Gap equation of BCS superconductivity

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In this note, we derive the self-consistency gap equation of conventional BCS superconductivity. We focus on the discretized tight-binding model for superconductivity, because our ultimate goal is to implement the self-consistency calculation on tight-binding models. Here, we consider the one-dimensional model of electrons, while generalization to two- and three-dimensional models is straightforward.

The microscopic Hamiltonian for electrons with attractive interaction is

$$H = H_0 + H_{\text{int}} = \sum_{j=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \left(-t\hat{c}^\dagger_{j+1\sigma}\hat{c}_{j\sigma} - t\hat{c}^\dagger_{j-1\sigma}\hat{c}_{j\sigma} + (2t-\mu)\hat{c}^\dagger_{j\sigma}\hat{c}_{j\sigma} \right) - g\sum_{j=1}^{N} \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow}, \tag{1}$$

where t is the hopping amplitude between the nearest-neighboring sites, μ is the chemical potential, and $g > 0$ is the strength of the local attraction among electrons. Note that in writing the interacting Hamiltonian, we keep the field operators of the same particle species (spin in our case) either in the outer two or the inner two positions of the quartic form. Here the 1D chain has N sites, and if we apply the periodic boundary condition on the chain, we will have the following Fourier transformation between real-space and momentum-space field operators:

$$\hat{c}_j = \frac{1}{\sqrt{N}} \sum_k \hat{c}_k e^{ikja}, \quad \hat{c}_k = \frac{1}{\sqrt{N}} \sum_j \hat{c}_j e^{-ikja}, \tag{2}$$

with a being the lattice constant. The periodic boundary condition $\hat{c}_{j+N} = \hat{c}_j$ would constrain the values of momentum k by

$$e^{ikNa} = e^{i2\pi m}, \tag{3}$$

such that

$$k = \frac{2\pi}{a} \cdot \frac{m}{N}, \quad m = 0, 1, \ldots, N-1. \tag{4}$$

The anti-commutation relation for the real-space field operators is

$$\{\hat{c}_i, \hat{c}^\dagger_j\} = \delta_{i,j}, \tag{5}$$

where $\delta_{i,j}$ is the Kronecker delta function, with

$$\delta_{i,j} = \begin{cases} 1 & \text{for} \quad i = j, \\ 0 & \text{otherwise.} \end{cases} \tag{6}$$

Thus the anti-commutation relation for the momentum-space field operators is

$$\{\hat{c}_k, \hat{c}^\dagger_q\} = \frac{1}{N} \sum_{j,n} e^{-ikja+iqna} \{\hat{c}_j, \hat{c}^\dagger_n\} = \frac{1}{N} \sum_j e^{-i(k-q)ja} = \delta_{k,q}. \tag{7}$$

The last equality holds because

$$\frac{1}{N} \sum_j e^{-ikja} = \begin{cases} 1 & \text{for} \quad k = 0, \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

for $k = 2\pi m/Na$.

1 Mean-field theory in momentum space

We now perform the Fourier transformation on the original real-space Hamiltonian, first the non-interacting part:

$$
\begin{aligned}
H_0 &= \sum_{j=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \left(-t\hat{c}^\dagger_{j+1\sigma}\hat{c}_{j\sigma} - t\hat{c}^\dagger_{j-1\sigma}\hat{c}_{j\sigma} + (2t-\mu)\hat{c}^\dagger_{j\sigma}\hat{c}_{j\sigma} \right) \\
&= \sum_{j=1}^{N} \sum_{\sigma=\uparrow,\downarrow} \frac{1}{N} \sum_{k,q} e^{-ikja} e^{iqja} \left(-te^{-ika} - te^{ika} + 2t - \mu \right) \hat{c}^\dagger_{k\sigma}\hat{c}_{q\sigma} \\
&= \sum_{\sigma=\uparrow,\downarrow} \sum_{k} \left(-2t\cos(ka) + 2t - \mu \right) \hat{c}^\dagger_{k\sigma}\hat{c}_{k\sigma}.
\end{aligned} \tag{9}
$$

