

—Chapter 4—

BdG Equations on a Lattice

4-1 Self-consistent BdG Equations

A. EQUATIONS OF MOTION

- (1) The BCS Hamiltonian on lattice

$$\hat{H} = \sum_{ij\sigma} \left(-t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} - \tilde{t}_{ij}^* \hat{c}_{j\sigma}^\dagger \hat{c}_{i\sigma} \right) + \sum_{ij} \left(\Delta_{ij} \hat{c}_{i\uparrow}^\dagger \hat{c}_{j\downarrow} + \Delta_{ij}^* \hat{c}_{j\downarrow} \hat{c}_{i\uparrow} \right)$$

Since the Hamiltonian should be a Hermitian operator, i.e.,

$$\hat{H}^\dagger = \hat{H} \Rightarrow t_{ij}^* = t_{ji} \text{ and } \Delta_{ij}^* = \Delta_{ji}$$

- (2) The equations of motion

Let the imaginary time $\tau = it$

$$-\frac{\partial}{\partial \tau} \hat{c}_{i\sigma} = [\hat{c}_{i\sigma}, \hat{H}]$$

$$-\frac{\partial}{\partial \tau} \hat{c}_{i\sigma}^\dagger = [\hat{c}_{i\sigma}^\dagger, \hat{H}]$$

OS:

$$[a, bc] = \{a, b\}c - b\{a, c\}$$

$$[ab, c] = a\{b, c\} - \{a, c\}b$$

$$\begin{aligned} [\hat{c}_{i\sigma}, \hat{H}] &= \sum_{uv} \left[\hat{c}_{i\sigma}, -t_{uv} \hat{c}_{u\sigma}^\dagger \hat{c}_{v\sigma} - t_{uv}^* \hat{c}_{v\sigma}^\dagger \hat{c}_{u\sigma} + \Delta_{uv} \hat{c}_{u\sigma}^\dagger \hat{c}_{v\bar{\sigma}} \right] \\ &= \sum_{uv} \left[-t_{uv} \hat{c}_{v\sigma} \delta_{iu} - t_{uv}^* \hat{c}_{u\sigma} \delta_{iv} + \sigma \Delta_{uv} \hat{c}_{v\bar{\sigma}}^\dagger \delta_{iu} \right] \\ &= \sum_j \left[-2t_{ij} \hat{c}_{j\sigma} + \sigma \Delta_{ij} \hat{c}_{j\bar{\sigma}}^\dagger \right] \\ &\xrightarrow{2t \rightarrow t} \sum_j \left[-t_{ij} \hat{c}_{j\sigma} + \sigma \Delta_{ij} \hat{c}_{j\bar{\sigma}}^\dagger \right] \end{aligned}$$

$$\begin{aligned}
[\hat{c}_{i\sigma}^\dagger, \hat{H}] &= \sum_{uv} [\hat{c}_{i\sigma}^\dagger, -t_{uv}\hat{c}_{u\sigma}^\dagger\hat{c}_{v\sigma} - t_{uv}^*\hat{c}_{v\sigma}^\dagger\hat{c}_{u\sigma} + \Delta_{uv}^*c_{v\bar{\sigma}}c_{u\sigma}] \\
&= \sum_{uv} t_{uv}\hat{c}_{u\sigma}^\dagger\delta_{iv} + t_{uv}^*\hat{c}_{v\sigma}^\dagger\delta_{iu} - \sigma\Delta_{uv}^*c_{v\bar{\sigma}}\delta_{iu} \\
&= \sum_j 2t_{ij}^*\hat{c}_{j\sigma}^\dagger - \sigma\Delta_{ij}^*c_{v\bar{\sigma}} \\
&\xrightarrow{2t \rightarrow t} \sum_j t_{ij}^*\hat{c}_{j\sigma}^\dagger - \sigma\Delta_{ij}^*c_{v\bar{\sigma}}
\end{aligned}$$

B. BOGOLIUBOV TRANSFORMATION

(1) Bogoliubov transformations

$$\begin{aligned}
\hat{c}_{i\sigma} &= \sum_n \left(u_i^n \hat{\gamma}_{n\sigma} - \sigma v_i^{n*} \hat{\gamma}_{n\bar{\sigma}}^\dagger \right) \\
\hat{c}_{i\sigma}^\dagger &= \sum_n \left(u_i^{n*} \hat{\gamma}_{n\sigma}^\dagger - \sigma v_i^n \hat{\gamma}_{n\bar{\sigma}} \right)
\end{aligned}$$

which are linear transformations of creation and annihilation operators that preserve the anticommutation relation, i.e.,

$$\hat{\gamma}_{n\sigma} \hat{\gamma}_{n\sigma}^\dagger + \hat{\gamma}_{n\sigma}^\dagger \hat{\gamma}_{n\sigma} = 1$$

(2) The Bogoliubov transformation in matrix form,

$$\begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \hat{c}_{N\uparrow} \\ \hat{c}_{1\downarrow}^\dagger \\ \vdots \\ \hat{c}_{N\downarrow}^\dagger \end{pmatrix} = \begin{pmatrix} u_1^1 & \cdots & u_1^N & -v_1^{1*} & \cdots & -v_1^{N*} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_N^1 & \cdots & u_N^N & -v_N^{1*} & \cdots & -v_N^{N*} \\ v_1^1 & \cdots & v_1^N & u_1^{1*} & \cdots & u_1^{N*} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ v_N^1 & \cdots & v_N^N & u_N^{1*} & \cdots & u_N^{N*} \end{pmatrix} \begin{pmatrix} \hat{\gamma}_{1\uparrow} \\ \vdots \\ \hat{\gamma}_{N\uparrow} \\ \hat{\gamma}_{1\downarrow}^\dagger \\ \vdots \\ \hat{\gamma}_{N\downarrow}^\dagger \end{pmatrix}$$

the transformation matrix is a $2N \times 2N$ matrix.

Let

$$\begin{aligned}
\mathbf{c}_\uparrow &= \begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \hat{c}_{N\uparrow} \end{pmatrix}, & \mathbf{c}_\downarrow^\dagger &= \begin{pmatrix} \hat{c}_{1\downarrow}^\dagger \\ \vdots \\ \hat{c}_{N\downarrow}^\dagger \end{pmatrix} \\
\mathbf{u} &= \begin{pmatrix} u_1^1 & \cdots & u_1^N \\ \vdots & \ddots & \vdots \\ u_N^1 & \cdots & u_N^N \end{pmatrix}, & \mathbf{v} &= \begin{pmatrix} v_1^1 & \cdots & v_1^N \\ \vdots & \ddots & \vdots \\ v_N^1 & \cdots & v_N^N \end{pmatrix}
\end{aligned}$$

$$\gamma_{\uparrow} = \begin{pmatrix} \hat{\gamma}_{1\uparrow} \\ \vdots \\ \hat{\gamma}_{N\uparrow} \end{pmatrix}, \quad \gamma_{\downarrow}^{\dagger} = \begin{pmatrix} \hat{\gamma}_{1\downarrow}^{\dagger} \\ \vdots \\ \hat{\gamma}_{N\downarrow}^{\dagger} \end{pmatrix}$$

The Bogoliubov transformation can be simplified as,

$$\begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix} \begin{pmatrix} \gamma_{\uparrow} \\ \gamma_{\downarrow}^{\dagger} \end{pmatrix}$$

(3) Since

$$\begin{aligned} \begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix} \begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix}^{\dagger} &= \begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix} \begin{pmatrix} u^{*} & v^{*} \\ -v & u \end{pmatrix} \\ &= \begin{pmatrix} |u|^2 + |v|^2 & uv^{*} - v^{*}u \\ vu^{*} - u^{*}v & |u|^2 + |v|^2 \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{1} \end{pmatrix} \end{aligned}$$

where

$$|u|^2 + |v|^2 = \mathbf{1} \Rightarrow \sum_n (|u_i^n|^2 + |v_i^n|^2) = 1 \dots\dots (a)$$

$$uv^{*} - v^{*}u = \mathbf{0} \Rightarrow \sum_n (u_i^n v_i^{n*} - v_i^{n*} u_i^n) = 0 \dots\dots (b)$$

$$vu^{*} - u^{*}v = \mathbf{0} \Rightarrow \sum_n (v_i^n u_i^{n*} - u_i^{n*} v_i^n) = 0$$

The Bogoliubov transformation matrix is a unitary matrix, i.e.,

$$\begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix}^{\dagger} = \begin{pmatrix} u & -v^{*} \\ v & u^{*} \end{pmatrix}^{-1}$$

C. BdG EQUATIONS

(1) Define a spinor operator

$$\psi = \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix}$$

The Hamiltonian in terms of ψ and $\psi^{\dagger}$

$$\mathbf{H} = \begin{pmatrix} \hat{c}_{1\uparrow}^\dagger & \cdots & \cdots & \hat{c}_{N\uparrow}^\dagger & \hat{c}_{1\downarrow} & \cdots & \cdots & \hat{c}_{N\downarrow} \end{pmatrix} \cdot \begin{pmatrix} 0 & -t_{12} & \cdots & -t_{1N} & \Delta_{11} & \cdots & \cdots & \Delta_{1N} \\ -t_{21} & 0 & \vdots & \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ -t_{N1} & \cdots & \cdots & 0 & \Delta_{N1} & \cdots & \cdots & \Delta_{NN} \\ \Delta_{11}^* & \cdots & \cdots & \Delta_{1N}^* & 0 & t_{12}^* & \cdots & t_{1N}^* \\ \vdots & \ddots & \vdots & \vdots & t_{21}^* & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ \Delta_{N1}^* & \cdots & \cdots & \Delta_{NN}^* & t_{N1}^* & \cdots & \cdots & 0 \end{pmatrix} \cdot \begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \vdots \\ \hat{c}_{N\uparrow} \\ \hat{c}_{1\downarrow}^\dagger \\ \vdots \\ \vdots \\ \hat{c}_{N\downarrow}^\dagger \end{pmatrix}.$$

Let

$$\mathbf{t} = \begin{pmatrix} 0 & t_{12} & \cdots & t_{1N} \\ t_{21} & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ t_{N1} & \cdots & \cdots & 0 \end{pmatrix}, \quad \Delta = \begin{pmatrix} \Delta_{11} & \cdots & \cdots & \Delta_{1N} \\ \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ \Delta_{N1} & \cdots & \cdots & \Delta_{NN} \end{pmatrix}$$

We obtain

$$\mathbf{H} = \begin{pmatrix} c_\uparrow^\dagger & c_\downarrow \end{pmatrix} \begin{pmatrix} -\mathbf{t} & \Delta \\ \Delta^* & \mathbf{t}^* \end{pmatrix} \begin{pmatrix} c_\uparrow \\ c_\downarrow^\dagger \end{pmatrix} \cdots \cdots (c)$$

