

## Chapter 2

# BdG Equations in Tight-Binding Model

**Abstract** In this chapter, I give an alternative derivation of the Bogoliubov-de Gennes equations for superconductors. It is based on a tight-binding model. A general symmetry of the equations is discussed. A few physically measurable quantities are derived in terms of the BdG eigenfunctions. The solutions to the BdG equations in the uniform case are provided. Finally, I also make its connection to the lattice Abrikosov-Gorkov equations.

### 2.1 Derivation of BdG Equations in a Tight-Bind Model

In the previous chapter, we have derived the BdG equations in the continuum model. The continuum model is reasonable to describe weak-coupling superconductors, especially when they have a wide-band metallic normal state. For the superconductors like high-temperature cuprates, the electronic band is quite narrow. Therefore, as we are encountered in solid state physics [1], the tight-binding model, either constructed from atomic orbitals or from Wannier orbitals, is appropriate to be used for studying narrow band behaviors arising from electronic correlation effects.

We generalize the second-quantized Hamiltonian given by Eq. (1.38) to include the spin-orbit coupling and spin-flip scattering interactions, in addition to the regular potential scattering. The single-particle part of the Hamiltonian is of the form:

$$H_0 = \int \int d\mathbf{r} d\mathbf{r}' \psi_{\alpha}^{\dagger}(\mathbf{r}) h_{\alpha\beta}(\mathbf{r}, \mathbf{r}') \psi_{\beta}(\mathbf{r}') \quad (2.1)$$

where  $h_{\alpha\beta}(\mathbf{r}, \mathbf{r}')$  is general enough to include the non-local and spin-flip effects. The field operators are now expressed in the localized-state basis as

$$\psi_{\alpha}(\mathbf{r}) = \sum_i w(\mathbf{r} - \mathbf{R}_i) c_{i\alpha}, \quad (2.2a)$$

$$\psi_{\alpha}^{\dagger}(\mathbf{r}) = \sum_i w^*(\mathbf{r} - \mathbf{R}_i) c_{i\alpha}^{\dagger}, \quad (2.2b)$$

where  $c_{i\alpha}^\dagger$  ( $c_{i\alpha}$ ) creates (annihilates) an electron of spin  $\alpha$  at site  $i$ , and  $w(\mathbf{r} - \mathbf{R}_i)$  is a localized orbital around the atomic site  $\mathbf{R}_i$ . The atomic orbitals or maximally localized Wannier orbitals are most amenable to have a physical interpretation. Substitution of these expressions into Eq. (2.1) gives

$$\begin{aligned} H_0 &= \sum_{ij, \sigma \sigma'} c_{i\sigma}^\dagger h_{i\sigma, j\sigma'} c_{j\sigma} \\ &= - \sum_{i \neq j, \sigma \sigma'} t_{i\sigma, j\sigma'} c_{i\sigma}^\dagger c_{j\sigma'} + \sum_{i\sigma} \epsilon_i c_{i\sigma}^\dagger c_{i\sigma} + \sum_{i, \sigma \sigma'} \Omega_{i, \sigma \sigma'} c_{i\sigma}^\dagger c_{i\sigma'} . \end{aligned} \quad (2.3)$$

Here the summation over the site indices  $ij$  in the kinetic energy (and also the nearest-neighbor interaction in Eq. 2.4 below) excludes those term with  $i = j$ . In the kinetic energy, the spin-orbit term has also been included by identifying the spin flip when an electron hops from one site to its nearest neighbor. The on-site single particle energy is introduced to consider the disorder or such inhomogeneity problems as those with a (non-magnetic) single impurity; while the third term accounts for the magnetic impurity effects (with the internal dynamics of the magnetic impurity neglected here).

We then follow the same ansatz for the extended Hubbard model [2], and write down an effective model Hamiltonian for superconductivity:

$$\begin{aligned} \mathcal{H} &= H_0 - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i \left( n_{i\uparrow} - \frac{1}{2} \right) \left( n_{i\downarrow} - \frac{1}{2} \right) - \frac{V}{2} \sum_{i \neq j} n_i n_j \\ &= \sum_{ij, \sigma \sigma'} c_{i\sigma}^\dagger \left[ h_{i\sigma, j\sigma'} - \left( \mu + \frac{U}{2} \right) \delta_{ij} \delta_{\sigma \sigma'} \right] c_{j\sigma'} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{V}{2} \sum_{i \neq j} n_i n_j . \end{aligned} \quad (2.4)$$

Here  $n_i = \sum_\sigma n_{i\sigma}$  with  $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$  is the particle number operator on site  $i$ . The on-site and nearest-neighbor electron-electron interaction strengths are, respectively,  $U$  and  $V$ . Positive values of  $U$  and negative values of  $V$  represent the repulsive interaction while negative values of  $U$  and positive values of  $V$  represent the attractive interaction since we have assigned a minus sign before the nearest-neighbor interaction term. Note that the single particle energy is measured with respect to the chemical potential  $\mu$ .

The derivation of the BdG equations for the on-site and nearest-neighbor pairing interaction is similar to that for the continuum model in Chap. 1. To be distinct, the above extended Hubbard model enables a description of possible competing orders. We show one example here by considering on-site repulsion ( $U > 0$ ), which drives magnetic instability, and nearest-neighbor attraction ( $V > 0$ ) for the  $d$ -wave pairing superconductivity. Therefore, we retain the standard Hartree-Fock term for the onsite repulsion and the anomalous Hartree-Fock terms for nearest-neighbor attraction. The inclusion of an onsite repulsion in the mean-field approximation

helps stabilize the  $d$ -wave pairing state, which comes from the nearest-neighbor pairing interaction. The effective mean-field Hamiltonian with a singlet pairing symmetry is now given by:

$$\mathcal{H}_{eff} = \sum_{ij, \sigma \sigma'} c_{i\sigma}^\dagger \tilde{h}_{i\sigma, j\sigma'} c_{j\sigma'} + \sum_{ij} [\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow}] + E_{const} . \quad (2.5)$$

Here the effective single-particle Hamiltonian is given by

$$\tilde{h}_{i\sigma, j\sigma'} = h_{i\sigma, j\sigma'} - \left( \mu + \frac{U}{2} - U \langle n_{i\bar{\sigma}} \rangle \right) \delta_{ij} \delta_{\sigma\sigma'} , \quad (2.6)$$

the singlet-pairing potential

$$\Delta_{ij} = \frac{V}{2} \left( \langle c_{i\uparrow} c_{j\downarrow} \rangle - \langle c_{i\downarrow} c_{j\uparrow} \rangle \right) , \quad (2.7)$$

$$\Delta_{ij}^* = \frac{V}{2} \left( \langle c_{j\downarrow}^\dagger c_{i\uparrow}^\dagger \rangle - \langle c_{j\uparrow}^\dagger c_{i\downarrow}^\dagger \rangle \right) , \quad (2.8)$$

and the constant energy term is given by

$$E_{const} = -U \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle + \sum_{ij} \frac{|\Delta_{ij}|^2}{V} . \quad (2.9)$$

It is evident that the singlet pairing potential satisfies the symmetry properties:  $\Delta_{ji} = \Delta_{ij}$ . Also we note again that the single particle energy is measured with respect to the chemical potential  $\mu$ .

We then obtain the following commutation relations:

$$[c_{i\uparrow}, \mathcal{H}_{eff}]_- = \sum_{j\sigma'} \tilde{h}_{i\uparrow, j\sigma'} c_{j\sigma'} + \sum_j \Delta_{ij} c_{j\downarrow}^\dagger , \quad (2.10a)$$

$$[c_{i\uparrow}^\dagger, \mathcal{H}_{eff}]_- = - \sum_{j\sigma'} \tilde{h}_{j\sigma', i\uparrow} c_{j\sigma'}^\dagger - \sum_j \Delta_{ij}^* c_{j\downarrow} , \quad (2.10b)$$

$$[c_{i\downarrow}, \mathcal{H}_{eff}]_- = \sum_{j\sigma'} \tilde{h}_{i\downarrow, j\sigma'} c_{j\sigma'} - \sum_j \Delta_{ji} c_{j\uparrow}^\dagger , \quad (2.10c)$$

$$[c_{i\downarrow}^\dagger, \mathcal{H}_{eff}]_- = - \sum_{j\sigma'} \tilde{h}_{j\sigma', i\downarrow} c_{j\sigma'}^\dagger + \sum_j \Delta_{ji}^* c_{j\uparrow} . \quad (2.10d)$$

Equations (2.10)(a)–(d) show that the electron field operator can be expressed as a linear combination of electron- and hole-like quasiparticle excitations, which

enables us to perform a Bogoliubov canonical transformation:

$$c_{i\sigma} = \sum_n' (u_{i\sigma}^n \gamma_n - \sigma v_{i\sigma}^{n*} \gamma_n^\dagger), \quad c_{i\sigma}^\dagger = \sum_n' (u_{i\sigma}^{n*} \gamma_n^\dagger - \sigma v_{i\sigma}^n \gamma_n), \quad (2.11)$$

where  $\sigma = \pm 1$  denotes the up and down spin orientations. The operators  $\gamma_n^\dagger$  ( $\gamma_n$ ) create (annihilate) a Bogoliubov quasiparticle at state  $n$ . The prime sign above the summation in the transformation means only those states with positive energy are counted. The quasiparticle operators satisfy the anti-commutation relations:

$$\{\gamma_n, \gamma_m^\dagger\} = \delta_{nm}, \quad (2.12)$$

$$\{\gamma_n, \gamma_m\} = \{\gamma_n^\dagger, \gamma_m^\dagger\} = 0. \quad (2.13)$$

These relations also guarantee the anti-commutation relations among the original electronic field operators.

