Doctoral Thesis

Number-Phase Fluctuations in Isolated Superconductors

(孤立超伝導体の粒子数*位相揺らぎ)

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1 Introduction

One of the most controversial issues in the Bardeen-Cooper-Schrieffer (BCS) theory[1]. which is remarkably successful in describing weak-coupling superconductors, may be the superposition over the number of condensed particles in their variational ground-state wave function.

This is apparently incompatible with particle-number conservation, which manifestly holds in any closed system, as noted by Schrieffer from the beginning[2] and emphasized by Peierls[3] and Leggett.[4]

On the other hand, the superposition was used by Anderson[5] in the context of Bose-Einstein condensation to discuss emergence of a well-defined macroscopic phase, called spontaneously broken gauge symmetry,[6, 7] as the key ingredient for superfluidity and the Josephson effect.

Thus, particle-number fluctuations seem indispensable for bringing macroscopic coherence to the system, which were originally traced by Anderson to the exchange of particles between subsystems.[5]

However, question may be raised regarding this identification because there are definitely no fluctuations in the total particle number in any closed system.[4, 7]

$$\Delta N = 0 \Rightarrow \Delta\Phi \to \infty?$$

If we consider that the fluctuations of particle number ΔN is absolutely zero, does that lead to an infinite fluctuation in the superconducting phase? Are the fluctuations real or a mere artifact in the mathematical treatment of superconductivity? If the former is the case, where do they originate from? How can we define a macroscopic wave function with a well-defined phase in isolated superconductors? We aim to answer these questions by improving the BCS wave function with a fixed particle number.

Weak-coupling superconductors have been described theoretically within the mean-field framework. The corresponding ground-state with N fermions has been identified as the anti-symmetrized product of $N/2$ Cooper-pairs with no superposition,

$$|\Phi_N^{\rm BCS}\rangle = A_N^{-1/2} \exp(\hat{\pi}_{\rm cp}^{\dagger})^{N/2}|0\rangle.$$

[4, 8, 9] which may thereby have no well-defined phase.[5]

Now, we will see what happens to this wave function when we incorporate many-body correlations beyond the mean-field treatment, which is given by

$$|\Phi_N^{\rm Corr.}\rangle = \mathscr{B}_N^{-1/2} \exp(\hat{\pi}_4^{\dagger})|\Phi_N^{\rm BCS}\rangle.$$

Our physical motivation lies in the following observation: the pair condensation energy in the weak-coupling region is exponentially small, $\sim \exp(-1/g)$ with $g > 0$ a dimensionless coupling constant, whereas the correlations energy is proportional to g^2 and also negative for any type of interactions, as seen by the second-order perturbation in terms of the interaction. In other words, the correlations lower the ground-state energy relatively far more than Cooper-pair condensation for $g \ll 1$.

This fact implies that, formally speaking, Cooper-pair condensation should be studied only after the correlations effects have been incorporated.

We incorporate the correlation effects to show explicitly that the correlations produce finite non-condensed particles in the ground-state, which work as a particle reservoir for the condensate to naturally yield the superposition, in exactly the same way as in the case of interacting Bose-Einstein condensates.[10]

Thus, the superposition is a real physical entity that exists in any isolated superconductor or superfluid. Note in this context that the superposition and coherence have so far been discussed mostly in terms of condensed particles alone.[5, 7, 11, 12]

This thesis is organized as follows;

We will discuss the improved ground-wave function with many-body correlations.

Section 2 presents formulation.

Section 3 gives numerical results.

Section 4 presents concluding remarks.

We also present details that deriving the formalism from Appendix.

Appendix A describes the mathematical properties of the inner-product of the BCS ground-state wave function as Q_n. The general expression and the asymptotic expression of Q_n plays an important role in evaluating the ground-state energy.

Appendix B provides a new method of using the asymptotic expression of Q_n, deriving the current canonical BCS formula, which is more mathematical treatable than the method emphasized by [4].

Appendix C points out the approximations we adopted in the process of deriving the formalism, and explain some difficulties it encountered.

Appendix D describes the process of deriving the quasi-particle operator $\hat{\gamma}$ and its inverse transformation.

Appendix E derives the equations to minimize the variational ground-state energy including the $\hat{\pi}_4$ correlations in detail.

Appendix F describes how to perform triple sums over wave vectors efficiently in numerical calculations.

Finally, in Appendix G, we present a possible formulation which enables us to evaluate the ground-state energy with relatively small number of total particles, and points out the numerical difficulty it may face.

2 Particle-Number Fluctuations in Isolated Superconductors

2.1 Model

We consider a system with N identical fermions (N ≫1, N:even) with mass m and spin $\pm\frac{1}{2}$. The Hamiltonian is given by

$$\hat{H}_{\text{BCS}} \equiv \hat{H}_0 + \hat{H}_{\text{int}}. \tag{2.1}$$

The kinetic energy $\hat{H}_0$ and the interaction energy $\hat{H}_{\text{int}}$ is given by

$$\hat{H}_0 \equiv \sum_{\mathbf{k}\alpha}^{\text{Fin.}} \varepsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\alpha} \hat{c}_{\mathbf{k}\alpha}, \quad \hat{H}_{\text{int}} \equiv \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\text{Fin.}} \sum_{\alpha\alpha'} U_q \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}\alpha} \hat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q}\alpha} \hat{c}_{\mathbf{k}'\alpha'} \hat{c}_{\mathbf{k}\alpha}, \tag{2.2}$$

where $\varepsilon_{\mathbf{k}}$ and U_q are given explicitly by

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}, \quad U_q = \int U(r) \mathrm{e}^{-i\mathbf{q}\mathbf{r}} d^3 r. \tag{2.3}$$

Basically, all summations in this thesis are performed over a finite number of particles, which we denote as "Fin".

Creation and annihilation operators satisfy the anti-communication relations of fermions:

$$\{\hat{c}_{\mathbf{k}\alpha}, \hat{c}^{\dagger}_{\mathbf{k}'\alpha'}\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\alpha'}, \quad \{\hat{c}_{\mathbf{k}\alpha}, \hat{c}_{\mathbf{k}'\alpha'}\} = 0, \tag{2.4}$$

with $\alpha = \uparrow, \downarrow$ for $\alpha = \frac{1}{2}, -\frac{1}{2}$, respectively.

This expression of BCS Hamiltonian is obtained through an expansion (see Appendix B.1) of basis functions satisfying:

$$\hat{\Psi}(\xi) = \sum_q \hat{c}(q)\varphi_q(\xi), \tag{2.5}$$

where $\hat{\Psi}(\xi)$ is the field operator and $\hat{c}(q)$ is the one-particle annihilation operator.

The expansion constant $\varphi_q(\xi)$ denotes particle wave function, where q denotes momentum and spin $\{\mathbf{k}, \alpha\}$.

2.2 Number-Fixed BCS wave function

We consider a homogenous system in a box of volume V with periodic boundary conditions and anticipate condensation with s-wave pairing for this model. We introduce the pair operator $\hat{\pi}^{\dagger}_{\text{cp}}$ by

$$\hat{\pi}^{\dagger}_{\text{cp}} \equiv \frac{1}{2} \sum_{\mathbf{k}\alpha}^{\text{Fin.}} \phi_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\alpha} \hat{c}^{\dagger}_{\mathbf{k}-\alpha}, \tag{2.6}$$

where $\phi_{\mathbf{k}}$ is the Fourier coefficient describes bound-state wave function, which describes a single Cooper pair.

The Number-fixed BCS wave function is given by the pair creation operator $\hat{\pi}^{\dagger}_{\text{cp}}$,

$$|\Phi^{\text{BCS}}_N\rangle = A^{-1/2}_{N/2}(\hat{\pi}^{\dagger}_{\text{cp}})^{N/2}|0\rangle, \tag{2.7}$$

where $A_{N/2}$ is the normalization constant defined by the inner product of the ket vector $\hat{\pi}^{\dagger}_{\text{cp}}|0\rangle$ as follows;

$$A_{N/2} \equiv \frac{\langle 0|(\hat{\pi}_{\text{cp}})^{N/2}(\hat{\pi}^{\dagger}_{\text{cp}})^{N/2}|0\rangle}{(N/2)!^2}. \tag{2.8}$$

The vacuum state defined by the annihilation operator satisfies

$$\hat{c}_{\mathbf{k}\alpha}|0\rangle = 0. \tag{2.9}$$

Eq.(2.7) can be treated as the N-paticle projection of the grand canonical BCS wave function

$$\begin{aligned} |\Phi\rangle &= A_{\text{n}}\sum_{n=0}^{\infty}\frac{(\hat{\pi}^{\dagger}_{\text{cp}})^n}{n!}|0\rangle \\ &= A_{\text{n}}\exp\left(\hat{\pi}^{\dagger}_{\text{cp}}\right)|0\rangle. \end{aligned} \tag{2.10}$$

where A_{n} is the normalization constant.

The exponential form of the wave function, Eq.(2.10), which represents an extension of the homogenous variational wave function emphasized by J.R. Schrieffer. The physical meaning of this wave function denotes linear combination of states with different particle number.

2.3 Number-conserving operators

Following the number-conserving BCS wave function, we introduce the number-conserving creation-annihilation operators as follows;

First, we introduce the creation and annihilation operators $(\hat{\beta}^{\dagger}_{\mathbf{k}\alpha}, \hat{\beta}_{\mathbf{k}\alpha})$ by

$$\hat{\beta}^{\dagger}_{\mathbf{k}\alpha}|\Phi^{\text{BCS}}_N\rangle = |\Phi^{\text{BCS}}_{N+2}\rangle, \quad \hat{\beta}_{\mathbf{k}\alpha}|\Phi^{\text{BCS}}_N\rangle = |\Phi^{\text{BCS}}_{N-2}\rangle. \tag{2.11}$$

The physical meaning of these operators is interpreted as increasing (decreasing) the number of Cooper pairs by one.

These operators is expressible by Cooper pair creation and annihilation operators $(\hat{\pi}^{\dagger}_{\text{cp}}, \hat{\pi}_{\text{cp}})$ as

$$\hat{\beta}^{\dagger} \equiv \sqrt{\frac{Q_{N/2}}{Q_{N/2+1}}}\frac{\hat{\pi}^{\dagger}_{\text{cp}}}{N/2+1}. \tag{2.12}$$

These operators follows Eq.(2.11) that

$$(\hat{\beta}_{\mathbf{k}\alpha})^{\nu}(\hat{\beta}^{\dagger}_{\mathbf{k}\alpha})^{\nu}|\Phi^{\text{BCS}}_N\rangle = |\Phi^{\text{BCS}}_N\rangle, \quad (\hat{\beta}^{\dagger}_{\mathbf{k}\alpha})^{\nu}(\hat{\beta}_{\mathbf{k}\alpha})^{\nu}|\Phi^{\text{BCS}}_N\rangle = \begin{cases} |\Phi^{\text{BCS}}_N\rangle : \nu \leq N/2 \\ 0 : \quad\quad \nu > N/2 \end{cases} \quad \forall \nu, N \in \mathbb{Z}^+. \tag{2.13}$$

so that

$$(\hat{\beta}_{\mathbf{k}\alpha})^{\nu}(\hat{\beta}^{\dagger}_{\mathbf{k}\alpha})^{\nu} = \hat{1}, \tag{2.14}$$

and

$$(\hat{\beta}^{\dagger}_{\mathbf{k}\alpha})^{\nu}(\hat{\beta}_{\mathbf{k}\alpha})^{\nu} \simeq \hat{1}. \tag{2.15}$$

The approximation in Eq.(2.15) becomes practically exact whenever the particle number condition $\nu \leq N/2$ is satisfied.

Then, we introduce the number-conserving Bogoliubov operator

$$\hat{\gamma}_{\mathbf{k}\alpha} \equiv u_{\mathbf{k}}\hat{c}_{\mathbf{k}\alpha} - (-1)^{\frac{1}{2}-\alpha} v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}, \tag{2.16}$$

which satisfies

$$\hat{\gamma}_{\mathbf{k}\alpha}|\Phi_N^{\mathrm{BCS}}\rangle = 0. \tag{2.17}$$

The functional $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ is denoted as

$$u_k \equiv \frac{1}{\sqrt{1+|\phi_k|^2}}, \quad v_k \equiv \frac{\phi_k}{\sqrt{1+|\phi_k|^2}}, \tag{2.18}$$

satisfying

$$|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2 = 1. \tag{2.19}$$

The inverse of Eq.(2.20) can be derived as

$$\hat{c}_{\mathbf{k}\alpha} = u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\alpha} + (-1)^{\frac{1}{2}-\alpha} v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}. \tag{2.20}$$

(See Appendix D).

We may use the number-conserving Bogoliubov operator $\hat{\gamma}_{\mathbf{k}\alpha}$ to characterize ket vector denoted by the BCS wave function $|\Phi_N^{\mathrm{BCS}}\rangle$ as the "vacuum of quasiparticles", which we used the same mathematical structure in Eq.(2.9).

Eq.(2.17) indicates that the Bogoliubov quasi-particles are absent from the mean-field BCS ground-state given by Eq.(2.7).

It is obvious that the number-conserving Bogoliubov operators also obeys the anti-symmetric commutation relation of fermions

$$\{\hat{\gamma}_{\mathbf{k}\alpha}, \hat{\gamma}^{\dagger}_{\mathbf{k}'\alpha'}\} = \delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\alpha'}, \quad \{\hat{\gamma}_{\mathbf{k}\alpha}, \hat{\gamma}_{\mathbf{k}'\alpha'}\} = 0. \tag{2.21}$$

(See Appendix D). We use the number-conserving Bogoliubov operator to create a dynamic particle changing process among cooper pairs and non-condensate particles in the following sections.

2.4 Improved wave function with correlations

We incorporate many-body correlations into the BCS wave function of Eq.(2.7). With this modification to the BCS ground-state, we investigate the possibility that some of quasi-particle state become occupied owing to many-body correlations.

Before we introduce our improved variational wave function, let us define the number-conserving correlations operator $\hat{\pi}_4^\dagger$ by

$$\hat{\pi}_4^\dagger \equiv \frac{1}{4!}\sum_{\kappa_1}\sum_{\kappa_2}\sum_{\kappa_3}\sum_{\kappa_4} w_{\kappa_1\kappa_2\kappa_3\kappa_4}\hat{\gamma}_{\kappa_1}^\dagger\hat{\gamma}_{\kappa_2}^\dagger\hat{\gamma}_{\kappa_3}^\dagger\hat{\gamma}_{\kappa_4}^\dagger\hat{\beta}^2, \tag{2.22}$$

where $\kappa_j \equiv \{\mathbf{k_j}, \alpha_\mathbf{j}\}_{j=1}^4$ denotes momentum and spin. The variational parameter $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$ is anti-symmetric with respect to any permutation of $\kappa_1\kappa_2\kappa_3\kappa_4$ by definition

$$\hat{P}w_{\kappa_1\kappa_2\kappa_3\kappa_4} = (-1)^P w_{\kappa_1\kappa_2\kappa_3\kappa_4}. \tag{2.23}$$

This number-conserving correlations operator describes the physical process that two Cooper pairs broken up into four quasi-particles.

Our improved variational wave function is given in terms of the BCS wave function Eq.(2.7) and the number-conserving correlations operator $\hat{\pi}_4^\dagger$ (2.22) by

$$|\Phi_N^{\text{Corr.}}\rangle = \mathscr{B}_N^{-1/2}\exp(\hat{\pi}_4^\dagger)|\Phi_N^{\text{BCS}}\rangle, \tag{2.24}$$

where the quantity $\mathscr{B}_N^{-1/2}$ denotes the normalization constant

$$\mathscr{B}_N \equiv \langle\Phi_N^{\text{BCS}}|\exp(\hat{\pi}_4)\exp(\hat{\pi}_4^\dagger)|\Phi_N^{\text{BCS}}\rangle \tag{2.25}$$

$$= \exp\Big(\frac{1}{4!}\sum_{\kappa_1}\sum_{\kappa_2}\sum_{\kappa_3}\sum_{\kappa_4}|w_{\kappa_1\kappa_2\kappa_3\kappa_4}|^2 + \mathrm{O}_{(|\mathrm{w}|^4)}\Big). \tag{2.26}$$

This improved variational wave function has finite occupations of quasi-particles when $w_{\kappa_1\kappa_2\kappa_3\kappa_4} \neq 0$ is realized. The exponent in Eq.(2.26) is expressible as Fig.1 in terms of connected Feynman diagrams. the first term denotes the lowest-order contribution. However, we ignored higher order terms of the normalization constant $\mathscr{B}_N$ in the weak-coupling region.

It will turn out below that Eq.(2.17), Eq.(2.22) and Eq.(2.26) suffice to perform an evaluation of the ground-state energy up to the first order in the correlations parameter $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$, which is beyond the framework of the mean-field theory.

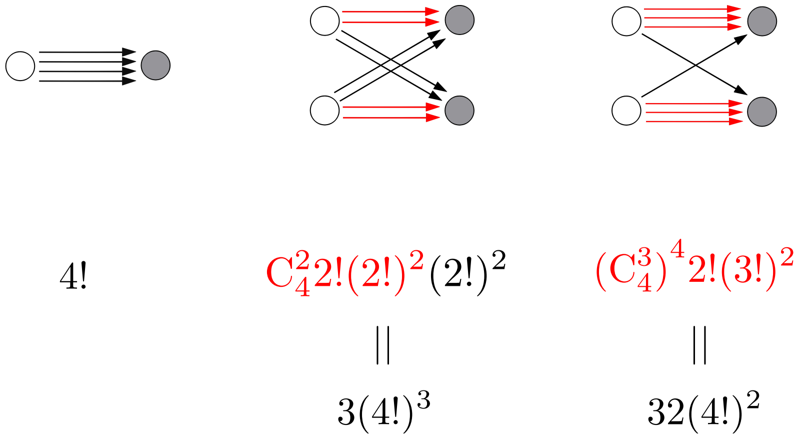

Figure 1: (Color online) Diagrammatic expansion of $\mathrm{Ln}\mathscr{B}_N$ up to the second order in π_4. An open (filled) circle with four outgoing (incoming) arrows denotes $\hat{\pi}_4^\dagger(\pi_4)$. The weight below each figure denotes the number of combinations to realize the connection.

2.5 Expression for the ground-state energy

We now evaluate the expectation of BCS Hamiltonian with the improved variation wave function of Eq.(2.24) follows

$$\varepsilon_{\text{Corr.}} \equiv \big\langle \Phi_N^{\text{Corr.}} | \hat{H}_{\text{BCS}} | \Phi_N^{\text{Corr.}} \big\rangle. \tag{2.27}$$

This ground-state energy can be performed exactly in the same way as that for the interacting Bose-Einstein condensates.

The inverse of the number-conserving Bogoliubov quasi-particle operator (2.20) follows

$$\hat{c}_{\mathbf{k}\alpha} = u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\alpha} + (-1)^{\frac{1}{2}-\alpha} v_{\mathbf{k}} \hat{\gamma}^\dagger_{-\mathbf{k}-\alpha}\hat{\beta}. \tag{2.28}$$

With the inverse transformation $(\hat{\gamma}^\dagger_{\mathbf{k}\alpha}, \hat{\gamma}_{\mathbf{k}\alpha}) \to (\hat{c}^\dagger_{\mathbf{k}\alpha}, \hat{c}_{\mathbf{k}\alpha})$, the evaluation of $\varepsilon_{\text{Corr.}}$ can be performed subsequently.