(2) Use the Bogoliubov transformation

$$\begin{aligned} \mathbf{H} &= \overbrace{\begin{pmatrix} c_\uparrow^\dagger & c_\downarrow \end{pmatrix}}^{\left(\begin{smallmatrix} c_\uparrow \\ c_\downarrow \end{smallmatrix} \right)} \cdot \begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix}^\dagger \cdot \begin{pmatrix} -\mathbf{t} & \Delta \\ \Delta^* & \mathbf{t}^* \end{pmatrix} \cdot \overbrace{\begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix} \begin{pmatrix} \gamma_\uparrow \\ \gamma_\downarrow^\dagger \end{pmatrix}}^{\left(\begin{smallmatrix} c_\uparrow \\ c_\downarrow \end{smallmatrix} \right)} \\ &= \begin{pmatrix} \gamma_\uparrow^\dagger & \gamma_\downarrow \end{pmatrix} \begin{pmatrix} \varepsilon_\uparrow & 0 \\ 0 & -\varepsilon_\downarrow \end{pmatrix} \begin{pmatrix} \gamma_\uparrow \\ \gamma_\downarrow^\dagger \end{pmatrix} \\ &= \sum_{\sigma} E_{\sigma} \gamma_{\sigma}^\dagger \gamma_{\sigma} + \varepsilon_0 \end{aligned}$$

where

$$\begin{aligned} &\begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix}^\dagger \begin{pmatrix} -\mathbf{t} & \Delta \\ \Delta^* & \mathbf{t}^* \end{pmatrix} \begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix} \\ &= \begin{pmatrix} -\mathbf{u}^* \mathbf{t} \mathbf{u} + \mathbf{u}^* \Delta \mathbf{v} + \mathbf{v}^* \Delta^* \mathbf{u} + \mathbf{v}^* \mathbf{t}^* \mathbf{v} & \mathbf{u}^* \mathbf{t} \mathbf{v}^* + \mathbf{u}^* \Delta \mathbf{u}^* - \mathbf{v}^* \Delta^* \mathbf{v}^* + \mathbf{v}^* \mathbf{t}^* \mathbf{u}^* \\ \mathbf{v} \mathbf{t} \mathbf{u} - \mathbf{v} \Delta \mathbf{v} + \mathbf{u} \Delta^* \mathbf{u} + \mathbf{u} \mathbf{t}^* \mathbf{v} & -\mathbf{v} \mathbf{t} \mathbf{v}^* - \mathbf{v} \Delta \mathbf{u}^* - \mathbf{u} \Delta^* \mathbf{v}^* + \mathbf{u} \mathbf{t}^* \mathbf{u}^* \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} &\mathbf{u}^* \mathbf{t} \mathbf{v}^* + \mathbf{u}^* \Delta \mathbf{u}^* - \mathbf{v}^* \Delta^* \mathbf{v}^* + \mathbf{v}^* \mathbf{t}^* \mathbf{u}^* = 0 \\ &\mathbf{v} \mathbf{t} \mathbf{u} - \mathbf{v} \Delta \mathbf{v} + \mathbf{u} \Delta^* \mathbf{u} + \mathbf{u} \mathbf{t}^* \mathbf{v} = 0 \\ &E_\uparrow = -\mathbf{t} \mathbf{u}^2 + \Delta \mathbf{u}^* \mathbf{v} + \Delta^* \mathbf{u} \mathbf{v}^* + \mathbf{t}^* \mathbf{v}^2 = -\mathbf{t} \mathbf{u}^2 + \mathbf{t}^* \mathbf{v}^2 + 2\Re\{\Delta \mathbf{u}^* \mathbf{v}\} \\ &E_\downarrow = -\mathbf{t}^* \mathbf{u}^2 + \Delta \mathbf{u}^* \mathbf{v} + \Delta^* \mathbf{u} \mathbf{v}^* + \mathbf{t} \mathbf{v}^2 = -\mathbf{t}^* \mathbf{u}^2 + \mathbf{t} \mathbf{v}^2 + 2\Re\{\Delta \mathbf{u}^* \mathbf{v}\} \end{aligned}$$

As $\mathbf{t}$ is real,

$$\begin{aligned}
E_{\uparrow} &= -t(u^2 + v^2) + 2\Re\{\Delta u^* v\} = -t + 2\Re\{\Delta u^* v\} \\
E_{\downarrow} &= -t(u^2 + v^2) + 2\Re\{\Delta u^* v\} = -t + 2\Re\{\Delta u^* v\} \\
\Rightarrow E_{\uparrow} &= E_{\downarrow}
\end{aligned}$$

- (3) The equations of motion in terms of c_{σ} and $c_{\sigma}^{\dagger}$

$$\begin{aligned}
[\hat{c}_{i\sigma}, \hat{H}] &= \sum_j -t_{ij} \hat{c}_{j\sigma} + \sigma \Delta_{ij} \hat{c}_{j\bar{\sigma}}^{\dagger} \\
[\hat{c}_{i\sigma}^{\dagger}, \hat{H}] &= \sum_j t_{ij}^* \hat{c}_{j\sigma}^{\dagger} - \sigma \Delta_{ij}^* \hat{c}_{j\bar{\sigma}} \\
\left[\begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \hat{c}_{N\uparrow} \\ \hat{c}_{1\downarrow}^{\dagger} \\ \vdots \\ \hat{c}_{N\downarrow}^{\dagger} \end{pmatrix}, \hat{H} \right] &= \begin{pmatrix} 0 & -t_{12} & \cdots & -t_{1N} & \Delta_{11} & \cdots & \cdots & \Delta_{1N} \\ -t_{21} & 0 & \vdots & \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ -t_{N1} & \cdots & \cdots & 0 & \Delta_{N1} & \cdots & \cdots & \Delta_{NN} \\ \Delta_{11}^* & \cdots & \cdots & \Delta_{1N}^* & 0 & t_{12}^* & \cdots & t_{1N}^* \\ \vdots & \ddots & \vdots & \vdots & t_{21}^* & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ \Delta_{N1}^* & \cdots & \cdots & \Delta_{NN}^* & t_{N1}^* & \cdots & \cdots & 0 \end{pmatrix} \begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \hat{c}_{N\uparrow} \\ \hat{c}_{1\downarrow}^{\dagger} \\ \vdots \\ \hat{c}_{N\downarrow}^{\dagger} \end{pmatrix} \\
\Rightarrow \left[\begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix}, H \right] &= \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix} \cdots \cdots (d)
\end{aligned}$$

- (4) The equations of motion in terms of γ_{σ} and $\gamma_{\sigma}^{\dagger}$

R.H.S. of equation (d):

$$\left[\begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix}, H \right] = \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} \gamma_{\uparrow} \\ \gamma_{\downarrow}^{\dagger} \end{pmatrix}, H = \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix} \begin{pmatrix} \gamma_{\uparrow} \\ \gamma_{\downarrow}^{\dagger} \end{pmatrix}$$

L.H.S. of equation (d):

$$\begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} c_{\uparrow} \\ c_{\downarrow}^{\dagger} \end{pmatrix} = \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} \gamma_{\uparrow} \\ \gamma_{\downarrow}^{\dagger} \end{pmatrix}$$

Thus, we obtain

$$\begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} = \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix}$$

The equations above are called the Bogoliubov-de Gennes' (BdG) equations.

- (5) Global Index in Code Implementation

From the equation (c), the Hamiltonian matrix is

$$\mathbf{H} = \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} = \begin{pmatrix} 0 & -t_{12} & \cdots & -t_{1N} & \Delta_{11} & \cdots & \cdots & \Delta_{1N} \\ -t_{21} & 0 & \vdots & \vdots & \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ -t_{N1} & \cdots & \cdots & 0 & \Delta_{N1} & \cdots & \cdots & \Delta_{NN} \\ \Delta_{11}^* & \cdots & \cdots & \Delta_{1N}^* & 0 & t_{12}^* & \cdots & t_{1N}^* \\ \vdots & \ddots & \vdots & \vdots & t_{21}^* & 0 & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots & \vdots & \cdots & \ddots & \vdots \\ \Delta_{N1}^* & \cdots & \cdots & \Delta_{NN}^* & t_{N1}^* & \cdots & \cdots & 0 \end{pmatrix}$$

Declare a matrix in code implementation:

$$\mathbf{H} = \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} = \begin{pmatrix} h_{1,1} & \cdots & h_{1,N} & h_{1,N+1} & \cdots & h_{1,2N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ h_{N,1} & \cdots & h_{N,N} & h_{N,N+1} & \cdots & h_{N,2N} \\ h_{N+1,1} & \cdots & h_{N+1,N} & h_{N+1,N+1} & \cdots & h_{N+1,2N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ h_{2N,1} & \cdots & h_{2N,N} & h_{2N,N+1} & \cdots & h_{2N,2N} \end{pmatrix}$$

Diagonalize $\mathbf{H}$ and obtain eigenvectors:

$$\begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix} = \begin{pmatrix} u_1^1 & \cdots & u_1^N & -v_1^{1*} & \cdots & -v_1^{N*} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_N^1 & \cdots & u_N^N & -v_N^{1*} & \cdots & -v_N^{N*} \\ v_1^1 & \cdots & v_1^N & u_1^{1*} & \cdots & u_1^{N*} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ v_N^1 & \cdots & v_N^N & u_N^{1*} & \cdots & u_N^{N*} \end{pmatrix} = \begin{pmatrix} \mathbf{u}_1 \\ \vdots \\ \mathbf{u}_N \\ \mathbf{v}_1 \\ \vdots \\ \mathbf{v}_N \end{pmatrix}$$

where we define the global indices

$$\mathbf{u}_i = (\overbrace{\mathbf{u}_i^1}^{u_i^1} \cdots \overbrace{\mathbf{u}_i^N}^{u_i^N} \overbrace{\mathbf{u}_i^{N+1}}^{-v_i^{1*}} \cdots \overbrace{\mathbf{u}_i^{2N}}^{-v_i^{N*}})$$

$$\mathbf{v}_i = (\overbrace{\mathbf{v}_i^1}^{v_i^1} \cdots \overbrace{\mathbf{v}_i^N}^{v_i^N} \overbrace{\mathbf{v}_i^{N+1}}^{u_i^{1*}} \cdots \overbrace{\mathbf{v}_i^{2N}}^{u_i^{N*}})$$

OS:

After diagonalization, we should use the normalization conditions to verify the global index as follows:

$$\sum_n (|u_i^n|^2 + |v_i^n|^2) = 1$$

$$\sum_n (u_i^n v_i^{n*} - v_i^{n*} u_i^n) = 0$$

eigenvalues:

$$\begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix} = \begin{pmatrix} E_1 & & & & \\ & \ddots & & & 0 \\ & & E_N & & \\ & & & E_{N+1} & \\ 0 & & & & \ddots \\ & & & & & E_{2N} \end{pmatrix}$$

where

$$\begin{pmatrix} E_1 \\ \vdots \\ E_N \\ E_{N+1} \\ \vdots \\ E_{2N} \end{pmatrix} = \begin{pmatrix} E_{1\uparrow} \\ \vdots \\ E_{N\uparrow} \\ -E_{1\downarrow} \\ \vdots \\ -E_{N\downarrow} \end{pmatrix}$$

D. SELF-CONSISTENT CONDITIONS AND ORDER PARAMETERS

(1) Electron density:

$$\begin{aligned} \langle \hat{n}_{i\uparrow} \rangle &= \langle \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\uparrow} \rangle \\ &= \sum_n \left\langle \left(u_i^{n*} \hat{\gamma}_{n\uparrow}^\dagger - v_i^n \hat{\gamma}_{n\downarrow} \right) \left(u_i^n \hat{\gamma}_{n\uparrow} - v_i^{n*} \hat{\gamma}_{n\downarrow}^\dagger \right) \right\rangle \\ &= \sum_n \left[|u_i^n|^2 \langle \hat{\gamma}_{n\uparrow}^\dagger \hat{\gamma}_{n\uparrow} \rangle + |v_i^n|^2 \langle \hat{\gamma}_{n\downarrow} \hat{\gamma}_{n\downarrow}^\dagger \rangle \right] \\ &= \sum_n \left[|u_i^n|^2 f(E_{n\uparrow}) + |v_i^n|^2 f(-E_{n\downarrow}) \right] \\ \langle n_{i\downarrow} \rangle &= \langle \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\downarrow} \rangle \\ &= \sum_n \left\langle \left(u_i^{n*} \hat{\gamma}_{n\downarrow}^\dagger + v_i^n \hat{\gamma}_{n\uparrow} \right) \left(u_i^n \hat{\gamma}_{n\downarrow} + v_i^{n*} \hat{\gamma}_{n\uparrow}^\dagger \right) \right\rangle \\ &= \sum_n \left[v_i^n v_i^{n*} \langle \hat{\gamma}_{n\uparrow} \hat{\gamma}_{n\uparrow}^\dagger \rangle + u_i^{n*} u_i^n \langle \hat{\gamma}_{n\downarrow}^\dagger \hat{\gamma}_{n\downarrow} \rangle \right] \\ &= \sum_n \left[|v_i^n|^2 f(-E_{n\uparrow}) + |u_i^n|^2 f(E_{n\downarrow}) \right] \end{aligned}$$

