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DOCTORAL THESIS

**Theoretical Study of Quasiparticle Excitations
in Bose-Einstein condensates**

(ボーズ・アインシュタイン凝縮相における
準粒子励起の研究)

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Part I

Preface

Bose-Einstein condensation (BEC) [1, 2, 3] is typical of the spontaneous symmetry breaking which is one of fundamental concepts in modern physics. BEC has been studied actively in both experimental and theoretical approaches. In the present thesis, we will confirm validities of results by previous studies. We first summarize the historical backgrounds of BEC and point out some issues.

In an assembly of N identical bosons, a macroscopic number of particles occupy the lowest single-particle state below a finite temperature T_c . If we assume an ideal Bose gas, all particles of the system lies in the lowest-energy state at $T = 0$. Such a phase transition is called Bose-Einstein condensation, which is one of typical examples of $U(1)$ symmetry breaking [4]. BEC was first pointed out in 1924. Bose reproduced concisely the Planck's formula by introducing a new occupation rule for the phase space of phonon [5]. The next year, Einstein predicted the existence of BEC by extending the theory to an ideal gas with mass [6, 7]. Afterward, superfluid ^4He was discovered by Kapitza in 1938 [8]. London pointed out that the superfluidity may be caused by BEC [9]. Superfluid ^4He also exhibits unique phenomena such as film flow and fountain effect. Tisza and Landau gave a phenomenological description called two fluid model, which regarded the condensate and excited phases as perfect and normal fluid respectively [10, 11, 12]. However, since ^4He particles interact strongly with each other, superfluid ^4He cannot be described qualitatively by the theory of Einstein. Thus, a realization of BEC in a weakly interacting system was desired. On the other hand, in 1947, Bogoliubov started a study of BEC with quantum field theory [13]. The perturbation theory of BEC in a dilute Bose system by using Green's function was constructed in 1958 by Beliaev [14]. This method is used even now. In experiments, the laser cooling method for atomic gases was invented by Hänsch and Shallow in 1975 [15]. Finally in 1995, Cornell and Wieman *et al.* realized the BEC in dilute ^{87}Rb gas [16]. The atomic gases are weakly interacting systems so that a good agreement between experimental and theoretical results are expected. The realization of atomic BEC has caused a revival of theoretical interest in BEC.

We next outline the previous results of theoretical studies on BEC. We here consider a weakly interacting Bose system, which was first considered by Bogoliubov as a microscopic model for superfluid ^4He . It considers identical bosons with mass m and spin 0 interacting via a contact potential $V(\mathbf{r} - \mathbf{r}') \equiv g\delta(\mathbf{r} - \mathbf{r}')$. The corresponding Hamiltonian \hat{H} in the second quantized form is given by

$$\hat{H} = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r})\hat{K}\hat{\psi}(\mathbf{r}) + \frac{g}{2} \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}),$$

where $\hat{K} \equiv \frac{\hat{p}^2}{2m} - \mu$ is the kinetic energy operator measured from the chemical potential μ . Bogoliubov considered the uniform system at $T \approx 0$. We express the field operator as a sum of the condensate wave function $\Psi(\mathbf{r}) \equiv \langle \hat{\psi}(\mathbf{r}) \rangle$ and the quasiparticle field $\hat{\phi}(\mathbf{r})$ as

$$\hat{\psi}(\mathbf{r}) = \Psi(\mathbf{r}) + \hat{\phi}(\mathbf{r}),$$

where $\langle \dots \rangle$ denotes the grand canonical average, and $\langle \hat{\phi} \rangle = 0$ by definition. We also introduce the condensate density $n_0 \equiv N_0/V$ with N_0 the condensate particle number. In uniform systems, we can set $\Psi(\mathbf{r}) \rightarrow n_0$. We then substitute the decomposed expression into the Hamiltonian and approximate it in bilinear forms in terms of $\hat{\phi}$. Diagonalizing the resulting Hamiltonian for uniform systems yields the famous Bogoliubov spectrum

$$E_{\mathbf{k}}^{(B)} \equiv \sqrt{\varepsilon_{\mathbf{k}}(\varepsilon_{\mathbf{k}} + 2gn_0)},$$

where $\varepsilon_{\mathbf{k}} \equiv \hbar^2\mathbf{k}^2/2m$. Note that the Bogoliubov mode has linear dispersion at $\mathbf{k} \rightarrow 0$.

In 1958, Beliaev constructed a perturbation theory for the quasiparticle field $\hat{\phi}$. Using this theory, the following theorems for excitation of BEC were "proved":

- (i): One-particle excitation, which corresponds to the pole of one-particle Green's function, must be a gapless excitation. (Hugenholtz-Pines theorem) [17]
- (ii): Two-particle Green's function share common poles with one-particle Green's function. Therefore the one-particle excitation is same as the two-particle excitation. (Gavoret, Nozières) [18]

The theorem (i) corresponds to the Goldstone’s theorem of quantum field theory [19, 20]. Also, the converse of the theorem (ii) doesn’t necessarily hold. However, the “proof” of the theorem (ii) has an ambiguity in the definition of Green’s functions, raising a fundamental question of whether their proof is really correct or not. This ambiguity originates from how to definite the skeleton diagrams under the existence of the condensate fields.

Next, we consider theories of BEC at finite temperatures. Girardeau and Arnowitt extended the Bogoliubov theory in 1959 so as to incorporate interaction between excitations approximately by a variational treatment (Girardeau-Arnouitt theory) [21]. It amount to retaining the pair correlation term $\langle \hat{\phi}\hat{\phi} \rangle$, which had been ignored in the Bogoliubov theory, and diagonalizing the quadratic Hamiltonian. The Girardeau-Arnouitt theory was renamed “Hartree-Fock-Bogoliubov theory” (HFB theory) by Griffin after the realization of the atomic BEC [22]. However, it gives rise to a finite energy gap in the single-particle excitation in contradiction to the Hugenholtz-Pines theorem. On the other hand, Shono proposed a theory which yields a gapless excitation for one-particle excitation [23, 24]. It omits the pair correlation term in the HFB theory by hand so as to satisfy the Hugenholtz-Pines theorem. However the pair correlation terms must be considered at finite temperatures, so it may lack the consistency. Also, this approximation cannot be used to describe a dynamical situation, because it breaks conservation laws such as particle number, momentum, energy, and so on. We also note that Griffin called this approximation “Popov” approximation [22], whose name becomes widely accepted today. However, there isn’t such an approximation in the literature by Popov [25] which was referenced by Griffin, so this approximation should be called more apparently as “Shono” approximation.

In 1965, on the other hand, Hohenberg and Martin [26] pointed out another important property:

(iii): Conservation laws should be satisfied.

Hohenberg and Martin classified the existing theories into “conserving” and “gapless” approximations. The conserving approximation, which is also called Φ -derivable approximation, was first formulated by Baym for a normal state in 1962 [27, 28]. The advantage is to satisfy conservation laws automatically when applying it to a time-dependent problem. It can be also used for the thermal equilibrium state by using the Matsubara form. The HFB theory belongs to this approximation scheme together with the Hartree-Fock theory and BCS theory [29]. Another advantage is to be able to construct the Dyson equation and Berthe-Salpeter equation from the same functional Φ . On the other hand, the gapless approximation such as the Bogoliubov theory and the Shono approximation may describe low-energy properties qualitatively, while it can’t be applied to time-dependent problems. Hohenberg and Martin named this situation “conserving v.s. gapless” dilemma, which was also emphasized by Griffin [22]. Thus, no theory that satisfies (i) and (ii) had been known until recently.

In 2009, Kita constructed a new perturbation theory for BEC which satisfies the Hugenholtz-Pines theorem and conservation laws simultaneously (conserving-gapless theory) [30]. This theory is the extension of the Φ -derivative approximation, which is summarized in the following two steps. First, we construct the functional Φ by including diagrams characteristic of BEC, whose numerical weights are still undetermined. Next, we determine these weights by using the Hugenholtz-Pines theorem. By considering the resulting Green’s function, it turns out that poles of the one- and the two-particle Green’s function are not shared. Therefore, the collective mode is not same as the one-particle excitation. The new one-particle excitation is called “bubbling mode” [31, 32]. Thus in BEC system, there still remain fundamental problems concerning the quasiparticle excitations. We are especially interested which of the conserving-gapless theory or that by Gavoret and Nozières (the theorem (ii)) is correct.

In this thesis, we will investigate the quasi-particle excitation by the conserving-gapless theory and the exact computational simulation. We here shortly summarize the results by our study. First, we will study the bubbling mode for weakly interacting Bose system at $T = 0$. We will find that the bubbling mode has a finite lifetime proportional to the s -wave scattering length a [33]. Also, the ground state energy proposed by Lee, Huang, Yang [34] should be modified as

$$\frac{\mathcal{E}}{N} = 4\pi an \left[1 + \frac{16}{5} \left(\frac{8}{3\sqrt{\pi}} + c_{ip} \right) \sqrt{na^3} \right],$$

where c_{ip} is the new additional term of $O(1)$ [35]. The result by Lee *et.al.* is reproduced by setting $c_{ip} \rightarrow 0$. We will find that these new results are given by a new class of Feynman diagrams which has been overlooked so far. We will see that they bring one-particle reducible diagrams for the self-energy.

Next, we will perform an exact calculation for a Bose system at $T = 0$ by using diffusion Monte Carlo method [36, 37, 38, 39, 40]. We will also apply the moment method [41, 42] to the one- and the two-particle excitations. This approximation is originally used for the analysis of collective modes such as those superfluid ^4He and magnon system, which corresponds to taking a first-order moment of the frequency ω of the dynamic structure factor $S(\mathbf{q}, \omega)$. In this thesis, we will extend it to the higher-order moments and apply it also to the case of the one-particle spectral function $A(\mathbf{k}, \varepsilon)$. We can thereby estimate the spectrum of the one- and the two-particle excitation and their lifetimes. We will obtain the result that these quasi-particle excitations have qualitatively different behavior in agreement with the conserving-gapless theory but against the theorem (ii).

This thesis is organized as follows: In chapter II, we summarized the conserving gapless theory and use it to estimate ground state energy and the lifetime of the bubbling mode. Next, in chapter III, we present how to simulate a Bose system by using the diffusion quantum Monte Carlo method, and give the expressions of the moments. Afterward, we show the results by these methods. Finally, we conclude and summarize those results in chapter IV.

Part II

Results of Conserving-Gapless Theory

Recently, a new self-consistent perturbation expansion (conserving-gapless theory [30]) has been formulated for condensed Bose systems which satisfies the Hugenholtz-Pines theorem[17] and conservation laws [27, 26] simultaneously. We will introduce results of the conserving-gapless theory, which produces several different results from the previous studies. Notations and equations in the following section are defined and derived in Appendix A. We also choose the following units:

$$\hbar = 1, \quad m = \frac{1}{2}, \quad k_B = 1, \quad T_c^0 = 1,$$

where m , k_B , and T_c^0 are the particle mass, the Boltzmann constant, the transition temperature of ideal Bose-Einstein condensation respectively.

1 Perturbation expansion for BEC

1.1 Notations

We consider N identical bosons with mass m and spin 0 and interacting with a two-body potential $V(\mathbf{r} - \mathbf{r}')$. The corresponding Hamiltonian \hat{H} is given by

$$\begin{aligned} \hat{H} &\equiv \hat{H}_0 + \hat{H}_{\text{int}} \\ &= \int d^3\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \hat{K}_1(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}), \end{aligned} \quad (1)$$

where $(\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}))$ are annihilation and creation operators satisfying the bosonic commutation relations, and $\hat{K}_1(\mathbf{r}) \equiv \hat{\mathbf{p}}^2/2m + U(\mathbf{r}) - \mu$ with $U(\mathbf{r})$ the external field and μ the chemical potential. Field operators in the Heisenberg representation are defined as

$$\psi_1(1) \equiv e^{-\tau_1 \hat{H}} \hat{\psi}(\mathbf{r}_1) e^{\tau_1 \hat{H}}, \quad \psi_2(1) \equiv e^{-\tau_1 \hat{H}} \hat{\psi}^\dagger(\mathbf{r}_1) e^{\tau_1 \hat{H}}, \quad (2)$$

respectively. We next divide these field operators into two parts as

$$\psi_i(1) = \Psi_i(1) + \phi_i(1), \quad (i = 1, 2), \quad (3)$$

where $\Psi_i(1) \equiv \langle \psi_i(1) \rangle$ and $\phi_i(1)$ are the condensate wave function and the quasiparticle operator respectively, and $\langle \dots \rangle$ is the grand-canonical average.

Next, we define the Matsubara Green's function in the Nambu space as

$$G_{ij} = -\langle T_\tau \phi_i(1) \phi_{3-j}(2) \rangle (-1)^{j-1}, \quad (4)$$

where T_τ is the time-ordering operator. G_{ij} also satisfies the following relations:

$$G_{ij}(1, 2) = (-1)^{i+j-1} G_{3-j, 3-i}(2, 1) = (-1)^{i+j} G_{ji}^*(\mathbf{r}_2 \tau_1, \mathbf{r}_1, \tau_2). \quad (5)$$

We can also express G_{ij} in a matrix form as

$$\hat{G}(1, 2) \equiv \begin{bmatrix} G_{11}(1, 2) & G_{12}(1, 2) \\ G_{21}(1, 2) & G_{22}(1, 2) \end{bmatrix} = \begin{bmatrix} G(1, 2) & F(1, 2) \\ -\bar{F}(1, 2) & -G(1, 2) \end{bmatrix}. \quad (6)$$

We now give the expression of the thermodynamic potential in a Luttinger-Ward form [28] for BEC as,

$$\Omega = -\frac{1}{\beta} \int d1 \int d2 \Psi_2(1) G_0^{-1}(1, 2) \Psi_1(2) + \frac{1}{2\beta} \text{Tr}[\ln(-\hat{G}_0^{-1} + \hat{\Sigma}) + \hat{\Sigma} \hat{G}] + \Phi, \quad (7)$$

where $\hat{G}_0^{-1} \equiv (-\hat{\sigma}_0 \partial / \partial \tau_1 - \hat{\sigma}_3 K_1) \delta(1, 2)$, and $\hat{\sigma}_0, \hat{\sigma}_3$ are 2×2 unit matrix and third Pauli matrix respectively, the self-energy $\hat{\Sigma} \equiv \Sigma_{ij}$ can be introduced as

$$\Sigma_{ij}(1, 2) \equiv -2\beta \frac{\delta \Phi}{\delta G_{ji}(2, 1)}, \quad (8)$$

also

$$\hat{\Sigma}(1, 2) \equiv \begin{bmatrix} \Sigma(1, 2) & \Delta(1, 2) \\ -\bar{\Delta}(1, 2) & -\bar{\Sigma}(1, 2) \end{bmatrix}. \quad (9)$$

And the trace $\text{Tr} \hat{\Sigma} \hat{G}$ is defined by

$$\text{Tr} \hat{\Sigma} \hat{G} \equiv \int d1 \int d2 \text{Tr} \begin{bmatrix} \Sigma(1, 2) & \Delta(1, 2) \\ -\bar{\Delta}(1, 2) & -\bar{\Sigma}(1, 2) \end{bmatrix} \begin{bmatrix} G(2, 1_+) & F(2, 1) \\ -\bar{F}(2, 1) & -\bar{G}(2, 1_-) \end{bmatrix}, \quad (10)$$

where the subscript of \pm denote presence of additional infinitesimal positive (negative) constant. The grand canonical average of \hat{H}_{int} is given by

$$\begin{aligned} \langle \hat{H}_{\text{int}} \rangle &= \frac{1}{4\beta} \int d1 \int d2 \{ 2\Sigma(1, 2) [\Psi(2)\bar{\Psi}(1) - G(2, 1_+)] \\ &\quad - \bar{\Delta}(1, 2) [\Psi(2)\Psi(1) - F(2, 1)] - \Delta(1, 2) [\bar{\Psi}(2)\bar{\Psi}(1) - \bar{F}(2, 1)] \}, \end{aligned} \quad (11)$$

which can be connected with the functional Φ order by order as

$$\Phi = -T \sum_{n=1}^{\infty} \frac{1}{2n} \text{Tr} \Sigma^{(n)} G. \quad (12)$$

By comparing Eqs. (11) and (12), we thus find the following relation:

$$\Phi^{(n)} = \frac{1}{n} \langle H_{\text{int}} \rangle^{(n)}. \quad (13)$$

\hat{G} and $\vec{\Psi} \equiv \Psi_i$ satisfy the following equations:

$$\int d3 [\hat{G}_0^{-1}(1, 2) - \hat{\Sigma}(1, 3)] \hat{G}(3, 2) = \hat{\sigma}_0 \delta(1, 2), \quad (14a)$$

$$\int d2 [\hat{G}_0^{-1}(1, 2) - \hat{\Sigma}(1, 2)] \vec{\Psi}(2) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad (14b)$$

which are the Dyson-Beliaev equation [14] and the Hugenholtz-Pines theorem [17] respectively.

For a later convenience, we define the symmetrized vertex as

$$\Gamma^{(0)}(11', 22') \equiv V(\mathbf{r}_1 - \mathbf{r}_2) \delta(\tau_1 - \tau_2) [\delta(1, 1') \delta(2, 2') + \delta(1, 2') \delta(2, 1')], \quad (15)$$

which also satisfies the following relations:

$$\Gamma^{(0)}(11', 22') = \Gamma^{(0)}(22', 11') = \Gamma^{(0)}(1'1, 2'2) = \Gamma^{(0)}(2'1, 21'). \quad (16)$$

By using Eq. (15), the expression of Φ can be written explicitly order by order in terms of the interaction as

$$\begin{aligned}\Phi^{(1)} &= \frac{T}{4} \int d1 \int d1' \int d2 \int d2' \Gamma^{(0)}(11', 22') \\ &\quad \times \{2G(1.1')G(2, 2') + c_{2b}^{(1)}F(1.2)\bar{F}(1', 2') + c_{1a}^{(1)}G(1, 1')\Psi(2)\bar{\Psi}(2') \\ &\quad + c_{1b}^{(1)}[F(1, 2)\bar{\Psi}(1')\bar{\Psi}(2') + \bar{F}(1', 2')\Psi(1)\Psi(2)] + \bar{\Psi}(1')\bar{\Psi}(2')\Psi(2)\Psi(1)\}\end{aligned}\quad (17a)$$

$$\begin{aligned}\Phi^{(2)} &= -\frac{T}{8} \int d1 \cdots \int d4' \Gamma^{(0)}(11', 22') \Gamma^{(0)}(33', 44') \\ &\quad \times \{G(2, 3')G(3, 2')G(1, 4')G(4', 1) + c_{4b}^{(2)}\bar{F}(2', 3')F(2, 3)G(1, 4')G(4, 1') \\ &\quad + c_{4c}^{(2)}\bar{F}(2', 3')F(2, 3)\bar{F}(1', 4')F(1, 4) + c_{3a}^{(2)}G(2, 3')G(3, 2')G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{3b}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]G(1, 4')G(4, 1') \\ &\quad + c_{3c}^{(2)}\bar{F}(2', 3')F(2, 3)G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{3d}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]\bar{F}(1', 4')F(1, 4) \\ &\quad + c_{2a}^{(2)}G(2, 3')G(3, 2')\Psi(1)\bar{\Psi}(4)\Psi(4')\bar{\Psi}(1') + c_{2b}^{(2)}G(2, 3')\Psi(3)\bar{\Psi}(2')G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2c}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2d}^{(2)}\bar{F}(2', 3')F(2, 3)\Psi(1)\bar{\Psi}(4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2e}^{(2)}[F(2, 3)\bar{\Psi}(3')\bar{\Psi}(2')F(1, 4)\bar{\Psi}(4')\bar{\Psi}(1') + \bar{F}(2', 3')\Psi(3)\Psi(2)\bar{F}(1', 4')\Psi(4)\Psi(1)]\},\end{aligned}\quad (17b)$$

where

$$c_{2b}^{(1)} = -1, \quad c_{1a}^{(1)} = -4, \quad c_{1b}^{(1)} = 1, \quad (18a)$$

$$\begin{aligned}c_{4b}^{(2)} &= -2, \quad c_{4c}^{(2)} = 1, \\ c_{3a}^{(2)} &= -4, \quad c_{3b}^{(2)} = 2, \quad c_{3c}^{(2)} = 4, \quad c_{3d}^{(2)} = -2, \\ c_{2a}^{(2)} &= c_{2b}^{(2)} = 2, \quad c_{2c}^{(2)} = -4, \quad c_{2d}^{(2)} = 2, \quad c_{2e}^{(2)} = 1.\end{aligned}\quad (18b)$$

1.2 Expressions of first and second self-energies

We introduce a matrix $\hat{\mathcal{G}} \equiv \mathcal{G}_{ij}$ [32] as

$$\mathcal{G}_{ij}(1, 2) \equiv G_{ij} - (-1)^{i-1}\Psi_i(1)\Psi_{3-j}(2). \quad (19)$$

Using this function, Eq. (11) can be rewritten as

$$\langle H_{\text{int}} \rangle = -\frac{1}{4\beta} \Sigma_{\bar{i}\bar{j}}(\bar{1}, \bar{2}) \mathcal{G}_{\bar{j}\bar{i}}(\bar{2}, \bar{1}), \quad (20)$$

where summation over barred arguments such as $\bar{1}$ and \bar{i} are implied.

We can construct Φ as a functional of $\hat{\mathcal{G}}$, which can be confirmed by considering the following conditions:

$$\begin{aligned}\Sigma_{ii'}(1, 1') &= -2\beta \frac{\delta\Phi}{\delta\mathcal{G}_{\bar{j}\bar{j}'}(\bar{2}, \bar{2}')} \frac{\delta\mathcal{G}_{\bar{j}\bar{j}'}(\bar{2}, \bar{2}')}{\delta G_{ii'}(1, 1')} \\ &= -2\beta \frac{\delta\Phi}{\delta\mathcal{G}_{ii'}(1, 1')},\end{aligned}\quad (21a)$$

$$\begin{aligned}
\beta \frac{\delta \Phi}{\delta \Psi_{3-i}(1)} &= \beta \frac{\delta \Phi}{\delta \mathcal{G}_{\bar{j}\bar{j}}(\bar{2}', \bar{2})} \frac{\delta \mathcal{G}_{\bar{j}\bar{j}}(\bar{2}', \bar{2})}{\delta \Psi_{3-i}(1)} \\
&= -\frac{1}{2} \frac{\delta \mathcal{G}_{\bar{j}\bar{j}}(\bar{2}', \bar{2})}{\delta \Psi_{3-i}(1)} \\
&= \frac{1}{2} [\Sigma_{i\bar{j}}(1, \bar{2}')(-1)^{\bar{j}-1} \Psi_{\bar{j}'}(\bar{2}') + \Sigma_{\bar{j}, 3-i}(\bar{2}, 1)(-1)^i \Psi_{3-\bar{j}}(\bar{2})] \\
&= \frac{1}{2} [\Sigma_{i\bar{j}}(1, \bar{2}')(-1)^{\bar{j}-1} \Psi_{\bar{j}'}(\bar{2}') + \Sigma_{i, 3-\bar{j}}(1, \bar{2})(-1)^{\bar{j}} \Psi_{3-\bar{j}}(\bar{2})] \\
&= \Sigma_{i\bar{j}}(1, \bar{2})(-1)^{\bar{j}-1} \Psi_{\bar{j}}(\bar{2})
\end{aligned} \tag{21b}$$

Let us introduce

$$\mathcal{G}(1, 2) \equiv \frac{\mathcal{G}_{11}(1, 2) - \mathcal{G}_{22}(2, 1)}{2}, \quad \mathcal{F}(1, 2) \equiv \frac{\mathcal{G}_{12}(1, 2) - \mathcal{G}_{12}(2, 1)}{2}, \quad \bar{\mathcal{F}}(1, 2) \equiv \frac{\mathcal{G}_{21}(1, 2) - \mathcal{G}_{21}(2, 1)}{2}. \tag{22}$$

Using these notations, we can transform Eq. (12) as

$$\begin{aligned}
\Phi^{(n)} &= \frac{1}{2n} \frac{\delta \Phi^{(n)}}{\delta \mathcal{G}_{\bar{i}\bar{j}}(\bar{2}, \bar{1})} \mathcal{G}_{\bar{i}\bar{j}}(\bar{2}, \bar{1}) \\
&= \frac{1}{2n} \left[\frac{\delta \Phi^{(n)}}{\delta \mathcal{G}(\bar{2}, \bar{1})} \mathcal{G}(\bar{2}, \bar{1}) + \frac{\delta \Phi^{(n)}}{\delta \mathcal{F}(\bar{2}, \bar{1})} \mathcal{F}(\bar{2}, \bar{1}) + \frac{\delta \Phi^{(n)}}{\delta \bar{\mathcal{F}}(\bar{2}, \bar{1})} \bar{\mathcal{F}}(\bar{2}, \bar{1}) \right].
\end{aligned} \tag{23}$$

We can rewrite Eq. (17a) and (17b) as

$$\Phi^{(1)} \equiv \frac{1}{4\beta} \Gamma^{(0)}(\bar{1}'\bar{1}, \bar{2}'\bar{2}) [2\mathcal{G}(\bar{1}, \bar{1}')\mathcal{G}(\bar{2}, \bar{2}') - \mathcal{F}(\bar{1}, \bar{2})\bar{\mathcal{F}}(\bar{1}', \bar{2}')], \tag{24a}$$

$$\begin{aligned}
\Phi^{(2)} &= -\frac{1}{8\beta} \Gamma^{(0)}(\bar{1}'\bar{1}, \bar{2}'\bar{2}) [\mathcal{G}(\bar{2}, \bar{3}')\mathcal{G}(\bar{3}, \bar{2}') - \mathcal{F}(\bar{2}', \bar{3}')\bar{\mathcal{F}}(\bar{2}, \bar{3})] \\
&\quad \times \Gamma^{(0)}(\bar{3}'\bar{3}, \bar{4}'\bar{4}) [\mathcal{G}(\bar{1}, \bar{4}')\mathcal{G}(\bar{4}, \bar{1}') - \mathcal{F}(\bar{1}', \bar{4}')\bar{\mathcal{F}}(\bar{1}, \bar{4})]
\end{aligned} \tag{24b}$$

respectively.

Using Eq. (21a), self-energies are also calculated as

$$\Sigma^{(1)}(1, 1') \equiv -T^{-1} \frac{\delta \Phi^{(1)}}{\delta \mathcal{G}(1', 1)} = -\Gamma^{(0)}(11', \bar{2}'\bar{2})\mathcal{G}(\bar{2}, \bar{2}'), \tag{25a}$$

$$\Delta^{(1)}(1, 1') \equiv 2T^{-1} \frac{\delta \Phi^{(1)}}{\delta \bar{\mathcal{F}}(1', 1)} = -\frac{1}{2} \Gamma^{(0)}(1\bar{2}', 1\bar{2})\bar{\mathcal{F}}(\bar{2}', \bar{2}), \tag{25b}$$

$$\begin{aligned}
\Sigma^{(2)}(1, 1') &\equiv -T^{-1} \frac{\delta \Phi^{(2)}}{\delta \mathcal{G}(1', 1)} \\
&= \frac{1}{2} \Gamma^{(0)}(1\bar{4}, \bar{2}'\bar{2}) \Gamma^{(0)}(\bar{3}'\bar{3}, \bar{4}'1') [\mathcal{G}(\bar{2}, \bar{3}')\mathcal{G}(\bar{3}, \bar{2}') - \bar{\mathcal{F}}(\bar{2}', \bar{3}')\mathcal{F}(\bar{2}, \bar{3})] \\
&= \frac{1}{2} \Gamma^{(0)}(1\bar{4}, \bar{2}'\bar{2}) \Gamma^{(0)}(\bar{3}'\bar{3}, \bar{4}'1') \\
&\quad \times \{G(\bar{2}, \bar{3}')G(\bar{3}, \bar{2}')G(\bar{4}, \bar{4}') - \bar{F}(\bar{2}', \bar{3}')\bar{F}(\bar{2}, \bar{3})G(\bar{4}, \bar{4}') \\
&\quad - 2\Psi(\bar{2})\bar{\Psi}(\bar{3}')G(\bar{3}, \bar{2}')G(\bar{4}, \bar{4}') - \Psi(\bar{3})\bar{\Psi}(\bar{2}')G(\bar{2}, \bar{3}')G(\bar{4}, \bar{4}') \\
&\quad + [\bar{F}(\bar{2}', \bar{3}')\Psi(\bar{2})\Psi(\bar{3}) + \bar{F}(\bar{2}', \bar{3}')\bar{\Psi}(\bar{2}')\bar{\Psi}(\bar{3}')]G(\bar{4}, \bar{4}') \\
&\quad + \bar{F}(\bar{2}', \bar{3}')\bar{F}(\bar{2}, \bar{3})\Psi(\bar{4})\Psi(\bar{4}') \\
&\quad + G(\bar{4}, \bar{4}')\Psi(\bar{2})\bar{\Psi}(\bar{3}')\Psi(\bar{3})\bar{\Psi}(\bar{2}') + G(\bar{3}, \bar{2}')\Psi(\bar{2})\bar{\Psi}(\bar{3}')\Psi(\bar{4})\bar{\Psi}(\bar{4}') \\
&\quad - [\bar{F}(\bar{2}', \bar{3}')\Psi(\bar{2})\Psi(\bar{3}) + \bar{F}(\bar{2}, \bar{3})\bar{\Psi}(\bar{2}')\bar{\Psi}(\bar{3}')] \Psi(\bar{4})\bar{\Psi}(\bar{4}') \},
\end{aligned} \tag{26a}$$

$$\begin{aligned}
\Delta^{(2)}(1, 1') &\equiv 2T^{-1} \frac{\delta\Phi^{(2)}}{\delta\bar{\mathcal{F}}(1', 1)} \\
&= \frac{1}{2} \Gamma^{(0)}(\bar{3}'\bar{3}, 1'\bar{2}) \Gamma^{(0)}(1\bar{2}', \bar{4}'\bar{4}) [\mathcal{G}(\bar{2}, \bar{3}') \mathcal{G}(\bar{3}, \bar{2}') - \bar{\mathcal{F}}(\bar{2}', \bar{3}') \mathcal{F}(\bar{2}, \bar{3})] \\
&= \frac{1}{2} \Gamma^{(0)}(\bar{3}'\bar{3}, 1'\bar{2}) \Gamma^{(0)}(1\bar{2}', \bar{4}'\bar{4}) \\
&\quad \times \{G(\bar{3}, \bar{4}') G(\bar{4}, \bar{3}') F(\bar{2}, \bar{2}') - \bar{F}(\bar{3}', \bar{4}') F(\bar{3}, \bar{4}) F(\bar{2}, \bar{2}') \\
&\quad - [G(\bar{3}, \bar{4}') \Psi(\bar{4}) \bar{\Psi}(\bar{3}') + G(\bar{4}, \bar{3}') \Psi(\bar{3}) \bar{\Psi}(\bar{4}')] F(\bar{2}, \bar{2}') \\
&\quad - G(\bar{3}, \bar{4}') G(\bar{4}, \bar{3}') \Psi(\bar{2}) \Psi(\bar{2}') \\
&\quad + 2\bar{F}(\bar{3}, \bar{4}') F(\bar{4}, \bar{3}') \Psi(\bar{2}) \Psi(\bar{2}') + F(\bar{3}, \bar{4}) \bar{\Psi}(\bar{3}') \bar{\Psi}(\bar{4}') F(\bar{2}, \bar{2}') \\
&\quad - [\bar{G}(\bar{3}, \bar{4}') \Psi(\bar{4}) \Psi(\bar{3}') + G(\bar{4}, \bar{3}') \bar{\Psi}(\bar{3}) \bar{\Psi}(\bar{4}')] \Psi(\bar{2}) \bar{\Psi}(\bar{2}') \\
&\quad - \Psi(\bar{3}) \bar{\Psi}(\bar{4}') \Psi(\bar{4}) \bar{\Psi}(\bar{3}') F(\bar{2}, \bar{2}') - \bar{F}(\bar{3}', \bar{4}') \Psi(\bar{4}) \bar{\Psi}(\bar{3}) \Psi(\bar{2}') \bar{\Psi}(\bar{2})\}, \tag{26b}
\end{aligned}$$

respectively.