With the above canonical transformation, the Hamiltonian is diagonalized in the following form:

$$H_{\text{eff}} = \sum_n E_n \gamma_n^\dagger \gamma_n + E'_{\text{const}}, \quad (2.14)$$

where the index  $n$  also includes the pseudo-spin state index. Upon substitution of Eq. (2.11) into Eq. (2.10), and with the aid of the following commutation relations,

$$[\gamma_n^\dagger, H_{\text{eff}}]_- = -E_n \gamma_n^\dagger, \quad (2.15)$$

$$[\gamma_n, H_{\text{eff}}]_- = E_n \gamma_n, \quad (2.16)$$

we compare the coefficients of the terms with  $\gamma_n$  and  $\gamma_n^\dagger$  and arrive at

$$E_n u_{i\uparrow}^n = \sum_{j\sigma'} \tilde{h}_{i\uparrow, j\sigma'} u_{j\sigma'}^n + \sum_j \Delta_{ij} v_{j\downarrow}^n, \quad (2.17)$$

$$E_n u_{i\downarrow}^n = \sum_{j\sigma'} \tilde{h}_{i\downarrow, j\sigma'} u_{j\sigma'}^n + \sum_j \Delta_{ji} v_{j\uparrow}^n, \quad (2.18)$$

$$E_n v_{i\uparrow}^n = -\sum_{j\sigma'} \sigma' \tilde{h}_{i\uparrow, j\sigma'}^* v_{j\sigma'}^n + \sum_j \Delta_{ij}^* u_{j\downarrow}^n, \quad (2.19)$$

$$E_n v_{i\downarrow}^n = \sum_{j\sigma'} \sigma' \tilde{h}_{i\downarrow, j\sigma'}^* v_{j\sigma'}^n + \sum_j \Delta_{ji}^* u_{j\uparrow}^n. \quad (2.20)$$

This set of BdG equations can be cast into a matrix form:

$$\sum_j \hat{M}_{ij} \hat{\phi}_j = E_n \hat{\phi}_i, \quad (2.21)$$

where

$$\hat{M}_{ij} = \begin{bmatrix} \tilde{h}_{i\uparrow j\uparrow} & \tilde{h}_{i\uparrow j\downarrow} & 0 & \Delta_{ij} \\ \tilde{h}_{i\downarrow j\uparrow} & \tilde{h}_{i\downarrow j\downarrow} & \Delta_{ji} & 0 \\ 0 & \Delta_{ij}^* & -\tilde{h}_{i\uparrow j\uparrow}^* & \tilde{h}_{i\uparrow j\downarrow}^* \\ \Delta_{ji}^* & 0 & \tilde{h}_{i\downarrow j\uparrow}^* & -\tilde{h}_{i\downarrow j\downarrow}^* \end{bmatrix}, \quad (2.22)$$

and

$$\hat{\phi}_i = \begin{pmatrix} u_{i\uparrow} \\ u_{i\downarrow} \\ v_{i\uparrow} \\ v_{i\downarrow} \end{pmatrix}. \quad (2.23)$$

This set of BdG equations is subjected to the self-consistency conditions:

$$n_{i\uparrow} = \sum_n^I [|u_{i\uparrow}^n|^2 f(E_n) + |v_{i\uparrow}^n|^2 f(-E_n)], \quad (2.24)$$

$$n_{i\downarrow} = \sum_n^I [|u_{i\downarrow}^n|^2 f(E_n) + |v_{i\downarrow}^n|^2 f(-E_n)], \quad (2.25)$$

and

$$\Delta_{ij} = \frac{V}{4} \sum_n^I [(u_{i\uparrow}^n v_{j\downarrow}^{n*} + u_{j\downarrow}^n v_{i\uparrow}^{n*}) + (u_{i\downarrow}^n v_{j\uparrow}^{n*} + u_{j\uparrow}^n v_{i\downarrow}^{n*})] \tanh\left(\frac{E_n}{2k_B T}\right), \quad (2.26)$$

where  $f(E)$  is the Fermi-Dirac distribution function defined in Eq. (1.72).

From Eqs. (2.17)–(2.20), it is not difficult to prove the following theorem:

If  $(u_{i\uparrow}^n, v_{i\downarrow}^n, u_{i\downarrow}^n, v_{i\uparrow}^n)$  is the solution to the BdG equations with eigenvalue  $E_n$ , then  $(-v_{i\uparrow}^{n*}, u_{i\downarrow}^{n*}, v_{i\downarrow}^{n*}, -u_{i\uparrow}^{n*})$  is the solution to the same equations with eigenvalue  $-E_n$ . Using this symmetry property, we can also rewrite Eqs. (2.24)–(2.26) as

$$n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n), \quad (2.27)$$

$$n_{i\downarrow} = \sum_n |v_{i\downarrow}^n|^2 f(-E_n), \quad (2.28)$$

and

$$\Delta_{ij} = \frac{V}{4} \sum_n [u_{i\uparrow}^n v_{j\downarrow}^{n*} + u_{j\uparrow}^n v_{i\downarrow}^{n*}] \tanh\left(\frac{E_n}{2k_B T}\right). \quad (2.29)$$

In the absence of spin-orbit coupling and other spin-flip scattering terms, that is  $\tilde{h}_{i\uparrow,j\downarrow} = \tilde{h}_{i\downarrow,j\uparrow} = 0$ , the BdG equations become block-diagonalized into two sets of equations:

$$\begin{cases} E_{\tilde{n}1} u_{i\uparrow}^{\tilde{n}1} = \sum_j \tilde{h}_{i\uparrow,j\uparrow} u_{j\uparrow}^{\tilde{n}1} + \sum_j \Delta_{ij} v_{j\downarrow}^{\tilde{n}1}, \\ E_{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1} = -\sum_j \tilde{h}_{i\downarrow,j\downarrow}^* v_{j\downarrow}^{\tilde{n}1} + \sum_j \Delta_{ji}^* u_{j\uparrow}^{\tilde{n}1}, \end{cases} \quad (2.30)$$

and

$$\begin{cases} E_{\tilde{n}2} u_{i\downarrow}^{\tilde{n}2} = \sum_j \tilde{h}_{i\downarrow,j\downarrow} u_{j\downarrow}^{\tilde{n}2} + \sum_j \Delta_{ji} v_{j\uparrow}^{\tilde{n}2}, \\ E_{\tilde{n}2} v_{i\uparrow}^{\tilde{n}2} = -\sum_j \tilde{h}_{i\uparrow,j\uparrow}^* v_{j\uparrow}^{\tilde{n}2} + \sum_j \Delta_{ij}^* u_{j\downarrow}^{\tilde{n}2}. \end{cases} \quad (2.31)$$

This block-diagonalization structure leads to a distinct nature of the canonical transformation:

$$c_{i\uparrow} = \sum_{\tilde{n}} (u_{i\uparrow}^{\tilde{n}1} \gamma_{\tilde{n}1} - v_{i\uparrow}^{\tilde{n}2*} \gamma_{\tilde{n}2}^\dagger), \quad c_{i\uparrow}^\dagger = \sum_{\tilde{n}} (u_{i\uparrow}^{\tilde{n}1*} \gamma_{\tilde{n}1}^\dagger - v_{i\uparrow}^{\tilde{n}2} \gamma_{\tilde{n}2}), \quad (2.32)$$

$$c_{i\downarrow} = \sum_{\tilde{n}} (u_{i\downarrow}^{\tilde{n}2} \gamma_{\tilde{n}2} + v_{i\downarrow}^{\tilde{n}1*} \gamma_{\tilde{n}1}^\dagger), \quad c_{i\downarrow}^\dagger = \sum_{\tilde{n}} (u_{i\downarrow}^{\tilde{n}2*} \gamma_{\tilde{n}2}^\dagger + v_{i\downarrow}^{\tilde{n}1} \gamma_{\tilde{n}1}). \quad (2.33)$$

The block diagonalization and the symmetry property suggest that we merely need to solve Eq. (2.30) subject to the self-consistency condition:

$$n_{i\uparrow} = \sum_{\tilde{n}} |u_{i\uparrow}^{\tilde{n}1}|^2 f(E_{\tilde{n}1}), \quad (2.34)$$

$$n_{i\downarrow} = \sum_{\tilde{n}} |v_{i\downarrow}^{\tilde{n}1}|^2 f(-E_{\tilde{n}1}), \quad (2.35)$$

and

$$\Delta_{ij} = \frac{V}{4} \sum_{\tilde{n}} [u_{i\uparrow}^{\tilde{n}1} v_{j\downarrow}^{\tilde{n}1*} + u_{j\uparrow}^{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1*}] \tanh\left(\frac{E_{\tilde{n}1}}{2k_B T}\right). \quad (2.36)$$

Therefore, by reducing the diagonalization of a  $4N$  by  $4N$  matrix down to that of a  $2N$  by  $2N$  matrix, the computational efficiency is improved significantly. Here  $N$  would be  $N_x N_y$  for a two-dimensional lattice while  $N_x N_y N_z$  for a three-dimensional lattice with  $N_x$ ,  $N_y$ , and  $N_z$  being the linear dimension of the system. When it is obvious that no spin-flip effect occurs, the reduced set of BdG equations, Eq. (2.30), will be used with the hat symbol on the energy eigenvalue index and the set index dropped. It will be encountered frequently in the later discussions.

It is straightforward for us to obtain the BdG equations for an  $s$ -wave superconductor in the lattice model. There we first replace  $U$  by  $-U$  ( $U > 0$ ) so that the Hamiltonian becomes

$$\mathcal{H} = \sum_{ij,\sigma\sigma'} c_{i\sigma}^\dagger \left[ h_{i\sigma,j\sigma'} - \mu \delta_{ij} \delta_{\sigma\sigma'} \right] c_{j\sigma'} - U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (2.37)$$

which leads to the BdG equations:

$$E_n u_{i\uparrow}^n = \sum_{j\sigma'} \tilde{h}_{i\uparrow,j\sigma'} u_{j\sigma'}^n + \Delta_{ii} v_{i\downarrow}^n, \quad (2.38)$$

$$E_n u_{i\downarrow}^n = \sum_{j\sigma'} \tilde{h}_{i\downarrow,j\sigma'} u_{j\sigma'}^n + \Delta_{ii} v_{i\uparrow}^n, \quad (2.39)$$

$$E_n v_{i\uparrow}^n = - \sum_{j\sigma'} \sigma' \tilde{h}_{i\uparrow,j\sigma'}^* v_{j\sigma'}^n + \Delta_{ii}^* u_{j\downarrow}^n, \quad (2.40)$$

$$E_n v_{i\downarrow}^n = \sum_{j\sigma'} \sigma' \tilde{h}_{i\downarrow,j\sigma'}^* v_{j\sigma'}^n + \Delta_{ii}^* u_{i\uparrow}^n. \quad (2.41)$$

Here

$$\tilde{h}_{i\sigma,j\sigma'} = h_{i\sigma,j\sigma'} - \mu \delta_{ij} \delta_{\sigma\sigma'}, \quad (2.42)$$

and the self-consistency condition

$$\Delta_{ii} = \frac{U}{2} \sum_n' [u_{i\uparrow}^n v_{i\downarrow}^{n*} + u_{i\downarrow}^n v_{i\uparrow}^{n*}] \tanh\left(\frac{E_n}{2k_B T}\right). \quad (2.43)$$

In the absence of spin-orbit coupling and spin-flip scattering, the BdG equations become

$$\begin{cases} E_{\tilde{n}1} u_{i\uparrow}^{\tilde{n}1} = \sum_j \tilde{h}_{i\uparrow,j\uparrow} u_{j\uparrow}^{\tilde{n}1} + \Delta_{ii} v_{i\downarrow}^{\tilde{n}1}, \\ E_{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1} = - \sum_j \tilde{h}_{i\downarrow,j\downarrow}^* v_{j\downarrow}^{\tilde{n}1} + \Delta_{ii}^* u_{i\uparrow}^{\tilde{n}1}, \end{cases} \quad (2.44)$$

and

$$\begin{cases} E_{\tilde{n}2} u_{i\downarrow}^{\tilde{n}2} = \sum_j \tilde{h}_{i\downarrow,j\downarrow} u_{j\downarrow}^{\tilde{n}2} + \Delta_{ii} v_{i\uparrow}^{\tilde{n}2}, \\ E_{\tilde{n}2} v_{i\uparrow}^{\tilde{n}2} = - \sum_j \tilde{h}_{i\uparrow,j\uparrow}^* v_{j\uparrow}^{\tilde{n}2} + \Delta_{ii}^* u_{i\downarrow}^{\tilde{n}2}. \end{cases} \quad (2.45)$$

with

$$\Delta_{ii} = \frac{U}{2} \sum_{\tilde{n}} u_{i\uparrow}^{\tilde{n}1} v_{i\downarrow}^{\tilde{n}1*} \tanh\left(\frac{E_{\tilde{n}1}}{2k_B T}\right). \quad (2.46)$$

Unless explicitly specified, we will focus on Eq. (2.44) with the tilde on the eigen-energy index and set index dropped.