Using global indices, we obtain

$$\langle n_{i\uparrow} \rangle = \sum_n \left[|u_i^n|^2 f(E_{n\uparrow}) + |v_i^n|^2 f(-E_{n\downarrow}) \right] = \sum_n |\mathbf{u}_i^n|^2 f(E_n)$$

$$\langle n_{i\downarrow} \rangle = \sum_n \left[|v_i^n|^2 f(-E_{n\uparrow}) + |u_i^n|^2 f(E_{n\downarrow}) \right] = \sum_n |\mathbf{v}_i^n|^2 [1 - f(E_n)]$$

Since

$$\begin{aligned} f(E_n) &= \frac{1}{e^{\beta E_n} + 1} \\ &= \frac{\frac{1}{2}}{\frac{1}{2} e^{\beta E_n} + 1} \\ &= \frac{1}{2} \left(1 - \frac{e^{\beta E_n} - 1}{e^{\beta E_n} + 1} \right) \\ &= \frac{1}{2} \left(1 - \frac{e^{\beta E_n/2} - e^{-\beta E_n/2}}{e^{\beta E_n/2} + e^{-\beta E_n/2}} \right) \\ &= \frac{1}{2} \left(1 - \tanh \frac{\beta E_n}{2} \right) \end{aligned}$$

we obtain

$$\begin{aligned} \langle n_{i\uparrow} \rangle &= \sum_{n=1}^{2N} |\mathbf{u}_i^n|^2 \frac{1}{2} \left(1 - \tanh \frac{\beta E_n}{2} \right) \\ \langle n_{i\downarrow} \rangle &= \sum_{n=1}^{2N} |\mathbf{v}_i^n|^2 \left[1 - \frac{1}{2} \left(1 - \tanh \frac{\beta E_n}{2} \right) \right] \\ &= \sum_{n=1}^{2N} |\mathbf{v}_i^n|^2 \frac{1}{2} \left(1 + \tanh \frac{\beta E_n}{2} \right) \end{aligned}$$

(2) Superconducting pairing:

$$\begin{aligned} \Delta_{ij} &= V \langle c_{i\uparrow} c_{j\downarrow} \rangle = \frac{V}{2} \langle c_{i\uparrow} c_{j\downarrow} - c_{j\downarrow} c_{i\uparrow} \rangle = \frac{V}{2} \left(\langle c_{i\uparrow} c_{j\downarrow} \rangle - \langle c_{j\downarrow} c_{i\uparrow} \rangle \right) \\ \langle c_{i\uparrow} c_{j\downarrow} \rangle &= \sum_n \left\langle \left(u_i^n \hat{\gamma}_{n\uparrow} - v_i^{n*} \hat{\gamma}_{n\downarrow}^\dagger \right) \left(u_j^n \hat{\gamma}_{n\downarrow} + v_j^{n*} \hat{\gamma}_{n\uparrow}^\dagger \right) \right\rangle \\ &= \sum_n \left[u_i^n v_j^{n*} \langle \hat{\gamma}_{n\uparrow} \hat{\gamma}_{n\uparrow}^\dagger \rangle - v_i^{n*} u_j^n \langle \hat{\gamma}_{n\downarrow}^\dagger \hat{\gamma}_{n\downarrow} \rangle \right] \\ &= \sum_n \left[u_i^n v_j^{n*} f(-E_{n\uparrow}) - v_i^{n*} u_j^n f(E_{n\downarrow}) \right] \end{aligned}$$

$$\begin{aligned}
\langle c_{i\uparrow} c_{j\downarrow} \rangle &= \sum_n \left\langle \left(u_j^n \hat{\gamma}_{n\downarrow} + v_j^{n*} \hat{\gamma}_{n\uparrow}^\dagger \right) \left(u_i^n \hat{\gamma}_{n\uparrow} - v_i^{n*} \hat{\gamma}_{n\downarrow}^\dagger \right) \right\rangle \\
&= \sum_n \left[-v_j^{n*} u_i^n \langle \hat{\gamma}_{n\uparrow}^\dagger \hat{\gamma}_{n\uparrow} \rangle + u_j^n v_i^{n*} \langle \hat{\gamma}_{n\downarrow} \hat{\gamma}_{n\downarrow}^\dagger \rangle \right] \\
&= \sum_n \left[-v_j^{n*} u_i^n f(E_{n\uparrow}) + u_j^n v_i^{n*} f(-E_{n\downarrow}) \right]
\end{aligned}$$

Using global indices, we obtain

$$\begin{aligned}
\Delta_{ij} &= \frac{V}{2} \sum_n \left[u_i^n v_j^{n*} f(-E_{n\uparrow}) - v_i^{n*} u_j^n f(E_{n\downarrow}) - v_j^{n*} u_i^n f(E_{n\uparrow}) + u_j^n v_i^{n*} f(-E_{n\downarrow}) \right] \\
&= \frac{V}{2} \sum_{n=1}^{2N} \left[\mathbf{u}_i^n \mathbf{v}_j^{n*} f(-E_n) - \mathbf{u}_i^n \mathbf{v}_j^{n*} f(E_n) \right] \\
&= \frac{V}{2} \sum_{n=1}^{2N} \mathbf{u}_i^n \mathbf{v}_j^{n*} [1 - 2f(E_n)]
\end{aligned}$$

Since

$$1 - 2f(E_n) = 1 - \frac{2}{e^{\beta E_n} + 1} = \frac{e^{\beta E_n} - 1}{e^{\beta E_n} + 1} = \tanh \frac{\beta E_n}{2}$$

we obtain

$$\Delta_{ij} = \frac{V}{2} \sum_{n=1}^{2N} \mathbf{u}_i^n \mathbf{v}_j^{n*} \tanh \frac{\beta E_n}{2}$$

EXAMPLES:

1. Solve the BdG equations for the d-wave superconductivity,

$$\begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix} = \begin{pmatrix} \mathbf{u} & -\mathbf{v}^* \\ \mathbf{v} & \mathbf{u}^* \end{pmatrix} \begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix}$$

We can then obtain the pairing using

$$\Delta_{ij} = \frac{V}{2} \sum_{n=1}^{2N} \mathbf{u}_i^n \mathbf{v}_j^{n*} \tanh \frac{\beta E_n}{2}$$

The d-wave superconductivity is

$$\Delta_i = \frac{1}{4} (\Delta_{i+x} + \Delta_{i-x} - \Delta_{i+y} - \Delta_{i-y})$$

- (3) D-density wave (DDW) order:

$$W_{ij\uparrow} = \frac{V}{2} \langle c_{i\uparrow}^\dagger c_{j\uparrow} - c_{j\uparrow}^\dagger c_{i\uparrow} \rangle = \frac{V}{2} \left(\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle - \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle^* \right) = V \cdot \Im \langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle$$

$$\begin{aligned}
W_{ij\downarrow} &= \frac{V}{2} \langle c_{i\downarrow}^\dagger c_{j\downarrow} - c_{j\downarrow}^\dagger c_{i\downarrow} \rangle = \frac{V}{2} \left(\langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle - \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle^* \right) = V \cdot \Im \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle \\
W_{ij} &= W_{ij\uparrow} + W_{ij\downarrow} = V \cdot \Im \left(\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle + \langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle \right) \\
\langle c_{i\uparrow}^\dagger c_{j\uparrow} \rangle &= \sum_n \left\langle \left(u_i^{n*} \gamma_{n\uparrow}^\dagger - v_i^n \gamma_{n\downarrow} \right) \left(u_j^n \gamma_{n\uparrow} - v_j^{n*} \gamma_{n\downarrow}^\dagger \right) \right\rangle \\
&= \sum_n \left\langle \left(u_i^{n*} \gamma_{n\uparrow}^\dagger - v_i^n \gamma_{n\downarrow} \right) \left(u_j^n \gamma_{n\uparrow} - v_j^{n*} \gamma_{n\downarrow}^\dagger \right) \right\rangle \\
&= \sum_n \left[u_i^{n*} u_j^n \langle \gamma_{n\uparrow}^\dagger \gamma_{n\uparrow} \rangle + v_i^n v_j^{n*} \langle \gamma_{n\downarrow} \gamma_{n\downarrow}^\dagger \rangle \right] \\
&= \sum_n \left[u_i^{n*} u_j^n f(E_{n\uparrow}) + v_i^n v_j^{n*} f(-E_{n\downarrow}) \right] \\
\langle c_{i\downarrow}^\dagger c_{j\downarrow} \rangle &= \sum_n \left\langle \left(u_i^{n*} \gamma_{n\downarrow}^\dagger + v_i^n \gamma_{n\uparrow} \right) \left(u_j^n \gamma_{n\downarrow} + v_j^{n*} \gamma_{n\uparrow}^\dagger \right) \right\rangle \\
&= \sum_n \left[u_i^{n*} u_j^n \langle \gamma_{n\downarrow}^\dagger \gamma_{n\downarrow} \rangle + v_i^n v_j^{n*} \langle \gamma_{n\uparrow} \gamma_{n\uparrow}^\dagger \rangle \right] \\
&= \sum_n \left[u_i^{n*} u_j^n f(E_{n\downarrow}) + v_i^n v_j^{n*} f(-E_{n\uparrow}) \right]
\end{aligned}$$

Using global indices, we obtain

$$\begin{aligned}
W_{ij} &= V \cdot \Im \sum_n \left[u_i^{n*} u_j^n f(E_{n\uparrow}) + v_i^n v_j^{n*} f(-E_{n\downarrow}) \right. \\
&\quad \left. + u_i^{n*} u_j^n f(E_{n\downarrow}) + v_i^n v_j^{n*} f(-E_{n\uparrow}) \right] \\
&= V \cdot \Im \sum_{n=1}^{2N} \left[\mathbf{u}_i^{n*} \mathbf{u}_j^n f(E_n) + \mathbf{v}_i^{n*} \mathbf{v}_j^n [1 - f(E_n)] \right]
\end{aligned}$$

4-2 Magnetic Field Effect

A. PEIERLS SUBSTITUTION IN TIGHT-BINDING MODEL

- (1) When apply an external magnetic field, the single-particle Hamiltonian and the Bloch eigenfunctions are

$$\begin{aligned}\hat{\mathcal{H}}_B &= \frac{1}{2m} \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right)^2 + V(\vec{r}) \\ \tilde{\psi}_k(\vec{r}) &= \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \tilde{w}(\vec{r} - \vec{R})\end{aligned}$$

Since in the presence of a magnetic field, the only term changed in the Hamiltonian is the momentum operator as

$$\vec{p} \rightarrow \vec{p} + \frac{e}{c} \vec{A}$$

Thus, we can assume the Wannier function as

$$\tilde{w}(\vec{r} - \vec{R}_i) = e^{i\varphi} w(\vec{r} - \vec{R})$$

The Schrödinger equation gives

$$\begin{aligned}\hat{\mathcal{H}}_B \tilde{\psi}_k(\vec{r}) &= \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \hat{\mathcal{H}} \tilde{w}(\vec{r} - \vec{R}) \\ &= \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} \left[\frac{1}{2m} \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right)^2 + V(\vec{r}) \right] \tilde{w}(\vec{r} - \vec{R})\end{aligned}$$

