}} = \int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\mathcal{A}_{\boldsymbol{k},\varepsilon}f(\varepsilon), \tag{110}$$

$$\begin{aligned} w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = {}& b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\int_{-\infty}^{\infty}\frac{d\varepsilon_1}{2\pi}\int_{-\infty}^{\infty}\frac{d\varepsilon_2}{2\pi}\int_{-\infty}^{\infty}\frac{d\varepsilon_3}{2\pi}\frac{\mathcal{A}_{\boldsymbol{k},\varepsilon_1}\mathcal{A}_{\boldsymbol{k},\varepsilon_2}\mathcal{A}_{\boldsymbol{k},\varepsilon_3}}{\varepsilon_1+\varepsilon_2+\varepsilon_3} \\ & \times\big[f(-\varepsilon_1)f(-\varepsilon_2)f(-\varepsilon_3) + f(\varepsilon_1)f(\varepsilon_2)f(\varepsilon_3)\big]. \end{aligned} \tag{111}$$

Here, we show that $\rho^{\rm qp}_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}$ reduces to the expressions obtained by zero-temperature formalism. To proceed calculations, we expand $\mathcal{G}$ assuming $\mathcal{S} \ll 1$ as

$$\begin{aligned}\mathcal{G}_{\boldsymbol{k},i\varepsilon_n} &= \frac{\mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n}}{1-\mathcal{S}_{\boldsymbol{k},i\varepsilon_n}\mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n}} \simeq \mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n}[1+\mathcal{S}^{(1)}_{\boldsymbol{k},i\varepsilon_n}\mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n}] \\ &\equiv \mathcal{G}^{(0)}_{\boldsymbol{k},i\varepsilon_n} + \mathcal{G}^{(1)}_{\boldsymbol{k},i\varepsilon_n}, \end{aligned} \tag{112}$$

where $\mathcal{S}^{(1)} \equiv \mathcal{S}[\mathcal{G}^{(0)}]$. Lehmann representation for $\mathcal{S}^{(1)}$ is given as

$$\begin{aligned}\mathcal{S}^{(1)}_{\boldsymbol{k},i\varepsilon_n} =& -\frac{1}{2}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2\int_{-\infty}^{\infty}\frac{d\varepsilon_2}{2\pi}\int_{-\infty}^{\infty}\frac{d\varepsilon_3}{2\pi}\frac{A^{(0)}_{\boldsymbol{k}_2}(\varepsilon_2)A^{(0)}_{\boldsymbol{k}_3}(\varepsilon_3)}{i\varepsilon_n+\varepsilon_2+\varepsilon_3}[f(-\varepsilon_2)f(-\varepsilon_3)-f(\varepsilon_2)f(\varepsilon_3)] \\ =& -\frac{1}{2}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2\frac{f(-E_{\boldsymbol{k}_2})f(-E_{\boldsymbol{k}_3})-f(E_{\boldsymbol{k}_2})f(E_{\boldsymbol{k}_3})}{i\varepsilon_n+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3}} = \int_{-\infty}^{\infty}\frac{d\varepsilon}{2\pi}\frac{\Gamma^{(1)}_{\boldsymbol{k},\varepsilon}}{i\varepsilon_n-\varepsilon} \\ \to \Gamma^{(1)}_{\boldsymbol{k},\varepsilon} =& -\pi\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2[f(-E_{\boldsymbol{k}_2})f(-E_{\boldsymbol{k}_3})-f(E_{\boldsymbol{k}_2})f(E_{\boldsymbol{k}_3})] \\ &\times\delta(\varepsilon+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3}), \end{aligned} \tag{113}$$

where $\Gamma^{(1)}_{\boldsymbol{k},\varepsilon}$ is the spectral function for $\mathcal{S}_{\boldsymbol{k},i\varepsilon_n}$.

Since the spectral function is also expressible as $A_{\boldsymbol{k},\varepsilon} \equiv -2{\rm Im}\mathcal{G}_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}$ and $\Gamma^{(1)}_{\boldsymbol{k},\varepsilon} \equiv -2{\rm Im}\mathcal{S}^{(1)}_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}$, we obtain $A^{(1)}_{\boldsymbol{k},\varepsilon}$ as

$$\begin{aligned}A^{(1)}_{\boldsymbol{k},\varepsilon} &\equiv -2{\rm Im}\mathcal{G}^{(1)}_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+} = -2{\rm Im}[{\mathcal{G}^{(0)}}^2_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}S^{(1)}_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}] \\ &\simeq -2{\rm Im}S^{(1)}_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}{\rm Re}{\mathcal{G}^{(0)}}^2_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+} \simeq \frac{\Gamma^{(1)}_{\boldsymbol{k},\varepsilon}}{(\varepsilon-E_{\boldsymbol{k}})^2} \\ &= -\pi\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2\frac{f(-E_{\boldsymbol{k}_2})f(-E_{\boldsymbol{k}_3})-f(E_{\boldsymbol{k}_2})f(E_{\boldsymbol{k}_3})}{(E_{\boldsymbol{k}}+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3})^2}\delta(\varepsilon+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3}), \end{aligned} \tag{114}$$

where we transformed the second into the third equation with ${\rm Im}\mathcal{G}^{(0)} \simeq 0$. This consideration is based on the assumption that ideal quasiparticles have infinite lifetimes due to the absence of interactions. On the other hand, in the presence of correlations between quasiparticles, such as 3/2-body correlations, finite lifetimes described by ${\rm Im}\mathcal{S}^{(1)}$ appear in the quasiparticles. Therefore, we obtain $\rho^{\rm qp}_{\boldsymbol{k}}$ as

$$\begin{aligned}\rho^{\rm qp}_{\boldsymbol{k}} &\simeq \int\frac{d\varepsilon}{2\pi}[A^{(0)}_{\boldsymbol{k},\varepsilon}+A^{(1)}_{\boldsymbol{k},\varepsilon}]f(\varepsilon) \\ &= f(E_{\boldsymbol{k}}) + \frac{1}{2}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\neq\boldsymbol{0}}|b_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2\frac{f(-E_{\boldsymbol{k}_2})f(-E_{\boldsymbol{k}_3})}{(E_{\boldsymbol{k}}+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3})^2} \end{aligned} \tag{115a}$$

On the other hand, by substituting $A \simeq A^{(0)}$ into Eq. (111), we obtain the expression of w as

$$w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} \simeq \frac{b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}}{E_{\boldsymbol{k}_1}+E_{\boldsymbol{k}_2}+E_{\boldsymbol{k}_3}}\big[f(-E_{\boldsymbol{k}_1})f(-E_{\boldsymbol{k}_2})f(-E_{\boldsymbol{k}_3})+f(E_{\boldsymbol{k}_1})f(E_{\boldsymbol{k}_2})f(E_{\boldsymbol{k}_3})\big]. \tag{115b}$$

Therefore, by taking $f(E_{\boldsymbol{k}\neq\boldsymbol{0}}) \to 0$ and $f(-E_{\boldsymbol{k}\neq\boldsymbol{0}}) \to -1$ in the limit $T \to 0$ in Eqs. (162a) and (162b), the finite-temperature formalism reduces to the zero-temperature formalism. We note the

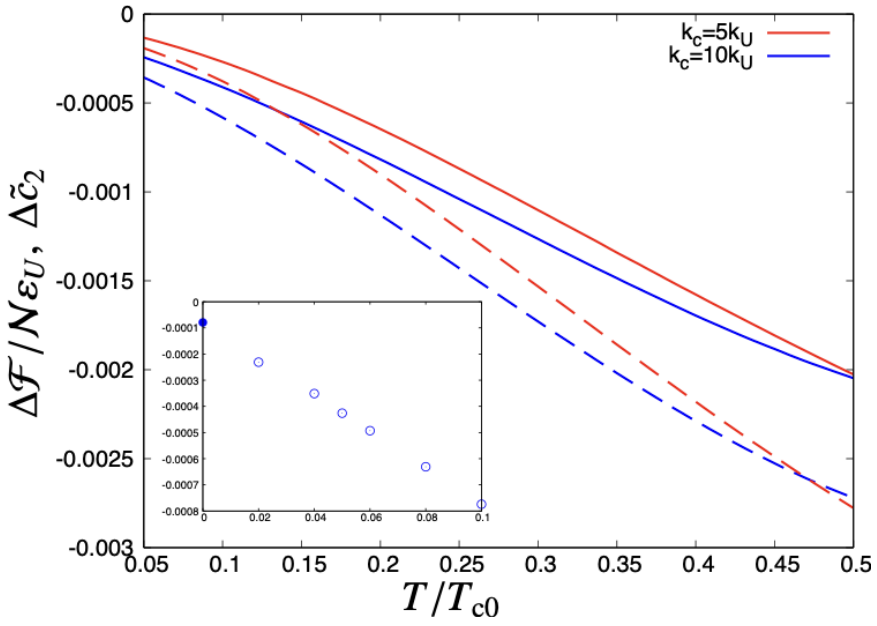

Figure 4: A picture from Ref. [26]: Temperature dependencies of $\Delta\mathcal{F}$ (solid) and $\Delta\tilde{c}_2 = \Delta c_2 \times \delta = (c_2 - c_2^{\mathrm{HFB}})\delta$ (dashed) for $\delta = 1.0 \times 10^{-6}$. The inset shows $\Delta\mathcal{F}$ near zero temperature for $k_{\mathrm{c}} = 10k_U$, and the filled circle is obtained by zero-temperature formalism in Ref. [17].

approximated spectral function given by $A^{(0)}_{\boldsymbol{k},\varepsilon} + A^{(1)}_{\boldsymbol{k},\varepsilon}$ does not satisfy the sum rule. To satisfy this sum rule completely, it is necessary to obtain $\mathcal{G}$ self-consistently.

Based on the finite-temperature formalism, we have evaluated the free-energy difference $\Delta\mathcal{F} \equiv \mathcal{F} - \mathcal{F}_{\mathrm{HFB}}$ in the region $T/T_{\mathrm{c0}} \leq 0.5$ in Ref. [26], where T_{c0} represents the critical temperature of an ideal BEC system. By numerical calculations, we have shown the 3/2-body correlations yield finite contribution to lower the free energy. In this sense, collisions between Bogoliubov quasiparticles introduced by 3/2-body correlations play roles to increase the entropy at finite temperature.

Before closing this section, we comment about the applicability of this theory, specifically in terms of the choice of $\hat{H}_{\mathrm{v}}$ in the variational density matrix. In this section, we have assumed that the 3/2-body correlations by quasiparticles given as $\hat{\gamma}\hat{\gamma}\hat{\gamma}$ and $\hat{\gamma}^\dagger\hat{\gamma}^\dagger\hat{\gamma}^\dagger$ are more important than other contributions on account of the consideration in the theory of the ground state. In this sense, it is possible to choose or add independent collisional processes by quasiparticles (e.g.,$\hat{\gamma}^\dagger\hat{\gamma}\hat{\gamma}$) in the density matrix with introducing the corresponding variational parameters. However, contributions except $\hat{\gamma}\hat{\gamma}\hat{\gamma}$ and $\hat{\gamma}^\dagger\hat{\gamma}^\dagger\hat{\gamma}^\dagger$ are neglected approximately at $T = 0$ and our zero-temperature formalism is valid. If the variational density matrix $\hat{\rho}_{\mathrm{v}}$ is chosen in terms of $\hat{H}_{\mathrm{v}}$ given by

$$\hat{H}_{\mathrm{v}} = \hat{H}^{\mathrm{MF}}_{\mathrm{v}} + \hat{H}^{2,1}_{\mathrm{v}}, \tag{116}$$

where $\hat{H}_{\rm v}^{2,1}$ is defined as

$$\hat{H}_{\rm v}^{2,1} \equiv \frac{1}{2!} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3 \neq \boldsymbol{0}} (b_{\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3} \hat{\gamma}_{\boldsymbol{k}_1}^\dagger \hat{\gamma}_{\boldsymbol{k}_2}^\dagger \hat{\gamma}_{-\boldsymbol{k}_3} + b_{\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3}^* \hat{\gamma}_{-\boldsymbol{k}_3}^\dagger \hat{\gamma}_{\boldsymbol{k}_2} \hat{\gamma}_{\boldsymbol{k}_1}). \tag{117}$$

$\rho_{\boldsymbol{k}}^{\rm qp} = {\rm Tr}\hat{\rho}_{\rm v}\hat{\gamma}_{\boldsymbol{k}}^\dagger\hat{\gamma}_{\boldsymbol{k}}$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} = {\rm Tr}\hat{\rho}_{\rm v}\hat{\gamma}_{\boldsymbol{k}_1}\hat{\gamma}_{\boldsymbol{k}_2}\hat{\gamma}_{\boldsymbol{k}_3}$ are calculated as

$$\rho_{\boldsymbol{k}}^{\rm qp} \simeq f(E_{\boldsymbol{k}}) + \sum_{\boldsymbol{k}_2\boldsymbol{k}_3 \neq \boldsymbol{0}} \left[\frac{|b_{\boldsymbol{k}_2\boldsymbol{k}_3;\boldsymbol{k}}|^2 f(E_{\boldsymbol{k}_2}) f(E_{\boldsymbol{k}_3})}{2(E_{\boldsymbol{k}} - E_{\boldsymbol{k}_2} - E_{\boldsymbol{k}_3})^2} - \frac{|b_{\boldsymbol{k}\boldsymbol{k}_2;\boldsymbol{k}_3}|^2 f(-E_{\boldsymbol{k}_2}) f(E_{\boldsymbol{k}_3})}{(E_{\boldsymbol{k}} + E_{\boldsymbol{k}_2} - E_{\boldsymbol{k}_3})^2} \right], \tag{118a}$$

$$w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} \simeq \frac{b_{\boldsymbol{k}_1\boldsymbol{k}_2;\boldsymbol{k}_3}}{E_{\boldsymbol{k}_1} + E_{\boldsymbol{k}_2} - E_{\boldsymbol{k}_3}} \big[f(-E_{\boldsymbol{k}_1}) f(-E_{\boldsymbol{k}_2}) f(E_{\boldsymbol{k}_3}) + f(E_{\boldsymbol{k}_1}) f(E_{\boldsymbol{k}_2}) f(-E_{\boldsymbol{k}_3}) \big]. \tag{118b}$$

Therefore, both of Eqs. (118) vanish in the limit $T \to 0$ due to the condition $f(E_{\boldsymbol{k}\neq\boldsymbol{0}}) = 0$.