The tight-binding model, from which the BdG equations are derived, has the origin from such strongly correlated models as the  $t$ - $J$  model [3] for high-temperature cuprates. The derived BdG equations in the tight-binding model have been used not only for unconventional superconductors with narrow electron band [4–9] but also for  $s$ -wave superconductors [10]. The calculated quantities range from the local density states to the superfluid density, which will be discussed in more details in later chapters.

### 2.1.1 Local Density of States and Bond Current in the Lattice Model

From Eqs. (2.24), (2.25), we extract the expression for the local density of states:

$$\rho_{i\sigma}(E) = \sum_n' [|u_{i\sigma}^n|^2 \delta(E_n - E) + |v_{i\sigma}|^2 \delta(E_n + E)] . \quad (2.47)$$

and the corresponding thermalized density of states

$$\rho_{i\sigma}(E) = - \sum_n' [|u_{i\sigma}^n|^2 f'(E_n - E) + |v_{i\sigma}|^2 f'(E_n + E)] . \quad (2.48)$$

The bond current can be derived in the following way. The Heisenberg equation of motion for  $\langle n_i \rangle = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle$  is:

$$\begin{aligned} i\hbar \frac{\partial \langle n_i \rangle}{\partial t} &= \langle [n_i, H]_- \rangle \\ &= \langle \{ - \sum_{j \neq i, \sigma, \sigma'} [-t(j\sigma', i\sigma) c_{j\sigma'}^\dagger c_{i\sigma} + t(i\sigma, j\sigma') c_{i\sigma}^\dagger c_{j\sigma'}] \} \rangle , \end{aligned} \quad (2.49)$$

where  $H$  is the system Hamiltonian given by Eq. (2.4). The electrical current operator from site  $j$  to site  $i$  is then found to be:

$$\hat{J}_{ij} = \frac{e}{i\hbar} \sum_{\sigma, \sigma'} [t(i\sigma, j\sigma') c_{i\sigma}^\dagger c_{j\sigma'} - t(j\sigma', i\sigma) c_{j\sigma'}^\dagger c_{i\sigma}] , \quad (2.50)$$

and the average bond current is given by:



$$J_{ij} = \frac{e}{i\hbar} \sum_{\sigma, \sigma'} \sum_n^I \{ t(i\sigma, j\sigma') [u_{i\sigma}^{n*} u_{j\sigma'}^n f(E_n) + \sigma \sigma' v_{i\sigma}^n v_{j\sigma'}^{n*} (1 - f(E_n))] - \text{c.c.} \} . \quad (2.51)$$

Using the symmetry property of the BdG equations, we can also write the physical quantities in the following form:

$$n_{i\sigma} = \sum_n |u_{i\sigma}^n|^2 f(E_n) = \sum_n |v_{i\sigma}^n|^2 [1 - f(E_n)] , \quad (2.52)$$

$$\begin{aligned} J_{ij} &= \frac{e}{i\hbar} \sum_{\sigma, \sigma'} \sum_n \{ t(i\sigma, j\sigma') u_{i\sigma}^{n*} u_{j\sigma'}^n f(E_n) - \text{c.c.} \} \\ &= \frac{e}{i\hbar} \sum_{\sigma, \sigma'} \sum_n \{ t(i\sigma, j\sigma') \sigma \sigma' v_{i\sigma}^n v_{j\sigma'}^{n*} (1 - f(E_n)) - \text{c.c.} \} , \end{aligned} \quad (2.53)$$

and

$$\rho_{i\sigma}(E) = - \sum_n |u_{i\sigma}^n|^2 f'(E_n - E) = - \sum_n |v_{i\sigma}^n|^2 f'(E_n + E) . \quad (2.54)$$

These new formulations are especially useful when we study the ferromagnetic impurity or Zeeman effect because the wavefunction of quasiparticles can be solved in a  $2 \times 2$  spin space.

### 2.1.2 Optical Conductivity and Superfluid Density in the Lattice Model

The BdG solutions can not only describe the local density of states, which is a direct measure of single particle properties, but also the eigenfunctions can be used to study the two-particle correlations. In particular, the optical superconductivity reveals the information about the coherent peak [11], while the superfluid stiffness [12] and its temperature dependence set a criterion for superconductivity. Both quantities are directly measurable in experiments. Theoretically, the formulae for these quantities, as derived from the BdG method, are also valid for inhomogeneous superconductors.

The formula of the superfluid density in a lattice model was first derived by Scalapino et al. [12, 13] in a Hubbard model. It was then used for calculations in other models. In the following, we give the derivation for the model with the Hamiltonian defined by Eq. (2.4) in the absence of spin-orbit coupling and other spin-flip scattering, that is,

$$\mathcal{H} = \sum_{ij, \sigma} c_{i\sigma}^\dagger \left[ -t_{ij} - \left( \mu + \frac{U}{2} - U_i^{\text{imp}} \right) \delta_{ij} \right] c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{V}{2} \sum_{i \neq j} n_i n_j .$$

$$(2.55)$$

Here the impurity potential is represented by  $U_i^{\text{imp}}$ .

In the presence of an electric field pointing to the  $x$ -direction,

$$E_x(\mathbf{r}_i, t) = \mathcal{E}_x e^{i(\mathbf{q}\cdot\mathbf{r}_i - \omega t)} . \quad (2.56)$$

The current density along the  $x$ -direction is defined as

$$J_x(\mathbf{r}_i, t) = \sigma_{xx}(\mathbf{r}_i, \omega) E_x(\mathbf{r}_i, t) , \quad (2.57)$$

where  $\sigma_{xx}(\mathbf{r}_i, \omega)$  is the local conductivity. In the Coulomb gauge, which dictates  $\nabla \cdot \mathbf{A} = 0$  and the scalar potential  $\phi = 0$ , the electric field can be expressed in terms of a vector potential

$$A_x(\mathbf{r}_i, t) = -\frac{i}{\omega} E_x(\mathbf{r}_i, t) . \quad (2.58)$$

Therefore, the total Hamiltonian becomes

$$H_t = - \sum_{ij, \sigma} \tilde{t}_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\sigma} (U_i^{\text{imp}} - \frac{U}{2} - \mu) c_{i\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \frac{V}{2} \sum_{ij} n_i n_j . \quad (2.59)$$

where

$$\tilde{t}_{ij} = t_{ij} e^{i\phi_{ij}(t)} , \quad (2.60)$$

with the gauge phase  $\phi_{ij}(t) = eA_{ij} = eA_x(\mathbf{r}_i, t)(x_i - x_j)$ . Hereafter the charge  $e$  for electrons includes the sign. In the linear response limit, we expand this hopping term up to the second order of  $A_x(\mathbf{r}_i, t)$ :

$$\tilde{t}_{ij} \approx t[1 + i\phi_{ij} + \frac{1}{2!}(i\phi_{ij})^2] . \quad (2.61)$$

The total Hamiltonian can then be rewritten as:

$$H_t = H - i \sum_{ij, \sigma} \phi_{ij}(t) t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{ij, \sigma} \phi_{ij}^2(t) t_{ij} c_{i\sigma}^\dagger c_{j\sigma} . \quad (2.62)$$

If we limit the hopping integral only between the nearest neighbors, we have

$$\begin{aligned} H_t = H - iea \sum_{i, \sigma} [-A_x(\mathbf{r}_i, t) t_{i, i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x}, \sigma} + A_x(\mathbf{r}_{i+\hat{x}}, t) t_{i+\hat{x}, i} c_{i+\hat{x}, \sigma}^\dagger c_{i\sigma}] \\ + \frac{e^2 a^2}{2} \sum_{i, \sigma} [A_x^2(\mathbf{r}_i, t) t_{i, i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x}, \sigma} + A_x^2(\mathbf{r}_{i+\hat{x}}, t) t_{i+\hat{x}, i} c_{i+\hat{x}, \sigma}^\dagger c_{i\sigma}] \end{aligned}$$

$$\begin{aligned}
& \approx H - iea \sum_{i,\sigma} A_x(\mathbf{r}_i, t) [-t_{i,i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x},\sigma} + t_{i+\hat{x},i} c_{i+\hat{x},\sigma}^\dagger c_{i\sigma}] \\
& \quad + \frac{e^2 a^2}{2} \sum_{i,\sigma} A_x^2(\mathbf{r}_i, t) [t_{i,i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x},\sigma} + t_{i+\hat{x},i} c_{i+\hat{x},\sigma}^\dagger c_{i\sigma}] \\
& \approx H - ea \sum_i A_x(\mathbf{r}_i, t) J_x^P(\mathbf{r}_i) - \frac{e^2 a^2}{2} \sum_i A_x^2(\mathbf{r}_i, t) K_x(\mathbf{r}_i) \\
& = H + H'(t) ,
\end{aligned} \tag{2.63}$$

where the particle current and the local kinetic energy associated with the  $x$ -oriented links are defined as

$$\begin{aligned}
J_x^P(\mathbf{r}_i) &= i \sum_{\sigma} [t_{i+\hat{x},i} c_{i+\hat{x},\sigma}^\dagger c_{i\sigma} - t_{i,i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x},\sigma}] \\
&= it \sum_{\sigma} [c_{i+\hat{x},\sigma}^\dagger c_{i\sigma} - c_{i\sigma}^\dagger c_{i+\hat{x},\sigma}] ,
\end{aligned} \tag{2.64}$$

and

$$\begin{aligned}
K_x(\mathbf{r}_i) &= - \sum_{\sigma} [t_{i,i+\hat{x}} c_{i\sigma}^\dagger c_{i+\hat{x},\sigma} + t_{i+\hat{x},i} c_{i+\hat{x},\sigma}^\dagger c_{i\sigma}] \\
&= -t \sum_{\sigma} [c_{i\sigma}^\dagger c_{i+\hat{x},\sigma} + c_{i+\hat{x},\sigma}^\dagger c_{i\sigma}] .
\end{aligned} \tag{2.65}$$

The  $x$ -oriented current density operator is then found to be

$$J_x^Q(\mathbf{r}_i) = - \frac{\delta H'(t)}{\delta A_x(\mathbf{r}_i, t)} = e J_x^P(\mathbf{r}_i) + e^2 K_x(\mathbf{r}_i) A_x(\mathbf{r}_i, t) . \tag{2.66}$$

Here we have set the lattice constant  $a = 1$ .