Since

$$\begin{aligned}\hat{\mathbf{p}} e^{i\varphi} w(\vec{r} - \vec{R}) &= -i\hbar \nabla e^{i\varphi} w(\vec{r} - \vec{R}) \\ &= -i\hbar \left[e^{i\varphi} \nabla w(\vec{r} - \vec{R}) + i e^{i\varphi} (\nabla \varphi) w(\vec{r} - \vec{R}) \right] \\ &= e^{i\varphi} (\hat{\mathbf{p}} + \hbar \nabla \varphi) w(\vec{r} - \vec{R}) \\ \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right)^2 \tilde{w}(\vec{r} - \vec{R}) &= \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right) \cdot \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right) e^{i\varphi} w(\vec{r} - \vec{R}) \\ &= \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} \right) \cdot e^{i\varphi} \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} + \hbar \nabla \varphi \right) w(\vec{r} - \vec{R}) \\ &= e^{i\varphi} \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} + \hbar \nabla \varphi \right)^2 w(\vec{r} - \vec{R})\end{aligned}$$

Thus, we obtain

$$\hat{\mathcal{H}}_B \tilde{\psi}_k(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k} \cdot \vec{R}} e^{i\varphi} \left[\frac{1}{2m} \left(\hat{\mathbf{p}} + \frac{e}{c} \vec{A} + \hbar \nabla \varphi \right)^2 + V(\vec{r}) \right] w(\vec{r} - \vec{R})$$

Since

$$\hat{\mathcal{H}}\psi_k(\vec{r}) = \left[\frac{\hat{p}^2}{2m} + V(\vec{r}) \right] \psi_k(\vec{r}) = \varepsilon_k \psi_k(\vec{r})$$

We need to set

$$\frac{e}{c} \vec{A} + \hbar \nabla \varphi = 0 \Rightarrow \varphi = -\frac{e}{\hbar c} \int_R^r \vec{A}(\vec{r}') \cdot d\vec{r}' \dots \dots \text{(a)}$$

Thus, we obtain

$$\hat{\mathcal{H}}_B \tilde{\psi}_k(\vec{r}) = e^{i\varphi} \hat{\mathcal{H}} \psi_k(\vec{r}) = e^{i\varphi} \varepsilon_k \psi_k(\vec{r}) = \varepsilon_k \tilde{\psi}_k(\vec{r})$$

$\Rightarrow$ The magnetic field has no effect on the eigenenergy at the scale of the crystal lattice and only adds a phase term in the Bloch wavefunction.

(2) Thus, the hopping integral is

$$\begin{aligned} \tilde{t}_{ij} &= - \int \tilde{w}^* (\vec{r} - \vec{R}_i) \hat{\mathcal{H}}_B \tilde{w} (\vec{r} - \vec{R}_j) d^3r \\ &= - \int e^{-i\varphi_i} w^* (\vec{r} - \vec{R}_i) e^{i\varphi_j} \hat{\mathcal{H}} w (\vec{r} - \vec{R}_j) d^3r \\ &= - \int e^{-i(\varphi_i - \varphi_j)} w^* (\vec{r} - \vec{R}_i) \hat{\mathcal{H}} w (\vec{r} - \vec{R}_j) d^3r \\ &= e^{-i(\varphi_i - \varphi_j)} t_{ij} \end{aligned}$$

Since

$$\begin{aligned} \varphi_i - \varphi_j &= -\frac{e}{\hbar c} \left(\int_{R_i}^r \vec{A}(\vec{r}') \cdot d\vec{r}' - \int_{R_j}^r \vec{A}(\vec{r}') \cdot d\vec{r}' \right) \\ &= -\frac{e}{\hbar c} \int_{R_i \rightarrow r \rightarrow R_j} \vec{A}(\vec{r}') \cdot d\vec{r}' \\ &= -\frac{e}{\hbar c} \oint_{\vec{R}_i \rightarrow \vec{r} \rightarrow \vec{R}_j \rightarrow \vec{R}_i} \vec{A}(\vec{r}') \cdot d\vec{r}' - \frac{e}{\hbar c} \int_{R_i}^{R_j} \vec{A}(\vec{r}') \cdot d\vec{r}' \end{aligned}$$

Since we assume $\vec{A}(\vec{r})$ is approximately uniform at the lattice scale - the scale at which the Wannier states are localized to the positions - we can approximate,

$$-\frac{e}{\hbar c} \oint_{\vec{R}_i \rightarrow \vec{r} \rightarrow \vec{R}_j \rightarrow \vec{R}_i} \vec{A}(\vec{r}') \cdot d\vec{r}' \approx 0$$

Let

$$\varphi_{ij} = \frac{e}{\hbar c} \int_{R_i}^{R_j} \vec{A}(\vec{r}') \cdot d\vec{r}' = \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}') \cdot d\vec{r}'$$

where Φ_0 is the single-particle flux quantum,

$$\Phi_0 = \frac{hc}{e} = 2.07 \times 10^{-15} \text{ Tm}^2$$

Thus, we obtain

$$\varphi_i - \varphi_j \approx -\varphi_{ij}$$

which is yielding the desired result,

$$\tilde{t}_{ij} = t_{ij} e^{i\varphi_{ij}}$$

$\Rightarrow$ Magnetic fields are incorporated in the tight-binding model by adding a phase to the hopping terms, i.e., the magnetic field enters the kinetic part of the Hamiltonian through a phase factor.

(3) Thus, the tight-binding Hamiltonian is

$$\hat{\mathcal{H}}_B = \sum_{ij\sigma} -\tilde{t}_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{ij} \Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}$$

Now, we can solve BdG equations as follows:

$$\begin{pmatrix} -\tilde{t} & \Delta \\ \Delta^* & \tilde{t}^* \end{pmatrix} \begin{pmatrix} \tilde{u} & -\tilde{v}^* \\ \tilde{v} & \tilde{u}^* \end{pmatrix} = \begin{pmatrix} \tilde{u} & -\tilde{v}^* \\ \tilde{v} & \tilde{u}^* \end{pmatrix} \begin{pmatrix} E_\uparrow & 0 \\ 0 & -E_\downarrow \end{pmatrix}$$

$$\sum_j \left[-\tilde{t}_{ij} \tilde{u}_j^n + \Delta_{ij} \tilde{v}_j^n \right] = E_{n\uparrow} \tilde{u}_i^n$$

$$\sum_j \left[-t_{ij} e^{-i(\varphi_i - \varphi_j)} \tilde{u}_j^n + \Delta_{ij} \tilde{v}_j^n \right] = E_{n\uparrow} \tilde{u}_i^n$$

Multiply $e^{i\varphi_i}$ on both sides

$$\sum_j \left[-t_{ij} e^{i\varphi_j} \tilde{u}_j^n + \Delta_{ij} \tilde{v}_j^n e^{i\varphi_i} \right] = E_{n\uparrow} \tilde{u}_i^n e^{i\varphi_i}$$

To make the equations covariant, let

$$\tilde{u}_j^n = u_j^n e^{-i\varphi_j}$$

$$\tilde{v}_j^n = v_j^n e^{-i\varphi_j}$$

$$\tilde{\Delta}_{ij} = \Delta_{ij} e^{i(\varphi_i - \varphi_j)}$$

We obtain

$$\sum_j \left[-t_{ij} e^{i\varphi_j} u_j^n e^{-i\varphi_j} + \Delta_{ij} v_j^n e^{-i\varphi_j} e^{i\varphi_i} \right] = E_{n\uparrow} u_i^n e^{i\varphi_i} e^{-i\varphi_i}$$

$$\sum_j \left[-t_{ij} u_j^n + \tilde{\Delta}_{ij} v_j^n \right] = E_{n\uparrow} u_i^n$$

EXAMPLES:

1. Solve the BdG equations for the d-wave superconductivity in the presence of a magnetic field,

$$\begin{pmatrix} -\tilde{t} & \Delta \\ \Delta^* & \tilde{t}^* \end{pmatrix} \begin{pmatrix} \tilde{u} & -\tilde{v}^* \\ \tilde{v} & \tilde{u}^* \end{pmatrix} = \begin{pmatrix} \tilde{u} & -\tilde{v}^* \\ \tilde{v} & \tilde{u}^* \end{pmatrix} \begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix}$$

We then obtain the pairing using

$$\tilde{\Delta}_{ij} = \frac{V}{2} \sum_{n=1}^{2N} \tilde{\mathbf{u}}_i^n \tilde{\mathbf{v}}_j^{n*} \tanh \frac{\beta E_n}{2} = \Delta_{ij} e^{i(\varphi_i - \varphi_j)}$$

Since the d-wave superconductivity is

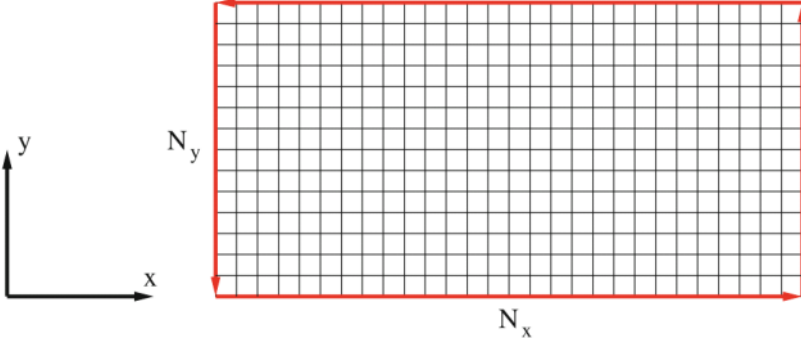
$$\Delta_i = \frac{1}{4} (\Delta_{i+x} + \Delta_{i-x} - \Delta_{i+y} - \Delta_{i-y})$$

We need calculate each pairing as

$$\Delta_{ij} = \tilde{\Delta}_{ij} e^{-i(\varphi_i - \varphi_j)} = \tilde{\Delta}_{ij} e^{i\varphi_{ij}}$$

B. RECTANGULAR VORTEX LATTICE

- (1) Consider a rectangular lattice with the linear dimensions N_x and N_y as a unit cell of the vortex lattice.



Since in the presence of a magnetic field, the magnetic effect is included through a Peierls phase factor as

$$\varphi_{ij} = \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r}$$

where $\nabla \times \vec{A} = B\hat{z}$. Thus, the flux density enclosed within one plaquette of the unit cell is given by

$$\sum_{\square} \varphi_{ij} = \sum_{\square} \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{2\pi}{\Phi_0} \sum_{\square} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r}$$

where $\square$ implies a closed loop

$$(x, y) \xrightarrow{\textcircled{1}} (x+1, y) \xrightarrow{\textcircled{2}} (x+1, y+1) \xrightarrow{\textcircled{3}} (x, y+1) \xrightarrow{\textcircled{4}} (x, y)$$

and

$$\sum_{\square} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \oint_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \int_S \nabla \times \vec{A} \cdot d\vec{S} = \int_S \vec{B} \cdot d\vec{S} = Ba^2$$

where S is the size of the plaquette and a is the lattice constant.

Thus, we obtain

$$\sum_{\square} \varphi_{ij} = \frac{2\pi}{\Phi_0} Ba^2$$

Since the single-particle flux enclosed in a unit cell is 2π such as

$$\sum_{\square} \varphi_{ij} = \sum_{i,j}^{N_x, N_y} \sum_{\square} \varphi_{ij} = \left(\frac{2\pi}{\Phi_0} Ba^2 \right) N_x N_y = 2\pi$$

where $\square$ implies a closed path around the rectangular lattice such as

$$(0,0) \xrightarrow{\textcircled{1}} (N_x a, 0) \xrightarrow{\textcircled{2}} (N_x a, N_y a) \xrightarrow{\textcircled{3}} (0, N_y a) \xrightarrow{\textcircled{4}} (0,0)$$

We then should obtain

$$B = \frac{\Phi_0}{N_x N_y a^2}$$

- (2) Since the rectangular lattice is a unit cell of the vortex lattice, we can introduce a translation operator $\hat{T}_{mn}$ such that

$$\vec{r}' = \hat{T}_{mn} \vec{r} = \vec{r} + \vec{R}$$

where $\vec{R} = mN_x a \hat{x} + nN_y a \hat{y}$.