1.3 Self-consistent equation in momentum space

We now construct the self-energy up to the second order in the momentum space. From here we consider particles interacting with a contact potential $V(\mathbf{r}-\mathbf{r}') \equiv g\delta(\mathbf{r}-\mathbf{r}')$ in a homogeneous system. The corresponding Hamiltonian is given by

$$\begin{aligned}
\hat{H} &\equiv \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} \hat{\psi}(\mathbf{r}) + \int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') g\delta(\mathbf{r}-\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \\
&= \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} + \frac{g}{2V} \sum_{\mathbf{p}\mathbf{p}'\mathbf{q}} \hat{a}_{\mathbf{p}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{p}'-\mathbf{q}}^\dagger \hat{a}_{\mathbf{p}'} \hat{a}_{\mathbf{p}}, \tag{27}
\end{aligned}$$

where $(\hat{a}_{\mathbf{p}}, \hat{a}_{\mathbf{p}}^\dagger)$ are bosonic annihilation and creation operators respectively. By introducing the cut-off momentum p_c , we can express g (see Appendix.C) as

$$g = \left(\frac{m}{4\pi a} - \frac{p_c}{4\pi^2} \right)^{-1} \tag{28}$$

If we set p_c as $0 \ll p_c \ll \pi m/a$, which can remove the cut-off dependence as

$$g = \frac{4\pi a}{m}. \tag{29}$$

We next introduce the Fourier transformation of \hat{G} as

$$\hat{G}(1, 2) = \sum_{\vec{p}} \hat{G}(\vec{p}) e^{i\vec{p}\cdot\vec{r}}, \tag{30}$$

where $\vec{r} \equiv (\mathbf{r}, i\tau)$, $\vec{p} \equiv (\mathbf{p}, z_\ell)$, and $z_\ell \equiv 2i\pi T\ell$ is the Matsubara frequency, and the summation over \vec{p} is given by

$$\sum_{\vec{p}} \equiv T \sum_{\ell=-\infty}^{\infty} \int \frac{d^3p}{(2\pi)^3}. \tag{31}$$

Function (5) has the following symmetry relations:

$$G_{ij}(\vec{p}) = (-1)^{i+j-1} G_{3-j, 3-i}(-\vec{p}) = (-1)^{i+j} G_{ji}^*(\vec{p}^*). \tag{32}$$

We define matrix Green's function and self-energy by

$$\hat{G}_{\vec{p}} \equiv \begin{bmatrix} G_{11}(\vec{p}) & G_{12}(\vec{p}) \\ G_{21}(\vec{p}) & G_{22}(\vec{p}) \end{bmatrix} = \begin{bmatrix} G_{\vec{p}} & F_{\vec{p}} \\ -F_{\vec{p}} & -G_{\vec{p}} \end{bmatrix}, \tag{33}$$

$$\hat{\Sigma}(\vec{p}) \equiv \begin{bmatrix} \Sigma_{11}(\vec{p}) & \Sigma_{12}(\vec{p}) \\ \Sigma_{21}(\vec{p}) & \Sigma_{22}(\vec{p}) \end{bmatrix} = \begin{bmatrix} \Sigma_{\vec{p}} & \Delta_{\vec{p}} \\ -\Delta_{\vec{p}} & -\bar{\Sigma}_{\vec{p}} \end{bmatrix}, \quad (34)$$

respectively, where lower elements with bars are connected with upper ones generally by

$$\bar{f}_{\vec{p}} = f_{-\vec{p}}^*. \quad (35)$$

We also give the Fourier transform of the vertex $\Gamma^{(0)}(11', 22')$ by

$$\Gamma^{(0)}(\vec{p}, \vec{p}', \vec{q}) = 2g. \quad (36)$$

In these notations, the Dyson-Beliaev equation (14a) can be expressed as

$$\hat{G}(\vec{p}) = \begin{bmatrix} z_{\ell} - \xi_{\mathbf{p}} - \Sigma_{\vec{p}} & -\Delta_{\vec{p}} \\ \Delta_{\vec{p}} & z_{\ell} + \xi_{\mathbf{p}} + \bar{\Sigma}_{\vec{p}} \end{bmatrix}^{-1} = \frac{1}{D_{\vec{p}}} \begin{bmatrix} z_{\ell} + \xi_{\mathbf{p}} + \bar{\Sigma}_{\vec{p}} & \Delta_{\vec{p}} \\ -\Delta_{\vec{p}} & z_{\ell} - \xi_{\mathbf{p}} - \Sigma_{\vec{p}} \end{bmatrix}, \quad (37)$$

where $\xi_{\mathbf{p}} \equiv p^2/2m - \mu$, and $D_{\vec{p}}$ is given by

$$\begin{aligned} D_{\vec{p}} &\equiv (z_{\ell} - \xi_{\mathbf{p}} - \Sigma_{\vec{p}})(z_{\ell} + \xi_{\mathbf{p}} + \bar{\Sigma}_{\vec{p}}) + \Delta_{\vec{p}}\bar{\Delta}_{\vec{p}} \\ &= z_{\ell}^2 - (\Sigma_{\vec{p}} - \bar{\Sigma}_{\vec{p}})z_{\ell} - \left(\xi_{\mathbf{p}} + \frac{\Sigma_{\vec{p}} + \bar{\Sigma}_{\vec{p}}}{2} \right)^2 + \left(\frac{\Sigma_{\vec{p}} - \bar{\Sigma}_{\vec{p}}}{2} \right)^2 + \Delta_{\vec{p}}\bar{\Delta}_{\vec{p}} \\ &= (z_{\ell} - E_{\vec{p}})(z_{\ell} + \bar{E}_{\vec{p}}), \end{aligned} \quad (38)$$

with

$$E_{\vec{p}} \equiv \frac{\Sigma_{\vec{p}} - \bar{\Sigma}_{\vec{p}}}{2} + \left[\left(\xi_{\mathbf{p}} + \frac{\Sigma_{\vec{p}} + \bar{\Sigma}_{\vec{p}}}{2} \right)^2 - \Delta_{\vec{p}}\bar{\Delta}_{\vec{p}} \right]^{1/2}, \quad (39a)$$

$$\bar{E}_{\vec{p}} \equiv \frac{\bar{\Sigma}_{\vec{p}} - \Sigma_{\vec{p}}}{2} + \left[\left(\xi_{\mathbf{p}} + \frac{\Sigma_{\vec{p}} + \bar{\Sigma}_{\vec{p}}}{2} \right)^2 - \Delta_{\vec{p}}\bar{\Delta}_{\vec{p}} \right]^{1/2}. \quad (39b)$$

The Hugenholtz-Pines theorem (14b) reduces to

$$\mu = \Sigma(\vec{0}) - \Delta(\vec{0}). \quad (40)$$

The particle density n is given by

$$n = n_0 - \sum_{\vec{p}} G_{\vec{p}}, \quad (41)$$

where n_0 is the condensate density $\Psi(1) \rightarrow n_0$.

Expressions of $\Sigma_{\vec{p}}$ and $\Delta_{\vec{p}}$ up to second order are written as

$$\begin{aligned} \Sigma_{\vec{p}} &= 2gn + 2[\Xi_{GGG}(\vec{p}) - \Xi_{GFF}(\vec{p})] \\ &\quad + 2gn_0[-2\Pi_{GG}(\vec{p}) - \Pi_{G\bar{G}}(\vec{p}) + 2\Pi_{GF}(\vec{p}) + \Pi_{FF}(\vec{p})] \\ &\quad + 2(gn_0)^2(G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}}) \end{aligned} \quad (42a)$$

$$\begin{aligned} \Delta_{\vec{p}} &= g \left(n_0 - \sum_{\vec{p}} F_{\vec{p}} \right) + 2[\Xi_{FGG}(\vec{p}) - \Xi_{FFF}(\vec{p})] \\ &\quad + 2gn_0[-\Pi_{FG}(\vec{p}) - \Pi_{FG}(-\vec{p}) - \Pi_{GG}(\vec{p}) + 3\Pi_{FF}(\vec{p})] \\ &\quad + 2(gn_0)^2(G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}}), \end{aligned} \quad (42b)$$

where we have introduced

$$\Pi_{GG}(\vec{q}) \equiv g \sum_{\vec{p}} G_{\vec{p}+\vec{q}} G_{\vec{p}} = \Pi_{GG}(-\vec{q}), \quad (43a)$$

$$\Pi_{G\bar{G}}(\vec{q}) \equiv g \sum_{\vec{p}} G_{\vec{p}+\vec{q}} G_{-\vec{p}} = \Pi_{\bar{G}G}(-\vec{q}), \quad (43b)$$

$$\Pi_{FF}(\vec{q}) \equiv g \sum_{\vec{p}} F_{\vec{p}+\vec{q}} F_{\vec{p}} = \Pi_{FF}(-\vec{q}), \quad (43c)$$

$$\Pi_{GF}(\vec{q}) \equiv g \sum_{\vec{p}} G_{\vec{p}+\vec{q}} F_{\vec{p}} = \Pi_{FG}(-\vec{q}), \quad (43d)$$

$$\Xi_{GGG}(\vec{p}) \equiv g \sum_{\vec{q}} G_{\vec{p}+\vec{q}} \Pi_{GG}(\vec{q}), \quad (43e)$$

$$\Xi_{GFF}(\vec{p}) \equiv g \sum_{\vec{q}} G_{\vec{p}+\vec{q}} \Pi_{FF}(\vec{q}), \quad (43f)$$

$$\Xi_{FGG}(\vec{p}) \equiv g \sum_{\vec{q}} F_{\vec{p}+\vec{q}} \Pi_{GG}(\vec{q}), \quad (43g)$$

$$\Xi_{FFF}(\vec{p}) \equiv g \sum_{\vec{q}} F_{\vec{p}+\vec{q}} \Pi_{FF}(\vec{q}). \quad (43h)$$

2 Analysis including 1PR diagrams

A notable prediction of the conserving-gapless theory is that there is a new class of Feynman diagrams [32] for the self-energy, *i.e.*, those that may be classified as one-particle reducible (1PR) following the conventional terminology [4, 20] and should certainly be excluded from its definition in the normal state.

In this section, we will estimate physical quantities by numerical calculation including those 1PR diagrams at $T = 0$. We present the numerical results for energy, condensate density, and lifetime of one-particle excitation.

2.1 Structure of 1PR diagrams

In previous studies, perturbation analysis has been performed by incorporating only irreducible (1PI) structures for the self-energy $\hat{\Sigma}$. Such diagrams are represented in Fig.1. However, as we can see in the previous section and Appendix.A, 1PR diagrams are essential to construct the Luttinger-Ward functional Φ satisfying the Hugenholtz-Pines theorem and conservation laws simultaneously. We note that these 1PR diagrams appear from second order as shown in Fig.2. Those of the second order are proportional to $(G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}})$. In the case of $T = 0$, we only need to consider a specific class of 1PR diagrams, whose structures are proportional to $(G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}})^{m-1}$ every m th-order self-energy, which are given by polygonal structures of $\Phi^{(\text{ip})}$ as shown in Fig.3. The other structures of Φ contribute only $g^m n_0^{m-1} (n - n_0)^1$, which is negligible near $T = 0$ ($n - n_0 \ll 1$). On the other hand, our 1PR diagrams are proportional to $(gn_0)^m$ (see also Eq. (42)). Therefore, we can approximate the functional Φ as

$$\Phi[\hat{G}, \vec{\Psi}] \approx \Phi^{(1)}[\hat{G}, \vec{\Psi}] + \Phi^{(\text{ip})}[\hat{G}, \vec{\Psi}]. \quad (44)$$

We estimate physical quantities containing the first-order self-energy and 1PR structures in the higher-order self-energies up to second and third-order and FLEX approximation. Such functionals are given by

$$\Phi^{(\text{ip})} \approx -V \sum_{\vec{p}} \frac{1}{2} (gn_0 f_{\vec{p}})^2, \quad (45a)$$

$$\Phi^{(\text{ip})} \approx -V \sum_{\vec{p}} \left[\frac{1}{2} (gn_0 f_{\vec{p}})^2 + \frac{5}{3} (gn_0 f_{\vec{p}})^3 \right], \quad (45b)$$

$$\Phi^{(\text{ip})} \approx -V \sum_{\vec{p}} \left[\frac{1}{2} (gn_0 f_{\vec{p}})^2 + \sum_{n=3}^{\infty} \frac{1 + 2^{n-1}}{n} (gn_0 f_{\vec{p}})^n \right], \quad (45c)$$

respectively [35, 45], where $f_{\vec{p}} \equiv (G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}})$. Let us estimate the internal energy \mathcal{E} and the condensate density n_0 in this approximation and compare the results to those by Lee, Huang, Yang [34, 35].

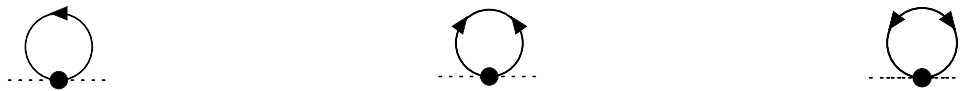


Fig 1: 1PI structures in $\hat{\Sigma}$.



Fig 2: 1PR structures in $\hat{\Sigma}$. These diagrams are characterized by straight line structures. Such structure had never been considered in previous studies.

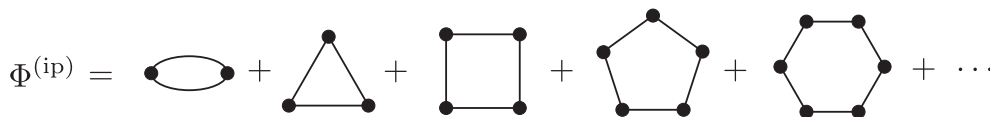


Fig 3: Polygonal structures in Φ . These diagrams have the dominant contribution to physical properties in BEC system for $T \approx 0$.

2.2 First-order analysis

To start with, we calculate the first-order self-energy, and confirm that the results by Bogoliubov [13] and Lee, Huang, Yang [34] can be reproduced appropriately. The first-order Green's functions $G^{(1)}$, $F^{(1)}$ and the self-energies $\Sigma^{(1)}$ and $\Delta^{(1)}$ are given by

$$G_{\vec{p}}^{(1)} \equiv \frac{z_{\ell} + p^2 + \Sigma^{(1)} - \mu^{(1)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta^{(1)})}, \quad (46a)$$

$$F_{\vec{p}}^{(1)} \equiv \frac{\Delta^{(1)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta^{(1)})}, \quad (46b)$$

$$\Sigma^{(1)} \equiv 2gn, \quad (47a)$$

$$\Delta^{(1)} \equiv g \left(n_0 - \sum_{\vec{p}} F_{\vec{p}}^{(1)} \right), \quad (47b)$$

respectively, where the chemical potential $\mu^{(1)}$ is given by

$$\mu^{(1)} \equiv \Sigma^{(1)} - \Delta^{(1)}. \quad (48)$$

Using Eq. (37), we can transform $G_{\vec{p}}^{(1)}$, $F_{\vec{p}}^{(1)}$ as

$$\begin{aligned} G_{\vec{p}}^{(1)} &= \frac{z_\ell + p^2 + \Delta^{(1)}}{(z_\ell - p\sqrt{p^2 + 2\Delta^{(1)}})(z_\ell + p\sqrt{p^2 + 2\Delta^{(1)}})} \\ &= \frac{1}{2E_{\mathbf{p}}^{(1)}} \left(\frac{p^2 + \Delta^{(1)} + E_{\mathbf{p}}^{(1)}}{z_\ell - E_{\mathbf{p}}^{(1)}} - \frac{p^2 + \Delta^{(1)} - E_{\mathbf{p}}^{(1)}}{z_\ell + E_{\mathbf{p}}^{(1)}} \right) \end{aligned} \quad (49a)$$

$$\begin{aligned} F_{\vec{p}}^{(1)} &= \frac{\Delta^{(1)}}{(z_\ell - p\sqrt{p^2 + 2\Delta^{(1)}})(z_\ell + p\sqrt{p^2 + 2\Delta^{(1)}})} \\ &= \frac{\Delta^{(1)}}{2E_{\mathbf{p}}^{(1)}} \left(\frac{1}{z_\ell - E_{\mathbf{p}}^{(1)}} - \frac{1}{z_\ell + E_{\mathbf{p}}^{(1)}} \right), \end{aligned} \quad (49b)$$

where $E_{\mathbf{p}}^{(1)}$ corresponds to the Bogoliubov mode as

$$E_{\mathbf{p}}^{(1)} \equiv p\sqrt{p^2 + 2\Delta^{(1)}}. \quad (50)$$

Summing over \vec{p} for Eq. (49), we obtain

$$\begin{aligned} \sum_{\vec{p}} G_{\vec{p}}^{(1)} &= \int \frac{d^3p}{(2\pi)^3} \int_C \frac{dz}{2\pi i} \frac{\bar{n}(z)}{2E_{\mathbf{p}}^{(1)}} \left(\frac{p^2 + \Delta^{(1)} + E_{\mathbf{p}}^{(1)}}{z - E_{\mathbf{p}}^{(1)}} - \frac{p^2 + \Delta^{(1)} - E_{\mathbf{p}}^{(1)}}{z + E_{\mathbf{p}}^{(1)}} \right) \\ &= - \int \frac{d^3p}{(2\pi)^3} \left[\frac{p^2 + \Delta^{(1)} + E_{\mathbf{p}}^{(1)}}{2E_{\mathbf{p}}^{(1)}} \bar{n}(E_{\mathbf{p}}^{(1)}) + \frac{p^2 + \Delta^{(1)} - E_{\mathbf{p}}^{(1)}}{2E_{\mathbf{p}}^{(1)}} (1 + \bar{n}(E_{\mathbf{p}}^{(1)})) \right] \\ &= - \frac{1}{2\pi^2} \int_0^\infty dp p^2 \left[\frac{p^2 + \Delta^{(1)}}{E_{\mathbf{p}}^{(1)}} \bar{n}(E_{\mathbf{p}}^{(1)}) + \frac{p^2 + \Delta^{(1)} - E_{\mathbf{p}}^{(1)}}{E_{\mathbf{p}}^{(1)}} \right] \\ &= - \frac{1}{4\pi^2} \int_0^\infty d\epsilon \epsilon^{1/2} \left[\frac{\epsilon + \Delta^{(1)}}{\sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}} \bar{n}(E_{\mathbf{p}}^{(1)}) + \frac{\epsilon + \Delta^{(1)} - \sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}}{2\sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}} \right], \end{aligned} \quad (51a)$$

$$\begin{aligned} \sum_{\vec{p}} F_{\vec{p}}^{(1)} &= \int \frac{d^3p}{(2\pi)^3} \int_C \frac{dz}{2\pi i} \frac{\bar{n}(z)\Delta^{(1)}}{2E_{\mathbf{p}}^{(1)}} \left(\frac{1}{z - E_{\mathbf{p}}^{(1)}} - \frac{1}{z + E_{\mathbf{p}}^{(1)}} \right) \\ &= - \int \frac{d^3p}{(2\pi)^3} \frac{\bar{n}(z)\Delta^{(1)}}{2E_{\mathbf{p}}^{(1)}} [1 + 2\bar{n}(E_{\mathbf{p}}^{(1)})] \\ &= - \frac{1}{2\pi^2} \int_0^{p_c} dp p^2 \frac{\Delta^{(1)}}{2E_{\mathbf{p}}^{(1)}} [1 + 2\bar{n}(E_{\mathbf{p}}^{(1)})] \\ &= - \frac{1}{4\pi^2} \int_0^{p_c^2} d\epsilon \epsilon^{1/2} \frac{\Delta^{(1)}}{\sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}} \left[\frac{1}{2} + \bar{n}(E_{\mathbf{p}}^{(1)}) \right]. \end{aligned} \quad (51b)$$

where $\bar{n}(z) \equiv (e^{\beta z} - 1)^{-1}$ and the integral path C has been taken as Fig.4 [43, 44].

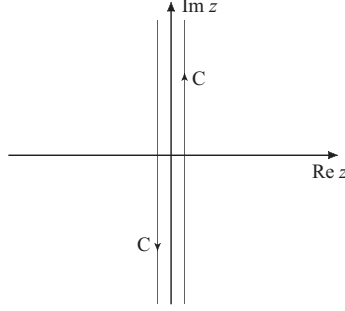


Fig 4: integration path C

Taking the limit $T \rightarrow 0$ for Eq. (51) gives the following:

$$\begin{aligned}
\sum_{\vec{p}} G_{\vec{p}}^{(1)} &\xrightarrow{T \rightarrow 0} -\frac{1}{4\pi^2} \int_0^\infty d\epsilon \epsilon^{1/2} \frac{\epsilon + \Delta^{(1)} - \sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}}{2\sqrt{\epsilon(\epsilon + 2\Delta^{(1)})}} \\
&= -\frac{(2\Delta^{(1)})^{3/2}}{8\pi^2} \int_0^\infty dx \left(\frac{x+1}{\sqrt{x+2}} - x^{1/2} \right) \\
&= -\frac{(2\Delta^{(1)})^{3/2}}{8\pi^2} \int_0^\infty dx \left[(x+2)^{1/2} - \frac{1}{(x+2)^{1/2}} - x^{1/2} \right] \\
&= -\frac{(2\Delta^{(1)})^{3/2}}{8\pi^2} \left[\frac{2}{3}(x+2)^{3/2} - 2(x+2)^{1/2} - \frac{2}{3}x^{3/2} \right] \\
&= -\frac{(2\Delta^{(1)})^{3/2}}{24\pi^2}, \tag{52a}
\end{aligned}$$

$$\sum_{\vec{p}} F_{\vec{p}}^{(1)} \xrightarrow{T \rightarrow 0} -\frac{\Delta^{(1)}}{8\pi^2} \int_0^{p_c^2} d\epsilon \epsilon^{1/2} \frac{1}{\sqrt{\epsilon + 2\Delta^{(1)}}} \approx -\frac{\Delta^{(1)}}{4\pi^2} (p_c - \sqrt{2\Delta^{(1)}}) = -\frac{\Delta^{(1)}}{4\pi^2} p_c + \frac{(\Delta^{(1)})^{3/2}}{8\pi^2}. \tag{52b}$$

By using these, Eq. (47) can be transformed as

$$\frac{n_0}{n} = 1 - \frac{(2\Delta^{(1)})^{3/2}}{24\pi^2 n}, \Delta^{(1)} = g \left[n_0 + \frac{\Delta^{(1)}}{4\pi^2} p_c - \frac{(2\Delta^{(1)})^{3/2}}{8\pi^2} \right] = gn \left[\frac{n_0}{n} + \frac{\Delta^{(1)}}{4\pi^2 n} p_c - \frac{(2\Delta^{(1)})^{3/2}}{8\pi^2 n} \right]. \tag{53}$$

Considering Eq. (28), we obtain

$$\Sigma^{(1)} \approx 16\pi an \left(1 + \frac{1}{\pi} p_c a \right), \tag{54a}$$

$$\begin{aligned}
\Delta^{(1)} &\approx 8\pi an \left(1 + \frac{2}{\pi} p_c a \right) \left[1 - \frac{2\Delta^{(1)}}{24\pi^2 n} + \frac{\Delta^{(1)}}{4\pi^2 n} p_c - \frac{(2\Delta^{(1)})^{3/2}}{8\pi^2 n} \right] \\
&\approx 8\pi an \left(1 + \frac{2}{\pi} p_c a \right) \left[1 + \frac{8\pi na}{4\pi^2 n} - \frac{(16\pi an)^{3/2}}{6\pi^2 n} \right] \\
&\approx 8\pi an \left[1 + \frac{4}{\pi} p_c a - \frac{32}{3\sqrt{\pi}} a^{3/2} n^{1/2} \right]. \tag{54b}
\end{aligned}$$

Substituting them into Eqs. (53) and (48), we obtain

$$\frac{n_0}{n} \approx 1 - \frac{(16\pi an)^{3/2}}{24\pi^2 n} = 1 - \frac{8}{3\sqrt{\pi}} \sqrt{na^3} \approx 1 - 1.504\sqrt{na^3}, \tag{55}$$

$$\mu^{(1)} = 8\pi an \left(1 + \frac{32}{3\pi^{1/2}} \sqrt{na^3} \right) \quad (56)$$

respectively. By using $\mu = \partial\mathcal{E}/\partial N$, we thereby obtain

$$\frac{\mathcal{E}^{(1)}}{N} \approx 4\pi an \left(1 + \frac{128}{15\sqrt{\pi}} \sqrt{na^3} \right) \approx 4\pi an \left(1 + 4.815\sqrt{na^3} \right). \quad (57)$$

We conclude that the first-order analysis reproduces the results by Lee, Huang, Yang [34].

2.3 Discussion for second order

We now construct Green's function containing 1PR diagrams up to second order. Using Eq. (47) and (45a), we obtain $\Sigma_{\vec{p}}^{(2)}$ and $\Delta_{\vec{p}}^{(2)}$

$$\Sigma_{\vec{p}}^{(2)} = \Sigma^{(1)} + \Delta_{\vec{p}}^{(2c)}, \quad (58a)$$

$$\Delta_{\vec{p}}^{(2)} = \Delta^{(1)} + \Delta_{\vec{p}}^{(2c)}, \quad (58b)$$

respectively, where $\Delta_{\vec{p}}^{(2c)}$ is defined by Eq. (42) as

$$\Delta_{\vec{p}}^{(2c)} \equiv 2(gn_0)^2 (G_{\vec{p}} + G_{-\vec{p}} - 2F_{\vec{p}}) = \Delta_{-\vec{p}}^{(2c)}. \quad (59)$$

The chemical potential $\mu^{(2)} = \Sigma^{(1)} - \Delta^{(1)}$ is equal to that of first-order Eq. (48).

The second-order Green's functions $G_{\vec{p}}^{(2)}$, $F_{\vec{p}}^{(2)}$ are expressible as

$$G_{\vec{p}}^{(2)} = \frac{z_\ell + p^2 + \Delta_{\vec{p}}^{(2)}}{z_\ell^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(2)})}, \quad (60a)$$

$$F_{\vec{p}}^{(2)} = \frac{z_\ell + p^2 + \Delta_{\vec{p}}^{(2)}}{z_\ell^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(2)})}, \quad (60b)$$

respectively.

Introducing $f_{\vec{p}}^{(2)} \equiv (G_{\vec{p}}^{(2)} + G_{-\vec{p}}^{(2)} - 2F_{\vec{p}}^{(2)})$ and using Eq. (60), we obtain

$$f_{\vec{p}}^{(2)} = \frac{2p^2}{z_\ell^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(2)})} = \frac{1}{\eta_{\vec{p}} - \Delta_{\vec{p}}^{(2c)}}, \quad (61)$$

where $\eta_{\vec{p}}$ is defined by

$$\eta_{\vec{p}} \equiv \frac{z_\ell^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(1)})}{2p^2}. \quad (62)$$

Thus we can construct a self-consistent equation for $\Delta_{\vec{p}}^{(2c)}$ by using Eq. (59) as

$$\Delta_{\vec{p}}^{(2c)} = \frac{2(gn_0)^2}{\eta_{\vec{p}} - \Delta_{\vec{p}}^{(2c)}}, \quad (63)$$

which reduces to the following quadratic equation:

$$(\Delta_{\vec{p}}^{(2c)})^2 - \eta_{\vec{p}}\Delta_{\vec{p}}^{(2c)} + 2(gn_0)^2 = 0. \quad (64)$$

Noting this equation contain only real coefficients and $\Delta^{(1)} \approx gn_0$, we can't find a solution which satisfies the symmetry relation (59). Therefore, we need to include higher-order contribution to self-energies.

2.4 Construction of third-order equations

We here include third-order 1PR diagrams whose numerical weights were given by [30]. We also choose series of the straight line diagrams. Such self-energies $\Sigma_{\bar{p}}^{(3)}$, $\Delta_{\bar{p}}^{(3)}$ and Green's functions $G_{\bar{p}}^{(3)}$, $F_{\bar{p}}^{(3)}$ can be written by

$$\Sigma_{\bar{p}}^{(3)} = \Sigma^{(1)} + \Delta_{\bar{p}}^{(2c)} + \Delta_{\bar{p}}^{(3c)} \equiv \Sigma^{(1)} + \tilde{\Delta}_{\bar{p}}^{(3c)}, \quad (65a)$$

$$\Delta_{\bar{p}}^{(3)} = \Delta^{(1)} + \Delta_{\bar{p}}^{(2c)} + \Delta_{\bar{p}}^{(3c)} \equiv \Delta^{(1)} + \tilde{\Delta}_{\bar{p}}^{(3c)}, \quad (65b)$$

and

$$G_{\bar{p}}^{(3)} = \frac{z_{\ell} + p^2 + \Delta_{\bar{p}}^{(3)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta_{\bar{p}}^{(3)})} \quad (66a)$$

$$F_{\bar{p}}^{(3)} = \frac{z_{\ell} + p^2 + \Delta_{\bar{p}}^{(3)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta_{\bar{p}}^{(3)})} \quad (66b)$$

respectively, where $\tilde{\Delta}_{\bar{p}}^{(3c)}$ can be represented by using Eq. (45b) as

$$\tilde{\Delta}_{\bar{p}}^{(3c)} \equiv 2(gn_0)^2 f_{\bar{p}}^{(3)} + \frac{5}{4}(2gn_0)^3 (f_{\bar{p}}^{(3)})^2, \quad (67)$$

with $f_{\bar{p}}^{(3)} \equiv (G_{\bar{p}}^{(3)} + G_{-\bar{p}}^{(3)} - 2F_{\bar{p}}^{(3)})$.

By using $\eta_{\bar{p}}$, the equation for $\tilde{\Delta}_{\bar{p}}^{(3c)}$ is given by

$$(\tilde{\Delta}_{\bar{p}}^{(3c)})^3 - 2\eta_{\bar{p}}(\tilde{\Delta}_{\bar{p}}^{(3c)})^2 + [\eta_{\bar{p}}^2 + 2(gn_0)^2]\tilde{\Delta}_{\bar{p}}^{(3c)} - 2(gn_0)^2(\eta_{\bar{p}} + 5gn_0) = 0, \quad (68)$$

which is a cubic equation. So, there is a real solution with $\tilde{\Delta}_{\bar{p}}^{(3c)}$ at least.

Here we perform the following transformation:

$$x_{\bar{p}} \equiv \tilde{\Delta}_{\bar{p}}^{(3c)}/gn_0, \quad (69)$$

$$a_{\bar{p}} \equiv \eta_{\bar{p}}/gn_0. \quad (70)$$

Equation (68) can be transformed into

$$x_{\bar{p}}^3 - 2a_{\bar{p}}x_{\bar{p}}^2 + (a_{\bar{p}}^2 + 2)x_{\bar{p}} - 2(a_{\bar{p}} + 5) = 0. \quad (71)$$

We can solve the equation by using the Cardano formula as

$$x_{\bar{p}} = \begin{cases} \frac{2}{3}a_{\bar{p}} + \left(-b_0 + \sqrt{b_0^2 + b_1^3}\right)^{1/3} + \left(-b_0 - \sqrt{b_0^2 + b_1^3}\right)^{1/3} & : |a_{\bar{p}}| \geq \sqrt{6} \\ \frac{2}{3}a_{\bar{p}} + \left(-b_0 + \sqrt{b_0^2 + b_1^3}\right)^{1/3} - \left(b_0 + \sqrt{b_0^2 + b_1^3}\right)^{1/3} & : |a_{\bar{p}}| < \sqrt{6}, \end{cases} \quad (72)$$

where

$$b_1 \equiv \frac{3(a_{\bar{p}}^2 + 2) - (-2a_{\bar{p}})^2}{9} = \frac{-a_{\bar{p}}^2 + 6}{9}, \quad (73)$$

$$b_0 \equiv \frac{27(-2)(a_{\bar{p}} + 5) - 9(-2a_{\bar{p}})(a_{\bar{p}}^2 + 2) + 2(-2a_{\bar{p}})^3}{54} = \frac{a_{\bar{p}}^3 - 9a_{\bar{p}} - 135}{27}, \quad (74)$$

respectively.

2.5 Equations for FLEX approximation

We next consider the case of the FLEX approximation. Self-energies $\Sigma_{\vec{p}}^{(Fc)}$, $\Delta_{\vec{p}}^{(Fc)}$ and Green's functions are given by

$$\Sigma_{\vec{p}}^{(Fc)} = \Sigma^{(1)} + \Delta_{\vec{p}}^{(Fc)}, \quad (75a)$$

$$\Delta_{\vec{p}}^{(Fc)} = \Delta^{(1)} + \Delta_{\vec{p}}^{(Fc)}, \quad (75b)$$

$$G_{\vec{p}}^{(Fc)} = \frac{z_{\ell} + p^2 + \Delta_{\vec{p}}^{(Fc)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(Fc)})}, \quad (76a)$$

$$F_{\vec{p}}^{(Fc)} = \frac{z_{\ell} + p^2 + \Delta_{\vec{p}}^{(Fc)}}{z_{\ell}^2 - p^2(p^2 + 2\Delta_{\vec{p}}^{(Fc)})}. \quad (76b)$$

The n th-order term of $\Delta_{\vec{p}}^{(Fc)}$ can be written by using Eqs. (67) and (45c) as

$$\Delta_{\vec{p}}^{(nc)} = \left(1 + \frac{1}{2^{n-1}}\right) (2gn_0)^n f_{\vec{p}}^{n-1} \quad (n \geq 3), \quad (77)$$

where $f_{\vec{p}}^{(Fc)}$ is defined by $f_{\vec{p}}^{(Fc)} \equiv (G_{\vec{p}}^{(Fc)} + G_{-\vec{p}}^{(Fc)} - 2F_{\vec{p}}^{(Fc)})$. Using Eqs. (59) and (77), we can transform it as

$$\begin{aligned} \Delta_{\vec{p}}^{(Fc)} &\equiv \Delta_{\vec{p}}^{(2c)} + \sum_{n=3}^{\infty} \Delta_{\vec{p}}^{(nc)} = 2(gn_0)^2 f_{\vec{p}}^{(Fc)} + \sum_{n=3}^{\infty} [(2gn_0)^n + 2(gn_0)^n] (f_{\vec{p}}^{(Fc)})^{n-1} \\ &= \frac{(2gn_0)^2 f_{\vec{p}}^{(Fc)}}{1 - 2gn_0 f_{\vec{p}}^{(Fc)}} + \frac{2(gn_0)^2 f_{\vec{p}}^{(Fc)}}{1 - gn_0 f_{\vec{p}}^{(Fc)}} - 4(gn_0)^2 f_{\vec{p}}^{(Fc)} \\ &= \frac{(2gn_0)^2}{\eta_{\vec{p}} - 2gn_0 - \Delta_{\vec{p}}^{(Fc)}} + \frac{2(gn_0)^2}{\eta_{\vec{p}} - gn_0 - \Delta_{\vec{p}}^{(Fc)}} - \frac{4(gn_0)^2}{\eta_{\vec{p}} - \Delta_{\vec{p}}^{(Fc)}}, \end{aligned} \quad (78)$$

where we have used $f_{\vec{p}}^{-1} = \eta_{\vec{p}} - \Delta_{\vec{p}}^{(Fc)}$. We then find that the equation for $\Delta_{\vec{p}}^{(Fc)}$ forms the fourth-order equation:

$$\begin{aligned} 0 &= -\Delta_{\vec{p}}^{(Fc)} (\eta_{\vec{p}} - 2gn_0 - \Delta_{\vec{p}}^{(Fc)}) (\eta_{\vec{p}} - gn_0 - \Delta_{\vec{p}}^{(Fc)}) (\eta_{\vec{p}} - \Delta_{\vec{p}}^{(Fc)}) \\ &\quad + 2(gn_0)^2 [2(\eta_{\vec{p}} - gn_0 - \Delta_{\vec{p}}^{(Fc)}) (\eta_{\vec{p}} - \Delta_{\vec{p}}^{(Fc)}) + (\eta_{\vec{p}} - 2gn_0 - \Delta_{\vec{p}}^{(Fc)}) (\eta_{\vec{p}} - \Delta_{\vec{p}}^{(Fc)}) \\ &\quad - 2(\eta_{\vec{p}} - 2gn_0 - \Delta_{\vec{p}}^{(Fc)}) (\eta_{\vec{p}} - gn_0 - \Delta_{\vec{p}}^{(Fc)})] \\ &= (\Delta_{\vec{p}}^{(Fc)})^4 - 3(\eta_{\vec{p}} - gn_0) (\Delta_{\vec{p}}^{(Fc)})^3 + [3\eta_{\vec{p}}^2 - 6gn_0\eta_{\vec{p}} + 4(gn_0)^2] (\Delta_{\vec{p}}^{(Fc)})^2 \\ &\quad - [\eta_{\vec{p}}^3 - 3gn_0\eta_{\vec{p}}^2 + 6(gn_0)^2\eta_{\vec{p}} + 4(gn_0)^3] \Delta_{\vec{p}}^{(Fc)} + 2(gn_0)^2 [\eta_{\vec{p}}^2 + 2gn_0\eta_{\vec{p}} - 4(gn_0)^2]. \end{aligned} \quad (79)$$

By introducing $\tilde{x}_{\vec{p}} \equiv \Delta_{\vec{p}}^{(Fc)}/gn_0$ and using $a_{\vec{p}}$ defined by Eq. (70), we can write down as

$$\tilde{x}_{\vec{p}}^4 - 3(a_{\vec{p}} - 1)\tilde{x}_{\vec{p}}^3 + (3a_{\vec{p}}^2 - 6a_{\vec{p}} + 4)\tilde{x}_{\vec{p}}^2 - (a_{\vec{p}}^3 - 3a_{\vec{p}}^2 + 6a_{\vec{p}} + 4)\tilde{x}_{\vec{p}} + 2(a_{\vec{p}}^2 + 2a_{\vec{p}} - 4) = 0. \quad (80)$$

Considering $a_{\vec{p}} \rightarrow -1$ for $|\vec{p}| \rightarrow 0$, a function $h(x) \equiv x^4 - 6x^3 + 13x^2 + 6x - 10$ satisfies $h(0) = -10 < 0$ for the limit $h(|x| \rightarrow \infty) \rightarrow \infty$. So, we can find there is a real solution in Eq. (80) for $a_{\vec{p}}$.