Chapter 3 Variational Theory out of Equilibrium States

In this chapter, we describe dynamics of interacting BEC systems with 3/2-body correlations and reconsider the relation between BEC and superfluidity in terms of macroscopic coherence. To do this, we introduce a time-evolutional variational wave function. Based on the wave function, we investigate the response of a weakly-interacting BEC system by changing of the s-wave scattering length (coupling constant) rapidly in order to observe the dynamical relaxation process [58]. Using the same method in this chapter, we also introduce the time-dependent theory of superconductivity beyond mean-field approximation in appendix B.

3.1 Variational Wave Function Derived from The Principle of Least Action

To observe 3/2-body correlations dynamically, we construct a variational wave function with time dependence imposing the following the principle of least action [55, 56, 57]:

$$\delta S = \delta \int_{t_0}^{t_1} dt' \, \langle \Phi(t') | \hat{\mathcal{L}}(t') | \Phi(t') \rangle = \delta \int_{t_0}^{t_1} dt' \, \langle \Phi(t') | i\hbar \frac{\partial}{\partial t'} - \hat{H} | \Phi(t') \rangle = 0, \tag{119}$$

where $\hat{\mathcal{L}}$ represents a Lagrangian operator and t_0, t_1 is arbitrary times. The Hamiltonian H is given by

$$\hat{H} = \sum_{\boldsymbol{k}} \varepsilon_k \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}} + \frac{1}{2\mathcal{V}} \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'} U_q \hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q}} \hat{c}^\dagger_{\boldsymbol{k}'-\boldsymbol{q}} \hat{c}_{\boldsymbol{k}'} \hat{c}_{\boldsymbol{k}}, \tag{120}$$

with $(\hat{c}, \hat{c}^\dagger)$ denoting a set of boson field operators with $[\hat{c}_{\boldsymbol{k}}, \hat{c}^\dagger_{\boldsymbol{k}'}] = \delta_{\boldsymbol{k},\boldsymbol{k}'}$, $\varepsilon_k = \hbar^2 k^2 / 2m$, and U_q the interaction potential. The Hamiltonian is categorized in terms of the number of $(\hat{c}_{\boldsymbol{0}}, \hat{c}^\dagger_{\boldsymbol{0}})$ as follows:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_{\frac{3}{2}} + \hat{H}_2, \tag{121a}$$

where

$$\hat{H}_0 = \frac{U_0}{2\mathcal{V}} \hat{c}^\dagger_{\boldsymbol{0}} \hat{c}^\dagger_{\boldsymbol{0}} \hat{c}_{\boldsymbol{0}} \hat{c}_{\boldsymbol{0}}, \tag{121b}$$

$$\hat{H}_1 = \sum_{\boldsymbol{k}\neq\boldsymbol{0}} \varepsilon_k \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} (U_0 + U_k) \hat{c}^\dagger_{\boldsymbol{0}} \hat{c}_{\boldsymbol{0}} \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}} + \frac{1}{2\mathcal{V}} \sum_{\boldsymbol{k}\neq\boldsymbol{0}} U_k (\hat{c}^\dagger_{\boldsymbol{0}} \hat{c}^\dagger_{\boldsymbol{0}} \hat{c}_{\boldsymbol{k}} \hat{c}_{-\boldsymbol{k}} + \hat{c}^\dagger_{-\boldsymbol{k}} \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{0}} \hat{c}_{\boldsymbol{0}}) \tag{121c}$$

$$\hat{H}_{\frac{3}{2}} = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3\neq\boldsymbol{0}} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\boldsymbol{0}} (\hat{c}^\dagger_{\boldsymbol{0}} \hat{c}^\dagger_{-\boldsymbol{k}_3} \hat{c}_{\boldsymbol{k}_2} \hat{c}_{\boldsymbol{k}_1} + \hat{c}^\dagger_{\boldsymbol{k}_1} \hat{c}^\dagger_{\boldsymbol{k}_2} \hat{c}_{-\boldsymbol{k}_3} \hat{c}_{\boldsymbol{0}}), \tag{121d}$$

$$\hat{H}_2 = \frac{1}{2\mathcal{V}} \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'\neq\boldsymbol{0}} U_q \hat{c}^\dagger_{\boldsymbol{k}+\boldsymbol{q}} \hat{c}^\dagger_{\boldsymbol{k}'-\boldsymbol{q}} \hat{c}_{\boldsymbol{k}'} \hat{c}_{\boldsymbol{k}}. \tag{121e}$$

The principle of least action in Eq. (119) for the variational parameters derives the time-dependent theories, such as the time-dependent Hartree–Fock–Bogoliubov (TDHFB) equations for BEC systems [57] and the time-dependent Bogoliubov–de–Genne (TDBdG) equations for superconductors

or superfluid Fermi systems[58], as shown later (regarding theory of superconductivity, the derivation is written in appendix B). Here, we start from Eq. (119) and generalize these time-dependent mean-field theories by improving the variational wave functions.

Using number-conserving operators $(\hat{\beta}_0, \hat{\beta}_0^\dagger)$, the field operators $(d, d^\dagger)$ for $\boldsymbol{k} \neq \boldsymbol{0}$ are expressed as

$$\hat{d}_{\boldsymbol{k}}^\dagger = \hat{c}_{\boldsymbol{k}}^\dagger \hat{\beta}_0, \hat{d}_{\boldsymbol{k}} = \hat{\beta}_0^\dagger \hat{c}_{\boldsymbol{k}}, \tag{122}$$

which satisfy $[\hat{d}_{\boldsymbol{k}}, \hat{d}_{\boldsymbol{k}'}^\dagger] = \delta_{\boldsymbol{k},\boldsymbol{k}'}$.

First, we introduce the Girardeau–Arnowitt variational wave function with time dependence as follows:

$$|\Phi_{\rm GA}(t)\rangle = A \exp[\hat{\pi}^\dagger(t)] \, |N\rangle_{\boldsymbol{0}} \, , \ \hat{\pi}^\dagger(t) \equiv \frac{1}{2} \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}}(t) \hat{d}_{\boldsymbol{k}}^\dagger \hat{d}_{-\boldsymbol{k}}^\dagger \tag{123}$$

with $A = \langle N_{\boldsymbol{0}} | e^{\hat{\pi}} e^{\hat{\pi}^\dagger} | N_{\boldsymbol{0}} \rangle^{-\frac{1}{2}}$. $|\Phi_{\rm GA}(t)\rangle$ corresponds to a "vacuum state" characterized by $\hat{\gamma}_{\boldsymbol{k}}(t) \, |\Phi_{\rm GA}(t)\rangle = 0$, where γ is defined by

$$\hat{\gamma}_{\boldsymbol{k}}(t) = u_{\boldsymbol{k}}(t) \hat{d}_{\boldsymbol{k}} - v_{\boldsymbol{k}}(t) \hat{d}_{-\boldsymbol{k}}^\dagger \tag{124a}$$

$$\gamma_{-\boldsymbol{k}}^\dagger(t) = -v_{\boldsymbol{k}}^*(t) \hat{d}_{\boldsymbol{k}} + u_{\boldsymbol{k}}(t) d_{-\boldsymbol{k}}^\dagger. \tag{124b}$$

with definitions $u_{\boldsymbol{k}} = \frac{1}{\sqrt{1-|\phi_{\boldsymbol{k}}|^2}} = u_{\boldsymbol{k}}^*$ and $v_{\boldsymbol{k}} = \frac{\phi_{\boldsymbol{k}}}{\sqrt{1-|\phi_{\boldsymbol{k}}|^2}}$. By these definitions, commutator relations are given by $[\hat{\gamma}_{\boldsymbol{k}}, \hat{\gamma}_{\boldsymbol{k}'}^\dagger] = \delta_{\boldsymbol{k}\boldsymbol{k}'}$ and $[\hat{\gamma}_{\boldsymbol{k}}, \hat{\gamma}_{\boldsymbol{k}'}] = 0$. The inverse transformations are given by

$$\hat{d}_{\boldsymbol{k}} = u_{\boldsymbol{k}}(t) \hat{\gamma}_{\boldsymbol{k}}(t) + v_{\boldsymbol{k}}(t) \gamma_{-\boldsymbol{k}}^\dagger(t), \tag{125a}$$

$$\hat{d}_{-\boldsymbol{k}}^\dagger = v_{\boldsymbol{k}}^*(t) \hat{\gamma}_{-\boldsymbol{k}}(t) + u_{\boldsymbol{k}}(t) \hat{\gamma}_{-\boldsymbol{k}}^\dagger(t). \tag{125b}$$

We note $\langle \Phi_{\rm GA}(t) | \hat{H}_{\frac{3}{2}} | \Phi_{\rm GA}(t) \rangle = 0$.

Before introducing our variational wave function, we reproduce the TDHFB at $T = 0$ within mean-field approximation. To do this, we evaluate $\langle \Phi_{\rm GA}(t) | \, i\hbar \partial / \partial t \, | \Phi_{\rm GA}(t) \rangle$ as

$$\begin{aligned} i\hbar \langle \Phi_{\rm GA}(t) | \frac{\partial}{\partial t} | \Phi_{\rm GA}(t) \rangle &= \frac{i\hbar}{2} \sum_{\boldsymbol{k}} \langle \Phi_{\rm GA}(t) | \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} \hat{d}_{\boldsymbol{k}}^\dagger \hat{d}_{-\boldsymbol{k}}^\dagger | \Phi_{\rm GA}(t) \rangle + i\hbar \frac{\partial \ln A(t)}{\partial t} \\ &= \frac{i\hbar}{2} \sum_{\boldsymbol{k}} F_{\boldsymbol{k}}^*(t) \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} + i\hbar \frac{\partial \ln A(t)}{\partial t}. \end{aligned} \tag{126}$$

Using this relation and $\partial(\phi^*/(1-|\phi|^2))/\partial\phi^* = (1-|\phi|^2)^{-2} = u^4$, we obtain

$$\frac{\delta}{\delta \phi_{\boldsymbol{k}}^*(t)} \int_{t_0}^{t_1} \mathcal{E}_{\rm GA}(t') dt' = \frac{i\hbar}{2} \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} u_{\boldsymbol{k}}^4(t), \tag{127}$$

where we used $\delta \ln A(t = t_0)/\delta \phi_{\boldsymbol{k}}^*(t) = \delta \ln A(t = t_1)/\delta \phi_{\boldsymbol{k}}^*(t)$ with $t \neq t_0, t_1$.

The expectation value of the Hamiltonian is given by

$$\begin{aligned}\mathcal{E}_{\rm GA} &= \langle\Phi_{\rm GA}(t)|\hat{H}_0+\hat{H}_1+\hat{H}_2|\Phi_{\rm GA}(t)\rangle \\ &= \frac{U_{\mathbf{0}}N^2}{2\mathcal{V}}+\sum_{\boldsymbol{k}\neq\mathbf{0}}\varepsilon_k\rho_{\boldsymbol{k}}+\frac{N_{\mathbf{0}}}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\mathbf{0}}U_k\rho_{\boldsymbol{k}}+\frac{N_{\mathbf{0}}}{2\mathcal{V}}\sum_{\boldsymbol{k}\neq\mathbf{0}}U_k(F_{\boldsymbol{k}}+F_{\boldsymbol{k}}^*) \\ &+\frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}\neq\mathbf{0}}U_{|\boldsymbol{k}-\boldsymbol{k}'|}(\rho_{\boldsymbol{k}}\rho_{\boldsymbol{k}'}+F_{\boldsymbol{k}}F_{\boldsymbol{k}'}^*),\end{aligned} \tag{128}$$

where we approximate $\langle\Phi_{\rm GA}(t)|(\hat{c}_{\mathbf{0}}^\dagger\hat{\beta}_0)^\nu(\hat{\beta}_0^\dagger\hat{c}_{\mathbf{0}})^\mu|\Phi_{\rm GA}(t)\rangle\simeq {N_{\mathbf{0}}}^{(\nu+\mu)/2}$, $N_{\mathbf{0}}=N-\sum_{\boldsymbol{k}}\rho_{\boldsymbol{k}}$, $\rho_{\boldsymbol{k}}\equiv\langle\hat{d}_{\boldsymbol{k}}^\dagger\hat{d}_{\boldsymbol{k}}\rangle$, and $F_{\boldsymbol{k}}\equiv\langle\hat{d}_{\boldsymbol{k}}\hat{d}_{-\boldsymbol{k}}\rangle$. $\rho_{\boldsymbol{k}}$ and $F_{\boldsymbol{k}}$ is given in terms of u and v as

$$\rho_{\boldsymbol{k}}=|v_{\boldsymbol{k}}|^2,\ F_{\boldsymbol{k}}=u_{\boldsymbol{k}}v_{-\boldsymbol{k}}.$$