The gauge transformation of the vector potential $\vec{A}$ under the translation operator is $\vec{A}(\hat{T}_{mn} \vec{r}) = \vec{A}(\vec{r}) + \nabla \chi(\vec{r})$

Now, consider a Landau gauge $\vec{A} = (-By, 0, 0)$ such that

$$\nabla \times \vec{A} = \begin{pmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ -By & 0 & 0 \end{pmatrix} = B\hat{z}$$

Thus, we have

$$\begin{aligned} \vec{A}(\hat{T}_{m0} \vec{r}) &= (-B\hat{T}_{m0}y, 0, 0) = (-By, 0, 0) = \vec{A}(\vec{r}) = \vec{A}(\vec{r}) + \nabla \chi(\vec{R}) \\ &\Rightarrow \nabla \chi(\vec{R}) = 0 \end{aligned}$$

and

$$\begin{aligned}
\vec{A}(\hat{T}_{0n}\vec{r}) &= (-B\hat{T}_{0n}y, 0, 0) \\
&= (-B(y + nN_y a), 0, 0) \\
&= (-By, 0, 0) + (-BnN_y a, 0, 0) \\
&= \vec{A}(\vec{r}) + \nabla\chi(\vec{R}) \\
\Rightarrow \nabla\chi(\vec{R}) &= -BnN_y a \hat{x} \\
\Rightarrow \chi(\vec{R}) &= -BnN_y ax
\end{aligned}$$

Thus, the Peierls phase factor becomes

$$\begin{aligned}
\varphi_{ij}(\vec{R}) &= \frac{2\pi}{\Phi_0} \int_{r_i}^{r_j+R} \vec{A}(\vec{r}') \cdot d\vec{r}' \\
&= \varphi_{ij} + \frac{2\pi}{\Phi_0} \int_0^R \nabla\chi(\vec{R}) \cdot d\vec{r}' \\
&= \varphi_{ij} + \frac{2\pi}{\Phi_0} (-BnN_y ax) \Big|_0^{R_x} \\
&= \varphi_{ij} + \frac{2\pi}{\Phi_0} (-BnN_y amN_x a) \\
&= \varphi_{ij} + \frac{2\pi}{\Phi_0} (-mn\Phi_0)
\end{aligned}$$

From 1-4-C,

$$\begin{aligned}
u'_i &= e^{i\frac{e}{\hbar c}\chi(R)} u_i = e^{i\frac{2\pi}{\Phi_0}\chi(R)} u_i \\
v'_i &= e^{-i\frac{e}{\hbar c}\chi(R)} v_i = e^{-i\frac{2\pi}{\Phi_0}\chi(R)} v_i \\
\Delta'_{ij} &= e^{i2\frac{e}{\hbar c}\chi(R)} \Delta_{ij} = e^{i\frac{4\pi}{\Phi_0}\chi(R)} \Delta_{ij}
\end{aligned}$$

we then obtain

$$\chi(\vec{R}) = -mn\Phi_0$$

By considering a closed path around the rectangular lattice,

$$(0,0) \xrightarrow{\textcircled{1}} (N_x a, 0) \xrightarrow{\textcircled{2}} (N_x a, N_y a) \xrightarrow{\textcircled{3}} (0, N_y a) \xrightarrow{\textcircled{4}} (0,0)$$

the acquired flux of the superconducting pairing is

$$\sum_{\square} \varphi = -\frac{4\pi}{\Phi_0} (-\Phi_0) = 4\pi$$

$\Rightarrow$ The flux enclosed by a unit cell has two superconducting flux quanta. Each vortex carries the flux quantum $\hbar c/2e$.

C. PERIODIC BOUNDARY CONDITIONS

- (1) Since a magnetic unit cell contains two vortices, conventionally, we set the dimension of the lattice as $N_x = 2N_y$. Thus, each vortex is enclosed in a square lattice with size $\frac{N_x}{2}N_y$.
- (2) For the nearest neighbor hopping term, the flux density in each plaquette is

$$\begin{aligned}
\sum_{\square} \varphi_{ij} &= \sum_{\square} \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \varphi_{\odot} + \varphi_{\ominus} + \varphi_{\circledast} + \varphi_{\circledcirc} \\
\varphi_{\odot} &= \frac{2\pi}{\Phi_0} \int_{x,y}^{x+1,y} \vec{A}(\vec{r}) \cdot d\vec{r} = -\frac{2\pi}{\Phi_0} B y a^2 \\
\varphi_{\ominus} &= \frac{2\pi}{\Phi_0} \int_{x+1,y}^{x+1,y+1} \vec{A}(\vec{r}) \cdot d\vec{r} = 0 \\
\varphi_{\circledast} &= \frac{2\pi}{\Phi_0} \int_{x+1,y+1}^{x,y+1} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{2\pi}{\Phi_0} B (y+1) a^2 \\
\varphi_{\circledcirc} &= \frac{2\pi}{\Phi_0} \int_{x,y+1}^{x,y} \vec{A}(\vec{r}) \cdot d\vec{r} = 0
\end{aligned}$$

For each plaquette, we have

$$\begin{aligned}
\sum_{\square} \varphi_{ij} &= -\frac{2\pi}{\Phi_0} B y a^2 + 0 + \frac{2\pi}{\Phi_0} B (y+1) a^2 + 0 \\
&= \frac{2\pi}{\Phi_0} \left(\frac{\Phi_0}{N_x N_y a^2} \right) a^2 \\
&= \frac{2\pi}{N_x N_y}
\end{aligned}$$

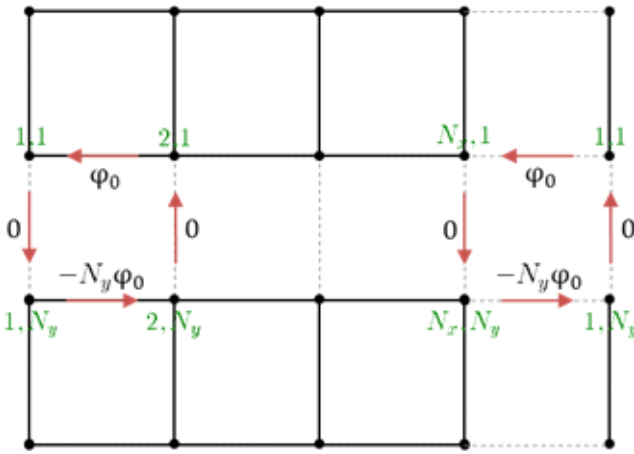
We then define a constant phase

$$\varphi_0 = \frac{2\pi}{N_x N_y}$$

The Peierls phase factors are

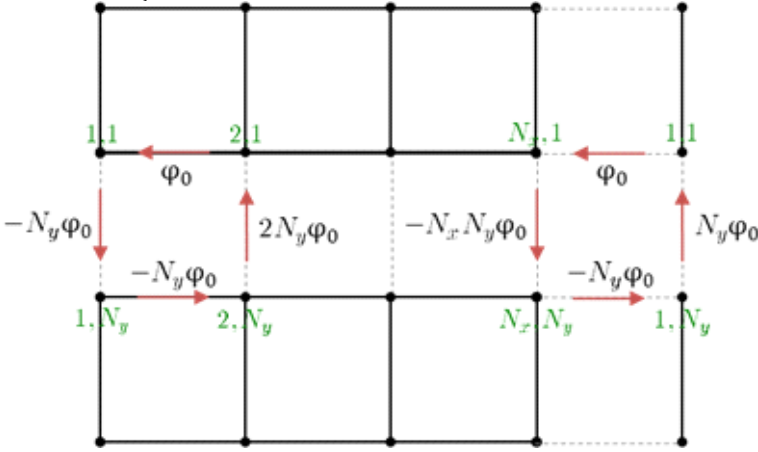
$$\varphi_{ij} = \begin{cases} \varphi_{\rightarrow} = -\frac{2\pi}{N_x N_y} y = -\varphi_0 y, & \text{along } +x \text{ direction} \\ \varphi_{\leftarrow} = \frac{2\pi}{N_x N_y} y = \varphi_0 y & , \quad \text{along } -x \text{ direction} \\ \varphi_{\uparrow} = 0 & , \quad \text{along } +y \text{ direction} \\ \varphi_{\downarrow} = 0 & , \quad \text{along } -y \text{ direction} \end{cases}$$

At the boundaries,



the flux of each plaquette is $-(N_y - 1)\varphi_0$. Thus, we need to manually compensate the phase to ensure that the flux equals to φ_0 . We then define the Peierls phase factors at the boundary as

$$\varphi_{ij} = \begin{cases} \varphi_0 N_y x, & \text{along } +y \text{ direction, at } y = N_y \\ -\varphi_0 N_y x, & \text{along } -y \text{ direction, at } y = 1 \end{cases}$$



- (3) For the next nearest neighbor hopping term, the flux density in each triangle-plaquette is

$$\begin{aligned} \sum_{\square} \varphi_{ij} &= \sum_{\square} \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \varphi_{\odot} + \varphi_{\otimes} + \varphi_{\ominus} \\ \varphi_{\odot} &= \frac{2\pi}{\Phi_0} \int_{x,y}^{x+1,y} \vec{A}(\vec{r}) \cdot d\vec{r} = -\frac{2\pi}{\Phi_0} B y a^2 \end{aligned}$$

$$\varphi_{\textcircled{2}} = \frac{2\pi}{\Phi_0} \int_{x+1,y}^{x+1,y+1} \vec{A}(\vec{r}) \cdot d\vec{r} = 0$$

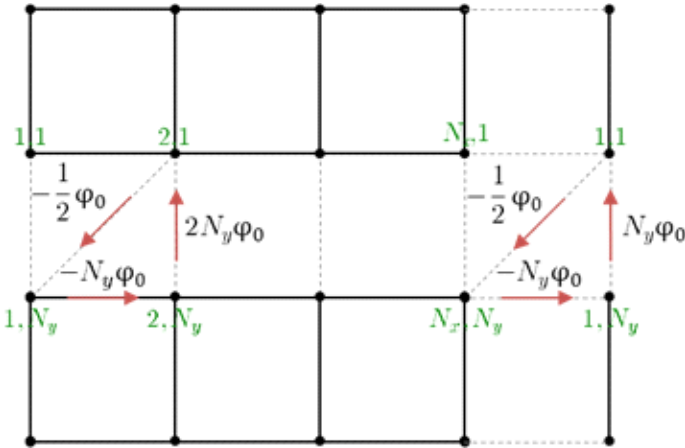
$$\begin{aligned} \varphi_{\textcircled{3}} &= \frac{2\pi}{\Phi_0} \int_{x+1,y+1}^{x,y} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{2\pi}{\Phi_0} B \frac{(y+1)^2 - y^2}{2} a^2 \\ &= \frac{2\pi}{\Phi_0} B \left(y + \frac{1}{2} \right) a^2 \end{aligned}$$

$$\sum_{\square} \varphi_{ij} = \frac{2\pi}{\Phi_0} B \frac{a^2}{2} = \frac{2\pi}{\Phi_0} \frac{\Phi_0}{N_x N_y a^2} \frac{a^2}{2} = \frac{1}{2} \frac{2\pi}{N_x N_y} = \frac{\varphi_0}{2}$$

The Peierls phase factors are

$$\varphi_{ij} = \begin{cases} \varphi_{\nearrow} = -\varphi_0 \left(y + \frac{1}{2} \right), & \text{along } +x + y \text{ direction} \\ \varphi_{\nwarrow} = \varphi_0 \left(y + \frac{1}{2} \right), & \text{along } -x + y \text{ direction} \\ \varphi_{\searrow} = -\varphi_0 \left(y - \frac{1}{2} \right), & \text{along } +x - y \text{ direction} \\ \varphi_{\swarrow} = \varphi_0 \left(y - \frac{1}{2} \right), & \text{along } -x - y \text{ direction} \end{cases}$$