3 Numerical results at $T = 0$

We now present the results of including 1PR diagrams for $T = 0$. We perform the calculation for the third-order and the FLEX approximations which are introduced in the previous section.

At first, we will discuss the energy per particle \mathcal{E}/N . 1PR diagrams add an extra term c_{ip} to the result by Lee, Huang, Yang [34]. Next, we estimate a lifetime of the one-particle excitation by using the one-particle spectral function $A_{\mathbf{p}}(\omega)$. We will see the one-particle excitation for BEC has a finite lifetime proportional to s -wave scattering length a .

3.1 Energy per particle

In this subsection, we first explain how to calculate the energy per particle in the third-order and the FLEX approximations. So, we introduce the self-energies $\bar{\Sigma}_{\vec{p}}$ and $\bar{\Delta}_{\vec{p}}$ by using first-order self-energies in Eq. (47) and its correction term $\Delta_{\vec{p}}^{(c)}$ as

$$\bar{\Sigma}_{\vec{p}} = \Sigma^{(1)} + \Delta_{\vec{p}}^{(c)}, \quad (81a)$$

$$\bar{\Delta}_{\vec{p}} = \Delta^{(1)} + \Delta_{\vec{p}}^{(c)}. \quad (81b)$$

We also express the corresponding Matsubara Green's functions by $\bar{G}_{\vec{p}}$, and $\bar{F}_{\vec{p}}$. Using first-order Green's functions in Eq. (46), we define difference functions for $\bar{G}_{\vec{p}}$, and $\bar{F}_{\vec{p}}$ as

$$\Delta\bar{G}_{\vec{p}} \equiv \bar{G}_{\vec{p}} - G_{\vec{p}}^{(1)}, \quad (82a)$$

$$\Delta\bar{F}_{\vec{p}} \equiv \bar{F}_{\vec{p}} - F_{\vec{p}}^{(1)}, \quad (82b)$$

respectively. We hence obtain

$$\bar{G}_{\vec{p}} = G_{\vec{p}}^{(1)} + \Delta\bar{G}_{\vec{p}}, \quad (83a)$$

$$\bar{F}_{\vec{p}} = F_{\vec{p}}^{(1)} + \Delta\bar{F}_{\vec{p}}. \quad (83b)$$

We can express the correction terms for non condensate density $\Delta\bar{n}^{(nc)}$ and the summation of $F_{\vec{p}}^{(1)}$ over \vec{p} , $\Delta\bar{F}_{\text{sum}}$ as

$$\begin{aligned} n^{(nc)} &= \sum_{\vec{p}} \bar{G}_{\vec{p}} = \sum_{\vec{p}} G_{\vec{p}}^{(1)} + \Delta\bar{n}^{(nc)} \\ &\equiv n^{(1)} + \Delta\bar{n}^{(nc)} \approx \frac{8}{3\sqrt{\pi}} a^{3/2} n^{3/2} + \Delta n^{(nc)}, \end{aligned} \quad (84a)$$

$$\sum_{\vec{p}} \bar{F}_{\vec{p}} = \sum_{\vec{p}} F_{\vec{p}}^{(1)} + \Delta\bar{F}_{\text{sum}}, \quad (84b)$$

where $n^{(1)}$ is the non condensate density of the first order as seen in Eq. (55). We note that the summations of $\Delta\bar{G}_{\vec{p}}$, $\Delta\bar{F}_{\vec{p}}$ are free from unphysical ultraviolet divergences for $\mathbf{p} \rightarrow 0$. So, we can replace $\Delta^{(1)}$ in $\Delta\bar{n}^{(nc)}$ and ΔF_{sum} in Eq. (84) as $\bar{g}n_0^{(1)} \equiv 8\pi a n_0^{(1)}$, and can ignore the p_c dependence in the summation over \vec{p} (taking the limit $p_c \rightarrow \infty$). Therefore, we can rewrite the summation over \vec{p} for $T \rightarrow 0$ as

$$\sum_{\vec{p}} \xrightarrow{T \rightarrow 0} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int \frac{d^3p}{(2\pi)^3} = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d\omega \int_0^{\infty} de \sqrt{e},$$

where the Matsubara frequency $i\epsilon_\ell$ and the one-particle kinetic energy p^2 are replaced by $i\omega$ and e respectively. Next we take the following transformation for ω and e :

$$\bar{\omega} = \omega/\bar{g}n_0^{(1)}, \quad \bar{e} = e/\bar{g}n_0^{(1)}.$$

Introducing

$$x_{\vec{p}} \equiv \bar{x}_{\bar{e}, i\bar{\omega}} = \Delta_{\vec{p}}^{(c)}/\bar{g}n_0^{(1)}, \quad (85)$$

we can transform $\Delta\bar{n}^{(nc)}$ and ΔF_{sum} as

$$\begin{aligned} \Delta\bar{n}^{(nc)} &= - \sum_{\vec{p}} \left(\frac{z_\ell + p^2 + \Delta_{\vec{p}}}{z_\ell^2 - p^2(p^2 + 2\Delta_{\vec{p}})} - \frac{z_\ell + p^2 + \Delta^{(1)}}{z_\ell^2 - p^2(p^2 + 2\Delta^{(1)})} \right) \\ &= - \frac{(\bar{g}n_0^{(1)})^{3/2}}{(2\pi)^3} \int_{-\infty}^{\infty} d\bar{\omega} \int_0^{\infty} d\bar{e} \sqrt{\bar{e}} \left(\frac{i\bar{\omega} + \bar{e} + 1 + \bar{x}_{\bar{e}, i\bar{\omega}}}{-\bar{\omega}^2 - \bar{e}\{\bar{e} + 2(1 + \bar{x}_{\bar{e}, i\bar{\omega}})\}} - \frac{i\bar{\omega} + \bar{e} + 1}{-\bar{\omega}^2 - \bar{e}(\bar{e} + 2)} \right) \\ &= (8\pi a n_0^{(1)})^{3/2} \times I_{\bar{G}} \approx (8\pi a n)^{3/2} \times I_{\bar{G}}, \end{aligned} \quad (86a)$$

$$\begin{aligned}
\Delta F_{\text{sum}} &= \sum_{\bar{p}} \left(\frac{\Delta_{\bar{p}}}{z_{\bar{p}}^2 - p^2(p^2 + 2\Delta_{\bar{p}})} - \frac{\Delta^{(1)}}{z_{\bar{p}}^2 - p^2(p^2 + 2\Delta^{(1)})} \right) \\
&= \frac{(\bar{g}n_0^{(1)})^{3/2}}{(2\pi)^3} \int_{-\infty}^{\infty} d\bar{\omega} \int_0^{\infty} d\bar{e} \sqrt{\bar{e}} \left(\frac{1 + \bar{x}_{\bar{e},i\bar{\omega}}}{-\bar{\omega}^2 - \bar{e}\{\bar{e} + 2(1 + \bar{x}_{\bar{e},i\bar{\omega}})\}} - \frac{1}{-\bar{\omega}^2 - \bar{e}(\bar{e} + 2)} \right) \\
&= (8\pi an_0^{(1)})^{3/2} \times I_{\bar{F}} \approx (8\pi an)^{3/2} \times I_{\bar{F}}
\end{aligned} \tag{86b}$$

respectively, where we have used Eq. (55) and $n_0 \approx n$ in the last equality, and also introduced

$$I_{\bar{G}} \equiv -\frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d\bar{\omega} \int_0^{\infty} d\bar{e} \sqrt{\bar{e}} \left(\frac{i\bar{\omega} + \bar{e} + 1 + \bar{x}_{\bar{e},i\bar{\omega}}}{-\bar{\omega}^2 - \bar{e}\{\bar{e} + 2(1 + \bar{x}_{\bar{e},i\bar{\omega}})\}} - \frac{i\bar{\omega} + \bar{e} + 1}{-\bar{\omega}^2 - \bar{e}(\bar{e} + 2)} \right), \tag{87a}$$

$$I_{\bar{F}} \equiv \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d\bar{\omega} \int_0^{\infty} d\bar{e} \sqrt{\bar{e}} \left(\frac{1 + \bar{x}_{\bar{e},i\bar{\omega}}}{-\bar{\omega}^2 - \bar{e}\{\bar{e} + 2(1 + \bar{x}_{\bar{e},i\bar{\omega}})\}} - \frac{1}{-\bar{\omega}^2 - \bar{e}(\bar{e} + 2)} \right). \tag{87b}$$

Therefore, we can express the condensate density \bar{n}_0 as

$$\begin{aligned}
\frac{\bar{n}_0}{n} &= \frac{(n - n^{(1)} - \Delta\bar{n}^{(nc)})}{n} \\
&= 1 - \left(\frac{8}{3\sqrt{\pi}} + (8\pi)^{3/2} \times (I_{\bar{G}} + I_{\bar{F}}) \right) \sqrt{na^3} \\
&\equiv 1 - \left(\frac{8}{3\sqrt{\pi}} + c_{ip} \right) \sqrt{na^3},
\end{aligned} \tag{88}$$

where c_{ip} is defined by

$$c_{ip} \equiv \frac{4\sqrt{2}}{\pi^{3/2}} \int_0^{\infty} d\bar{\omega} \int_0^{\infty} d\bar{e} \frac{(\bar{\omega}^2 - \bar{e}^2)\bar{x}_{\bar{e},i\bar{\omega}}}{[\bar{\omega}^2 + \bar{e}(\bar{e} + 2\bar{x}_{\bar{e},i\bar{\omega}})][\bar{\omega}^2 + \bar{e}(\bar{e} + 2\bar{x}_{\bar{e},i\bar{\omega}})]}. \tag{89}$$

The chemical potential $\bar{\mu}$ is also given by

$$\begin{aligned}
\bar{\mu} = \Sigma^{(1)} - \Delta^{(1)} &= gn \left\{ 1 - \frac{1}{n} \sum_{\bar{p}} \left(G_{\bar{p}}^{(1)} - F_{\bar{p}}^{(1)} \right) - \frac{1}{n} \sum_{\bar{p}} \left(\Delta\bar{G}_{\bar{p}} - \Delta\bar{F}_{\bar{p}} \right) \right\} \\
&= \mu^{(1)} - g \sum_{\bar{p}} \left(\Delta\bar{G}_{\bar{p}} - \Delta\bar{F}_{\bar{p}} \right) \\
&\approx \mu^{(1)} + \bar{g}(\bar{g}n)^{3/2} (I_{\bar{G}} + I_{\bar{F}}) \\
&\approx 8\pi an \left[1 + \left(\frac{32}{3\sqrt{\pi}} + c_{ip} \right) n^{1/2} a^{3/2} \right],
\end{aligned} \tag{90}$$

where we have used Eq. (56) and

$$\begin{aligned}
\Delta^{(1)} &= g \left(n_0 - \sum_{\bar{p}} \bar{F}_{\bar{p}} \right) \\
&= gn \left\{ 1 + \frac{1}{n} \sum_{\bar{p}} \left(\bar{G}_{\bar{p}} - \bar{F}_{\bar{p}} \right) \right\} \\
&= gn \left\{ 1 + \frac{1}{n} \sum_{\bar{p}} \left(G_{\bar{p}}^{(1)} - F_{\bar{p}}^{(1)} \right) + \frac{1}{n} \sum_{\bar{p}} \left(\Delta\bar{G}_{\bar{p}} - \Delta\bar{F}_{\bar{p}} \right) \right\}.
\end{aligned} \tag{91}$$

We hence obtain the energy per particle $\bar{\mathcal{E}}/N$ as

$$\frac{\bar{\mathcal{E}}}{N} = 4\pi an \left[1 + \frac{16}{5} \left(\frac{8}{3\sqrt{\pi}} + c_{ip} \right) \sqrt{na^3} \right]. \tag{92}$$

We here present numerical results for c_{ip} in each approximation, which can be obtained as

$$c_{ip}^{(3)} = 0.412, \quad c_{ip}^{(F)} = 0.563, \quad (93)$$

where superscripts (3) and (F) denote the third-order and FLEX approximations respectively [35].

Thus c_{ip} for the two approximations are both of order 1. The exact value of c_{ip} can only be obtained by collecting all the leading-order 1PR terms, however, meaning that further studies are required for a quantitative estimate of c_{ip} . On the other hand, a diffusion Monte Carlo study [47] was performed on Eq. (57); the data in Table I for $na^3 \leq 10^{-2}$ yield the value 4.3(1), rather than $128/15\sqrt{\pi} = 4.815$ from Eq. (57), thus showing a clear deviation from the Lee-Huang-Yang expression beyond the numerical uncertainty. However, the exact estimation of the energy by the diffusion Monte Carlo simulation needs certain approximations for removing finite size effects [37] (see also Appendix.B.3). On the other hand, an experiment on Eq. (57) in a trap potential [48] reported a value 4.5(7), which still requires improvement.

3.2 Lifetime of one-particle excitation

We here estimate lifetime of the one-particle excitation in BEC system by using the conserving-gapless theory. The one-particle spectral function is obtained by performing the analytic continuation for $G_{\vec{p}}$ from imaginary axis to real axis:

$$A_p(\omega) = -2 \operatorname{Im} G_{\vec{p}} \Big|_{z_\ell \rightarrow \omega + i\eta}. \quad (94)$$

The resultant values on the imaginary axis are used subsequently to calculate Eq. (94) based on Thiele's reciprocal difference algorithm for Padé approximation [49]. Function $A_p(\omega)$ thereby calculated can be checked numerically with a couple of exact relations as

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} A_p(\omega) = 1, \quad (95a)$$

$$G_{\vec{p}} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A_p(\omega)}{z_\ell - \omega}. \quad (95b)$$

We have confirmed that sum rule Eq. (95a) is satisfied beyond 99.7% and Green's function on the imaginary axis are reproduced with an error of less than 0.02%.

To begin with, let us review the spectral function of the Bogoliubov theory, which is obtained by inserting Eq. (46) into Eq. (94). It yields

$$A_p^{(1)}(\omega) = \pi[(\alpha_p + 1)\delta(\omega - E_{\mathbf{p}}^{(B)}) - (\alpha_p - 1)\delta(\omega + E_{\mathbf{p}}^{(B)})], \quad (96)$$

where $E_{\mathbf{p}}^{(B)} \equiv \sqrt{\varepsilon_{\mathbf{p}}(\varepsilon_{\mathbf{p}} + 2\Delta^{(1)})}$ is the Bogoliubov mode with a linear dependence for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} \ll 1$, and $\alpha_p \equiv (\varepsilon_{\mathbf{p}} + \Delta^{(1)})/E_{\mathbf{p}}^{(B)}$. Thus, $A_p^{(1)}(\omega)$ has a couple of sharp δ -function peaks at $\omega = \pm E_{\mathbf{p}}^{(B)}$ corresponding to well-defined quasiparticles with the infinite lifetime.

However, the 1PR self-energy brings about a qualitative change in the spectral function. To see this explicitly, let us consider the second-order approximation of Eq. (63), which can be solved analytically as

$$\Delta_{\vec{p}}^{(2c)} = \frac{D_{\vec{p}}^{(1)}}{4\varepsilon_{\mathbf{p}}} - \left[\left(\frac{D_{\vec{p}}^{(1)}}{4\varepsilon_{\mathbf{p}}} \right)^2 - 2(\Delta^{(1)})^2 \right]^{1/2} \quad (97)$$

with

$$D_{\vec{p}}^{(1)} \equiv (z_\ell - E_{\mathbf{p}}^{(B)})(z_\ell + E_{\mathbf{p}}^{(B)}). \quad (98)$$

Using this $\Delta_{\vec{p}}^{(2c)}$ in Eq. (60a) and substituting resultant $G_{\vec{p}}$ into Eq. (94), we can obtain the spectral function in the second-order approximation as

$$A_p^{(2)}(\omega) = \theta(\omega^2 - E_{p-}^2)\theta(E_{p+}^2 - \omega^2)[\theta(\omega) - \theta(\omega)] \frac{(\omega + \varepsilon_{\mathbf{p}})^2}{(4\Delta^{(1)})^2 \varepsilon_{\mathbf{p}}^3} \sqrt{(E_{p+}^2 - \omega^2)(\omega^2 - E_{p-}^2)}, \quad (99)$$

where $E_{p\pm} \equiv \sqrt{\varepsilon_{\mathbf{p}}[\varepsilon_{\mathbf{p}} + (2 \pm 4\sqrt{2})\Delta^{(1)}]}$. Figure.5 exhibits $A_p^{(2)}(\omega)$ for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} = 4$. as seen clearly, the quasi-particle excitation peaks are broadened due to $\Delta_p^{(2c)}$. The half-width $\delta\omega_p^{(2)}$ is proportional to the inverse of its lifetime τ^{-1} . The main peak of $A_p^{(2)}(\omega)$ for $\omega > 0$ is clearly of the order of a and approaches $57.3an$ as $\varepsilon_{\mathbf{p}} \rightarrow \infty$ as seen in Fig.6. However, Eq. (99) is valid only for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} \geq -2 + 4\sqrt{2}$; the second-order approximation fails to describe the low-momentum region adequately.

This unphysical behavior is removed in the third-order and the FLEX approximation. First, Fig.7 plots the spectral function $A_p^{(3)}(\omega)$ in the third-order approximation for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} = 4$ around its peak for $\omega > 0$. As seen clearly, this peak also has a finite lifetime $\tau \propto a^{-1}$. Figure.8 shows $\varepsilon_{\mathbf{p}}$ dependence of $\delta\omega_p^{(3)} \propto \tau^{-1}$. It apparently develops from zero as $\varepsilon_{\mathbf{p}}$ is increased, has the maximum around $\varepsilon_{\mathbf{p}}/\Delta^{(1)} \approx 300$, and starts to decrease thereafter towards 0. A qualitatively similar behavior is obtained by the FLEX approximation as shown in Fig.9, 10. However, both the magnitude of $\delta\omega_p^{(F)}$ and its peak location are quantitatively different from $\delta\omega_p^{(3)}$. To resolve this point requires a better treatment of the infinite series of Fig.3.

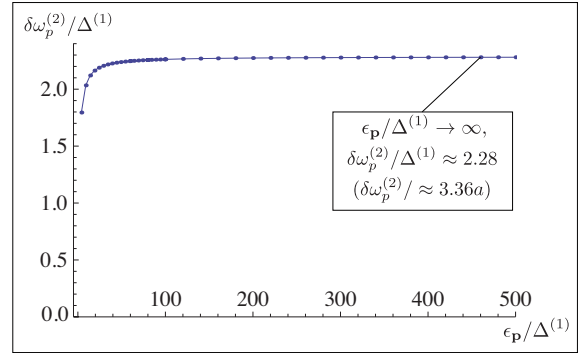
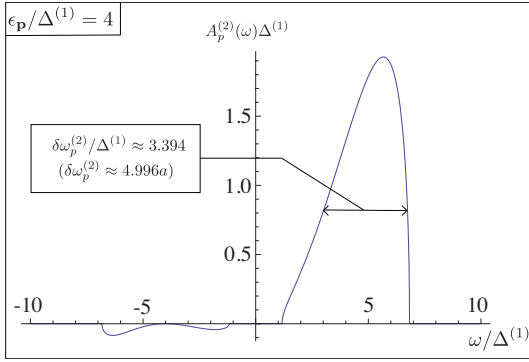


Fig 5: Plot of the spectral function $A_p^{(2)}(\omega)$ in the second-order approximation for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} = 4$. The half-width $\delta\omega_p^{(2)}$ is proportional to a .

Fig 6: Plot of the half-width $\delta\omega_p^{(2)}/p$ of $A_p^{(2)}(\omega)$. It increasing with $\varepsilon_{\mathbf{p}}/\Delta^{(1)}$, and approaches $57.3an$ for $\varepsilon_{\mathbf{p}} \rightarrow \infty$.

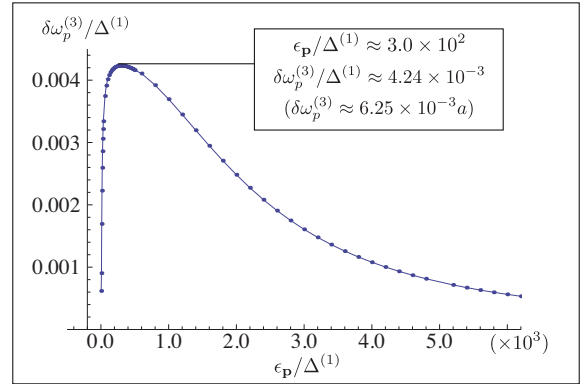
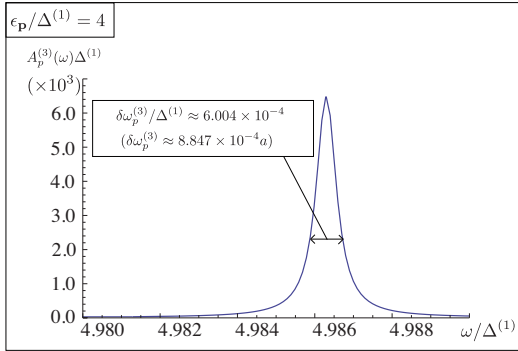


Fig 7: Plot of the spectral function $A_p^{(3)}(\omega)$ in the third-order approximation for $\varepsilon_{\mathbf{p}}/\Delta^{(1)} = 4$. The half-width $\delta\omega_p^{(3)}$ is proportional to a .

Fig 8: Plot of the half-width $\delta\omega_p^{(3)}/p$ of $A_p^{(3)}(\omega)$. It increasing with $\varepsilon_{\mathbf{p}}/\Delta^{(1)}$, and approaches 0 for $\varepsilon_{\mathbf{p}} \rightarrow \infty$.

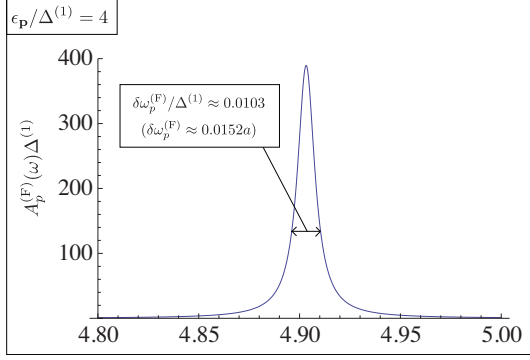


Fig 9: Plot of the spectral function $A_p^{(F)}(\omega)$ in the second-order approximation for $\epsilon_{\mathbf{p}}/\Delta^{(1)} = 4$. The half-width $\delta\omega_p^{(F)}$ is proportional to a .

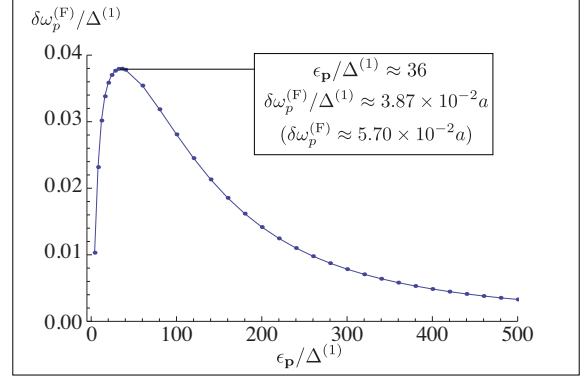


Fig 10: Plot of the half-width $\delta\omega_p^{(F)}/p$ of $A_p^{(F)}(\omega)$. It increasing with $\epsilon_{\mathbf{p}}/\Delta^{(1)}$, and approaches 0 for $\epsilon_{\mathbf{p}} \rightarrow \infty$.

Part III

Monte Carlo Study of Quasiparticle Excitations

In the previous part, we discussed the one-particle excitation of BEC by using the conserving-gapless theory. We concluded that the one-particle excitation has the finite lifetime proportional to s -wave scattering length a within perturbation theory (the bubbling mode). In this chapter, we will estimate the one- and the two-particle excitations by combining the Green's function Monte Carlo (GFMC) method [36, 37, 38, 39, 40] and the moment method [41, 42], which are introduced in Appendix.B.

For performing the Monte Carlo (MC) simulation, we need the trial wave function. So, we will first construct the Bijl-Jastraw type trial wave function [53] by solving two particle scattering problem (see also Appendix.C). Afterward, we will present results and conditions of MC simulations.

4 Construction of trial wave function

4.1 Hamiltonian and Units

We consider a system of N identical bosons with mass m and spin 0 interacting with a two-body potential $U(r)$ in a box of volume \mathcal{V} . The Hamiltonian is given by

$$\begin{aligned}\hat{H} &\equiv \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} \hat{\psi}(\mathbf{r}) + \int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') U(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) \\ &= \sum_{\mathbf{p}} \varepsilon_{\mathbf{p}} + \frac{1}{2V} \sum_{\mathbf{p}\mathbf{p}'\mathbf{q}} U_q \hat{c}_{\mathbf{p}+\mathbf{q}}^\dagger \hat{c}_{\mathbf{p}'-\mathbf{q}}^\dagger \hat{c}_{\mathbf{p}'} \hat{c}_{\mathbf{p}},\end{aligned}\quad (100)$$

where the potential can be expanded as

$$U(r) = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} U_q e^{i\mathbf{q}\cdot\mathbf{r}} \quad \longleftrightarrow \quad U_q = \int d\mathbf{r} U(r) e^{-i\mathbf{q}\cdot\mathbf{r}}. \quad (101)$$

Here we use the following potential:

$$U(r) = \frac{U_0}{8\pi r_0^3} e^{-r/r_0}, \quad (102)$$

for which U_q is given by $U_q = U_0/(1 + q^2 r_0^2)^2$. We can construct Bijl-Jastraw type trial wave function for \hat{H} by solving a two-particle scattering problem. We present the procedures as follows.

4.2 Variational optimization

We start from the following Schrödinger equation:

$$\left[-\frac{\hbar^2}{2m_{\text{red}}} \frac{1}{r} \frac{d^2}{dr^2} r + U(r) \right] \psi(r) = E\psi(r), \quad (103)$$

where $m_{\text{red}} \equiv m/2$. By introducing $u(r) \equiv r\psi(r)$, we obtain

$$\left[-\frac{\hbar^2}{2m_{\text{red}}} \frac{d^2}{dr^2} + U(r) \right] u(r) = Eu(r). \quad (104)$$

We also introduce dimensionless length $\xi \equiv r/a$ in terms of the s -wave scattering length a . Equation (104) can be rewritten as

$$\frac{d^2 u(\xi)}{d\xi^2} = \frac{1}{2D} [U(\xi) - E] u(\xi), \quad (105)$$

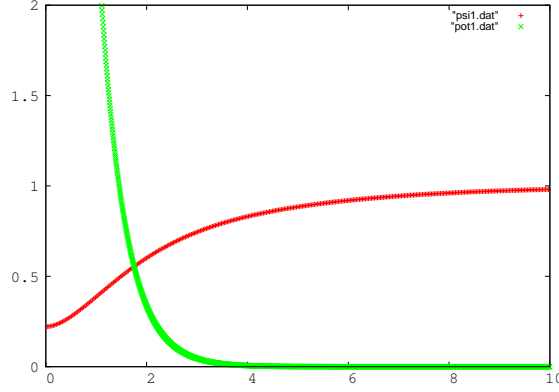


Fig 11: Plots of $f(\xi)$ (red line) and its potential $U(\xi)$ (green line).

where $D \equiv \hbar^2/2ma^2$ and $U(\xi) \equiv (U_0/8\pi r_0^3)e^{-(a/r_0)\xi}$. We can solve this equation numerically by using Runge-Kutta method. We also set $\hbar = 1$, $m = 1/2$ respectively.

We can also estimate the s -wave scattering length a by solving the following equation:

$$a = \frac{m}{4\pi} U^{(\text{eff})}(0, 0), \quad (106)$$

with

$$\begin{aligned} U^{(\text{eff})}(p, p') &= U_0(p, p') - \int \frac{d^3 p_1}{(2\pi)^3} U_0(p, p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U^{(\text{eff})}(p_1, p') \\ &= U_0(p, p') - \frac{1}{4\pi^2} \int_0^\infty dp_1 U_0(p, p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U^{(\text{eff})}(p_1, p'), \end{aligned} \quad (107)$$

where $U_0(p, p')$ can be given by

$$U_0(p, p') = \frac{U_0}{(1 + r_0^2 p^2 + r_0^2 p'^2)^2 - 4r_0^4 p^2 p'^2}, \quad (108)$$

for our potential. Using this equations, we can set s -wave scattering length by fixing r_0 and U_0 . We set $a = 1$ and $r_0 = 0.5$, then U_0 can be calculated $U_0 \approx 57.7465$ numerically.

We first construct a function as $f_0(\xi) \rightarrow 1$ for large ξ , so we try to connect $\psi(\xi)$ to a constant ψ_0 at $\xi = \xi_{\text{max}}$ which satisfies $\psi'(\xi_{\text{max}}) = 0$. By normalizing it, we obtain $f_0(\xi)$ as

$$f_0(\xi) = \begin{cases} \psi(\xi)/\psi_0 & (\xi \leq \xi_{\text{max}}) \\ 1 & (\xi > \xi_{\text{max}}), \end{cases} \quad (109)$$

Next, we connect $f_0(\xi)$ ($\xi_s \leq \xi_{\text{max}}$) to another function at $\xi = \xi_s$. We choose the function $f_1(\xi)$ as

$$f_1(\xi) \equiv 1 - A \exp\left(-\frac{\xi}{\alpha}\right) \quad (\xi \geq \xi_s), \quad (110)$$

where the variational parameters A, α and ξ_s can be obtained by variational optimization. Then we match $f_0(\xi)$ and $f_1(\xi)$ at $\xi = \xi_s$ up to the second derivative, which can be represented as

$$f_0(\xi_s) = f_1(\xi_s), \quad f_0'(\xi_s) = f_1'(\xi_s), \quad f_0''(\xi_s) = f_1''(\xi_s).$$

These conditions can be transformed into

$$\alpha = \frac{1 - f_0(\xi_s)}{f_0'(\xi_s)}, \quad (111a)$$

$$A = (1 - f_0(\xi_s)) \exp\left(\frac{\xi_s}{\alpha}\right), \quad (111b)$$

$$\frac{f_0(\xi_s)}{f_0''(\xi_s)} + \alpha^2 \left(\frac{1}{A} \exp\left(\frac{\xi_s}{\alpha}\right) - 1\right) = 0, \quad (111c)$$

with which we seek the solution in $1 > A, \alpha > 0$ and $\xi_{\max} > \xi_s$. If we fix the value of ξ_{\max} , then other variational parameters yield automatically. ξ_{\max} can be optimized by using VQMC method, which can be estimated as $\xi_{\max} \approx 14.8867$. Other parameters are also determined as $\xi_s = 6.0512, E = 2.06124 \times 10^{-3}, A = 0.702866, \alpha = 2.76514$, respectively. The function $f(\xi)$ is plotted in Fig.11. We also present the results of VQMC calculation, which are shown in Fig.12. Our conditions are the following: Walker number is 400, and prestep count and observation count are 10^5 and 2.0×10^5 respectively. We adopt the rigid boundary condition for a cubic box and particle number $N = 50$, and particle density $na^3 = 1.0 \times 10^{-3}$. We obtained the value of energy per particle $\mathcal{E}^{(\text{VQMC})}/N \approx 8.751(1) \times 10^{-3}$ at $\xi_{\max} = 14.8867$.

Thus we can construct N -body trial wave function $\Psi(\mathbf{R})$ in the Bijl-Jastrow form as

$$\Psi(\mathbf{R}) \equiv \prod_{i < j} f(r_{ij}), \quad (112)$$

with

$$f(\xi) = \begin{cases} \psi(\xi)/\psi_0 & (\xi \leq \xi_s) \\ 1 - A \exp\left(-\frac{\xi}{\alpha}\right) & (\xi > \xi_s), \end{cases} \quad (113)$$

where \mathbf{R} denotes positions of particles $\mathbf{R} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$, and $r_{ij} = |\mathbf{r}_{ij}|, \mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$.