Therefore,

$$\frac{\delta\mathcal{E}_{\rm GA}}{\delta\phi_{\boldsymbol{k}}^*}=\sum_{\boldsymbol{k}'\neq\mathbf{0}}\Big[\frac{\delta\mathcal{E}_{\rm GA}}{\delta\rho_{\boldsymbol{k}'}}\frac{\delta\rho_{\boldsymbol{k}'}}{\delta\phi_{\boldsymbol{k}}^*}+\frac{\delta\mathcal{E}_{\rm GA}}{\delta F_{\boldsymbol{k}'}}\frac{\delta F_{\boldsymbol{k}'}}{\delta\phi_{\boldsymbol{k}}^*}+\frac{\delta\mathcal{E}_{\rm GA}}{\delta F_{\boldsymbol{k}'}^*}\frac{\delta F_{\boldsymbol{k}'}^*}{\delta\phi_{\boldsymbol{k}}^*}\Big]=\xi_{\boldsymbol{k}}\phi_{\boldsymbol{k}}+\frac{\Delta_{\boldsymbol{k}}^*\phi_{\boldsymbol{k}}^2}{2}+\frac{\Delta_{\boldsymbol{k}}}{2},$$

where

$$\xi_{\boldsymbol{k}}=\varepsilon_k+\frac{N_{\mathbf{0}}U_k}{\mathcal{V}}+\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'\neq\mathbf{0}}(U_{|\boldsymbol{k}-\boldsymbol{k}'|}-U_{k'})\rho_{\boldsymbol{k}'}-\frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}'}U_{k'}(F_{\boldsymbol{k}'}+F_{\boldsymbol{k}'}^*), \tag{129a}$$

$$\Delta_{\boldsymbol{k}}=\frac{N_{\mathbf{0}}U_k}{\mathcal{V}}+\frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'}U_{|\boldsymbol{k}-\boldsymbol{k}'|}F_{\boldsymbol{k}'}. \tag{129b}$$

By these calculations, we obtain

$$i\hbar\frac{\partial\phi_{\boldsymbol{k}}}{\partial t}=2\xi_{\boldsymbol{k}}\phi_{\boldsymbol{k}}+\Delta_{\boldsymbol{k}}^*\phi_{\boldsymbol{k}}^2+\Delta_{\boldsymbol{k}}. \tag{130}$$

Here, we confirm the equivalence between the TDHFB theory and Eq. (130). Recalling the relations for $u_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}}=\phi_{\boldsymbol{k}}u_{\boldsymbol{k}}$, we can express Eq. (130) in the following form:

$$\begin{aligned}i\hbar\frac{\partial v_{\boldsymbol{k}}}{\partial t}&=i\hbar u_{\boldsymbol{k}}\frac{\partial\phi_{\boldsymbol{k}}}{\partial t}+i\hbar\frac{\partial u_{\boldsymbol{k}}}{\partial t}\phi_{\boldsymbol{k}} \\ &=[2\xi_{\boldsymbol{k}}\phi_{\boldsymbol{k}}+\Delta_{\boldsymbol{k}}^*\phi_{\boldsymbol{k}}^2+\Delta_{\boldsymbol{k}}]u_{\boldsymbol{k}}+i\hbar\frac{\partial u_{\boldsymbol{k}}}{\partial t}\phi_{\boldsymbol{k}}.\end{aligned} \tag{131}$$

On the other hand, the TDHFB theory at $T=0$ is given as [57]

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{pmatrix}=\begin{pmatrix}\xi_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}}\\ -\Delta_{\boldsymbol{k}}^* & -\xi_{\boldsymbol{k}}\end{pmatrix}\begin{pmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{pmatrix}. \tag{132}$$

Substituting Eq. (132) into Eq. (131), we can see the equivalence easily.

Next, we incorporate the effect by 3/2-body correlations into the wave function.

$$|\Phi\rangle=A_3\exp(\hat{\pi}_3^\dagger)\,|\Phi_{\rm GA}\rangle\,,\ \hat{\pi}_3^\dagger\equiv\frac{1}{3!}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\hat{\gamma}_{\boldsymbol{k}_1}^\dagger\hat{\gamma}_{\boldsymbol{k}_2}^\dagger\hat{\gamma}_{\boldsymbol{k}_3}^\dagger. \tag{133}$$

We extend this wave function using the same manner as that by mean-field theory. The expectation value of Hamiltonian is given by

$$i\hbar \langle \Phi(t)| \frac{\partial}{\partial t} |\Phi(t)\rangle = \frac{i\hbar}{2} \sum_{\boldsymbol{k}} u_{\boldsymbol{k}} v^*_{\boldsymbol{k}} \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} + i\hbar \langle \Phi(t)| \frac{\partial \hat{\pi}^\dagger_3(t)}{\partial t} |\Phi(t)\rangle + i\hbar \frac{\partial (\ln A + \ln A_3)}{\partial t}. \tag{134}$$

The first term is evaluated as

$$\begin{aligned}
&i\hbar \langle \Phi(t)| \frac{\partial \hat{\pi}^\dagger_3(t)}{\partial t} |\Phi(t)\rangle \\
&= \frac{i\hbar}{3!} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \neq \boldsymbol{0}} w^*_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} \frac{\partial w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}(t)}{\partial t} \\
&+ \frac{i\hbar}{3!} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \neq \boldsymbol{0}} w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} \langle \Phi(t)| \frac{\partial \hat{\gamma}^\dagger_{\boldsymbol{k}_1}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}_2}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}_3}(t)}{\partial t} |\Phi(t)\rangle \\
&\simeq \frac{i\hbar}{3!} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \neq \boldsymbol{0}} w^*_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} \frac{\partial w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}(t)}{\partial t} + \frac{i\hbar}{(3!)^2} \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3 \boldsymbol{k}'_1 \boldsymbol{k}'_2 \boldsymbol{k}'_3 \neq \boldsymbol{0}} w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} w^*_{\boldsymbol{k}'_1 \boldsymbol{k}'_2 \boldsymbol{k}'_3} \\
&\times \langle \Phi_{\mathrm{GA}}(t)| \hat{\gamma}_{\boldsymbol{k}'_3}(t) \hat{\gamma}_{\boldsymbol{k}'_2}(t) \hat{\gamma}_{\boldsymbol{k}'_1}(t) \frac{\partial \hat{\gamma}^\dagger_{\boldsymbol{k}_1}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}_2}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}_3}(t)}{\partial t} |\Phi_{\mathrm{GA}}(t)\rangle .
\end{aligned}$$

Using the following relation,

$$\begin{aligned}
&\langle \Phi_{\mathrm{GA}}(t)| \hat{\gamma}_{\boldsymbol{k}_3}(t) \hat{\gamma}_{\boldsymbol{k}_2}(t) \hat{\gamma}_{\boldsymbol{k}_1}(t) \frac{\partial \hat{\gamma}^\dagger_{\boldsymbol{k}'_1}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}'_2}(t) \hat{\gamma}^\dagger_{\boldsymbol{k}'_3}(t)}{\partial t} |\Phi_{\mathrm{GA}}(t)\rangle \\
&= \sum_P \delta_{\boldsymbol{k}_1, \boldsymbol{k}'_{1P}} \delta_{\boldsymbol{k}_2, \boldsymbol{k}'_{2P}} \delta_{\boldsymbol{k}_3, \boldsymbol{k}'_{3P}} (f_{\boldsymbol{k}_{1P}} + f_{\boldsymbol{k}_{2P}} + f_{\boldsymbol{k}_{3P}}),
\end{aligned}$$

with definition of f as

$$[\hat{\gamma}_{\boldsymbol{k}}(t), \frac{\partial \hat{\gamma}^\dagger_{\boldsymbol{k}'}(t)}{\partial t}] = \delta_{\boldsymbol{k}, \boldsymbol{k}'} \Big(v^*_{\boldsymbol{k}} \frac{\partial v_{\boldsymbol{k}}}{\partial t} - u_{\boldsymbol{k}} \frac{\partial u_{\boldsymbol{k}}}{\partial t} \Big) \equiv \delta_{\boldsymbol{k}, \boldsymbol{k}'} \frac{f_{\boldsymbol{k}}}{i\hbar},$$

Eq. (134) is transformed into

$$\begin{aligned}
i\hbar \langle \Phi(t)| \frac{\partial}{\partial t} |\Phi(t)\rangle \simeq \frac{i\hbar}{2} \sum_{\boldsymbol{k}} u_{\boldsymbol{k}} v^*_{\boldsymbol{k}} \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} + \frac{i\hbar}{3!} \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3} w^*_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} \frac{\partial w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}(t)}{\partial t} \\
+ \frac{1}{3!} \sum_{\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{k}_3} |w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}|^2 \Big[f_{\boldsymbol{k}_1} + f_{\boldsymbol{k}_2} + f_{\boldsymbol{k}_3} \Big] + i\hbar \frac{\partial (\ln A + \ln A_3)}{\partial t}.
\end{aligned} \tag{135}$$

Therefore, we obtain the following equations:

$$\frac{\delta \mathcal{E}}{\delta \phi^*_{\boldsymbol{k}}} = \frac{i\hbar}{2} \frac{\partial \phi_{\boldsymbol{k}}}{\partial t} \left[1 + \sum_{\boldsymbol{k}_2, \boldsymbol{k}_3} |w_{\boldsymbol{k} \boldsymbol{k}_2 \boldsymbol{k}_3}|^2 \right] u^4_{\boldsymbol{k}}, \tag{136a}$$

$$\frac{\delta \mathcal{E}}{\delta w^*_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}} = i\hbar \frac{\partial w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}}{\partial t} + w_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3} \Big[f_{\boldsymbol{k}_1} + f_{\boldsymbol{k}_2} + f_{\boldsymbol{k}_3} \Big], \tag{136b}$$

where $\mathcal{E} = \langle\Phi(t)|\hat{H}|\Phi(t)\rangle$ given by

$$\begin{aligned}\mathcal{E} &= \langle\Phi(t)|\hat{H}_0 + \hat{H}_1 + \hat{H}_{\frac{3}{2}} + \hat{H}_2|\Phi(t)\rangle \\ &= \frac{U_{\mathbf{0}}N^2}{2\mathcal{V}} + \sum_{\boldsymbol{k}\neq\mathbf{0}}\varepsilon_k\rho_{\boldsymbol{k}} + \frac{N_{\mathbf{0}}}{\mathcal{V}}\sum_{\boldsymbol{k}\neq\mathbf{0}}U_k\rho_{\boldsymbol{k}} + \frac{N_{\mathbf{0}}}{2\mathcal{V}}\sum_{\boldsymbol{k}\neq\mathbf{0}}U_k(F_{\boldsymbol{k}} + F^*_{\boldsymbol{k}}) \\ &+ \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k},\boldsymbol{k}',\boldsymbol{q}\neq\mathbf{0}}U_{|\boldsymbol{k}-\boldsymbol{k}'|}(\rho_{\boldsymbol{k}}\rho_{\boldsymbol{k}'} + F_{\boldsymbol{k}}F^*_{\boldsymbol{k}'}) \\ &+ \frac{\sqrt{N_{\mathbf{0}}}}{\mathcal{V}}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3\neq\mathbf{0}}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\mathbf{0}}U_{k_1}(W_{\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_3} + W^*_{\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_3}),\end{aligned} \tag{137}$$

with

$$\rho_{\boldsymbol{k}} = |v_{\boldsymbol{k}}|^2 + \frac{|v_{\boldsymbol{k}}|^2}{2}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3}|w_{-\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2 + \frac{u^2_{\boldsymbol{k}}}{2}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3}|w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2, \tag{138a}$$

$$F_{\boldsymbol{k}} = u_{\boldsymbol{k}}v_{\boldsymbol{k}}\Big[1 + \frac{1}{2}\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3}(|w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2 + |w_{-\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2)\Big], \tag{138b}$$

$$W_{\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_3} \equiv \langle\Phi|\hat{d}^\dagger_{-\boldsymbol{k}_3}\hat{d}_{\boldsymbol{k}_2}\hat{d}_{\boldsymbol{k}_1}|\Phi\rangle = u_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2}v^*_{\boldsymbol{k}_3}w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} + v_{\boldsymbol{k}_1}v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}w^*_{-\boldsymbol{k}_1-\boldsymbol{k}_2-\boldsymbol{k}_3}, \tag{138c}$$