At the boundaries



we define the Peierls phase factors as

$$\varphi_{ij} = \begin{cases} \varphi_0 \left(N_y x - \frac{1}{2} \right) & , \text{ along } +x + y \text{ direction, at } y = N_y \\ \varphi_0 \left(N_y x + \frac{1}{2} \right) & , \text{ along } -x + y \text{ direction, at } y = N_y \\ -\varphi_0 \left(N_y (x + 1) + \frac{1}{2} \right) & , \text{ along } +x - y \text{ direction, at } y = 1 \\ -\varphi_0 \left(N_y (x - 1) - \frac{1}{2} \right) & , \text{ along } -x - y \text{ direction, at } y = 1 \end{cases}$$

OS:

For some computer language, the index conventionally starts from 0. Thus, we need to modify the boundary conditions as follows:

$$\varphi_{ij} = \begin{cases} \varphi_0 \left(N_y x + \frac{1}{2} \right) & , \text{ along } +x + y \text{ direction, at } y = N_y - 1 \\ \varphi_0 \left(N_y x - \frac{1}{2} \right) & , \text{ along } -x + y \text{ direction, at } y = N_y - 1 \\ -\varphi_0 \left(N_y (x + 1) - \frac{1}{2} \right) & , \text{ along } +x - y \text{ direction, at } y = 0 \\ -\varphi_0 \left(N_y (x - 1) + \frac{1}{2} \right) & , \text{ along } -x - y \text{ direction, at } y = 0 \end{cases}$$

- (4) For the 3rd nearest neighbor hopping term, the flux density in each triangle-plaquette is

$$\sum_{\square} \varphi_{ij} = \sum_{\square} \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \varphi_{\odot} + \varphi_{\ominus} + \varphi_{\circledast} + \varphi_{\circledcirc}$$

$$\varphi_{\textcircled{1}} = \frac{2\pi}{\Phi_0} \int_{x,y}^{x+2,y} \vec{A}(\vec{r}) \cdot d\vec{r} = -\frac{2\pi}{\Phi_0} B 2y a^2$$

$$\varphi_{\textcircled{2}} = \frac{2\pi}{\Phi_0} \int_{x+2,y}^{x+2,y+1} \vec{A}(\vec{r}) \cdot d\vec{r} = 0$$

$$\varphi_{\textcircled{3}} = \frac{2\pi}{\Phi_0} \int_{x+2,y+1}^{x,y+1} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{2\pi}{\Phi_0} B 2(y+1) a^2$$

$$\varphi_{\textcircled{4}} = \frac{2\pi}{\Phi_0} \int_{x,y+1}^{x,y} \vec{A}(\vec{r}) \cdot d\vec{r} = 0$$

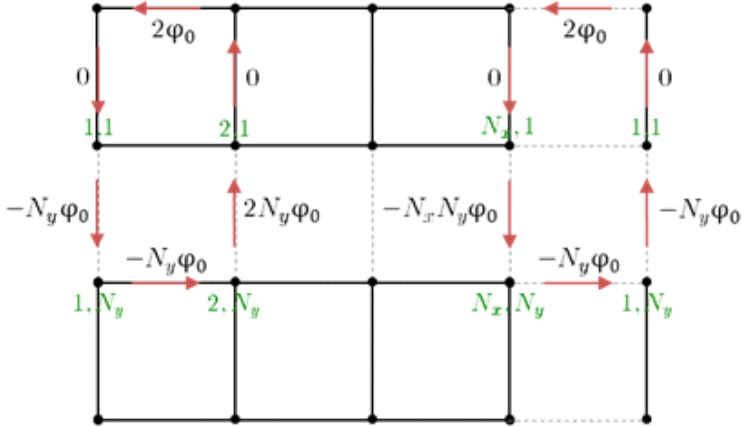
$$\sum_{\square} \varphi_{ij} = \frac{2\pi}{\Phi_0} B 2a^2 = \frac{2\pi}{\Phi_0} \frac{2\Phi_0}{N_x N_y a^2} a^2 = 2 \frac{2\pi}{N_x N_y} = 2\varphi_0$$

The Peierls phase factors are

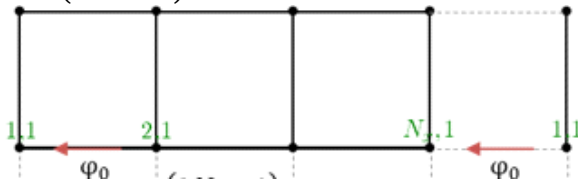
$$\varphi_{ij} = \begin{cases} -\varphi_0 2y, & \text{along } +x \text{ direction} \\ \varphi_0 2y, & \text{along } -x \text{ direction} \\ 0, & \text{along } +y \text{ direction} \\ 0, & \text{along } -y \text{ direction} \end{cases}$$

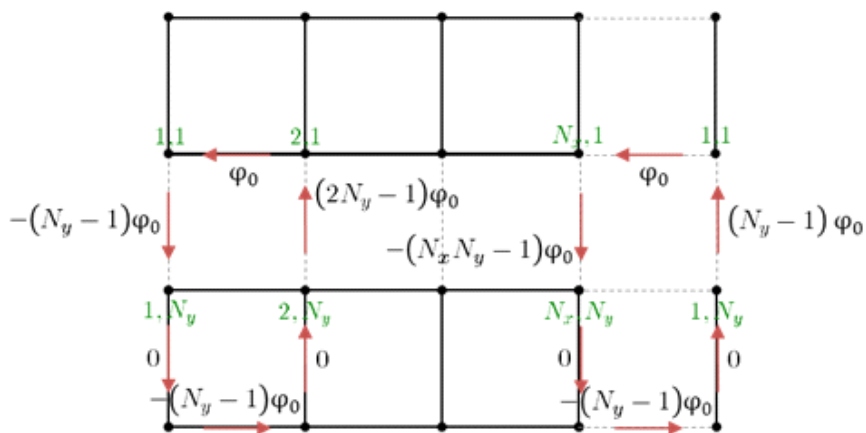
At the boundaries, we define the Peierls phase factors as

$$\varphi_{ij} = \begin{cases} \varphi_0 N_y x, & \text{along } +y \text{ direction, at } y = N_y \\ -\varphi_0 N_y x, & \text{along } -y \text{ direction, at } y = 2 \end{cases}$$



$$\varphi_{ij} = \begin{cases} \varphi_0 (N_y x - 1), & \text{along } +y \text{ direction, at } y = N_y - 1 \\ -\varphi_0 (N_y x - 1), & \text{along } -y \text{ direction, at } y = 1 \end{cases}$$





4-3 Local Density of States

A. GREEN'S FUNCTIONS ON LATTICE

(1) Matsubara Green's function

$$\begin{aligned}
 G_{ij\uparrow}(\tau) &= -\left\langle \hat{T} \left[\hat{c}_{i\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right] \right\rangle = -\Theta(\tau) \left\langle \hat{c}_{i\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right\rangle + \Theta(-\tau) \left\langle \hat{c}_{j\uparrow}^\dagger(0) \hat{c}_{i\uparrow}(\tau) \right\rangle \\
 G_{ij\downarrow}^*(\tau) &= -\left\langle \hat{T} \left[\hat{c}_{i\downarrow}^\dagger(\tau) \hat{c}_{j\downarrow}(0) \right] \right\rangle \\
 &= -\Theta(\tau) \left\langle \hat{c}_{i\downarrow}^\dagger(\tau) \hat{c}_{j\downarrow}(0) \right\rangle + \Theta(-\tau) \left\langle \hat{c}_{j\downarrow}(0) \hat{c}_{i\downarrow}^\dagger(\tau) \right\rangle \\
 F_{ij}(\tau) &= -\left\langle \hat{T} \left[\hat{c}_{i\uparrow}(\tau) \hat{c}_{j\downarrow}(0) \right] \right\rangle = -\Theta(\tau) \left\langle \hat{c}_{i\uparrow}(\tau) \hat{c}_{j\downarrow}(0) \right\rangle + \Theta(-\tau) \left\langle \hat{c}_{j\downarrow}(0) \hat{c}_{i\uparrow}(\tau) \right\rangle \\
 F_{ij}^*(\tau) &= -\left\langle \hat{T} \left[\hat{c}_{i\downarrow}^\dagger(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right] \right\rangle = -\Theta(\tau) \left\langle \hat{c}_{i\downarrow}^\dagger(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right\rangle + \Theta(-\tau) \left\langle \hat{c}_{j\uparrow}^\dagger(0) \hat{c}_{i\downarrow}^\dagger(\tau) \right\rangle
 \end{aligned}$$

The equations of motion of Green's function

$$\begin{aligned}
 \frac{\partial}{\partial \tau} G_{ij\uparrow}(\tau) &= -\frac{\partial}{\partial \tau} \Theta(\tau) \left\langle \hat{c}_{i\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right\rangle + \frac{\partial}{\partial \tau} \Theta(-\tau) \left\langle \hat{c}_{j\uparrow}^\dagger(0) \hat{c}_{i\uparrow}(\tau) \right\rangle \\
 &\quad - \Theta(\tau) \left\langle \frac{\partial}{\partial \tau} \hat{c}_{i\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right\rangle + \Theta(-\tau) \left\langle \hat{c}_{j\uparrow}^\dagger(0) \frac{\partial}{\partial \tau} \hat{c}_{i\uparrow}(\tau) \right\rangle
 \end{aligned}$$

Since $\frac{\partial}{\partial \tau} \Theta(\tau) = \delta(\tau)$ and $\frac{\partial}{\partial \tau} \Theta(-\tau) = -\delta(-\tau)$

$$\frac{\partial}{\partial \tau} G_{ij\uparrow}(\tau) = -\delta(\tau) \left\langle \left\{ \hat{c}_{i\uparrow}(\tau), \hat{c}_{j\uparrow}^\dagger(0) \right\} \right\rangle - \left\langle \hat{T} \left[\frac{\partial}{\partial \tau} \hat{c}_{i\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right] \right\rangle$$

Use

$$\begin{aligned}
 -\frac{\partial}{\partial \tau} \hat{c}_{i\sigma}^\dagger(\tau) &= [\hat{c}_{i\sigma}^\dagger(\tau), \hat{H}] = \sum_j t_{ij}^* \hat{c}_{j\sigma}^\dagger - \sigma \Delta_{ij}^* c_{v\bar{\sigma}} \\
 -\frac{\partial}{\partial \tau} c_{i\sigma}(\tau) &= [c_{i\sigma}(\tau), \hat{H}] = \sum_l -t_{il} \hat{c}_{l\sigma}(\tau) + \sigma \Delta_{il} \hat{c}_{l\bar{\sigma}}^\dagger(\tau)
 \end{aligned}$$

We obtain

$$\begin{aligned}
 \frac{\partial}{\partial \tau} G_{ij\uparrow}(\tau) &= -\delta(\tau) \delta_{ij} + \sum_l \left\langle \hat{T} \left[-t_{il} c_{l\uparrow}(\tau) \hat{c}_{j\uparrow}^\dagger(0) + \Delta_{il} \hat{c}_{l\downarrow}^\dagger(\tau) \hat{c}_{j\uparrow}^\dagger(0) \right] \right\rangle \\
 &= -\delta(\tau) \delta_{ij} + \sum_l \left(t_{il} G_{lj\uparrow}(\tau) - \Delta_{il} F_{lj}^*(\tau) \right)
 \end{aligned}$$

$$\begin{aligned}
\frac{\partial}{\partial \tau} G_{ij\downarrow}^*(\tau) &= -\delta(\tau) \left\langle \{c_{i\downarrow}^\dagger(\tau), c_{j\downarrow}(0)\} \right\rangle - \left\langle \hat{T} \left[\frac{\partial}{\partial \tau} c_{i\downarrow}^\dagger(\tau) c_{j\downarrow}(0) \right] \right\rangle \\
&= \delta(\tau) \delta_{ij} + \sum_l \left(-t_{il}^* G_{lj\downarrow}^*(\tau) - \Delta_{il}^* F_{lj}(\tau) \right) \\
\frac{\partial}{\partial \tau} F_{ij}(\tau) &= -\delta(\tau) \left\langle \{c_{i\uparrow}(\tau), c_{j\downarrow}(0)\} \right\rangle - \left\langle \hat{T} \left[\frac{\partial}{\partial \tau} c_{i\uparrow}(\tau) c_{j\downarrow}(0) \right] \right\rangle \\
&= \sum_l \left(t_{il} F_{lj}(\tau) - \Delta_{il} G_{lj\downarrow}^*(\tau) \right) \\
\frac{\partial}{\partial \tau} F_{ij}^*(\tau) &= -\delta(\tau) \left\langle \{c_{i\downarrow}^\dagger(\tau), c_{j\uparrow}^\dagger(0)\} \right\rangle - \left\langle \hat{T} \left[\frac{\partial}{\partial \tau} c_{i\downarrow}^\dagger(\tau) c_{j\uparrow}^\dagger(0) \right] \right\rangle \\
&= \sum_l \left(-\Delta_{il}^* G_{lj\uparrow}(\tau) - t_{il}^* F_{lj}^*(\tau) \right)
\end{aligned}$$