Finally, we show the energy estimated by GFMC method. We chose the unit of time as $\tau \equiv \hbar(\mathcal{E}^{(\text{VQMC})}/N)^{-1}$ and set $\Delta\tau = 1.0 \times 10^{-3}\tau$. We also set walker number 400, prestep number 30000 and main step number 100000 respectively. Then, we obtain the energy per particle $\mathcal{E}/N \approx 8.3455(2) \times 10^{-3}$.

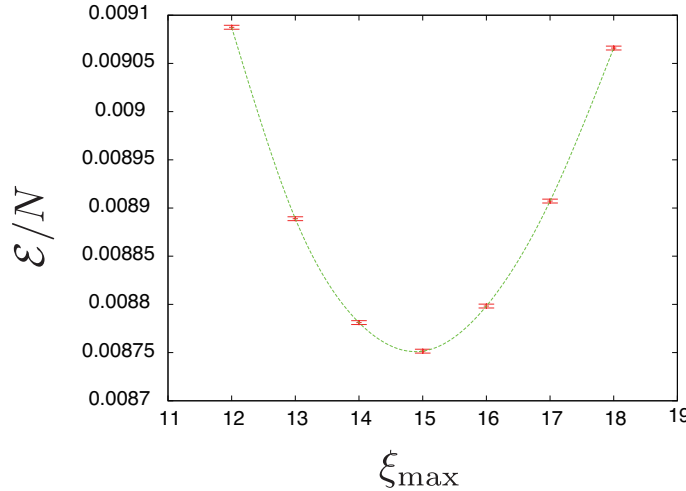


Fig 12: Plots of the energy per particle \mathcal{E}/N to variational parameter ξ_{\max} .

5 Expression of quasiparticle excitations by moments

We next present how to estimate quasiparticle excitation in N identical bosons. We introduce the moment method, which was used for investigating two-particle excitation spectrum for superfluid ^4He and magnon

systems. Previously, it has been used only for estimating the peak position of the dynamic structure factor $S(\mathbf{q}, \omega)$ with frequency ω based on the first moment. However, by extending the method to higher moments, we can estimate lifetime of the two-particle excitation. And we can also obtain details of the one-particle excitation by using it for the one-particle spectral function $A(\mathbf{k}, \varepsilon)$. Here we will outline the method. These details are given in Appendix B.

5.1 Density correlation function and Dynamic structure factor

We first introduce the one-particle spectral function $A(\mathbf{k}, \varepsilon)$ and the dynamic structure factor $S(\mathbf{q}, \omega)$ for $T = 0$ as

$$A(\mathbf{k}, \varepsilon) = \sum_{\nu} |\langle \Psi_{\nu} | \hat{a}_{\mathbf{k}}^{\dagger} | \Psi_G \rangle|^2 \delta(\varepsilon - E_{\nu} + E_G), \quad (114a)$$

$$S(\mathbf{q}, \omega) \equiv \sum_{\nu} |\langle \Psi_{\nu} | \hat{\rho}_{\mathbf{q}}^{\dagger} | \Psi_G \rangle|^2 \delta(\omega - E_{\nu} + E_G). \quad (114b)$$

respectively, where $|\Psi_{\nu}\rangle$ is the eigenket of our system, and E_{ν} is its eigenenergy. We also express the ground state ket and its eigen energy $|\Psi_G\rangle$, E_G respectively. The operator $\hat{\rho}_{\mathbf{q}}$ is given by

$$\hat{\rho}_{\mathbf{q}} \equiv \sum_{\mathbf{k}} \hat{a}_{\mathbf{q}+\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}}. \quad (115)$$

We also introduce the moments of $A(\mathbf{k}, \varepsilon)$ and $S(\mathbf{q}, \omega)$ as

$$J_n(\mathbf{k}) \equiv \int_{-\infty}^{\infty} d\varepsilon \varepsilon^n A(\mathbf{k}, \varepsilon) = \sum_{\nu} |\langle \Psi_{\nu} | \hat{a}_{\mathbf{k}}^{\dagger} | \Psi_G \rangle|^2 (E_{\nu} - E_G)^n, \quad (116a)$$

$$I_n(\mathbf{q}) \equiv \int_{-\infty}^{\infty} d\omega \omega^n S(\mathbf{q}, \omega) = \sum_{\nu} |\langle \Psi_{\nu} | \hat{\rho}_{\mathbf{q}}^{\dagger} | \Psi_G \rangle|^2 (E_G - E_{\nu})^n. \quad (116b)$$

respectively.

We first review how to estimate the two-particle excitation. The dynamic structure factor $S(\mathbf{q}, \omega)$ includes the information of two-particle excitation. The pole of $S(\mathbf{q}, \omega)$ and its half-width correspond to the spectrum and its lifetime at the frequency ω respectively. So, we can find that the integration of $S(\mathbf{q}, \omega)$ over ω is the distribution function for mode \mathbf{q} . Thus the first-order moment $I_1(\mathbf{q})$ is proportional to the two-particle dispersion $\omega_{\mathbf{q}}$. However, $I_1(\mathbf{q})$ is not normalized, so we here introduce the following functions:

$$\tilde{S}_n(\mathbf{q}, \omega) \equiv \frac{S(\mathbf{q}, \omega) \omega^n}{I_0(\mathbf{q})}, \quad \tilde{I}_n(\mathbf{q}) \equiv \frac{I_n(\mathbf{q})}{I_0(\mathbf{q})}. \quad (117)$$

Noting that the function $\tilde{S}_n(\mathbf{q}, \omega)$ is normalized, we realize that $\tilde{I}_1(\mathbf{q})$ signifies the peak position of the two-particle excitation $\omega_{\mathbf{q}}$. In addition, the second moment includes information about the width of the mode $S(\mathbf{q}, \omega)$. To be more specific, the two-particle excitation spectrum $\omega_{\mathbf{q}}$ and its half-width of $S(\mathbf{q}, \omega)$ can be expressed as

$$\omega_{\mathbf{q}} = \tilde{I}_1(\mathbf{q}), \quad (118a)$$

$$\delta\omega_{\mathbf{q}} = \sqrt{\tilde{I}_2(\mathbf{q}) - \tilde{I}_1(\mathbf{q})^2}. \quad (118b)$$

This consideration can be extended for the one-particle excitation by replacing $S(\mathbf{q}, \omega)$ by $A(\mathbf{k}, \varepsilon)$. Defining the normalized moments of $A(\mathbf{k}, \varepsilon)$ as

$$\tilde{A}_n(\mathbf{k}, \varepsilon) \equiv \frac{A(\mathbf{k}, \varepsilon) \varepsilon^n}{J_0(\mathbf{k})}, \quad \tilde{J}_n(\mathbf{k}) \equiv \frac{J_n(\mathbf{k})}{J_0(\mathbf{k})}. \quad (119)$$

We also obtain the one-particle excitation spectrum $\varepsilon_{\mathbf{k}}$ and its lifetime $\delta\varepsilon_{\mathbf{k}}$ as

$$\varepsilon_{\mathbf{k}} = \tilde{J}_1(\mathbf{k}), \quad (120a)$$

$$\delta\varepsilon_{\mathbf{k}} = \sqrt{\tilde{J}_2(\mathbf{k}) - \tilde{J}_1(\mathbf{k})^2}, \quad (120b)$$

respectively. So, we have to calculate the moments up to the second order for both the one- and two- particle channels.

5.2 Expressions of moments

We can construct moments of $A(\mathbf{k}, \varepsilon)$ as

$$J_0(\mathbf{k}) = 1 + \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad (121a)$$

$$J_1(\mathbf{k}) = \frac{\hbar^2 k^2}{2m} \left[1 + \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \right] + nU_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} U(\mathbf{r}) g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}, \quad (121b)$$

$$\begin{aligned} J_2(\mathbf{k}) &= \left(\frac{\hbar^2 k^2}{2m} \right)^2 \left[1 + \int d\mathbf{r} e^{i\mathbf{k}\cdot\mathbf{r}} g_1(\mathbf{r}) \right] + \frac{\hbar^2 k^2}{2m} \left[nU_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} U(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \right] \\ &+ \frac{\hbar^2 k^2}{2m} \left[nU_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} U(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \right]^* \\ &+ n \int d\mathbf{r} [U(\mathbf{r})]^2 + \int d\mathbf{r} [U(\mathbf{r})]^2 g_1(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + \int d\mathbf{r} \int d\mathbf{r}' U(\mathbf{r} - \mathbf{r}') U(\mathbf{r}) g_2(\mathbf{r}') \\ &+ N(N-1) \left[\int d\mathbf{r} U(\mathbf{r}) S_A(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + \left(\int d\mathbf{r} U(\mathbf{r}) S_A(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} \right)^* \right] \\ &+ N(N-1) \int d\mathbf{r} S_B(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}} + N(N-1)(N-2) \int d\mathbf{r} S_C(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \end{aligned} \quad (121c)$$

where $g_1(\mathbf{r})$ and $g_2(\mathbf{r})$ are the one-particle and the two-particle density matrices respectively, and the functions S_A, S_B, S_C are given by

$$S_A(\mathbf{r}) \equiv \frac{1}{V} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N U(\mathbf{r}_1 + \mathbf{r} - \mathbf{r}_2) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N), \quad (122a)$$

$$S_B(\mathbf{r}) \equiv \frac{1}{V} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N U(\mathbf{r}_1 - \mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{r}) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \quad (122b)$$

$$S_C(\mathbf{r}) \equiv \frac{1}{V} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N U(\mathbf{r}_1 - \mathbf{r}_2) U(\mathbf{r}_1 - \mathbf{r}_3 + \mathbf{r}) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N), \quad (122c)$$

respectively, where $\Psi_G(\mathbf{R})$ is the ground state wave function.

Next, the moments of $S(\mathbf{q}, \omega)$ can be represented as

$$I_0(\mathbf{q}) = N \left\{ \frac{1}{n} \int d\mathbf{r} [g_2(\mathbf{r}) - 1] e^{i\mathbf{q}\cdot\mathbf{r}} + \frac{V}{n} \delta_{\mathbf{q}\mathbf{0}} + 1 \right\}, \quad (123a)$$

$$I_1(\mathbf{q}) = N \frac{\hbar^2 q^2}{2m}, \quad (123b)$$

$$I_2(\mathbf{q}) = N \left(\frac{\hbar^2 q^2}{2m} \right)^2 + \frac{\hbar^2 q^2}{3m} \sum_{\mathbf{k}} k^2 \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}}. \quad (123c)$$

We can see that these moments (121) and (123) have apparently different forms. We estimate these functions by using GFMC and VQMC methods.

Finally, we introduce the unit of moments $(\tilde{\mathbf{k}}, \tilde{\mathbf{q}}) \equiv (a\mathbf{k}, a\mathbf{q})$.

6 Numerical results

We will here present our numerical results obtained by using the Bijl-Jastrow type wave function constructed in Sec. 4.2. We need to calculate the one- and the two- particle density matrices and several functions to obtain the quasi-particle excitation.

6.1 Density matrices and some functions

To estimate lifetimes, we need to calculate the density matrices and functions in Eq. (122). So, we here present plots of these functions estimated by VQMC and GFMC methods. The conditions of the simulations are as

follows: Particle number N , density na^3 , some variational parameters for the trial wave function, and units are used the same as in Sec. 4.2. For VQMC simulation, we usually set the number of walker $n^{(v)} = 400$, prestep count 10^5 and main step count 3×10^4 . But for two-particle density matrix, we set the main step count 9×10^4 , because it has the worst convergence property. For GFMC calculations, we set the same walker number and step for main sampling as the VQMC calculation. We give the plots of the one- and two- particle density matrices and other basic functions in Figs.13-17. We obtain the values of functions by GFMC and VQMC samplings. We apply the “extrapolated” estimation for each of these functions. Finally we calculate the moments (121), (123) numerically.

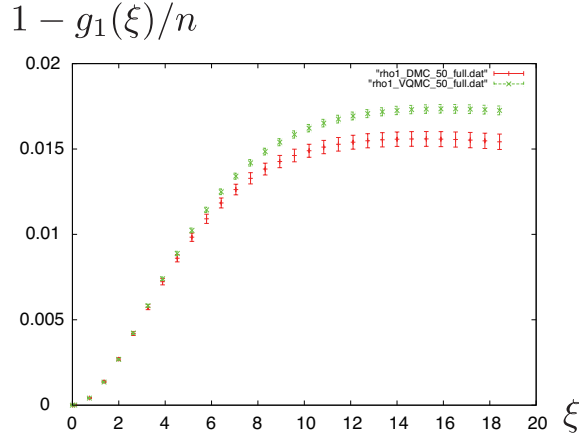


Fig 13: Plots of the one-particle density matrices per the density n with their errorbars. The red and the green lines are estimated by GFMC and VQMC methods respectively.

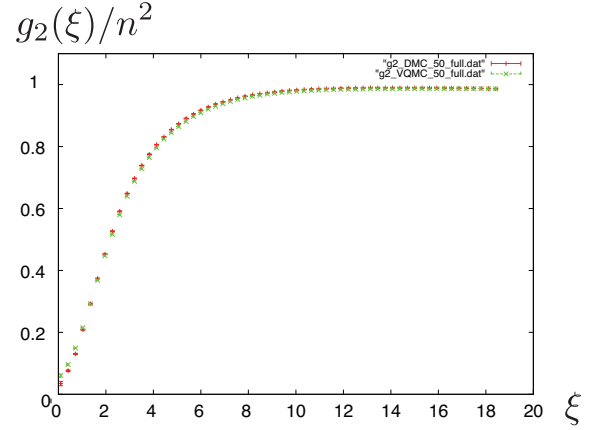


Fig 14: Plots of the the two-particle density matrices per square of the density n^2 with their errorbars. The red and the green lines are estimated by GFMC and VQMC methods respectively. These lines have good agreement for large ξ .

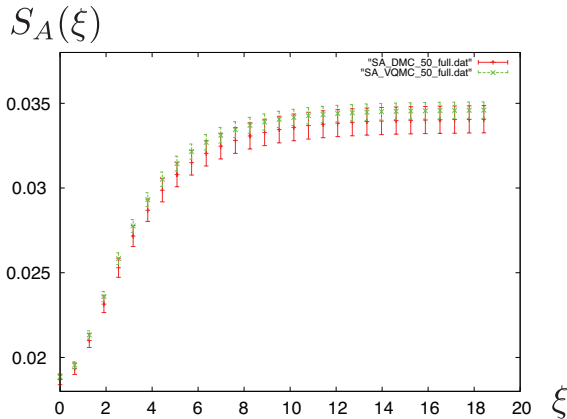


Fig 15: Plots of $S_A(\xi)$ with their errorbars. The red and the green lines are estimated by GFMC and VQMC methods respectively.

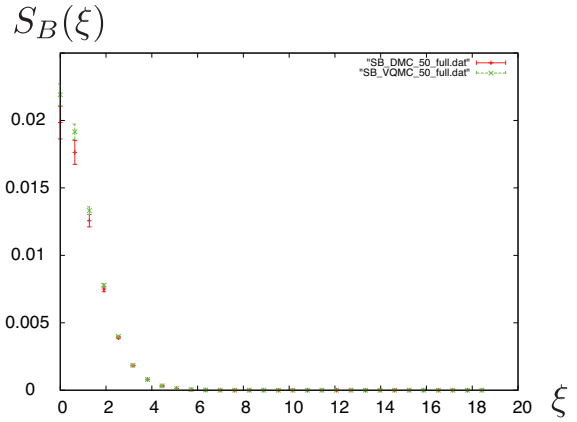


Fig 16: Plots of $S_B(\xi)$ with their errorbars. The red and the green lines are estimated by GFMC and VQMC methods respectively. $S_B(\xi)$ goes to rapidly 0 for large ξ .

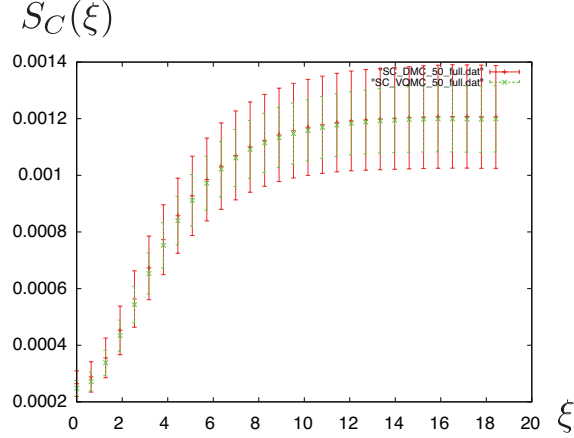


Fig 17: Plots of $S_C(\xi)$ with their errorbars. The red and the green lines are estimated by GFMC and VQMC methods respectively.

6.2 lifetime estimation

Before we present the final results, we comment on the first moment of the one-particle spectral function (120a). We note that the first-order moment $\tilde{J}_1(\tilde{\mathbf{k}})$ is apparently nonzero at $\tilde{\mathbf{k}} = \tilde{\mathbf{0}}$ as seen in Eq. (121b). However, this is not inconsistent with the Hugenholtz-Pines theorem. To confirm it, we start from the following expression of $\tilde{J}_1(\tilde{\mathbf{k}})$:

$$\tilde{J}_1(\tilde{\mathbf{0}}) = \frac{\langle \Psi_G | \hat{a}_0 [\hat{H}, \hat{a}_0^\dagger] | \Psi_G \rangle}{\langle \Psi_G | \hat{a}_0 \hat{a}_0^\dagger | \Psi_G \rangle} = \frac{\langle \Psi_G | \hat{a}_0 \hat{H} \hat{a}_0^\dagger | \Psi_G \rangle - \langle \Psi_G | \hat{H} \hat{a}_0 \hat{a}_0^\dagger | \Psi_G \rangle}{\langle \Psi_G | \hat{a}_0 \hat{a}_0^\dagger | \Psi_G \rangle}. \quad (124)$$

As seen in the above calculation, $\tilde{J}_1(\tilde{\mathbf{0}})$ consists of two different expectations with dimension of energy. If we consider a system of the grand canonical ensemble and take the Lehman representation for the one-particle Green's function [44, 51], a similar term remains at $\tilde{\mathbf{k}} = \mathbf{0}$, which corresponds to the chemical potential μ . In the present case where we fix the particle number (the canonical ensemble), the term obtained in Eq. (124) is not exactly the chemical potential in this system. However, we are interested in the lifetime of the one-particle excitation. This term only specify the position of the one-particle spectral function. So, when we consider the second-order moment for the one-particle excitation, this term is removed. We show the plots of $J_n(\tilde{\mathbf{k}})$ in Fig. 18, 19, 20.

Next, we show the results of the half-widths of the one- and the two-particle excitation in Fig.23. For low momentum region the two-particle excitation cannot be calculated. It turns out impossible to obtain a reliable result for the second moment in the low-momentum region due to the lack of enough accuracy in the large ξ region in the coordinate space. However, $I_0(\tilde{\mathbf{q}})$ approaches to N at the high momentum regime as seen in Fig.22. So we can obtain the half-width in the high momentum regime. That is derived from the limit for $\xi \rightarrow \infty$. At this regime, using the Eq. (123), the half-width $\delta\omega_{\tilde{\mathbf{q}}}$ can be approximated by

$$\begin{aligned} \delta\omega_{\tilde{\mathbf{q}}} &= \sqrt{\frac{I_2(\tilde{\mathbf{q}})}{I_0(\tilde{\mathbf{q}})} - \left(\frac{I_1(\tilde{\mathbf{q}})}{I_0(\tilde{\mathbf{q}})}\right)^2} \\ &\approx \sqrt{na^3 \frac{2D\tilde{q}^2}{3} \int \frac{d\tilde{\mathbf{k}}}{(2\pi)^3} \tilde{k}^2 \int d\xi g_1(\xi) e^{-i\tilde{\mathbf{k}}\cdot\xi}} \propto \tilde{q}. \end{aligned} \quad (125)$$

Actually, we can see the linear behavior of $\delta\omega_{\tilde{\mathbf{q}}}$ in Fig 23. On the other hand, the half-width of the one-particle excitation $\delta\varepsilon_{\tilde{\mathbf{k}}}$ has an apparently different behavior, which decreases monotonously as a function of $\tilde{\mathbf{k}}$.

Therefore, we conclude that these half-widths are qualitatively different, which contradicts the statement Gavoret and Nozières [18] but agrees with that of the conserving-gapless theory.

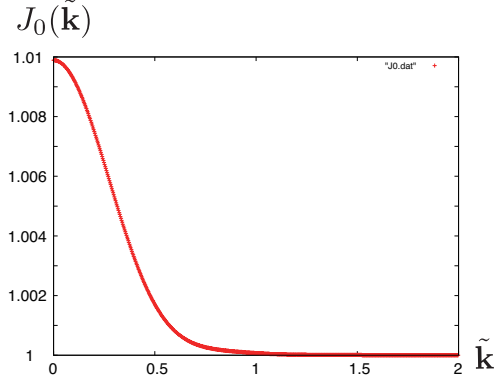


Fig 18: Plot of $J_0(\tilde{k})$.

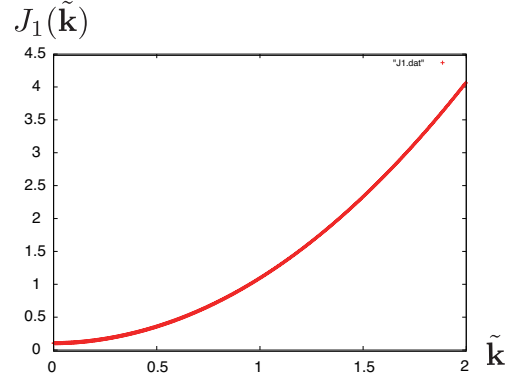


Fig 19: Plot of $J_1(\tilde{k})$.

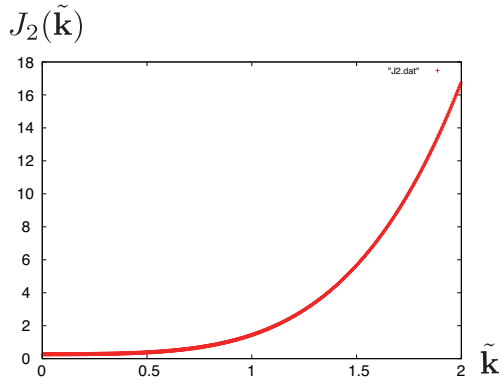


Fig 20: Plots of $J_2(\tilde{k})$.

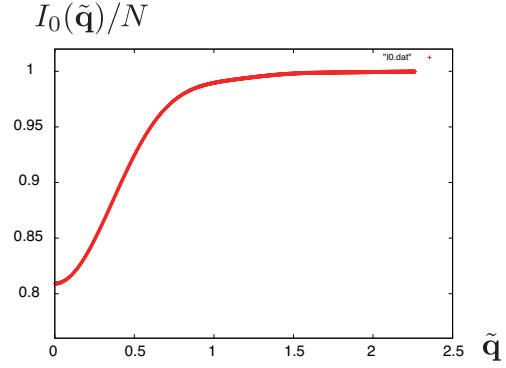


Fig 21: Plots of $I_0(\tilde{q})$ per particle number N . It converges to 1 for large momentum.

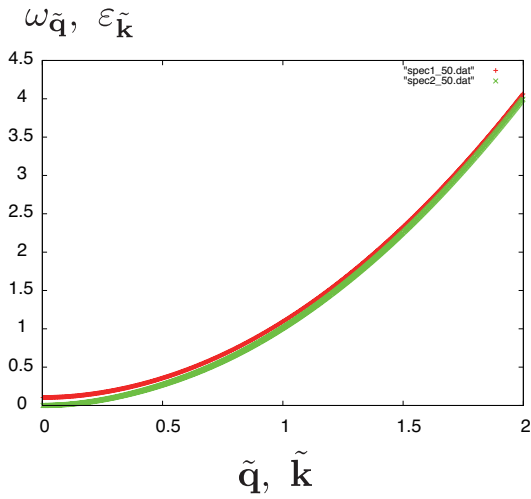


Fig 22: Plots of $\varepsilon_{\tilde{k}}$ and $\omega_{\tilde{q}}$. The red and the green lines are results for the one- and the two-particle excitations. $\varepsilon_{\tilde{k}}$ starts from a finite value corresponding to the chemical potential. They have similar behavior for large momentum region.

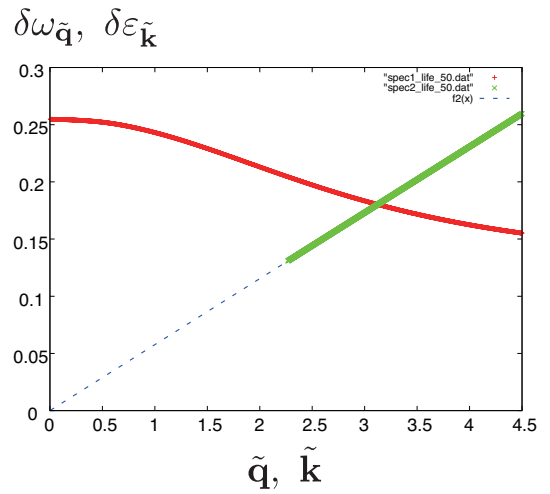


Fig 23: Plots of the half-widths of the quasi-particle excitations. The red, the green and the dashed lines are results the one- and the two-particle excitations and the auxiliary line $f(\xi) = 0.0577\tilde{q}$ for $\delta\omega_{\tilde{q}}$. The low momentum region of the two-particle excitation cannot be calculated because we couldn't estimate the two-particle density matrix for large ξ .

Part IV

Summary and Conclusion

7 Summary and Conclusion

In this thesis, we have investigated the details of the quasiparticle excitation of BEC. Our motivations of the study are summarized concisely as follows. Bogoliubov theory predicts that the one-particle excitation has an infinite lifetime and a linear dispersion at $\mathbf{k} \rightarrow \mathbf{0}$ [13]. Also, Gavoret and Nozières claim that the one-particle Green's function for BEC share its pole with that of the two-particle Green's function [18]. Thus, they conclude that the Bogoliubov mode is a collective mode. However, the proof by Gavoret and Nozières has an ambiguity in the definition of the Green's functions. Moreover, the Bogoliubov theory has some difficulties. One is relevant to its extension for the finite temperature system (HFB theory) [21, 22]. It gives a gap the one-particle excitation, which is inconsistent with the Hugenholtz-Pines (Goldstone) theorem [17, 19]. There is the approximation of setting the gap zero by hand (Shono approximation [23, 24]). However, such a procedure breaks the conservation laws when used in dynamical problems. Such a situation is called "conserving v.s. gapless dilemma" by Hohenberg and Martin. Recently, conserving-gapless theory was constructed by Kita [30]. It corresponds to the extension of the Luttinger-Ward [28] theory for BEC. It also predicts that the one- and the two-particle excitation are different [31]. Especially, the one-particle excitation is not the Bogoliubov mode but the bubbling mode, which has the finite lifetime.

We have studied the one-particle excitation by using the conserving-gapless theory for weak interacting system at $T = 0$. We have obtained the result that the lifetime of the one-particle excitation is proportional to the s -wave scattering length a [33]. We have found that the physical quantities proposed by Lee, Huang, Yang [34] are also modified [35]. These properties originate from the 1PR diagrams which are overlooked so far in the previous studies. Next, we have studied the one- and the two-particle excitation of BEC system at $T = 0$ by using the Monte Carlo method [37, 54]. We have used the moment method [41, 42] extended to higher orders, which is a powerful method to estimate them quantitatively. We have obtained the results that the one- and two-particle excitation have qualitatively different behavior, which implies the proof by Gavoret and Nozières are incorrect and justifies the statement of the conserving-gapless theory. The Bogoliubov theory and statement by Gavoret and Nozières have some flaws. On the other hand, the conserving-gapless theory describes more realistic situation given by the Monte Carlo simulation. We are confident that the conserving-gapless theory is one of powerful tools to understand BEC theoretically.

Part V

Appendix

A Conserving-Gapless Theory

A.1 Notations

A.1.1 Hamiltonian

We introduce some notations to calculate thermodynamical properties of BEC. Here we consider N identical bosons with mass m and spin 0 and interacting with a two-body potential $V(\mathbf{r} - \mathbf{r}')$. The corresponding Hamiltonian \hat{H} is given by [50]

$$\hat{H} \equiv \int d^3\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) \hat{K}_1(\mathbf{r}) \hat{\psi}(\mathbf{r}) + \frac{1}{2} \int d^3\mathbf{r} \int d^3\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}), \quad (\text{A.1})$$

where $(\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}))$ are annihilation and creation operators satisfying the bosonic commutation relations, and $\hat{K}_1(\mathbf{r}) \equiv \hat{\mathbf{p}}^2/2m + U(\mathbf{r}) - \mu$ with $U(\mathbf{r})$ the external field and μ the chemical potential. Then, we introduce field operators of Heisenberg representation as

$$\psi_1(1) \equiv e^{-\tau_1 \hat{H}} \hat{\psi}(\mathbf{r}_1) e^{\tau_1 \hat{H}}, \quad \psi_2(1) \equiv e^{-\tau_1 \hat{H}} \hat{\psi}^\dagger(\mathbf{r}_1) e^{\tau_1 \hat{H}}, \quad (\text{A.2})$$

where the arabic number 1 is defined by $1 \equiv (\mathbf{r}_1, \tau_1)$, and τ is the imaginary time ($0 \leq \tau \leq \beta$) with $\beta \equiv (k_B T)^{-1}$ and temperature T . In BEC system, we must divide these field operators into two parts as

$$\psi_i(1) = \Psi_i(1) + \phi_i(1), \quad (i = 1, 2), \quad (\text{A.3})$$

where $\Psi_i(1) \equiv \langle \psi_i(1) \rangle$ and $\phi_i(1)$ are the condensate wave function and quasi-particle operator respectively, and $\langle \dots \rangle$ is the grand-canonical average. They have the following properties: (i) $\Psi_1(1) = \Psi^*(2) \equiv \Psi(\mathbf{r}_1)$, (ii) $\langle \phi_i(1) \rangle = 0$.

A.1.2 Matsubara Green's function

By using these operators, we define the Matsubara Green's function in the Nambu space as

$$G_{ij} = -\langle T_\tau \phi_i(1) \phi_{3-j}(2) \rangle (-1)^{j-1}, \quad (\text{A.4})$$

with the time-ordering operator T_τ . The off-diagonal elements G_{ij} ($i = 1, j = 2$) and ($i = 2, j = 1$) represent expectations of pair annihilation and pair creation respectively, which are characteristic terms of BEC system. We can also write the particle number N as

$$N = \int d^3\mathbf{r}_1 [\Psi_2(1) \Psi_1(1) - G_{11}(1, 1_+)], \quad (\text{A.5})$$

with $1_\pm \equiv (\mathbf{r}_1, \tau_1 \pm \eta)$, where η is the infinitesimal positive constant. Then, we find symmetry relations for G_{ij} as

$$G_{ij}(1, 2) = (-1)^{i+j-1} G_{3-j, 3-i}(2, 1) = (-1)^{i+j} G_{ji}^*(\mathbf{r}_2 \tau_1, \mathbf{r}_1, \tau_2). \quad (\text{A.6})$$

Using these notations, we will give a representation of the thermodynamic potential Ω as a functional of the Matsubara Green's function and formulate a self-consistent perturbation expansion.

A.2 Relations for BEC system

Here we derive basic relations for BEC to carry out the perturbation expansion for the thermodynamic potential Ω [30].

A.2.1 Time evolution operator

First, we introduce the extra perturbation to \hat{H} as

$$\hat{H}_{\text{ext}}(\tau_1) \equiv \int d^3 \mathbf{r}_1 [\hat{\psi}^\dagger(\mathbf{r}_1) \eta_{\text{ext}}(1) + \hat{\psi}(\mathbf{r}_1) \eta_{\text{ext}}^*(1)], \quad (\text{A.7})$$

where $\eta_{\text{ext}}(1)$ is the periodic function in τ_1 with period β . The total Hamiltonian in this section is defined by

$$\hat{\mathcal{H}}(\tau_1) \equiv \hat{H} + \hat{H}_{\text{ext}}(\tau_1). \quad (\text{A.8})$$

By using this extra perturbation, we will derive exact relations for BEC, and finally η_{ext} will be set equal to 0. To begin with, we introduce the time evolution operator $\hat{\mathcal{U}}$ for $\hat{\mathcal{H}}$ as

$$\begin{aligned} \hat{\mathcal{U}}(\tau, \tau_0) &\equiv 1 + \sum_{n=1}^{\infty} (-1)^n \int_{\tau_0}^{\tau} d\tau_n \cdots \int_{\tau_0}^{\tau_2} d\tau_1 \hat{\mathcal{H}}(\tau_n) \cdots \hat{\mathcal{H}}(\tau_1) \\ &= \begin{cases} T_{\tau} \exp \left[- \int_{\tau_0}^{\tau} d\tau_1 \hat{\mathcal{H}}(\tau_1) \right] & (\tau \geq \tau_0) \\ T_{\tau}^a \exp \left[- \int_{\tau_0}^{\tau} d\tau_1 \hat{\mathcal{H}}(\tau_1) \right] & (\tau < \tau_0), \end{cases} \end{aligned} \quad (\text{A.9})$$

where T_{τ} and T_{τ}^a are time-ordering and anti-time ordering operators respectively. We also confirm that $\hat{\mathcal{U}}$ satisfies $\hat{\mathcal{U}}(\tau_0, \tau_0) = 1$, $\hat{\mathcal{U}}^{-1}(\tau, \tau_0) = \hat{\mathcal{U}}(\tau_0, \tau)$, and

$$\hat{\mathcal{U}}(\tau, \tau_1) \hat{\mathcal{U}}(\tau_1, \tau_0) = \hat{\mathcal{U}}(\tau, \tau_0). \quad (\text{A.10})$$

Moreover, it also satisfies following equations:

$$\frac{d\hat{\mathcal{U}}(\tau, \tau_0)}{d\tau} = -\hat{\mathcal{H}}(\tau) \hat{\mathcal{U}}(\tau, \tau_0), \quad (\text{A.11a})$$

$$\frac{d\hat{\mathcal{U}}(\tau, \tau_0)}{d\tau_0} = \hat{\mathcal{U}}(\tau, \tau_0) \hat{\mathcal{H}}(\tau_0). \quad (\text{A.11b})$$

We note that $\hat{\mathcal{U}}$ reduces to the normal time evolution operator for $\eta_{\text{ext}} \rightarrow 0$.