An alternative derivation of the current density operator is to start with the electric polarization operator:

$$\mathbf{P} = e \sum_i \mathbf{r}_i n_i \tag{2.67}$$

with its  $x$ -component

$$P_x = e \sum_i x_i n_i . \tag{2.68}$$

The time-derivative is

$$\begin{aligned}
 J_x^Q(\mathbf{r}_i) &= i[H_t, P_x] \\
 &= ie \sum_{ij,\sigma} x_i [\tilde{t}_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \tilde{t}_{ji} c_{j\sigma}^\dagger c_{i\sigma}] \\
 &= ie \sum_{ij,\sigma} (x_i - x_j) \tilde{t}_{ij} c_{i\sigma}^\dagger c_{j\sigma} \\
 &= ie \sum_{ij,\sigma} (x_i - x_j) t_{ij} (1 + i\phi_{ij}) c_{i\sigma}^\dagger c_{j\sigma} \\
 &= eJ_x^P(\mathbf{r}_i) + e^2 K_x(\mathbf{r}_i) A_x(\mathbf{r}_i, t) .
 \end{aligned} \tag{2.69}$$

Now let us calculate the expectation value of the current density operator. In the linear response theory, the statistical operator in the interaction picture is given by:

$$\hat{\rho}_I(t) = \hat{\rho}_I(-\infty) - \frac{i}{\hbar} \int_{-\infty}^t [H'_I(t'), \hat{\rho}_I(-\infty)]_- dt' . \tag{2.70}$$

The expectation of a physical variable is found to be:

$$\langle \hat{O} \rangle = \text{Tr}[\hat{\rho}_I(-\infty) \hat{O}_I] - \frac{i}{\hbar} \int_{-\infty}^t \text{Tr}\{\hat{\rho}_I(-\infty) [\hat{O}_I(t), H'_I(t')]_-\} dt' \tag{2.71}$$

$$= \langle \hat{O}_I \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^t \langle [\hat{O}_I(t), H'_I(t')]_- \rangle_0 dt' , \tag{2.72}$$

where

$$\hat{O}_I = e^{iHt} \hat{O} e^{-iHt} , \tag{2.73}$$

and

$$H'_I(t) = e^{iHt} H'(t) e^{-iHt} . \tag{2.74}$$

with the term proportional to  $A^2(t)$  in  $H'(t)$  neglected. The particle current density is then given by

$$\langle J_x^P(\mathbf{r}_i) \rangle = -i \int_{-\infty}^t \langle [J_x^P(\mathbf{r}_i, t), H'_I(t)] \rangle , \tag{2.75}$$

where the particle operator and the perturbation term in the Heisenberg picture with respect to the unperturbed Hamiltonian  $H$  are given by, respectively,

$$J_x^P(\mathbf{r}_i, t) = e^{iHt} J_x^P(\mathbf{r}_i) e^{-iHt} . \tag{2.76}$$

We notice that the first term in  $H'(t)$  can be rewritten as

$$-e \sum_{i,\sigma} A_x(\mathbf{r}_i, t) J_x^P(\mathbf{r}_i) = \frac{ie}{\omega} J_x^P(-\mathbf{q}) \mathcal{E}_x e^{-i\omega t}, \quad (2.77)$$

where the Fourier transform of the particle density operator is given by

$$J_x^P(\mathbf{q}) = \sum_i e^{-i\mathbf{q}\cdot\mathbf{r}_i} J_x^P(\mathbf{r}_i). \quad (2.78)$$

We then obtain

$$\langle J_x^P(\mathbf{r}_i) \rangle = \frac{e}{\omega} E_x(\mathbf{r}_i, t) e^{-i\mathbf{q}\cdot\mathbf{r}_i} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle. \quad (2.79)$$

Finally, the current density is found to be

$$\begin{aligned} \langle J_x^Q(\mathbf{r}_i) \rangle &= \frac{e^2}{\omega} E_x(\mathbf{r}_i, t) e^{-i\mathbf{q}\cdot\mathbf{r}_i} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle \\ &\quad - \frac{ie^2}{\omega} \langle K_x(\mathbf{r}_i) \rangle E_x(\mathbf{r}_i, t). \end{aligned} \quad (2.80)$$

The local conductivity is then given by

$$\begin{aligned} \sigma_{xx}(\mathbf{r}_i, \omega) &= \frac{\langle J_x^Q(\mathbf{r}_i) \rangle}{E_x(\mathbf{r}_i, t)} \\ &= \frac{e^2}{\omega} e^{-i\mathbf{q}\cdot\mathbf{r}_i} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle \\ &\quad - \frac{ie^2}{\omega} \langle K_x(\mathbf{r}_i) \rangle. \end{aligned} \quad (2.81)$$

To eliminate the atomic fluctuations, we take an average over the spatial variable  $\mathbf{r}_i$  and obtain the conductivity

$$\sigma_{xx}(\mathbf{q}, \omega) = \frac{e^2}{N\omega} \int_{-\infty}^t dt' e^{i\omega(t-t')} \langle [J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, t')] \rangle - \frac{ie^2}{\omega} \langle K_x \rangle.$$

where

$$\langle K_x \rangle = \frac{1}{N} \sum_i \langle K_x(\mathbf{r}_i) \rangle. \quad (2.82)$$

Since the correlation function in Eq. (2.82) is only a function of the time difference  $t - t'$ , we can express the conductivity as

$$\begin{aligned}\sigma_{xx}(\mathbf{q}, \omega) &= \frac{e^2}{N\omega} \int_0^\infty dt e^{i\omega t} \langle [J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, 0)] \rangle - \frac{ie^2}{\omega} \langle K_x \rangle \\ &= \frac{e^2}{i\omega} \left[ \frac{i}{N} \int_{-\infty}^\infty dt \theta(t) e^{i\omega t} \langle [J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, 0)] \rangle + \langle K_x \rangle \right] \\ &= \frac{e^2}{i\omega} [-\Pi_{xx}(\mathbf{q}, \omega) + \langle K_x \rangle],\end{aligned}\quad (2.83)$$

where we define the retarded correlation function of the particle current operator as

$$\Pi_{xx}(\mathbf{q}, t) = -\frac{i}{N} \theta(t) \langle [J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, 0)] \rangle, \quad (2.84)$$

with its Fourier transform

$$\Pi_{xx}(\mathbf{q}, \omega) = \int_{-\infty}^\infty dt e^{i\omega t} \Pi_{xx}(\mathbf{q}, t). \quad (2.85)$$

The frequency-dependent, uniform electrical conductivity is given by taking the limit  $\mathbf{q} \rightarrow 0$ :

$$\sigma_{xx}(\omega) = \frac{e^2}{i\omega} [-\Pi_{xx}(\mathbf{q} = 0, \omega) + \langle K_x \rangle]. \quad (2.86)$$

The dc conductivity is obtained by taking first the limit  $\mathbf{q} \rightarrow 0$  and then the limit  $\omega \rightarrow 0$ .

$$\sigma_{xx} = -\lim_{\omega \rightarrow 0} \frac{e^2}{i\omega} [-\Pi_{xx}(\mathbf{q} = 0, \omega) + \langle K_x \rangle]. \quad (2.87)$$

Be reminded that the order of these limits cannot be reversed.

Similarly the transverse conductivity can also be derived as:

$$\sigma_{xy}(\mathbf{q}, \omega) = \frac{e^2}{i\omega} [-\Pi_{xy}(\mathbf{q}, \omega)]. \quad (2.88)$$

It is convenient to calculate the retarded correlation function in the Matsubara formalism. First define the equivalent current-current correlation function in the Matsubara formalism:

$$\Pi_{xx}(\mathbf{q}, \tau) = -\frac{1}{N} \langle T_\tau [J_x^P(\mathbf{q}, \tau) J_x^P(-\mathbf{q}, 0)] \rangle, \quad (2.89)$$

$$\Pi_{xx}(\mathbf{q}, i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \Pi_{xx}(\mathbf{q}, \tau), \quad (2.90)$$

where  $\omega_n = 2n\pi T$  since the current density operator is regarded as a bosonic operator acting as a composite particle. The Matsubara function is evaluated as best one can. Then the desired retarded function is obtained by performing the analytical continuation  $i\omega_n \rightarrow \omega + i\delta$ :

$$\Pi_{xx}(\mathbf{q}, \omega) = \Pi_{xx}(\mathbf{q}, i\omega_n \rightarrow \omega + i\delta) . \quad (2.91)$$

Technically, we always write the conductivity formula as:

$$\sigma_{xx}(\mathbf{q}, \omega) = \frac{e^2}{i(\omega + i\delta)} [-\Pi_{xx}(\mathbf{q}, \omega) + \langle K_x \rangle] , \quad (2.92)$$

and its uniform counterpart

$$\sigma_{xx}(\omega) = \frac{e^2}{i(\omega + i\delta)} [-\Pi_{xx}(\mathbf{q} = 0, \omega) + \langle K_x \rangle] . \quad (2.93)$$

If the numerator approaches a finite limit as  $\omega \rightarrow 0$ , the real part of  $\sigma_{xx}(\omega)$  will contain a delta function contribution  $D\delta(\omega)$  with the “Drude weight” given by

$$\frac{D}{\pi e^2} \equiv \frac{\rho^*}{4\pi} = -\langle K_x \rangle + \Pi_{xx}(\mathbf{q} = 0, \omega \rightarrow 0) , \quad (2.94)$$

with  $\rho^*$  an effective density of the mobile charge carriers in units of their mass. This implies a zero resistance state.

In a superconductor, the Meissner effect is the current response to a static, i.e.,  $\omega = 0$  and transverse gauge potential  $\mathbf{q} \cdot \mathbf{A}(\mathbf{q}, \omega = 0) = 0$ . In this case, the electric field  $\mathbf{E} = 0$ . When we only apply a transverse electric field along the  $x$ -direction, we should have  $q_x A_x(\mathbf{q}, \omega = 0) = 0$ , which requires  $q_x = 0$ . Following the same procedure as before, we can find the expectation value of the electrical current operator

$$\begin{aligned} \langle J_x^Q(\mathbf{r}_i) \rangle &= ie^2 A_x(\mathbf{r}_i) e^{-i\mathbf{q} \cdot \mathbf{r}_i} \int_{-\infty}^t dt' \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle \\ &\quad + e^2 \langle K_x(\mathbf{r}_i) \rangle A_x(\mathbf{r}_i) . \end{aligned} \quad (2.95)$$

We then have

$$\frac{\langle J_x^Q(\mathbf{r}_i) \rangle}{e^2 A_x(\mathbf{r}_i)} = ie^{-i\mathbf{q} \cdot \mathbf{r}_i} \int_{-\infty}^t dt' \langle [J_x^P(\mathbf{r}_i, t), J_x^P(-\mathbf{q}, t')] \rangle + \langle K_x(\mathbf{r}_i) \rangle . \quad (2.96)$$

By performing an average over the spatial variable  $\mathbf{r}_i$  to eliminate the atomic fluctuations, we define an effective “Drude weight” as

$$\frac{D_s}{\pi e^2} = \frac{\rho_s^*}{4\pi} = -\langle K_x \rangle + \Pi_{xx}(q_x = 0, q_y \rightarrow 0, \omega = 0) . \quad (2.97)$$

The quantity  $D_s$  measures the superfluid density in units of the mass. The crucial difference between  $\rho^*$  and  $\rho_s^*$  is the order in which the momentum and frequency approach zero.