Next, we perform the Fourier transformation on the interacting term:

$$
\begin{aligned}
H_{\text{int}} &= -g \sum_{j=1}^{N} \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} \\
&= -g \sum_{j=1}^{N} \frac{1}{\sqrt{N}} \sum_{l} e^{-ilja}\hat{c}^\dagger_{l\uparrow} \frac{1}{\sqrt{N}} \sum_{q} e^{-iqja}\hat{c}^\dagger_{q\downarrow} \frac{1}{\sqrt{N}} \sum_{p} e^{ipja}\hat{c}_{p\downarrow} \frac{1}{\sqrt{N}} \sum_{k} e^{ikja}\hat{c}_{k\uparrow} \\
&= -\frac{g}{N} \sum_{k,p,q,l} \delta_{-l+q+p+k,0}\hat{c}^\dagger_{l\uparrow}\hat{c}^\dagger_{-q\downarrow}\hat{c}_{p\downarrow}\hat{c}_{k\uparrow} \\
&= -\frac{g}{N} \sum_{k,p,q} \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow}\hat{c}_{p\downarrow}\hat{c}_{k\uparrow}.
\end{aligned} \tag{10}
$$

Now we start to make the mean-field approximation on the interaction term. The assumption is that we only consider the fluctuations on top of the pairing order parameter, i.e.,

$$
H_{\text{int}} \approx -\frac{g}{N} \sum_{k,p,q} \langle \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \hat{c}_{p\downarrow}\hat{c}_{k\uparrow} - \frac{g}{N} \sum_{k,p,q} \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow} \langle \hat{c}_{p\downarrow}\hat{c}_{k\uparrow} \rangle + \frac{g}{N} \sum_{k,p,q} \langle \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \langle \hat{c}_{p\downarrow}\hat{c}_{k\uparrow} \rangle. \tag{11}
$$

Note that within such a mean-field approximation, we have

$$
\langle H_{\text{int}} \rangle \approx -\frac{g}{N} \sum_{k,p,q} \langle \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \langle \hat{c}_{p\downarrow}\hat{c}_{k\uparrow} \rangle, \tag{12}
$$

which is the product of the mean-field order parameters. Another observation based on physical arguments is that the ground state is spatially homogeneous without any density wave, because the original Hamiltonian is homogeneous in space and we are considering the formation of superconductivity instead of crystal. Therefore

$$
\langle \hat{c}^\dagger_{k+p+q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle = \langle \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \delta_{k+p,0}, \tag{13}
$$

and the interaction term becomes

$$
H_{\text{int}} \approx -\frac{g}{N} \sum_{k,q} \langle \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \frac{g}{N} \sum_{k,q} \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow} \langle \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} \rangle + \frac{g}{N} \sum_{k,q} \langle \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle \langle \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} \rangle. \tag{14}
$$

If we define the order parameter as

$$
\Delta^* = \frac{g}{N} \sum_{q} \langle \hat{c}^\dagger_{q\uparrow}\hat{c}^\dagger_{-q\downarrow} \rangle, \quad \Delta = \frac{g}{N} \sum_{k} \langle \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} \rangle, \tag{15}
$$

then

$$H_{\text{int}}^{\text{MF}} = -\Delta^* \sum_k \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \Delta \sum_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger + \frac{N|\Delta|^2}{g}. \tag{16}$$

So in the end, the total Hamiltonian at the mean-field level becomes

$$H = \sum_k \left(\xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} + \xi_k \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} - \Delta^* \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \Delta \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \right) + \frac{N|\Delta|^2}{g}. \tag{17}$$

We now rewrite the total Hamiltonian into the BdG form by doubling the degrees of freedom, i.e.,

$$\begin{aligned} H = &\frac{1}{2}\sum_k \left(\xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} + \xi_k \hat{c}_{k\downarrow}^\dagger \hat{c}_{k\downarrow} - \Delta^* \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow} - \Delta \hat{c}_{k\uparrow}^\dagger \hat{c}_{-k\downarrow}^\dagger \right) \\ &+ \frac{1}{2}\sum_k \left(-\xi_k \hat{c}_{-k\uparrow}\hat{c}_{-k\uparrow}^\dagger - \xi_k \hat{c}_{-k\downarrow}\hat{c}_{-k\downarrow}^\dagger + \Delta^* \hat{c}_{-k\uparrow}\hat{c}_{k\downarrow} + \Delta \hat{c}_{k\downarrow}^\dagger \hat{c}_{-k\uparrow}^\dagger \right) + \frac{1}{2}\sum_k (\xi_{k\uparrow} + \xi_{k\downarrow}) + N|\Delta|^2/g \end{aligned} \tag{18}$$