A.2.2 Equation of motion

We introduce the Heisenberg representation for $\hat{\mathcal{H}}$ by using $\hat{\mathcal{U}}$ as

$$\begin{cases} \psi(1) \equiv \hat{\mathcal{U}}^{-1}(\tau_1) \hat{\psi}(\mathbf{r}_1) \hat{\mathcal{U}}(\tau_1) \\ \bar{\psi}(1) \equiv \hat{\mathcal{U}}^{-1}(\tau_1) \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\mathcal{U}}(\tau_1), \end{cases} \quad (\text{A.12})$$

where $0 \leq \tau_1 \leq \beta$. Equations of motion for these operators are given by

$$\left(-\frac{\partial}{\partial \tau_1} - K_1 \right) \psi(1) = \eta_{\text{ext}}(1) + \int d1' \bar{V}(1, 1') \bar{\psi}(1') \psi(1') \psi(1), \quad (\text{A.13a})$$

$$\left(\frac{\partial}{\partial \tau_1} - K_1 \right) \bar{\psi}(1) = \eta_{\text{ext}}^*(1) + \int d1' \bar{V}(1, 1') \bar{\psi}(1) \bar{\psi}(1') \psi(1'), \quad (\text{A.13b})$$

with $\bar{V}(1, 2) \equiv \delta(\tau_1 - \tau_2) V(\mathbf{r}_1 - \mathbf{r}_2)$.

The expectation value of $\mathcal{O}(1) \equiv \hat{\mathcal{U}}^{-1}(\tau_1) \hat{\mathcal{O}}(\mathbf{r}_1) \hat{\mathcal{U}}(\tau_1)$ is also defined by

$$\langle \mathcal{O}(1) \rangle \equiv \frac{\text{Tr} T_{\tau} \hat{\mathcal{U}}(\beta) \mathcal{O}(1)}{\text{Tr} \hat{\mathcal{U}}(\beta)}, \quad (\text{A.14})$$

where $\langle \mathcal{O}(1) \rangle$ reduces to the normal form of the grand canonical average if we put $\eta_{\text{ext}} \rightarrow 0$. By using this notation, we take thermodynamic average of Eqs. (A.13) to obtain

$$\left(-\frac{\partial}{\partial \tau_1} - K_1\right)\Psi(1) = \eta_{\text{ext}}(1) + \eta(1), \quad (\text{A.15a})$$

$$\left(\frac{\partial}{\partial \tau_1} - K_1\right)\bar{\Psi}(1) = \eta_{\text{ext}}^*(1) + \bar{\eta}(1), \quad (\text{A.15b})$$

respectively, where we also define expectation values for $\psi(1)$, $\bar{\psi}(1)$ as

$$\Psi(1) \equiv \langle \psi(1) \rangle, \quad \bar{\Psi}(1) \equiv \langle \bar{\psi}(1) \rangle, \quad (\text{A.16})$$

respectively, and we used the following notations:

$$\eta(1) \equiv \int d1' \bar{V}(1, 1') \langle \bar{\psi}(1') \psi(1') \psi(1) \rangle, \quad (\text{A.17a})$$

$$\bar{\eta}(1) \equiv \int d1' \bar{V}(1, 1') \langle \bar{\psi}(1) \bar{\psi}(1') \psi(1') \rangle. \quad (\text{A.17b})$$

We note that the condensate wave function in this section is given as the expectation value of the field operator different from that introduced in the previous section.

A.2.3 Dyson-Beliaev equation

In this section, we will derive the Dyson-Beliaev equation [14] by using equations in the previous sections. First, we differentiate $\Psi(1)$ in Eq. (A.16) with $\eta_{\text{ext}}(2)$. By using the definition Eq. (A.14), we then obtain

$$\frac{\delta \Psi(1)}{\delta \eta_{\text{ext}}(2)} = -\langle T_\tau \psi(1) \bar{\psi}(2) \rangle + \Psi(1) \bar{\Psi}(2) \equiv G(1, 2). \quad (\text{A.18})$$

where we can see that this quantity is equal to $\langle T_\tau \phi_1(1) \phi_2(2) \rangle$ by using the definition of Eq. (A.3). Similarly, we introduce

$$\frac{\delta \Psi(1)}{\delta \eta_{\text{ext}}(2)} \equiv G(1, 2), \quad \frac{\delta \Psi(1)}{\delta \eta_{\text{ext}}^*(2)} \equiv -F(1, 2) \quad (\text{A.19a})$$

$$\frac{\delta \bar{\Psi}(1)}{\delta \eta_{\text{ext}}(2)} \equiv -\bar{F}(1, 2), \quad \frac{\delta \bar{\Psi}(1)}{\delta \eta_{\text{ext}}^*(2)} \equiv \bar{G}(1, 2). \quad (\text{A.19b})$$

Next, the self energies are defined by

$$\Sigma(1, 2) \equiv \frac{\delta \eta(1)}{\delta \Psi(2)}, \quad \Delta(1, 2) \equiv \frac{\delta \eta(1)}{\delta \bar{\Psi}(2)}, \quad (\text{A.20a})$$

$$\bar{\Delta}(1, 2) \equiv \frac{\delta \bar{\eta}(1)}{\delta \Psi(2)}, \quad \bar{\Sigma}(1, 2) \equiv \frac{\delta \bar{\eta}(1)}{\delta \bar{\Psi}(2)}. \quad (\text{A.20b})$$

By using these functions, the functional differentiation of $\eta(1)$ with respect to $\eta_{\text{ext}}(2)$ is transformed as

$$\begin{aligned} \frac{\delta \eta(1)}{\delta \eta_{\text{ext}}(2)} &= \int d3 \left[\frac{\delta \eta(1)}{\delta \Psi(3)} \frac{\delta \Psi(3)}{\delta \eta_{\text{ext}}(2)} + \frac{\delta \eta(1)}{\delta \bar{\Psi}(3)} \frac{\delta \bar{\Psi}(3)}{\delta \eta_{\text{ext}}(2)} \right] \\ &= \int d3 [\Sigma(1, 3)G(3, 2) - \Delta(1, 3)\bar{F}(3, 2)]. \end{aligned} \quad (\text{A.21a})$$

And, similarly,

$$\frac{\delta \eta(1)}{\delta \eta_{\text{ext}}^*(2)} = \int d3 [-\Sigma(1, 3)F(3, 2) + \Delta(1, 3)\bar{G}(3, 2)], \quad (\text{A.21b})$$

$$\frac{\delta \bar{\eta}(1)}{\delta \eta_{\text{ext}}(2)} = \int d3 [\bar{\Delta}(1, 3)G(3, 2) - \bar{\Sigma}(1, 3)\bar{F}(3, 2)], \quad (\text{A.21c})$$

$$\frac{\delta \bar{\eta}(1)}{\delta \eta_{\text{ext}}^*(2)} = \int d3 [-\bar{\Delta}(1, 3)F(3, 2) + \bar{\Sigma}(1, 3)\bar{G}(3, 2)]. \quad (\text{A.21d})$$

The functional differentiation of Eq. (A.15a) with respect to $\eta_{\text{ext}}(2)$ is given by

$$\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\frac{\delta\Psi(1)}{\delta\eta_{\text{ext}}(2)} = \delta(1,2) + \frac{\delta\eta(1)}{\delta\eta_{\text{ext}}(2)}. \quad (\text{A.22})$$

Substituting this equation to Eq. (A.21a) and using the notation of Eq. (A.18), we obtain

$$\left(-\frac{\partial}{\partial\tau_1} - K_1\right)G(1,2) = \delta(1,2) + \int d3 [\Sigma(1,3)G(3,2) - \Delta(1,3)\bar{F}(3,2)], \quad (\text{A.23a})$$

where $\delta(1,2) \equiv \delta(\tau_1 - \tau_2)\delta(\mathbf{r}_1 - \mathbf{r}_2)$. And, with similar procedures, we also obtain

$$-\left(-\frac{\partial}{\partial\tau_1} - K_1\right)F(1,2) = \int d3 [-\Sigma(1,3)F(3,2) + \Delta(1,3)\bar{G}(3,2)], \quad (\text{A.23b})$$

$$-\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\bar{F}(1,2) = \int d3 [-\bar{\Delta}(1,3)G(3,2) - \bar{\Sigma}(1,3)\bar{F}(3,2)], \quad (\text{A.23c})$$

$$-\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\bar{G}(1,2) = \delta(1,2) + \int d3 [\bar{\Delta}(1,3)F(3,2) + \bar{\Sigma}(1,3)\bar{G}(3,2)]. \quad (\text{A.23d})$$

By combining these equations, we finally arrive at the Dyson-Beliaev equation in a matrix representation as

$$\int d3 [\hat{G}_0^{-1}(1,2) - \hat{\Sigma}(1,3)]\hat{G}(3,2) = \hat{\sigma}_0\delta(1,2), \quad (\text{A.24})$$

where $\hat{\sigma}_0$ is a 2×2 unit matrix, and we define

$$\hat{G}_0^{-1}(1,2) \equiv \left(-\hat{\sigma}_0\frac{\partial}{\partial\tau_1} - \hat{\sigma}_3K_1\right)\delta(1,2), \quad (\text{A.25a})$$

$$\hat{\Sigma}(1,2) \equiv \begin{bmatrix} \Sigma(1,2) & \Delta(1,2) \\ -\bar{\Delta}(1,2) & -\bar{\Sigma}(1,2) \end{bmatrix}, \quad (\text{A.25b})$$

$$\hat{G}(1,2) \equiv \begin{bmatrix} G(1,2) & F(1,2) \\ -\bar{F}(1,2) & -\bar{G}(1,2) \end{bmatrix}. \quad (\text{A.25c})$$

A.2.4 Hugenholtz-Pines relation

Here we will derive the Hugenholtz-Pines relation. This relation states that the quasi-particle excitation in BEC system has gapless (massless) mode, which was proved by Hugenholtz and Pines in 1959 [17]. It is regarded as Goldstone's theorem for the $U(1)$ symmetry breaking.

We first consider the following gauge transformation:

$$\eta_{\text{ext}}(1) \rightarrow e^{i\chi}\eta_{\text{ext}}(1), \quad \hat{\psi}(\mathbf{r}_1) \rightarrow e^{i\chi}\hat{\psi}(\mathbf{r}_1), \quad (\text{A.26})$$

where χ is a constant. By using Eq. (A.15) and (A.21), we obtain

$$\begin{aligned} 0 &= \left(-\frac{\partial}{\partial\tau_1} - K_1\right)\delta\Psi(1) - \delta\eta_{\text{ext}}(1) - \delta\eta(1) \\ &= i\chi\left\{\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\Psi(1) - \eta_{\text{ext}}(1) - \int d2 [\Sigma(1,2)\Psi(2) - \Delta(1,2)\bar{\Psi}(2)]\right\}, \end{aligned} \quad (\text{A.27})$$

$$0 = i\chi\left\{\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\bar{\Psi}(1) - \eta_{\text{ext}}^*(1) - \int d2 [\bar{\Delta}(1,2)\Psi(2) - \bar{\Sigma}(1,2)\bar{\Psi}(2)]\right\}, \quad (\text{A.28})$$

where we used the following variational relations: $\delta\eta_{\text{ext}}(1) = i\chi\eta_{\text{ext}}(1)$, $\delta\eta_{\text{ext}}^*(1) = -i\chi\eta_{\text{ext}}^*(1)$, $\delta\Psi(1) = i\chi\Psi(1)$, $\delta\bar{\Psi}(1) = -i\chi\bar{\Psi}(1)$. By considering an arbitrariness of χ and taking the limit $\eta_{\text{ext}} \rightarrow 0$, we can represent above equations in a combined form as

$$\int d2 [\hat{G}_0^{-1}(1,2) - \hat{\Sigma}(1,2)]\bar{\Psi}(2) = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad (\text{A.29})$$

where we also define the vector $\vec{\Psi}(1)$ by

$$\vec{\Psi}(1) \equiv \begin{bmatrix} \Psi(1) \\ -\bar{\Psi}(1) \end{bmatrix}. \quad (\text{A.30})$$

This equation is the inhomogeneous extension of the Hugenholtz-Pines relation. By imposing the uniform condition $U(\mathbf{r}) \rightarrow 0$, $\Psi(1) \rightarrow n_0$ (n_0 : condensate density), we can express it as

$$\mu = \int d2 [\Sigma(1, 2) - \Delta(1, 2)]. \quad (\text{A.31})$$

Then by performing the Fourier transform to this relation, we arrive at the well-known form [44, 51]:

$$\mu = \Sigma_{\vec{p}=\vec{0}} - \Delta_{\vec{p}=\vec{0}}, \quad (\text{A.32})$$

where $\vec{p} = (\mathbf{p}, i\epsilon_n \equiv 2\pi i n \beta^{-1})$ and n is an integer.

A.3 Construction of Luttinger-Ward functional Φ for BEC

In this section, we derive the expression of the Luttinger-Ward functional for BEC. Our goal is to construct the Luttinger-Ward functional which satisfies the Dyson-Beliaev equation (A.24) and the Hugenholtz-Pines relation (A.29) simultaneously.

A.3.1 Interaction Energy

We first give an expression of a thermodynamic average of interaction term \hat{H}_{int} . Let us introduce \hat{H}_{int} by

$$\hat{H}_{\text{int}} \equiv \frac{1}{2} \int d\mathbf{r} \int d\mathbf{r}' \hat{\psi}(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') V(\mathbf{r} - \mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}). \quad (\text{A.33})$$

By taking the limit $\eta_{\text{ext}} \rightarrow 0$ for Eqs. (A.13a,b), then multiplying $\phi_2(1')$, $\bar{\phi}_2(1')$ from the right sides respectively, and operating T_τ and finally taking the thermodynamic average, we obtain the following two equations

$$-\left(-\frac{\partial}{\partial\tau_1} - K_1\right)G(1, 1') + \delta(1, 1') = \int d2 \bar{V}(1, 2) \langle T_\tau \bar{\psi}(2) \psi(1) \psi(2) \phi_2(1') \rangle, \quad (\text{A.34a})$$

$$-\left(-\frac{\partial}{\partial\tau_1} - K_1\right)\bar{G}(1, 1') + \delta(1, 1') = \int d2 \bar{V}(1, 2) \langle T_\tau \bar{\psi}(2) \psi(1) \psi(2) \phi_1(1') \rangle, \quad (\text{A.34b})$$

respectively, where we used the definition of quasi particle operator $\langle \phi_i \rangle = 0$ and the relation

$$-\langle T_\tau \frac{\partial \phi_1(1)}{\partial \tau_1} \phi_2(1') \rangle = \frac{\partial}{\partial \tau_1} \langle T_\tau \phi_1(1) \phi_2(1') \rangle + \delta(1, 1').$$

We also take the same limit for Eqs. (A.17a,b), and multiply $\bar{\Psi}(1)$, $\Psi(1)$ from the left sides respectively. We add these equations and Eqs. (A.34a,b) to obtain

$$\begin{aligned} & \bar{\Psi}(1) \left(-\frac{\partial}{\partial\tau_1} - K_1 \right) \Psi(1) + \Psi(1) \left(\frac{\partial}{\partial\tau_1} - K_1 \right) \bar{\Psi}(1) \\ & + \left[-\left(-\frac{\partial}{\partial\tau_1} - K_1 \right) G(1, 1') + \delta(1, 1') \right]_{1'=1_+} + \left[-\left(\frac{\partial}{\partial\tau_1} - K_1 \right) \bar{G}(1, 1') + \delta(1, 1') \right]_{1'=1_-} \\ & = \int d2 \bar{V}(1, 2) \left[\langle T_\tau \bar{\psi}(2) \psi(2) \psi(1) \phi_2(1_+) \rangle + \langle T_\tau \bar{\psi}(1) \bar{\psi}(2) \psi(2) \phi_1(1_-) \rangle \right. \\ & \quad \left. + \Psi(1) \langle T_\tau \bar{\psi}(2) \bar{\psi}(2) \psi(1) \rangle + \bar{\Psi}(1) \langle T_\tau \bar{\psi}(1) \bar{\psi}(2) \psi(2) \rangle \right], \quad (\text{A.35}) \end{aligned}$$

where we take $1' \rightarrow 1_+$, $1' \rightarrow 1_-$.

Next we integrate these equations over 1. Then we can find the results multiplied by $1/4\beta$ is equal to the thermodynamic average of Eq. (A.33). Also considering $\bar{V}(1, 2) = V(\mathbf{r}_2 - \mathbf{r}_1)\delta(\tau_2 - \tau_1)$ and $\int d\tau_1\delta(\tau_1) = \beta$, we obtain

$$\begin{aligned} \langle \hat{H}_{\text{int}} \rangle = & \frac{1}{4\beta} \int d1 \left\{ \bar{\Psi}(1) \left(-\frac{\partial}{\partial\tau_1} - K_1 \right) \Psi(1) + \Psi(1) \left(\frac{\partial}{\partial\tau_1} - K_1 \right) \bar{\Psi}(1) \right. \\ & \left. + \left[-\left(-\frac{\partial}{\partial\tau_1} - K_1 \right) G(1, 1') + \delta(1, 1') \right]_{1'=1_+} + \left[-\left(\frac{\partial}{\partial\tau_1} - K_1 \right) \bar{G}(1, 1') + \delta(1, 1') \right]_{1'=1_-} \right\}. \end{aligned} \quad (\text{A.36})$$

Subsequently, we use the Dyson-Beliaev equation (A.24) and the Hugenholtz-Pines relation (A.29). Hence we can transform Eq. (A.36) into

$$\begin{aligned} \langle \hat{H}_{\text{int}} \rangle = & \frac{1}{4\beta} \int d1 \int d2 \{ 2\Sigma(1, 2)[\Psi(2)\bar{\Psi}(1) - G(2, 1_+)] \\ & - \bar{\Delta}(1, 2)[\Psi(2)\Psi(1) - F(2, 1)] - \Delta(1, 2)[\bar{\Psi}(2)\bar{\Psi}(1) - \bar{F}(2, 1)] \}, \end{aligned} \quad (\text{A.37})$$

where we use Eq. (A.6), and $\Sigma(2, 1) = \bar{\Sigma}(1, 2)$, $G(1_-, 2) = G(1, 2_+)$.

A.3.2 Luttinger-Ward functional

Luttinger and Ward [28] gave an expression of the thermodynamic potential $\Omega \equiv -\beta \ln \text{Tr}[\exp(-\beta\hat{H})]$ for a normal Fermi system as a functional of the self energy Σ . Their formulation can be easily extended for the normal Bose system. For convenience, we regard our thermodynamic potential in normal state Ω_{nom} as a functional of G , which can be written as

$$\Omega_{\text{nom}} \equiv -\beta^{-1} \text{Tr}[\ln(-G_0^{-1} + \Sigma) + \Sigma G] + \Phi_{\text{nom}} \quad (\text{A.38})$$

where the trace is defined by $\text{Tr}AB \equiv \int d1 \int d2 A(1, 2)B(2, 1_+)$ and

$$G_0^{-1}(1, 2) \equiv \left(-\frac{\partial}{\partial\tau_1} - \hat{K}_1 \right) \delta(1, 2). \quad (\text{A.39})$$

The functional Φ_{nom} denotes all contribution of skelton diagrams in the perturbation expansion for Ω_{nom} with the replacement $G_0 \rightarrow G$. The functional differentiation of Φ_{nom} with respect to G give the self energy Σ as

$$\Sigma(1, 2) = -\beta^{-1} \frac{\partial \Phi_{\text{nom}}}{\partial G(2, 1)}. \quad (\text{A.40})$$

The stationary condition $\delta\Omega/\delta G(2, 1) = 0$ yields the Dyson equation $G = (G_0^{-1} - \Sigma)^{-1}$. We can also express the functional Φ_{nom} order by order as

$$\Phi_{\text{nom}} = -\beta^{-1} \sum_{n=1}^{\infty} \frac{1}{2n} \text{Tr} \Sigma^n G \quad (\text{A.41})$$

where we note $\Sigma^{(n)}$ has $2n - 1$ Green's function lines. Comparing it with Eq. (A.37) for the normal state limit $F, \Psi \rightarrow 0$, we obtain the following relation for $\langle \hat{H}_{\text{int}} \rangle$ order by order:

$$\langle \hat{H}_{\text{int}} \rangle^{(n)} = \frac{1}{n} \Phi^{(n)}, \quad (\text{A.42})$$

where the factor $1/n$ is due to the extra \hat{H}_{int} present in the evaluation of $\langle \hat{H}_{\text{int}} \rangle^{(n)}$ as compared with that of $\Phi^{(n)}$.

A.3.3 De Dominicis-Martin theorem

Now we construct the Luttinger-Ward functional for $\vec{\Psi} \neq 0$. Dominicis and Martin [52] prove that the thermodynamic potential in thermal equilibrium is expressible as a functional such as $\Omega[T, \mu, \hat{G}, \vec{\Psi}]$. Like the Luttinger-Ward functional in the normal state, the exact Ω for BEC system is stationary with respect to variations for \hat{G} and $\vec{\Psi}$:

$$\frac{\delta\Omega}{\delta G(2,1)} = \frac{\delta\Omega}{\delta \bar{G}(2,1)} = \frac{\delta\Omega}{\delta F(2,1)} = \frac{\delta\Omega}{\delta \bar{F}(2,1)} = 0, \quad \frac{\delta\Omega}{\delta \Psi(1)} = \frac{\delta\Omega}{\delta \bar{\Psi}(1)} = 0. \quad (\text{A.43})$$

Note that our desirable thermodynamic potential Ω must satisfy both Dyson-Beliaev equation (A.24) and Hugenholtz-Pines relation (A.29), and reduce to the normal-state functional Ω_{nom} in the limit of $\vec{\Psi} \rightarrow 0$. Such a functional is given by

$$\Omega = -\frac{1}{\beta} \int d1 \int d2 \Psi_2(1) G_0^{-1}(1,2) \Psi_1(2) + \frac{1}{2\beta} \text{Tr}[\ln(-\hat{G}_0^{-1} + \hat{\Sigma}) + \hat{\Sigma} \hat{G}] + \Phi, \quad (\text{A.44})$$

where $\hat{G}_0^{-1} \equiv (-\hat{\sigma}_0 \partial / \partial \tau_1 - \hat{\sigma}_3 K_1) \delta(1,2)$, $\hat{\sigma}_0$, $\hat{\sigma}_3$ are 2×2 unit matrix and third Pauli matrix respectively, and the trace $\text{Tr} \hat{\Sigma} \hat{G}$ is defined by

$$\text{Tr} \hat{\Sigma} \hat{G} \equiv \int d1 \int d2 \text{Tr} \begin{bmatrix} \Sigma(1,2) & \Delta(1,2) \\ -\bar{\Delta}(1,2) & -\bar{\Sigma}(1,2) \end{bmatrix} \begin{bmatrix} G(2,1_+) & F(2,1) \\ -\bar{F}(2,1) & -\bar{G}(2,1_-) \end{bmatrix}. \quad (\text{A.45})$$

We also give an expression of the self energy $\hat{\Sigma} \equiv (\Sigma_{ij})$ similarly as in the case of the normal state (A.40) as

$$\Sigma_{ij}(1,2) \equiv -2\beta \frac{\delta\Phi}{\delta G_{ji}(2,1)}, \quad (\text{A.46a})$$

where we used notations $\hat{G} \equiv (G_{ij})$, $\vec{\Psi} \equiv (\Psi_i)$, and $\Phi = \Phi[\hat{G}, \vec{\Psi}]$ in Eq. (A.44). By using this definition, we can obtain the following relation:

$$\beta \frac{\delta\Phi}{\delta \Psi_{3-i}(1)} = \Sigma_{i\bar{j}}(1, \bar{2}) (-1)^{\bar{j}-1} \Psi_{\bar{j}}(\bar{2}), \quad (\text{A.46b})$$

where summation and integration over barred indices \bar{j} , $\bar{2}$ are implied. We haven't found how Φ can be constructed as the functional of \hat{G} and $\vec{\Psi}$ yet. However, differentiating Eq. (A.44) with respect to \hat{G} and $\vec{\Psi}$, these reduce to the Dyson-Beliaev equation (A.24) and Hugenholtz-Pines relation (A.29) respectively.

A.3.4 Exact relations with Φ

We derive exact relations for BEC. Substituting the n th-order contribution of Eq. (A.37) into Eq. (A.42) and using Eq. (A.46a), we obtain

$$2n\Phi^{(n)} + \int d1 \int d2 \left\{ \frac{\delta\Phi^{(n)}}{\delta G(2,1)} [\Psi(2)\bar{\Psi}(1) - G(2,1)] + \frac{\delta\Phi^{(n)}}{\delta F(2,1)} [\Psi(2)\Psi(1) - F(2,1)] + \frac{\delta\Phi^{(n)}}{\delta \bar{F}(2,1)} [\bar{\Psi}(2)\bar{\Psi}(1) - \bar{F}(2,1)] \right\} = 0. \quad (\text{A.47})$$

We also substitute Eq. (A.46a) into Eq. (A.46b) to obtain

$$\frac{\delta\Phi}{\delta \bar{\Psi}(1)} + \int d2 \left[\frac{\delta\Phi}{\delta G(2,1)} \Psi(2) + 2 \frac{\delta\Phi}{\delta \bar{F}(2,1)} \bar{\Psi}(2) \right] = 0. \quad (\text{A.48})$$

By using these equations, we can determine the specific structure of Φ order by order. For a later convenience, we define the symmetrized vertex as

$$\Gamma^{(0)}(11', 22') \equiv V(\mathbf{r}_1 - \mathbf{r}_2) \delta(\tau_1 - \tau_2) [\delta(1,1') \delta(2,2') + \delta(1,2') \delta(2,1')], \quad (\text{A.49})$$

which also satisfies the following relations:

$$\Gamma^{(0)}(11', 22') = \Gamma^{(0)}(22', 11') = \Gamma^{(0)}(1'1, 2'2) = \Gamma^{(0)}(2'1, 21'). \quad (\text{A.50})$$

A.3.5 Constructing Φ

We here present how to construct Φ which satisfies the Dyson-Beliaev equation (A.24) and the Hugenholtz-Pines relation (A.29). Feynman diagrams of G, F, \bar{F} are expressible in the same way as those of superconductivity [51] and $\Gamma^{(0)}$ is denoted by a filled circle. And we suppress drawing the condensate wave function $\Psi, \bar{\Psi}$ following Popov [25], which can be easily recovered by considering the relation between the number of Green's function lines and its perturbative order. We summarize the steps for constructing n th-order functional $\Phi^{(n)}$ as follows:

- (i) : Draw all the normal-state diagrams contributing to $\Phi^{(n)}$, whose numerical weights are equal to those of the perturbation analysis for the normal state.
- (ii) : Draw all the distinct diagrams obtained from those of (i) by successively replacing G by F, \bar{F} , whose numerical weights are still undetermined.
- (iii) : Draw all the distinct diagrams constructed by the steps (i) and (ii) by successively removing a Green's function line so as to satisfy the condition that a further removal of any line from each diagram would not break itself into two unconnected parts.
- (iv) : Determine numerical weights of these diagrams by using Eqs. (A.47), (A.48).

By following these procedures, we can construct the Luttinger-Ward functional order by order. We draw the diagrams $\Phi^{(1)}$ and $\Phi^{(2)}$ as Fig.24 and 25 respectively. Finally, we note that the diagram with only vertex in $\Phi^{(1)}$ has the weight $T/4$.

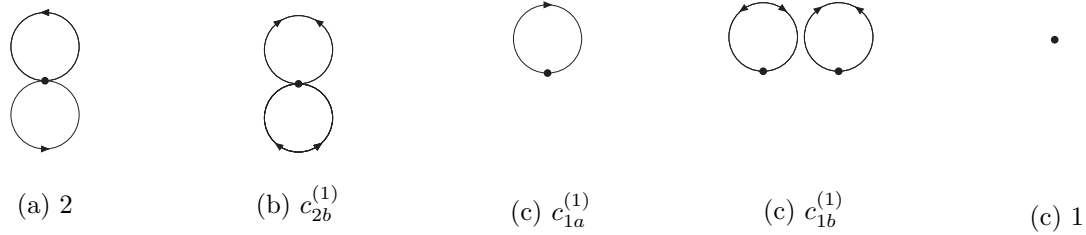


Fig 24: Diagrammatic expression of $\Phi^{(1)}$

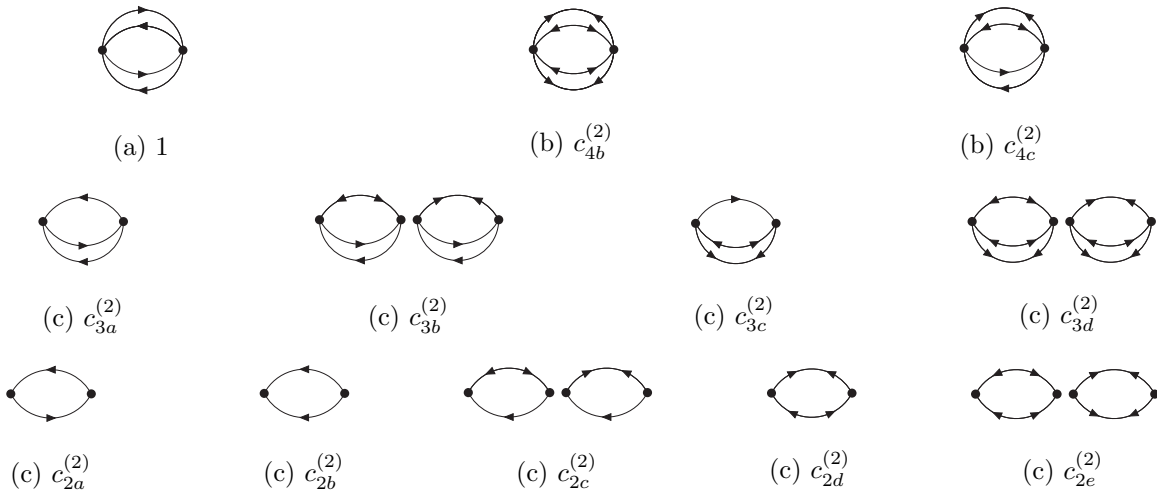


Fig 25: Diagrammatic expression of $\Phi^{(2)}$

Based on these diagrammatic expressions, we can express $\Phi^{(1)}$ and $\Phi^{(2)}$ as

$$\begin{aligned}\Phi^{(1)} &= \frac{T}{4} \int d1 \int d1' \int d2 \int d2' \Gamma^{(0)}(11', 22') \\ &\quad \times \{2G(1.1')G(2, 2') + c_{2b}^{(1)}F(1.2)\bar{F}(1', 2') + c_{1a}^{(1)}G(1, 1')\Psi(2)\bar{\Psi}(2') \\ &\quad + c_{1b}^{(1)}[F(1, 2)\bar{\Psi}(1')\bar{\Psi}(2') + \bar{F}(1', 2')\Psi(1)\Psi(2)] + \bar{\Psi}(1')\bar{\Psi}(2')\Psi(2)\Psi(1)\} \end{aligned} \quad (\text{A.51})$$

$$\begin{aligned}\Phi^{(2)} &= -\frac{T}{8} \int d1 \dots \int d4' \Gamma^{(0)}(11', 22') \Gamma^{(0)}(33', 44') \\ &\quad \times \{G(2, 3')G(3, 2')G(1, 4')G(4', 1) + c_{4b}^{(2)}\bar{F}(2', 3')F(2, 3)G(1, 4')G(4, 1') \\ &\quad + c_{4c}^{(2)}\bar{F}(2', 3')F(2, 3)\bar{F}(1', 4')F(1, 4) + c_{3a}^{(2)}G(2, 3')G(3, 2')G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{3b}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]G(1, 4')G(4, 1') \\ &\quad + c_{3c}^{(2)}\bar{F}(2', 3')F(2, 3)G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{3d}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]\bar{F}(1', 4')F(1, 4) \\ &\quad + c_{2a}^{(2)}G(2, 3')G(3, 2')\Psi(1)\bar{\Psi}(4)\Psi(4')\bar{\Psi}(1') + c_{2b}^{(2)}G(2, 3')\Psi(3)\bar{\Psi}(2')G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2c}^{(2)}[\bar{F}(2', 3')\Psi(2)\Psi(3) + F(2, 3)\bar{\Psi}(2')\bar{\Psi}(3')]G(1, 4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2d}^{(2)}\bar{F}(2', 3')F(2, 3)\Psi(1)\bar{\Psi}(4')\Psi(4)\bar{\Psi}(1') \\ &\quad + c_{2e}^{(2)}[F(2, 3)\bar{\Psi}(3')\bar{\Psi}(2')F(1, 4)\bar{\Psi}(4')\bar{\Psi}(1') + \bar{F}(2', 3')\Psi(3)\Psi(2)\bar{F}(1', 4')\Psi(4)\Psi(1)]\}, \end{aligned} \quad (\text{A.52})$$

respectively. By imposing Eq. (A.47) for Eq. (A.51), we obtain

$$4 + c_{1a}^{(1)} = 0, \quad c_{2b}^{(1)} + c_{1b}^{(1)} = 0, \quad c_{1a}^{(1)} + 2c_{1b}^{(1)} + 2 = 0,$$

which can be solved easily as

$$c_{2b}^{(1)} = -1, \quad c_{1a}^{(1)} = -4, \quad c_{1b}^{(1)} = 1 \quad (\text{A.53})$$

Similarly, we also obtain the equations for Eq. (A.52) as

$$\begin{aligned}0 &= c_{3a}^{(2)} + 4 = c_{3b}^{(2)} + c_{4b}^{(2)} = c_{3c}^{(2)} + 2c_{4b}^{(2)} = c_{3d}^{(2)} + 2c_{4c}^{(2)}, \\ 0 &= c_{2a}^{(2)} + c_{3a}^{(2)} + c_{3b}^{(2)} = 2c_{2b}^{(2)} + c_{3a}^{(2)} = 2c_{2c}^{(2)} + c_{3c}^{(2)} + 2c_{3b}^{(2)} \\ &= 2c_{2b}^{(2)} + c_{3c}^{(2)} + 4c_{3d}^{(2)} = 2c_{2e}^{(2)} + c_{3d}^{(2)}, \\ 0 &= c_{2a}^{(2)} + c_{2b}^{(2)} + c_{2c}^{(2)} = c_{2c}^{(2)} + c_{2d}^{(2)} + 2c_{2e}^{(2)}.\end{aligned}$$

We solve these equations as

$$\begin{aligned}c_{4b}^{(2)} &= -2, \quad c_{4c}^{(2)} = 1 \\ c_{3a}^{(2)} &= -4, \quad c_{3b}^{(2)} = 2, \quad c_{3c}^{(2)} = 4, \quad c_{3d}^{(2)} = -2 \\ c_{2a}^{(2)} &= c_{2b}^{(2)} = 2, \quad c_{2c}^{(2)} = -4, \quad c_{2d}^{(2)} = 2, \quad c_{2e}^{(2)} = 1.\end{aligned} \quad (\text{A.54})$$

Thus we can determine numerical weights of the Feynman diagrams uniquely by using exact relations for BEC (A.47), (A.48). We note that we can obtain the same numerical weights by using either of them [30].