These equations are rearranged

$$\begin{aligned}
-\frac{\partial}{\partial \tau} G_{ij\uparrow}(\tau) - \sum_l \left(-t_{il} G_{lj\uparrow}(\tau) + \Delta_{il} F_{lj}^*(\tau) \right) &= \delta(\tau) \delta_{ij} \\
-\frac{\partial}{\partial \tau} F_{ij}(\tau) - \sum_l \left(-t_{il} F_{lj}(\tau) + \Delta_{il} G_{lj\downarrow}^*(\tau) \right) &= 0 \\
-\frac{\partial}{\partial \tau} F_{ij}^*(\tau) - \sum_l \left(\Delta_{il}^* G_{lj\uparrow}(\tau) + t_{il}^* F_{lj}^*(\tau) \right) &= 0 \\
-\frac{\partial}{\partial \tau} G_{ij\downarrow}^*(\tau) - \sum_l \left(t_{il}^* G_{lj\downarrow}^*(\tau) + \Delta_{il}^* F_{lj}(\tau) \right) &= \delta(\tau) \delta_{ij}
\end{aligned}$$

We now write these equations in a matrix form

$$-\frac{\partial}{\partial \tau} \begin{pmatrix} G_{11\uparrow} & \cdots & G_{1N\uparrow} & F_{11} & \cdots & F_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ G_{N1\uparrow} & \cdots & G_{NN\uparrow} & F_{N1} & \cdots & F_{NN} \\ F_{11}^* & \cdots & F_{1N}^* & G_{11\downarrow}^* & \cdots & G_{1N\downarrow}^* \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ F_{N1}^* & \cdots & F_{NN}^* & G_{N1\downarrow}^* & \cdots & G_{NN\downarrow}^* \end{pmatrix} - \begin{pmatrix} -t_{11} & \cdots & -t_{1N} & \Delta_{11} & \cdots & \Delta_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -t_{N1} & \cdots & -t_{NN} & \Delta_{N1} & \cdots & \Delta_{NN} \\ \Delta_{11}^* & \cdots & \Delta_{1N}^* & t_{11}^* & \cdots & t_{1N}^* \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \Delta_{11}^* & \cdots & \Delta_{1N}^* & t_{N1}^* & \cdots & t_{NN}^* \end{pmatrix} \begin{pmatrix} G_{11\uparrow} & \cdots & G_{1N\uparrow} & F_{11} & \cdots & F_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ G_{N1\uparrow} & \cdots & G_{NN\uparrow} & F_{N1} & \cdots & F_{NN} \\ F_{11}^* & \cdots & F_{1N}^* & G_{11\downarrow}^* & \cdots & G_{1N\downarrow}^* \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ F_{N1}^* & \cdots & F_{NN}^* & G_{N1\downarrow}^* & \cdots & G_{NN\downarrow}^* \end{pmatrix}$$

$$= \delta(\tau) \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

Let

$$G_{\sigma} = \begin{pmatrix} G_{11\sigma} & \cdots & G_{1N\sigma} \\ \vdots & \ddots & \vdots \\ G_{N1\sigma} & \cdots & G_{NN\sigma} \end{pmatrix}, \quad F = \begin{pmatrix} F_{11} & \cdots & F_{1N} \\ \vdots & \ddots & \vdots \\ F_{N1} & \cdots & F_{NN} \end{pmatrix}$$

The equations can be rewritten as

$$\begin{aligned} & -\frac{\partial}{\partial \tau} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(\tau) - \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(\tau) = \delta(\tau) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \Rightarrow & \left[-\frac{\partial}{\partial \tau} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \right] \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(\tau) = \delta(\tau) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

This equation is known as Gor'kov equations.

(2) Fourier transform of the Green's functions

$$\begin{aligned} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(\tau) &= \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) \\ \delta(\tau) &= \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} \end{aligned}$$

Substituting into Gor'kov equations, we obtain

$$\begin{aligned} & \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} \left[i\omega \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \right] \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) = \frac{1}{\beta} \sum_{\omega} e^{-i\omega\tau} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \Rightarrow & \left[\begin{pmatrix} i\omega & 0 \\ 0 & i\omega \end{pmatrix} - \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \right] \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

Insert Bogoliubov unitary transformation matrix

$$\left[\begin{pmatrix} i\omega & 0 \\ 0 & i\omega \end{pmatrix} - \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix} \right] \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix}^{\dagger} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The solutions of BdG equations give us

$$\begin{aligned} & \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \left[\begin{pmatrix} i\omega & 0 \\ 0 & i\omega \end{pmatrix} - \begin{pmatrix} E_{\uparrow} & 0 \\ 0 & -E_{\downarrow} \end{pmatrix} \right] \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix}^{\dagger} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ \Rightarrow & \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} i\omega - E_{\uparrow} & 0 \\ 0 & i\omega + E_{\downarrow} \end{pmatrix} \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix}^{\dagger} \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

$$\begin{aligned}
\Rightarrow \begin{pmatrix} G_{\uparrow} & F \\ F^* & G_{\downarrow}^* \end{pmatrix} (i\omega) &= \left[\begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} i\omega - E_{\uparrow} & 0 \\ 0 & i\omega + E_{\downarrow} \end{pmatrix} \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix}^{\dagger} \right]^{-1} \\
&= \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix} \begin{pmatrix} \frac{1}{i\omega - E_{\uparrow}} & 0 \\ 0 & \frac{1}{i\omega + E_{\downarrow}} \end{pmatrix} \begin{pmatrix} u^* & v^* \\ -v & u \end{pmatrix} \\
&= \begin{pmatrix} \frac{uu^*}{i\omega - E_{\uparrow}} + \frac{v^*v}{i\omega + E_{\downarrow}} & \frac{uv^*}{i\omega - E_{\uparrow}} - \frac{v^*u}{i\omega + E_{\downarrow}} \\ \frac{vu^*}{i\omega - E_{\uparrow}} - \frac{u^*v}{i\omega + E_{\downarrow}} & \frac{v^*v}{i\omega - E_{\uparrow}} + \frac{uu^*}{i\omega + E_{\downarrow}} \end{pmatrix}
\end{aligned}$$

Use global indices $\mathbf{u}_i^n$, $\mathbf{v}_i^n$, and E_n , i.e,

$$\begin{aligned}
\mathbf{u}_i &= (\underbrace{u_i^1}_{\mathbf{u}_i^1} \dots \underbrace{u_i^N}_{\mathbf{u}_i^N} \underbrace{-v_i^{1*}}_{\mathbf{u}_i^{N+1}} \dots \underbrace{-v_i^{N*}}_{\mathbf{u}_i^{2N}}) \\
\mathbf{v}_i &= (\underbrace{v_i^1}_{\mathbf{v}_i^1} \dots \underbrace{v_i^N}_{\mathbf{v}_i^N} \underbrace{u_i^{1*}}_{\mathbf{v}_i^{N+1}} \dots \underbrace{u_i^{N*}}_{\mathbf{v}_i^{2N}}) \\
\begin{pmatrix} E_1 \\ \vdots \\ E_N \\ E_{N+1} \\ \vdots \\ E_{2N} \end{pmatrix} &= \begin{pmatrix} E_{1\uparrow} \\ \vdots \\ E_{N\uparrow} \\ -E_{1\downarrow} \\ \vdots \\ -E_{N\downarrow} \end{pmatrix}
\end{aligned}$$

Thus, we obtain

$$\begin{pmatrix} G_{i\uparrow} & F_{ij} \\ F_{ij}^* & G_{i\downarrow}^* \end{pmatrix} (i\omega) = \sum_n \begin{pmatrix} \frac{\mathbf{u}_i^n \mathbf{u}_j^{n*}}{i\omega - E_n} & \frac{\mathbf{u}_i^n \mathbf{v}_j^{n*}}{i\omega - E_n} \\ \frac{\mathbf{v}_i^n \mathbf{u}_j^{n*}}{i\omega - E_n} & \frac{\mathbf{v}_i^n \mathbf{v}_j^{n*}}{i\omega - E_n} \end{pmatrix}$$

B. LOCAL DENSITY OF STATES

(1) The local density of states at zero temperature

$$\begin{aligned}
\rho_i(\omega) &= -\frac{1}{\pi} \Im(G_{ii\uparrow} + G_{ii\downarrow}) \\
-\frac{1}{\pi} \Im(G_{ii\uparrow}) &= -\frac{1}{\pi} \sum_n \Im \left(\frac{\mathbf{u}_i^n \mathbf{u}_i^{n*}}{i\omega - E_n} \right) = -\sum_n |\mathbf{u}_i^n|^2 \delta(E_n - \omega) \\
-\frac{1}{\pi} \Im(G_{ii\downarrow}) &= -\frac{1}{\pi} \sum_n \Im \left(\frac{\mathbf{v}_i^{n*} \mathbf{v}_i^n}{i\omega + E_n} \right) = -\sum_n |\mathbf{v}_i^n|^2 \delta(E_n + \omega)
\end{aligned}$$

$$\rho_i(\omega) = - \sum_n |\mathbf{u}_i^n|^2 \delta(E_n - \omega) + |\mathbf{v}_i^n|^2 \delta(E_n + \omega)$$

OS:

$$\frac{1}{\pi} \Im \left(\frac{1}{i\omega - E_n} \right) = \delta(E_n - \omega)$$

- (2) The local density of states at finite temperature T

Using the property of δ -function

$$\begin{aligned} \delta(E_n - \omega) &= -f'(E_n - \omega) = -\frac{df(\omega)}{d\omega} \\ \rho_i(\omega) &= \sum_n |\mathbf{u}_i^n|^2 f'(E_n - \omega) + |\mathbf{v}_i^n|^2 f'(E_n + \omega) \end{aligned}$$

Since

$$\begin{aligned} f(E_n \pm \omega) &= \frac{1}{1 + e^{\beta(E_n \pm \omega)}} \\ &= \frac{1}{1 + \frac{1 + \tanh\left(\frac{\beta(E_n \pm \omega)}{2}\right)}{1 - \tanh\left(\frac{\beta(E_n \pm \omega)}{2}\right)}} \\ &= \frac{1}{2} \left(1 - \tanh\left(\frac{\beta(E_n \pm \omega)}{2}\right) \right) \end{aligned}$$

The derivative of the Fermi function is

$$-\frac{\partial}{\partial \omega} f(E_n \pm \omega) = \frac{\beta}{4} \left[1 - \tanh^2 \left(\frac{\beta(E_n \pm \omega)}{2} \right) \right]$$

The local density of states at the temperature T is

$$\begin{aligned} \rho_i(\omega) &= \frac{\beta}{4} \sum_n \left\{ |\mathbf{u}_i^n|^2 \left[1 - \tanh^2 \left(\frac{\beta(E_n - \omega)}{2} \right) \right] \right. \\ &\quad \left. + |\mathbf{v}_i^n|^2 \left[1 - \tanh^2 \left(\frac{\beta(E_n + \omega)}{2} \right) \right] \right\} \end{aligned}$$

C. SUPERCCELL

- (1) Let $M_i L_i$ be the length of a crystal and $L_i = N_i a_i$ be the length of a supercell.