with $\xi_{-k} = \xi_k$. In Eq. (18), we double the degrees of freedom and have an additional flipped energy branch $-\xi_k$, and we want to know the physical implications of the flipped energy branch. As an example, we consider the normal metal and switching off Δ. In the normal picture without doubling the degrees of freedom, we have

$$H_{\text{N}} = \sum_k \xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow}, \tag{19}$$

where we only consider the spin-up electrons. The ground state is the Fermi sea for which all the states below the Fermi energy are filled by electrons while those above are empty. Thus the ground state energy is

$$E_{\text{gs}} = \sum_{|k|<k_F} \xi_k. \tag{20}$$

On the other hand, in the BdG picture,

$$H_{\text{BdG}} = \frac{1}{2}\sum_k (\xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} - \xi_k \hat{c}_{-k\uparrow}\hat{c}_{-k\uparrow}^\dagger) + \frac{1}{2}\sum_k \xi_k. \tag{21}$$

Now there is a flipped "hole branch" $-\xi_k$. Although this "hole branch" is an artificial reproduction of the original electron branch, we can regard them as an independent particles, as if there is a second particle species

$$\begin{aligned} \hat{c}_{-k\uparrow} &\to \hat{b}_{k\downarrow}^\dagger, \\ \hat{c}_{-k\uparrow}^\dagger &\to \hat{b}_{k\downarrow}, \end{aligned} \tag{22}$$

so that

$$H_{\text{BdG}} = \frac{1}{2}\sum_k (\xi_k \hat{c}_{k\uparrow}^\dagger \hat{c}_{k\uparrow} - \xi_k \hat{b}_{k\downarrow}^\dagger \hat{b}_{k\downarrow}) + \frac{1}{2}\sum_k \xi_k. \tag{23}$$

For c-particles, the state energy is negative for $|k| < k_F$, while for b-particles, the state energy is negative for $|k| > k_F$, so the ground-state energy is

$$E_{\text{gs}} = \frac{1}{2}\sum_{|k|<k_F} \xi_k - \frac{1}{2}\sum_{|k|>k_F} \xi_k + \frac{1}{2}\sum_k \xi_k = \sum_{|k|<k_F} \xi_k, \tag{24}$$

which is consistent with the normal picture. It means that we can understand the BdG system by regarding each branch as an independent particle. This is very helpful for understanding the derivations later on. The BdG Hamiltonian for BCS superconductor is

$$\begin{aligned}
H &= \frac{1}{2}\sum_k \Psi_k^\dagger H_{\mathrm{BdG}}(k)\Psi_k \\
&= \frac{1}{2}\sum_k \begin{pmatrix} \hat{c}_{k\uparrow}^\dagger \\ \hat{c}_{k\downarrow}^\dagger \\ \hat{c}_{-k\uparrow} \\ \hat{c}_{-k\downarrow} \end{pmatrix}^T \begin{pmatrix} \xi_k & 0 & 0 & -\Delta \\ 0 & \xi_k & \Delta & 0 \\ 0 & \Delta^* & -\xi_k & 0 \\ -\Delta^* & 0 & 0 & -\xi_k \end{pmatrix} \begin{pmatrix} \hat{c}_{k\uparrow} \\ \hat{c}_{k\downarrow} \\ \hat{c}_{-k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow}^\dagger \end{pmatrix} \\
&= \frac{1}{2}\sum_k \begin{pmatrix} \hat{\gamma}_{k1}^\dagger \\ \hat{\gamma}_{k2}^\dagger \\ \hat{\gamma}_{k3}^\dagger \\ \hat{\gamma}_{k4}^\dagger \end{pmatrix}^T \begin{pmatrix} E_{k1} & & & \\ & E_{k2} & & \\ & & E_{k3} & \\ & & & E_{k4} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{k1} \\ \hat{\gamma}_{k2} \\ \hat{\gamma}_{k3} \\ \hat{\gamma}_{k4} \end{pmatrix} \\
&.
\end{aligned} \tag{25}$$