A.4 Two-particle Geen's function

Here, we discuss two-particle Green's function [31]. First, we introduce an extra perturbation \hat{U} given in an S -matrix form. And, we differentiate it with respect to \hat{U} , then take limit of $\hat{U} \rightarrow 0$. The procedure yields the Bethe-Salpeter equation for BEC.

A.4.1 Extra perturbation

First, we define two-particle Green's function by using Eq. (A.3) as

$$\begin{aligned} \mathcal{K}_{ij,kl}(12, 34) &\equiv \langle T_\tau \psi_i(1) \psi_k(3) \psi_{3-l}(4) \psi_{3-j}(2) \rangle (-1)^{j+l} \\ &\quad - \langle T_\tau \psi_i(1) \psi_{3-j}(2) \rangle \langle T_\tau \psi_k(3) \psi_{3-l}(4) \rangle (-1)^{j+l}, \end{aligned} \quad (\text{A.55})$$

with the nonlocal potential $\hat{U} \equiv U_{ij}$. We note that collective modes correspond to the two-particle Green' function.

Second, we introduce an extra perturbation described by the S -matrix as

$$\mathcal{S}(\beta) \equiv T_\tau \exp \left[-\frac{1}{2} \psi_{\bar{i}}(\bar{1}) \psi_{3-\bar{j}}(\bar{2}) (-1)^{\bar{j}-1} U_{\bar{i}\bar{j}}(\bar{2}, \bar{1}) \right]. \quad (\text{A.56})$$

The full Matsubara Green's function is also defined by

$$\begin{aligned} \mathcal{G}_{ij}(1, 2) &\equiv -\frac{\langle T_\tau \mathcal{S}(\beta) \psi_i(1) \psi_{3-j}(2) \rangle}{\mathcal{S}(\beta)} (-1)^{j-1} \\ &= -\langle T_\tau \mathcal{S}(\beta) \psi_i(1) \psi_{3-j}(2) \rangle_c (-1)^{j-1}, \end{aligned} \quad (\text{A.57a})$$

where the subscript c represents contribution of Feynman diagrams which are connected with $\psi_i(1)$ and (or) $\psi_{3-j}(2)$, and $\Psi_i(1)$ is rewritten as $\Psi_i(1) \equiv \langle T_\tau \mathcal{S}(\beta) \psi_i(1) \rangle_c$. Equation (A.57a) is also expressible as

$$\mathcal{G}_{ij} = G_{ij}(1, 2) - \Psi_i(1) \Psi_{3-j}(2) (-1)^{j-1}, \quad (\text{A.57b})$$

where $G_{ij}(12) \equiv -\langle T_\tau \mathcal{S}(\beta) \phi_i(1) \phi_{3-j}(2) \rangle_c (-1)^{j-1}$. Note this quantity reduces to Eq. (A.4) for $\hat{U} \rightarrow \hat{0}$. From Eq. (A.57a), it can be seen that two-particle Green's function (A.55) is given by

$$\mathcal{K}_{ij,kl}(12, 34) = 2 \frac{\delta \mathcal{G}_{ij}(1, 2)}{\delta U_{lk}(4, 3)}, \quad (\text{A.58})$$

where taking the limit $\hat{U} \rightarrow \hat{0}$ after differentiation is implied. We will use this procedure implicitly below. Next, substituting Eq. (A.57b) into Eq. (A.58), we obtain

$$\mathcal{K}_{ij,kl}(12, 34) = 2 \frac{\delta G_{ij}(1, 2)}{\delta U_{lk}(4, 3)} - 2 \left[\Psi_i(1) \frac{\delta \Psi_{3-j}(2)}{\delta U_{lk}(4, 3)} + \frac{\delta \Psi_i(1)}{\delta U_{lk}(4, 3)} \Psi_{3-j}(2) \right] (-1)^{j-1}, \quad (\text{A.59})$$

where we find that we only need to know linear responses of \hat{G} and $\vec{\Psi}$ to \hat{U} for writing \mathcal{K} down explicitly.

A.4.2 Linear response of \hat{G} and $\vec{\Psi}$

First we note that an extra term appear in $\hat{G}^{-1}(1, 2) \equiv \hat{G}_0^{-1}(1, 2) - \hat{\Sigma}(1, 2)$ by adding the perturbation \hat{U} as

$$\hat{G}^{-1}(1, 2) = \left(-\hat{\sigma}_0 \frac{\partial}{\partial \tau_1} - \hat{\sigma}_3 \hat{K}_1 \right) \delta(1, 2) - \hat{\Sigma}(1, 2) - \hat{U}'(1, 2), \quad (\text{A.60})$$

where the extra $\hat{U}' \equiv (U'_{ij})$ is given by

$$U'_{ij}(1, 2) \equiv \frac{U_{ij}(1, 2) + (-1)^{i+j+1} U_{3-j, 3-i}(2, 1)}{2}. \quad (\text{A.61})$$

By varying $\hat{U} \rightarrow \hat{U} + \delta \hat{U}$, then setting $\hat{U} = \hat{0}$ for Dyson-Beliaev equation (A.24) and Hugenholtz-Pines relation (A.29), we obtain the following equations as

$$\hat{G}^{-1}(1, \bar{3}) \delta \hat{G}(\bar{3}, 2) = [\delta \hat{U}(1, \bar{3}) + \delta \hat{\Sigma}(1, \bar{2})] \hat{G}(\bar{3}, 2), \quad (\text{A.62a})$$

$$\hat{G}^{-1}(1, \bar{3}) \delta \vec{\Psi}(\bar{3}) = [\delta \hat{U}(1, \bar{3}) + \delta \hat{\Sigma}(1, \bar{2})] \hat{\sigma}_3 \vec{\Psi}(\bar{2}), \quad (\text{A.62b})$$

respectively. Let us introduce the following vertices for a later convenience:

$$\Gamma_{ij,kl}^{(4)}(12, 34) \equiv -\frac{1}{2} \frac{\delta \Sigma_{ij}(1, 2)}{\delta G_{lk}(4, 3)} = \frac{1}{T} \frac{\delta^2 \Phi}{\delta G_{ij}(2, 1) \delta G_{lk}(4, 3)}, \quad (\text{A.63a})$$

$$\begin{aligned} \Gamma_{ij,k}^{(3)}(12, 3) &\equiv \frac{1}{2} (-1)^{k-1} \frac{\delta \Sigma_{ij}(1, 2)}{\delta \Psi_k(3)} \\ &= 2(-1)^{k+\bar{l}} \Gamma^{(4)}_{ij, 3-k\bar{l}}(12, 3\bar{4}) \Psi_{\bar{l}}(\bar{4}), \end{aligned} \quad (\text{A.63b})$$

$$\tilde{\Gamma}_{i,jk}^{(3)}(1, 23) \equiv 2(-1)^{\bar{l}-1} \Gamma^{(4)}(1\bar{4}, 23) \Psi_{\bar{l}}(\bar{4}) = (-1)^i \Gamma_{jk, 3-i}^{(3)}(23, 1), \quad (\text{A.63c})$$

$$\Gamma_{ij}^{(2)} \equiv 2(-1)^{\bar{k}-1} \Gamma_{i\bar{k}, j}^{(3)}(1\bar{3}, 2) \Psi_{\bar{k}}(\bar{3}), \quad (\text{A.63d})$$

where we used Eq. (A.46) for deriving the second expression of $\Gamma^{(3)}$, $\Gamma^{(4)}$. These are the irreducible vertices of our condensed Bose system, as seen below. In Fig.26, we give the diagrammatic expressions of them. By considering Eq. (A.6) and $\Phi = \Phi^*$, we can find symmetry relations of vertices such as $\Gamma_{ij,kl}^{(4)}(12, 34) = \Gamma_{kl,ij}^{(4)}(34, 12) = (-1)^{i+j-1} \Gamma_{3-j, 3-i, kl}^{(4)}(21, 34)$ etc. Note that our $\Gamma^{(3)}$, $\Gamma^{(4)}$ correspond to I and J of Gavoret and Nozières [18], respectively. Our formulations may have an advantage over theirs because the vertices can be obtained from a single functional Φ with clear relations among them.

By using $\Gamma^{(4)}$, $\Gamma^{(3)}$, we can express $\delta \tilde{\Sigma}$ in Eq. (A.62) as

$$\delta \Sigma_{ij}(1, 2) = -2\Gamma_{ij, \bar{l}\bar{k}}^{(4)}(12, \bar{4}\bar{3}) \delta G_{\bar{k}\bar{l}}(\bar{3}, \bar{4}) + 2\Gamma_{ij, \bar{k}}^{(3)}(12, \bar{3}) (-1)^{\bar{k}-1} \delta \tilde{\Psi}_{\bar{k}}(\bar{3}). \quad (\text{A.64})$$

This relation enables us to obtain closed equations for $\delta \hat{G}$ and $\delta \tilde{\Psi}$. To be specific, we multiply Eq. (A.62) by \hat{G} from the left, substitute Eq. (A.64), and use Eqs. (A.63c,d). The procedure yields

$$\begin{aligned} \delta G_{ij}(1, 2) &= G_{i\bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) \delta U'_{\bar{l}\bar{k}}(\bar{4}, \bar{3}) - 2G_{i\bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) \Gamma_{\bar{l}\bar{k}, \bar{m}\bar{n}}^{(4)}(\bar{4}\bar{3}, \bar{6}\bar{5}) \delta G_{\bar{m}\bar{n}}(\bar{5}, \bar{6}) \\ &\quad + 2G_{i\bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) \Gamma_{\bar{l}\bar{k}, \bar{m}}^{(3)}(\bar{4}\bar{3}, \bar{5}) (-1)^{\bar{m}-1} \delta \Psi_{\bar{m}}(\bar{5}), \end{aligned} \quad (\text{A.65a})$$

$$\begin{aligned} (-1)^{i-1} \delta \Psi_i(1) &= G_{i\bar{k}}(1, \bar{3}) (-1)^{\bar{j}-1} \Psi_{\bar{j}}(\bar{2}) \delta U'_{\bar{k}\bar{j}}(\bar{3}, \bar{2}) - G_{i\bar{j}}(1, \bar{3}) \tilde{\Gamma}_{\bar{i}, \bar{j}\bar{k}}^{(3)}(\bar{2}, \bar{4}\bar{3}) \delta G_{\bar{k}\bar{l}}(\bar{3}, \bar{4}) \\ &\quad + G_{i\bar{j}}(1, \bar{2}) \Gamma_{\bar{j}\bar{k}}^{(2)}(\bar{2}, \bar{3}) (-1)^{\bar{k}-1} \delta \Psi_{\bar{k}}(\bar{3}). \end{aligned} \quad (\text{A.65b})$$

We also obtain from Eq. (A.61) the relation

$$G_{i\bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) \delta U'_{\bar{l}\bar{k}}(\bar{4}, \bar{3}) = \frac{1}{2} [G_{i\bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) + (-1)^{\bar{k}+\bar{l}-1} G_{i, 3-\bar{k}}(1, \bar{3}) G_{3-\bar{l}, j}(\bar{4}, 2)] \delta U_{\bar{l}\bar{k}}(\bar{4}, \bar{3}). \quad (\text{A.66})$$

We can also transform

$$G_{i, \bar{l}}(1, \bar{4}) G_{\bar{k}j}(\bar{3}, 2) \Gamma^{(4)}(\bar{4}\bar{3}, 56) = (-1)^{\bar{k}+\bar{l}-1} G_{i, 3-\bar{k}}(1, \bar{3}) G_{3-\bar{l}, j}(\bar{4}, 2) \Gamma_{\bar{l}\bar{k}m\bar{n}}^{(4)}(\bar{4}\bar{3}, 56), \quad (\text{A.67})$$

by using

$$\Gamma_{ij,kl}^{(4)}(12, 34) = (-1)^{i+j-1} \Gamma_{3-j, 3-i, kl}^{(4)}(21, 34). \quad (\text{A.68})$$

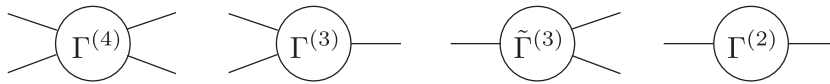


Fig 26: Irreducible vertices

A.4.3 Bethe-Salpeter equation for BEC

We can express Eq. (A.65). We start to introduce the following notations for $\delta\vec{G}$ and $\delta\vec{U}$ as

$$\langle 12_{ij} | \delta\vec{G} \rangle = \delta G_{ij}(1, 2), \quad \langle 12_{ij} | \delta\vec{U} \rangle = \delta U_{ij}(1, 2). \quad (\text{A.69})$$

We also introduce the matrices $\underline{\mathcal{K}}$, $\underline{\Gamma}^{(4)}$, $\underline{\chi}^{(0)}$, $\underline{1}$, $\underline{\Gamma}^{(3)}$, $\tilde{\underline{\Gamma}}^{(3)}$, $\underline{\Psi}^{(3)}$, $\tilde{\underline{\Psi}}^{(3)}$, and $\underline{\Gamma}^{(2)}$ as

$$\langle 12_{ij} | \underline{\mathcal{K}} | 43_{lk} \rangle \equiv \mathcal{K}_{ij,kl}(12, 34), \quad (\text{A.70a})$$

$$\langle 12_{ij} | \underline{\Gamma}^{(4)} | 43_{lk} \rangle \equiv \Gamma^{(4)}_{ij,kl}(12, 34), \quad (\text{A.70b})$$

$$\langle 12_{ij} | \underline{\chi}^{(0)} | 43_{lk} \rangle \equiv G_{il}(1, 4)G_{kj}(3, 2) + (-1)^{k+l-1}G_{i,3-k}(1, 3)G_{3-l,j}(4, 2), \quad (\text{A.70c})$$

$$\langle 12_{ij} | \underline{1} | 43_{lk} \rangle \equiv \delta_{il}\delta_{kj}\delta(1, 4)\delta(3, 2), \quad (\text{A.70d})$$

$$\langle 12_{ij} | \underline{\Gamma}^{(3)} | 3_k \rangle \equiv \Gamma^{(3)}_{ij,k}(12, 3), \quad (\text{A.70e})$$

$$\langle 1_i | \tilde{\underline{\Gamma}}^{(3)} | 32_{kj} \rangle \equiv \tilde{\Gamma}^{(3)}_{i,jk}(1, 23), \quad (\text{A.70f})$$

$$\langle 12_{ij} | \underline{\Psi}^{(3)} | 3_k \rangle \equiv (-1)^{j+k}[\Psi_i(1)\delta_{k,3-j}\delta(3, 2) + \delta_{ki}\delta(3, 1)\Psi_{3-j}(3)], \quad (\text{A.70g})$$

$$\langle 1_i | \tilde{\underline{\Psi}}^{(3)} | 32_{kj} \rangle \equiv (-1)^{j-1}[\delta_{lk}\delta(1, 3)\Psi_j(2) + \delta_{i,3-j}\delta(1, 2)\Psi_{3-k}(3)], \quad (\text{A.70h})$$

$$\langle 1_i | \underline{\Gamma}^{(2)} | 2_j \rangle \equiv \Gamma^{(2)}_{ij}(1, 2), \quad (\text{A.70i})$$

where the quantity $\underline{\chi}^{(0)}$ expresses independent propagation of two particles.

Using Eqs. (A.69) and (A.70), we can obtain the equations $\delta\vec{G} = \frac{1}{2}\underline{\chi}^{(0)}\delta\vec{U} - \underline{\chi}^{(0)}\underline{\Gamma}^{(4)}\delta\vec{G} + \underline{\chi}^{(0)}\underline{\Gamma}^{(3)}\hat{\sigma}_3\delta\vec{\Psi}$ and $\hat{\sigma}_3\delta\vec{\Psi} = \frac{1}{2}\hat{G}\hat{\underline{\Psi}}^{(3)}\delta\vec{U} - \hat{G}\hat{\underline{\Gamma}}^{(3)}\delta\vec{G} + \hat{G}\hat{\underline{\Gamma}}^{(2)}\hat{\sigma}_3\delta\vec{\Psi}$ from Eq. (A.65). We finally obtain

$$\delta\vec{G} = \frac{1}{2}\underline{\chi}^{(4)}\delta\vec{U} + \underline{\chi}^{(4)}\underline{\Gamma}^{(3)}\hat{\sigma}_3\delta\vec{\Psi}, \quad (\text{A.71a})$$

$$\hat{\sigma}_3\delta\vec{\Psi} = \frac{1}{2}\hat{\chi}^{(2)}\tilde{\underline{\Psi}}^{(3)}\delta\vec{U} - \hat{\chi}^{(2)}\tilde{\underline{\Gamma}}^{(3)}\delta\vec{G}, \quad (\text{A.71b})$$

where

$$\underline{\chi}^{(4)} \equiv (\underline{1} + \underline{\chi}^{(0)}\underline{\Gamma}^{(4)})^{-1}\underline{\chi}^{(0)} = (\underline{\chi}^{(0)-1} + \underline{\Gamma}^{(4)})^{-1}, \quad (\text{A.72a})$$

$$\hat{\chi}^{(2)} \equiv (\hat{1} - \hat{G}\hat{\underline{\Gamma}}^{(2)})^{-1}\hat{G} = (\hat{G}^{-1} - \hat{\Gamma}^{(2)})^{-1}. \quad (\text{A.72b})$$

It is convenient to define the quantities:

$$\underline{\chi}^{(q)} \equiv (\underline{\chi}^{(4)-1} + \underline{\Gamma}^{(3)}\hat{\chi}^{(2)}\tilde{\underline{\Gamma}}^{(3)})^{-1}, \quad (\text{A.72c})$$

$$\hat{\chi}^{(c)} \equiv (\hat{\chi}^{(2)-1} + \tilde{\underline{\Gamma}}^{(3)}\underline{\chi}^{(4)}\underline{\Gamma}^{(3)})^{-1} = (\hat{G}^{-1} - \hat{\Gamma}^{(2)} + \tilde{\underline{\Gamma}}^{(3)}\underline{\chi}^{(4)}\underline{\Gamma}^{(3)})^{-1}, \quad (\text{A.72d})$$

where the superscripts q and c means ‘‘quasiparticle’’ and ‘‘condensate’’ respectively. These quantities are represented diagrammatically in Fig. 27. We thus obtain solution of Eq. (A.71) in terms of $\underline{\chi}^{(q)}$ and $\hat{\chi}^{(c)}$ as

$$\delta\vec{G} = \frac{1}{2}\underline{\chi}^{(q)}(\underline{1} + \underline{\Gamma}^{(3)}\hat{\chi}^{(2)}\tilde{\underline{\Psi}}^{(3)})\delta\vec{U}, \quad (\text{A.73a})$$

$$\delta\vec{\Psi} = \frac{1}{2}\hat{\sigma}_3\hat{\chi}^{(c)}(\tilde{\underline{\Psi}}^{(3)} - \tilde{\underline{\Gamma}}^{(3)}\underline{\chi}^{(4)})\delta\vec{U}. \quad (\text{A.73b})$$

By substituting Eq. (A.73) into Eq. (A.59) and using the notations of Eq. (A.70) and $\underline{\chi}^{(q)}\underline{\Gamma}^{(3)}\hat{\chi}^{(2)} = \underline{\chi}^{(4)}\underline{\Gamma}^{(3)}\hat{\chi}^{(c)}$ in Eq. (A.72), we obtain the Bethe-Salpeter equation:

$$\underline{\mathcal{K}} = \underline{\chi}^{(q)} + \underline{\chi}^{(4)}\underline{\Gamma}^{(3)}\hat{\chi}^{(c)}\tilde{\underline{\Psi}}^{(3)} + \underline{\Psi}^{(3)}\hat{\chi}^{(c)}\tilde{\underline{\Gamma}}^{(3)}\underline{\chi}^{(4)} - \underline{\Psi}^{(3)}\hat{\chi}^{(c)}\tilde{\underline{\Psi}}^{(3)}. \quad (\text{A.74})$$

$$\begin{aligned}
\chi^{(4)} &= \chi^{(0)} + \chi^{(0)} \Gamma^{(4)} \chi^{(0)} + \dots \\
\chi^{(2)} &= \text{---} + \text{---} \Gamma^{(2)} \text{---} + \dots \\
\chi^{(4)} &= \chi^{(4)} + \chi^{(4)} \Gamma^{(3)} \chi^{(2)} \tilde{\Gamma}^{(3)} \chi^{(4)} + \dots \\
\chi^{(c)} &= \chi^{(2)} + \chi^{(2)} \tilde{\Gamma}^{(3)} \chi^{(4)} \Gamma^{(3)} \chi^{(2)} + \dots
\end{aligned}$$

Fig 27: Diagrammatic structure of Eq. (A.72). Every long straight line in the second equation denotes \hat{G} .

We now discuss poles of two-particle Green's function \mathcal{K} . Poles of $\underline{\chi}^{(4)}$ in Eq. (A.74) are cancelled by those of $\underline{\chi}^{(4)}$ in the denominator of $\underline{\chi}^{(c)}$ in Eq. (A.72). It can be also seen that the poles of $\underline{\chi}^{(c)}$ are generally not identical to those of the one particle Green's function \hat{G} due to the additional terms $\hat{\Gamma}^{(2)} - \tilde{\Gamma}^{(3)} \underline{\chi}^{(4)} \tilde{\Gamma}^{(3)}$, which contradicts with the statement by Gavoret and Nozières [18]. They erroneously identified $\underline{\chi}^{(c)}$ as the one particle Green's function's line [31].

B Quantum Monte Carlo Methods

B.1 Green's Function Monte Carlo Method

Here we will introduce the Green's function Monte Carlo (GFMC) method [37, 54], which is one of the diffusion quantum Monte Carlo (DQMC) methods [55]. DQMC methods give exact results which have no dependences on trial functions in principle. The GFMC method is a powerful tool for calculations in quantum many-body systems, especially for bosonic cases.

B.1.1 Outline of DQMC method

First, we consider a system of N identical bosons with mass m and spin 0 interacting via a two-body potential $V(\mathbf{r} - \mathbf{r}')$. The corresponding Hamiltonian \hat{H} is given by

$$\hat{H} \equiv \sum_{i=1}^N \left[\frac{\hbar^2}{2m} \Delta_i + U(\mathbf{r}_i) \right] + \sum_{i < j} V(\mathbf{r}_i - \mathbf{r}_j), \quad (\text{B.1})$$

where $\mathbf{r}_i \equiv (x_i, y_i, z_i)$, $\Delta_i \equiv \nabla_i \cdot \nabla_i = (\partial_{x_i}^2 + \partial_{y_i}^2 + \partial_{z_i}^2)$, and $U(\mathbf{r}_i)$ is the external field. The exact N -body wave function $\Psi(\mathbf{R}, t)$ satisfies the time-dependent Schrödinger equation as

$$i\hbar \frac{\partial \Psi(\mathbf{R}, t)}{\partial t} = \hat{H} \Psi(\mathbf{R}, \tau), \quad (\text{B.2})$$

with $\mathbf{R} \equiv (\mathbf{r}_1, \dots, \mathbf{r}_N)$. Next, we introduce the imaginary time $\tau \equiv -it/\hbar$ and a constant energy shift E . Then we can rewrite Eq. (B.2) as

$$-\frac{\partial \Psi(\mathbf{R}, \tau)}{\partial \tau} = (\hat{H} - E) \Psi(\mathbf{R}, \tau), \quad (\text{B.3})$$

whose formal solution can be written as $\Psi(\mathbf{R}, \tau) = e^{-(\hat{H}-E)\tau} \Psi(\mathbf{R}, 0)$. By introducing eigenfunctions and eigenvalues as $\phi_n(\mathbf{R}, \tau)$ and E_n which are ordered by increasing order $E_0 < E_1 < \dots$ respectively, $\Psi(\mathbf{R}, \tau)$ can be expanded as

$$\Psi(\mathbf{R}, \tau) = \sum_{n=0}^{\infty} c_n \phi_n(\mathbf{R}, 0) e^{-(E_n - E)\tau}, \quad (\text{B.4})$$

with c_n the expansion prefactor. In the limit of $\tau \rightarrow \infty$, excited states vanish and the ground state eigenfunction will have dominant contribution as,

$$\Psi(\mathbf{R}, \tau) \rightarrow c_0 \phi_0(\mathbf{R}, 0) e^{-(E_0 - E)\tau}. \quad (\text{B.5})$$

If the energy shift E we choose is equal to the exact ground state energy E_0 , only the ground state eigenfunction will survive. Finally, we can determine the ground state eigenfunction ϕ_0 and energy E_0 . We can also estimate other physical quantities.

B.1.2 GFMC method

In this subsection, we introduce the GFMC method which needs a trial wave function $\psi_T(\mathbf{R})$, but final results are exact for physical quantities which commute with \hat{H} . This will be explained later. We start from Eq. (B.3), which is expressible in terms of the distribution function $f(\mathbf{R}, \tau) \equiv \langle \mathbf{R} | f(\tau) \rangle \equiv \psi_T(\mathbf{R}) \Psi(\mathbf{R}, \tau)$ as

$$\begin{aligned} -\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau} &= \sum_{i=1}^N [-D \Delta_i f(\mathbf{R}, \tau) + D \nabla_i \cdot (\mathbf{F}_i f(\mathbf{R}, \tau))] + (E_{loc}(\mathbf{R}) - E) f(\mathbf{R}, \tau) \\ &\equiv (\hat{A}_1 + \hat{A}_2 + \hat{A}_3) f(\mathbf{R}, \tau) \equiv \hat{A} f(\mathbf{R}, \tau), \end{aligned} \quad (\text{B.6})$$

where $D \equiv \hbar^2/2m$, the drift force \mathbf{F}_i and the local energy $E_{loc}(\mathbf{R})$ are defined by $\mathbf{F}_i \equiv (2\nabla_i\psi_T(\mathbf{R}))/\psi_T(\mathbf{R})$, $E_{loc}(\mathbf{R}) \equiv (\hat{H}\psi_T(\mathbf{R}))/\psi_T(\mathbf{R})$ respectively [56], and we have used the following relation:

$$\begin{aligned}\Delta_i \left(\frac{f(\mathbf{R}, \tau)}{\psi_T(\mathbf{R})} \right) &= \nabla_i \cdot \left[\frac{\nabla_i f(\mathbf{R}, \tau)}{\psi_T(\mathbf{R})} - \frac{1}{[\psi_T(\mathbf{R})]^2} (\nabla_i \psi_T(\mathbf{R})) f(\mathbf{R}, \tau) \right] \\ &= \frac{1}{\psi_T(\mathbf{R})} \left[\Delta_i f(\mathbf{R}, \tau) - \nabla_i \cdot \left(\frac{2\nabla_i \psi_T(\mathbf{R})}{\psi_T(\mathbf{R})} f(\mathbf{R}, \tau) \right) + \frac{\Delta_i \psi_T(\mathbf{R})}{\psi_T(\mathbf{R})} f(\mathbf{R}, \tau) \right].\end{aligned}\quad (\text{B.7})$$

Its formal solution is given by

$$f(\mathbf{R}', \tau + \Delta\tau) = \int d\mathbf{R} G(\mathbf{R}', \mathbf{R}; \Delta\tau) f(\mathbf{R}, \tau), \quad (\text{B.8})$$

where the Green's function can be written as

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) \equiv \langle \mathbf{R}' | \exp(-\hat{A}\Delta\tau) | \mathbf{R} \rangle. \quad (\text{B.9})$$

Now we approximate $\exp(-\hat{A}\Delta\tau)$ by using Baker-Campbell-Hausdorff formula [56] as

$$\exp(-\hat{A}\Delta\tau) \approx \exp\left(-\hat{A}_3\Delta\frac{\tau}{2}\right) \exp\left(-\hat{A}_2\Delta\frac{\tau}{2}\right) \exp\left(-\hat{A}_1\Delta\tau\right) \exp\left(-\hat{A}_2\Delta\frac{\tau}{2}\right) \exp\left(-\hat{A}_3\Delta\frac{\tau}{2}\right), \quad (\text{B.10})$$

which is an exact transformation up to $(\Delta\tau)^2$ order. So, Eq. (B.8) can be expressed by using Green's functions G_1 , G_2 and G_3 for \hat{A}_1 , \hat{A}_2 , \hat{A}_3 respectively as

$$\begin{aligned}f(\mathbf{R}', \tau + \Delta\tau) &= \int d\mathbf{R} d\mathbf{R}_1 \cdots d\mathbf{R}_4 G_3\left(\mathbf{R}', \mathbf{R}_1; \frac{\Delta\tau}{2}\right) G_2\left(\mathbf{R}_1, \mathbf{R}_2; \frac{\Delta\tau}{2}\right) G_1(\mathbf{R}_2, \mathbf{R}_3; \Delta\tau) \\ &\quad \times G_2\left(\mathbf{R}_3, \mathbf{R}_4; \frac{\Delta\tau}{2}\right) G_3\left(\mathbf{R}_4, \mathbf{R}; \frac{\Delta\tau}{2}\right) f(\mathbf{R}, \tau),\end{aligned}\quad (\text{B.11})$$

with

$$G_1(\mathbf{R}', \mathbf{R}; \tau) \equiv \frac{1}{(4\pi D\tau)^{3N/2}} \exp\left(-\frac{(\mathbf{R}' - \mathbf{R})^2}{4D\tau}\right), \quad (\text{B.12a})$$

$$G_2(\mathbf{R}', \mathbf{R}; \tau) \equiv \delta(\mathbf{R}' - \mathbf{R}(\tau)), \quad \text{where} \begin{cases} \mathbf{R}(0) = \mathbf{R} \\ \frac{d\mathbf{R}(\tau)}{d\tau} = D\mathbf{F}(\mathbf{R}(\tau)), \end{cases} \quad (\text{B.12b})$$

$$G_3(\mathbf{R}', \mathbf{R}; \tau) = \exp(-(E_{loc}(\mathbf{R}) - E)\tau) \delta(\mathbf{R} - \mathbf{R}'), \quad (\text{B.12c})$$

where \mathbf{F} in Eq. (B.12b) is the vector of the drift forces defined as $\mathbf{F} \equiv (\mathbf{F}_1, \dots, \mathbf{F}_N)$. Especially, the validity of Eq. (B.12b) can be confirmed as follows: We introduce $\tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau)$ as the Fourier transform of $G_2(\mathbf{R}', \mathbf{R}; \tau)$. It can be written as

$$\begin{aligned}\int d\mathbf{k} \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau) e^{i\mathbf{k}\cdot\mathbf{R}'} &= \int d\mathbf{k} e^{i\mathbf{k}\cdot(\mathbf{R}' - \mathbf{R}(\tau))}, \\ \therefore \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau) &= e^{i\mathbf{k}\cdot\mathbf{R}(\tau)}.\end{aligned}\quad (\text{B.13})$$

By differentiating both sides with respect to τ , we obtain the following equation

$$\begin{aligned}\frac{\partial \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau)}{\partial \tau} &= (-i\mathbf{k}) \cdot \frac{\partial \mathbf{R}(\tau)}{\partial \tau} \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau), \\ \frac{\partial \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau)}{\partial \tau} e^{i\mathbf{k}\cdot\mathbf{R}'} &= \nabla_{\mathbf{R}'} \cdot \left(\frac{\partial \mathbf{R}(\tau)}{\partial \tau} \tilde{G}_2(\mathbf{k}, \mathbf{R}; \tau) e^{-i\mathbf{k}\cdot\mathbf{R}'} \right).\end{aligned}\quad (\text{B.14})$$

Next, we integrate this equation with respect to \mathbf{k} and use the condition $d\mathbf{R}(\tau)/d\tau = D\mathbf{F}(\mathbf{R}(\tau))$. It can be transformed into

$$\frac{\partial G_2(\mathbf{R}', \mathbf{R}; \tau)}{\partial \tau} = D\nabla_{\mathbf{R}'} \cdot (\mathbf{F}(\mathbf{R}(\tau))G_2(\mathbf{R}', \mathbf{R}; \tau)),$$

with $\nabla_{\mathbf{R}'} \equiv (\nabla_{1'}, \dots, \nabla_{N'})$ for $\mathbf{R}' = (\mathbf{r}'_1, \dots, \mathbf{r}'_N)$. Noting the definition $G_2(\mathbf{R}', \mathbf{R}; \tau) = \delta(\mathbf{R}' - \mathbf{R}(\tau))$, we obtain

$$\frac{\partial G_2(\mathbf{R}', \mathbf{R}; \tau)}{\partial \tau} = D\nabla_{\mathbf{R}'} \cdot (\mathbf{F}(\mathbf{R}')G_2(\mathbf{R}', \mathbf{R}; \tau)). \quad (\text{B.15})$$

Thus, we have confirmed that G_2 is the correct expression of the Green's function of the operator \hat{A}_2 .