Particularly, with Eq.(2.28), the interaction energy $\hat{H}_{\text{int}}$ can be performed as

$$\begin{aligned}
&\big\langle \Phi_N^{\text{Corr.}} | \hat{H}_{\text{int}} | \Phi_N^{\text{Corr.}} \big\rangle \\
=&\frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\text{Fin.}}\sum_{\alpha\alpha'} U_q \big\langle \Phi_N^{\text{Corr.}} | \big[u_{\mathbf{k}+\mathbf{q}}\hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},\alpha}\big] + (-1)^{\frac{1}{2}-\alpha} v^*_{\mathbf{k}+\mathbf{q}}\hat{\gamma}_{-\mathbf{k}-\mathbf{q},-\alpha}\hat{\beta}^\dagger\big] \\
&\times \big[u_{\mathbf{k}'-\mathbf{q}}\hat{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},\alpha'}\big] + (-1)^{\frac{1}{2}-\alpha'} v^*_{\mathbf{k}'-\mathbf{q}}\hat{\gamma}_{-\mathbf{k}'+\mathbf{q},-\alpha'}\hat{\beta}^\dagger\big] \\
&\times \big[u_{\mathbf{k}'}\hat{\gamma}_{\mathbf{k}'\alpha'} + (-1)^{\frac{1}{2}-\alpha} v_{\mathbf{k}'}\hat{\gamma}^\dagger_{-\mathbf{k}'-\alpha'}\hat{\beta}\big] \times \big[u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\alpha} + (-1)^{\frac{1}{2}-\alpha} v_{\mathbf{k}}\hat{\gamma}^\dagger_{-\mathbf{k}-\alpha}\hat{\beta}\big] | \Phi_N^{\text{Corr.}} \big\rangle.
\end{aligned} \tag{2.29}$$

With careful calculation of Eq.(2.29), we obtain the following terms as

$$
\begin{aligned}
&\big\langle \Phi_N^{\text{Corr.}} | \hat{H}_{\text{int}} | \Phi_N^{\text{Corr.}} \big\rangle \\
=&\frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}'-\mathbf{q}} u_{\mathbf{k}'} u_{\mathbf{k}} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},\alpha} \hat{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},\alpha'} \hat{\gamma}_{\mathbf{k}'\alpha'} \hat{\gamma}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} v_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'} v_{\mathbf{k}} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}_{-\mathbf{k}-\mathbf{q},-\alpha} \hat{\gamma}_{-\mathbf{k}'+\mathbf{q},-\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}'-\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}-\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} v_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}'-\mathbf{q}} u_{\mathbf{k}'} v_{\mathbf{k}} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}_{-\mathbf{k}-\mathbf{q},-\alpha} \hat{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},\alpha'} \hat{\gamma}_{\mathbf{k}'\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}-\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'} u_{\mathbf{k}} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},\alpha} \hat{\gamma}_{-\mathbf{k}'+\mathbf{q},\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}'-\alpha'} \hat{\gamma}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} v_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'} u_{\mathbf{k}} (-1)^{1-\alpha-\alpha'} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}_{-\mathbf{k}-\mathbf{q},-\alpha} \hat{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},-\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}'-\alpha'} \hat{\gamma}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} u_{\mathbf{k}'} v_{\mathbf{k}} (-1)^{1-\alpha-\alpha'} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},\alpha} \hat{\gamma}_{-\mathbf{k}'+\mathbf{q},-\alpha'} \hat{\gamma}_{\mathbf{k}'\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}-\alpha} | \Phi_N^{\text{Corr.}} \big\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k}+\mathbf{q}} u_{\mathbf{k}'-\mathbf{q}} v_{\mathbf{k}'} v_{\mathbf{k}} (-1)^{1-\alpha-\alpha'} \big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^\dagger_{\mathbf{k}+\mathbf{q},\alpha} \hat{\gamma}^\dagger_{\mathbf{k}'-\mathbf{q},\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}'-\alpha'} \hat{\gamma}^\dagger_{-\mathbf{k}-\alpha} (\hat{\beta})^2 | \Phi_N^{\text{Corr.}} \big\rangle
\end{aligned} \tag{2.30a}
$$

$$
+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}} U_q \sum_{\alpha\alpha'} v_{\mathbf{k}+\mathbf{q}} v_{\mathbf{k}'-\mathbf{q}} u_{\mathbf{k}'} u_{\mathbf{k}} (-1)^{1-\alpha-\alpha'} \big\langle \Phi_N^{\text{Corr.}} | (\hat{\beta}^\dagger)^2 \hat{\gamma}_{-\mathbf{k}-\mathbf{q},-\alpha} \hat{\gamma}_{-\mathbf{k}'+\mathbf{q},-\alpha'} \hat{\gamma}_{\mathbf{k}'\alpha'} \hat{\gamma}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \big\rangle. \tag{2.30b}
$$

Firstly, compared with the mean-field BCS theory is the finite average, a new pair of ingredient which includes its conjugate, emerged from the evaluation of $\varepsilon_{\text{Corr.}}$, precisely the terms colored red in the evaluation of $\hat{H}_{\text{int}}$, i.e.(2.30a) and (2.30b), which can be performed as

$$
\big\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^\dagger_{\kappa_1} \hat{\gamma}^\dagger_{\kappa_2} \hat{\gamma}^\dagger_{\kappa_3} \hat{\gamma}^\dagger_{\kappa_4} \hat{\beta}^2 | \Phi_N^{\text{Corr.}} \big\rangle = \frac{\delta \text{Ln} \mathscr{B}_N}{\delta w_{\kappa_1\kappa_2\kappa_3\kappa_4}} \approx w^*_{\kappa_1\kappa_2\kappa_3\kappa_4}, \tag{2.31}
$$

where we used Eq.(2.26) in the second approximation.

We also notice the following calculation

$$
\begin{aligned}
\hat{\gamma}_\kappa | \Phi_N^{\text{Corr.}} \big\rangle &= \mathscr{B}_N^{-1/2} \{\hat{\gamma}_\kappa, \exp(\hat{\pi}_4^\dagger)\} | \Phi_N^{\text{BCS}} \big\rangle \\
&= \{\hat{\gamma}_\kappa, (\hat{\pi}_4^\dagger)\} | \Phi_N^{\text{Corr.}} \big\rangle \\
&= \frac{1}{3!} \sum_{\kappa_2\kappa_3\kappa_4} w_{\kappa\kappa_2\kappa_3\kappa_4} \hat{\gamma}^\dagger_{\kappa_2} \hat{\gamma}^\dagger_{\kappa_3} \hat{\gamma}^\dagger_{\kappa_4} | \Phi_N^{\text{Corr.}} \big\rangle.
\end{aligned} \tag{2.32}
$$

holds. Moreover, we define another finite average $\eta_{\mathbf{k}}$, which denotes a important quantity as

$$\eta_{\mathbf{k}} \equiv \left\langle \Phi_N^{\text{Corr.}} | \hat{\gamma}^{\dagger}_{\mathbf{k}\alpha} \hat{\gamma}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \right\rangle \simeq \frac{1}{3!} \sum_{\kappa_2\kappa_3\kappa_4} |w_{\kappa\kappa_2\kappa_3\kappa_4}|^2. \tag{2.33}$$

We assume that both variational parameter $\phi_{\mathbf{k}}$ and $w_{\kappa 1\kappa_2\kappa_3\kappa_4}$ are real number through the calculation.

It is convinent to introduce two basic expectations with the improved variational wave function $|\Phi_N^{\text{Corr.}}\rangle$

$$\bar{n}_{\mathbf{k}} \equiv \left\langle \Phi_N^{\text{Corr.}} | \hat{c}^{\dagger}_{\mathbf{k}\alpha} \hat{c}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \right\rangle = v_{\mathbf{k}}^2 + (u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2)\eta_{\mathbf{k}}, \tag{2.34}$$

$$\bar{F}_{\mathbf{k}} \equiv \left\langle \Phi_N^{\text{Corr.}} | \hat{\beta}^{\dagger} \hat{c}_{-\mathbf{k}-\alpha} \hat{c}_{\mathbf{k}\alpha} | \Phi_N^{\text{Corr.}} \right\rangle = u_{\mathbf{k}} v_{\mathbf{k}} (1 - 2\eta_{\mathbf{k}}). \tag{2.35}$$

Using Eq.(2.31), Eq.(2.33), Eq.(2.34) and Eq.(2.35), we obtain an expression of the ground-state energy estimated with improved variational wave function $|\Phi_N^{\text{Corr.}}\rangle$ (see Appendix E) in the weak-coupling region as

$$\begin{aligned} \varepsilon_{\text{Corr.}} &\equiv \left\langle \Phi_N^{\text{Corr.}} | \hat{H}_{\text{BCS}} | \Phi_N^{\text{Corr.}} \right\rangle \\ &= 2\sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \bar{n}_{\mathbf{k}} + \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} (2U_0 - U_{|\mathbf{k}-\mathbf{k}'|}) \bar{n}_{\mathbf{k}} \bar{n}_{\mathbf{k}'} + \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} U_{|\mathbf{k}-\mathbf{k}'|} \bar{F}_{\mathbf{k}} \bar{F}^*_{\mathbf{k}'} + \sum_{\mathbf{k}} \zeta_{\mathbf{k}}, \end{aligned} \tag{2.36}$$

where the last term $\zeta_{\mathbf{k}}$,

$$\zeta_{\mathbf{k}} \equiv \frac{1}{V} \sum_{\mathbf{k_1 k_2 k_3 k_4}} \delta_{\mathbf{k_1+k_2+k_3+k_4,0}} U_{|\mathbf{k_1+k_3}|} u_{\mathbf{k_1}} u_{\mathbf{k_2}} v_{\mathbf{k_3}} v_{\mathbf{k_4}} \times \sum_{\alpha\alpha'} (-1)^{1-\alpha-\alpha'} w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha'\mathbf{k_4}-\alpha'\mathbf{k_3}-\alpha}. \tag{2.37}$$

denotes the correlations energy.

The first term denotes the kinetic energy, the second term denotes the Hartree-Fock energy, the third term denotes the pair-condensation energy.

Moreover, we should recognize that the characteristic function " $\bar{n}_{\mathbf{k}}$" and "$\bar{F}_{\mathbf{k}}$ ", as shown in Eq.(2.34) and Eq.(2.35), also influenced by many-body correlations numerically, which eventually influenced the kinetic energy, the Hartree-Fock energy and the pair-condensation energy.

Setting $w_{\kappa\kappa_2\kappa_3\kappa_4}$ to zero, we can reproduces the BCS expression for the ground-state energy including the Hartree-Fock contribution.

2.6 Minimization of the ground-state energy

Let us minimize the ground-state energy for a fixed total particle number N.
First we incorporate the constraint condition

$$N = 2\sum_{\mathbf{k}}^{\mathbf{Fin.}} \bar{n}_{\mathbf{k}}, \tag{2.38}$$

in terms of Eq.(2.34) by the method of Lagrange multipliers. We introduce the energy functional

$$\bar{\varepsilon} \equiv \varepsilon + \mu \sum_{\mathbf{k}}^{\mathbf{Fin.}} (N - 2\bar{n}_{\mathbf{k}}), \tag{2.39}$$

with μ denoting the Lagrange multiplier.

Then, we set the energy functional $\bar{\varepsilon}$ with respect to the variational parameters (μ, $\phi_{\mathbf{k}}$, $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$) simultaneously

$$\frac{\delta\bar{\varepsilon}}{\delta\phi_{\mathbf{k}}} = 0, \tag{2.40}$$

$$\frac{\delta\bar{\varepsilon}}{\delta w_{\kappa_1\kappa_2\kappa_3\kappa_4}} = 0. \tag{2.41}$$

The resultant expression of the variation with respect to μ yields the constraint condition Eq.(2.38), the resultant expression of the variation with respect to $\phi_{\mathbf{k}}$ yields

$$\phi_{\mathbf{k}} = \frac{-\xi_{\mathbf{k}} + E_{\mathbf{k}}}{\Delta^*_{\mathbf{k}}}, \quad E_{\mathbf{k}} \equiv \sqrt{\xi^2_{\mathbf{k}} + |\Delta_{\mathbf{k}}|^2}. \tag{2.42}$$

which Eq.(2.18) acquires the standard BCS expression

$$u_k = \sqrt{\frac{1}{2}\big(1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\big)}, \quad v_k = \sqrt{\frac{1}{2}\big(1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}}\big)}. \tag{2.43}$$

However, many-body correlations are incorporated into the single particle energy $\xi_{\mathbf{k}}$ and gap energy $\Delta_{\mathbf{k}}$ as

$$\xi_{\mathbf{k}} = \xi^{(0)}_{\mathbf{k}} + \xi^{(1)}_{\mathbf{k}}, \tag{2.44}$$

$$\Delta_{\mathbf{k}} = \Delta^{(0)}_{\mathbf{k}} + \Delta^{(1)}_{\mathbf{k}}, \tag{2.45}$$

where we define

$$\xi^{(0)}_{\mathbf{k}} \equiv \varepsilon_k - \mu + \frac{1}{V}\sum_{\mathbf{k}'}^{\mathbf{Fin.}} (2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\bar{n}_{\mathbf{k}'}, \tag{2.46a}$$

$$\Delta^{(0)}_{\mathbf{k}} \equiv -\frac{1}{V}\sum_{\mathbf{k}'}^{\mathbf{Fin.}} U_{|\mathbf{k}-\mathbf{k}'|}\bar{F}^*_{\mathbf{k}'}, \tag{2.46b}$$

$$
\begin{aligned}
\xi_{\mathbf{k}}^{(1)} \equiv (1-2\eta_{\mathrm{k}})^{-1}\frac{1}{V^2}\sum_{\mathrm{k}_2\mathrm{k}_3\mathrm{k}_4}\frac{\delta_{\mathbf{k}+\mathbf{k_2}+\mathbf{k_3}+\mathbf{k_4},\mathbf{0}}}{E_{\mathbf{k}}^{(0)}+E_{\mathbf{k_2}}^{(0)}+E_{\mathbf{k_3}}^{(0)}+E_{\mathbf{k_4}}^{(0)}} \\
\times U_{|\mathbf{k}+\mathbf{k_2}|}\{U_{|\mathbf{k}+\mathbf{k_2}|}(v_{\mathbf{k_2}}^2-u_{\mathbf{k_2}}^2)(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})^2 \\
-U_{|\mathbf{k}+\mathbf{k_3}|}(v_{\mathbf{k_2}}v_{\mathbf{k_3}}-u_{\mathbf{k_2}}u_{\mathbf{k_3}})(u_{\mathbf{k_2}}v_{\mathbf{k_4}}+v_{\mathbf{k_2}}u_{\mathbf{k_4}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})\},
\end{aligned}
\tag{2.47a}
$$

$$
\begin{aligned}
\Delta_{\mathbf{k}}^{(1)} \equiv (1-2\eta_{\mathrm{k}})^{-1}\frac{2}{V^2}\sum_{\mathrm{k}_2\mathrm{k}_3\mathrm{k}_4}\frac{\delta_{\mathbf{k}+\mathbf{k_2}+\mathbf{k_3}+\mathbf{k_4},\mathbf{0}}}{E_{\mathbf{k}}^{(0)}+E_{\mathbf{k_2}}^{(0)}+E_{\mathbf{k_3}}^{(0)}+E_{\mathbf{k_4}}^{(0)}} \\
\times U_{|\mathbf{k}+\mathbf{k_2}|}\{U_{|\mathbf{k}+\mathbf{k_2}|}u_{\mathbf{k_2}}v_{\mathbf{k_2}}(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})^2 \\
-U_{|\mathbf{k}+\mathbf{k_3}|}u_{\mathbf{k_2}}v_{\mathbf{k_3}}(u_{\mathbf{k_2}}v_{\mathbf{k_4}}+v_{\mathbf{k_2}}u_{\mathbf{k_4}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})\},
\end{aligned}
\tag{2.47b}
$$

where $E_{\mathbf{k}}^{(0)}$ is defined as

$$
E_{\mathbf{k}}^{(0)} \equiv (u_{\mathbf{k}}^2-v_{\mathbf{k}}^2)\xi_{\mathbf{k}}^{(0)}+2u_{\mathbf{k}}v_{\mathbf{k}}\Delta_{\mathbf{k}}^{(0)}, \tag{2.48}
$$

in terms of $\xi_{\mathbf{k}}^{(0)}$ and $\Delta_{\mathbf{k}}^{(0)}$.

The Eqs.(2.46) follows the same mathematical structure as the mean-field BCS theory, and Eqs.(2.47) denotes the correlations energy with respect to the single-particle energy and the gap energy.

The solution of Eq.(2.41), variation with respect to $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$ can be calculated explicitly as

$$
\begin{aligned}
w_{\kappa_1\kappa_2\kappa_3\kappa_4} = -\frac{\delta_{\mathbf{k_1}+\mathbf{k_2}+\mathbf{k_3}+\mathbf{k_4},\mathbf{0}}}{E_{\mathbf{k_1}}^{(0)}+E_{\mathbf{k_2}}^{(0)}+E_{\mathbf{k_3}}^{(0)}+E_{\mathbf{k_4}}^{(0)}}\frac{1}{V}\big[\delta_{\alpha_1,-\alpha_2}\delta_{\alpha_3,-\alpha_4}(-1)^{1-\alpha_1-\alpha_3} \\
\times U_{|\mathbf{k_1}+\mathbf{k_3}|}(u_{\mathbf{k_1}}v_{\mathbf{k_2}}+v_{\mathbf{k_1}}u_{\mathbf{k_2}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})+(\text{two terms})\big],
\end{aligned}
\tag{2.49}
$$

where the two terms obtain from the first term in the square brackets by the two cyclic permutations of (2,3,4) (see Appendix E).

Since we assume spin-singlet during the calculation, the variational parameter $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$ reduces to four dimensional anti-symmetric tensor, which is only relates to the momentum space.

We now summarize our self-consistent equations. Eq.(2.33), Eq.(2.34), Eq.(2.35), Eq.(2.43), Eq.(2.44), Eq.(2.45) and Eq.(2.48), combined with Eq.(2.38), form the closed non-linear equations, which can be used to evaluate the ground-state energy of s-wave Cooper pair condensation for any given potential $U(r)$.

Moreover, the corresponding normal state energy can be obtained by replacing $(u_{\mathbf{k}}, v_{\mathbf{k}})$ with the step function $\theta(x)$

$$
(u_{\mathbf{k}}, v_{\mathbf{k}}) \to (\theta(k-k_{\mathrm{F}}), \theta(k_{\mathrm{F}}-k)), \tag{2.50}
$$

which eventually gives us the normal state distribution functional

$$
n_{\mathbf{k}}^{0} \equiv \theta(k_{\mathrm{F}}-k), \tag{2.51a}
$$

$$
n_{\mathbf{k}}^{\mathrm{n}} = (1-\eta_{\mathbf{k}}^{\mathrm{n}})\theta(k_{\mathrm{F}}-k)+\eta_{\mathbf{k}}^{\mathrm{n}}\theta(k-k_{\mathrm{F}}). \tag{2.51b}
$$

The Eq.(2.51a) denotes the normal state functional of non-interacting expression, and Eq.(2.51b) denotes denotes the normal state functional with correlations, where k_{F} is the Fermi wave number, which exhibits a discontinuity. It should be noted that, in the limit of Eqs.(2.51) and $\eta_{\mathrm{k}} \to 0$ reduces the normal ground-state energy evaluated by the second-order perturbation expansion.

2.7 Superposition over the number of Cooper pairs

In the preceding sections, we discussed the correlations operator $\hat{\pi}_4^\dagger$ decreases the Cooper pairs into quasi-particles by two. We then realize that the improved wave function $|\Phi_N^{\mathrm{Corr.}}\rangle$ is made up of superpositions over different number of Cooper pairs.

The superposition can be quantified as follows;

First, the normalization constant $\mathscr{B}_N$ of $|\Phi_N^{\mathrm{Corr.}}\rangle$ can be expanded by $(\hat{\pi}_4, \hat{\pi}_4^\dagger)$ as

$$\mathscr{B}_N = \exp\Big(\sum_{l=1}^{\infty} J_{4l}\Big), \tag{2.52}$$

where J_{4l} is defined as

$$J_{4l} \equiv \frac{\langle \Phi_N^{\mathrm{BCS}} | (\exp(\hat{\pi}_4))^l \exp(\hat{\pi}_4^\dagger)^l | \Phi_N^{\mathrm{BCS}} \rangle}{(l!)^2}, \lambda \in \mathbb{Z}^+. \tag{2.53}$$

We may neglect terms of $l \geq 2$, only incorporate the $l = 1$ contribution as justified in the weak-coupling region. According to Eq.(2.26), quantity J_{4l} can be expressed as

$$J_4 \equiv \frac{1}{2} \sum_{\mathrm{k}} \eta_{\mathrm{k}}, \tag{2.54}$$

where we used Eq.(2.33).

We thereby estimate the overlap $|\langle \frac{N}{2} - 2n | \Phi_N^{\mathrm{Corr.}} \rangle|^2$, which denotes the resultant probability of having Cooper pairs in the fixed system by Poisson distribution

$$P_{(\frac{N}{2} - 2n)} = \frac{J_4^n \mathrm{e}^{-\mathrm{J}_4}}{n!}. \tag{2.55}$$

We note that $P_{(\frac{N}{2} - 2n)}$ approaches a Gaussian distribution in the thermodynamic limit as seen that J_4 is proportional to total particle number N.

3 Numerical Calculation

3.1 Model potential

We consider a model with attractive potential

$$U(r) = \frac{\hbar^2 a_0}{2mr_0^3} e^{-r/r_0}, \tag{3.1}$$

with parameters (a_0, r_0), where $a_0 < 0$ and $r_0 > 0$.

This potential can be expanded in plane waves as

$$U(k) = \frac{4\pi\hbar^2 a_0}{m(1 + r_0^2 k^2)}. \tag{3.2}$$

It is also convenient to express the potential $U(|\mathbf{k_1} - \mathbf{k_2}|)$ as

$$U(k) = U(|\mathbf{k_1} - \mathbf{k_2}|) = \sum_{l=0}^{\infty} U_l(k_1, k_2) \sum_{m=-l}^{l} 4\pi Y_{lm}(\mathbf{k_1}) Y_{lm}^*(\mathbf{k_2}), \tag{3.3}$$

where Y_{lm} and Y_{lm}^* are spherical harmonics function.

Then, we set the expansion coefficient in Eq.(3.3) for $l = 0$, then we get

$$U_0(k, k') = \frac{4\pi\hbar^2}{m} \frac{a_0}{(1 + r_0^2 k^2 + r_0^2 k'^2)^2 - 4r_0^4 k^2 k'^2}. \tag{3.4}$$

There are several reasons that we finally choose such potential model like Eq.(3.2) with a finite range, instead of the contact attractive model, which is frequently used in the literatures[4].