Straightforwardly, the variational conditions are calculated as

$$\begin{aligned}\frac{\delta\mathcal{E}}{\delta\phi^*_{\boldsymbol{k}}} &= \frac{1+\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3}|w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2}{2}(2\xi_{\boldsymbol{k}}\phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\phi^2_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} + \chi_{\boldsymbol{k}})u^4_{\boldsymbol{k}} \\ \frac{\delta\mathcal{E}}{\delta w^*_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}} &= b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} + w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}(E^0_{\boldsymbol{k}_1} + E^0_{\boldsymbol{k}_2} + E^0_{\boldsymbol{k}_3}),\end{aligned}$$

where

$$\begin{aligned}\xi_{\boldsymbol{k}} =& \varepsilon_k + \frac{N_{\mathbf{0}}U_k}{\mathcal{V}} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'\neq\mathbf{0}}(U_{|\boldsymbol{k}-\boldsymbol{k}'|} - U_{k'})\rho_{\boldsymbol{k}'} - \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}'}U_{k'}(F_{\boldsymbol{k}'} + F^*_{\boldsymbol{k}'}) \\ &+ \frac{1}{2\mathcal{V}\sqrt{N_{\mathbf{0}}}}\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{k}_3\neq\mathbf{0}}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\mathbf{0}}U_{k_1}(W_{\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_3} + W^*_{\boldsymbol{k}_1,\boldsymbol{k}_2;\boldsymbol{k}_3})\end{aligned} \tag{139a}$$

$$\Delta_{\boldsymbol{k}} = \frac{N_{\mathbf{0}}U_k}{\mathcal{V}} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}'\neq\mathbf{0}}U_{|\boldsymbol{k}-\boldsymbol{k}'|}F_{\boldsymbol{k}'}, \tag{139b}$$

$$\begin{aligned}\chi_{\boldsymbol{k}} =& \frac{\sqrt{N_{\mathbf{0}}}}{1+\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3}|w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}|^2}\frac{1}{\mathcal{V}} \\ &\times\sum_{\boldsymbol{k}_2,\boldsymbol{k}_3\neq\mathbf{0}}\delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3}\frac{u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}}{u_{\boldsymbol{k}}}\Big[(U_k + U_{k_2})\big[\phi_{\boldsymbol{k}}(\phi_{\boldsymbol{k}_3} + \phi_{\boldsymbol{k}}\phi_{\boldsymbol{k}_2})w^*_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3} \\ &+ [2(1-|\phi_{\boldsymbol{k}}|^2)\phi^*_{\boldsymbol{k}_2} + \phi_{\boldsymbol{k}}(\phi^*_{\boldsymbol{k}_3} + \phi^*_{\boldsymbol{k}}\phi^*_{\boldsymbol{k}_2})]w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}\big] + U_{k_2}[2(1-|\phi_{\boldsymbol{k}}|^2)w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3} \\ &+ \phi_{\boldsymbol{k}}(\phi^*_{\boldsymbol{k}} + \phi^*_{\boldsymbol{k}_2}\phi^*_{\boldsymbol{k}_3})w_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3} + \phi_{\boldsymbol{k}}(\phi_{\boldsymbol{k}} + \phi_{\boldsymbol{k}_2}\phi_{\boldsymbol{k}_3})w^*_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3}]\Big].\end{aligned} \tag{139c}$$

$$E^0_{\boldsymbol{k}} = \xi_{\boldsymbol{k}}(u^2_{\boldsymbol{k}} + |v_{\boldsymbol{k}}|^2) + \Delta^*_{\boldsymbol{k}}u_{\boldsymbol{k}}v_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}}u_{\boldsymbol{k}}v^*_{\boldsymbol{k}}, \tag{139d}$$

$$\begin{aligned}b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} =& \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3,\mathbf{0}}\frac{\sqrt{N_{\mathbf{0}}}}{\mathcal{V}}u_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}\Big[(U_{k_1} + U_{k_2})(\phi_{\boldsymbol{k}_3} + \phi_{\boldsymbol{k}_1}\phi_{\boldsymbol{k}_2}) \\ &+ (U_{k_1} + U_{k_3})(\phi_{\boldsymbol{k}_2} + \phi_{\boldsymbol{k}_1}\phi_{\boldsymbol{k}_3}) + (U_{k_2} + U_{k_3})(\phi_{\boldsymbol{k}_1} + \phi_{\boldsymbol{k}_2}\phi_{\boldsymbol{k}_3})\Big].\end{aligned} \tag{139e}$$

Therefore, we obtain the dynamical equations as follows:

$$i\hbar\frac{\partial\phi_{\boldsymbol{k}}}{\partial t} = 2\xi_{\boldsymbol{k}}\phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\phi^2_{\boldsymbol{k}} + \Delta_{\boldsymbol{k}} + \chi_{\boldsymbol{k}}, \tag{140a}$$

$$i\hbar\frac{\partial w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}}{\partial t} = b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3} + w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}\sum_{i=1,2,3}\Big[E^0_{\boldsymbol{k}_i} - f_{\boldsymbol{k}_i}\Big]. \tag{140b}$$

By solving these equations simultaneously, we obtain the dynamical state given by $\phi_{\boldsymbol{k}}(t)$ and $w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3}(t)$.

3.2 Numerical Calculations

In the following, we introduce the model and method for numerical calculations and present the numerical results.

3.2.1 Model : rapid change for s-wave scattering length

By solving the TDBdG theory, Scott et al., [58] investigated the dynamical response of superfluid Fermi gases to rapid changes of the s-wave scattering length. Here, we perform the numerical calculation for the contact interaction potential $U_k = U(t)$ with units for energy and wave number given in Eq. (70) and consider the rapid changes of interaction potential. In terms of coupling constant $\delta(t) \equiv a^3_{U(t)}\bar{n}$, we control the interaction potential using the following model:

$$\delta(t) = \delta_1 f(t/t_0),\ \delta(t=0) \equiv \delta(t=dt) \equiv \delta_0, \tag{141}$$

where f is a dimensionless model function giving time dependence for interaction potential with $f(t=0) \ll 1$ and $f(t\to\infty) = 1$ and t_0 represents a time scale for the change of interaction potential. Therefore, the initial condition for $(\phi(t=0), w(t=0))$ are set to be the solution for equilibrium solution for $\delta = \delta_0$. On the other hand, the behaviors of $(\phi(t\to\infty), w(t\to\infty))$ are expected to approach to the equilibrium solution for $\delta = \delta_1$ through relaxation process. In our numerical calculation, we use $\delta(t) = \delta_1 \tanh(t/t_0)$. The unit for time is set as $t_U \equiv \hbar/\bar{n}U_1$. The schematic drawing for the present numerical model is described in Fig. 5.

3.2.2 Numerical results

In the following, we show the numerical results calculated with $\Delta t = 5.0\times10^{-5}t_U$, $\Delta k = 2.0\times10^{-2}k_U$ (interval of wave numbers), $t_0 = 0.1t_U$, $\delta_1 = 1.0\times10^{-5}$, $(\therefore \delta_0 \simeq 5.0\times10^{-9})$, $k_{\rm c} = 5k_U$.

Before discussing the numerical results, we give a comment about a method to solve dynamical equations by using second-order differential method in terms of t. For instance, assuming a time-evolutional equation given by

$$i\frac{\partial\psi}{\partial t} = X(t), \tag{142a}$$

we evaluate $\partial\psi/\partial t$ by taking the central difference with discretizing t as $\psi(t)\to\psi_i$ ($i \geq 0$: integer) as follows:

$$\left.\frac{\partial\psi}{\partial t}\right|_{t=t_i} \simeq i\frac{\psi_{i+1}-\psi_{i-1}}{2\Delta t} = X_i \to \psi_{i+1} \simeq \psi_{i-1} - i2X_i\Delta t. \tag{142b}$$

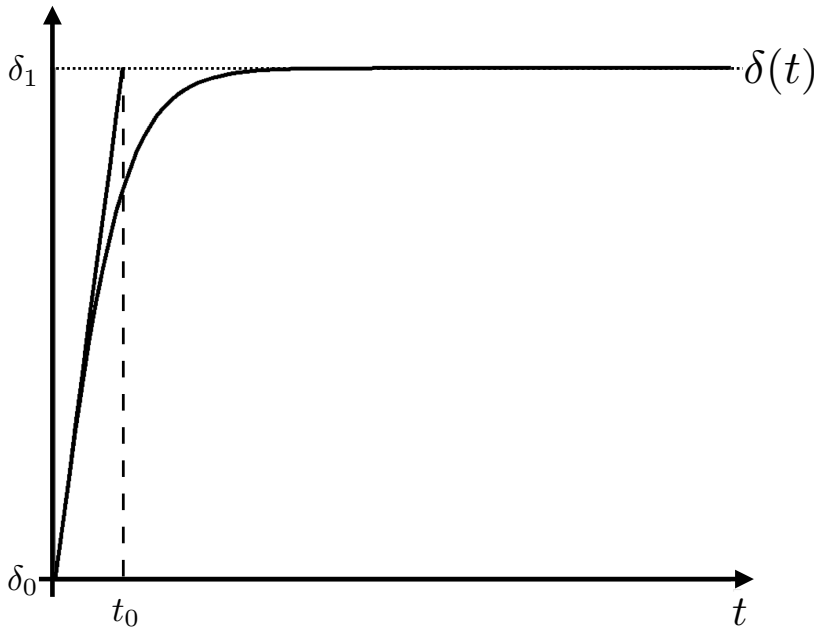

Figure 5: The schematic drawing for the present model. We change interaction potential (coupling constant) rapidly, and stop increasing it around $t = t_0$. By this procedure, we can observe the relaxation processes of physical quantities in a homogeneous system.

where Δt denotes time interval between $\psi(t_i)$ and $\psi(t_{i+1})$. Solving Eq. (142b) recursively from $\psi_0 = \psi_1 = \psi^{\rm eq}$, we obtain $\psi(t)$. This algorithm is effective if Δt is small enough to neglect numerical errors of order $O(\Delta t^3)$.

First, we show the time dependencies of expectation values of Hamiltonian by the TDHFB theory and our theory subtracted by $UN^2/2\mathcal{V} = N\varepsilon_U/2$, which we call "dynamical energy" here, in Fig. 6. As seen in this figure, both dynamical energies saturate to constant values towards the region where the interaction potential is constant. Thus, both theories satisfy the dynamical energy conservation law in the relaxation process. In addition, our theory with 3/2-body correlations yields lower dynamical energy than that by TDHFB, i.e., the stable state is realized by incorporating 3/2-body correlations. In the same figure, we also plot the corresponding ground-state energies. Although their dynamical energies approach to the equilibrium energies, they do not saturate to their values strictly. One of the reasons for this undesirable property may be the model for rapid changes of interaction potential. We observed that the models with larger t_0 yield smaller dynamical energies. However, taking large t_0 also yields a difficulty in carrying out the numerical calculations in terms of accumulation of numerical error characteristic of dynamical simulations.

Next, we show the profiles of $\rho_{\boldsymbol{k}}$ at various times in Fig. 7. Left figure corresponds to the result by the TDHFB theory and right corresponds to the result by our theory with 3/2-body correlations. As seen in the left figure, the profile of $\rho_{\boldsymbol{k}}$ changes substantially as time proceeds, specifically $|\boldsymbol{k}| = k \gtrsim 0$. Our observation is described in the schematic drawing in the graph, i.e.,

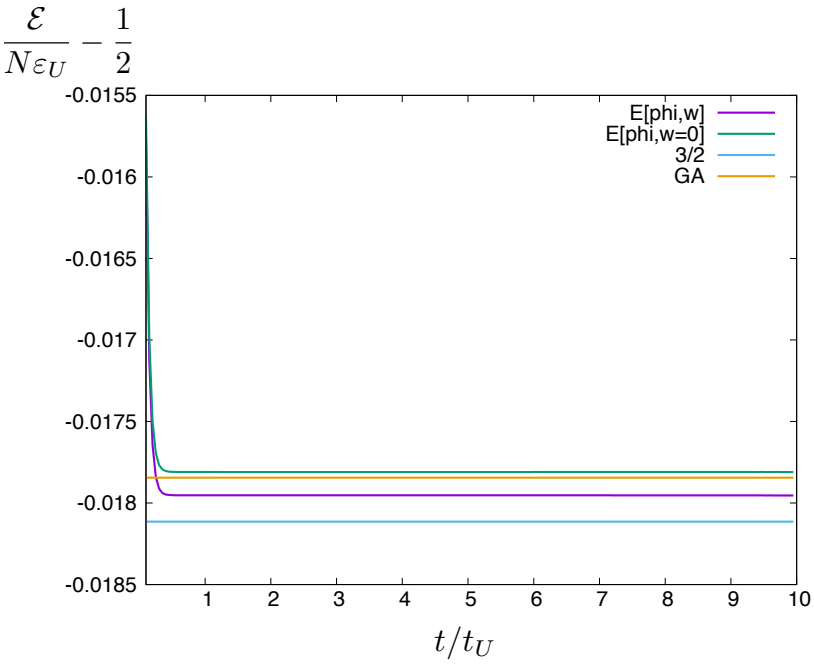

Figure 6: The expectation values of Hamiltonian evaluated by our theory (purple) and the TDHFB theory (green) subtracted by $N\varepsilon_U/2$ as a function of time. Cyan (orange) lines plot the ground state energies by the wave function with 3/2-body correlations (GA wave function).

noncondensates move collectively without collisions with condensates once they are excited due to the rapid change of interaction potential. On the other hand, $\rho_{\boldsymbol{k}}$ by the theory with 3/2-body correlations always has a peak at the smallest $\boldsymbol{k}$. This behavior indicates that local momentum-exchange processes between condensates and noncondensates are incorporated successfully in the wave function.

Finally, we discuss the noncondensates' wave function. The variational parameter $\phi_{\boldsymbol{k}}$ characterizes the pair excitations with wave numbers $\boldsymbol{k}$ and $-\boldsymbol{k}$ from condensates. Thus, $\varphi_{\boldsymbol{k}}$ given by $\varphi_{\boldsymbol{k}} = \tan^{-1}\mathrm{Im}\phi_{\boldsymbol{k}}/\mathrm{Re}\phi_{\boldsymbol{k}}$ (strictly, $\varphi_{\boldsymbol{k}}/2$) directly corresponds to the phase of noncondensates' or quasiparticles' wave function. Figure 8 shows the k dependencies of $\tan\varphi_k$ at $t = 0.5t_U$, $2.5t_U$, $5.0t_U$ and $7.5t_U$. The left figure corresponds to the result by TDHFB theory and the right corresponds to the result by our theory. In our calculation, the phase of condensate wave function was fixed as $\varphi_{\mathrm{c}} = 0$, i.e., $\langle\hat{c}_{\boldsymbol{0}}\hat{\beta}_0^\dagger\rangle = \langle\hat{c}_{\boldsymbol{0}}^\dagger\hat{\beta}_0\rangle = \sqrt{N_{\boldsymbol{0}}}$. As seen in the left figure, $\tan\varphi_{\boldsymbol{k}}$ oscillates around 0 as time proceeds, particularly around $k \gtrsim 0$. In this sense, $\varphi_{\mathrm{c}} \neq \varphi_{\boldsymbol{k}}$ within the TDHFB theory. On the other hand, such phase oscillation around $k \gtrsim 0$ is suppressed substantially by 3/2-body correlations, as seen in the right figure. Compared to the result by the TDHFB theory, we apparently observe the relation $\varphi_{\boldsymbol{k}} \simeq \varphi_{\mathrm{c}} = 0$ in every k.