In the last line, we have diagonalized the BdG Hamiltonian, and $\hat{\gamma}_i$ is the field operator for the i-th branch. The relation between the electron field operators and the Bogoliubov quasiparticle operators is

$$\begin{aligned}
&\Psi = U\Gamma, \\
&\begin{pmatrix} \hat{c}_{k\uparrow} \\ \hat{c}_{k\downarrow} \\ \hat{c}_{-k\uparrow}^\dagger \\ \hat{c}_{-k\downarrow}^\dagger \end{pmatrix} = (\phi_1, \phi_2, \phi_3, \phi_4) \begin{pmatrix} \hat{\gamma}_{k1} \\ \hat{\gamma}_{k2} \\ \hat{\gamma}_{k3} \\ \hat{\gamma}_{k4} \end{pmatrix},
\end{aligned} \tag{26}$$

where $\phi_i = (u_{i\uparrow}, u_{i\downarrow}, v_{i\uparrow}, v_{i\downarrow})^T$ is the i-th eigenstate of H_{BdG}. Now we come back to the self-consistency gap equation, and we have

$$\begin{aligned}
\Delta &= \frac{g}{N}\sum_k \langle \hat{c}_{-k\downarrow}\hat{c}_{k\uparrow}\rangle \\
&= \frac{g}{N}\sum_k \langle \left(\sum_{n=1}^4 v_{kn\downarrow}^* \hat{\gamma}_{kn}^\dagger\right)\left(\sum_{m=1}^4 u_{km\uparrow}(k)\hat{\gamma}_{km}\right)\rangle \\
&= \frac{g}{N}\sum_k \sum_{n,m} v_{kn\downarrow}^* u_{km\uparrow} \langle \hat{\gamma}_{kn}^\dagger \hat{\gamma}_{km}\rangle \\
&= \frac{g}{N}\sum_k \sum_n v_{kn\downarrow}^* u_{kn\uparrow} \langle \hat{\gamma}_{kn}^\dagger \hat{\gamma}_{kn}\rangle.
\end{aligned} \tag{27}$$

Therefore, the self-consistency equation is

$$\Delta = \frac{g}{N}\sum_k \sum_{n=1}^4 v_{kn\downarrow}^* u_{kn\uparrow} n_F(E_{kn}) \tag{28}$$

with $n_F(E) = \frac{1}{e^{E/k_BT}+1}$ is the Fermi-Dirac distribution. Besides the pairing gap calculated self-consistently, another important quantity is the free energy difference between the superconducting and the normal-state phase.

$$F_{sn} = F_s - F_n. \tag{29}$$

If we are interested in the system at the zero-temperature limit, the free energy is equal to the ground-state energy. As we discussed previously, for the normal state, the ground-state energy is

$$F_n(T=0) = \frac{1}{2}\sum_k \sum_{E_{ki}<0} E_{ki}(\Delta=0) + \frac{1}{2}\sum_k (\xi_{k\uparrow} + \xi_{k\downarrow}), \tag{30}$$

while for the superconducting phase, the free energy is

$$F_s(T=0) = \frac{1}{2}\sum_k \sum_{E_{ki}<0} E_{ki}(\Delta) + \frac{1}{2}\sum_k (\xi_{k\uparrow} + \xi_{k\downarrow}) + \frac{N|\Delta|^2}{g}. \tag{31}$$

Thus the free energy difference is

$$F_{sn}(T=0) = F_s - F_n = \frac{1}{2}\sum_k \sum_{E_{ki}<0} [E_{ki}(\Delta) - E_{ki}(0)] + \frac{N|\Delta|^2}{g}. \tag{32}$$

By definition, the system is superconducting when $F_{sn} < 0$, while normal metal when $F_{sn} > 0$.

2 Mean-field theory in real space

Next, we derive the mean-field theory and the self-consistency equation in real space.

$$\begin{aligned}
H &= H_0 - g\sum_{j=1}^{N} \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} \\
&\approx H_0 - g\sum_{j=1}^{N}\langle \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\rangle \hat{c}_{j\downarrow}\hat{c}_{j\uparrow} - g\sum_{j=1}^{N}\hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\langle \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}\rangle + g\sum_{j=1}^{N}\langle \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\rangle\langle \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}\rangle \\
&= H_0 - \sum_{j=1}^{N}\left(\Delta^*_j \hat{c}_{j\downarrow}\hat{c}_{j\uparrow} + \Delta \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\right) + \sum_{j=1}^{N}|\Delta_j|^2/g,
\end{aligned} \tag{33}$$

where the pairing potential is local and defined as

$$\Delta_j = g\langle \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}\rangle, \quad \Delta^*_j = g\langle \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{j\downarrow}\rangle. \tag{34}$$