For a superconductor, we perform the BdG transformation:

$$c_{i\sigma} = \sum_{n(E_n \geq 0)} (u_{i\sigma}^n \gamma_n - \sigma v_{i\sigma}^{n*} \gamma_n^\dagger) . \quad (2.98)$$

The kinetic energy can be found readily:

$$\langle K_x \rangle = -\frac{t}{N} \sum_{i,n,\sigma} \{f(E_n)[u_{i+x,\sigma}^{n*} u_{i\sigma}^n + \text{c.c.}] + (1-f(E_n))[v_{i+x,\sigma}^{n*} v_{i\sigma}^n + \text{c.c.}]\} . \quad (2.99)$$

However, the re-expression of the current-current correlation function is much more tedious. In the expansion form, the commutator:

$$[J_x^P(\mathbf{q}, t), J_x^P(-\mathbf{q}, 0)] = (it)^2 \sum_{i\sigma} \sum_{i'\sigma'} e^{-i\mathbf{q} \cdot (\mathbf{r}_i - \mathbf{r}_{i'})} [\hat{A} + \hat{B} + \hat{C} + \hat{D}] , \quad (2.100)$$

where

$$\hat{A} = [c_{i+\hat{x},\sigma}^\dagger(t) c_{i\sigma}(t), c_{i'+\hat{x},\sigma'}^\dagger c_{i'\sigma'}] , \quad (2.101)$$

$$\hat{B} = -[c_{i+\hat{x},\sigma}^\dagger(t) c_{i\sigma}(t), c_{i'\sigma'}^\dagger c_{i'+\hat{x},\sigma'}] , \quad (2.102)$$

$$\hat{C} = -[c_{i\sigma}^\dagger(t) c_{i+\hat{x},\sigma}(t), c_{i'+\hat{x},\sigma'}^\dagger c_{i'\sigma'}] , \quad (2.103)$$

$$\hat{D} = [c_{i\sigma}^\dagger(t) c_{i+\hat{x},\sigma}(t), c_{i'\sigma'}^\dagger c_{i'+\hat{x},\sigma'}] , \quad (2.104)$$

with

$$\begin{aligned} c_{i+\hat{x},\sigma}^\dagger(t) c_{i\sigma}(t) &= \sum_{n_1, n_2} [(u_{i+\hat{x},\sigma}^{n_1*} \gamma_{n_1}^\dagger(t) - \sigma v_{i+\hat{x},\sigma}^{n_1} \gamma_{n_1}(t)) (u_{i\sigma}^{n_2} \gamma_{n_2}(t) - \sigma v_{i\sigma}^{n_2*} \gamma_{n_2}^\dagger(t))] \\ &= \sum_{n_1, n_2} [u_{i+\hat{x},\sigma}^{n_1*} u_{i\sigma}^{n_2} e^{i(E_{n_1} - E_{n_2})t} \gamma_{n_1}^\dagger \gamma_{n_2} - \sigma u_{i+\hat{x},\sigma}^{n_1*} v_{i\sigma}^{n_2*} e^{i(E_{n_1} + E_{n_2})t} \gamma_{n_1}^\dagger \gamma_{n_2}^\dagger \\ &\quad - \sigma v_{i+\hat{x},\sigma}^{n_1} u_{i\sigma}^{n_2} e^{-i(E_{n_1} + E_{n_2})t} \gamma_{n_1} \gamma_{n_2} + v_{i+\hat{x},\sigma}^{n_1} v_{i\sigma}^{n_2*} e^{-i(E_{n_1} - E_{n_2})t} \gamma_{n_1} \gamma_{n_2}^\dagger] , \end{aligned} \quad (2.105)$$



and

$$\begin{aligned}
c_{i\sigma}^\dagger(t)c_{i+\hat{x},\sigma}(t) &= \sum_{n_1, n_2} [(u_{i\sigma}^{n_1*} \gamma_{n_1}^\dagger(t) - \sigma v_{i\sigma}^{n_1} \gamma_{n_1}(t))(u_{i+\hat{x},\sigma}^{n_2} \gamma_{n_2}(t) - \sigma v_{i+\hat{x},\sigma}^{n_2*} \gamma_{n_2}^\dagger(t))] \\
&= \sum_{n_1, n_2} [u_{i\sigma}^{n_1*} u_{i+\hat{x},\sigma}^{n_2} e^{i(E_{n_1}-E_{n_2})t} \gamma_{n_1}^\dagger \gamma_{n_2} - \sigma u_{i\sigma}^{n_1*} v_{i+\hat{x},\sigma}^{n_2*} e^{i(E_{n_1}+E_{n_2})t} \gamma_{n_1}^\dagger \gamma_{n_2}^\dagger \\
&\quad - \sigma v_{i\sigma}^{n_1} u_{i+\hat{x},\sigma}^{n_2} e^{-i(E_{n_1}+E_{n_2})t} \gamma_{n_1} \gamma_{n_2} + v_{i\sigma}^{n_1} v_{i+\hat{x},\sigma}^{n_2*} e^{-i(E_{n_1}-E_{n_2})t} \gamma_{n_1} \gamma_{n_2}^\dagger] .
\end{aligned} \tag{2.106}$$

Using the following relations

$$\langle [\gamma_{n_1}^\dagger \gamma_{n_2}, \gamma_{n_3}^\dagger \gamma_{n_4}] \rangle = (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \delta_{n_1 n_4} \delta_{n_2 n_3} , \tag{2.107}$$

$$\langle [\gamma_{n_1}^\dagger \gamma_{n_2}, \gamma_{n_3} \gamma_{n_4}^\dagger] \rangle = -(\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \delta_{n_1 n_3} \delta_{n_2 n_4} , \tag{2.108}$$

$$\langle [\gamma_{n_1}^\dagger \gamma_{n_2}, \gamma_{n_3} \gamma_{n_4}] \rangle = (\delta_{n_1 n_4} \delta_{n_2 n_3} - \delta_{n_1 n_3} \delta_{n_2 n_4}) (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) , \tag{2.109}$$

$$\langle [\gamma_{n_1} \gamma_{n_2}, \gamma_{n_3}^\dagger \gamma_{n_4}^\dagger] \rangle = (\delta_{n_1 n_4} \delta_{n_2 n_3} - \delta_{n_1 n_3} \delta_{n_2 n_4}) (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) , \tag{2.110}$$

$$\langle [\gamma_{n_1} \gamma_{n_2}, \gamma_{n_3}^\dagger \gamma_{n_4}] \rangle = -(\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \delta_{n_1 n_3} \delta_{n_2 n_4} , \tag{2.111}$$

$$\langle [\gamma_{n_1} \gamma_{n_2}, \gamma_{n_3} \gamma_{n_4}^\dagger] \rangle = (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \delta_{n_1 n_4} \delta_{n_2 n_3} , \tag{2.112}$$

we obtain

$$\begin{aligned}
\langle \hat{A} \rangle &= \sum_{n_1, n_2} [u_{i+\hat{x},\sigma}^{n_1*} u_{i\sigma}^{n_2} e^{i(E_{n_1}-E_{n_2})t} u_{i'+\hat{x},\sigma}^{n_2*} u_{i'\sigma'}^{n_1} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \\
&\quad - u_{i+\hat{x},\sigma}^{n_1*} u_{i\sigma}^{n_2} e^{i(E_{n_1}-E_{n_2})t} v_{i'+\hat{x},\sigma'}^{n_2*} v_{i'\sigma'}^{n_1} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \\
&\quad + \sigma \sigma' u_{i+\hat{x},\sigma}^{n_1*} v_{i\sigma}^{n_2*} e^{i(E_{n_1}+E_{n_2})t} v_{i'+\hat{x},\sigma'}^{n_2} u_{i'\sigma'}^{n_1} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \\
&\quad - \sigma \sigma' u_{i+\hat{x},\sigma}^{n_1*} v_{i\sigma}^{n_2*} e^{i(E_{n_1}+E_{n_2})t} v_{i'+\hat{x},\sigma'}^{n_1} u_{i'\sigma'}^{n_2} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \\
&\quad + \sigma \sigma' v_{i+\hat{x},\sigma}^{n_1} u_{i\sigma}^{n_2} e^{-i(E_{n_1}+E_{n_2})t} u_{i'+\hat{x},\sigma'}^{n_2*} v_{i'\sigma'}^{n_1*} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \\
&\quad - \sigma \sigma' v_{i+\hat{x},\sigma}^{n_1} u_{i\sigma}^{n_2} e^{-i(E_{n_1}+E_{n_2})t} u_{i'+\hat{x},\sigma'}^{n_1*} v_{i'\sigma'}^{n_2*} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \\
&\quad - v_{i+\hat{x},\sigma}^{n_1} v_{i\sigma}^{n_2*} e^{-i(E_{n_1}-E_{n_2})t} u_{i'+\hat{x},\sigma'}^{n_1*} u_{i'\sigma'}^{n_2} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \\
&\quad + v_{i+\hat{x},\sigma}^{n_1} v_{i\sigma}^{n_2*} e^{-i(E_{n_1}-E_{n_2})t} v_{i'+\hat{x},\sigma'}^{n_2} v_{i'\sigma'}^{n_1*} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle)] , \tag{2.113}
\end{aligned}$$



$$\begin{aligned}
& -v_{i\sigma}^{n_1} v_{i+\hat{x},\sigma}^{n_2*} e^{-i(E_{n_1}-E_{n_2})t} u_{i'\sigma'}^{n_1*} u_{i'+\hat{x},\sigma'}^{n_2} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \\
& + v_{i\sigma}^{n_1} v_{i+\hat{x},\sigma}^{n_2*} e^{-i(E_{n_1}-E_{n_2})t} v_{i'\sigma'}^{n_2} v_{i'+\hat{x},\sigma'}^{n_1*} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) . \quad (2.116)
\end{aligned}$$