In Refs. [17] and [27], superposition over different condensed-particle-number states due to the interaction was regarded as the essential factor for the macroscopic coherence. On the other hand,

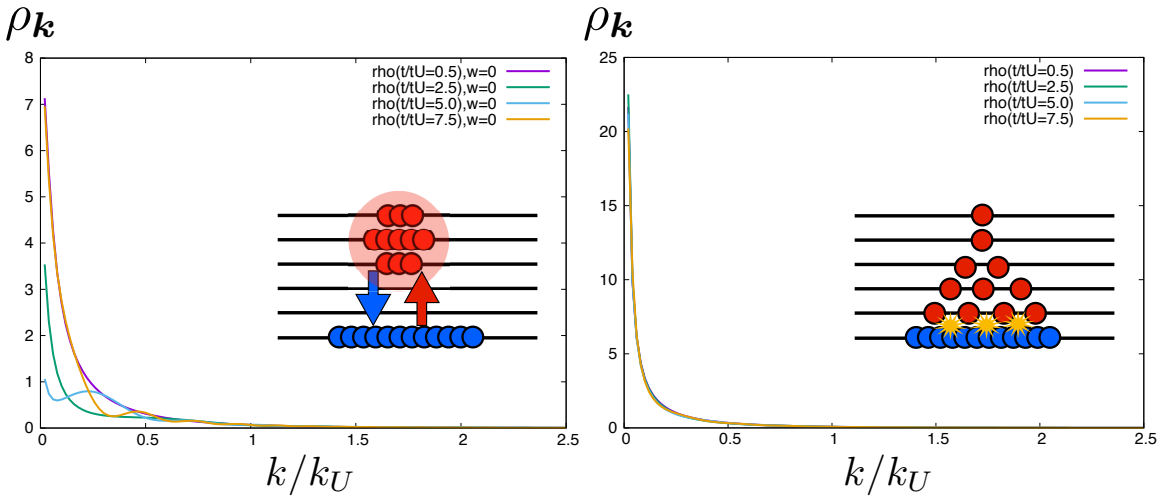

Figure 7: Numerical results of the dynamics of noncondensate densities. The left figure corresponds to the result by TDHFB theory and right figure corresponds to the result by our variational theory with 3/2-body correlations. Purple, green, cyan, and orange lines corresponds to the results at $t = 0.5t_U$, $2.5t_U$, $5.0t_U$ and $7.5t_U$, respectively. Two figures in the graphs show their respective dynamics schematically.

our calculation shows that the wave function of noncondensate within self-consistent mean-field approximation has large oscillations around $k \gtrsim 0$. Such oscillations are caused by the unphysical energy gap at $k = 0$ in the excitation spectrum because the energy gap prevents noncondensates from interacting with condensates. In our calculation, we have observed that the variational wave function with 3/2-body correlations described the collisions between noncondensates and condensate reservoir. In addition, the dynamical oscillations in the phase of noncondensate wave function is strongly suppressed. As shown in Fig. 2 in the introduction part, it also played a role to decrease the unphysical energy gaps due to the mean-field approximations. With these facts, one can see that the excited particles can exchange their momentums with condensates without energy barrier owing to the 3/2-body processes and the macroscopic phase is maintained dynamically. In this sense, not only "superposition", but also "gapless excitation" seems to be one of the crucial points for discussing the origin of macroscopic coherence. Strictly speaking, however, very small energy gap remains even if we incorporate 3/2-body correlations successfully as seen in Fig. 2. The small variation of $\varphi_{k\gtrsim 0}(t \to \infty)$ observed in the right figure may be due to such small energy gap between condensates and noncondensates.

Associated with this problem, the other independent studies based on functional renormalization group theory have been carried out very recently [59, 60]. In this study, the author derived general conditions among n-point vertices for gapless excitation in BEC and showed that the lowest-order condition corresponds to the Hugenholtz-Pines theorem. In addition, the effective coupling constant g_Λ at the energy cut-off Λ was also obtained by solving the exact renormalization-group equations for

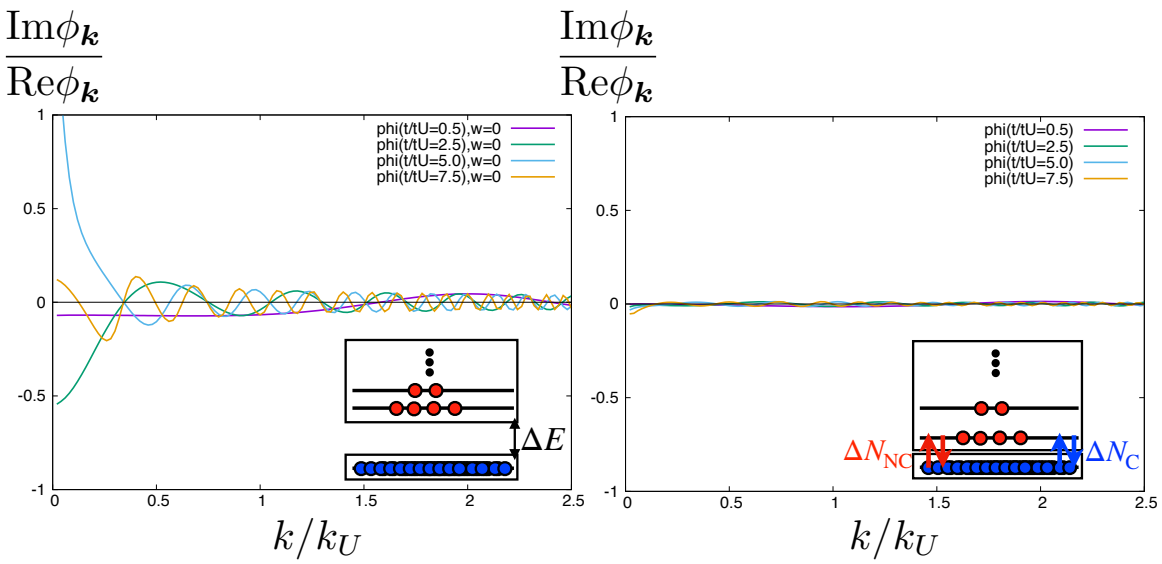

Figure 8: Numerical results of the dynamics of $\mathrm{Im}\phi_k/\mathrm{Re}\phi_k$. The left figure corresponds to the result by the TDHFB theory and right figure corresponds to the result by our variational theory with 3/2-body correlations. Purple, green, cyan, and orange lines corresponds to the results at $t = 0.5t_U$, $2.5t_U$, $5.0t_U$ and $7.5t_U$, respectively. Two figures in the graphs draw their respective particle-number fluctuations schematically with considering their gaps in excitation spectrums.

the n-point vertices and showed $g_{\Lambda\to 0} \to 0$ under $d < 4$ ($d < 3$) at finite (zero) temperature, where d denotes a dimension of the system. This vanishing of g_Λ, caused by the many-body correlations (n-point vertices) beyond mean-field treatment, indicates that the Bogoliubov mode with linear dispersion is absent in one-particle excitations in BEC systems. Even if there are no Bogoliubov modes with linear dispersion, the origin of superfluidity in BEC systems can be explained using the present idea based on the macroscopic coherence. In this sense, many-body correlations such as 3/2-body correlations should be a key factor for investigating interacting BEC systems definitely.

Chapter 4 Concluding Remarks

In this thesis, we have developed variational theories to describe equilibrium and nonequilibrium systems. Conclusions in respective chapters are summarized as follows.

In the first chapter, we have introduced a variational method to incorporate the correlations between condensates and noncondensates with dividing 3 equilibrium systems : (1) inhomogeneous systems, (2) Bose–Bose mixtures, (3) finite-temperature systems. These 3 analysis have a common conclusion that 3/2-body correlations decrease the ground-state energies and free energies, and their contributions are comparable to those of 2-body correlations. Therefore, the mean-field approximation for BEC systems may not be effective quantitatively even in the weak-coupling region. As shown in appendix A, we can also apply the same method to superconducting states beyond mean-field approximations. Our variational theories introduced here are expected to give physical pictures beyond mean-field contributions in various BEC and superconducting systems.

In the second chapter, we have derived time-evolutional equations of variational parameters with 3/2-body correlations from the principle of least action and investigated the dynamical response of weakly-interacting BEC systems to change the s-wave scattering length rapidly. Specifically, we have focused on the dynamics of noncondensates' density and the noncondensates' wave function. To summarize, our observation in this chapter is as follows: (1) not only particle-number fluctuations but also gapless one-particle excitation (not necessary to be linear) seems also crucial for the macroscopic coherence (2) 3/2-body correlations play an essential role to maintain coherence in interacting BEC systems. If the macroscopic phase in a BEC system is maintained dynamically at $T = 0$ as $\varphi_{\rm c} = \varphi_{\rm nc}$, we can explain the experimental results of the relation between superfluid density and condensate density [37, 38] without contradictions. In addition, the "equivalence" between one and collective excitations in the long-wave-length limit, which has been believed to be essential for the relation between BEC and superfluidity, may not be necessary.

Appendix A Variational Theory of Superconductivity with Many-Body Correlations at Finite Temperature

By using a formalism based on the variational density matrix $\hat{\rho}_{\rm v}$ introduced in Ref. [26], we extend the variational theory for superconductors given in Ref. [27] to finite-temperature formalism.

We start from the following Hamiltonian:

$$\hat{H} = \sum_{\alpha} \sum_{\boldsymbol{k}} \varepsilon_k \hat{c}^{\dagger}_{\boldsymbol{k}\alpha} \hat{c}_{\boldsymbol{k}\alpha} + \frac{1}{2\mathcal{V}} \sum_{\alpha,\beta} \sum_{\boldsymbol{q},\boldsymbol{k},\boldsymbol{k}'} U_q \hat{c}^{\dagger}_{\boldsymbol{k}+\boldsymbol{q}\alpha} \hat{c}^{\dagger}_{\boldsymbol{k}'-\boldsymbol{q}\beta} \hat{c}_{\boldsymbol{k}'\beta} \hat{c}_{\boldsymbol{k}\alpha}, \tag{143}$$

where $(\hat{c}, \hat{c}^{\dagger})$ is a set of fermion field operators satisfying $\{\hat{c}_{\boldsymbol{k}\alpha}, \hat{c}^{\dagger}_{\boldsymbol{k}'\alpha'}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\alpha\alpha'}$, α and β spin indices, $\varepsilon_k = \hbar^2 k^2/2m$, and $U_q < 0$ the interaction potential.

Now, we introduce the BCS variational wave function with time dependence as follows:

$$|\Phi_{\rm BCS}\rangle = A \exp(\hat{\pi}^{\dagger}_{\rm BCS}) |0\rangle , \tag{144}$$

where $\hat{\pi}^{\dagger} \equiv \sum_{\boldsymbol{k}} \phi_{\boldsymbol{k}} \hat{c}^{\dagger}_{\boldsymbol{k}\uparrow} \hat{c}^{\dagger}_{-\boldsymbol{k}\downarrow}$, A is the normalization constant determined by $\langle \Phi_{\rm BCS} | \Phi_{\rm BCS} \rangle = 1$, and $\phi_{\boldsymbol{k}}$ is a variational parameters. $|\Phi_{\rm BCS}\rangle$ corresponds to a "vacuum state" characterized by $\hat{\gamma}_{\boldsymbol{k}\alpha} |\Phi_{\rm BCS}\rangle = 0$, where $(\hat{\gamma}, \hat{\gamma}^{\dagger})$ is a set of quasiparticle operators defined by

$$\hat{\gamma}_{\boldsymbol{k}\alpha} = u_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}\alpha} + (-1)^{\alpha+\frac{1}{2}} v_{\boldsymbol{k}} \hat{c}^{\dagger}_{-\boldsymbol{k}-\alpha} \tag{145a}$$

$$\hat{\gamma}^{\dagger}_{-\boldsymbol{k}-\alpha} = (-1)^{-\alpha+\frac{1}{2}} v^{*}_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}\alpha} + u_{\boldsymbol{k}} \hat{c}^{\dagger}_{-\boldsymbol{k}-\alpha}. \tag{145b}$$

with definitions $u_{\boldsymbol{k}} = \frac{1}{\sqrt{1+|\phi_{\boldsymbol{k}}|^2}} = u^{*}_{\boldsymbol{k}}$ and $v_{\boldsymbol{k}} = \frac{\phi_{\boldsymbol{k}}}{\sqrt{1+|\phi_{\boldsymbol{k}}|^2}}$. By these definitions, commutator relations are given by $\{\hat{\gamma}_{\boldsymbol{k}\alpha}, \hat{\gamma}^{\dagger}_{\boldsymbol{k}'\alpha'}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\alpha\alpha'}$ and $\{\hat{\gamma}_{\boldsymbol{k}\alpha}, \hat{\gamma}_{\boldsymbol{k}'\alpha'}\} = 0$. The inverse transformations are given by

$$\hat{c}_{\boldsymbol{k}\alpha} = u_{\boldsymbol{k}} \hat{\gamma}_{\boldsymbol{k}\alpha} - (-1)^{\alpha+\frac{1}{2}} v_{\boldsymbol{k}} \hat{\gamma}^{\dagger}_{-\boldsymbol{k}-\alpha}, \tag{145c}$$

$$\hat{c}^{\dagger}_{-\boldsymbol{k}-\alpha} = -(-1)^{-\alpha+\frac{1}{2}} v^{*}_{\boldsymbol{k}} \hat{\gamma}_{-\boldsymbol{k}} + u_{\boldsymbol{k}} \hat{\gamma}^{\dagger}_{-\boldsymbol{k}}. \tag{145d}$$