The contact attractive model can only have an equivalent, however artificial mathematical approximation towards momentum integral range around Fermi's surface. Compared to the contact attractive model, the exponential type model can have a un-artificial integral range corresponds to a certain combination of the potential parameter (a_0, r_0), in accordance with the solution of gap equation. It naturally make our calculation free from the ultraviolet divergences inherent.

Also, such artificial mathematical approximation of the momentum space in the contact attractive model does not contain any information about many-body correlations, precisely does not contain the variational parameter $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$. It is essential to test whether our improved variational wave function $|\Phi_N^{\text{Corr.}}\rangle$ actually decreases the ground-state energy compare to the current BCS wave function $|\Phi_N^{\text{BCS}}\rangle$, which is directly caused by many-body correlations rather than other artificial reasons.

3.2 Numerical procedures

For example, setting the potential parameter $(a_0, r_0) = (-0.12k_{\rm F}^{-1}, 0.1k_{\rm F}^{-1})$ yields a weak-coupling transition temperature $T_c \approx 1.16 \times 10^{-4}\varepsilon_{\rm F}^0/k_{\rm B}$, where $\varepsilon_{\rm F}^0$ is the non-interacting Fermi energy and $k_{\rm B}$ is the Boltzmann constant.

In order to make the evaluation of correlations energy more tractable with high accuracy numerically, we have chosen

$$(a_0, r_0) = (-0.19k_{\rm F}^{-1}, 0.1k_{\rm F}^{-1}), \tag{3.5}$$

which yields a weak-coupling transition temperature $T_c \approx 2.0 \times 10^{-2}\varepsilon_{\rm F}^0/k_{\rm B}$. The sums over $(\kappa_2\kappa_3\kappa_4)$ in Eq.(2.44) can be expressed into vectors of triple radial and double angular integrals, which simplifies in Appendix(F). The radial integrals were performed on the interval of $0 \leq k \leq k_{\rm cut}$, where the integer upper limit $k_{\rm cut} \approx 50k_{\rm F}$.

We express the momentum $k = k_{\rm F}(1 + \sinh(\mathrm{x})^3)$, and discretizing variable x at interval equally, so that can accumulate integration points around the Fermi's surface $k_{\rm F}$. It turned out that the quantity E_{k0} defined in Eq.(2.48) can be negative, which cause instability when evaluating quintuple sum. This numerical problem was eventually moved by replacing E_{k0} to the absolute value $|\xi_{\mathbf{k}}^n|$, where $|\xi_{\mathbf{k}}^n|$ denotes the normal state single-particle energy follows the replacement of distribution functions in Eq.(2.51b). This numerical procedure corresponds to choosing the parameter $w_{\kappa_1\kappa_2\kappa_3\kappa_4}$ slightly away from extremal value for numerical stability at the expense of increasing the variational ground-state energy. Our numerical calculation was performed by setting the natural unit

$$\hbar = k_{\rm B} = k_{\rm F} = 2m = 1. \tag{3.6}$$

We have confirmed convergence of the solution of self-consistent equations within $\approx 1\%$ error in the pair condensation energy by choosing 130 points for each radial integral and 20 points for each angular integral.

3.3 Numerical results

Let us present the numerical results for $(a_0, r_0) = (-0.19k_{\rm F}^{-1}, 0.1k_{\rm F}^{-1})$ self-consistently. Fig. 2 plots the gap energy $\Delta_{\rm k}/\varepsilon_{\rm F}^0$ as a function of momentum $\rm k/k_F$. The red line denotes the gap energy $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^{(0)} + \Delta_{\mathbf{k}}^{(1)}$, which includes $\hat{\pi}_4$ correlations. The blue line denotes the gap energy $\Delta_{\rm k}^{\rm BCS}/\varepsilon_{\rm F}^0$ by the mean-field BCS theory without $\hat{\pi}_4$ correlations. We observe that the correlations reduce gap energy from the mean-field value, and also produce a small dip around Fermi's surface $k = k_{\rm F}$.

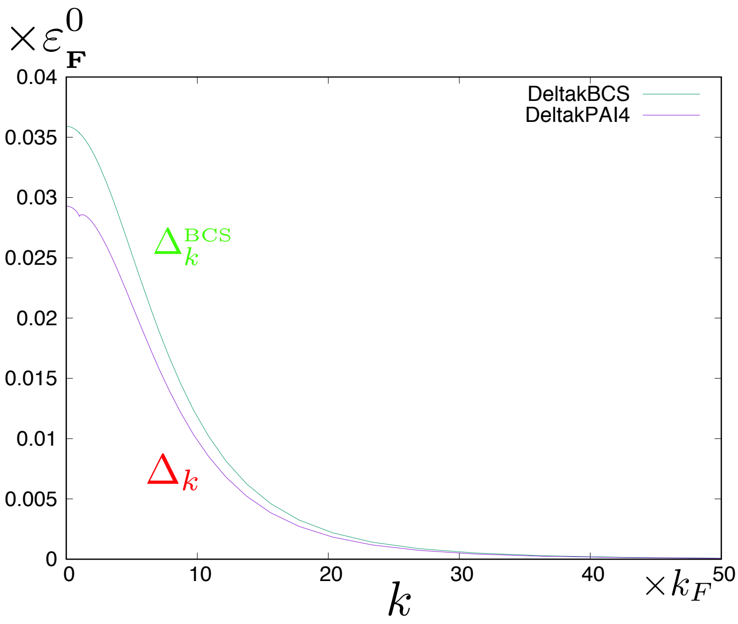

Figure 2: Energy gap $\Delta_{\rm k}$ in unit of $\varepsilon_{\rm F}^0$ as a function of momentum k in comparison with $\Delta_{\rm k}^{\rm BCS}$ without $\hat{\pi}_4$ correlations

Table 1 summarizes the normal-state energy and pair condensation energy of both theories. We choose non-interaction kinetic energy $\varepsilon_0 \equiv 2\sum_k \varepsilon_k \theta(k_{\rm F} - k)$ as unit to evaluate the normal-state energy and pair condensation energy. As expected, the correlation energy is seen to be much larger in magnitude than pair condensation energy due to $\hat{\pi}_4$ correlations.

表 1: Normal-state energy and pair condensation energy in unit of non–interaction kinetic energy ε_0 for parameters $(a_0, r_0) = (-0.19k_{\mathrm{F}}^{-1}, 0.1k_{\mathrm{F}}^{-1})$.

	$(\varepsilon_{\mathrm{n}} - \varepsilon_0)/\varepsilon_0$	$(\varepsilon - \varepsilon_{\mathrm{n}})/\varepsilon_0$
Mean-field BCS theory	-6.877×10^{-2}	-7.81×10^{-4}
Theory with $\hat{\pi}_4$ correlations	-1.033×10^{-1}	-5.06×10^{-4}

It should be noted that the mean-field condensation energy is in excellent still agreement with the BCS prediction

$$\begin{aligned} E_{\mathrm{cond.}} &= 2N(\varepsilon_{\mathrm{F}}) \int_0^\infty \big(\xi_{\mathrm{k}} - E_{\mathrm{k}} + \frac{(\Delta_{\mathrm{k_F}}^{\mathrm{BCS}})^2}{E_{\mathrm{k}}}\big) \mathrm{d}\xi_{\mathrm{k}} \\ &= -\frac{1}{2} N(\varepsilon_{\mathrm{F}}) (\Delta_{\mathrm{k_F}}^{\mathrm{BCS}})^2 \\ &= -7.81 \times 10^{-4} \varepsilon_0, \end{aligned} \tag{3.7}$$

which is given in terms of the energy gap $\Delta_{\mathrm{k_F}}^{\mathrm{BCS}} = 0.0354\varepsilon_{\mathrm{F}}^0$ at the Fermi level and the density of states $N(\varepsilon_{\mathrm{F}}) = m\mathrm{k_F}\mathrm{V}/2\pi^2\hbar^2$.

The quantity η_{k} is essential to characterizes the $\hat{\pi}_4$ correlations. In the normal state, it describes the deviation of Eq.(2.51b) from the non-interacting expression Eq.(2.51a), and the reultant reduction of the discontinuty of $k = k_{\mathrm{F}}$ from 1.

Fig. 3 plots η_{k} in the pair condensed state in comparison with normal state. The latter exhibits a discontinuity $\Delta\eta^{\mathrm{n}}_{\mathrm{k}} = 3.48 \times 10^{-3}$ of at $k = k_{\mathrm{F}}$, which is blurred in η_{k} due to condensation.

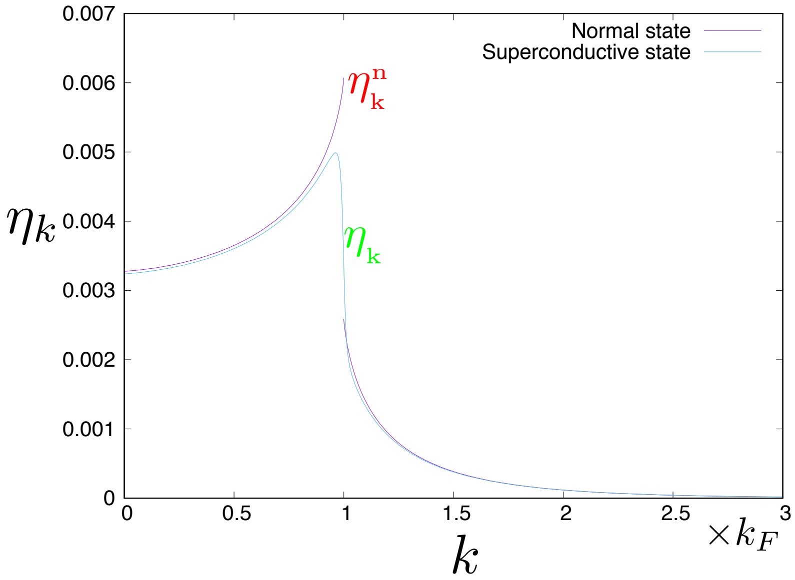

Figure 3: Plots of superconducting η_{k} (blue line) as a function of in the pair condensed state in comparison with $\eta^{\mathrm{n}}_{\mathrm{k}}$ (red line) of normal state.

This finite quantity η_{k} also produce a superposition over the number of Cooper pairs in the condensate which is expressible as Eq.(2.55) in the weak-coupling region.

Fig. 4 and Fig. 5 show the Poisson distribution of number of Cooper pairs for a total particle number from a relatively small number $N = 1000$ to larger number $N = 20000$. We observed that the distribution shifts to the right as total particle number increasing. Especially the redline of Fig. 3 which denotes the total particle number $N = 20000$ already has the appearance of a complete Gaussian.

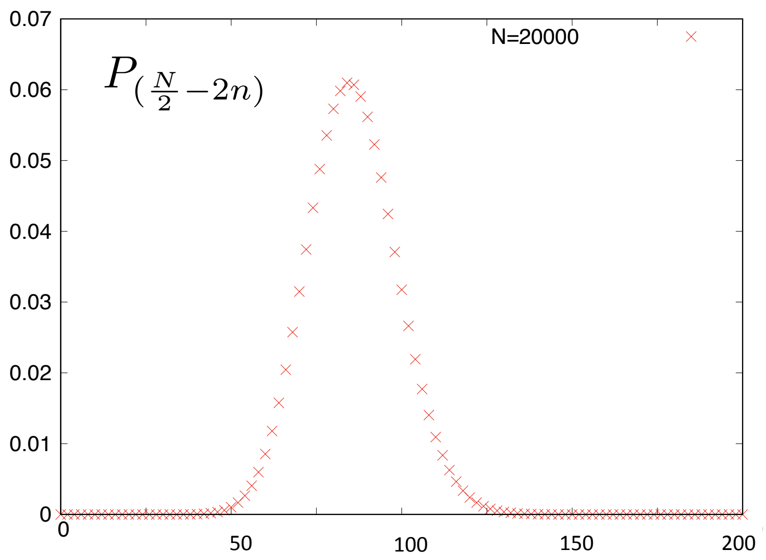

Figure 4: (Redline) Plots of probability $P_{(\frac{N}{2}-2n)}$ of having Cooper pairs in the ket $|\Phi_N^{\text{Corr.}}\rangle$ for the total particle number N=20000.

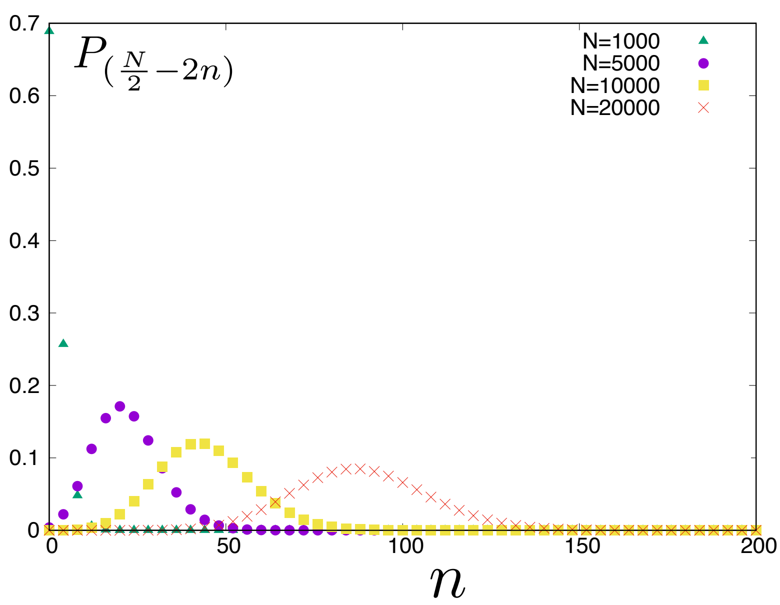

Figure 5: Plots of probability $P_{(\frac{N}{2}-2n)}$ of having Cooper pairs in the ket $|\Phi_N^{\text{Corr.}}\rangle$ for a certain total particle number N. We observe that the distribution shifts to the right as total particle number increasing.

4 Summary and Conclusion

The present research has clarified the correlations naturally produce a superposition over number of Cooper pairs in the ground-state wave function. This superposition, which is given by Eq.(2.55) and shown in Fig.4, enables us define the "anomalous" average unambiguously as Eq.(2.35) within the number-conserving formalism, in contrast to the mean-field BCS theory, where the average becomes finite only between states with different particle numbers as $\langle \Phi^{\rm BCS}_{N-2}|\hat{c}_{-\mathbf{k}-\alpha}\hat{c}_{\mathbf{k}\alpha}|\Phi^{\rm BCS}_{N}\rangle$.[4] Indeed, the destruction of a single Cooper pair in our improved wave function $|\Phi^{\rm Corr.}_{N}\rangle$ is accompanied by the creation of a pair of non-condensed particles.

Moreover, the gauge transformation $\{\phi_{\rm k}, w_{\kappa_1\kappa_2\kappa_3\kappa_4}\} \stackrel{g(\forall\chi\in{\rm R})}{\rightarrow} \{\phi_{\rm k}{\rm e}^{2i\chi}, w_{\kappa_1\kappa_2\kappa_3\kappa_4}, {\rm e}^{4i\chi}\}$ in Eq.(2.7) and Eq.(2.24) changes Eq.(2.35) as $F_{\mathbf{k}} \to F_{\mathbf{k}}{\rm e}^{2i\chi}$ without affecting the ground-state energy. Thus $F(\mathbf{r_1}-\mathbf{r_2}) \equiv \sum_k F_{\mathbf{k}} e^{i\mathbf{k}(\mathbf{r_1}-\mathbf{r_2})}$ has the property of a macroscopic wave function with a well-defined phase. It follows from Eq.(2.24) that the superposition is realized and sustained energetically by the exchange of quasi-particles between states with different numbers of Cooper pairs, similarly to the way that two weakly coupled superconductors is realized and mediated by the exchange process between them.[4, 5] Thus the correlations are identified as being responsible for the emergence of macroscopic coherence in isolated superconductors. The present study also makes it clear that fluctuations in the number of condensed particles $\Delta N_{\rm cond.}$, instead of those in the total particle number as discussed frequently, are responsible for the appearance of a macroscopic well-defined phase, in accordance with the concept of coherence in optics,[18] and also the gauge invariance.

Thus, the present theory supports the mean-field description of superconductivity using grand-canonical ensemble[1, 8, 9, 15] in the thermodynamic limit. For systems with a small number of particles or with low dimensions, on the other hand, the fluctuations $\Delta N_{\rm cond.}$ are expected to have substantial effects on the physical properties and realization of coherence. However, the present theory cannot be applied directly to finite systems because of the mathematical approximation introduced around Eq.(2.11) (see Appendix C), which becomes valid for $N \gg 1$. We are planing to report some progress in removing the approximations in the future research (see Appendix G).

Appendix

A Mathematical Preparation for Deviating the Formalism

A.1 General expression of Q_n

First, we introduce the pair operator $\hat{\pi}^\dagger$ as

$$\hat{\pi}^\dagger \equiv \sum_{q_1 q_2} \phi_{q_1 q_2} \hat{c}^\dagger_{q_1} \hat{c}^\dagger_{q_2}, \tag{A.1}$$

where $\{q_i\}_{i=1,2} \equiv \{\mathbf{k_i}, \alpha_\mathbf{i}\}_\mathbf{i=1,2}$ denotes momentum and spin, and $\phi_{q_1 q_2}$ is assumed to have the symmetry $\phi_{q_1 q_2} = \sigma \phi_{q_1 q_2}$, with $\sigma = \pm 1$ denotes statistical properties for bosons and fermions respectively.

Let us define the canonical commutation relation for bosons ($\sigma = +1$) and fermions ($\sigma = -1$) as

$$[\hat{A}, \hat{B}]_{\sigma=+1} \equiv [\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}, \tag{A.2a}$$

$$[\hat{A}, \hat{B}]_{\sigma=-1} \equiv \{\hat{A}, \hat{B}\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}. \tag{A.2b}$$

It is straightforward to prove that the pair operator and its Hermitian conjugate operator satisfies the following canonical commutation relations (A.2):

$$\{\hat{c}_q, \hat{\pi}^\dagger\} = \sum_{q_1} \phi_{q q_1} \hat{c}^\dagger_{q_1}, \tag{A.3a}$$

$$\{\hat{\pi}, \hat{\pi}^\dagger\} = \frac{1}{2}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger + \sigma \sum_{q_1 q_1'} \hat{c}^\dagger_{q_1} \left(\underline{\phi}\underline{\phi}^\dagger\right)_{q_1 q_1'} \hat{c}_{q_1'}. \tag{A.3b}$$

It is also convenient to express the commutation relation $\{\hat{\pi}, (\hat{\pi}^\dagger)^n\}$ as follows;

$$\begin{aligned}
&\{\hat{\pi}, (\hat{\pi}^\dagger)^n\} \\
=&\{\hat{\pi}, (\hat{\pi}^\dagger)\}(\hat{\pi}^\dagger)^{n-1} + \hat{\pi}\{\hat{\pi}, (\hat{\pi}^\dagger)\}(\hat{\pi}^\dagger)^{n-1} \ldots + (\hat{\pi})^{n-2}\{\hat{\pi}, (\hat{\pi}^\dagger)\}(\hat{\pi}^\dagger)^{n-1} + (\hat{\pi})^{n-1}\{\hat{\pi}, (\hat{\pi}^\dagger)\}(\hat{\pi}^\dagger)^{n-1} \\
=&\frac{n}{2}(\hat{\pi}^\dagger)^{n-1}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger + \sigma\frac{n(n-1)}{2}(\hat{\pi}^\dagger)^{n-2}\sum_{q_1 q_2}\left(\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\right)_{q_1 q_2}\hat{c}^\dagger_{q_1}\hat{c}^\dagger_{q_2} + \sigma n(\hat{\pi}^\dagger)^{n-1}\sum_{q_1 q_1'}\hat{c}^\dagger_{q_1}\left(\underline{\phi}\underline{\phi}^\dagger\right)_{q_1 q_1'}\hat{c}_{q_1'}
\end{aligned} \tag{A.4}$$

With these preparation, we define the following quantities:

$$Q_n \equiv \frac{\langle 0|(\hat{\pi})^n(\hat{\pi}^\dagger)^n|0\rangle}{(n!)^2}, \tag{A.5a}$$

$$P_n \equiv \frac{\langle 0|(\hat{\pi})^{n-1}\hat{c}_{q_1}\hat{c}_{q_2}(\hat{\pi}^\dagger)^n|0\rangle}{(n!)^2}, \tag{A.5b}$$

$$I_n \equiv \frac{\sigma^{n-1}}{2}\mathrm{Tr}(\underline{\phi}\underline{\phi}^\dagger)^n. \tag{A.5c}$$