By defining

$$A_{n_1,n_2}(\mathbf{q}) = \sum_{i\sigma} e^{-i\mathbf{q}\cdot\mathbf{r}_i} [u_{i+\hat{x},\sigma}^{n_1*} u_{i\sigma}^{n_2} - u_{i\sigma}^{n_1*} u_{i+\hat{x},\sigma}^{n_2}] , \quad (2.117)$$

$$B_{n_1,n_2}(\mathbf{q}) = \sum_{i\sigma} \sigma e^{-i\mathbf{q}\cdot\mathbf{r}} [u_{i+\hat{x},\sigma}^{n_1*} v_{i\sigma}^{n_2*} - u_{i\sigma}^{n_1*} v_{i+\hat{x},\sigma}^{n_2*}] , \quad (2.118)$$

$$C_{n_1,n_2}(\mathbf{q}) = \sum_{i\sigma} \sigma e^{-i\mathbf{q}\cdot\mathbf{r}} [v_{i+\hat{x},\sigma}^{n_1} u_{i\sigma}^{n_2} - v_{i\sigma}^{n_1} u_{i+\hat{x},\sigma}^{n_2}] , \quad (2.119)$$

$$D_{n_1,n_2}(\mathbf{q}) = \sum_{i\sigma} e^{-i\mathbf{q}\cdot\mathbf{r}_i} [v_{i+\hat{x},\sigma}^{n_1} v_{i\sigma}^{n_2*} - v_{i\sigma}^{n_1} v_{i+\hat{x},\sigma}^{n_2*}] , \quad (2.120)$$

we find the current-current correlation function

$$\begin{aligned}
\Pi_{xx}(\mathbf{q}, \omega) &= -\frac{1}{N} \sum_{n_1, n_2} \left\{ \frac{A_{n_1, n_2}(\mathbf{q}) [-A_{n_1, n_2}^*(\mathbf{q}) - D_{n_1, n_2}(-\mathbf{q})]}{\omega + (E_{n_1} - E_{n_2}) + i\delta} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \right. \\
&+ \frac{B_{n_1, n_2}(\mathbf{q}) [-B_{n_1, n_2}^*(\mathbf{q}) - C_{n_1, n_2}(-\mathbf{q})]}{\omega + (E_{n_1} + E_{n_2}) + i\delta} (\langle \gamma_{n_1}^\dagger \gamma_{n_1} \rangle - \langle \gamma_{n_2}^\dagger \gamma_{n_2} \rangle) \\
&+ \frac{C_{n_1, n_2}(\mathbf{q}) [-C_{n_1, n_2}^*(\mathbf{q}) - B_{n_1, n_2}(-\mathbf{q})]}{\omega - (E_{n_1} + E_{n_2}) + i\delta} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \\
&+ \left. \frac{D_{n_1, n_2}(\mathbf{q}) [-D_{n_1, n_2}^*(\mathbf{q}) - A_{n_1, n_2}(-\mathbf{q})]}{\omega - (E_{n_1} - E_{n_2}) + i\delta} (\langle \gamma_{n_1} \gamma_{n_1}^\dagger \rangle - \langle \gamma_{n_2} \gamma_{n_2}^\dagger \rangle) \right\} \\
&= \frac{1}{N} \sum_{n_1, n_2} \left\{ \frac{A_{n_1, n_2}(\mathbf{q}) [A_{n_1, n_2}^*(\mathbf{q}) + D_{n_1, n_2}(-\mathbf{q})]}{\omega + (E_{n_1} - E_{n_2}) + i\delta} [f(E_{n_1}) - f(E_{n_2})] \right. \\
&+ \frac{B_{n_1, n_2}(\mathbf{q}) [B_{n_1, n_2}^*(\mathbf{q}) + C_{n_1, n_2}(-\mathbf{q})]}{\omega + (E_{n_1} + E_{n_2}) + i\delta} [f(E_{n_1}) - f(-E_{n_2})] \\
&+ \frac{C_{n_1, n_2}(\mathbf{q}) [C_{n_1, n_2}^*(\mathbf{q}) + B_{n_1, n_2}(-\mathbf{q})]}{\omega - (E_{n_1} + E_{n_2}) + i\delta} [f(-E_{n_1}) - f(E_{n_2})] \\
&+ \left. \frac{D_{n_1, n_2}(\mathbf{q}) [D_{n_1, n_2}^*(\mathbf{q}) + A_{n_1, n_2}(-\mathbf{q})]}{\omega - (E_{n_1} - E_{n_2}) + i\delta} [f(-E_{n_1}) - f(-E_{n_2})] \right\} . \quad (2.121)
\end{aligned}$$

Using the symmetry relation of eigenstates for positive and negative eigenvalues in the BdG equation, we can write the  $\Pi_{xx}$  in a simplified form:

$$\Pi_{xx}(\mathbf{q}, \omega) = \frac{1}{N} \sum_{n_1, n_2} \left\{ \frac{A_{n_1, n_2}(\mathbf{q})[A_{n_1, n_2}^*(\mathbf{q}) + D_{n_1, n_2}(-\mathbf{q})]}{\omega + (E_{n_1} - E_{n_2}) + i\delta} [f(E_{n_1}) - f(E_{n_2})] \right\}, \quad (2.122)$$

where  $E_n$  cover all eigenvalues from the BdG equation.

For the optical conductivity and charge stiffness, we set  $\mathbf{q} = 0$  and obtain:

$$\Pi_{xx}(\omega) = \frac{1}{N} \sum_{n_1, n_2} \left\{ \frac{A_{n_1, n_2}[A_{n_1, n_2}^* + D_{n_1, n_2}]}{\omega + (E_{n_1} - E_{n_2}) + i\delta} [f(E_{n_1}) - f(E_{n_2})] \right\}, \quad (2.123)$$

where  $A = A(\mathbf{q} = 0)$  and  $D = D(\mathbf{q} = 0)$ .

For the superfluid density, we first set  $\omega = 0$  and obtain

$$\begin{aligned} \Pi_{xx}(\mathbf{q} \rightarrow 0) = \frac{1}{N} \sum_{n_1, n_2} \left\{ \frac{A_{n_1, n_2}(\mathbf{q} \rightarrow 0)[A_{n_1, n_2}^*(\mathbf{q} \rightarrow 0) + D_{n_1, n_2}(-\mathbf{q} \rightarrow 0)]}{E_{n_1} - E_{n_2}} \right. \\ \left. \times [f(E_{n_1}) - f(E_{n_2})] \right\}. \end{aligned} \quad (2.124)$$

An alternative derivation of the optical conductivity and superfluid can be carried out within the Green function method, which is left for the readers to explore as an exercise. The above formulae for optical conductivity and superfluid density are particularly useful for the study of inhomogeneous superconductors.

## 2.2 Solution to the BdG Equations in the Lattice Model for a Uniform Superconductor

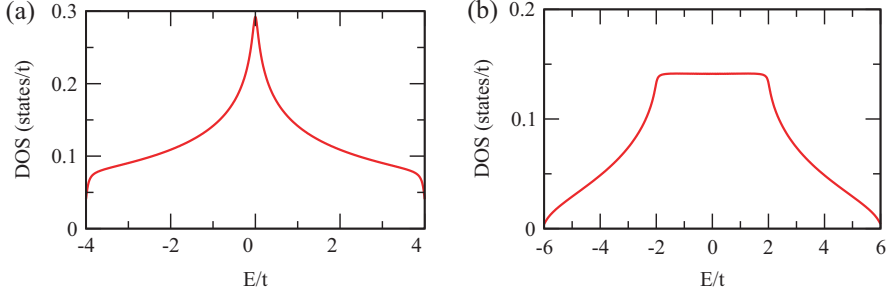
We consider the case in the absence of spin-orbit coupling and other spin-flip scattering effect, and assume only a superconducting order is present in the system. In the nearest-neighbor hopping approximation for the tight-binding model of a cubic system, the normal-state single-particle energy dispersion is given by

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a + \cos k_z a), \quad (2.125)$$

for a three-dimensional cubic lattice, while

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a), \quad (2.126)$$

for a two-dimensional square lattice. Here  $a$  is the lattice constant and  $t$  is the nearest-neighbor hopping integral. From these dispersions, the normal-state density



**Fig. 2.1** Normal-state single-particle density of states for a two-dimensional (a) and three-dimensional (b) system. Lattice size is chosen to be  $400 \times 400$  for the 2D system and  $200 \times 200 \times 200$  for the 3D system. The intrinsic lifetime broadening  $\Gamma = 0.05$  is used for the calculation

of states can be numerically evaluated. The results of normal-state density of states are shown in Fig. 2.1. As one can see, for the 2D system, the DOS exhibits the van Hove singularity. The strong energy dependence of this DOS will influence the magnitude of the superconducting order parameter. For high-temperature cuprate superconductors, the electrons are mostly confined into a two-dimensional Cu square lattice and the energy dispersion for the low-energy Cu-3d electrons usually includes the next-nearest-neighbor hopping

$$\epsilon_{\mathbf{k}} = -2t(\cos k_x a + \cos k_y a) - 4t' \cos k_x a \cos k_y a . \quad (2.127)$$

We consider a pristine 2D superconductor with an  $s$ -wave or  $d_{x^2-y^2}$ -wave pairing symmetry. In this case, the system is invariant under a translation with a lattice constant  $a$  of the square lattice, and the BdG wave functions take the Bloch wavelike:

$$u_i = \frac{1}{\sqrt{N_L}} u_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} , \quad (2.128)$$

$$v_i = \frac{1}{\sqrt{N_L}} v_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_i} , \quad (2.129)$$

which gives rise to

$$E_{\mathbf{k}} u_{\mathbf{k}} = \xi_{\mathbf{k}} u_{\mathbf{k}} + \Delta_{\mathbf{k}} v_{\mathbf{k}} , \quad (2.130a)$$

$$E_{\mathbf{k}} v_{\mathbf{k}} = -\xi_{\mathbf{k}} v_{\mathbf{k}} + \Delta_{\mathbf{k}}^* u_{\mathbf{k}} . \quad (2.130b)$$

Here

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \quad (2.131)$$

and

$$\Delta_{\mathbf{k}} = \Delta_s \quad (2.132)$$

for the  $s$ -wave pairing symmetry while

$$\Delta_{\mathbf{k}} = (\Delta_d/2)(\cos k_x a - \cos k_y a) \quad (2.133)$$

for the  $d$ -wave pairing symmetry.