In Ref. [27], a variational wave function that describes dynamical annihilation and creation processes of Cooper pairs has been constructed by extending the conventional mean-field BCS wave function. According to this study, the augmented variational wave function is introduced as follows:

$$|\Phi\rangle \equiv A_4 \exp(\hat{\pi}^{\dagger}_4) |\Phi_{\rm BCS}\rangle , \quad \hat{\pi}^{\dagger}_4 = \frac{1}{4!} \sum_{\kappa_1\kappa_2\kappa_3\kappa_4} w_{\kappa_1\kappa_2\kappa_3\kappa_4} \hat{\gamma}^{\dagger}_{\kappa_1} \hat{\gamma}^{\dagger}_{\kappa_2} \hat{\gamma}^{\dagger}_{\kappa_3} \hat{\gamma}^{\dagger}_{\kappa_4}, \tag{146}$$

where $\kappa \equiv (\boldsymbol{k}, \alpha)$, $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$ is a variational parameter characterizing the dynamical annihilation and creation processes of Cooper pairs, and A_4 is a normalization constant defined by $\langle \Phi | \Phi \rangle = 1$. Here, we generalize the theory for ground state to describe finite-temperature systems. To do this,

we introduce the variational density matrix. Following the manner in the theory of BEC, we choose the form of $\hat{\rho}_{\rm v}$ as follows:

$$\hat{\rho}_{\rm v} = \exp[\beta(\Omega_{\rm vLW} - \hat{H}_{\rm v})],\ \Omega_{\rm vLW} \equiv -\beta^{-1} \ln {\rm Tr} e^{-\beta \hat{H}_{\rm v}}, \tag{147a}$$

with

$$\begin{aligned} \hat{H}_{\rm v} &= \hat{H}_{\rm v}^{\rm MF} + \hat{H}_{\rm v}^4 \\ &\equiv \sum_{\kappa} E_\kappa \hat{\gamma}_\kappa^\dagger \hat{\gamma}_\kappa + \frac{1}{4!} \sum_{\kappa_1\kappa_2\kappa_3\kappa_4} (b_{\kappa_1\kappa_2\kappa_3\kappa_4} \hat{\gamma}_{\kappa_1}^\dagger \hat{\gamma}_{\kappa_2}^\dagger \hat{\gamma}_{\kappa_3}^\dagger \hat{\gamma}_{\kappa_4}^\dagger + {\rm H.C}), \end{aligned} \tag{147b}$$

where E_κ and $b_{\kappa_1\kappa_2\kappa_3\kappa_4}$ represent variational parameters.

The quasiparticle Green's function is introduced as follows:

$$\mathcal{G}_\kappa(\tau_1, \tau_2) = -{\rm Tr}\rho_{\rm v} \hat{T}_\tau \hat{\gamma}_\kappa(\tau_1) \hat{\gamma}_\kappa^\dagger(\tau_2) = -{\rm Tr}\rho_{\rm v} \hat{T}_\tau \hat{\gamma}_\kappa(\tau_1 - \tau_2) \hat{\gamma}_\kappa^\dagger \equiv \mathcal{G}_\kappa(\tau_1 - \tau_2), \tag{148}$$

$$\mathcal{G}_\kappa(\tau) = \frac{1}{\beta} \sum_{n=-\infty}^{\infty} e^{-i\varepsilon_n \tau} \mathcal{G}_{\kappa, i\varepsilon_n}, \tag{149}$$

where $\hat{T}_\tau$ is a time-ordered operator for imaginary time τ and $\hat{\gamma}_\kappa(\tau) \equiv e^{\tau \hat{H}_{\rm v}} \hat{\gamma}_\kappa e^{-\tau \hat{H}_{\rm v}}$, $\hat{\gamma}_\kappa^\dagger(\tau) \equiv e^{\tau \hat{H}_{\rm v}} \hat{\gamma}_\kappa^\dagger e^{-\tau \hat{H}_{\rm v}}$ are the Heisenberg representation for quasiparticle operators, and $\varepsilon_n \equiv (2n+1)\pi/\beta$ (n: integer) is the Matsubara energy for fermions.

To construct the self-consistent equations for $\mathcal{G}_{\kappa, i\varepsilon_n}$, we define a self energy $\mathcal{S}$ expressed by $\mathcal{G}_{\kappa, i\varepsilon_n}$. As shown by Luttinger and Ward, $\Omega_{\rm vLW} = \Omega_{\rm vLW}[\mathcal{G}]$ can be expressed in terms of $\mathcal{G}_{\kappa, i\varepsilon_n}$ as

$$\Omega_{\rm vLW}[\mathcal{G}] = -\frac{1}{\beta} \sum_n \sum_\kappa \left[e^{i\varepsilon_n 0_+} \ln[-{\mathcal{G}^{(0)}}^{-1}_{\kappa, i\varepsilon_n} + \mathcal{S}_{\kappa, i\varepsilon_n}] + \mathcal{S}_{\kappa, i\varepsilon_n} \mathcal{G}_{\kappa, i\varepsilon_n} \right] + \Phi_{\rm vLW}[\mathcal{G}] \tag{150}$$

where $\Phi_{\rm vLW}$ consists of all the skeleton diagrams in the simple perturbation expansion with respect to $\hat{H}_{\rm v}^4$ for $\Omega_{\rm vLW}$ with replacement of free quasiparticle's propagator $\mathcal{G}^{(0)}$ with $\mathcal{G}_{\kappa, i\varepsilon_n}$. Here, $\mathcal{G}^{(0)}$ is defined by

$$\mathcal{G}^{(0)}_{\kappa, i\varepsilon_n} = \frac{1}{i\varepsilon_n - E_\kappa}. \tag{151}$$

The equation for $\mathcal{G}_{\kappa, i\varepsilon_n}$ is determined by $\delta\Omega_{\rm vLW}/\delta\mathcal{G}_{\kappa, i\varepsilon_n} = 0$. From this condition, we obtain the Dyson equation for $\mathcal{G}_{\kappa, i\varepsilon_n}$

$$\mathcal{G}_{\kappa, i\varepsilon_n} = \frac{1}{i\varepsilon_n - E_\kappa - \mathcal{S}_{\kappa, i\varepsilon_n}}, \tag{152}$$

where $\mathcal{S}_{\kappa, i\varepsilon_n}$ is the self-energy defined by

$$\mathcal{S}_{\kappa, i\varepsilon_n} = \beta \frac{\delta \Phi_{\rm vLW}}{\delta \mathcal{G}_{\kappa, i\varepsilon_n}}. \tag{153}$$

Following the manner of Φ-derivative approximation, we introduce $\Phi_{\rm vLW}$ as follows:

$$\Phi_{\rm vLW} = -\frac{1}{\beta} [\langle \hat{S}(\beta) \rangle_{\rm BCS, connect} - 1]_{{\rm skeleton}, \mathcal{G}^{(0)} \to \mathcal{G}}, \tag{154}$$

where $\langle\cdots\rangle_{\rm BCS}$ denotes the average by $\hat{\rho}_{\rm v}[b=b^*=0]$ and $\hat{S}(\beta)$ is an operator to carry out the perturbation expansion defined by

$$\hat{S}(\beta)\equiv e^{\beta\hat{H}_{\rm v}^{\rm MF}}e^{-\beta\hat{H}_{\rm v}}=1+\sum_{m=1}^{\infty}\frac{1}{n!}\int_0^\beta d\tau_1\int_0^\beta d\tau_2\cdots\int_0^\beta d\tau_m\hat{T}_\tau\hat{H}_{\rm v}^4(\tau_1)\cdots\hat{H}_{\rm v}^4(\tau_m). \tag{155}$$

Thus, $\Phi_{\rm vLW}=\sum_{n=1}^{\infty}\Phi_{\rm vLW}^n$ formally consists of infinite closed skeleton diagrams with $\mathcal{G}_0$ replaced by $\mathcal{G}$. In order to obtain an explicit expression for $\mathcal{S}$, we use the lowest-order approximation for $\Phi_{\rm vLW}$ as $\Phi_{\rm vLW}\simeq\Phi_{\rm vLW}^{(2)}$, where $\Phi_{\rm vLW}^{(2)}$ is expressed by

$$\begin{aligned}\Phi_{\rm vLW}^{(2)}=&-\frac{1}{4!\beta^3}\sum_{n_1n_2n_3n_4}\sum_{\kappa_1\kappa_2\kappa_3\kappa_4}|b_{\kappa_1\kappa_2\kappa_3\kappa_4}|^2\delta_{\varepsilon_{n_1}+\varepsilon_{n_2}+\varepsilon_{n_3}+\varepsilon_{n_4},0}\\&\times\mathcal{G}_{\kappa_1,i\varepsilon_{n_1}}\mathcal{G}_{\kappa_2,i\varepsilon_{n_2}}\mathcal{G}_{\kappa_3,,i\varepsilon_{n_3}}\mathcal{G}_{\kappa_4,i\varepsilon_{n_4}}\end{aligned} \tag{156}$$

Therefore, the self energy is

$$\mathcal{S}_{\kappa,i\varepsilon_n}\simeq-\frac{1}{3!\beta^2}\sum_{n_2n_3n_4}\sum_{\kappa_2\kappa_3\kappa_4}|b_{\kappa\kappa_2\kappa_3}|^2\delta_{\varepsilon_n+\varepsilon_{n_2}+\varepsilon_{n_3}+\varepsilon_{n_4},0}\mathcal{G}_{\kappa_2,i\varepsilon_{n_2}}\mathcal{G}_{\kappa_3,i\varepsilon_{n_3}}\mathcal{G}_{\kappa_4,i\varepsilon_{n_4}}. \tag{157}$$

Using $\mathcal{G}_{\kappa,i\varepsilon_n}$, we obtain $\rho_\kappa^{\rm qp}$ and $w_{\kappa_1\kappa_2\kappa_3}$ as follows:

$$\rho_\kappa^{\rm qp}=\frac{1}{\beta}\sum_n\mathcal{G}_{\kappa,i\varepsilon_n} \tag{158a}$$

$$w_{\kappa_1\kappa_2\kappa_3\kappa_4}=\frac{b_{\kappa_1\kappa_2\kappa_3\kappa_4}}{\beta^3}\sum_{n_1n_2n_3n_4}\delta_{\varepsilon_{n_1}+\varepsilon_{n_2}+\varepsilon_{n_3}+\varepsilon_{n_4},0}\mathcal{G}_{\kappa_1,i\varepsilon_{n_1}}\mathcal{G}_{\kappa_2,i\varepsilon_{n_2}}\mathcal{G}_{\kappa_3,i\varepsilon_{n_3}}\mathcal{G}_{\kappa_4,i\varepsilon_{n_4}}. \tag{158b}$$

We also show that our theory reproduces the results in Ref. [27] by taking $T\to0$. To proceed calculations, we expand $\mathcal{G}$ assuming $\mathcal{S}\ll1$ as

$$\begin{aligned}\mathcal{G}_{\kappa,i\varepsilon_n}&\simeq\mathcal{G}^{(0)}_{\kappa,i\varepsilon_n}[1+\mathcal{S}^{(1)}_{\kappa,i\varepsilon_n}\mathcal{G}^{(0)}_{\kappa,i\varepsilon_n}]\\&\equiv\mathcal{G}^{(0)}_{\kappa,i\varepsilon_n}+\mathcal{G}^{(1)}_{\kappa,i\varepsilon_n},\end{aligned} \tag{159}$$

where $\mathcal{S}^{(1)}\equiv\mathcal{S}[\mathcal{G}^{(0)}]$. Lehmann representation for $\mathcal{S}^{(1)}$ is given as

$$\begin{aligned}\mathcal{S}^{(1)}_{\kappa,i\varepsilon_n}=&\frac{1}{3!}\sum_{\kappa_2\kappa_3\kappa_4}|b_{\kappa\kappa_2\kappa_3\kappa_4}|^2\int_{-\infty}^{\infty}\frac{d\varepsilon_2}{2\pi}\int_{-\infty}^{\infty}\frac{d\varepsilon_3}{2\pi}\int_{-\infty}^{\infty}\frac{d\varepsilon_4}{2\pi}\\&\times\frac{A^{(0)}_{\kappa_2,\varepsilon_2}A^{(0)}_{\kappa_3,\varepsilon_3}A^{(0)}_{\kappa_4,\varepsilon_4}}{i\varepsilon_n+\varepsilon_2+\varepsilon_3+\varepsilon_4}[f(\varepsilon_2)f(\varepsilon_3)f(\varepsilon_4)+f(-\varepsilon_2)f(-\varepsilon_3)f(-\varepsilon_4)]\\=&\frac{1}{3!}\sum_{\kappa_2\kappa_3\kappa_4}|b_{\kappa\kappa_2\kappa_3\kappa_4}|^2\frac{1-f(E_{\kappa_2})-f(E_{\kappa_3})-f(E_{\kappa_4})}{i\varepsilon_n+E_{\kappa_2}+E_{\kappa_3}+E_{\kappa_4}}\\\to\Gamma^{(1)}_{\kappa,\varepsilon}=&\frac{\pi}{3}\sum_{\kappa_2\kappa_3\kappa_4}|b_{\kappa\kappa_2\kappa_3\kappa_4}|^2[f(\varepsilon_2)f(\varepsilon_3)f(\varepsilon_4)+f(-\varepsilon_2)f(-\varepsilon_3)f(-\varepsilon_4)]\\&\times\delta(\varepsilon+E_{\kappa_2}+E_{\kappa_3}+E_{\kappa_4}),\end{aligned} \tag{160}$$

where $A^{(0)}_{\kappa,\varepsilon}(\Gamma^{(1)}_{\kappa,\varepsilon})$ is the spectral function for $\mathcal{G}^{(0)}_{\kappa,i\varepsilon_n}(\mathcal{S}^{(1)}_{\kappa,i\varepsilon_n})$.