It is easy to prove the following equation

$$P_n(q_1,q_2) = \frac{1}{n}\frac{\delta Q_n}{\delta \phi^*_{q_2 q_1}} = \sigma P_n(q_2,q_1). \tag{A.6}$$

holds. Then, we obtain the recurrence formula for Q_n and P_n by using Eq.(A.4) and the definition of vacuum $\hat{c}_q|0\rangle = 0$ as

$$Q_n = \frac{\langle 0|(\hat{\pi})^{n-1}\{\hat{\pi},(\hat{\pi}^\dagger)^n\}|0\rangle}{(n!)^2} = ... = \frac{1}{n}(Q_{n-1}I_1 + \frac{n-1}{2}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{P}^\dagger_{n-1}), \tag{A.7a}$$

$$P_n = \frac{\langle 0|(\hat{\pi})^{n-1}\{\hat{c}_{q_1}\hat{c}_{q_2},(\hat{\pi}^\dagger)^n\}|0\rangle}{(n!)^2} = ... = \frac{\sigma}{n}\big(Q_{n-1}\underline{\phi} + (n-1)\underline{\phi}\underline{P}^\dagger_{n-1}\underline{\phi}\big)_{q_1 q_2}. \tag{A.7b}$$

We give examples to calculate the first few terms of Eq.(A.7) as

$$
\begin{aligned}
n=0,\quad & Q_0 = 1,\quad \underline{P}_0 = \underline{0};\\
n=1,\quad & Q_1 = I_1,\quad \underline{P}_1 = \sigma\underline{\phi};\\
n=2,\quad & Q_2 = \frac{1}{2}(Q_1 I_1 + \frac{1}{2}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger)\\
& \quad = \frac{Q_1 I_1 + I_2}{2},\\
& \underline{P}_2 = \frac{\sigma}{2}\big(Q_1\underline{\phi} + \underline{\phi}\underline{P}_1^\dagger\underline{\phi}\big);\\
n=3,\quad & Q_3 = \frac{1}{3}\big(Q_2 I_1 + \frac{2}{2}\frac{\sigma}{2}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger\underline{\phi}(Q_1\underline{\phi}^\dagger + \sigma\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger)\big)\\
& \quad = \frac{Q_2 I_1 + Q_1 I_1 + I_3}{3},\\
& \underline{P}_3 = \frac{\sigma}{3}\big(Q_2\underline{\phi} + 2\frac{\sigma}{2}\underline{\phi}(Q_1\underline{\phi}^\dagger + \sigma\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger)\underline{\phi}\big)\\
& \quad = \frac{\sigma}{3}\big(Q_2\underline{\phi} + \sigma Q_1\underline{\phi}\underline{\phi}^\dagger\underline{\phi} + \sigma^2\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\big);\\
n=4,\quad & Q_4 = \frac{1}{4}\big(Q_3 I_1 + \frac{3}{2}\mathrm{Tr}\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\big(\frac{\sigma}{3}Q_2^\dagger\underline{\phi}^\dagger + 2\frac{\sigma}{2}\underline{\phi}^\dagger(Q_1\underline{\phi} + \underline{\phi}\sigma\underline{\phi}^\dagger\underline{\phi})\underline{\phi}^\dagger\big)\\
& \quad = \frac{1}{4}\big(Q_3 I_1 + \frac{3}{3}(Q_2 I_2 + Q_1 I_3 + I_4)\big)\\
& \quad = \frac{Q_3 I_1 + Q_2 I_2 + Q_1 I_3 + Q_0 I_4}{4},\\
& \underline{P}_4 = \frac{\sigma}{4}\big(Q_3\underline{\phi} + 3\underline{\phi}\ \big(\frac{\sigma}{3}(Q_2\underline{\phi} + \sigma Q_1\underline{\phi}\underline{\phi}^\dagger\underline{\phi} + \sigma^2\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger\underline{\phi})\big)\underline{\phi}\ \big)\\
& \quad = \frac{\sigma}{4}\big(Q_3\underline{\phi} + \sigma Q_2\underline{\phi}\underline{\phi}^\dagger\underline{\phi} + \sigma^2 Q_1\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger\underline{\phi} + \sigma^3 Q_0\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\underline{\phi}^\dagger\underline{\phi}\big);\\
n=4,\quad & Q_4 = \frac{Q_4 I_1 + Q_3 I_2 + Q_2 I_3 + Q_1 I_4 + Q_0 I_5}{5},\\
& \underline{P}_5 = ...;
\end{aligned}
$$

From these results, we suggest that P_n and Q_n may be expressed generally as

$$Q_n = \frac{1}{n}\sum_{l=1}^{n} Q_{n-l} I_l, \tag{A.8a}$$

$$\underline{P}_n = \frac{1}{n}\sum_{l=1}^{n} Q_{n-l}\underline{\phi}(\underline{\phi}^{\dagger}\underline{\phi})^{l-1}\sigma^l. \tag{A.8b}$$

These two expression can be proved by induction as follows; First, it is obviously that the expressions holds for $n = 1$. Then we suppose that they are vaild for $n \leq m-1$, we obtain that for $n = m$,

$$\begin{aligned} Q_m &= \frac{1}{m}\big[Q_{m-1}I_1 + \sum_{l=1}^{m-1} Q_{m-1-l}\frac{\sigma^l}{2}\mathrm{Tr}(\underline{\phi\phi}^{\dagger})^{l+1}\big] \\ &= \frac{1}{m}\big[Q_{m-1}I_1 + \sum_{l=1}^{m-1} Q_{m-1-l}I_{l+1}\big] \\ &= \frac{1}{m}\sum_{l=1}^{m} Q_{m-l}I_l, \end{aligned} \tag{A.9a}$$

$$\begin{aligned} \underline{P}_m &= \frac{\sigma}{m}\big[Q_{m-1}\underline{\phi} + \sum_{l=1}^{m-1} Q_{m-1-l}\underline{\phi}(\underline{\phi}^{\dagger}\underline{\phi})^l\sigma^l\big] \\ &= \frac{\sigma}{m}\big[Q_{m-1}\underline{\phi}\sigma + \sum_{l=2}^{m-1} Q_{m-1}\underline{\phi}(\underline{\phi}^{\dagger}\underline{\phi})^{l-1}\sigma^l\big] \\ &= \frac{1}{m}\sum_{l=1}^{m} Q_{m-l}\underline{\phi}(\underline{\phi}^{\dagger}\underline{\phi})^{l-1}\sigma^l. \end{aligned} \tag{A.9b}$$

Moreover, we set $q \to \{\mathbf{k}, \alpha\}$ which denotes the relations between Eqs.(A.9) can be expressed as

$$\begin{aligned} Q_n(\mathbf{k}) &= \frac{1}{n}\sum_{l=1}^{n} Q_{n-l}\sum_{\mathbf{k}}|\phi_{\mathbf{k}}|^{2l}(-1)^{l-1}, \\ &= -\sum_{\mathbf{k}}\phi_{\mathbf{k}}{}^{*}P_n(\mathbf{k}), \end{aligned} \tag{A.10a}$$

$$P_n(\mathbf{k}) = \frac{1}{n}\sum_{l=1}^{n} Q_{n-l}\phi_{\mathbf{k}}|\phi_{\mathbf{k}}|^{2(l-1)}(-1)^l. \tag{A.10b}$$

with

$$I_l = (-1)^{n-1}\sum_{\mathbf{k}}|\phi_{\mathbf{k}}|^{2l}.$$

An alternative expression of Q_n is expressible as follows;

$$Q_n = \sum_{\nu_1,\nu_2,...,\nu_n} W(\nu_1,\nu_2,...,\nu_n) I_1^{\nu_1} I_2^{\nu_2} \dots I_n^{\nu_n}$$
$$= \sum_{\nu_1,\nu_2,...,\nu_n} \delta_{\nu_1+2\nu_2,...,+n\nu_n,n} \prod_{l=1}^{n} \frac{(I_l/l)^{\nu_l}}{\nu_l!}, \quad \text{(A.11)}$$

where the weight $W(\nu_1,\nu_2,...,\nu_n)$ is obtained as

$$W(\nu_1,\nu_2,...,\nu_n) = \frac{\delta_{\nu_1+2\nu_2,...,+n\nu_n,n}}{(n!)^2}\Big[\frac{n!}{\nu_1(1!)^{\nu_1}\nu_2(2!)^{\nu_2}\dots\nu_n(n!)^{\nu_n}}\Big]^2$$
$$\times \nu_1!\nu_2!\dots\nu_n!(1!0!)^{\nu_1}(2!1!)^{\nu_2}\dots(n!(n-1)!)^{\nu_n}$$
$$= \frac{\delta_{\nu_1+2\nu_2,...,+n\nu_n,n}}{\nu_1!\nu_2!\dots\nu_n!1^{\nu_1}2^{\nu_2}\dots n^{\nu_n}}. \quad \text{(A.12)}$$

The factor of square bracket denotes the number of combinations to distribute n persons into $(\nu_1,\nu_2,...,\nu_n)$ rooms, where ν_l denotes the number of rooms with l beds. Factor $\nu_l!$ denotes the number of combinations for connecting ν_l pairs of operators $(\hat{\pi}^l,(\hat{\pi}^\dagger)^l)$. Factor $(l!(l-1)!)$ denotes the number of possible connections within each $(\hat{\pi}^l,(\hat{\pi}^\dagger)^l)$ pair.

A.2 Asymptotic expression of Q_n

The generating function of Q_n can be constructed as follows;

$$Q_{(\theta)} \equiv \sum_{n=0}^{\infty} Q_n e^{in\theta}$$
$$= \exp\Big[\frac{\sigma}{2}\sum_{l=0}^{\infty}(\sigma e^{i\theta})^l \frac{\mathrm{Tr}(\underline{\phi\phi^\dagger})^l}{l}\Big]$$
$$= \exp\Big[-\frac{\sigma}{2}\mathrm{Tr}(\underline{1}-\sigma e^{i\theta}\underline{\phi\phi^\dagger})^l\Big]. \quad \text{(A.13)}$$

The inverse transform of $Q_n \to Q_{(\theta)}$ is given by

$$Q_n = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{-in\theta}Q_{(\theta)}. \quad \text{(A.14)}$$

The differential of Logorthm Q_θ with respect to $(\phi_{q_1q_2},\phi^*_{q_1q_2})$ yields

$$\frac{\delta \mathrm{Ln} Q_{(\theta)}}{\phi_{q_1q_2}} = \big[\underline{\phi}^\dagger(\underline{1}-\sigma e^{i\theta}\underline{\phi\phi^\dagger})^{-1/2}\big]_{q_1q_2}, \quad \frac{\delta \mathrm{Ln} Q_{(\theta)}}{\phi^*_{q_1q_2}} = \big[(\underline{1}-\sigma e^{i\theta}\underline{\phi\phi^\dagger})^{-1/2}\underline{\phi}\big]_{q_1q_2}. \quad \text{(A.15a)}$$

Using the generating function $Q_{(\theta)}$, we derive an asymptotic expression of Q_n which holds for $n \in \mathbb{Z}^+$. We have assumed homogeneous system with spin-singlet pairing. We set $q_i \to \{k_i,\alpha_i\}$, then according to Eq.(A.13) and Eq.(A.14), the Q_n is expressible as

$$Q_n = \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{-in\theta}\exp\big[\sum_{\mathbf{k}}\mathrm{Ln}(1+e^{i\theta}|\phi_{\mathbf{k}}|^2)\big],$$
$$= \int_{-\pi}^{\pi}\frac{d\theta}{2\pi}e^{f_n(\theta)}, \quad \text{(A.16)}$$

where we define

$$f_n(\theta) \equiv -in\theta + \sum_{\mathbf{k}} \mathrm{Ln}(1 + e^{i\theta}|\phi_{\mathbf{k}}|^2). \tag{A.17}$$

For future purpose, we calculate the first two derivatives with respect to θ as

$$f_n^{'}(\theta) = -i\big(-n + \sum_{\mathbf{k}} \frac{e^{i\theta}|\phi_{\mathbf{k}}|^2}{1 + e^{i\theta}|\phi_{\mathbf{k}}|^2}\big), \tag{A.18a}$$

$$f_n^{''}(\theta) = (-i)^2 \sum_{\mathbf{k}} \frac{e^{i\theta}|\phi_{\mathbf{k}}|^2}{1 + e^{i\theta}|\phi_{\mathbf{k}}|^2}. \tag{A.18b}$$

We suppose that $f_{(N/2)}^{'}(\theta) = 0$ satisfies at $\theta = 0$

$$\begin{aligned} f_{(N/2)}^{'}(\theta) = 0 \leftrightarrow -i\big(-N/2 + \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\phi_{\mathbf{k}}|^2}\big) = 0, \\ \leftrightarrow N - 2\sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\phi_{\mathbf{k}}|^2} = 0. \end{aligned} \tag{A.19}$$

This mathematical suggestion corresponds to the constrain condition, in which the total particle number is fixed. The expansion of $f_{(N/2)}(\theta)$ at $\theta = 0$ can be expressed as

$$\begin{aligned} f_{(N/2)}(\theta) &= f_{(N/2)}(0) + \frac{1}{2!} f_{(N/2)}^{'}(0)\theta^2 + O(\theta^n) \\ &= \sum_{\mathbf{k}} \mathrm{Ln}(1 + |\phi_{\mathbf{k}}|^2) - \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\phi_{\mathbf{k}}|^2} \frac{\theta^2}{2} + O(\theta^n). \end{aligned} \tag{A.20}$$

We substitute this Taylor expression into Q_n (A.16), and performing the integration over θ asymptotically, we obtain that

$$\begin{aligned} Q_n &= \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} e^{f_n(\theta)} \\ &\approx e^{f_{N/2}(0)} \int_{-\infty}^{\infty} \frac{d\theta}{2\pi} e^{\frac{1}{2!} f_{N/2}^{''}(0)\theta^2} \\ &= \exp\big[\sum_{\mathbf{k}} \mathrm{Ln}(1 + |\phi_{\mathbf{k}}|^2)\big] \big[2\pi \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\phi_{\mathbf{k}}|^2}\big]^{-1/2}. \end{aligned} \tag{A.21}$$

Thus the logarithm of $Q_{N/2}$ is given by

$$\begin{aligned} \mathrm{Ln} Q_{N/2} &= \sum_{\mathbf{k}} \mathrm{Ln}(1 + |\phi_{\mathbf{k}}|^2) - \frac{1}{2} \mathrm{Ln}\big[2\pi \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1 + |\phi_{\mathbf{k}}|^2}\big] \\ &\approx \sum_{\mathbf{k}} \mathrm{Ln}(1 + |\phi_{\mathbf{k}}|^2), \end{aligned} \tag{A.22}$$

where we neglect the second term of order LnN in comparison with the first term with order N in the last approximate equality.

This asymptotic expression of Q_n (A.22) enables us deriving the canonical BCS formulation mathematical properly (see Appendix B) compared to other methods, which are frequently emphasized.[2, 3, 4]

B Mathematical Reconstruction of Canonical BCS Formalism

B.1 Deviation of the BCS Hamiltonian

We consider a system of N (even) identical particles ($N \gg 1$), with mass m and spin $\pm 1/2$ ($\sigma = -1$) described by Hamiltonian

$$\hat{H} \equiv \int d\xi \hat{\Psi}^{\dagger}(\xi)\big[\frac{\hbar^2 k^2}{2m} + U(r)\big]\Psi(\xi) + \frac{1}{2}\int d\xi_1 \int d\xi_2 \hat{\Psi}^{\dagger}(\xi_1)\hat{\Psi}^{\dagger}(\xi_2)U(|r_1 - r_2|)\hat{\Psi}(\xi_1)\hat{\Psi}(\xi_2). \tag{B.1}$$

Here $(\Psi^{\dagger}(\xi), \Psi(\xi))$ are field operators obeying the Fermion communication relations.

The field operator can be expressed as a linear combination of one-particle creation-annihilation operator form, with coefficients given by basis functions $\varphi_q(\xi) \equiv \langle \xi | q \rangle$ as

$$\hat{\Psi}(\xi) = \sum_q \hat{c}(q)\varphi_q(\xi). \tag{B.2}$$

The basis functions $\varphi_q(\xi) \equiv \langle \xi | q \rangle$, satisfying

$$\sum_q \langle q | q^{'} \rangle = \delta_{qq^{'}}, \ \sum_q |q\rangle\langle q| = 1. \tag{B.3}$$

which forms a complete orthonormal system.

Hence the Hamiltonian (B.1) is expressible into the form given by

$$\hat{H} \equiv \sum_{q^{'}q} K_{q^{'}q}\hat{c}^{\dagger}_{q^{'}}\hat{c}_q + \frac{1}{2V}\sum_{q_1 q_2} \sum_{q^{'}_1 q^{'}_2} U_{q_1 q_2; q^{'}_1 q^{'}_2}\hat{c}^{\dagger}_{q^{'}_1}\hat{c}^{\dagger}_{q^{'}_2}\hat{c}_{q_2}\hat{c}_{q_1}, \tag{B.4}$$

where $K_{q^{'}q}$ and $U_{q_1 q_2; q^{'}_1 q^{'}_2}$ are given by

$$K_{q^{'}q} \equiv \int d\xi \hat{\phi}^{\dagger}_{q^{'}}(\xi)\big[\frac{p^2}{2m} + U(r)\big]\phi_q(\xi), \tag{B.5a}$$

$$U_{q_1 q_2; q^{'}_1 q^{'}_2} \equiv \frac{1}{2}\int d\xi_1 \int d\xi_2 U(|r_1 - r_2|)\hat{\phi}^{*}_{q^{'}_1}(r_1)\hat{\phi}^{*}_{q^{'}_2}(r_2)\hat{\phi}_{q_2}(r_1)\hat{\phi}_{q_1}(r_2). \tag{B.5b}$$

We denote $q_i \to \{k_i, \alpha_i\}$ for momentum and spin, then we have the form of BCS Hamiltonian mentioned in section(2.1) as

$$\hat{H} \equiv \sum_{\mathbf{k}\alpha}^{\textbf{Fin.}} \varepsilon_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}-\alpha} + \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\textbf{Fin.}}\sum_{\alpha\alpha'} U_q \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}\alpha}\hat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q}\alpha}\hat{c}_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}\alpha},$$

where

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}, \text{and } U_q = \int U(r)\mathrm{e}^{-i\mathbf{q}\mathbf{r}}d^3r.$$

B.2 Homogeneous system

We replace q by k,α in Eq.(B.5), and consider the system in a box of volume V with periodic boundary conditions. Thus, the basic matrix elements are given by

$$K_{q'q} \rightarrow K_{\mathbf{k_1}\alpha_1,\mathbf{k_2}\alpha_2} = \delta_{\mathbf{k_1}\mathbf{k_2}}\delta_{\alpha_1\alpha_2}\varepsilon_{\mathbf{k_1}}, \quad \varepsilon_{\mathbf{k_1}}, = \frac{\hbar^2 k_1^2}{2m} \tag{B.6a}$$

$$U_{q_1q_2;q_1'q_2'} \rightarrow U_{\mathbf{k_1}\alpha_1,\mathbf{k_2}\alpha_2;\mathbf{k}_1'\alpha_1',\mathbf{k}_2'\alpha_2'} = \frac{1}{V}\delta_{\mathbf{k}_1'+\mathbf{k}_2';\mathbf{k_1}+\mathbf{k_2}}\delta_{\alpha_1'\alpha_1}\delta_{\alpha_2'\alpha_2}U(|\mathbf{k}_1' - \mathbf{k_1}|). \tag{B.6b}$$

We assume the pair wave function for spin-singlet pairing is expressible as

$$\phi_{\mathbf{k_1}\alpha_1,\mathbf{k_2}\alpha_2} = \delta_{\mathbf{k_1},-\mathbf{k_2}}\delta_{\alpha_2,-\alpha_1}(-1)^{\alpha_1-1/2}\phi_{\mathbf{k_1}} \tag{B.7}$$

$$= (\delta_{\alpha_1\uparrow}\delta_{\alpha_2\downarrow} - \delta_{\alpha_2\uparrow}\delta_{\alpha_1\downarrow})\delta_{\mathbf{k_1},-\mathbf{k_2}}\phi_{\mathbf{k_1}}, \tag{B.8}$$

with the assumption of $\phi_{-\mathbf{k}} = \phi_{\mathbf{k}}$.

Thus the matrix representation for the spin degrees of freedom is given by

$$\underline{\phi_{\mathbf{k_1}\mathbf{k_2}}} \equiv \left(\phi_{\mathbf{k_1}\alpha_1,\mathbf{k_2}\alpha_2}\right) = \delta_{\mathbf{k_1},-\mathbf{k_2}}\begin{pmatrix} 0 & \phi_{\mathbf{k_1}} \\ -\phi_{\mathbf{k_1}} & 0 \end{pmatrix} = \delta_{\mathbf{k_1},-\mathbf{k_2}}\phi_{\mathbf{k_1}}i\underline{\sigma}_2, \tag{B.9}$$

where $\underline{\sigma}_2$ is the second Pauli matrix.