We will summarize the algorithm of GFMC method below. First, we prepare the initial state \mathbf{R} which is called walker, then we replicate a set of n_w walkers. Now we label these n_w walkers as $\{\mathbf{R}\}_i$, ($i = 1, \dots, n_w$), and these walkers will move following Eq. (B.11) to $\tau \rightarrow \infty$ in steps of $\Delta\tau$. The corresponding GFMC simulation can be performed as follows:

1. Choose a walker $\{\mathbf{R}\}_i$, and calculate its local energy $E_{loc}(\mathbf{R})$.
2. Move the walker under the drift force $\mathbf{F}(\mathbf{R})$ which can be obtained from Eq. (B.12b) as $\mathbf{R}' \rightarrow \mathbf{R} + \mathbf{F}(\mathbf{R})\Delta\tau/2$.
3. Take Gaussian steps for all components of $\{\mathbf{R}\}_i$. Those steps are derivable from Eq. (B.12a) as $R''_i \rightarrow R'_i + \Delta R_i$ for each $3N$ coordinates, where ΔR_i is generated by random numbers obeying a Gaussian distribution function $\exp(-\Delta R_i^2/4D\Delta\tau)$.
4. Repeat procedure 2 for \mathbf{R}'' (then we obtain \mathbf{R}'''), and calculate $E_{loc}(\mathbf{R}''')$.
5. Replicate the walker with $\langle n \rangle_i$ times. $\langle n \rangle_i$ can be calculated by the following relation,

$$\langle n \rangle_i = \text{int} \left[\exp \left(-\Delta\tau \left(\frac{E_{loc}(\mathbf{R}) + E_{loc}(\mathbf{R}''')}{2} - E \right) \right) + \text{ran}() \right], \quad (\text{B.16})$$

where $\text{ran}()$ is a uniform random number lying between 0 to 1.

6. By repeating above procedures for all walkers, we obtain a new set of walkers with the total number $n'_w = \sum_i \langle n \rangle_i$. We then update the new value of E_{new} as

$$E_{new} = E + \frac{1}{\Delta\tau} \left(1 - \frac{n'_w}{n_w} \right), \quad (\text{B.17})$$

where $1/\Delta\tau$ doesn't always have to be used as the prefactor of $(1 - n'_w/n_w)$ [55].

By repeating these procedures to large τ , walkers start to follow the distribution $\psi_T\phi_0$ where ϕ_0 is the exact ground state wave function. We can estimate the ground state energy as an average of $E_{loc}(\mathbf{R})$ and its static error $\sigma(\hat{H})$. It can be expressed as

$$\sigma^2(\hat{H}) \equiv \frac{1}{N_I - 1} \left\{ \frac{1}{N_I} \sum_{j=1}^{N_I} E_{loc}^2(\mathbf{R}_j) - \left(\frac{1}{N_I} \sum_{j=1}^{N_I} E_{loc}(\mathbf{R}_j) \right)^2 \right\}, \quad (\text{B.18})$$

where N_I is the number of observations and here j is the label of each observations. In addition, we can also estimate other physical quantities. If we want to observe an expectation value of an operator \hat{A} which commute with \hat{H} , we have only to take an average of $A_{loc}(\mathbf{R}) \equiv (\hat{A}\psi_T(\mathbf{R}))/\psi_T(\mathbf{R})$. That's because the estimation of the total energy $\langle \hat{H} \rangle$ by using GFMC method (taking the average of $E_{loc}(\mathbf{R})$) is nothing but the calculation of the following integration

$$\langle \hat{H} \rangle_m \equiv \frac{\int d\mathbf{R} \phi_0(\mathbf{R}) \hat{H} \psi_T(\mathbf{R})}{\int d\mathbf{R} \phi_0(\mathbf{R}) \psi_T(\mathbf{R})} = \frac{\langle \phi_0(\mathbf{R}) | \hat{H} | \psi_T(\mathbf{R}) \rangle}{\langle \phi_0(\mathbf{R}) | \psi_T(\mathbf{R}) \rangle}, \quad (\text{B.19})$$

where such estimations are called ‘‘mixed’’ estimation. Therefore, we can simulate accurately expectation values of any operators which commute with \hat{H} by mixed estimation (not biased by trial wave function ψ_T).

For ageneral operator $\hat{B} \equiv B(\mathbf{R})$, estimations are more complicated. An average of \hat{B} which does not commute with \hat{H} are biased in using mixed estimation. Then we use the ‘‘pure’’ estimation $\langle \hat{B} \rangle_p$ which is defined by [46]

$$\langle \hat{B} \rangle_p \equiv \frac{\int d\mathbf{R} \phi_0(\mathbf{R})B(\mathbf{R})\phi_0(\mathbf{R})}{\int d\mathbf{R} \phi_0(\mathbf{R})\phi_0(\mathbf{R})} = \frac{\langle \phi_0(\mathbf{R})|B(\mathbf{R})\phi_0(\mathbf{R})/\psi_T(\mathbf{R})|\psi_T(\mathbf{R}) \rangle}{\langle \phi_0(\mathbf{R})|\phi_0/\psi_T(\mathbf{R})|\psi_T(\mathbf{R}) \rangle} \quad (\text{B.20})$$

In $\tau \rightarrow \infty$ regime, $\langle \hat{B} \rangle_p$ can be transformed as

$$\langle \hat{B} \rangle_p = \frac{\sum_i B(\mathbf{R}_i)W(\mathbf{R}_i)}{\sum_i W(\mathbf{R}_i)}, \quad (\text{B.21})$$

where the weight $W(\mathbf{R})$ is proportional to the number of future descendants at \mathbf{R} as

$$W(\mathbf{R}) \propto n(\mathbf{R}, \tau \rightarrow \infty), \quad (\text{B.22})$$

as proved by Liu *et.al.* [58, 57]. How to perform the pure estimation is summarized as follows. First, we perform GFMC simulation for the system from $\tau = 0$ to large τ' . Then, we continue GFMC steps with sampling \hat{B} as,

$$\begin{aligned} \{\mathbf{R}\}_i &\rightarrow \{\mathbf{R}'\}_i \\ \{\hat{B}\}_i &\rightarrow \{\hat{B}'\}_i, \end{aligned}$$

in the same time interval $\Delta\tau$, and the number of walker N changes to N' in this step. We also introduce an auxiliary variable $\{P\}_i$ which is evolved by the following law,

$$\{P\}_i \rightarrow \{\hat{B}'\}_i + \{P^t\}_i, \quad (\text{B.23})$$

where $\{P^t\}_i$ is the previous configuration of $\{P\}_i$. At the first step, $\{P^t\}_i$ is set 0 for all i . If we have obtained a set of N_f values $\{P\}_i$ after additional M steps, the pure estimation of \hat{B} can be written as

$$\langle \hat{B} \rangle_p = \sum_{i=1}^{N_f} \frac{\{P\}_i}{MN_f}. \quad (\text{B.24})$$

Finally in this subsection, we introduce an approximate estimation called ‘‘extrapolated’’ [54], which is given by

$$\langle \hat{A} \rangle_e \equiv 2\langle \hat{A} \rangle_m - \langle \hat{A} \rangle_v, \quad (\text{B.25})$$

where $\langle \hat{A} \rangle_v$ is variational estimation of \hat{A} which is defined by

$$\langle \hat{A} \rangle_v \equiv \frac{\int d\mathbf{R} \psi_T(\mathbf{R})\hat{A}\psi_T(\mathbf{R})}{\int d\mathbf{R} \psi_T(\mathbf{R})\psi_T(\mathbf{R})} = \frac{\langle \psi_T(\mathbf{R})|\hat{A}|\psi_T(\mathbf{R}) \rangle}{\langle \psi_T(\mathbf{R})|\psi_T(\mathbf{R}) \rangle}. \quad (\text{B.26})$$

The next subsection explains how we can estimate $\langle \hat{A} \rangle_v$. On the other hand, Eq. (B.25) can be obtained by the following procedure. Let us change the trial wave function ψ_T as $\psi_T \rightarrow \phi_0 + \delta\psi_T$. By using it, the pure estimation of \hat{A} can be expressed as

$$\langle \hat{A} \rangle_p = \frac{\langle \phi_0|\hat{A}|\phi_0 \rangle}{\langle \phi_0|\phi_0 \rangle} = \frac{1}{\langle \phi_0|\phi_0 \rangle} \left(\langle \psi_T|\hat{A}|\psi_T \rangle + 2\langle \psi_T|\hat{A}|\delta\psi_T \rangle + \langle \delta\psi_T|\hat{A}|\delta\psi_T \rangle \right). \quad (\text{B.27})$$

If we can neglect the second-order term $\langle \delta\psi_T|\hat{A}|\delta\psi_T \rangle$, $\langle \hat{A} \rangle_p$ can be approximated as

$$\langle \hat{A} \rangle_p \approx 2\frac{\langle \phi_0|\hat{A}|\psi_T \rangle}{\langle \phi_0|\psi_T \rangle} - \frac{\langle \psi_T|\hat{A}|\psi_T \rangle}{\langle \psi_T|\psi_T \rangle} = \langle \hat{A} \rangle_e, \quad (\text{B.28})$$

where we also used $\langle \phi_0|\hat{A}|\delta\psi_T \rangle = \langle \psi_T|\hat{A}|\phi_0 \rangle - \langle \psi_T|\hat{A}|\psi_T \rangle$. Advantages of this estimation are twofold. First, it is easier than the pure estimation; second, we can observe derivative operators such as $\hat{p} = -i\hbar\nabla$.

B.2 Variational Quantum Monte Carlo Method

Next we will introduce the variational Monte Carlo (VQMC) method [37, 39]. By using this method, we can estimate a many body integration, such as

$$E_v \equiv \langle \hat{H} \rangle_v = \frac{\langle \psi_T | \hat{H} | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle} = \frac{\int d\mathbf{R} E_{loc}(\mathbf{R}) |\psi_T(\mathbf{R})|^2}{\int d\mathbf{R} |\psi_T(\mathbf{R})|^2} \quad (\text{B.29})$$

If we try to perform this integration directly, we have to solve a numerical $3N$ -dimensional integration, which is too difficult. Here $|\psi_T(\mathbf{R})|^2$ is proportional to the stochastic density at \mathbf{R} , so it can be used for the importance sampling. An appropriate choice of the trial wave function ψ_T is also very important to estimate the ground state energy E_0 because the value of E_v satisfies the following variational principle,

$$E_T \geq E_0. \quad (\text{B.30})$$

Moreover, if we use the exact eigenstate wave function ϕ_k with eigenenergy E_k of \hat{H} , the corresponding static error is equal to 0 exactly.

In the next subsection, we will summarize the algorithm of VQMC sampling with a trial ψ_T . Next, we will introduce the trial wave function for many-body systems called ‘‘Bijl-Jastraw’’ type [53].

B.2.1 Algorithm of VQMC method

Here we summarize the VQMC calculation. First, we want to observe values of physical quantities such as \hat{H} and so on. Their expectations are denoted by $\langle \hat{H} \rangle_v$, which can be rewritten by using the probability density $p(\mathbf{R}) \equiv |\psi_T(\mathbf{R})|^2 / \int d\mathbf{R} |\psi_T(\mathbf{R})|^2$ as

$$\langle \hat{H} \rangle_v = \int d\mathbf{R} E_{loc}(\mathbf{R}) p(\mathbf{R}) \approx \sum_{i=1}^{N_I} E_{loc}(\mathbf{R}_i). \quad (\text{B.31})$$

where N_I is the total number of observations, and the final form can be calculated by importance sampling. The algorithm of VQMC calculation is summarized as follows:

1. Set up a Initial state $\mathbf{R}^{(0)}$.
2. Take a movement $\mathbf{R}^{(1)} \rightarrow \mathbf{R}^{(0)} + (2 \times \text{ran}() - 1) \Delta\mathbf{R}$, where $\Delta\mathbf{R}$ is the maximum distance for each step.
3. If $|\psi_T(\mathbf{R}^{(1)})|^2 / |\psi_T(\mathbf{R}^{(0)})|^2 > \text{ran}()$, then $\mathbf{R}^{(0)} = \mathbf{R}^{(1)}$. Unless, $\mathbf{R}^{(0)} = \mathbf{R}^{(0)}$ (Metropolis step).
4. Sample physical quantities such as energy and its static error *etc.*
5. Go back to step 2.

By repeating these procedures, we can estimate various expectation values.

B.2.2 Trial wave function for bosons

Here we introduce one of many body trial wave functions for the ground sate, called Bijl-Jastraw type wave function $\Psi_T(\mathbf{R})$. For bosonic systems, it can be given by

$$\Psi_T(\mathbf{R}) \equiv \prod_{i=1}^N u(\mathbf{r}_i) \prod_{i<j} f(r_{ij}), \quad (\text{B.32})$$

where $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$, functions $u(\mathbf{r}_i)$ and $f(r_{ij})$ are constructed so as to incorporate the external field and the interaction potential respectively.

We can write down the expression of $E_{loc}(\mathbf{R})$ for the Hamiltonian Eq. (B.1) as

$$E_{loc}(\mathbf{R}) = \sum_{i=1}^N \left[-\frac{\hbar^2}{2m} \left\{ \left(\frac{\nabla_i u(\mathbf{r}_i)}{u(\mathbf{r}_i)} + \sum_{j \neq i} \frac{\mathbf{r}_{ij}}{r_{ij}} \frac{f'(r_{ij})}{f(r_{ij})} \right)^2 + \left(\frac{\Delta_i u(\mathbf{r}_i)}{u(\mathbf{r}_i)} - \left(\frac{\nabla_i u(\mathbf{r}_i)}{u(\mathbf{r}_i)} \right)^2 \right) \right. \right. \\ \left. \left. + \sum_{j \neq i} \left(\frac{2}{r_{ij}} \frac{f'(r_{ij})}{f(r_{ij})} + \frac{f''(r_{ij})}{f(r_{ij})} - \left(\frac{f'(r_{ij})}{f(r_{ij})} \right)^2 \right) \right\} + U(\mathbf{r}_i) + \sum_{j>i} V(\mathbf{r}_i - \mathbf{r}_j) \right], \quad (\text{B.33})$$

where $f'(r) \equiv \partial f(r)/\partial r$ and $f''(r) \equiv \partial^2 f(r)/\partial r^2$.

B.3 Finite size effect

We now discuss finite size effects for the Monte Carlo simulation [37, 54, 56].

We consider the size effect of the volume V . If we want to estimate an energy for a homogeneous system, we have to remove a “tail” effect. One of the methods is to adopt “uniform” approximation[37] as follows: We perform a simulation, we set particle number N , and fix the density ρ . The maximum length $L = (\rho/N)^{1/3}$ can be obtained automatically. Here we assume that we can extract the information of the energy to the distance $L/2$. The tail contributions of the potential energy $(V/N)_t(\rho)$ and the kinetic energy $(K/N)_t(\rho)$ from the region larger than $L/2$ can be included by the following integrals as

$$\left(\frac{V}{N} \right)_t(\rho) = 2\pi\rho \int_{L/2}^{\infty} dr r^2 V(r) g(r) = 2\pi\rho \int_{L/2}^{\infty} dr r^2 V(r), \quad (\text{B.34a})$$

$$\left(\frac{K}{N} \right)_t(\rho) = -\frac{\hbar^2}{m} 2\pi\rho \int_{L/2}^{\infty} dr r^2 \left(\frac{2}{r} \frac{f'(r)}{f(r)} + \frac{f''(r)}{f(r)} \right), \quad (\text{B.34b})$$

respectively, where we have assumed that the two-body radial distribution function [60] $g(r) = 1$ for $r > L/2$, and $f(r)$ is the part of the Bijl-Jastrow type wave function in Eq. (B.32). There is also a dependence on particle number N . So, we have to consider the effect by performing several simulations changing the number N . We can adopt the lowest value of N where the energy is nearly constant.

B.4 Expressions of Physical Quantities for Sampling

We will introduce several expressions of basic physical quantities for importance sampling.

B.4.1 Density matrix

In the second quantized formulation, the one-particle density matrix [50] is given by

$$g_1(\mathbf{r}', \mathbf{r}) \equiv \langle \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') \rangle, \quad (\text{B.35})$$

where $\hat{\psi}(\mathbf{r})$ is the annihilation operator at \mathbf{r} , and $\hat{\psi}(\mathbf{r})$, $\hat{\psi}^\dagger(\mathbf{r})$ obey commutation relations $[\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')] = \delta(\mathbf{r} - \mathbf{r}')$, $[\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')] = 0$. When a N -body normalized ground state $|\Psi_G\rangle$ is considered, we can express g_1 as

$$g_1(\mathbf{r}', \mathbf{r}) = \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') | \Psi_G \rangle \\ = \int d\mathbf{R} \int d\mathbf{R}' \Psi_G^*(\mathbf{R}) \langle \mathbf{R} | \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}') | \mathbf{R}' \rangle \Psi_G(\mathbf{R}') \\ = N \int d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \int d\mathbf{r}'_2 d\mathbf{r}'_3 \cdots d\mathbf{r}'_N \Psi_G^*(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N) \\ \times \langle \mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N | \mathbf{r}', \mathbf{r}'_2, \mathbf{r}'_3, \cdots, \mathbf{r}'_N \rangle \Psi_G(\mathbf{r}', \mathbf{r}'_2, \mathbf{r}'_3, \cdots, \mathbf{r}'_N) \\ = N \int d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \Psi_G^*(\mathbf{r}, \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}', \mathbf{r}_2, \mathbf{r}_3, \cdots, \mathbf{r}_N), \quad (\text{B.36})$$

where $\Psi_G(\mathbf{R}) \equiv \langle \mathbf{R} | \Psi_G \rangle$ and $\mathbf{R} \equiv (\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)$. Then we transform Eq. (B.36) into a form suitable for GFMC and VMC methods. In a homogeneous system, we can express the one-particle density matrix for the ground state by variational estimation as

$$g_1^{var}(\mathbf{r}) \equiv N \frac{\int d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \psi_T^*(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \psi_T(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\int d\mathbf{R} |\psi_T(\mathbf{R})|^2} \quad (\text{B.37a})$$

We here adopt the extrapolated method (B.25) for the GFMC estimation, which is given by

$$g_1^{(e)} \equiv 2\tilde{g}_1^{mix}(\mathbf{r}) - g_1^{var}(\mathbf{r}), \quad (\text{B.37b})$$

where $\tilde{g}_1^{mix}(\mathbf{r})$ can be written as

$$\tilde{g}_1^{mix}(\mathbf{r}) \equiv N \frac{\int d\mathbf{r}_2 d\mathbf{r}_3 \cdots d\mathbf{r}_N \psi_T^*(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \phi_0(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\int d\mathbf{R} \psi_T(\mathbf{R}) \phi_0(\mathbf{R})} \quad (\text{B.37c})$$

These expressions can be approximated [54] as

$$g_1^{var}(\mathbf{r}) = n \left\langle \frac{\psi_T^*(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\psi_T(\mathbf{R})} \right\rangle_v, \quad (\text{B.38a})$$

$$\begin{aligned} \tilde{g}_1^{mix}(\mathbf{r}) &\approx n \frac{\int d\mathbf{R} \{\psi_T^*(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) (\psi_T(\mathbf{R}))^{-1}\} f(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\int d\mathbf{R} f(\mathbf{R})} \\ &= n \left\langle \frac{\psi_T^*(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N)}{\psi_T(\mathbf{R})} \right\rangle_m, \end{aligned} \quad (\text{B.38b})$$

respectively, where n is the particle density $n \equiv N/V$.

Next, we introduce two-particle density matrix $g_2(\mathbf{r}, \mathbf{r}')$ as

$$\begin{aligned} g_2(\mathbf{r}, \mathbf{r}') &\equiv \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}') \hat{\psi}(\mathbf{r}') \hat{\psi}(\mathbf{r}) | \Psi_G \rangle \\ &= N(N-1) \int d\mathbf{r}_3 \cdots d\mathbf{r}_N |\Psi_G(\mathbf{r}, \mathbf{r}', \mathbf{r}_3 \cdots \mathbf{r}_N)|^2. \end{aligned} \quad (\text{B.39})$$

In homogeneous cases, we can express $g_2(\mathbf{r}, \mathbf{r}') \rightarrow g_2(\mathbf{r} - \mathbf{r}')$, which can be transformed as

$$\begin{aligned} g_2(\mathbf{r}) &= \frac{N(N-1)}{V} \int d\mathbf{r}_2 \cdots d\mathbf{r}_N |\Psi_G(\mathbf{r} + \mathbf{r}_2, \mathbf{r}_2, \mathbf{r}_3 \cdots \mathbf{r}_N)|^2 \\ &= \frac{2}{V} \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N \sum_{i < j} \delta(\mathbf{r}_{ij} - \mathbf{r}) |\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 \cdots \mathbf{r}_N)|^2. \end{aligned} \quad (\text{B.40})$$

Introducing the step function $\theta_h(z)$, which is 1 if $z < h$ and 0 otherwise, Eq. (B.40) can be written by [61]

$$g_2(\mathbf{r}) \approx \frac{2}{V} \frac{1}{4\pi r^2 h} \int d\mathbf{r}_1 d\mathbf{r}_2 \cdots d\mathbf{r}_N \sum_{i < j} \theta_h(|r_{ij} - r|) |\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 \cdots \mathbf{r}_N)|^2. \quad (\text{B.41})$$

B.4.2 The moment method for two-particle excitation

We want to know details of quasiparticle excitation for a system of N particles. The moment method, developed mainly for the two-particle excitations, forms a tractable and reliable tool for this purpose [41, 42, 59, 60]. In this subsection we first summarize the moment method. Then we extend it up to second-order moment and apply to the one-particle excitation. We also give expressions of these excitation for sampling.

We start from the density correlation function $S(\mathbf{q}, t)$ for the ground state $|\Psi_G\rangle$ given by

$$S(\mathbf{q}, t) \equiv \sum_{\nu} \langle \Psi_G | e^{i\hat{H}t/\hbar} \hat{\rho}_{\mathbf{q}} e^{-i\hat{H}t/\hbar} \hat{\rho}_{\mathbf{q}}^\dagger | \Psi_G \rangle, \quad (\text{B.42})$$

where the particle density operator $\hat{\rho}_{\mathbf{q}}$ is defined by

$$\hat{\rho}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r}) = \frac{1}{\mathcal{V}} \sum_{\mathbf{q}} \hat{\rho}_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}}, \quad \hat{\rho}_{\mathbf{q}} \equiv \sum_{\mathbf{k}} \hat{a}_{\mathbf{q}+\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}, \quad (\text{B.43})$$

with

$$\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}. \quad (\text{B.44})$$

Its Fourier transform with respect to t ,

$$S(\mathbf{q}, \omega) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dt S(\mathbf{q}, t) e^{i\omega t}, \quad (\text{B.45a})$$

defines the dynamic form factor. Let us insert the complete set $\sum_{\nu} |\Psi_{\nu}\rangle \langle\Psi_{\nu}|$ between $e^{i\hat{H}t/\hbar}$ and $\hat{\rho}_{\mathbf{q}}^\dagger$ in Eq. (B.42), transform $\langle\Psi_{\nu}| e^{i\hat{H}t/\hbar} = \langle\Psi_{\nu}| e^{iE_{\nu}t/\hbar}$ and $e^{-i\hat{H}t/\hbar} |\Psi_G\rangle = e^{-i\hat{E}_G t/\hbar} |\Psi_G\rangle$, and substitute the resulting expression of $S(\mathbf{q}, t)$ into Eq. (B.45a) to perform the time integration. We thereby obtain

$$S(\mathbf{q}, \omega) = \sum_{\nu} |\langle\Psi_{\nu}|\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle|^2 \delta(\omega - E_{\nu} + E_G). \quad (\text{B.45b})$$

We next introduce the moments of $S(\mathbf{q}, \omega)$ as

$$I_n(\mathbf{q}) \equiv \int_{-\infty}^{\infty} d\omega \omega^n S(\mathbf{q}, \omega) = \sum_{\nu} |\langle\Psi_{\nu}|\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle|^2 (E_G - E_{\nu})^n. \quad (\text{B.46})$$

Substituting Eq. (B.45a) into the first expression and performing partial integrations with respect to t , we can express $I_n(\mathbf{q})$ alternatively as

$$\begin{aligned} I_n(\mathbf{q}) &= \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} \frac{dt}{2\pi} S(\mathbf{q}, t) \left(-i \frac{d}{dt}\right)^n e^{i\omega t} \\ &= \int_{-\infty}^{\infty} \frac{dt}{2\pi} \int_{-\infty}^{\infty} d\omega e^{i\omega t} \left(i \frac{d}{dt}\right)^n S(\mathbf{q}, t) \\ &= \left(i \frac{d}{dt}\right)^n S(\mathbf{q}, t) \Big|_{t \rightarrow 0} \end{aligned} \quad (\text{B.47})$$

By using Eq. (B.42), we can express the first few series of $I_n(\mathbf{q})$ as

$$I_0(\mathbf{q}) = \langle\Psi_G|\hat{\rho}_{\mathbf{q}}\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle \quad (\text{B.48a})$$

$$I_1(\mathbf{q}) = \langle\Psi_G|[\hat{\rho}_{\mathbf{q}}, \hat{H}]\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle \quad (\text{B.48b})$$

$$I_2(\mathbf{q}) = \langle\Psi_G|[[\hat{\rho}_{\mathbf{q}}, \hat{H}], \hat{H}]\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle. \quad (\text{B.48c})$$

$I_0(\mathbf{q})$ can be transformed by using Eq. (B.43) as

$$\begin{aligned} I_0(\mathbf{q}) &= \langle\Psi_G|\hat{\rho}_{\mathbf{q}}\hat{\rho}_{\mathbf{q}}^\dagger|\Psi_G\rangle = \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle\Psi_G|\hat{\rho}(\mathbf{r}_1)\hat{\rho}(\mathbf{r}_2)|\Psi_G\rangle e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\ &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 \langle\Psi_G|\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_2)|\Psi_G\rangle e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\ &= \int d\mathbf{r}_1 \int d\mathbf{r}_2 [\langle\Psi_G|\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}^\dagger(\mathbf{r}_2)\hat{\psi}(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_2)|\Psi_G\rangle + \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle\Psi_G|\hat{\psi}^\dagger(\mathbf{r}_1)\hat{\psi}(\mathbf{r}_2)|\Psi_G\rangle] e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\ &= \mathcal{V} \int d\mathbf{r} g_2(\mathbf{r}) e^{-\mathbf{q}\cdot\mathbf{r}} + N \\ &= N \left\{ \frac{1}{n} \int d\mathbf{r} [g_2(\mathbf{r}) - 1] e^{i\mathbf{q}\cdot\mathbf{r}} + \frac{\mathcal{V}}{n} \delta_{\mathbf{q}\mathbf{0}} + 1 \right\}. \end{aligned} \quad (\text{B.49})$$

We next give an alternative expression of I_1 . We consider the following quantity:

$$\begin{aligned}
\mathcal{I}_1 &\equiv \langle \Psi_G | [[\hat{\rho}_{\mathbf{q}}, \hat{H}], \hat{\rho}_{\mathbf{q}}^\dagger] | \Psi_G \rangle \\
&= \sum_{\nu} \left[\langle \Psi_G | (\hat{\rho}_{\mathbf{q}} \hat{H} - \hat{H} \hat{\rho}_{\mathbf{q}}) | \Psi_{\nu} \rangle \langle \Psi_{\nu} | \hat{\rho}_{\mathbf{q}}^\dagger | \Psi_G \rangle - \langle \Psi_G | \hat{\rho}_{\mathbf{q}}^\dagger | \Psi_{\nu} \rangle \langle \Psi_{\nu} | (\hat{\rho}_{\mathbf{q}} \hat{H} - \hat{H} \hat{\rho}_{\mathbf{q}}) | \Psi_G \rangle \right] \\
&= \sum_{\nu} (|\langle \Psi_G | \hat{\rho}_{\mathbf{q}}^\dagger | \Psi_G \rangle|^2 + |\langle \Psi_G | \hat{\rho}_{\mathbf{q}} | \Psi_G \rangle|^2) (E_{\nu} - E_G) \\
&= I_1(\mathbf{q}) + I_1(-\mathbf{q}).
\end{aligned} \tag{B.50}$$

The time reversal symmetry implies

$$I_1(\mathbf{q}) = I_1(-\mathbf{q}). \tag{B.51}$$

Hence, we can express Eq. (B.48b) as

$$I_1(\mathbf{q}) = \frac{1}{2} \langle \Psi_G | [[\hat{\rho}_{\mathbf{q}}, \hat{H}], \hat{\rho}_{\mathbf{q}}^\dagger] | \Psi_G \rangle. \tag{B.52}$$

Noting $[\hat{\rho}_{\mathbf{q}}, \hat{H}_{int}] = 0$ in Eq. (B.46), we can transform $[\hat{\rho}_{\mathbf{q}}, \hat{H}]$ as

$$\begin{aligned}
[\hat{\rho}_{\mathbf{q}}, \hat{H}] &= [\hat{\rho}_{\mathbf{q}}, \hat{H}_0] = \sum_{\mathbf{k}\mathbf{k}'} \varepsilon_{\mathbf{k}} [\hat{a}_{\mathbf{k}'}^\dagger, \hat{a}_{\mathbf{k}'+\mathbf{q}}, \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}] = \sum_{\mathbf{k}\mathbf{k}'} \varepsilon_{\mathbf{k}} \left(\hat{a}_{\mathbf{k}'}^\dagger [\hat{a}_{\mathbf{k}'+\mathbf{q}}, \hat{a}_{\mathbf{k}}^\dagger] \hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}}^\dagger [\hat{a}_{\mathbf{k}'}^\dagger, \hat{a}_{\mathbf{k}}] \hat{a}_{\mathbf{k}'+\mathbf{q}} \right) \\
&= \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}} = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}/2} - \varepsilon_{\mathbf{k}-\mathbf{q}/2}) \hat{a}_{\mathbf{k}-\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}/2} \\
&= \frac{\hbar \mathbf{q}}{m} \cdot \sum_{\mathbf{k}} \hbar \mathbf{k} a_{\mathbf{k}-\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}/2} \equiv \hat{J}_{\mathbf{q}},
\end{aligned} \tag{B.53}$$

where $\hat{J}_{\mathbf{q}}$ is the current operator [62].