Since the spectral functions are given by $A_{\kappa,\varepsilon} \equiv -2\mathrm{Im}G_{\boldsymbol{k},i\varepsilon_n\to\varepsilon+i0_+}$ and $\Gamma^{(1)}_{\kappa,\varepsilon} \equiv -2\mathrm{Im}\mathcal{S}^{(1)}_{\kappa,i\varepsilon_n\to\varepsilon+i0_+}$, we obtain $A^{(1)}_{\kappa,\varepsilon}$ as

$$A^{(1)}_{\kappa,\varepsilon} \simeq \frac{\Gamma^{(1)}_{\kappa,\varepsilon}}{(\varepsilon - E_\kappa)^2} = \frac{\pi}{3}\sum_{\kappa_2\kappa_3\kappa_4} |b_{\kappa\kappa_2\kappa_3\kappa_4}|^2 \frac{f(\varepsilon_2)f(\varepsilon_3)f(\varepsilon_4) + f(-\varepsilon_2)f(-\varepsilon_3)f(-\varepsilon_4)}{(E_\kappa + E_{\kappa_2} + E_{\kappa_3} + E_{\kappa_4})^2} \times \delta(\varepsilon + E_{\kappa_2} + E_{\kappa_3} + E_{\kappa_4}), \tag{161}$$

where we transformed the second into the third equation with $\mathrm{Im}\mathcal{G}^{(0)} \simeq 0$. This consideration is based on the assumption that ideal quasiparticles have infinite lifetimes due to the absence of interactions. On the other hand, in the presence of correlations between quasiparticles, such as 3/2-body correlations, finite lifetimes described by $\mathrm{Im}\mathcal{S}^{(1)}$ appear in the quasiparticles. Therefore, we obtain $\rho^{\mathrm{qp}}_\kappa$ as

$$\begin{aligned}\rho^{\mathrm{qp}}_\kappa &\simeq \int \frac{d\varepsilon}{2\pi}[A^{(0)}_{\kappa,\varepsilon} + A^{(1)}_{\kappa,\varepsilon}]f(\varepsilon) \\ &= f(E_\kappa) + \frac{1}{3!}\sum_{\kappa_2\kappa_3\kappa_4} |b_{\kappa\kappa_2\kappa_3\kappa_4}|^2 \frac{f(-E_{\kappa_2})f(-E_{\kappa_3})f(-E_{\kappa_4})}{(E_\kappa + E_{\kappa_2} + E_{\kappa_3} + E_{\kappa_4})^2}\end{aligned} \tag{162a}$$

On the other hand, we obtain the expression of w in the lowest order as

$$\begin{aligned}w_{\kappa_1\kappa_2\kappa_3\kappa_4} \simeq -\frac{b_{\kappa_1\kappa_2\kappa_3\kappa_4}}{E_{\kappa_1} + E_{\kappa_2} + E_{\kappa_3} + E_{\kappa_4}}\big[&f(-E_{\kappa_1})f(-E_{\kappa_2})f(-E_{\kappa_3})f(-E_{\kappa_4}) \\ &- f(E_{\kappa_1})f(E_{\kappa_2})f(E_{\kappa_3})f(E_{\kappa_4})\big].\end{aligned} \tag{162b}$$

Therefore, the zero-temperature formalism is reproduced in the limit $T \to 0$ ($f(E_\kappa) \to 0$ and $f(-E_\kappa) \to 1$).

The stationary condition for variational parameters are determined by $\delta\Omega_{\mathrm{v}} = 0$. By this procedure, we obtain

$$\phi_{\boldsymbol{k}} = \frac{-(\varepsilon_k - \mu + U^{\mathrm{HF}}_{\boldsymbol{k}}) + \sqrt{(\varepsilon_k - \mu + U^{\mathrm{HF}}_{\boldsymbol{k}})^2 + \Delta_{\boldsymbol{k}}(\Delta_{\boldsymbol{k}} - \chi_{\boldsymbol{k}})}}{\Delta_{\boldsymbol{k}}}, \tag{163a}$$

$$E_\kappa = E_{\boldsymbol{k}} = (u^2_{\boldsymbol{k}} - v^2_{\boldsymbol{k}})(\varepsilon_k - \mu + U^{\mathrm{HF}}_{\boldsymbol{k}}) + 2\Delta_{\boldsymbol{k}}u_{\boldsymbol{k}}v_{\boldsymbol{k}}, \tag{163b}$$

$$\begin{aligned}b_{\boldsymbol{k}_1\alpha_1\boldsymbol{k}_2\alpha_2\boldsymbol{k}_3\alpha_3\boldsymbol{k}_4\alpha_4} = \frac{\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4\boldsymbol{0}}}{\mathcal{V}} \\ \times\Big[U_{|\boldsymbol{k}_1+\boldsymbol{k}_4|}\delta_{\alpha_1-\alpha_4}\delta_{\alpha_2-\alpha_3}(-1)^{1-\alpha_1-\alpha_2}(u_{\boldsymbol{k}_1}v_{\boldsymbol{k}_4} + v_{\boldsymbol{k}_1}u_{\boldsymbol{k}_4})(u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3} + v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}) \\ +U_{|\boldsymbol{k}_1+\boldsymbol{k}_2|}\delta_{\alpha_1-\alpha_2}\delta_{\alpha_3-\alpha_4}(-1)^{1-\alpha_1-\alpha_3}(u_{\boldsymbol{k}_1}v_{\boldsymbol{k}_2} + v_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2})(u_{\boldsymbol{k}_3}v_{\boldsymbol{k}_4} + v_{\boldsymbol{k}_3}u_{\boldsymbol{k}_4}) \\ +U_{|\boldsymbol{k}_1+\boldsymbol{k}_3|}\delta_{\alpha_1-\alpha_3}\delta_{\alpha_2-\alpha_4}(-1)^{1-\alpha_1-\alpha_4}(u_{\boldsymbol{k}_1}v_{\boldsymbol{k}_3} + v_{\boldsymbol{k}_1}u_{\boldsymbol{k}_3})(u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_4} + v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_4})\Big],\end{aligned} \tag{163c}$$

where

$$U_{\boldsymbol{k}}^{\mathrm{HF}} = \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}'} (2U_0 - U_{|\boldsymbol{k}-\boldsymbol{k}'|}) \rho_{\boldsymbol{k}'}, \tag{163d}$$

$$\Delta_{\boldsymbol{k}} = -\frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}'} U_{|\boldsymbol{k}-\boldsymbol{k}'|} F_{\boldsymbol{k}'}, \tag{163e}$$

$$\chi_{\boldsymbol{k}} = \frac{1}{\mathcal{V}(1 - \sum_{\kappa} \rho_{\kappa}^{\mathrm{qp}})} \sum_{\boldsymbol{k}_2 \boldsymbol{k}_3 \boldsymbol{k}_4} \delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4, \mathbf{0}} U_{|\boldsymbol{k}+\boldsymbol{k}_4|} \Big[(\phi_{\boldsymbol{k}_2} - \phi_{\boldsymbol{k}} \phi_{\boldsymbol{k}_3} \phi_{\boldsymbol{k}_4}) \frac{u_{\boldsymbol{k}_2} u_{\boldsymbol{k}_3} u_{\boldsymbol{k}_4}}{u_{\boldsymbol{k}}}$$
$$\times \sum_{\alpha\alpha'} (-1)^{1-\alpha-\alpha'} w_{\boldsymbol{k}\alpha \boldsymbol{k}_2 \alpha' \boldsymbol{k}_3 - \alpha' \boldsymbol{k}_4 - \alpha}. \tag{163f}$$

Appendix B Time-Dependent Variational Theory of Superconductivity beyond Mean-Field Approximation

We construct a time-dependent variational theory of superconductivity based on the principle of least action :

$$\delta S = \delta \int_{t_0}^{t_1} dt \, \langle \Phi(t) | i\hbar \frac{\partial}{\partial t} - \hat{H} | \Phi(t) \rangle = 0, \tag{164}$$

where t_0, t_1 is arbitrary times. Here, we consider the Hamiltonian given by Eq. (143).

First, we consider within the TDBdG theory with defining $\mathcal{E}_{\rm BCS}(t) \equiv \langle \Phi_{\rm BCS}(t) | \hat{H} | \Phi_{\rm BCS}(t) \rangle$. To modify $|\Phi_{\rm BCS}\rangle$ as $|\Phi_{\rm BCS}(t)\rangle$, we only need to consider the time dependence of $\phi_{\boldsymbol{k}}(t)$ in Eq. (144). Calculating $\langle \Phi_{\rm BCS}(t) | \partial_t | \Phi_{\rm BCS}(t) \rangle$, we obtain

$$i\hbar \langle \Phi_{\rm BCS}(t) | \frac{\partial}{\partial t} | \Phi_{\rm BCS}(t) \rangle = i\hbar \frac{\partial \ln A(t)}{\partial t} + i\hbar \sum_{\boldsymbol{k}} u_{\boldsymbol{k}}(t) v^*_{\boldsymbol{k}}(t) \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t}, \tag{165}$$

Using this relation and $\partial / \partial \phi^* (\phi^* / (1 + |\phi|^2)) = (1 + |\phi|^2)^{-2} = u^4$, Eq. (164) is transformed into

$$\frac{\delta \mathcal{E}_{\rm BCS}}{\delta \phi^*_{\boldsymbol{k}}(t)} = i\hbar \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} u^4_{\boldsymbol{k}}, \tag{166}$$

where we used $\delta \ln A(t = t_0) / \delta \phi^*_{\boldsymbol{k}}(t) = \delta \ln A(t = t_1) / \delta \phi^*_{\boldsymbol{k}}(t)$ with $t \neq t_0, t_1$.

The expression of ground-state energy $\mathcal{E}_{\rm BCS}$ is given by

$$\mathcal{E}_{\rm BCS} = 2 \sum_{\boldsymbol{k}} \varepsilon_k \rho_{\boldsymbol{k}} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}, \boldsymbol{k}'} (2U_0 - U_{|\boldsymbol{k} - \boldsymbol{k}'|}) \rho_{\boldsymbol{k}} \rho_{\boldsymbol{k}'} + \frac{1}{\mathcal{V}} \sum_{\boldsymbol{k}, \boldsymbol{k}'} U_{|\boldsymbol{k} - \boldsymbol{k}'|} F_{\boldsymbol{k}} F^*_{\boldsymbol{k}'}, \tag{167}$$

where $\rho_{\boldsymbol{k}} \equiv \langle \hat{c}^\dagger_{\boldsymbol{k}} \hat{c}_{\boldsymbol{k}} \rangle = |v_{\boldsymbol{k}}|^2$, and $F_{\boldsymbol{k}} \equiv \langle \hat{c}_{\boldsymbol{k}} \hat{c}_{-\boldsymbol{k}} \rangle = u_{\boldsymbol{k}} v_{-\boldsymbol{k}}$. Therefore, Eq. (166) is transformed into

$$i\hbar \frac{\partial \phi_{\boldsymbol{k}}(t)}{\partial t} = 2(\varepsilon_k + U^{\rm HF}_{\boldsymbol{k}}) \phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}} \phi^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}}. \tag{168}$$

The TdBdG equation with familiar form is also derived, starting from the original BCS wave function [28]

$$|\Phi_{\rm BCS}(t)\rangle = \prod_{\boldsymbol{k}} [u_{\boldsymbol{k}}(t) + v_{\boldsymbol{k}}(t) \hat{c}^\dagger_{\boldsymbol{k}\uparrow} \hat{c}^\dagger_{-\boldsymbol{k}\downarrow}] \, |0\rangle \, , \ |u_{\boldsymbol{k}}|^2 + |v_{\boldsymbol{k}}|^2 = 1, \tag{169}$$

which is equivalent to the state by Eq. (144) with definitions for u and v in terms of ϕ. Based on this variational state, the principle of least action $\delta S = 0$ yields

$$\begin{aligned} &\frac{\delta \mathcal{E}_{\rm BCS}(t)}{\delta u^*_{\boldsymbol{k}}(t)} = i\hbar \frac{\partial u_{\boldsymbol{k}}(t)}{\partial t}, \ \frac{\delta \mathcal{E}_{\rm BCS}(t)}{\delta v^*_{\boldsymbol{k}}(t)} = i\hbar \frac{\partial v_{\boldsymbol{k}}(t)}{\partial t} \\ \rightarrow &i\hbar \frac{\partial}{\partial t} \begin{pmatrix} u_{\boldsymbol{k}} \\ v_{\boldsymbol{k}} \end{pmatrix} = \begin{pmatrix} \varepsilon_k + U^{\rm HF}_{\boldsymbol{k}} & \Delta_{\boldsymbol{k}} \\ \Delta^*_{\boldsymbol{k}} & -\varepsilon_k - U^{\rm HF}_{\boldsymbol{k}} \end{pmatrix} \begin{pmatrix} u_{\boldsymbol{k}} \\ v_{\boldsymbol{k}} \end{pmatrix}. \end{aligned} \tag{170}$$