Thus, the Cooper-pair annihilation operator Eq.(2.6) is expressible as

$$\hat{\pi}^\dagger_{\text{cp}} = \frac{1}{2}\sum_{\mathbf{k}}^{\text{Fin.}}\phi_{\mathbf{k}}\left(\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow}\hat{c}^\dagger_{-\mathbf{k}\uparrow}\right) = \frac{1}{2}\sum_{\mathbf{k}}^{\text{Fin.}}\phi_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \frac{1}{2}\sum_{\mathbf{k}}^{\text{Fin.}}\phi_{\mathbf{k}}\hat{c}^\dagger_{-\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\downarrow} = \sum_{\mathbf{k}}^{\text{Fin.}}\phi_{\mathbf{k}}\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow}. \tag{B.10}$$

Now, we calculate basic expectations with the BCS ground wave function $|\Phi_N^{\text{BCS}}\rangle$ as

$$\varepsilon_{\text{BCS}} \equiv \left\langle\Phi_N^{\text{BCS}}|\hat{H}_{\text{BCS}}|\Phi_N^{\text{BCS}}\right\rangle = \left\langle\Phi_N^{\text{BCS}}|\hat{H}_0 + \hat{H}_{\text{int}}|\Phi_N^{\text{BCS}}\right\rangle. \tag{B.11}$$

First, the kinetic energy can be transformed as

$$\begin{aligned}\left\langle\Phi_N^{\text{BCS}}|\hat{H}_0|\Phi_N^{\text{BCS}}\right\rangle \equiv& \sum_{\mathbf{k}\alpha}^{\text{Fin.}}\varepsilon_{\mathbf{k}}\left\langle\Phi_N^{\text{BCS}}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\text{BCS}}\right\rangle \\ =& Q_{N/2}^{-1}\sum_{\mathbf{k}\alpha}^{\text{Fin.}}\varepsilon_{\mathbf{k}}\frac{\left\langle 0|\hat{\pi}^{N/2}\left(\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} - \hat{c}^\dagger_{\mathbf{k}\downarrow}\hat{c}^\dagger_{-\mathbf{k}\uparrow}\right)(\hat{\pi}^\dagger)^{(N/2-1)}|0\right\rangle}{\left[(N/2)!\right]^2}\frac{N}{2}\phi_{\mathbf{k}} \\ =& Q_{N/2}^{-1}\sum_{\mathbf{k}\alpha}^{\text{Fin.}}\varepsilon_{\mathbf{k}}\frac{\left\langle 0|\hat{\pi}^{N/2}\left(\hat{c}^\dagger_{\mathbf{k}\uparrow}\hat{c}^\dagger_{-\mathbf{k}\downarrow} + \hat{c}^\dagger_{-\mathbf{k}\uparrow}\hat{c}^\dagger_{\mathbf{k}\downarrow}\right)(\hat{\pi}^\dagger)^{(N/2-1)}|0\right\rangle}{\left[(N/2)!\right]^2}\frac{N}{2}\phi_{\mathbf{k}} \\ =& Q_{N/2}^{-1}\sum_{\mathbf{k}\alpha}^{\text{Fin.}}\varepsilon_{\mathbf{k}}\phi_{\mathbf{k}}\frac{\delta Q_{N/2}}{\delta\phi_{\mathbf{k}}} \\ =& \sum_{\mathbf{k}\alpha}^{\text{Fin.}}\varepsilon_{\mathbf{k}}\phi_{\mathbf{k}}\frac{\delta \text{Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}.\end{aligned} \tag{B.12}$$

where we also used the assumption of $\phi_{-\mathbf{k}} = \phi_{\mathbf{k}}$. Next, we evaluate the interaction energy as follows;

$$\begin{aligned}
&\langle \Phi_N^{\rm BCS}|\hat{H}_{\rm int}|\Phi_N^{\rm BCS}\rangle \\
&\equiv \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_q \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}+\mathbf{q}\alpha}\hat{c}^\dagger_{\mathbf{k}'-\mathbf{q}\alpha'}\hat{c}_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle \\
&= \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_0 \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}^\dagger_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle + \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_q \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}+\mathbf{q}\alpha}\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}+\mathbf{q}\alpha}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_q \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}+\mathbf{q}\alpha}\hat{c}^\dagger_{-\mathbf{k}-\mathbf{q}\alpha'}\hat{c}_{-\mathbf{k}\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle \\
&= \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_0 \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}^\dagger_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle - \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_{|\mathbf{k}-\mathbf{k}'|} \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}'\alpha}\hat{c}^\dagger_{\mathbf{k}\alpha'}\hat{c}_{\mathbf{k}\alpha'}\hat{c}_{\mathbf{k}'\alpha}|\Phi_N^{\rm BCS}\rangle \\
&+ \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} U_{|\mathbf{k}-\mathbf{k}'|} \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}'\alpha}\hat{c}^\dagger_{\mathbf{k}'\alpha'}\hat{c}_{\mathbf{k}\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle \\
&\approx \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} (-1)^{\alpha-\frac{1}{2}}(-1)^{\alpha'-\frac{1}{2}} U_0 \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}^\dagger_{-\mathbf{k}-\alpha}\hat{c}_{\mathbf{k}'\alpha'}\hat{c}_{-\mathbf{k}'-\alpha'}|\Phi_{N-2}^{\rm BCS}\rangle \phi_{\mathbf{k}}\phi_{\mathbf{k}'}\frac{Q^{1/2}_{(N/2)-1}}{Q^{1/2}_{N/2}} \\
&\quad - \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} (-1)^{2(\alpha-\frac{1}{2})} U_{|\mathbf{k}-\mathbf{k}'|} \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}^\dagger_{-\mathbf{k}-\alpha'}\hat{c}_{\mathbf{k}'\alpha}\hat{c}_{-\mathbf{k}'-\alpha}|\Phi_{N-2}^{\rm BCS}\rangle \phi_{\mathbf{k}}\phi_{\mathbf{k}'}\frac{Q^{1/2}_{(N/2)-1}}{Q^{1/2}_{N/2}} \\
&\quad + \frac{1}{2V}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q}}^{\rm Fin.}\sum_{\alpha\alpha'} \delta_{\alpha',-\alpha} U_{|\mathbf{k}-\mathbf{k}'|} \langle \Phi_N^{\rm BCS}|\hat{c}^\dagger_{\mathbf{k}'\alpha}\hat{c}^\dagger_{-\mathbf{k}'\alpha'}\hat{c}_{-\mathbf{k}\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\rm BCS}\rangle
\end{aligned}$$

$$= Q^{-1}_{N/2}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\frac{\phi_{\mathbf{k}}\phi_{\mathbf{k}'}}{2^2}\frac{\delta^2 Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}} + Q^{-1}_{N/2}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k}'|}\frac{1}{2^2}\frac{\delta^2 Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}'}\phi_{\mathbf{k}}} \tag{B.13}$$

$$\begin{aligned}
&= Q^{-1}_{N/2}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\frac{\phi_{\mathbf{k}'}}{2}\frac{\delta}{\phi_{\mathbf{k}'}}\big(Q_{N/2}\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\big) \\
&+ Q^{-1}_{N/2}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k}'|}\frac{1}{2}\frac{\delta}{\phi^*_{\mathbf{k}'}}\big(Q_{(N/2)+1}\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\big) \\
&= \frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\big[\big(\frac{\phi_{\mathbf{k}'}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}'}}\big)\big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\big) + \frac{\phi_{\mathbf{k}'}}{2}\frac{\delta}{\delta\phi_{\mathbf{k}'}}\big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\big)\big] \\
&\quad + \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k}'|}\big[\big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k}'}}\big)\big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\big) + \frac{1}{2}\frac{\delta}{\delta\phi^*_{\mathbf{k}'}}\big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\big)\big] \\
&\approx \frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\big[\big(\frac{\phi_{\mathbf{k}'}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}'}}\big)\big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\big)\big] \\
&\quad + \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum_{\mathbf{k}\mathbf{k}'}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k}'|}\big[\big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k}'}}\big)\big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\big)\big].
\end{aligned} \tag{B.14}$$

Where, we neglect two-fold differential of $\phi_{\mathbf{k}}$ in the last equality, since these terms are proportional to $\delta_{kk'}$, which are negligible in the thermodynamic limit.

Thus, with Eq.(B.12) and Eq.(B.13), we obtain an estimation of the ground-state energy with $|\Phi_N^{\rm BCS}\rangle$ as

$$\begin{aligned}\varepsilon_{\rm BCS} \equiv& \langle \Phi_N^{\rm BCS}|\hat{H}_{\rm BCS}|\Phi_N^{\rm BCS}\rangle \\ \simeq& \sum_{\mathbf{k}\alpha}^{\rm Fin.} \varepsilon_{\mathbf{k}} \phi_{\mathbf{k}} \frac{\delta {\rm Ln} Q_{N/2}}{\delta \phi_{\mathbf{k}}} + \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} (2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\Big[\Big(\frac{\phi_{\mathbf{k'}}}{2}\frac{\delta {\rm Ln} Q_{N/2}}{\delta \phi_{\mathbf{k'}}}\Big)\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln} Q_{N/2}}{\delta \phi_{\mathbf{k}}}\Big)\Big] \\ &+ \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k'}|}\Big[\Big(\frac{1}{2}\frac{\delta {\rm Ln} Q_{(N/2)+1}}{\delta \phi^*_{\mathbf{k'}}}\Big)\Big(\frac{1}{2}\frac{\delta {\rm Ln} Q_{(N/2)+1}}{\delta \phi_{\mathbf{k}}}\Big)\Big]. \end{aligned} \tag{B.15}$$

B.3 Minimization of the ground-state energy

We have discussed the asymptotic expression of Q_n (A.22) as

$${\rm Ln} Q_{N/2} \approx \sum_{\mathbf{k}} {\rm Ln}(1+\phi_{\mathbf{k}}^2),$$

thus, we can rewrite the ground-state energy Eq.(B.15) using the logarithm of Q_n as

$$\begin{aligned}\varepsilon_{\rm BCS} \equiv& \langle \Phi_N^{\rm BCS}|\hat{H}_{\rm BCS}|\Phi_N^{\rm BCS}\rangle \\ \simeq& 2\sum_{\mathbf{k}}^{\rm Fin.} \varepsilon_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2} + \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} (2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\frac{|\phi_{\mathbf{k'}}|^2}{1+|\phi_{\mathbf{k'}}|^2}\frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2} \\ &+ \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k'}|}\frac{\phi_{\mathbf{k'}}}{1+|\phi_{\mathbf{k'}}|^2}\frac{\phi^*_{\mathbf{k}}}{1+|\phi_{\mathbf{k}}|^2} \\ \approx& 2\sum_{\mathbf{k}}^{\rm Fin.} \varepsilon_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2} + \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} (2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\frac{|\phi_{\mathbf{k'}}|^2}{1+|\phi_{\mathbf{k'}}|^2}\frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2} \\ &+ \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k'}|}\frac{\phi_{\mathbf{k'}}}{1+|\phi_{\mathbf{k'}}|^2}\frac{\phi^*_{\mathbf{k}}}{1+|\phi_{\mathbf{k}}|^2} \\ =& 2\sum_{\mathbf{k}}^{\rm Fin.} \varepsilon_{\mathbf{k}} \bar{n}_{\mathbf{k}} + \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} (2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\bar{n}_{\mathbf{k}}\bar{n}_{\mathbf{k'}} + \frac{1}{V}\sum_{\mathbf{kk'}}^{\rm Fin.} U_{|\mathbf{k}-\mathbf{k'}|}\bar{F}_{\mathbf{k}}\bar{F}^*_{\mathbf{k'}}, \end{aligned} \tag{B.16}$$

with

$$\bar{n}_{\mathbf{k}} \equiv \frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2}\Big(=\phi_{\mathbf{k}}\frac{\delta {\rm Ln} Q_{N/2}}{\delta \phi_{\mathbf{k}}}\Big), \quad \bar{F}_{\mathbf{k}} \equiv \frac{1}{1+|\phi_{\mathbf{k}}|^2}\Big(=\frac{\delta {\rm Ln} Q_{N/2}}{\delta \phi_{\mathbf{k}}}\Big),$$

where $Q_{N/2}$ is denoted as

$$Q_{N/2} = \frac{\langle 0|(\hat{\pi}_{\rm cp})^{N/2}(\hat{\pi}^\dagger_{\rm cp})^{N/2}|0\rangle}{(N/2)!}.$$

Let us define the following quantity $\bar{\varepsilon}$ under the constraint condition of total particle number conservation $N = 2\sum_{\mathbf{k}}^{\rm Fin.} \bar{n}_{\mathbf{k}}$ as

$$\bar{\varepsilon} \equiv \varepsilon_{\rm BCS} + \mu \sum_{\mathbf{k}}^{\rm Fin.} (N - 2\bar{n}_{\mathbf{k}}), \tag{B.17}$$

where μ is the Lagrange multiplier. Then we minimize $\bar{\varepsilon}$ with respect to $(\mu, \phi_{\mathbf{k}})$ as

$$2\big[\varepsilon_k - \mu + \frac{1}{V}\sum_{\mathbf{k}'}^{\text{Fin.}}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\bar{n}_{\mathbf{k}'}\big]\phi_{\mathbf{k}} - \frac{1}{V}\sum_{\mathbf{k}'}^{\text{Fin.}} U_{|\mathbf{k}-\mathbf{k}'|}\bar{F}^*_{\mathbf{k}'}\phi_{\mathbf{k}}^2 + \frac{1}{V}\sum_{\mathbf{k}'}^{\text{Fin.}} U_{|\mathbf{k}-\mathbf{k}'|}\bar{F}_{\mathbf{k}'} = 0. \tag{B.18}$$

This equation can be written concisely by introducing the following quantities as

$$\xi_{\mathbf{k}} \equiv \varepsilon_k - \mu + \frac{1}{V}\sum_{\mathbf{k}'}^{\text{Fin.}}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\bar{n}_{\mathbf{k}'}, \tag{B.19}$$

$$\Delta_{\mathbf{k}} \equiv -\frac{1}{V}\sum_{\mathbf{k}'}^{\text{Fin.}} U_{|\mathbf{k}-\mathbf{k}'|}\bar{F}^*_{\mathbf{k}'}, \tag{B.20}$$

where $\xi_{\mathbf{k}}$ denotes the single particle energy, and $\Delta_{\mathbf{k}}$ denotes the gap energy.

Thus Eq.(B.18) becomes

$$\Delta_k^*|\phi_{\mathbf{k}}|^2 + 2\xi_k\phi_{\mathbf{k}} - \Delta_k = 0, \tag{B.21}$$

and it can be easily solved formally by imposing $\phi_{\mathbf{k}} \to 0$ for $k \to \infty$ as

$$\phi_{\mathbf{k}} = \frac{-\xi_{\mathbf{k}} + E_{\mathbf{k}}}{\Delta^*_{\mathbf{k}}}, \quad E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}, \tag{B.22}$$

With this expression, we can transform the quantities $\bar{n}_{\mathbf{k}}$ and $\bar{F}_{\mathbf{k}}$ as

$$\bar{n}_{\mathbf{k}} = \frac{E_{\mathbf{k}} - \xi_{\mathbf{k}}}{E_{\mathbf{k}}}, \quad \bar{F}_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}. \tag{B.23}$$

C Approximation in the Current Formulation

Several approximations are necessary for deriving the current BCS formalism.

1) First approximation was performed in the process of deriving the quasi-particle operators $(\hat{\beta}_{\mathbf{k}\alpha}, \hat{\beta}^\dagger_{\mathbf{k}\alpha})$. Let us operate $\hat{c}_q$ on the ket vector $|\Phi_N\rangle \equiv Q_{N/2}^{-1/2}(\hat{\pi}^\dagger)^{N/2}|0\rangle$, and transform the resulting expression as

$$\begin{aligned}\hat{c}_q|\Phi_N\rangle &= \frac{Q_{N/2}^{-1/2}}{(N/2)!}\{\hat{c}_q, (\hat{\pi}^\dagger)^{N/2}\}|0\rangle \\ &= \frac{Q_{N/2}^{-1/2}}{(N/2-1)!}\sum_{q_1}\phi_{qq_1}\hat{c}^\dagger_{q_1}(\hat{\pi}^\dagger)^{(N/2)-1}|0\rangle \\ &= \sqrt{\frac{Q_{N/2-1}}{Q_{N/2}}}\sum_{q_1}\phi_{qq_1}\hat{c}^\dagger_{q_1}|\Phi_{N-2}\rangle.\end{aligned} \tag{C.1}$$

This Equation can be written as

$$\Big(\hat{c}_q - \sqrt{\frac{Q_{N/2-1}}{Q_{N/2}}}\sum_{q_1}\phi_{qq_1}\hat{c}^\dagger_{q_1}\hat{\beta}\Big)|\Phi_N\rangle = 0. \tag{C.2}$$

As we mentioned in Section(2.3), the explicit expression of $(\hat{\beta}_{\mathbf{k}\alpha}, \hat{\beta}^{\dagger}_{\mathbf{k}\alpha})$ is given by

$$\hat{\beta}^{\dagger}_{\mathbf{k}\alpha}|\Phi_N\rangle = |\Phi_{N+2}\rangle, \quad \hat{\beta}_{\mathbf{k}\alpha}|\Phi_N\rangle = |\Phi_{N-2}\rangle, \quad \hat{\beta}^{\dagger} \equiv \sqrt{\frac{Q_{N/2}}{Q_{N/2+1}}}\frac{\hat{\pi}^{\dagger}}{N/2+1}.$$

We multiply Eq.(C.2) by $u_{qq'} \equiv (\underline{1} - \sigma\underline{\phi\phi^{\dagger}})^{-1/2}_{qq'}$ and subsequently sum it over q. Then the resulting equation is expressible as

$$\sum_{q'}\left(u_{qq'}\hat{c}_q - \sqrt{\frac{Q_{N/2-1}}{Q_{N/2}}}v_{qq'}\hat{c}^{\dagger}_{q'}\hat{\beta}\right)|\Phi_N\rangle = 0. \tag{C.3}$$

Here we introduce the approximation $Q_{N/2-1}/Q_{N/2}\approx 1$, which holds in thermodynamic limit as $N \to \infty$. If so, we can express Eq.(C.3) as

$$\hat{\gamma}_q|\Phi_N\rangle = 0, \tag{C.4}$$

with the definition of $\hat{\gamma}_q$ as

$$\hat{\gamma}_q \equiv \sum_{q'}\left(u_{qq'}\hat{c}_q - v_{qq'}\hat{c}^{\dagger}_{q'}\hat{\beta}\right). \tag{C.5}$$

We set $q \to \{\mathbf{k}, \alpha\}$, then we obtain Eq.(2.20).

Similar approximation also performed in Eq.(B.16), where we evaluate the ground-state energy by using the approximation of $Q_{N/2+1}/Q_{N/2}\approx 1$ as for $N \to \infty$.

2) As we mentioned in Appendix B.2, another approximation was performed in deriving the interaction energy as Eq.(B.13)

$$\begin{aligned}
&\langle\Phi^{\rm BCS}_N|\hat{H}_{\rm int}|\Phi^{\rm BCS}_N\rangle \\
=&\frac{1}{V}\sum^{\rm Fin.}_{\mathbf{kk'}}(2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\Big[\Big(\frac{\phi_{\mathbf{k'}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k'}}}\Big)\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big) + \frac{\phi_{\mathbf{k'}}}{2}\frac{\delta}{\phi_{\mathbf{k'}}}\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big)\Big] \\
&+ \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum^{\rm Fin.}_{\mathbf{kk'}}U_{|\mathbf{k}-\mathbf{k'}|}\Big[\Big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}}\Big)\Big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\Big) + \frac{1}{2}\frac{\delta}{\phi^*_{\mathbf{k'}}}\Big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\Big)\Big] \\
\approx&\frac{1}{V}\sum^{\rm Fin.}_{\mathbf{kk'}}(2U_0 - U_{|\mathbf{k}-\mathbf{k'}|})\Big[\Big(\frac{\phi_{\mathbf{k'}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k'}}}\Big)\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta {\rm Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big)\Big] \\
&+ \frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum^{\rm Fin.}_{\mathbf{kk'}}U_{|\mathbf{k}-\mathbf{k'}|}\Big[\Big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}}\Big)\Big(\frac{1}{2}\frac{\delta {\rm Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\Big)\Big].
\end{aligned} \tag{C.6}$$

We suggest that the red terms are negligible in the thermodynamic limit since they are proportional to the delta function.

3) Finally, we also expressed the quantity Q_n asymptotically Eq.(A.22) in Appendix A.2 as

$$
\begin{aligned}
\text{Ln}Q_{N/2} &= \sum_{\mathbf{k}} \text{Ln}(1+|\phi_{\mathbf{k}}|^2) - \frac{1}{2}\text{Ln}\big[2\pi \sum_{\mathbf{k}} \frac{|\phi_{\mathbf{k}}|^2}{1+|\phi_{\mathbf{k}}|^2}\big] \\
&\approx \sum_{\mathbf{k}} \text{Ln}(1+|\phi_{\mathbf{k}}|^2).
\end{aligned}
$$

We neglect the second term of order LnN in comparison with the first term with order N.

We aim to remove these mathematical approximation mentioned, and develop new set of formula to evaluate the ground-state energy more properly from a relatively small number of particles to the thermodynamic limit, as for the particle-number-fixed model (see Appendix G).