We also transform the double commutator in Eq. (B.52) as

$$\begin{aligned}
[[\hat{\rho}_{\mathbf{q}}, \hat{H}], \hat{\rho}_{\mathbf{q}}^\dagger] &= \sum_{\mathbf{k}\mathbf{k}'} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}} [\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}}, \hat{a}_{\mathbf{k}'+\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}'}] \\
&= \sum_{\mathbf{k}\mathbf{k}'} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \left(\hat{a}_{\mathbf{k}}^\dagger [\hat{a}_{\mathbf{k}+\mathbf{q}}, \hat{a}_{\mathbf{k}'+\mathbf{q}}^\dagger] \hat{a}_{\mathbf{k}'} + \hat{a}_{\mathbf{k}'+\mathbf{q}}^\dagger [\hat{a}_{\mathbf{k}}^\dagger, \hat{a}_{\mathbf{k}'}] \hat{a}_{\mathbf{k}+\mathbf{q}} \right) \\
&= \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) \left(\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} + \hat{a}_{\mathbf{k}+\mathbf{q}}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}} \right) \\
&= \sum_{\mathbf{k}} [(\varepsilon_{\mathbf{k}+\mathbf{q}} - \varepsilon_{\mathbf{k}}) - (\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})] \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} \\
&= \frac{\hbar^2 q^2}{m} \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}} = N \frac{\hbar^2 q^2}{m}.
\end{aligned} \tag{B.54}$$

Substituting the result into Eq. (B.52), we obtain the f -sum rule

$$I_1(\mathbf{q}) = N \frac{\hbar^2 \mathbf{q}^2}{2m}. \tag{B.55}$$

By using

$$\hat{a}_{\mathbf{k}} = \frac{1}{\sqrt{\mathcal{V}}} \int d\mathbf{r} \hat{\psi}(\mathbf{r}) e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{B.56}$$

and substituting Eq. (B.53) into Eq. (B.48b), $I_1(\mathbf{q})$ can be transformed as

$$\begin{aligned}
I_1(\mathbf{q}) &= \frac{\hbar\mathbf{q}}{m} \cdot \sum_{\mathbf{k}\mathbf{k}'} \hbar\mathbf{k} \langle \Psi_G | \hat{a}_{\mathbf{k}-\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}/2} \hat{a}_{\mathbf{k}'+\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}/2} | \Psi_G \rangle \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{k}'} \hbar\mathbf{k} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad \times e^{-i(\mathbf{k}-\mathbf{q}/2)\cdot\mathbf{r}'_1 - i(\mathbf{k}+\mathbf{q}/2)\cdot\mathbf{r}_1 + i(\mathbf{k}'+\mathbf{q}/2)\cdot\mathbf{r}'_2 - i(\mathbf{k}'-\mathbf{q}/2)\cdot\mathbf{r}_2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{V^2} \sum_{\mathbf{k}\mathbf{k}'} \hbar\mathbf{k} \left[\langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle + \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \right] \\
&\quad \times e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{k}\cdot(\mathbf{r}_2 - \mathbf{r}'_2) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - \mathbf{r}_2 - \mathbf{r}'_2)/2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{V^2} \sum_{\mathbf{k}} \hbar\mathbf{k} \left[\langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle + \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \right] \\
&\quad \times e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - \mathbf{r}_2 - \mathbf{r}'_2)/2} \delta(\mathbf{r}_2 - \mathbf{r}'_2) \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{V} \sum_{\mathbf{k}} \hbar\mathbf{k} \left[\langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \right] \\
&\quad \times e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - 2\mathbf{r}_2)/2}. \tag{B.57a}
\end{aligned}$$

The second term in the square bracket can be transformed as

$$\begin{aligned}
&\frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{V} \sum_{\mathbf{k}} \hbar\mathbf{k} \delta(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - 2\mathbf{r}_2)/2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \sum_{\mathbf{k}} \hbar\mathbf{k} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}'_1 + \mathbf{r}_1)/2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \sum_{\mathbf{k}} \hbar\mathbf{k} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 g_1(\mathbf{r}_1 - \mathbf{r}'_1) e^{-i(\mathbf{k}-\mathbf{q}/2)\cdot(\mathbf{r}_1 - \mathbf{r}'_1)} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \sum_{\mathbf{k}} \hbar \left(\mathbf{k} + \frac{\mathbf{q}}{2} \right) \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} = \frac{\hbar^2 \mathbf{q}^2}{2m} \int d\mathbf{r} g_1(\mathbf{r}) \delta(\mathbf{r}) = N \frac{\hbar^2 \mathbf{q}^2}{2m} \tag{B.57b}
\end{aligned}$$

On the other hand, the first term in the square bracket of Eq. (B.57a) can be transformed as

$$\begin{aligned}
&\frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{V} \sum_{\mathbf{k}} \hbar\mathbf{k} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - 2\mathbf{r}_2)/2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{V} \sum_{\mathbf{k}} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \hbar \frac{\nabla_1 - \nabla_{1'}}{2i} e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - 2\mathbf{r}_2)/2} \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{V} \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot(\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}'_1 - 2\mathbf{r}_2)/2} \hbar \frac{\nabla_1 - \nabla_{1'}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \\
&= \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \delta(\mathbf{r}_1 - \mathbf{r}'_1) e^{-i\mathbf{q}\cdot(\mathbf{r}_1 - \mathbf{r}_2)} \hbar \frac{\nabla_1 - \nabla_{1'}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle. \tag{B.57c}
\end{aligned}$$

Substituting Eqs. (B.57b) and (B.57c) into Eq. (B.57a), we obtain

$$I_1(\mathbf{q}) = N \frac{\hbar^2 \mathbf{q}^2}{2m} + \frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}_2)} \hbar \frac{\nabla_1 - \nabla_{1'}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \Big|_{\mathbf{r}'_1 \rightarrow \mathbf{r}_1}. \tag{B.57d}$$

Comparing Eq. (B.55) with (B.57c), we obtain

$$\frac{\hbar\mathbf{q}}{m} \cdot \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}_2)} \hbar \frac{\nabla_1 - \nabla_{1'}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \Big|_{\mathbf{r}'_1 \rightarrow \mathbf{r}_1} = 0. \tag{B.58}$$

The second moment I_2 can be also written as

$$I_2(\mathbf{q}) = \langle \Psi_G | \hat{J}_{\mathbf{q}} \hat{J}_{\mathbf{q}}^\dagger | \Psi_G \rangle = \langle \Psi_G | [\hat{\rho}_{\mathbf{q}}, \hat{H}] [\hat{\rho}_{\mathbf{q}}, \hat{H}]^\dagger | \Psi_G \rangle. \quad (\text{B.59})$$

Let us substitute Eq. (B.53) into Eq. (B.59):

$$\begin{aligned} I_2(\mathbf{q}) &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \langle \Psi_G | \hat{a}_{\mathbf{k}-\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}+\mathbf{q}/2} \hat{a}_{\mathbf{k}'+\mathbf{q}/2}^\dagger \hat{a}_{\mathbf{k}'-\mathbf{q}/2} | \Psi_G \rangle \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\ &\quad \times e^{-i(\mathbf{k}-\mathbf{q}/2) \cdot \mathbf{r}'_1 - i(\mathbf{k}+\mathbf{q}/2) \cdot \mathbf{r}_1 + i(\mathbf{k}'+\mathbf{q}/2) \cdot \mathbf{r}'_2 - i(\mathbf{k}'-\mathbf{q}/2) \cdot \mathbf{r}_2} \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu [\langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\ &\quad + \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle] e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{k} \cdot (\mathbf{r}_2 - \mathbf{r}'_2) - i\mathbf{q} \cdot (\mathbf{r}_1 + \mathbf{r}'_1 - \mathbf{r}_2 - \mathbf{r}'_2)/2}. \end{aligned} \quad (\text{B.60a})$$

The second term in the square bracket can be transformed as

$$\begin{aligned} &\sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\ &\quad \times e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{k} \cdot (\mathbf{r}_2 - \mathbf{r}'_2) - i\mathbf{q} \cdot (\mathbf{r}_1 + \mathbf{r}'_1 - \mathbf{r}_2 - \mathbf{r}'_2)/2} \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1) - i\mathbf{k} \cdot (\mathbf{r}_2 - \mathbf{r}_1) - i\mathbf{q} \cdot (\mathbf{r}'_1 - \mathbf{r}_2)/2} \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle e^{i\mathbf{k} \cdot \mathbf{r}'_1 - i\mathbf{k}' \cdot \mathbf{r}_2 - i\mathbf{q} \cdot (\mathbf{r}'_1 - \mathbf{r}_2)/2} \int d\mathbf{r}_1 e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{r}_1} \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \frac{1}{\mathcal{V}} \sum_{\mathbf{k}} k_\mu k_\nu \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle e^{i(\mathbf{k}-\mathbf{q}/2) \cdot (\mathbf{r}'_1 - \mathbf{r}_2)} \\ &= \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} \left(k_\mu + \frac{q_\mu}{2} \right) \left(k_\nu + \frac{q_\nu}{2} \right) \int d\mathbf{r}'_1 \int d\mathbf{r}_2 g_1(\mathbf{r}_2 - \mathbf{r}'_1) e^{-i(\mathbf{k}') \cdot (\mathbf{r}_2 - \mathbf{r}'_1)} \\ &= \left(\frac{\hbar^2 q^2}{2m} \right)^2 \int d\mathbf{r} g_1(\mathbf{r}) \sum_{\mathbf{k}'} e^{-i\mathbf{k}' \cdot \mathbf{r}} + \sum_{\mu, \nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \sum_{\mathbf{k}'} k'_\mu k'_\nu \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}' \cdot \mathbf{r}} \\ &= N \left(\frac{\hbar^2 q^2}{2m} \right)^2 + \frac{\hbar^2 q^2}{3m^2} \sum_{\mathbf{k}} k^2 \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}. \end{aligned} \quad (\text{B.60b})$$

On the other hand, the first term in the square bracket of Eq. (B.60a) can be written as

$$\begin{aligned}
& \sum_{\mu,\nu=x,y,z} \hbar^4 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} k_\mu k'_\nu \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& \times e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}'_1) - i\mathbf{k}\cdot(\mathbf{r}_2-\mathbf{r}'_2) - i\mathbf{q}\cdot(\mathbf{r}_1+\mathbf{r}'_1-\mathbf{r}_2-\mathbf{r}'_2)/2} \\
& = \sum_{\mu,\nu=x,y,z} \hbar^2 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& \times \hbar \frac{\nabla'_{1\mu} - \nabla_{1\mu}}{2i} \hbar \frac{\nabla'_{2\nu} - \nabla_{2\nu}}{2i} e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}'_1) - i\mathbf{k}\cdot(\mathbf{r}_2-\mathbf{r}'_2) - i\mathbf{q}\cdot(\mathbf{r}_1+\mathbf{r}'_1-\mathbf{r}_2-\mathbf{r}'_2)/2} \\
& = \sum_{\mu,\nu=x,y,z} \hbar^2 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \frac{1}{\mathcal{V}^2} \sum_{\mathbf{k}\mathbf{k}'} e^{-i\mathbf{k}\cdot(\mathbf{r}_1-\mathbf{r}'_1) - i\mathbf{k}\cdot(\mathbf{r}_2-\mathbf{r}'_2) - i\mathbf{q}\cdot(\mathbf{r}_1+\mathbf{r}'_1-\mathbf{r}_2-\mathbf{r}'_2)/2} \\
& \times \hbar \frac{\nabla'_{1\mu} - \nabla_{1\mu}}{2i} \hbar \frac{\nabla'_{2\nu} - \nabla_{2\nu}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& = \sum_{\mu,\nu=x,y,z} \hbar^2 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \delta(\mathbf{r}_1 - \mathbf{r}'_1) \delta(\mathbf{r}_2 - \mathbf{r}'_2) e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \\
& \times \hbar \frac{\nabla'_{1\mu} - \nabla_{1\mu}}{2i} \hbar \frac{\nabla'_{2\nu} - \nabla_{2\nu}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle. \tag{B.60c}
\end{aligned}$$

Substituting Eqs. (B.60b) and Eq. (B.60c) into Eq. (B.60a), we obtain

$$\begin{aligned}
I_2(\mathbf{q}) & = N \left(\frac{\hbar^2 q^2}{2m} \right)^2 + \frac{\hbar^2 q^2}{3m^2} \sum_{\mathbf{k}} k^2 \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\
& + \sum_{\mu,\nu=x,y,z} \hbar^2 \frac{q_\mu q_\nu}{m^2} \int d\mathbf{r}_1 \int d\mathbf{r}_2 e^{-i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)} \hbar \frac{\nabla'_{1\mu} - \nabla_{1\mu}}{2i} \hbar \frac{\nabla'_{2\nu} - \nabla_{2\nu}}{2i} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \Big|_{\mathbf{r}'_1 \rightarrow \mathbf{r}_1, \mathbf{r}'_2 \rightarrow \mathbf{r}_2}. \tag{B.61}
\end{aligned}$$

We note that if we choose the real wave function, the third term is equal to 0.

We introduce the following functions:

$$\tilde{S}_n(\mathbf{q}, \omega) \equiv \frac{S(\mathbf{q}, \omega) \omega^n}{I_0(\mathbf{q})}, \quad \tilde{I}_n(\mathbf{q}) \equiv \frac{I_n(\mathbf{q})}{I_0(\mathbf{q})}. \tag{B.62}$$

which satisfies the sum rule

$$\int d\omega \tilde{S}_0(\mathbf{q}, \omega) = 1. \tag{B.63}$$

$\tilde{S}_0(\mathbf{q}, \omega)$ can be regarded as the momentum distribution function for ω with mode \mathbf{q} . We can see easily that \tilde{I}_1 and \tilde{I}_2 correspond to expectation values for $\omega_{\mathbf{q}}$ and $\omega_{\mathbf{q}}^2$ respectively. Therefore, we can estimate the two-particle excitation spectrum $\omega_{\mathbf{q}}$ and its lifetime $\delta\omega_{\mathbf{q}}$ as

$$\omega_{\mathbf{q}} = \tilde{I}_1(\mathbf{q}), \tag{B.64a}$$

$$\delta\omega_{\mathbf{q}} = \sqrt{\tilde{I}_2(\mathbf{q}) - \tilde{I}_1(\mathbf{q})^2}. \tag{B.64b}$$

respectively.

B.4.3 Extensiton for one-particle excitation

We next consider the one-particle excitation. We start from the one-particle correlation function $A(\mathbf{k}, t)$ defined by

$$A(\mathbf{k}, t) \equiv \langle \Psi_G | e^{i\hat{H}t/\hbar} \hat{a}_{\mathbf{k}} e^{-i\hat{H}t/\hbar} \hat{a}_{\mathbf{k}}^\dagger | \Psi_G \rangle, \tag{B.65}$$

whose Fourier transform defines the one-particle spectral function as

$$A(\mathbf{k}, \varepsilon) = \frac{1}{2\pi} \int dt A(\mathbf{k}, t) e^{i\varepsilon t}. \quad (\text{B.66})$$

Using a similar procedure for deriving Eq. (B.45b), we obtain an expression for $A(\mathbf{k}, \varepsilon)$ as

$$A(\mathbf{k}, \varepsilon) = \sum_{\nu} |\langle \Psi_{\nu} | \hat{a}_{\mathbf{k}}^{\dagger} | \Psi_G \rangle|^2 \delta(\varepsilon - E_{\nu} + E_G). \quad (\text{B.67})$$

The moment of $A(\mathbf{k}, \varepsilon)$ is defined by

$$J_n(\mathbf{k}) = \int d\varepsilon A(\mathbf{k}, \varepsilon) \varepsilon^n = \sum_{\nu} |\langle \Psi_{\nu} | \hat{a}_{\mathbf{k}}^{\dagger} | \Psi_G \rangle|^2 (E_{\nu} - E_G)^n. \quad (\text{B.68})$$

It can be expressed in an alternative form similarly as in Eq. (B.47) as

$$J_n(\mathbf{k}) = \left(i \frac{d}{dt} \right)^n A(\mathbf{k}, t) \Big|_{t \rightarrow 0}. \quad (\text{B.69})$$

The first few series of $J_n(\mathbf{k})$ are given by

$$J_0(\mathbf{k}) \equiv \langle \Psi_G | \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{k}}^{\dagger} | \Psi_G \rangle, \quad (\text{B.70a})$$

$$J_1(\mathbf{k}) \equiv \langle \Psi_G | \hat{a}_{\mathbf{k}} [\hat{H}, \hat{a}_{\mathbf{k}}^{\dagger}] | \Psi_G \rangle, \quad (\text{B.70b})$$

$$J_2(\mathbf{k}) \equiv \langle \Psi_G | \hat{a}_{\mathbf{k}} [\hat{H}, [\hat{H}, \hat{a}_{\mathbf{k}}^{\dagger}]] | \Psi_G \rangle. \quad (\text{B.70c})$$

So we can find the details of the one-particle excitation by these moments.

We next transform them into forms suitable for importance sampling. To this end, we use the following commutation relations for convenience:

$$[\hat{H}_0, \hat{\psi}(\mathbf{r})] = -\hat{h}^{(1)}(\mathbf{r}) \hat{\psi}(\mathbf{r}), \quad (\text{B.71a})$$

$$[\hat{H}_{int}, \hat{\psi}(\mathbf{r})] = - \int d\mathbf{r}_1 V(\mathbf{r} - \mathbf{r}_1) \hat{\psi}^{\dagger}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}), \quad (\text{B.71b})$$

$$[\hat{H}_0, \hat{\psi}^{\dagger}(\mathbf{r})] = \hat{h}^{(1)}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}), \quad (\text{B.71c})$$

$$[\hat{H}_{int}, \hat{\psi}^{\dagger}(\mathbf{r})] = \int d\mathbf{r}_1 V(\mathbf{r} - \mathbf{r}_1) \hat{\psi}^{\dagger}(\mathbf{r}) \hat{\psi}^{\dagger}(\mathbf{r}_1) \hat{\psi}(\mathbf{r}_1), \quad (\text{B.71d})$$

where $\hat{h}^{(1)}(\mathbf{r}) \equiv \hbar^2 \nabla_{\mathbf{r}}^2 / 2m$ is the one-particle operator [50]. We now give the expression of $J_0(\mathbf{k})$, which can be written by

$$\begin{aligned} J_0(\mathbf{k}) &= 1 + \frac{1}{\mathcal{V}} \int d\mathbf{r} \int d\mathbf{r}' g_1(\mathbf{r}, \mathbf{r}') e^{-i\mathbf{k} \cdot (\mathbf{r} - \mathbf{r}')} \\ &= 1 + \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}. \end{aligned} \quad (\text{B.72})$$

Next, we consider $J_1(\mathbf{k})$. Using Eq. (B.71), we can transform it as

$$\begin{aligned}
J_1(\mathbf{k}) &= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \hat{h}^{(1)}(\mathbf{r}_1) \langle \Psi_G | \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) | \Psi_G \rangle e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) | \Psi_G \rangle e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \hat{h}^{(1)}(\mathbf{r}_1) [\delta(\mathbf{r}_1 - \mathbf{r}'_1) + g_1(\mathbf{r}_1 - \mathbf{r}'_1)] e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) [\delta(\mathbf{r}_1 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad + \delta(\mathbf{r}_2 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle] e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 [\delta(\mathbf{r}_1 - \mathbf{r}'_1) + g_1(\mathbf{r}_1 - \mathbf{r}'_1)] \frac{\hbar^2 \mathbf{k}^2}{2m} e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)}. \tag{B.73}
\end{aligned}$$

Noting $\langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle = N/\mathcal{V}$, we obtain $J_1(\mathbf{k})$ in terms of

$$S_A(\mathbf{r}_1 - \mathbf{r}'_1) \equiv \frac{1}{N(N-1)} \int d\mathbf{r}_1 V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle, \tag{B.74}$$

as

$$\begin{aligned}
J_1(\mathbf{k}) &= \frac{\hbar^2 k^2}{2m} \left[1 + \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \right] + nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \\
&\quad + \frac{N(N-1)}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 S_A(\mathbf{r}_1 - \mathbf{r}'_1) e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
&= \frac{\hbar^2 k^2}{2m} \left[1 + \int d\mathbf{r} g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} \right] + nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{r}}. \tag{B.75}
\end{aligned}$$

Note that the second and the third terms are the Hartree and Fock energies, respectively.

We next transform J_2 as

$$\begin{aligned}
J_2(\mathbf{k}) &= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \hat{h}^{(1)}(\mathbf{r}_1) \hat{h}^{(1)}(\mathbf{r}'_1) \langle \Psi_G | \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) | \Psi_G \rangle \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \hat{h}^{(1)}(\mathbf{r}'_1) V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \hat{h}^{(1)}(\mathbf{r}_1) V(\mathbf{r}'_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}'_2) \\
&\quad \times e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
&= \left(\frac{\hbar^2 k^2}{2m} \right)^2 \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} [\delta(\mathbf{r}_1 - \mathbf{r}'_1) + g_1(\mathbf{r}_1 - \mathbf{r}'_1)] \\
&\quad + \frac{\hbar^2}{2m} \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} V(\mathbf{r}_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}_2) | \Psi_G \rangle \\
&\quad + \frac{\hbar^2}{2m} \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \hat{h}^{(1)}(\mathbf{r}_1) V(\mathbf{r}'_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}'_2) [\delta(\mathbf{r}_1 - \mathbf{r}'_1) \delta(\mathbf{r}_2 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& + \delta(\mathbf{r}'_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \delta(\mathbf{r}_1 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& + \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \delta(\mathbf{r}_2 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \\
& + \delta(\mathbf{r}_2 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle] \\
& \times e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \\
& = \left(\frac{\hbar^2 k^2}{2m} \right)^2 \left[1 + \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} g_1(\mathbf{r}) \right] + \frac{\hbar^2 k^2}{2m} \left[nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \right] \\
& + \frac{\hbar^2 k^2}{2m} \left[nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \right]^* \\
& + \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \int d\mathbf{r}'_1 \int d\mathbf{r}_2 \int d\mathbf{r}'_2 V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}'_2) [\delta(\mathbf{r}_1 - \mathbf{r}'_1) \delta(\mathbf{r}_2 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& + \delta(\mathbf{r}'_1 - \mathbf{r}_2) \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \delta(\mathbf{r}_1 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) | \Psi_G \rangle \\
& + \delta(\mathbf{r}_1 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \delta(\mathbf{r}_2 - \mathbf{r}'_1) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle \\
& + \delta(\mathbf{r}_2 - \mathbf{r}'_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle + \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle] \\
& \times e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}'_1)} \tag{B.76}
\end{aligned}$$

We now introduce the following functions:

$$S_B(\mathbf{r}_1 - \mathbf{r}'_1) \equiv \frac{1}{N(N-1)} \int d\mathbf{r}_2 V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}_2) \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle, \tag{B.77}$$

$$S_C(\mathbf{r}_1 - \mathbf{r}'_1) \equiv \frac{1}{N(N-1)(N-2)} \int d\mathbf{r}_2 \int d\mathbf{r}'_2 V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}'_2) \times \langle \Psi_G | \hat{\psi}^\dagger(\mathbf{r}'_1) \hat{\psi}^\dagger(\mathbf{r}_2) \hat{\psi}^\dagger(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}'_2) \hat{\psi}(\mathbf{r}_2) \hat{\psi}(\mathbf{r}_1) | \Psi_G \rangle. \tag{B.78}$$

Using them, we can express Eq. (B.70) concisely as

$$\begin{aligned}
J_2(\mathbf{k}) & = \left(\frac{\hbar^2 k^2}{2m} \right)^2 \left[1 + \int d\mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}} g_1(\mathbf{r}) \right] + \frac{\hbar^2 k^2}{2m} \left[nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \right] \\
& + \frac{\hbar^2 k^2}{2m} \left[nV_{\mathbf{q}=\mathbf{0}} + \int d\mathbf{r} V(\mathbf{r}) g_1(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + N(N-1) \int d\mathbf{r} S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \right]^* \\
& + n \int d\mathbf{r} [V(\mathbf{r})]^2 + \int d\mathbf{r} [V(\mathbf{r})]^2 g_1(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + \int d\mathbf{r} \int d\mathbf{r}' V(\mathbf{r} - \mathbf{r}') V(\mathbf{r}) g_2(\mathbf{r}') \\
& + N(N-1) \left[\int d\mathbf{r} V(\mathbf{r}) S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + \left(\int d\mathbf{r} V(\mathbf{r}) S_A(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \right)^* \right] \\
& + N(N-1) \int d\mathbf{r} S_B(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} + N(N-1)(N-2) \int d\mathbf{r} S_C(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}. \tag{B.79}
\end{aligned}$$

We note that the functions $S_A(\mathbf{r})$, $S_B(\mathbf{r})$, $S_C(\mathbf{r})$ are expressible in forms suitable for the sampling as

$$\begin{aligned}
S_A(\mathbf{r}_1 - \mathbf{r}'_1) & = \int d\mathbf{r}_2 \cdots \int d\mathbf{r}_N V(\mathbf{r}_1 - \mathbf{r}_2) \Psi_G^*(\mathbf{r}'_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \\
S_A(\mathbf{r}) & = \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N V(\mathbf{r}_1 + \mathbf{r} - \mathbf{r}_2) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \\
& = \frac{1}{\mathcal{V}} \frac{2}{N(N-1)} \sum_{i < j} \left\langle V(\mathbf{r}_i - \mathbf{r}_j + \mathbf{r}) \frac{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_i + \mathbf{r}, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_N)}{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)} \right\rangle, \tag{B.80}
\end{aligned}$$

$$\begin{aligned}
S_B(\mathbf{r}) &= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{r}) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \\
&= \frac{1}{\mathcal{V}} \frac{2}{N(N-1)} \sum_{i < j} \left\langle V(\mathbf{r}_i - \mathbf{r}_j) V(\mathbf{r}_i - \mathbf{r}_j + \mathbf{r}) \frac{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_i + \mathbf{r}, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_N)}{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)} \right\rangle, \tag{B.81}
\end{aligned}$$

$$\begin{aligned}
S_C(\mathbf{r}_1 - \mathbf{r}'_1) &= \int d\mathbf{r}_2 \int d\mathbf{r}'_2 \int d\mathbf{r}_4 \cdots \int d\mathbf{r}_N V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}'_1 - \mathbf{r}'_2) \\
&\quad \times \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_2, \mathbf{r}_4, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}'_2, \mathbf{r}_4, \cdots, \mathbf{r}_N) \\
S_C(\mathbf{r}) &= \frac{1}{\mathcal{V}} \int d\mathbf{r}_1 \cdots \int d\mathbf{r}_N V(\mathbf{r}_1 - \mathbf{r}_2) V(\mathbf{r}_1 - \mathbf{r}_3 + \mathbf{r}) \Psi_G^*(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) \Psi_G(\mathbf{r}_1 + \mathbf{r}, \mathbf{r}_2, \cdots, \mathbf{r}_N) \\
&= \frac{1}{\mathcal{V}} \frac{2}{N(N-1)(N-2)} \sum_{k \neq i, j} \sum_{i < j} \left\langle V(\mathbf{r}_i - \mathbf{r}_j) V(\mathbf{r}_i - \mathbf{r}_k + \mathbf{r}) \frac{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_i + \mathbf{r}, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N)}{\Psi_G(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)} \right\rangle \tag{B.82}
\end{aligned}$$

respectively.

Finally we introduce the following functions:

$$\tilde{A}_n(\mathbf{k}, \varepsilon) \equiv \frac{A(\mathbf{k}, \varepsilon) \varepsilon^n}{J_0(\mathbf{k})}, \quad \tilde{J}_n(\mathbf{k}) \equiv \frac{J_n(\mathbf{k})}{J_0(\mathbf{k})}. \tag{B.83}$$

Hence we can express the one-particle excitation spectrum $\varepsilon_{\mathbf{k}}$ and its lifetime $\delta\varepsilon_{\mathbf{k}}$ as

$$\varepsilon_{\mathbf{k}} = \tilde{J}_1(\mathbf{k}), \tag{B.84a}$$

$$\delta\varepsilon_{\mathbf{k}} = \sqrt{\tilde{J}_2(\mathbf{k}) - \tilde{J}_1^2(\mathbf{k})}, \tag{B.84b}$$

respectively.

C Two-particle scattering theory

C.1 Formalism

We consider a two-particle scattering problem of identical particles with mass m described by reduced Hamiltonian for the relative coordinate ($\hbar = 1$),

$$\hat{H} \equiv -\frac{\nabla^2}{2m_{\text{red}}} + U(r), \quad m_{\text{red}} = \frac{m}{2}, \quad (\text{C.1})$$

which in the momentum representation reads

$$\langle \mathbf{p}' | \hat{H} | \mathbf{p} \rangle = \varepsilon_{\mathbf{p}}^{\text{red}} \delta_{\mathbf{p}'\mathbf{p}} + \frac{U_{\mathbf{p}'-\mathbf{p}}}{(2\pi)^3}, \quad \varepsilon_{\mathbf{p}}^{\text{red}} = \frac{p^2}{2m_{\text{red}}}, \quad U_{\mathbf{p}} \equiv \int d^3r U(r) e^{i\mathbf{p}\cdot\mathbf{r}}. \quad (\text{C.2})$$

The transition matrix T is given by Eq. (37.25) of Schiff, *Quantum Mechanics* [64]. It is expressed in the momentum representation as

$$\begin{aligned} & \langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle \\ & \equiv \langle \mathbf{p}' | U | \mathbf{p} \rangle + \langle \mathbf{p}' | U (\varepsilon_{\mathbf{p}}^{\text{red}} - \hat{H} - i0_+)^{-1} U | \mathbf{p} \rangle \\ & = \langle \mathbf{p}' | U | \mathbf{p} \rangle + \langle \mathbf{p}' | U (\varepsilon_{\mathbf{p}}^{\text{red}} - \hat{H}_0 - i0_+)^{-1} U | \mathbf{p} \rangle \\ & \quad + \langle \mathbf{p}' | U (\varepsilon_{\mathbf{p}}^{\text{red}} - \hat{H}_0 - i0_+)^{-1} U (\varepsilon_{\mathbf{p}}^{\text{red}} - \hat{H}_0 - i0_+)^{-1} U | \mathbf{p} \rangle + \dots \\ & = \frac{1}{(2\pi)^3} U_{\mathbf{p}'-\mathbf{p}} + \frac{1}{(2\pi)^6} \int d^3p_1 U_{\mathbf{p}'-\mathbf{p}_1} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_1-\mathbf{p}} + \frac{1}{(2\pi)^9} \int d^3p_1 \int d^3p_2 \\ & \quad \times U_{\mathbf{p}'-\mathbf{p}_1} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_1-\mathbf{p}_2} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_2}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_2-\mathbf{p}} + \dots \\ & = \frac{1}{(2\pi)^3} \left[U_{\mathbf{p}'-\mathbf{p}} + \frac{1}{(2\pi)^3} \int d^3p_1 U_{\mathbf{p}'-\mathbf{p}_1} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_1-\mathbf{p}} + \frac{1}{(2\pi)^6} \int d^3p_1 \int d^3p_2 \right. \\ & \quad \left. \times U_{\mathbf{p}'-\mathbf{p}_1} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_1-\mathbf{p}_2} (\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_2}^{\text{red}} - i0_+)^{-1} U_{\mathbf{p}_2-\mathbf{p}} + \dots \right] \end{aligned} \quad (\text{C.3})$$

We also introduce the scattering amplitude $f(\mathbf{p}', \mathbf{p})$ by Eq. (37.21) of Schiff with $C = (2\pi)^{-3/2}$ and $\mu = m_{\text{red}}$, i.e.,

$$-\frac{2\pi}{m_{\text{red}}} f(\mathbf{p}', \mathbf{p}) \equiv (2\pi)^3 \langle \mathbf{p}' | \hat{T} | \mathbf{p} \rangle. \quad (\text{C.4})$$

We note that $k' = k$ in Eq. (C.3) and (C.4) for the relevant potential scattering by $U(r)$. Next, we expand $U_{\mathbf{p}'-\mathbf{p}}$ and $f(\mathbf{p}', \mathbf{p})$ in spherical harmonics as

$$U_{\mathbf{p}'-\mathbf{p}} = 4\pi \sum_{\ell=0}^{\infty} U_{\ell}(k', p) \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{\mathbf{p}}') Y_{\ell m}^*(\hat{\mathbf{p}}), \quad (\text{C.5a})$$

$$f(\mathbf{p}', \mathbf{p}) = 4\pi \sum_{\ell=0}^{\infty} f_{\ell}(p) \sum_{m=-\ell}^{\ell} Y_{\ell m}(\hat{\mathbf{p}}') Y_{\ell m}^*(\hat{\mathbf{p}}). \quad (\text{C.5b})$$

Substituting them into Eq. (C.4) and carrying out the angular integrations with

$$\int d\Omega_{\mathbf{p}} Y_{\ell m}(\hat{\mathbf{p}}) Y_{\ell' m'}^*(\hat{\mathbf{p}}) = \delta_{\ell, \ell'} \delta_{m, m'}. \quad (\text{C.6})$$

Therefore we obtain

$$\begin{aligned} & \frac{-2\pi}{m_{\text{red}}} f_{\ell}(p) \\ & = U_{\ell}(p, p) + \int \frac{d^3p_1}{(2\pi)^3} U_{\ell}(p, p_1) \frac{1}{\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+} U_{\ell}(p_1, p) + \int \frac{d^3p_1}{(2\pi)^3} \int \frac{d^3p_2}{(2\pi)^3} U_{\ell}(p, p_1) \\ & \quad \times \frac{1}{\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_1}^{\text{red}} - i0_+} U_{\ell}(p_1, p_2) \frac{1}{\varepsilon_{\mathbf{p}}^{\text{red}} - \varepsilon_{\mathbf{p}_2}^{\text{red}} - i0_+} U_{\ell}(p_2, p) + \dots \end{aligned} \quad (\text{C.7})$$

We now consider the low-energy limit $p \rightarrow 0$, where $f_{\ell=0}(p)$ reduces to the s -wave scattering length a as [see, Landau and Lifschitz, *Quantum Mechanics*, Eq. (130.9) [63]]

$$\lim_{p \rightarrow 0} f_0(p) = -a, \quad (\text{C.8})$$

and $\ell > 0$ channels can be neglected. Taking this limit in Eq. (C.7), we obtain

$$\begin{aligned} \frac{4\pi}{m}a &= U_0(0,0) - \int \frac{d^3 p_1}{(2\pi)^3} U_0(0,p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U_0(p_1,0) \\ &+ \int \frac{d^3 p_1}{(2\pi)^3} \int \frac{d^3 p_2}{(2\pi)^3} U_0(0,p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U_0(p_1,p_2) \frac{1}{2\varepsilon_{\mathbf{p}_2}} U_0(p_2,0) + \dots, \end{aligned} \quad (\text{C.9})$$

where we have used $m_{\text{red}} = m/2$ and $\varepsilon_{\mathbf{p}}^{\text{red}} = 2\varepsilon_{\mathbf{p}}$ with

$$\varepsilon_{\mathbf{p}} \equiv \frac{p^2}{2m}. \quad (\text{C.10})$$

Let us introduce $U^{(\text{eff})}(p, p')$ that satisfies the integral equation:

$$\begin{aligned} U^{(\text{eff})}(p, p') &= U_0(p, p') - \int \frac{d^3 p_1}{(2\pi)^3} U_0(p, p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U^{(\text{eff})}(p_1, p') \\ &= U_0(p, p') - \frac{1}{4\pi^2} \int_0^\infty dp_1 U_0(p, p_1) \frac{1}{2\varepsilon_{\mathbf{p}_1}} U^{(\text{eff})}(p_1, p'). \end{aligned} \quad (\text{C.11})$$

Then, Eq. (C.9) can be expressed concisely as

$$a = \frac{m}{4\pi} U^{(\text{eff})}(0, 0). \quad (\text{C.12})$$

C.2 Applications

First, we consider the following potential:

$$U(\mathbf{r}) = U_0 \delta(\mathbf{r}), \quad (\text{C.13})$$

whose Fourier transformation is given by $U_{\mathbf{p}} = U_0$. It has no dependence on momentum \mathbf{p} , so we also obtain $U_0(p, p') = U_0$. By introducing the cut-off momentum p_c for the integration in Eq. (C.11), we can solve it as

$$U_0 = \left(\frac{m}{4\pi a} - \frac{p_c}{4\pi^2} \right)^{-1}. \quad (\text{C.14})$$

If we set p_c as $0 \ll p_c \ll \pi m/a$, we can remove the cut-off dependence as

$$U_0 = \frac{4\pi a}{m}. \quad (\text{C.15})$$

Next, we consider a finite-range potential (see reference [50], Chapter 6.):

$$U(r) \equiv \frac{U_0}{8\pi r_0^3} e^{-r/r_0}. \quad (\text{C.16})$$

By performing Fourier transform for $U(r)$, we obtain

$$U_{\mathbf{p}} = \frac{U_0}{(1 + r_0^2 p^2)^2}. \quad (\text{C.17a})$$

We then expand it in spherical harmonics and use Eq. (C.6) to obtain

$$U_0(p, q) = \frac{U_0}{(1 + r_0^2 p^2 + r_0^2 q^2)^2 - 4r_0^4 p^2 q^2}. \quad (\text{C.17b})$$

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