The relation between the electron and Bogoliubov operators is $\Psi = U\Gamma$, i.e.,

$$\begin{aligned}
\hat{c}_{j\uparrow} &= \sum_{n=1}^{4N} u_{j\uparrow}\hat{\gamma}_n, \\
\hat{c}_{j\downarrow} &= \sum_{n=1}^{4N} v^*_{j\downarrow}\hat{\gamma}^\dagger_n.
\end{aligned} \tag{35}$$

If we plug them into the self-consistency equation, we have

$$\begin{aligned}
\Delta_j &= g\langle \hat{c}_{j\downarrow}\hat{c}_{j\uparrow}\rangle \\
&= g\langle \left(\sum_{m=1}^{4N} v^*_{j\downarrow}\hat{\gamma}^\dagger_m\right)\left(\sum_{n=1}^{4N} u_{j\uparrow}\hat{\gamma}_n\right)\rangle \\
&= g\sum_{n=1}^{4N} v^*_{j\downarrow}u_{j\uparrow}\langle \hat{\gamma}^\dagger_n\hat{\gamma}_n\rangle,
\end{aligned} \tag{36}$$

and finally we obtain the self-consistency gap equation in real space as

$$\Delta_j = g\sum_{n=1}^{4N} v^*_{j\downarrow}u_{j\uparrow}n_F(E_n), \tag{37}$$

with $n_F(E) = \frac{1}{e^{E/k_BT}+1}$ being the Fermi-Dirac distribution.

3 Mean-field theory in real and momentum space

We now consider a 3D system in which translational symmetry is present along z-axis. Thus we treat the degrees of freedom in the xy-plane in real space, while those in the z-axis in momentum space. The original Hamiltonian in real space is

$$
\begin{aligned}
H =& H_0 + H_{\text{int}} \\
=& \sum_{\mathbf{r}} \sum_{j=1}^{N_z} \sum_{\sigma=\uparrow,\downarrow} \Big(-t\hat{c}^\dagger_{\mathbf{r}+\hat{x},j,\sigma}\hat{c}_{\mathbf{r},j,\sigma} - t\hat{c}^\dagger_{\mathbf{r}-\hat{x},j,\sigma}\hat{c}_{\mathbf{r},j,\sigma} - t\hat{c}^\dagger_{\mathbf{r}+\hat{y},j,\sigma}\hat{c}_{\mathbf{r},j,\sigma} - t\hat{c}^\dagger_{\mathbf{r}-\hat{y},j,\sigma}\hat{c}_{\mathbf{r},j,\sigma} \Big) \\
&+ \sum_{\mathbf{r}} \sum_{j=1}^{N_z} \sum_{\sigma=\uparrow,\downarrow} \Big(-t\hat{c}^\dagger_{\mathbf{r},j+1,\sigma}\hat{c}_{\mathbf{r},j,\sigma} - t\hat{c}^\dagger_{\mathbf{r},j-1,\sigma}\hat{c}_{\mathbf{r},j,\sigma} \Big) \\
&+ \sum_{\mathbf{r}} \sum_{j=1}^{N_z} \sum_{\sigma=\uparrow,\downarrow} (6t-\mu)\hat{c}^\dagger_{\mathbf{r},j,\sigma}\hat{c}_{\mathbf{r},j,\sigma} \\
&- g \sum_{\mathbf{r}} \sum_{j=1}^{N_z} \hat{c}^\dagger_{\mathbf{r},j\uparrow}\hat{c}^\dagger_{\mathbf{r},j\downarrow}\hat{c}_{\mathbf{r},j\downarrow}\hat{c}_{\mathbf{r},j\uparrow}.
\end{aligned} \tag{38}
$$

Because there is translational symmetry along z-axis direction, we can perform Fourier transformation along z-direction as follows

$$
\hat{c}_{\mathbf{r},j,\sigma} = \frac{1}{\sqrt{N_z}} \sum_k \hat{c}_{\mathbf{r},k,\sigma} e^{ikja}, \quad \hat{c}^\dagger_{\mathbf{r},j,\sigma} = \frac{1}{\sqrt{N_z}} \sum_k \hat{c}^\dagger_{\mathbf{r},k,\sigma} e^{-ikja}. \tag{39}
$$