Now, we introduce the dynamical theory with many-body correlations following the manner by Ref. [27], i.e., we start from the variational state given in Eq. (146) with considering its time dependence. Calculating $\langle\Phi(t)|\partial_t|\Phi(t)\rangle$, we obtain

$$\begin{aligned} i\hbar\langle\Phi(t)|\frac{\partial}{\partial t}|\Phi(t)\rangle &= i\hbar\frac{\partial[\ln A(t)+\ln A_4(t)]}{\partial t} + i\hbar\langle\Phi(t)|\frac{\partial\hat{\pi}_4^\dagger(t)}{\partial t}|\Phi(t)\rangle + i\hbar\sum_{\boldsymbol{k}} u_{\boldsymbol{k}}v_{\boldsymbol{k}}^*\frac{\partial\phi_{\boldsymbol{k}}(t)}{\partial t} \\ &\simeq \frac{\partial[\ln A(t)+\ln A_4(t)]}{\partial t} + \frac{i\hbar}{4!}\sum_{\kappa_1,\kappa_2,\kappa_3,\kappa_4} w^*_{\kappa_1\kappa_2\kappa_3\kappa_4}\frac{\partial w_{\kappa_1\kappa_2\kappa_3\kappa_4}(t)}{\partial t} \\ &-\frac{1}{4!}\sum_{\kappa_1,\kappa_2,\kappa_3,\kappa_4}|w_{\kappa_1\kappa_2\kappa_3\kappa_4}|^2[f_{\boldsymbol{k}_1}+f_{\boldsymbol{k}_2}+f_{\boldsymbol{k}_3}+f_{\boldsymbol{k}_4}] + i\hbar\sum_{\boldsymbol{k}} u_{\boldsymbol{k}}v_{\boldsymbol{k}}^*\frac{\partial\phi_{\boldsymbol{k}}(t)}{\partial t}. \end{aligned} \tag{171a}$$

where we define f as follows:

$$f_{\boldsymbol{k}} = i\hbar\Big(v_{\boldsymbol{k}}^*\frac{\partial v_{\boldsymbol{k}}}{\partial t} + u_{\boldsymbol{k}}\frac{\partial u_{\boldsymbol{k}}}{\partial t}\Big). \tag{171b}$$

Defining $\mathcal{E} = \langle\Phi(t)|H|\Phi(t)\rangle$, we obtain the following equations:

$$\frac{\delta\mathcal{E}}{\delta\phi_{\boldsymbol{k}}^*(t)} = i\hbar\frac{\partial\phi_{\boldsymbol{k}}(t)}{\partial t}\left[1-2\sum_{\kappa_2,\kappa_3,\kappa_4}|w_{\kappa\kappa_2\kappa_3\kappa_4}|^2\right]u_{\boldsymbol{k}}^4 \tag{172a}$$

$$\frac{\delta\mathcal{E}}{\delta w^*_{\kappa_1\kappa_2\kappa_3\kappa_4}(t)} = i\hbar\frac{\partial w_{\kappa_1\kappa_2\kappa_3\kappa_4}(t)}{\partial t} - w_{\kappa_1\kappa_2\kappa_3\kappa_4}\Big[f_{\boldsymbol{k}_1}+f_{\boldsymbol{k}_2}+f_{\boldsymbol{k}_3}+f_{\boldsymbol{k}_4}\Big]. \tag{172b}$$

The expectation value of $\hat{H}$ with w is calculated as

$$\begin{aligned} \mathcal{E} &= \langle\Phi|\hat{H}|\Phi\rangle = 2\sum_{\boldsymbol{k}}\varepsilon_{\boldsymbol{k}}\rho_{\boldsymbol{k}} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'}(2U_0-U_{|\boldsymbol{k}-\boldsymbol{k}'|})\rho_{\boldsymbol{k}}\rho_{\boldsymbol{k}'} + \frac{1}{\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'}U_{|\boldsymbol{k}-\boldsymbol{k}'|}F_{\boldsymbol{k}}F^*_{\boldsymbol{k}'} \\ &+ \frac{1}{2\mathcal{V}}\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}\sum_{\alpha\alpha'}U_{|\boldsymbol{k}_1+\boldsymbol{k}_4|}(-1)^{1-\alpha-\alpha'}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4,\boldsymbol{0}} \\ &\times(u_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3}v_{\boldsymbol{k}_4}w^*_{\boldsymbol{k}_1\alpha\boldsymbol{k}_2\alpha'\boldsymbol{k}_3-\alpha'\boldsymbol{k}_4-\alpha} + v^*_{\boldsymbol{k}_1}v^*_{\boldsymbol{k}_2}u^*_{\boldsymbol{k}_3}u^*_{\boldsymbol{k}_4}w_{\boldsymbol{k}_1\alpha\boldsymbol{k}_2\alpha'\boldsymbol{k}_3-\alpha'\boldsymbol{k}_4-\alpha}), \end{aligned} \tag{173a}$$

where

$$\rho_{\boldsymbol{k}} = |v_{\boldsymbol{k}}|^2 + (|u_{\boldsymbol{k}}|^2-|v_{\boldsymbol{k}}|^2)\eta_{\boldsymbol{k}} = \frac{1}{2}\big[1+(|u_{\boldsymbol{k}}|^2-|v_{\boldsymbol{k}}|^2)(1-2\eta_{\boldsymbol{k}})\big] \tag{173b}$$

$$F_{\boldsymbol{k}} = u_{\boldsymbol{k}}v^*_{\boldsymbol{k}}(1-2\eta_{\boldsymbol{k}}) \tag{173c}$$

$$\eta_{\boldsymbol{k}} = \eta_\kappa = \frac{1}{3!}\sum_{\kappa_2\kappa_3\kappa_4}|w_{\kappa\kappa_2\kappa_3\kappa_4}|^2. \tag{173d}$$

Thus, the variational conditions are given by

$$\frac{\delta\mathcal{E}}{\delta\phi_{\boldsymbol{k}}^*} = [2(\varepsilon_k+U_{\boldsymbol{k}}^{\mathrm{HF}})\phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\phi^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}} + \chi_{\boldsymbol{k}}](1-2\eta_{\boldsymbol{k}})u^4_{\boldsymbol{k}}, \tag{174a}$$

$$\begin{aligned} \frac{\delta\mathcal{E}}{\delta w^*_{\boldsymbol{k}_1\alpha_1\boldsymbol{k}_2\alpha_2\boldsymbol{k}_3\alpha_3\boldsymbol{k}_4\alpha_4}} &= b_{\boldsymbol{k}_1\alpha_1\boldsymbol{k}_2\alpha_2\boldsymbol{k}_3\alpha_3\boldsymbol{k}_4\alpha_4} \\ &+ w_{\boldsymbol{k}_1\alpha_1\boldsymbol{k}_2\alpha_2\boldsymbol{k}_3\alpha_3\boldsymbol{k}_4\alpha_4}(E^0_{\boldsymbol{k}_1}+E^0_{\boldsymbol{k}_2}+E^0_{\boldsymbol{k}_3}+E^0_{\boldsymbol{k}_4}), \end{aligned} \tag{174b}$$

where

$$E^{(0)}_{\boldsymbol{k}} \equiv (u^2_{\boldsymbol{k}} - |v_{\boldsymbol{k}}|^2)(\varepsilon_k + U^{\rm HF}_{\boldsymbol{k}}) + 2{\rm Re}\Delta^*_{\boldsymbol{k}} u_{\boldsymbol{k}} v_{\boldsymbol{k}} \tag{175a}$$

$$\begin{aligned}\chi_{\boldsymbol{k}} &= \frac{1}{(1-2\eta_{\boldsymbol{k}})u^4_{\boldsymbol{k}}}\frac{1}{2\mathcal{V}}\frac{\delta}{\delta\phi^*_{\boldsymbol{k}}}\Bigg[\sum_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}\sum_{\alpha\alpha'} U_{|\boldsymbol{k}_1+\boldsymbol{k}_4|}(-1)^{1-\alpha-\alpha'}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4,\boldsymbol{0}} \\ &\times (u_{\boldsymbol{k}_1}u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3}v_{\boldsymbol{k}_4}w^*_{\boldsymbol{k}_1\alpha\boldsymbol{k}_2\alpha'\boldsymbol{k}_3-\alpha'\boldsymbol{k}_4-\alpha} + v^*_{\boldsymbol{k}_1}v^*_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}u_{\boldsymbol{k}_4}w_{\boldsymbol{k}_1\alpha\boldsymbol{k}_2\alpha'\boldsymbol{k}_3-\alpha'\boldsymbol{k}_4-\alpha})\Bigg] \\ &= \frac{1}{\mathcal{V}(1-2\eta_{\boldsymbol{k}})}\sum_{\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}\delta_{\boldsymbol{k}+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4,\boldsymbol{0}}U_{|\boldsymbol{k}+\boldsymbol{k}_4|}\Big[\phi^*_{\boldsymbol{k}_2} - \phi_{\boldsymbol{k}}({\rm Re}\phi_{\boldsymbol{k}_3}\phi_{\boldsymbol{k}_4} + i{\rm Im}\phi_{\boldsymbol{k}}\phi_{\boldsymbol{k}_2}) \\ &\times (w^*_{\boldsymbol{k}\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} + w^*_{\boldsymbol{k}\boldsymbol{k}_3\boldsymbol{k}_2\boldsymbol{k}_4} + w^*_{\boldsymbol{k}_4\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}} + w^*_{\boldsymbol{k}_4\boldsymbol{k}_3\boldsymbol{k}_2\boldsymbol{k}})\Big]\frac{u_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}u_{\boldsymbol{k}_4}}{u_{\boldsymbol{k}}},\end{aligned} \tag{175b}$$

$$w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} \equiv w_{\boldsymbol{k}_1\uparrow\boldsymbol{k}_2\uparrow\boldsymbol{k}_3\downarrow\boldsymbol{k}_4\downarrow}. \tag{175c}$$

Therefore, we obtain

$$i\hbar\frac{\partial\phi_{\boldsymbol{k}}}{\partial t} = 2(\varepsilon_k + U^{\rm HF}_{\boldsymbol{k}})\phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\phi^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}} + \chi_{\boldsymbol{k}}, \tag{176a}$$

$$i\hbar\frac{\partial w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}}{\partial t} = b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} + w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}\sum_{i=1}^{4}(E^0_{\boldsymbol{k}_i} + f_{\boldsymbol{k}_i}), \tag{176b}$$

with

$$\begin{aligned}b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} = b_{\boldsymbol{k}_1\uparrow\boldsymbol{k}_2\uparrow\boldsymbol{k}_3\downarrow\boldsymbol{k}_4\downarrow} &= \frac{\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2+\boldsymbol{k}_3+\boldsymbol{k}_4\boldsymbol{0}}}{\mathcal{V}}\Big[U_{|\boldsymbol{k}_1+\boldsymbol{k}_4|}(u_{\boldsymbol{k}_1}v_{\boldsymbol{k}_4} + v_{\boldsymbol{k}_1}u_{\boldsymbol{k}_4})(u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_3} + v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_3}) \\ &- U_{|\boldsymbol{k}_1+\boldsymbol{k}_3|}(u_{\boldsymbol{k}_1}v_{\boldsymbol{k}_3} + v_{\boldsymbol{k}_1}u_{\boldsymbol{k}_3})(u_{\boldsymbol{k}_2}v_{\boldsymbol{k}_4} + v_{\boldsymbol{k}_2}u_{\boldsymbol{k}_4})\Big].\end{aligned} \tag{176c}$$

Under the gauge transformation as $\phi \to \phi e^{-i2\mu t/\hbar}$ and $w \to we^{-i4\mu t/\hbar}$ (μ: arbitrary constant), the dynamics of variational parameters are given by

$$i\hbar\frac{\partial\phi_{\boldsymbol{k}}}{\partial t} = 2(\varepsilon_k - \mu + U^{\rm HF}_{\boldsymbol{k}})\phi_{\boldsymbol{k}} + \Delta^*_{\boldsymbol{k}}\phi^2_{\boldsymbol{k}} - \Delta_{\boldsymbol{k}} + \chi_{\boldsymbol{k}}, \tag{177a}$$

$$i\hbar\frac{\partial w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}}{\partial t} = b_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4} + w_{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3\boldsymbol{k}_4}\sum_{i=1}^{4}(\tilde{E}^0_{\boldsymbol{k}_i} + f_{\boldsymbol{k}_i}), \tag{177b}$$

where $\tilde{E}^{(0)}_{\boldsymbol{k}} \equiv (u^2_{\boldsymbol{k}} - |v_{\boldsymbol{k}}|^2)(\varepsilon_k + U^{\rm HF}_{\boldsymbol{k}} - \mu) + 2{\rm Re}\Delta^*_{\boldsymbol{k}}u_{\boldsymbol{k}}v_{\boldsymbol{k}}$. Assuming μ is chemical potential and setting $\partial_t\phi = \partial_t w = 0$ and $(\phi, w) = (\phi^*, w^*)$, we reproduce the equilibrium solutions of ϕ and w in Ref. [27].

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