D Quasi-particle Operator and its Inverse Operator

We derived the quasi-particle operator in Appendix C. Here we introduce the method of deriving the inverse of quasi-particle operators $(\hat{\gamma}_{\mathbf{k}\alpha}\hat{\gamma}^{\dagger}_{\mathbf{k}\alpha})$.

The operator of Eq.(C.5) is now given by

$$\hat{\gamma}_{\mathbf{k}\uparrow} = u_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta}, \tag{D.1a}$$

$$\hat{\gamma}_{\mathbf{k}\downarrow} = u_{\mathbf{k}}\hat{c}_{\mathbf{k}\downarrow} - v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\uparrow}\hat{\beta}. \tag{D.1b}$$

Note that $\alpha = \uparrow, \downarrow$ does denote the eigenstate of $\hat{s}_z$ but is only used here to distinguish the two quasi-particle operators conveniently. In Section 2, we have rewritten Eqs.(D.1) into Eq.(2.20) as $\hat{\gamma}_{\mathbf{k}\alpha} \equiv u_{\mathbf{k}}\hat{c}_{\mathbf{k}\alpha} - (-1)^{\frac{1}{2}-\alpha}v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}$.

Using Eq.(2.12), we can show that

$$\{\hat{c}_{\mathbf{k}\alpha}, \hat{\beta}^{\dagger}\}|\Phi_N\rangle = \sqrt{\frac{Q_{N/2}/Q_{N/2+1}}{N/2+1}}\{\hat{c}_{\mathbf{k}\alpha}, \hat{\pi}^{\dagger}\}|\Phi_N\rangle \approx 0, \tag{D.2}$$

holds in the thermodynamic limit. Hence, we set

$$\{\hat{c}_{\mathbf{k}\alpha}, \hat{\beta}^{\dagger}\} = \{\hat{c}^{\dagger}_{\mathbf{k}\alpha}, \hat{\beta}\} = 0. \tag{D.3}$$

Hence Eq.(D.1b) with $\mathbf{k} \to -\mathbf{k}$ and its Hermitian conjugate can be approximated as

$$\hat{\gamma}_{-\mathbf{k}\downarrow} = u_{\mathbf{k}}\hat{c}_{-\mathbf{k}\downarrow} + v_{\mathbf{k}}\hat{\beta}\hat{c}^{\dagger}_{\mathbf{k}\uparrow}, \tag{D.4a}$$

$$\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow} = v^{*}_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow}\hat{\beta}^{\dagger} + u_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}. \tag{D.4b}$$

We multiply the operator (D.4b) by $\hat{\beta}$ from the right side, then we obtain

$$\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta} = v^{*}_{\mathbf{k}}\hat{c}_{\mathbf{k}\uparrow} + u_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta}. \tag{D.5}$$

Then Eq.(D.1a) and Eq.(D.5) can be written as

$$\begin{pmatrix} \hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow} \\ \hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & -v_{\mathbf{k}} \\ v^{*}_{\mathbf{k}} & u_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta} \end{pmatrix}. \tag{D.6}$$

The inverse of Eq.(D.6) is given by

$$\begin{pmatrix} \hat{c}_{\mathbf{k}\uparrow} \\ \hat{c}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}} & v_{\mathbf{k}} \\ -v^{*}_{\mathbf{k}} & -v^{*}_{\mathbf{k}} \end{pmatrix} \begin{pmatrix} \hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow} \\ \hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}\hat{\beta} \end{pmatrix}. \tag{D.7}$$

The second row is given explicitly by

$$\hat{c}^{\dagger}_{-\mathbf{k}\downarrow} = -v^{*}_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\uparrow}\hat{\beta}^{\dagger} + u_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}\downarrow}, \tag{D.8}$$

from which we obtain

$$\hat{c}_{-\mathbf{k}\downarrow} = -v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{\mathbf{k}\uparrow}\hat{\beta} + u_{\mathbf{k}}\hat{\gamma}_{-\mathbf{k}\downarrow}. \tag{D.9}$$

Thus, the expression of Eq.(D.8) and Eq.(D.9) can be written together as

$$\hat{c}_{\mathbf{k}\alpha} = u_{\mathbf{k}}\hat{\gamma}_{\mathbf{k}\alpha} + (-1)^{\frac{1}{2}-\alpha}v_{\mathbf{k}}\hat{\gamma}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}. \tag{D.10}$$

It is also straightforward to prove the anti-symmetric commutation relation of the quasi-particle operator as follows;

$$\begin{aligned} &\{\hat{\gamma}_{\mathbf{k}\alpha}, \hat{\gamma}^{\dagger}_{\mathbf{k}'\alpha'}\} \\ =&\{u_{\mathbf{k}}\hat{c}_{\mathbf{k}\alpha} - (-1)^{\frac{1}{2}-\alpha}v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}, u_{\mathbf{k}}\hat{c}^{\dagger}_{\mathbf{k}'\alpha'} - (-1)^{\frac{1}{2}-\alpha'}v^{*}_{\mathbf{k}'}\hat{c}_{-\mathbf{k}'-\alpha'}\hat{\beta}^{\dagger}\} \\ =&u_{\mathbf{k}}u_{\mathbf{k}'}\{\hat{c}_{\mathbf{k}\alpha}, \hat{c}^{\dagger}_{\mathbf{k}'\alpha'}\} + (-1)^{1-\alpha-\alpha'}v_{\mathbf{k}}v^{*}_{\mathbf{k}'}\{\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}, \hat{c}_{-\mathbf{k}'-\alpha'}\} \\ =&\delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\alpha'}(|u_{\mathbf{k}}|^2 + |v_{\mathbf{k}}|^2) \\ =&\delta_{\mathbf{k}\mathbf{k}'}\delta_{\alpha\alpha'}, \end{aligned} \tag{D.11}$$

$$\begin{aligned} &\{\hat{\gamma}_{\mathbf{k}\alpha}, \hat{\gamma}_{\mathbf{k}'\alpha'}\} \\ =&\{u_{\mathbf{k}}\hat{c}_{\mathbf{k}\alpha} - (-1)^{\frac{1}{2}-\alpha}v_{\mathbf{k}}\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}\hat{\beta}, u_{\mathbf{k}'}\hat{c}_{\mathbf{k}'\alpha'} - (-1)^{\frac{1}{2}-\alpha'}v_{\mathbf{k}'}\hat{c}^{\dagger}_{-\mathbf{k}'-\alpha'}\hat{\beta}\} \\ =&-(-1)^{\frac{1}{2}-\alpha'}u_{\mathbf{k}}v_{\mathbf{k}'}\{\hat{c}_{\mathbf{k}\alpha}, \hat{c}^{\dagger}_{-\mathbf{k}'-\alpha'}\}\hat{\beta} - (-1)^{\frac{1}{2}-\alpha}v_{\mathbf{k}}u_{\mathbf{k}'}\{\hat{c}^{\dagger}_{-\mathbf{k}-\alpha}, \hat{c}_{\mathbf{k}'\alpha'}\}\hat{\beta} \\ =&\delta_{\mathbf{k},-\mathbf{k}'}\delta_{\alpha,-\alpha'}(-1)^{\frac{3}{2}-\alpha}u_{\mathbf{k}}v_{\mathbf{k}}[(-1)^{2\alpha} + 1] \\ =&0. \end{aligned} \tag{D.12}$$

E Extremal Conditions of $\hat{\pi}_4$ Correlation Theory

The variation of Eq.(2.39) can be calculated concisely with chain rule.

Let us introduce following quantities in terms of the explicit dependences of $\bar{\varepsilon}$.

$$\xi_{\mathbf{k}}^{(0)} \equiv \frac{1}{2}\frac{\delta\bar{\varepsilon}}{\bar{n}_k} = \varepsilon_k - \mu + \frac{1}{V}\sum_{\mathbf{k}'}^{\mathbf{Fin.}}(2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\bar{n}_{\mathbf{k}'}, \tag{E.1}$$

$$\Delta_{\mathbf{k}}^{(0)} \equiv -\frac{1}{2}\frac{\delta\bar{\varepsilon}}{\bar{F}_k} = -\frac{1}{V}\sum_{\mathbf{k}'}^{\mathbf{Fin.}} U_{|\mathbf{k}-\mathbf{k}'|}\bar{F}^*_{\mathbf{k}'}, \tag{E.2}$$

$$\frac{\delta\bar{\varepsilon}}{u_k} = \frac{2}{V}\sum_{\mathbf{k_2k_3k_4}} \delta_{\mathbf{k+k_2+k_3+k_4,0}} U_{|\mathbf{k+k_3}|} u_{\mathbf{k_2}} v_{\mathbf{k_3}} v_{\mathbf{k_4}} \times \sum_{\alpha\alpha'} (-1)^{1-\alpha-\alpha'} w_{\mathbf{k}\alpha\mathbf{k_2}\alpha'\mathbf{k_4}-\alpha'\mathbf{k_3}-\alpha}, \tag{E.3}$$

$$\frac{\delta\bar{\varepsilon}}{v_k} = \frac{2}{V}\sum_{\mathbf{k_2k_3k_4}} \delta_{\mathbf{k+k_2+k_3+k_4,0}} U_{|\mathbf{k+k_3}|} v_{\mathbf{k_2}} u_{\mathbf{k_3}} u_{\mathbf{k_4}} \times \sum_{\alpha\alpha'} (-1)^{1+\alpha+\alpha'} w_{\mathbf{k}\alpha\mathbf{k_2}\alpha'\mathbf{k_4}-\alpha'\mathbf{k_3}-\alpha}. \tag{E.4}$$

Subsequently, we use of Eq.(2.34) and Eq.(2.35) to differentiate $(\bar{n}_{k\alpha}, \bar{F}_{k\alpha}, u_k, v_k)$ with respect to $\phi_{\mathbf{k}}$ and $w_{\mathbf{k}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}$.

First, the differentiation with respect to $\phi_{\mathbf{k}}$ can be performed as

$$\begin{aligned}\frac{\delta\bar{n}_{k\alpha}}{\delta\phi_{\mathbf{k}}} &= \frac{2\phi_{\mathbf{k}}}{(1+|\phi_{\mathbf{k}}|^2)^2}\Big(1 - \frac{2}{3!}\sum_{\kappa_2\kappa_3\kappa_4} w^2_{\mathbf{k}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}\Big) \\ &= 2\phi_{\mathbf{k}} u_k^4(1-2\eta_k),\end{aligned} \tag{E.5}$$

$$\begin{aligned}\frac{\delta\bar{F}_{k\alpha}}{\delta\phi_{\mathbf{k}}} &= \frac{1-|\phi_{\mathbf{k}}|^2}{(1+|\phi_{\mathbf{k}}|^2)^2}\Big(1 - \frac{2}{3!}\sum_{\kappa_2\kappa_3\kappa_4} w^2_{\mathbf{k}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}\Big) \\ &= (1-\phi_{\mathbf{k}}^2) u_k^4(1-2\eta_k),\end{aligned} \tag{E.6}$$

$$\begin{aligned}\frac{\delta u_k}{\delta\phi_{\mathbf{k}}} &= -\frac{\phi_{\mathbf{k}}/u_k}{(1+|\phi_{\mathbf{k}}|^2)^2} \\ &= -u_k^2 v_k,\end{aligned} \tag{E.7}$$

$$\begin{aligned}\frac{\delta u_k}{\delta\phi_{\mathbf{k}}} &= -\frac{1/u_k}{(1+|\phi_{\mathbf{k}}|^2)^2} \\ &= v_k^3.\end{aligned} \tag{E.8}$$

Next, we consider the stationary condition of Equation with respect to $w_{\mathbf{k}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}$.

The basic differentiation of $(\bar{n}_k, \bar{F}_k, \zeta_k)$ can be performed as follows;

$$\frac{\delta\bar{n}_k}{\delta w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}} = \sum_{j=1}^{4}\delta_{k_jk}(u_{k_j}^2 - v_{k_j}^2) w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}, \tag{E.9}$$

$$\frac{\delta\bar{F}_k}{\delta w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}} = -2\sum_{j=1}^{4}\delta_{k_jk}(u_{k_j}v_{k_j}) w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}, \tag{E.10}$$

$$
\begin{aligned}
&\frac{\delta\zeta_{\mathbf{k}}}{\delta w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}}\\
=&\delta\Big(\frac{1}{V}\sum_{\mathbf{k_1k_2k_3k_4}}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}U_{|\mathbf{k_1+k_3}|}u_{\mathbf{k_1}}u_{\mathbf{k_2}}v_{\mathbf{k_3}}v_{\mathbf{k_4}}\\
&\times\sum_{\alpha\alpha'}(-1)^{1-\alpha-\alpha'}w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha'\mathbf{k_4}-\alpha'\mathbf{k_3}-\alpha}\Big)/\delta\big(w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}\big)\\
=&\frac{2}{V}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}\\
&\times\big[\delta_{\alpha_1,-\alpha_2}\delta_{\alpha_3,-\alpha_4}(-1)^{1-\alpha_1-\alpha_3}\times U_{|\mathbf{k_1+k_2}|}(u_{\mathbf{k_1}}v_{\mathbf{k_2}}+v_{\mathbf{k_1}}u_{\mathbf{k_2}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_3}\delta_{\alpha_4,-\alpha_2}(-1)^{1-\alpha_1-\alpha_4}\times U_{|\mathbf{k_1+k_3}|}(u_{\mathbf{k_1}}v_{\mathbf{k_3}}+v_{\mathbf{k_1}}u_{\mathbf{k_3}})(u_{\mathbf{k_2}}v_{\mathbf{k_4}}+v_{\mathbf{k_2}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_4}\delta_{\alpha_2,-\alpha_3}(-1)^{1-\alpha_1-\alpha_2}\times U_{|\mathbf{k_1+k_4}|}(u_{\mathbf{k_1}}v_{\mathbf{k_4}}+v_{\mathbf{k_1}}u_{\mathbf{k_4}})(u_{\mathbf{k_2}}v_{\mathbf{k_3}}+v_{\mathbf{k_2}}u_{\mathbf{k_3}})\big].
\end{aligned}
\tag{E.11}
$$

In deriving the differentiation of ζ_k with respect to $w_{\mathbf{k}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}$, we used the identities $(-1)^{\alpha-\alpha'}\delta_{\alpha,-\alpha'}=-\delta_{\alpha,-\alpha'}$ and $(-1)^{\alpha+\alpha'}=(-1)^{-\alpha-\alpha'}$ for $\alpha,\alpha'=\pm\frac{1}{2}$.

Then, we can transform $\delta\bar{\varepsilon}/\delta\phi_{\mathbf{k}}=0$ the extremal condition into

$$
\Delta_k^{(0)*}|\phi_{\mathbf{k}}|^2+2\xi_k^{(0)}\phi_{\mathbf{k}}-\Delta_k^{(0)}+\chi_k=0,
\tag{E.12}
$$

with the expression of χ_k as

$$
\begin{aligned}
\chi_{\mathbf{k}}\equiv&(1-2\eta_{\mathbf{k}})^{-1}\frac{1}{V}\sum_{\mathbf{k_2k_3k_4}}U_{|\mathbf{k+k_3}|}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}U_{|\mathbf{k_1+k_3}|}\\
&\times\frac{u_{\mathbf{k_2}}u_{\mathbf{k_3}}u_{\mathbf{k_4}}}{u_{\mathbf{k}}}(\phi_{\mathbf{k_2}}-\phi_{\mathbf{k}}\phi_{\mathbf{k_3}}\phi_{\mathbf{k_4}})\sum_{\alpha\alpha'}(-1)^{1-\alpha-\alpha'}w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha'\mathbf{k_3}-\alpha'\mathbf{k_4}-\alpha},
\end{aligned}
\tag{E.13}
$$

where we used $(-1)^{\alpha+\alpha'}=(-1)^{-\alpha-\alpha'}$ for $\alpha,\alpha'=\pm\frac{1}{2}$.

Also, using Equations from Eq.(E.1) to Eq.(E.4), and Equations from Eq.(E.9) to Eq.(E.11), the extremal condition of $\delta\bar{\varepsilon}/\delta w_{\kappa_1\kappa_2\kappa_3\kappa_4}=0$ can be performed as

$$
\begin{aligned}
&2\sum_{j=1}^{4}\big[(u_{k_j}^2-v_{k_j}^2)\xi_{k_j}^{(0)}+2u_{k_j}v_{k_j}\Delta_{k_j}^{(0)}\big]w_{\mathbf{k_1}\alpha\mathbf{k_2}\alpha_2\mathbf{k_3}\alpha_3\mathbf{k_4}\alpha_4}+\frac{2}{V}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}\\
&\times\big[\delta_{\alpha_1,-\alpha_2}\delta_{\alpha_3,-\alpha_4}(-1)^{1-\alpha_1-\alpha_3}\times U_{|\mathbf{k_1+k_2}|}(u_{\mathbf{k_1}}v_{\mathbf{k_2}}+v_{\mathbf{k_1}}u_{\mathbf{k_2}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_3}\delta_{\alpha_4,-\alpha_2}(-1)^{1-\alpha_1-\alpha_4}\times U_{|\mathbf{k_1+k_3}|}(u_{\mathbf{k_1}}v_{\mathbf{k_3}}+v_{\mathbf{k_1}}u_{\mathbf{k_3}})(u_{\mathbf{k_2}}v_{\mathbf{k_4}}+v_{\mathbf{k_2}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_4}\delta_{\alpha_2,-\alpha_3}(-1)^{1-\alpha_1-\alpha_2}\times U_{|\mathbf{k_1+k_4}|}(u_{\mathbf{k_1}}v_{\mathbf{k_4}}+v_{\mathbf{k_1}}u_{\mathbf{k_4}})(u_{\mathbf{k_2}}v_{\mathbf{k_3}}+v_{\mathbf{k_2}}u_{\mathbf{k_3}})\big]=0.
\end{aligned}
\tag{E.14}
$$

Thus, the equation can be easily solved as

$$
\begin{aligned}
w_{\kappa_1\kappa_2\kappa_3\kappa_4}=&-\frac{\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}}{E_{\mathbf{k_1}}^{(0)}+E_{\mathbf{k_2}}^{(0)}+E_{\mathbf{k_3}}^{(0)}+E_{\mathbf{k_4}}^{(0)}}\frac{1}{V}\\
&\times\big[\delta_{\alpha_1,-\alpha_2}\delta_{\alpha_3,-\alpha_4}(-1)^{1-\alpha_1-\alpha_3}\times U_{|\mathbf{k_1+k_2}|}(u_{\mathbf{k_1}}v_{\mathbf{k_2}}+v_{\mathbf{k_1}}u_{\mathbf{k_2}})(u_{\mathbf{k_3}}v_{\mathbf{k_4}}+v_{\mathbf{k_3}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_3}\delta_{\alpha_4,-\alpha_2}(-1)^{1-\alpha_1-\alpha_4}\times U_{|\mathbf{k_1+k_3}|}(u_{\mathbf{k_1}}v_{\mathbf{k_3}}+v_{\mathbf{k_1}}u_{\mathbf{k_3}})(u_{\mathbf{k_2}}v_{\mathbf{k_4}}+v_{\mathbf{k_2}}u_{\mathbf{k_4}})\\
&+\delta_{\alpha_1,-\alpha_4}\delta_{\alpha_2,-\alpha_3}(-1)^{1-\alpha_1-\alpha_2}\times U_{|\mathbf{k_1+k_4}|}(u_{\mathbf{k_1}}v_{\mathbf{k_4}}+v_{\mathbf{k_1}}u_{\mathbf{k_4}})(u_{\mathbf{k_2}}v_{\mathbf{k_3}}+v_{\mathbf{k_2}}u_{\mathbf{k_3}})\big].
\end{aligned}
$$

Let us substitute Eq.(E.15) into Eq.(E.13). We use the identities

$$\sum_{\alpha\alpha'}(-1)^{2-2\alpha}\delta_{\alpha,-\alpha'} = \sum_{\alpha\alpha'}(-1)^{2-\alpha-\alpha'}\delta_{\alpha\alpha'} = -2, \quad \sum_{\alpha\alpha'}(-1)^{2-2\alpha-2\alpha'}\delta_{\alpha\alpha'} = 4. \tag{E.15}$$

and exchange variables such as $\mathbf{k_2} \leftrightarrow \mathbf{k_4}$ several times. Therefore, we figure out that Eq.(E.13) can be divided into two parts, which are proportional to $\phi_{\mathbf{k}}$ and $(\phi_{\mathbf{k}}^2 - 1)$ respectively as

$$\chi_{\mathbf{k}} = 2\xi_{\mathbf{k}}^{(1)}\phi_{\mathbf{k}} + (\phi_{\mathbf{k}}^2 - 1)\Delta_{\mathbf{k}}^{(1)}, \tag{E.16}$$

where $\xi_{\mathbf{k}}^{(1)}$ and $\Delta_{\mathbf{k}}^{(1)}$ denote correlation parts of Eq.(2.44) and Eq.(2.45) respectively, which are proportional to V^{-2}.