Therefore the Hamiltonian becomes

$$
\begin{aligned}
H_0 =& \sum_{\mathbf{r}} \sum_k \sum_{\sigma=\uparrow,\downarrow} \Big(-t\hat{c}^\dagger_{\mathbf{r}+\hat{x},k,\sigma}\hat{c}_{\mathbf{r},k,\sigma} - t\hat{c}^\dagger_{\mathbf{r}-\hat{x},k,\sigma}\hat{c}_{\mathbf{r},k,\sigma} - t\hat{c}^\dagger_{\mathbf{r}+\hat{y},k,\sigma}\hat{c}_{\mathbf{r},k,\sigma} - t\hat{c}^\dagger_{\mathbf{r}-\hat{y},k,\sigma}\hat{c}_{\mathbf{r},k,\sigma} \Big) \\
&+ \sum_{\mathbf{r}} \sum_k \sum_{\sigma=\uparrow,\downarrow} \Big(-2t\cos(ka) + 6t - \mu \Big) \hat{c}^\dagger_{\mathbf{r},k,\sigma}\hat{c}_{\mathbf{r},k,\sigma}.
\end{aligned} \tag{40}
$$

The interaction term is

$$
\begin{aligned}
H_{\text{int}} &= -\frac{g}{N_z} \sum_{\mathbf{r}} \sum_{kpq} \hat{c}^\dagger_{\mathbf{r},k+p+q\uparrow}\hat{c}^\dagger_{\mathbf{r},-q\downarrow}\hat{c}_{\mathbf{r},p\downarrow}\hat{c}_{\mathbf{r},k\uparrow} \\
&\approx -\frac{g}{N_z} \sum_{\mathbf{r}} \sum_{kq} \langle \hat{c}^\dagger_{\mathbf{r},q\uparrow}\hat{c}^\dagger_{\mathbf{r},-q\downarrow}\rangle \hat{c}_{\mathbf{r},-k\downarrow}\hat{c}_{\mathbf{r},k\uparrow} - \frac{g}{N_z} \sum_{\mathbf{r}} \sum_{kq} \hat{c}^\dagger_{\mathbf{r},q\uparrow}\hat{c}^\dagger_{\mathbf{r},-q\downarrow} \langle \hat{c}_{\mathbf{r},-k\downarrow}\hat{c}_{\mathbf{r},k\uparrow}\rangle \\
&+ \frac{g}{N_z} \sum_{\mathbf{r}} \sum_{kq} \langle \hat{c}^\dagger_{\mathbf{r},q\uparrow}\hat{c}^\dagger_{\mathbf{r},-q\downarrow}\rangle \langle \hat{c}_{\mathbf{r},-k\downarrow}\hat{c}_{\mathbf{r},k\uparrow}\rangle \\
&= \sum_{\mathbf{r}} \sum_k \Big(-\Delta^*(\mathbf{r})\hat{c}_{\mathbf{r},-k\downarrow}\hat{c}_{\mathbf{r},k\uparrow} - \Delta(\mathbf{r})\hat{c}^\dagger_{\mathbf{r},k\uparrow}\hat{c}^\dagger_{\mathbf{r},-k\downarrow} \Big) + \frac{N_z}{g} \sum_{\mathbf{r}} |\Delta(\mathbf{r})|^2,
\end{aligned} \tag{41}
$$

where the pairing potential is self-consistently defined as

$$
\Delta(\mathbf{r}) = \frac{g}{N_z} \sum_k \langle \hat{c}_{\mathbf{r},-k\downarrow}\hat{c}_{\mathbf{r},k\uparrow}\rangle = \frac{g}{N_z} \sum_k \sum_{n=1}^{4N_{xy}} v^*_{k,n,\mathbf{r},\downarrow} u_{k,n,\mathbf{r},\uparrow} n_F(E_{kn}). \tag{42}
$$

In the numerical calculation, the Nambu field operator is defined as

$$
\Psi(\mathbf{r},k) = (c_{\mathbf{r},k,\uparrow}, c_{\mathbf{r},k,\downarrow}, c^\dagger_{\mathbf{r},-k,\uparrow}, c^\dagger_{\mathbf{r},-k,\downarrow})^T. \tag{43}
$$