A little algebra yields to the eigensolutions

$$\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} u_{\mathbf{k}}^{(0)} e^{i\varphi_{\mathbf{k}}} \\ v_{\mathbf{k}}^{(0)} \end{pmatrix} \quad (2.134)$$

corresponding to the eigenvalue

$$E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}. \quad (2.135)$$

and

$$\begin{pmatrix} u_{\mathbf{k}} \\ v_{\mathbf{k}} \end{pmatrix} = \begin{pmatrix} -v_{\mathbf{k}}^{(0)} e^{i\varphi_{\mathbf{k}}} \\ u_{\mathbf{k}}^{(0)} \end{pmatrix} \quad (2.136)$$

corresponding to the eigenvalue  $-E_{\mathbf{k}}$ . Here the BdG wave function amplitude is given by

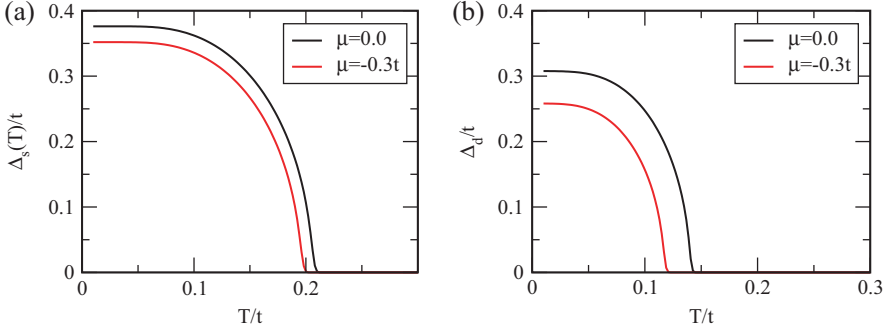
$$\begin{pmatrix} u_{\mathbf{k}}^{(0)} \\ v_{\mathbf{k}}^{(0)} \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{1}{2} \left( 1 + \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right)} \\ \sqrt{\frac{1}{2} \left( 1 - \frac{\xi_{\mathbf{k}}}{E_{\mathbf{k}}} \right)} \end{pmatrix}, \quad (2.137)$$

and  $\varphi_{\mathbf{k}}$  is the phase angle of  $\Delta_{\mathbf{k}}$ . Therefore, we obtain the self-consistency equation for the pair potential

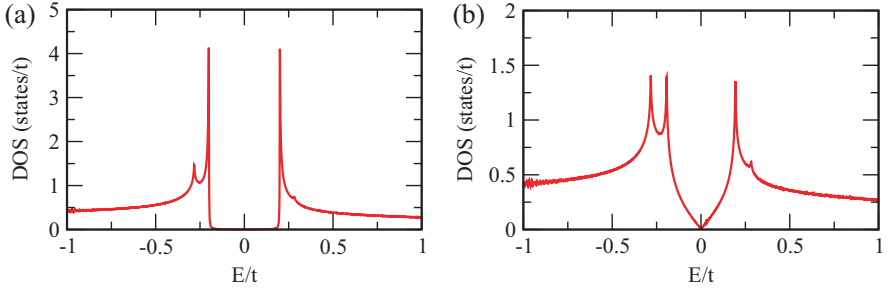
$$\Delta_s = \frac{1}{N_L} \sum_{\mathbf{k}} V_s \frac{\Delta_s}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (2.138)$$

for a three-dimensional  $s$ -wave superconductor with the quasiparticle excitation energy  $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_s^2}$ ; and

$$\Delta_d = \frac{1}{N_L} \sum_{\mathbf{k}} V_d (\cos k_x a - \cos k_y a)^2 \frac{\Delta_d}{2E_{\mathbf{k}}} \tanh\left(\frac{E_{\mathbf{k}}}{2k_B T}\right), \quad (2.139)$$



**Fig. 2.2** Temperature dependence of the superconducting order parameter for an  $s$ -wave (a) and  $d_{x^2-y^2}$ -wave (b) pairing symmetry for various values of chemical potential in a 2D tight-binding lattice model with nearest-neighbor hopping. Lattice size is chosen to be  $400 \times 400$  for the calculations. The energy and temperature ( $k_B T$  and  $k_B$  is set to 1) are measured in units of  $t$



**Fig. 2.3** Density of states for a pristine 2D superconductor with  $s$ -wave (a) and  $d_{x^2-y^2}$ -wave (b) pairing symmetry. A square-lattice tight-binding model with normal-state single-particle energy dispersion given by Eq. (2.127) is used. The parameter  $t' = -0.3t$  and  $\mu = -t$ , and  $\Delta_s = \Delta_d = 0.2t$  are taken. Lattice size is chosen to be  $4096 \times 4096$  and  $\Gamma = 0.001t$  is used for the calculations

for a two-dimensional  $d_{x^2-y^2}$ -wave superconductor with the quasiparticle excitation energy  $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + [\frac{\Delta_d}{2}(\cos k_x a - \cos k_y a)]^2}$ . In Fig. 2.2, the temperature dependence of superconducting order parameter for various values of chemical potential is shown. The results show that the zero-temperature superconducting pair potential and transition temperature are dependent on the location of the chemical potential, at which the intensity of density of states is tuned. In the 2D tight-binding model with nearest-neighbor hopping, the van Hove singularity occurs at the normal state energy  $\epsilon = 0$ . In Fig. 2.3, we show the typical feature of density of states for a 2D superconductor described by a square-lattice tight-binding model. The normal-state single-particle energy dispersion given by Eq. (2.127) with  $t' = -0.3t$  and a chemical potential  $\mu = -t$  are considered. For the  $s$ -wave pairing symmetry, a well-shape characteristic as marked by the superconducting coherent peaks around the Fermi energy at  $E = 0$  is exhibited in the density of states. Instead, for

the  $d_{x^2-y^2}$ -wave pairing symmetry, a V-shape characteristic is exhibited in the density of states around the Fermi energy, which arises from the gapless nodal quasiparticles. In addition, the normal-state van Hove singularity peak is shifted by the superconducting gap opening.

### 2.3 Abrikosov-Gorkov Equations in the Lattice Model

Similar to the continuum model, we can also establish the Abrikosov-Gorkov theory in the lattice model. Here we generalize it to include the effects of spin-orbit coupling and spin-flip scattering. We first define a 4-component spinor field operator in the Nambu space

$$\hat{\Psi}_i(\tau) = \begin{pmatrix} c_{i\uparrow}(\tau) \\ c_{i\downarrow}(\tau) \\ c_{i\uparrow}^\dagger(\tau) \\ c_{i\downarrow}^\dagger(\tau) \end{pmatrix}, \quad (2.140)$$

and

$$\hat{\Psi}_i^\dagger(\tau) = \begin{pmatrix} c_{i\uparrow}^\dagger(\tau) & c_{i\downarrow}^\dagger(\tau) & c_{i\uparrow}(\tau) & c_{i\downarrow}(\tau) \end{pmatrix}, \quad (2.141)$$

where the electronic operators

$$c_{i\sigma}(\tau) = e^{\mathcal{H}_{\text{eff}}\tau/\hbar} c_{i\sigma} e^{-\mathcal{H}_{\text{eff}}\tau/\hbar}, \quad (2.142)$$

$$c_{i\sigma}^\dagger(\tau) = e^{\mathcal{H}_{\text{eff}}\tau/\hbar} c_{i\sigma}^\dagger e^{-\mathcal{H}_{\text{eff}}\tau/\hbar}, \quad (2.143)$$

are defined in the imaginary-time space and  $\mathcal{H}_{\text{eff}}$  is given by Eq. (2.5). Note that  $c_{i\sigma}^\dagger(\tau) \neq [c_{i\sigma}(\tau)]^\dagger$ . We then introduce the real-space Green's function in the lattice model as

$$\begin{aligned} \mathcal{G}(i\tau; j\tau') &= -\langle T_\tau (\hat{\Psi}_i(\tau) \otimes \hat{\Psi}_j^\dagger(\tau')) \rangle, \\ &= -\theta(\tau - \tau') \langle \hat{\Psi}_i(\tau) \otimes \hat{\Psi}_j^\dagger(\tau') \rangle + \theta(\tau' - \tau) \langle \hat{\Psi}_j^\dagger(\tau') \otimes \hat{\Psi}_i(\tau) \rangle. \end{aligned} \quad (2.144)$$

Therefore, in an expanded form, it becomes

$$\begin{aligned} \mathcal{G}(i\tau; j\tau') &= \begin{pmatrix} -\langle T_\tau (c_{i\uparrow}(\tau) c_{j\uparrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}(\tau) c_{j\downarrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}(\tau) c_{j\uparrow}(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}(\tau) c_{j\downarrow}(\tau')) \rangle \\ -\langle T_\tau (c_{i\downarrow}(\tau) c_{j\uparrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}(\tau) c_{j\downarrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}(\tau) c_{j\uparrow}(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}(\tau) c_{j\downarrow}(\tau')) \rangle \\ -\langle T_\tau (c_{i\uparrow}^\dagger(\tau) c_{j\uparrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}^\dagger(\tau) c_{j\downarrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}^\dagger(\tau) c_{j\uparrow}(\tau')) \rangle & -\langle T_\tau (c_{i\uparrow}^\dagger(\tau) c_{j\downarrow}(\tau')) \rangle \\ -\langle T_\tau (c_{i\downarrow}^\dagger(\tau) c_{j\uparrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}^\dagger(\tau) c_{j\downarrow}^\dagger(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}^\dagger(\tau) c_{j\uparrow}(\tau')) \rangle & -\langle T_\tau (c_{i\downarrow}^\dagger(\tau) c_{j\downarrow}(\tau')) \rangle \end{pmatrix}. \end{aligned} \quad (2.145)$$



Since the trace is unchanged upon a cyclic variation of operators, we can easily prove that the Green's function is a function of the difference  $\tau - \tau'$ , that is,

$$\mathcal{G}(i\tau; j\tau') = \mathcal{G}(i, j; \tau - \tau') , \quad (2.146)$$

with  $\tau - \tau'$  restricted in the range of  $[-\beta, \beta]$  and the factor  $\beta = 1/k_B T$ . Therefore, the Fourier transform is given by

$$\mathcal{G}(i, j; i\omega_n) = \int_0^\beta d\tau e^{i\omega_n \tau} \mathcal{G}(i, j; \tau) , \quad (2.147)$$

$$\mathcal{G}(i, j; \tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} \mathcal{G}(i, j; i\omega_n) , \quad (2.148)$$

where the Matsubara frequency  $\omega_n = (2n + 1)\pi k_B T / \hbar$  with  $n = -\infty, \dots, -1, 0, 1, \dots, \infty$ .