We substitute Eq.(E.16) into Eq.(E.12), obtain the equation for $\phi_{\mathbf{k}}$ as

$$\Delta_k^*|\phi_{\mathbf{k}}|^2 + 2\xi_k\phi_{\mathbf{k}} - \Delta_k = 0, \tag{E.17}$$

in terms of $\xi_{\mathbf{k}} = \xi_{\mathbf{k}}^{(0)} + \xi_{\mathbf{k}}^{(1)}$ and $\Delta_{\mathbf{k}} = \Delta_{\mathbf{k}}^{(0)} + \Delta_{\mathbf{k}}^{(1)}$ respectively. The solution of this Equation satisfies $\phi_{\mathbf{k}} \to 0$ for $k \to \infty$ is given by

$$\phi_{\mathbf{k}} = \frac{-\xi_{\mathbf{k}} + E_{\mathbf{k}}}{\Delta_{\mathbf{k}}^*}, \quad E_{\mathbf{k}} \equiv \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}.$$

which exactly the same structure as the mean-field BCS theory.

In what follows, we present an elaborate derivation of the expectation of the interaction energy H_{int}.

For simplicity, we consider the first term on the right hand side of Eq.(2.30),

$$\frac{1}{2V}\sum_{\mathbf{kk'q}}^{\text{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k+q}}u_{\mathbf{k'-q}}u_{\mathbf{k'}}u_{\mathbf{k}}\langle\Phi_N^{\text{Corr.}}|\hat{\gamma}^\dagger_{\mathbf{k+q},\alpha}\hat{\gamma}^\dagger_{\mathbf{k'-q},\alpha'}\hat{\gamma}_{\mathbf{k'}\alpha'}\hat{\gamma}_{\mathbf{k}\alpha}|\Phi_N^{\text{Corr.}}\rangle$$

$$= \frac{1}{2V}\sum_{\mathbf{q}} U_q \sum_{\mathbf{k}_1\alpha_1\ldots\mathbf{k}_4\alpha_4}\ \sum_{\mathbf{k}'_1\alpha'_1\ldots\mathbf{k}'_4\alpha'_4} u_{\mathbf{k_1+q}}u_{\mathbf{k}'_1-\mathbf{q}}u_{\mathbf{k}'_1}u_{\mathbf{k}_1}\frac{w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}}{3!}\frac{w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}}{3!}$$

$$\times\langle\Phi_N^{\text{Corr.}}|\hat{\gamma}^\dagger_{\kappa_1}\hat{\gamma}^\dagger_{\kappa_2}\hat{\gamma}^\dagger_{\kappa_3}\hat{\gamma}^\dagger_{\kappa_4}\hat{\gamma}^\dagger_{\kappa_1}\hat{\gamma}^\dagger_{\kappa_2}\hat{\gamma}^\dagger_{\kappa_3}\hat{\gamma}^\dagger_{\kappa_4}|\Phi_N^{\text{Corr.}}\rangle. \tag{E.18}$$

We assume that $w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}$ is proportional to $\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}$, then we obtain

$$= \frac{1}{2V}\sum_{\mathbf{q}} U_q \sum_{\mathbf{k}_1\alpha_1\ldots\mathbf{k}_4\alpha_4}\ \sum_{\mathbf{k}'_1\alpha'_1\ldots\mathbf{k}'_4\alpha'_4} u_{\mathbf{k_1+q}}u_{\mathbf{k}'_1-\mathbf{q}}u_{\mathbf{k}'_1}u_{\mathbf{k}_1}\frac{|w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}|^2}{3!}\frac{|w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}|^2}{3!}$$

$$\times\left(\delta_{q,0}-\delta_{k_1+q,k'_1}\delta_{\alpha_1,\alpha'_1}\right), \tag{E.19}$$

which gives

$$= \frac{1}{2V}\sum_{\mathbf{q}} U_q \sum_{\mathbf{k}_1\alpha_1\ldots\mathbf{k}_4\alpha_4}\ \sum_{\mathbf{k}'_1\alpha'_1\ldots\mathbf{k}'_4\alpha'_4} u_{\mathbf{k_1+q}}u_{\mathbf{k}'_1-\mathbf{q}}u_{\mathbf{k}'_1}u_{\mathbf{k}_1}\frac{|w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}|^2}{3!}\frac{|w_{\mathbf{k}_1\alpha_1\mathbf{k}_2\alpha\mathbf{k}_3\alpha_3\mathbf{k}_4\alpha_4}|^2}{3!}. \tag{E.20}$$

Others terms besides the last two terms in Eq.(2.30), are derivable using the same proceedure.

Furthermore, we show how we obtain the expectation of the new emerged terms, Eq.(2.30a) and Eq.(2.30b) as follows;

$$\frac{1}{2V}\sum_{\mathbf{kk'q}}^{\text{Fin.}} U_q \sum_{\alpha\alpha'} u_{\mathbf{k+q}}u_{\mathbf{k'-q}}v_{\mathbf{k'}}v_{\mathbf{k}}(-1)^{1-\alpha-\alpha'}\langle\Phi_N^{\text{Corr.}}|\hat{\gamma}^\dagger_{\mathbf{k+q},\alpha}\hat{\gamma}^\dagger_{\mathbf{k'-q},\alpha'}\hat{\gamma}^\dagger_{\mathbf{-k'}-\alpha'}\hat{\gamma}^\dagger_{\mathbf{-k}-\alpha}(\hat{\beta})^2|\Phi_N^{\text{Corr.}}\rangle$$

$$+\frac{1}{2V}\sum_{\mathbf{kk'q}}^{\text{Fin.}} U_q \sum_{\alpha\alpha'} v_{\mathbf{k+q}}v_{\mathbf{k'-q}}u_{\mathbf{k'}}u_{\mathbf{k}}(-1)^{1-\alpha-\alpha'}\langle\Phi_N^{\text{Corr.}}|(\hat{\beta}^\dagger)^2\hat{\gamma}_{\mathbf{-k-q},-\alpha}\hat{\gamma}_{\mathbf{-k'+q},-\alpha'}\hat{\gamma}_{\mathbf{k'}\alpha'}\hat{\gamma}_{\mathbf{k}\alpha}|\Phi_N^{\text{Corr.}}\rangle$$

$$=\frac{1}{2V}\sum_{\mathbf{k_1k_2k_3k_4}}\sum_{\alpha\alpha'}U_{|\mathbf{k_1+k_3}|}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}$$

$$\times\Big[u_{\mathbf{k}_1}u_{\mathbf{k}_2}v_{\mathbf{k}_3}v_{\mathbf{k}_4}\langle\Phi_N^{\text{Corr.}}|(\hat{\beta}^\dagger)^2\hat{\gamma}_{\mathbf{k}_1,\alpha}\hat{\gamma}_{\mathbf{k}_2,\alpha'}\hat{\gamma}_{\mathbf{k}_4,-\alpha'}\hat{\gamma}_{\mathbf{k}_3,-\alpha}|\Phi_N^{\text{Corr.}}\rangle$$

$$+v^*_{\mathbf{k}_1}v^*_{\mathbf{k}_2}u_{\mathbf{k}_3}u_{\mathbf{k}_4}\langle\Phi_N^{\text{Corr.}}|(\hat{\beta}^\dagger)^2\hat{\gamma}_{\mathbf{k}_1,-\alpha}\hat{\gamma}_{\mathbf{k}_2,-\alpha'}\hat{\gamma}_{\mathbf{k}_4,\alpha'}\hat{\gamma}_{\mathbf{k}_3,\alpha}|\Phi_N^{\text{Corr.}}\rangle\Big],$$

which finally becomes

$$=\frac{1}{2V}\sum_{\mathbf{k_1k_2k_3k_4}}\sum_{\alpha\alpha'}U_{|\mathbf{k_1+k_3}|}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}}$$

$$\times\Big[u_{\mathbf{k}_1}u_{\mathbf{k}_2}v_{\mathbf{k}_3}v_{\mathbf{k}_4}w_{\mathbf{k}_1\alpha\mathbf{k}_2\alpha'\mathbf{k}_4-\alpha'\mathbf{k}_3-\alpha}+v^*_{\mathbf{k}_1}v^*_{\mathbf{k}_2}u_{\mathbf{k}_3}u_{\mathbf{k}_4}w_{\mathbf{k}_1-\alpha\mathbf{k}_2-\alpha'\mathbf{k}_4\alpha'\mathbf{k}_3\alpha}\Big].$$

Therefore, using the mathematical properties of the anti-symmetric tensor

$$\hat{P} w_{\kappa_1 \kappa_2 \kappa_3 \kappa_4} = (-1)^P w_{\kappa_1 \kappa_2 \kappa_3 \kappa_4}, \tag{E.21}$$

we can rewrite the correlation energy into a more compact form, for which we denote the functional $\zeta_{\mathbf{k}}$, for algebraic convenience as follows;

$$\zeta_{\mathbf{k}} \equiv \frac{1}{V} \sum_{\mathbf{k_1 k_2 k_3 k_4}} \delta_{\mathbf{k_1}+\mathbf{k_2}+\mathbf{k_3}+\mathbf{k_4},\mathbf{0}} U_{|\mathbf{k_1}+\mathbf{k_3}|} u_{\mathbf{k_1}} u_{\mathbf{k_2}} v_{\mathbf{k_3}} v_{\mathbf{k_4}} \times \sum_{\alpha\alpha'} (-1)^{1-\alpha-\alpha'} w_{\mathbf{k_1}\alpha \mathbf{k_2}\alpha' \mathbf{k_4} -\alpha' \mathbf{k_3} -\alpha}. \tag{E.22}$$

F Expression of Sums Over $(\kappa_2\kappa_3\kappa_4)$

We now introduce the way to evaluate the triple sums efficiently

$$f(k) \equiv \frac{1}{V^2} \sum_{\mathbf{k_2 k_3 k_4}} U_{|\mathbf{k}+\mathbf{k_2}|} U_{|\mathbf{k}+\mathbf{k_3}|} \delta_{\mathbf{k_1}+\mathbf{k_2}+\mathbf{k_3}+\mathbf{k_4},\mathbf{0}} \times g(k, k_2, k_3, k_4). \tag{F.1}$$

First, we choose $\mathbf{k}$ along the z-axis and express $\mathbf{k_2}$ in the polar coordinates. The vector $\mathbf{k} + \mathbf{k_2}$ is given by

$$\begin{aligned} \mathbf{k} + \mathbf{k_2} &= (k_2 \mathrm{sin}\theta_2 \mathrm{cos}\theta_2, k_2 \mathrm{sin}\theta_2 \mathrm{sin}\theta_2, k + k_2 \mathrm{cos}\theta_2) \\ &= (k_{12} \mathrm{sin}\theta_{12} \mathrm{cos}\theta_{12}, k_{12} \mathrm{sin}\theta_{12} \mathrm{sin}\theta_{12}, k_{12} \mathrm{cos}\theta_{12}), \end{aligned} \tag{F.2}$$

where we define k_{12} and θ_{12} as follows;

$$k_{12} \equiv |\mathbf{k_1} + \mathbf{k_2}| = \sqrt{k^2 + k_2^2 + 2kk_2 \mathrm{cos}\theta_2}, \tag{F.3}$$

$$\theta_{12} \equiv \tan^{-1} \frac{k_2 \mathrm{sin}\theta_2}{k + k_2 \mathrm{cos}\theta_2}. \tag{F.4}$$

The vector $\mathbf{k} + \mathbf{k_2}$ can be also written in terms of the orthogonal matrix as

$$\mathbf{k_1} + \mathbf{k_2} = R_{12} \begin{pmatrix} 0 \\ 0 \\ k_{12} \end{pmatrix}, \tag{F.5}$$

where the orthogonal matrix R_{12} is expressible as

$$R_{12} \equiv \begin{pmatrix} \mathrm{cos}\theta_{12}\mathrm{cos}\theta_2 & -\mathrm{sin}\theta_2 & \mathrm{sin}\theta_{12}\mathrm{cos}\theta_2 \\ \mathrm{cos}\theta_{12}\mathrm{sin}\theta_2 & \mathrm{cos}\theta_2 & \mathrm{sin}\theta_{12}\mathrm{sin}\theta_2 \\ \mathrm{sin}\theta_{12} & 0 & \mathrm{cos}\theta_{12} \end{pmatrix}. \tag{F.6}$$

We can also express $\mathbf{k_3}$ in terms of the matrix R_{12} by

$$\mathbf{k_3} = R_{12} \begin{pmatrix} k_3 \mathrm{sin}\bar{\theta}_3 \mathrm{cos}\bar{\phi}_3 \\ k_3 \mathrm{sin}\bar{\theta}_3 \mathrm{sin}\bar{\phi}_3 \\ k_3 \mathrm{cos}\bar{\theta}_3 \end{pmatrix}, \tag{F.7}$$

where $(\bar{\theta}_3, \bar{\phi}_3)$ are polar angles in the coordinate system when $\mathbf{k} + \mathbf{k_2}$ lies along the z-axis.

This representation enables us to write $(\mathbf{k_1} + \mathbf{k_2}) \cdot \mathbf{k_3}$ and $|\mathbf{k_1} + \mathbf{k_3}|$ concisely as

$$(\mathbf{k_1} + \mathbf{k_2}) \cdot \mathbf{k_3} = k_{12} k_3 \mathrm{cos}\bar{\theta}_3, \tag{F.8}$$

$$\mathrm{k}_{13} \equiv |\mathbf{k_1} + \mathbf{k_3}| = \sqrt{\mathrm{k}^2 + \mathrm{k}_3^2 + 2\mathrm{k}\mathrm{k}_3(-\mathrm{sin}\theta_{12}\mathrm{sin}\bar{\theta}_3\mathrm{cos}\bar{\phi}_3 + \mathrm{cos}\theta_{12}\mathrm{cos}\bar{\theta}_3)}. \tag{F.9}$$

Thereby, we can perform the triple sums as follows;

$$f(k) \equiv \frac{1}{V^2}\sum_{\mathbf{k_2k_3k_4}} U_{|\mathbf{k+k_2}|}U_{|\mathbf{k+k_3}|}\delta_{\mathbf{k_1+k_2+k_3+k_4,0}} \times g(k,k_2,k_3,k_4)$$
$$= \frac{1}{(2\pi)^6}\int_0^\infty \mathrm{dk_2k_2^2}\int_0^\pi \mathrm{d}\theta_2\mathrm{sin}\theta_2\int_0^{2\pi}\mathrm{d}\phi_2\int_0^\infty \mathrm{dk_3k_3^2}\int_0^\pi \mathrm{d}\bar{\theta}_3\mathrm{sin}\bar{\theta}_3\int_0^{2\pi}\mathrm{d}\bar{\phi}_3 U_{k_{12}}U_{k_{13}}$$
$$\times\, g(\mathrm{k},\mathrm{k_2},\mathrm{k_3},\sqrt{k_{12}^2+k_3^2+2kk_2k_{12}k_3\mathrm{cos}\bar{\theta}_3}). \tag{F.10}$$

Integration over ϕ_2 can be easily performed from lower-limit 0 to upper-limit 2π. Subsequently, we make a variable exchange as follows;

$$\bar{\theta}_3 \to k_4 \equiv \sqrt{k_{12}^2+k_3^2+2kk_2k_{12}k_3\mathrm{cos}\bar{\theta}_3}, \tag{F.11}$$
$$d\bar{\theta}_3 \to dk_4 = -\frac{k_{13}k_2}{k_4}\mathrm{sin}\theta_3 d\bar{\theta}_3. \tag{F.12}$$

Then we can express Eq.(F.10) as

$$f(k) = \frac{1}{(2\pi)^5}\int_0^\infty \mathrm{dk_2k_2}\int_0^\infty \mathrm{dk_3k_3}\int_0^\pi \mathrm{d}\theta_2\frac{\mathrm{k_2sin}\theta_2}{\mathrm{k_{12}}}U_{k_{12}}\int_{|k_{12}-k_3|}^{k_{12}+k_3} dk_4k_4 g(\mathrm{k},\mathrm{k_2},\mathrm{k_3}k_4)\int_0^{2\pi}\mathrm{d}\bar{\phi}_3 U_{k_{13}}. \tag{F.13}$$

Further, we exchange the order of integrations over θ_2 and k_4 by noting that

$$|k_{12}-k_3| \le k_4 \le k_{12}+k_3$$
$$\Rightarrow |k_3-k_4| \le k_{12} \le k_3+k_4$$
$$\Rightarrow \frac{(k_4-k_3)^2-k^2-k_2^2}{2kk_2} \le \mathrm{cos}\theta_2 \le \frac{(k_4+k_3)^2-k^2-k_2^2}{2kk_2}. \tag{F.14}$$
$$\tag{F.15}$$

The last to inequalities are satisfied when the domain

$$\frac{(k_4-k_3)^2-k^2-k_2^2}{2kk_2} \le 1, \quad \frac{(k_4+k_3)^2-k^2-k_2^2}{2kk_2} \ge -1, \tag{F.16}$$

are simultaneously met.

Thus, we can transform the upper and lower limit of k_4 as

$$k_{4\mathrm{i}} \le k_4 \le k_{4\mathrm{f}}, \tag{F.17}$$

where $k_{4\mathrm{i}}$ and $k_{4\mathrm{f}}$ are written as

$$k_{4\mathrm{i}} \equiv \max(0,\mathrm{k_2}-\mathrm{k}-\mathrm{k_3},|\mathrm{k}-\mathrm{k_3}|-\mathrm{k_2}), \tag{F.18}$$
$$k_{4\mathrm{f}} \equiv \min(\mathrm{k}+\mathrm{k_2}+\mathrm{k_3},\mathrm{k_{max}}). \tag{F.19}$$

In addition, Eq.(F.16) is expressible in terms of two angles as

$$\theta_{2\mathrm{i}} \le \theta_2 \le \theta_{2\mathrm{f}}, \tag{F.20}$$

where the definition of $(\theta_{2\rm i}, \theta_{2\rm f})$ is denoted as

$$\begin{aligned}
\cos\theta_{2\rm i} &\equiv \min\big(1, \frac{(\rm k_4 + k_3)^2 - k^2 - k_2^2}{2kk_2}\big), \\
\cos\theta_{2\rm f} &\equiv \max\big(-1, \frac{(\rm k_4 - k_3)^2 - k^2 - k_2^2}{2kk_2}\big).
\end{aligned} \tag{F.21}$$

With transformation of variables mentioned, we can transform Eq.(F.13) into

$$f(k) = \frac{1}{(2\pi)^5} \int_0^\infty \rm dk_2 k_2 \int_0^\infty dk_3 k_3 \int_{k_{4i}}^{k_{4f}} dk_4 k_4 \mathit{f}(k, k_2, k_3, k_4) \int_{\theta_{2i}}^{\theta_{2f}} d\theta_2 \sin\theta_2 \frac{k_2}{k_{12}} \mathit{U}_{\mathit{k}_{12}} \int_0^{2\pi} d\bar{\phi}_3 \mathit{U}_{\mathit{k}_{13}}. \tag{F.22}$$

The momentum k_{12} is defined by Eq.(F.3), and the momentum k_{13} is defined by Eq.(F.9), in terms of θ_{12} and $\bar{\theta}_3$ which defined by Eq.(F.4) and

$$\bar{\theta}_3 \equiv \cos^{-1} \frac{\rm k_4^2 - k_{12}^2 - k_3^2}{2k_{12}k_3}, \tag{F.23}$$

respectively.

G A Potential Formula for Evaluating the Ground-state Energy of Particle-Number Conserved System with Minimal Mathematical Approximation

As we mentioned in the Conclusion, we aim to construct a formulation removed the mathematical approximation we talked in Appendix C, which still inside the framework of the mean-field theory.

G.1 Formulation

First, we introduce the BCS Hamiltonian with exactly the same structure as we used in the preceding chapters

$$\hat{H} \equiv \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} \hat{c}^{\dagger}_{\mathbf{k}\alpha} \hat{c}_{\mathbf{k}-\alpha} + \frac{1}{2V} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \sum_{\alpha\alpha'} U_q \hat{c}^{\dagger}_{\mathbf{k}+\mathbf{q}\alpha} \hat{c}^{\dagger}_{\mathbf{k}'-\mathbf{q}\alpha} \hat{c}_{\mathbf{k}'\alpha'} \hat{c}_{\mathbf{k}\alpha}, \tag{G.1}$$

where

$$\varepsilon_{\mathbf{k}} = \frac{\hbar^2 k^2}{2m}, \text{and } U_q = \int U(r) \mathrm{e}^{-i\mathbf{q}\mathbf{r}} d^3 r.$$

We choose the BCS wave function

$$|\Phi_N^{\text{BCS}}\rangle = A_{N/2}^{-1/2} (\hat{\pi}^{\dagger}_{\text{cp}})^{N/2} |0\rangle.$$

to evaluate the ground-state energy.