Using the equation of motion for  $c_{i\sigma}(\tau)$  and  $c_{i\sigma}^\dagger(\tau)$ :

$$-\hbar \frac{\partial c_{i\sigma}(\tau)}{\partial \tau} = [c_{i\sigma}(\tau), \mathcal{H}_{eff}]_- , \quad (2.149)$$

$$-\hbar \frac{\partial c_{i\sigma}^\dagger(\tau)}{\partial \tau} = [c_{i\sigma}^\dagger(\tau), \mathcal{H}_{eff}]_- , \quad (2.150)$$

and Eq. (2.10), we can obtain the equation of motion for the Green's function

$$\sum_{j'} \hat{M}_{ij'}(\tau) \mathcal{G}(j'\tau; j\tau') = \delta_{ij} \delta(\tau - \tau') \hat{1} , \quad (2.151)$$

with

$$\hat{M}_{ij}(\tau) = \begin{pmatrix} -\frac{\partial}{\partial \tau} \delta_{ij} - \tilde{h}_{i\uparrow j\uparrow} & -\tilde{h}_{i\uparrow j\downarrow} & 0 & -\Delta_{ij} \\ -\tilde{h}_{i\downarrow j\uparrow} & -\frac{\partial}{\partial \tau} \delta_{ij} - \tilde{h}_{i\downarrow j\downarrow} & -\Delta_{ji} & 0 \\ 0 & -\Delta_{ij}^* & -\frac{\partial}{\partial \tau} \delta_{ij} + \tilde{h}_{i\uparrow j\uparrow}^* & -\tilde{h}_{i\uparrow j\downarrow}^* \\ -\Delta_{ji}^* & 0 & -\tilde{h}_{i\uparrow j\downarrow}^* & -\frac{\partial}{\partial \tau} \delta_{ij} + \tilde{h}_{i\downarrow j\downarrow}^* \end{pmatrix} . \quad (2.152)$$

for the spin-singlet pairing case, and subject to the self-consistency condition:

$$\Delta_{ij} = -\frac{V}{2} [\mathcal{G}_{14}(i\tau \rightarrow \tau' + 0^+, j\tau') - \mathcal{G}_{23}(i\tau \rightarrow \tau' + 0^+, j\tau')] , \quad (2.153)$$

$$\Delta_{ij}^* = -\frac{V}{2} [\mathcal{G}_{41}(i\tau \rightarrow \tau' + 0^+, j\tau') - \mathcal{G}_{32}(i\tau \rightarrow \tau' + 0^+, j\tau')] . \quad (2.154)$$

In the absence of the spin-orbit coupling and spin-flip scattering, we can decouple the equation of motion for the Green's function into two sets:

$$\sum_{j'} \begin{pmatrix} -\frac{\partial}{\partial \tau} \delta_{ij'} - \tilde{h}_{i\uparrow j'\uparrow} & -\Delta_{ij'} \\ -\Delta_{j'i}^* & -\frac{\partial}{\partial \tau} \delta_{ij'} + \tilde{h}_{i\downarrow j'\downarrow}^* \end{pmatrix} \begin{pmatrix} \mathcal{G}_{11}(j'\tau; j\tau') & \mathcal{G}_{14}(j'\tau; j\tau') \\ \mathcal{G}_{41}(j'\tau; j\tau') & \mathcal{G}_{44}(j'\tau; j\tau') \end{pmatrix} \\ = \delta_{ij} \delta(\tau - \tau') \hat{1} , \quad (2.155)$$

and

$$\sum_{j'} \begin{pmatrix} -\frac{\partial}{\partial \tau} \delta_{ij'} - \tilde{h}_{i\downarrow j'\downarrow} & -\Delta_{j'i} \\ -\Delta_{ij'}^* & -\frac{\partial}{\partial \tau} \delta_{ij'} + \tilde{h}_{i\uparrow j'\uparrow}^* \end{pmatrix} \begin{pmatrix} \mathcal{G}_{22}(j'\tau; j\tau') & \mathcal{G}_{23}(j'\tau; j\tau') \\ \mathcal{G}_{32}(j'\tau; j\tau') & \mathcal{G}_{33}(j'\tau; j\tau') \end{pmatrix} \\ = \delta_{ij} \delta(\tau - \tau') \hat{1} . \quad (2.156)$$

In this case, either one of the above two sets of equations of motion is sufficient to solve the whole problem. More interestingly, there exists a close relation between the Green's function and the BdG eigenfunctions. Specifically, with the time dependence of the quasiparticle operators:

$$\gamma_n(\tau) = \gamma_n e^{-E_n \tau / \hbar} , \quad (2.157)$$

$$\gamma_n^\dagger(\tau) = \gamma_n^\dagger e^{E_n \tau / \hbar} . \quad (2.158)$$

and the canonical transformation, we can obtain for the most general case the following matrix elements of the Green's function

$$\mathcal{G}_{11}(i, j; \tau) = -\theta(\tau) \sum_n [u_{i\uparrow}^n u_{j\uparrow}^{n*} f(-E_n) e^{-E_n \tau / \hbar} + v_{i\uparrow}^{n*} v_{j\uparrow}^n f(E_n) e^{E_n \tau / \hbar}] \\ + \theta(-\tau) \sum_n [u_{j\uparrow}^{n*} u_{i\uparrow}^n f(E_n) e^{-E_n \tau / \hbar} + v_{j\uparrow}^n v_{i\uparrow}^n f(-E_n) e^{E_n \tau / \hbar}] , \quad (2.159)$$

and

$$\mathcal{G}_{44}(i, j; \tau) = -\theta(\tau) \sum_n [u_{i\downarrow}^{n*} u_{j\downarrow}^n f(E_n) e^{E_n \tau / \hbar} + v_{i\downarrow}^n v_{j\downarrow}^{n*} f(-E_n) e^{-E_n \tau / \hbar}] \\ + \theta(-\tau) \sum_n [u_{j\downarrow}^n u_{i\downarrow}^{n*} f(-E_n) e^{E_n \tau / \hbar} + v_{j\downarrow}^{n*} v_{i\downarrow}^n f(E_n) e^{-E_n \tau / \hbar}] . \quad (2.160)$$

It is straightforward to obtain the Green's function in the frequency domain

$$\begin{aligned}
\mathcal{G}_{11}(i, j; i\omega_n) &= \int_0^{\beta\hbar} d\tau e^{i\omega_n\tau} \mathcal{G}_{11}(i, j; \tau) \\
&= - \sum_n' [u_{i\uparrow}^n u_{j\uparrow}^{n*} f(-E_n) \int_0^{\beta\hbar} d\tau e^{(i\omega_n - E_n/\hbar)\tau} \\
&\quad + v_{i\uparrow}^{n*} v_{j\uparrow}^n f(E_n) \int_0^{\beta\hbar} d\tau e^{(i\omega_n + E_n/\hbar)\tau}] \\
&= - \sum_n' \left\{ \frac{u_{i\uparrow}^n u_{j\uparrow}^{n*}}{i\omega_n - E_n/\hbar} f(-E_n) (e^{\beta\hbar(i\omega_n - E_n/\hbar)} - 1) \right. \\
&\quad \left. + \frac{v_{i\uparrow}^{n*} v_{j\uparrow}^n}{i\omega_n + E_n/\hbar} f(E_n) (e^{\beta\hbar(i\omega_n + E_n/\hbar)} - 1) \right\} \\
&= \sum_n' \left[ \frac{u_{i\uparrow}^n u_{j\uparrow}^{n*}}{i\omega_n - E_n/\hbar} + \frac{v_{i\uparrow}^{n*} v_{j\uparrow}^n}{i\omega_n + E_n/\hbar} \right], \tag{2.161}
\end{aligned}$$

and

$$\begin{aligned}
\mathcal{G}_{44}(i, j; i\omega_n) &= \int_0^{\beta\hbar} d\tau e^{i\omega_n\tau} \mathcal{G}_{44}(i, j; \tau) \\
&= - \sum_n' [u_{i\downarrow}^{n*} u_{j\downarrow}^n f(E_n) \int_0^{\beta\hbar} d\tau e^{(i\omega_n + E_n/\hbar)\tau} \\
&\quad + v_{i\downarrow}^n v_{j\downarrow}^{n*} f(-E_n) \int_0^{\beta\hbar} d\tau e^{(i\omega_n + E_n/\hbar)\tau}] \\
&= - \sum_n' \left\{ \frac{u_{i\downarrow}^{n*} u_{j\downarrow}^n}{i\omega_n + E_n/\hbar} f(E_n) (e^{\beta\hbar(i\omega_n + E_n/\hbar)} - 1) \right. \\
&\quad \left. + \frac{v_{i\downarrow}^n v_{j\downarrow}^{n*}}{i\omega_n - E_n/\hbar} f(-E_n) (e^{\beta\hbar(i\omega_n - E_n/\hbar)} - 1) \right\} \\
&= \sum_n' \left[ \frac{u_{i\downarrow}^{n*} u_{j\downarrow}^n}{i\omega_n + E_n/\hbar} + \frac{v_{i\downarrow}^n v_{j\downarrow}^{n*}}{i\omega_n - E_n/\hbar} \right]. \tag{2.162}
\end{aligned}$$

Other matrix elements of the Green's function can be evaluated in the same way, which are left for exercise.

In the absence of the spin-orbit coupling and spin-flip scattering, we can rewrite the Green's matrix elements as

$$\mathcal{G}_{11}(i, j; i\omega_n) = \sum_{\tilde{n}}' \left[ \frac{u_{i\uparrow}^{\tilde{n}1} u_{j\uparrow}^{\tilde{n}1*}}{i\omega_n - E_{\tilde{n}1}/\hbar} + \frac{v_{i\uparrow}^{\tilde{n}2*} v_{j\uparrow}^{\tilde{n}2}}{i\omega_n + E_{\tilde{n}2}/\hbar} \right], \quad (2.163)$$

and

$$\mathcal{G}_{44}(i, j; i\omega_n) = \sum_{\tilde{n}}' \left[ \frac{u_{i\downarrow}^{\tilde{n}2*} u_{j\downarrow}^{\tilde{n}2}}{i\omega_n + E_{\tilde{n}2}/\hbar} + \frac{v_{i\downarrow}^{\tilde{n}1} v_{j\downarrow}^{\tilde{n}1*}}{i\omega_n - E_{\tilde{n}1}/\hbar} \right]. \quad (2.164)$$

In summary, we have demonstrated that once we know the eigensolution of the BdG equations, the Abrikosov-Gorkov Green's function can be expressed rigorously. Conversely, if we know the solution to the Abrikosov-Gorkov equations of motion for the Green's functions, the local density of states can be calculated as

$$\begin{aligned} \rho_{i,\uparrow}(E) &= -\frac{1}{\hbar\pi} \text{Im}[\mathcal{G}_{11}(i, i; i\omega_n \rightarrow E/\hbar + i0^+)] \\ &= \sum_{\tilde{n}}' [|u_{i\uparrow}^{\tilde{n}1}|^2 \delta(E - E_{\tilde{n}1}) + |v_{i\uparrow}^{\tilde{n}2}|^2 \delta(E + E_{\tilde{n}2})], \end{aligned} \quad (2.165)$$

and

$$\begin{aligned} \rho_{i,\downarrow}(E) &= \frac{1}{\hbar\pi} \text{Im}[\mathcal{G}_{44}(i, i; -i\omega_n \rightarrow -(E/\hbar + i0^+))] \\ &= \sum_{\tilde{n}}' [|u_{i\downarrow}^{\tilde{n}2}|^2 \delta(E - E_{\tilde{n}2}) + |v_{i\downarrow}^{\tilde{n}1}|^2 \delta(E + E_{\tilde{n}1})]. \end{aligned} \quad (2.166)$$

The above expressions for the local density of states are the same as those given in terms of the eigensolution to the BdG equations (2.47). As we will show in later chapters, the Green's function technique is very useful and convenient for some situations.

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