Moreover, as we mentioned in the preceding sections, we set $q \to \{\mathbf{k}, \alpha\}$, the relations between Eqs.(A.9) can be expressed as

$$\begin{aligned} Q_n(\mathbf{k}) &= \frac{1}{n} \sum_{l=1}^{n} Q_{n-l} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2l} (-1)^{l-1}, \\ &= -\sum_{\mathbf{k}} \phi_{\mathbf{k}}{}^* P_n(\mathbf{k}) \end{aligned} \tag{G.2a}$$

$$P_n(\mathbf{k}) = \frac{1}{n} \sum_{l=1}^{n} Q_{n-l} \phi_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^l. \tag{G.2b}$$

with

$$I_l = (-1)^{n-1} \sum_{\mathbf{k}} |\phi_{\mathbf{k}}|^{2l}.$$

G.2 Evaluation of the ground-state energy

In Appendix B.2, the kinetic energy can be also written as

$$\begin{aligned}\langle\Phi_N^{\mathrm{BCS}}|\hat{H}_0|\Phi_N^{\mathrm{BCS}}\rangle \equiv& \sum_{\mathbf{k}\alpha}\varepsilon_{\mathbf{k}}\langle\Phi_N^{\mathrm{BCS}}|\hat{c}^\dagger_{\mathbf{k}\alpha}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\mathrm{BCS}}\rangle\\ =&Q_{N/2}^{-1}\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}\phi_{\mathbf{k}}\frac{\delta Q_{N/2}}{\delta\phi_{\mathbf{k}}}\\ =&\sum_{\mathbf{k}}\varepsilon_{\mathbf{k}}\phi_{\mathbf{k}}\frac{\delta \mathrm{Ln} Q_{N/2}}{\delta\phi_{\mathbf{k}}}.\end{aligned} \tag{G.3}$$

Here, we choose the second equality in (G.3) for convenience.

Next, we evaluate the interaction energy as follows;

$$\begin{aligned}&\langle\Phi_N^{\mathrm{BCS}}|\hat{H}_{\mathrm{int}}|\Phi_N^{\mathrm{BCS}}\rangle\\ &\equiv\frac{1}{2V}\sum_{\mathbf{kk'q}}^{\mathrm{Fin.}}\sum_{\alpha\alpha'}U_q\langle\Phi_N^{\mathrm{BCS}}|\hat{c}^\dagger_{\mathbf{k+q}\alpha}\hat{c}^\dagger_{\mathbf{k'-q}\alpha'}\hat{c}_{\mathbf{k'}\alpha'}\hat{c}_{\mathbf{k}\alpha}|\Phi_N^{\mathrm{BCS}}\rangle\\ &=\frac{1}{V}\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}(2U_0-U_{|\mathbf{k}-\mathbf{k'}|})\Big[\Big(\frac{\phi_{\mathbf{k'}}}{2}\frac{\delta\mathrm{Ln}Q_{N/2}}{\delta\phi_{\mathbf{k'}}}\Big)\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta\mathrm{Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big)+\frac{\phi_{\mathbf{k'}}}{2}\frac{\delta}{\delta\phi_{\mathbf{k'}}}\Big(\frac{\phi_{\mathbf{k}}}{2}\frac{\delta\mathrm{Ln}Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big)\Big]\\ &\quad+\frac{Q_{(N/2)+1}}{Q_{N/2}}\frac{1}{V}\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}U_{|\mathbf{k}-\mathbf{k'}|}\Big[\Big(\frac{1}{2}\frac{\delta\mathrm{Ln}Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}}\Big)\Big(\frac{1}{2}\frac{\delta\mathrm{Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\Big)+\frac{1}{2}\frac{\delta}{\delta\phi^*_{\mathbf{k'}}}\Big(\frac{1}{2}\frac{\delta\mathrm{Ln}Q_{(N/2)+1}}{\delta\phi_{\mathbf{k}}}\Big)\Big].\end{aligned}$$

For convenience, we focus on Eq.(B.13), two steps backwards of Eq.(B.15), which includes the neglected terms as follows;

$$\begin{aligned}&\langle\Phi_N^{\mathrm{BCS}}|\hat{H}_{\mathrm{int}}|\Phi_N^{\mathrm{BCS}}\rangle\\ &=Q_{N/2}^{-1}\frac{1}{V}\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}(2U_0-U_{|\mathbf{k}-\mathbf{k'}|})\frac{\phi_{\mathbf{k}}\phi_{\mathbf{k'}}}{2^2}\frac{\delta^2Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k'}}}+Q_{N/2}^{-1}\frac{1}{V}\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}U_{|\mathbf{k}-\mathbf{k'}|}\frac{1}{2^2}\frac{\delta^2Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}\phi_{\mathbf{k}}}.\end{aligned} \tag{G.4}$$

Then, we can rewrite the ground-state energy functional based on Eq.(G.3) and Eq.(G.4) as

$$\begin{aligned}\varepsilon\equiv&\langle\Phi_N^{\mathrm{BCS}}|\hat{H}|\Phi_N^{\mathrm{BCS}}\rangle\\ =&Q_{N/2}^{-1}\Big\{\sum_{\mathbf{k}\alpha}^{\mathrm{Fin.}}\varepsilon_{\mathbf{k}}\phi_{\mathbf{k}}\frac{\delta Q_{N/2}}{\delta\phi_{\mathbf{k}}}+\frac{1}{4V}\Big[\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}(2U_0-U_{|\mathbf{k}-\mathbf{k'}|})\phi_{\mathbf{k}}\phi_{\mathbf{k'}}\frac{\delta^2Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k'}}}+\sum_{\mathbf{kk'}}^{\mathrm{Fin.}}U_{|\mathbf{k}-\mathbf{k'}|}\frac{\delta^2Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}\phi_{\mathbf{k}}}\Big]\Big\}.\end{aligned}$$

Therefore, the energy functional ε is expressible in terms of the differential of $\phi_{\mathbf{k}}$, i.e.

$$\varepsilon\{\phi_{\mathbf{k}},\phi^*_{\mathbf{k}}\}=\varepsilon\Big\{\mathscr{L}\Big(\frac{\delta Q_{N/2}}{\delta\phi_{\mathbf{k}}}\Big),\mathscr{L}\Big(\frac{\delta^2Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k'}}}\Big),\mathscr{L}\Big(\frac{\delta^2Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k'}}\phi_{\mathbf{k}}}\Big)\Big\}. \tag{G.5}$$

where the notation $\mathscr{L}$ denotes the summation to the differential of Q_n with respect to $(\phi_{\mathbf{k}},\phi_{\mathbf{k'}})$ in the energy functional.

Now, it is clear to calculate the differential terms respectively.

First, it is straightforward to calculate the differential of the quantity Q_n with respect to $\phi_{\mathbf{k}}$ as

$$\frac{\delta Q_{N/2}(\mathbf{k})}{\delta\phi_{\mathbf{k}}} = \Big[\delta\big(\frac{1}{n}\sum_{l=1}^{n} Q_{n-l}\sum_{\mathbf{k}}|\phi_{\mathbf{k}}|^{2l}(-1)^{l-1}\big)/\delta\phi_{\mathbf{k}}\Big]_{n=N/2},$$
$$= 2\phi^*_{\mathbf{k}}\sum_{l=1}^{N/2} Q_{N/2-l}|\phi_{\mathbf{k}}|^{2(l-1)}(-1)^{l-1}. \qquad \text{(G.6)}$$

Next, note that the differential of the interaction energy can be expressed as the second-order differential of the quantity Q_n with respect to $\phi_{\mathbf{k}}$, it is convenient to denote and calculate the second-order differential $\mathscr{L}\left(\frac{\delta^2 Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}}\right), \mathscr{L}\left(\frac{\delta^2 Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k}'}\phi_{\mathbf{k}}}\right)$ as

$$\mathscr{L}\left(\frac{\delta^2 Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}}\right) \equiv \sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'}\frac{\delta^2 Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}}, \qquad \text{(G.7a)}$$
$$\mathscr{L}\left(\frac{\delta^2 Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k}'}\phi_{\mathbf{k}}}\right) \equiv \sum_{\mathbf{k}\mathbf{k}'} g_{\mathbf{k},\mathbf{k}'}\frac{\delta^2 Q_{(N/2)+1}}{\delta\phi^*_{\mathbf{k}}\phi_{\mathbf{k}'}}. \qquad \text{(G.7b)}$$

where we define the quantities $f_{\mathbf{k},\mathbf{k}'}$ and $g_{\mathbf{k},\mathbf{k}'}$ as

$$f_{\mathbf{k},\mathbf{k}'} \equiv (2U_0 - U_{|\mathbf{k}-\mathbf{k}'|})\phi_{\mathbf{k}}\phi_{\mathbf{k}'}, \qquad \text{(G.8a)}$$
$$g_{\mathbf{k},\mathbf{k}'} \equiv U_{|\mathbf{k}-\mathbf{k}'|}. \qquad \text{(G.8b)}$$

Let us calculate Eq.(G.7a) using Eq.(G.6) .

$$
\begin{aligned}
\text{Eq.(G.7a)} &= \sum_{\mathbf{k}\mathbf{k}'} \mathrm{f}_{\mathbf{k},\mathbf{k}'} \frac{\delta^2 \mathrm{Q}_{\mathrm{N}/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}} \\
&= \sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \frac{\delta}{\delta\phi_{\mathbf{k}'}} \left(2\phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \right) \\
&= 2\sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \left(\frac{\delta\phi_{\mathbf{k}}^*}{\delta\phi_{\mathbf{k}'}} \right) \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 2\sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} \left(\frac{\delta Q_{N/2-l}}{\delta\phi_{\mathbf{k}'}} \right) |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 2\sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} Q_{N/2-l} \left(\frac{\delta |\phi_{\mathbf{k}}|^{2(l-1)}}{\delta\phi_{\mathbf{k}'}} \right) (-1)^{l-1} \\
&= 2\sum_{\mathbf{k}\mathbf{k}'} \left[(f_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (f_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 4\sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} \left(\phi_{\mathbf{k}'}^* \sum_{m=1}^{N/2-l} Q_{N/2-l-m} |\phi_{\mathbf{k}'}|^{2(m-1)} (-1)^{m-1} \right) |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 2\sum_{\mathbf{k}} \left[(f_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (f_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} \left(Q_{N/2-l} 2(l-1) |\phi_{\mathbf{k}}|^{2(l-2)} \phi_{\mathbf{k}}^* \right) (-1)^{l-1} \\
&= 2\sum_{\mathbf{k}\mathbf{k}'} \left[(f_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (f_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 4\sum_{\mathbf{k}\mathbf{k}'} f_{\mathbf{k},\mathbf{k}'} \phi_{\mathbf{k}}^* \phi_{\mathbf{k}'}^* \sum_{l=1}^{N/2} \sum_{m=1}^{N/2-l} Q_{N/2-l-m} |\phi_{\mathbf{k}'}|^{2(m-1)} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l+m} \\
&\quad + 2\sum_{\mathbf{k}} \left[(f_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (f_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \phi_{\mathbf{k}}^* \phi_{\mathbf{k}}^* \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-2)} 2(l-1)(-1)^{l-1}. \qquad \text{(G.9)}
\end{aligned}
$$

Similarly, Eq.(G.7b) can be also calculated as follows;

$$
\begin{aligned}
\text{Eq.(G.7b)} &= \sum_{\mathbf{kk'}} \mathrm{g}_{\mathbf{k},\mathbf{k'}} \frac{\delta^2 \mathrm{Q}_{(\mathrm{N}/2)+1}}{\delta\phi^*_{\mathbf{k}}\phi_{\mathbf{k'}}} \\
&= \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \frac{\delta}{\delta\phi^*_{\mathbf{k'}}} \left(2\phi^*_{\mathbf{k}} \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \right) \\
&= 2 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \left(\frac{\delta\phi^*_{\mathbf{k}}}{\delta\phi^*_{\mathbf{k'}}} \right) \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 2 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \phi^*_{\mathbf{k}} \sum_{l=1}^{(N/2)+1} \left(\frac{\delta Q_{(N/2)+1-l}}{\delta\phi^*_{\mathbf{k'}}} \right) |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 2 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \phi^*_{\mathbf{k}} \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} \left(\frac{\delta |\phi_{\mathbf{k}}|^{2(l-1)}}{\delta\phi^*_{\mathbf{k'}}} \right) (-1)^{l-1} \\
&= 2 \sum_{\mathbf{kk'}} \left[(g_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (g_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \\
&\quad + 4 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \phi^*_{\mathbf{k}} \phi_{\mathbf{k'}} \sum_{l=1}^{(N/2)+1} \sum_{m=1}^{(N/2)+1-l} Q_{(N/2)+1-l-m} |\phi_{\mathbf{k'}}|^{2(m-1)} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l+m} \\
&\quad + 2 \sum_{\mathbf{k}} \left[(g_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (g_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \phi_{\mathbf{k}} \phi^*_{\mathbf{k}} \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} |\phi_{\mathbf{k}}|^{2(l-2)} 2(l-1)(-1)^{l}.
\end{aligned}
\tag{G.10}
$$

First, we decompose the second term of Eq.(G.10) into two terms, for $l = 1$ and $2 \le l \le N/2$ respectively. Then we combine the first and the third term of Eq.(G.10), we obtain that

$$
\begin{aligned}
&\text{Eq.(G.10)} \\
&= 4 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \phi^*_{\mathbf{k}} \phi_{\mathbf{k'}} \sum_{l=1}^{N/2} \sum_{m=1}^{(N/2)-l} Q_{(N/2)-l-m} |\phi_{\mathbf{k'}}|^{2(m-1)} |\phi_{\mathbf{k}}|^{2l} (-1)^{l+m+1} \\
&\quad + 4 \sum_{\mathbf{kk'}} g_{\mathbf{k},\mathbf{k'}} \phi^*_{\mathbf{k}} \phi_{\mathbf{k'}} \sum_{m=1}^{N/2} Q_{(N/2)-m} |\phi_{\mathbf{k'}}|^{2(m-1)} (-1)^{m+1} \\
&\quad + 2 \sum_{\mathbf{k}} \left[(g_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (g_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \phi_{\mathbf{k}} \phi^*_{\mathbf{k}} \sum_{l=1}^{(N/2)+1} Q_{(N/2)+1-l} |\phi_{\mathbf{k}}|^{2(l-2)} (2l-1)(-1)^{l}.
\end{aligned}
\tag{G.11}
$$

Finally, we also decompose the last term of Eq.(G.11) into two terms, for $l = 1$ and $2 \le l \le N/2$ respectively, and reset the index of the summation $l \to l+1$ for algebraic convenience. Therefore, the last term of Eq.(G.11) is expressible as

$$
\begin{aligned}
&= 2\sum_{\mathbf{k}} \left[(g_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (g_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] Q_{N/2} \\
&+ 2\sum_{\mathbf{k}} \left[(g_{\mathbf{k},\mathbf{k}}|_{k=k'}) + (g_{\mathbf{k},-\mathbf{k}}|_{k=-k'}) \right] \phi_{\mathbf{k}}\phi^*_{\mathbf{k}} \sum_{l=1}^{N/2} Q_{(N/2)-l}|\phi_{\mathbf{k}}|^{2(l-1)}(2l+1)(-1)^l. \qquad \text{(G.12)}
\end{aligned}
$$

We substitute Eq.(G.7a) for $f_{\mathbf{k},\mathbf{k}'}$, Eq.(G.7b) for $g_{\mathbf{k},\mathbf{k}'}$, and we rewrite the ground-state energy using Eq.(G.3), Eq.(G.9), Eq.(G.10) and Eq.(G.13) as follows;

$$
\begin{aligned}
\varepsilon \equiv& \langle \Phi_N^{\text{BCS}} | \hat{H} | \Phi_N^{\text{BCS}} \rangle \\
=& Q^{-1}_{N/2} \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} \phi_{\mathbf{k}} \frac{\delta Q_{N/2}}{\delta \phi_{\mathbf{k}}} + \frac{Q^{-1}_{N/2}}{4V} \left[\sum_{\mathbf{k}\mathbf{k}'} (2U_0 - U_{|\mathbf{k}-\mathbf{k}'|}) \phi_{\mathbf{k}}\phi_{\mathbf{k}'} \frac{\delta^2 Q_{N/2}}{\delta\phi_{\mathbf{k}}\phi_{\mathbf{k}'}} + \sum_{\mathbf{k}\mathbf{k}'} U_{|\mathbf{k}-\mathbf{k}'|} \frac{\delta^2 Q_{(N/2)+1}}{\delta \phi^*_{\mathbf{k}'}\phi_{\mathbf{k}}} \right] \\
=& 2Q^{-1}_{N/2} \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \phi_{\mathbf{k}} \left(2\phi^*_{\mathbf{k}} \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \right) \qquad \text{(G.13a)} \\
&+ Q^{-1}_{N/2} \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} (3U_0 - U_{\mathbf{2k}}) \phi_{\mathbf{k}}\phi_{\mathbf{k}'} \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l-1} \qquad \text{(G.13b)} \\
&+ Q^{-1}_{N/2} \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} (2U_0 - U_{|\mathbf{k}-\mathbf{k}'|}) \phi^*_{\mathbf{k}}\phi^*_{\mathbf{k}'} \sum_{l=1}^{N/2} \sum_{m=1}^{N/2-l} Q_{N/2-l-m} |\phi_{\mathbf{k}'}|^{2(m-1)} |\phi_{\mathbf{k}}|^{2(l-1)} (-1)^{l+m} \\
& \qquad \text{(G.13c)} \\
&+ Q^{-1}_{N/2} \frac{1}{V} \sum_{\mathbf{k}} (3U_0 - U_{\mathbf{2k}}) \phi^*_{\mathbf{k}}\phi^*_{\mathbf{k}} \sum_{l=1}^{N/2} Q_{N/2-l} |\phi_{\mathbf{k}}|^{2(l-2)} (l-1)(-1)^{l-1} \qquad \text{(G.13d)} \\
&+ Q^{-1}_{N/2} \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} U_{|\mathbf{k}-\mathbf{k}'|} \phi^*_{\mathbf{k}}\phi_{\mathbf{k}'} \sum_{l=1}^{N/2} \sum_{m=1}^{(N/2)-l} Q_{(N/2)-l-m} |\phi_{\mathbf{k}'}|^{2(m-1)} |\phi_{\mathbf{k}}|^{2l} (-1)^{l+m+1} \qquad \text{(G.13e)} \\
&+ Q^{-1}_{N/2} \frac{1}{V} \sum_{\mathbf{k}\mathbf{k}'} U_{|\mathbf{k}-\mathbf{k}'|} \phi^*_{\mathbf{k}}\phi_{\mathbf{k}'} \sum_{m=1}^{N/2} Q_{(N/2)-m} |\phi_{\mathbf{k}'}|^{2(m-1)} (-1)^{m+1} \qquad \text{(G.13f)} \\
&+ Q^{-1}_{N/2} \frac{1}{2V} \sum_{\mathbf{k}} (U_0 + U_{\mathbf{2k}}) Q_{N/2} \qquad \text{(G.13g)} \\
&+ Q^{-1}_{N/2} \frac{1}{2V} \sum_{\mathbf{k}} (U_0 + U_{\mathbf{2k}}) \phi_{\mathbf{k}}\phi^*_{\mathbf{k}} \sum_{l=1}^{N/2} Q_{(N/2)-l} |\phi_{\mathbf{k}}|^{2(l-1)} (2l+1)(-1)^l. \qquad \text{(G.13h)}
\end{aligned}
$$

Compared with the current canonical BCS ground-state energy, several new terms, the Hartree-Fock potential with $(3U_0 - U_{\mathbf{2k}})$, and the pair potential with $(U_0 + U_{\mathbf{2k}})$, emerge from the second-order differential of $Q_{(N/2)}$ with respect to $(\phi_{\mathbf{k}}, \phi_{\mathbf{k}'})$.

Using Eq.(G.6) and the same way we derived the ground-state energy Eq.(G.13), it is straightforward to derive the differential of the ground-state energy ε with respect to the variational parameter $\phi_{\mathbf{k}}$ according to the variational principle,

$$\frac{\delta \mathrm{Eq.(G.13)}}{\delta \phi_{\mathbf{k}}} = 0. \tag{G.14}$$

Compared with the current canonical BCS formula, which is valid in the thermodynamic limit, this method may cause our formula become quite complex eventually. However, this potential formula can be solved numerically using cumulation method for the total particle number N. Our numerical procedure is based on the following concept. Once we set a total particle number N, we obtain a specified variational condition for that total particle number. We substitute the total particle number to the variational condition Eq.(G.14) from N=1 to a relatively large number in a sequential order, with which we can solve Eq.(G.14) and therefore evaluate the ground-state energy cumulatively.

Theoretically Eq.(G.14) offers a possible solution to evaluate the ground-state energy with any total number of particles, which from a relative small number ($N = 1, 2, 3 \ldots$) to a large total number of particles ($N \approx 10^4$). Moreover, the current formulation which was frequently mentioned in [1, 2, 4, 8], only hold in the thermodynamic limit. We can also check if the ground-state energy agree with the current canonical BCS formulation in the thermodynamic limit.

However, to solve Eq.(G.14), we need specific a program for every total particle number, which is theoretically possible but takes a large amount of time. Thus, we are searching for a formulation, otherwise a more elegant algorithm, which is simple and elegant enough both on the mathematical structure and numerical procedures, which still needs further research.

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