Apply the periodic boundary conditions

$$\begin{aligned} \mathbf{u}_k(\vec{r} + M\vec{L}) &= e^{i\vec{k} \cdot M\vec{L}} \mathbf{u}_k(\vec{r}) = \mathbf{u}_k(\vec{r}) \\ \Rightarrow e^{ik_i M_i L_i} &= 1 \\ \Rightarrow k_i &= \frac{2\pi \ell_i}{M_i L_i} = \frac{\ell_i}{M_i} \frac{2\pi}{L_i} \text{ where } \ell_i = 0, \dots, M_i - 1 \end{aligned}$$

The Bloch wavefunctions for each supercell are

$$\mathbf{u}_k(\vec{r}) = e^{i \frac{\ell_i}{M_i} \frac{2\pi}{L_i} \cdot \vec{r}_i} \mathbf{u}(\vec{r})$$

Define the supercell Bloch states wave vector as $\vec{k}$, according to Bloch's theorem, BdG wavefunctions are

$$\begin{aligned} \mathbf{u}_k &= e^{i\vec{k} \cdot \vec{r}} \mathbf{u} \\ \mathbf{v}_k &= e^{i\vec{k} \cdot \vec{r}} \mathbf{v} \end{aligned}$$

(2) BdG equations are

$$\begin{aligned} \begin{pmatrix} -\mathbf{t}_k & \Delta_k \\ \Delta_k^* & \mathbf{t}_k^* \end{pmatrix} \begin{pmatrix} \mathbf{u}_k & -\mathbf{v}_k^* \\ \mathbf{v}_k & \mathbf{u}_k^* \end{pmatrix} &= \begin{pmatrix} \mathbf{u}_k & -\mathbf{v}_k^* \\ \mathbf{v}_k & \mathbf{u}_k^* \end{pmatrix} \begin{pmatrix} E_{k\uparrow} & 0 \\ 0 & -E_{k\downarrow} \end{pmatrix} \\ \sum_j \left[-t_{ij}(k) u_j^n(k) + \Delta_{ij}(k) v_j^n(k) \right] &= E_{n\uparrow}(k) u_i^n(k) \\ \sum_j \left[-t_{ij}(k) e^{i\vec{k} \cdot \vec{r}_j} u_j^n + \Delta_{ij}(k) e^{i\vec{k} \cdot \vec{r}_j} v_j^n \right] &= E_{n\uparrow}(k) e^{i\vec{k} \cdot \vec{r}_i} u_i^n \\ \sum_j \left[-t_{ij}(k) e^{-i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} u_j^n + \Delta_{ij}(k) e^{-i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} v_j^n \right] &= E_{n\uparrow}(k) u_i^n \end{aligned}$$

Let $t_{ij}(k) = e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} t_{ij}$ and $\Delta_{ij}(k) = e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} \Delta_{ij}$

$$\Rightarrow \sum_j \left[-t_{ij} u_j^n + \Delta_{ij} v_j^n \right] = E_{n\uparrow} u_i^n$$

(3) The local density of states in terms of supercell Bloch states

$$\begin{aligned} \rho_i(\omega) &= \frac{\beta}{4} \frac{1}{M_x M_y} \sum_k \sum_n \left\{ |\mathbf{u}_i^n(k)|^2 \left[1 - \tanh^2 \left(\frac{\beta(E_n(k) - \omega)}{2} \right) \right] \right. \\ &\quad \left. + |\mathbf{v}_i^n(k)|^2 \left[1 - \tanh^2 \left(\frac{\beta(E_n(k) + \omega)}{2} \right) \right] \right\} \end{aligned}$$

4-4 Superfluid Density

OS:

Inspired by Scalapino et. al. [Phy. Rev. Lett. 68, 2830 (1992)] for the Hubbard model on a lattice.

A. CURRENT DENSITY OPERATOR

- (1) We expand the Hamiltonian to include the interactions of electrons coupled to an electromagnetic field.

$$\hat{H} = - \sum_{ij\sigma} \left(\tilde{t}_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.} \right) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \frac{V}{2} \sum_{i \neq j} \hat{n}_i \hat{n}_j = \hat{H}_0 + \hat{H}'$$

Here, $\hat{H}'(t)$ describes such a minimal coupling

$$\hat{H}'(t) = -ea \sum_i A_x(\vec{r}_i, t) \hat{j}_x^P(\vec{r}_i) - \frac{e^2 a^2}{2} \sum_i A_x^2(\vec{r}_i, t) \hat{K}_x(\vec{r}_i)$$

where a is the lattice constant, A_x is the vector potential along the x -axis, and the particle current operator is defined as

$$\hat{j}_x^P(\vec{r}_i) = -i \sum_{\sigma} \left(t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - t_{ij}^* c_{j\sigma}^\dagger c_{i\sigma} \right)$$

and the kinetic energy operator is defined as

$$\hat{K}_x(\vec{r}_i) = - \sum_{\sigma} \left(t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + t_{ij}^* c_{j\sigma}^\dagger c_{i\sigma} \right)$$

- (2) The charge current density operator along the x -axis is found to be

$$\hat{j}_x(\vec{r}_i) = - \frac{\delta \hat{H}'(t)}{\delta A_x(\vec{r}_i, t)} = ea \hat{j}_x^P(\vec{r}_i) + e^2 a^2 \hat{K}_x(\vec{r}_i) A_x(\vec{r}_i, t)$$

OS:

An alternative derivation of the charge current density operator
The electric polarization operator

$$\hat{P} = e \sum_i \vec{r}_i \hat{n}_i$$

The x -component

$$\hat{P}_x = e \sum_i x_i \hat{n}_i$$

The time derivative is

$$\begin{aligned}
\hat{j}_x(\vec{r}) &= \frac{\partial \hat{P}_x}{\partial t} = \frac{i}{\hbar} [\hat{H}, \hat{P}_x] \\
&= ie \sum_{\sigma} \left[x_i \tilde{t}_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - x_i \tilde{t}_{ji} c_{j\sigma}^{\dagger} c_{i\sigma} \right] \\
&= ie \sum_{\sigma} (x_i - x_j) \tilde{t}_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} \\
&= ie \sum_{\sigma} (x_i - x_j) t_{ij} (1 + i\phi_{ij}) c_{i\sigma}^{\dagger} c_{j\sigma}
\end{aligned}$$

With the phase $\phi_{ij} = eA_{ij} = eA_x(\vec{r}_i, t)(x_i - x_j)$, in the limit that the hopping integral only between the nearest neighbors, i.e., $x_i - x_j = a$.

$$\begin{aligned}
\hat{j}_x(\vec{r}) &= ie \sum_{\sigma} at_{ij} (1 + ieA_x(\vec{r}_i, t)a) c_{i\sigma}^{\dagger} c_{j\sigma} \\
&= eai \sum_{\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - e^2 a^2 \sum_{\sigma} t_{ij} A_x(\vec{r}_i, t) c_{i\sigma}^{\dagger} c_{j\sigma} \\
&= ea\hat{j}_x^P(\vec{r}) + e^2 a^2 \hat{K}_x(\vec{r}) A_x(\vec{r}, t)
\end{aligned}$$

B. KUBO FORMULA

- (1) In the linear response theory, the statistical operator in the interaction picture is given by

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

The expectation of a physical variable is found to be

$$\begin{aligned}
\langle \hat{O} \rangle &= \text{Tr} [\hat{\rho}(-\infty) \hat{O}] - \frac{i}{\hbar} \int_{-\infty}^t \text{Tr} \{ \hat{\rho}(-\infty) [\hat{O}(t'), \hat{H}'(t')] \} dt' \\
&= \langle \hat{O} \rangle_0 - \frac{i}{\hbar} \int_{-\infty}^t \langle [\hat{O}(t'), \hat{H}'(t')] \rangle dt'
\end{aligned}$$

where

$$\begin{aligned}
\hat{O}(t') &= e^{i\hat{H}_0 t'} \hat{O} e^{-i\hat{H}_0 t'} \\
\hat{H}'(t') &= e^{i\hat{H}_0 t'} \hat{H}' e^{-i\hat{H}_0 t'}
\end{aligned}$$

- (2) The paramagnetic component of the electric current density to first order in A_x is

$$\langle \hat{J}_x^P(\vec{r}) \rangle = -i \int_{-\infty}^t \langle [\hat{J}_x^P(\vec{r}, t), \hat{H}'(t)] \rangle dt'$$

where

$$\hat{J}_x^P(\vec{r}, t) = e^{i\hat{H}_0 t} \hat{J}_x^P(\vec{r}) e^{-i\hat{H}_0 t}$$

The diamagnetic part in $\langle \hat{K}_x \rangle_0$ only to zeroth order; $\langle \cdots \rangle_0$ represents a thermodynamic average with respect to $\hat{H}_0$.

C. SUPERFLUID DENSITY

(1) Diamagnetic response to an external magnetic field

$$\begin{aligned} \langle \hat{K}_{ij}^x \rangle &= \langle -t_{ij} c_{i\uparrow}^\dagger c_{j\uparrow} - t_{ij} c_{i\downarrow}^\dagger c_{j\downarrow} + \text{H.c.} \rangle \\ &= \sum_n \langle -t_{ij} (u_i^{n*} \gamma_{n\uparrow}^\dagger - v_i^n \gamma_{n\downarrow}) (u_j^n \gamma_{n\uparrow} - v_j^{n*} \gamma_{n\downarrow}^\dagger) \\ &\quad - t_{ij} (u_i^{n*} \gamma_{n\downarrow}^\dagger + v_i^n \gamma_{n\uparrow}) (u_j^n \gamma_{n\downarrow} + v_j^{n*} \gamma_{n\uparrow}^\dagger) + \text{H.c.} \rangle \\ &= -t_{ij} \sum_n \left[u_i^{n*} u_j^n \langle \gamma_{n\uparrow}^\dagger \gamma_{n\uparrow} \rangle + v_i^n v_j^{n*} \langle \gamma_{n\downarrow} \gamma_{n\downarrow}^\dagger \rangle \right. \\ &\quad \left. + u_i^{n*} u_j^n \langle \gamma_{n\downarrow}^\dagger \gamma_{n\downarrow} \rangle + v_i^n v_j^{n*} \langle \gamma_{n\uparrow} \gamma_{n\uparrow}^\dagger \rangle + \text{H.c.} \right] \end{aligned}$$

Use global indices $\mathbf{u}_i^n$, $\mathbf{v}_i^n$, and E_n , i.e.,

$$\begin{aligned} \mathbf{u}_i &= (\overbrace{\mathbf{u}_i^1}^{u_i^1} \cdots \overbrace{\mathbf{u}_i^N}^{u_i^N} \overbrace{\mathbf{u}_i^{N+1}}^{-v_i^{1*}} \cdots \overbrace{\mathbf{u}_i^{2N}}^{-v_i^{N*}}) \\ \mathbf{v}_i &= (\overbrace{\mathbf{v}_i^1}^{v_i^1} \cdots \overbrace{\mathbf{v}_i^N}^{v_i^N} \overbrace{\mathbf{v}_i^{N+1}}^{u_i^{1*}} \cdots \overbrace{\mathbf{v}_i^{2N}}^{u_i^{N*}}) \\ \begin{pmatrix} E_1 \\ \vdots \\ E_N \\ E_{N+1} \\ \vdots \\ E_{2N} \end{pmatrix} &= \begin{pmatrix} E_{1\uparrow} \\ \vdots \\ E_{N\uparrow} \\ -E_{1\downarrow} \\ \vdots \\ -E_{N\downarrow} \end{pmatrix} \end{aligned}$$

Thus, we obtain

$$\langle \hat{K}_{ij}^x \rangle = -t_{ij} \sum_n [\mathbf{u}_i^{n*} \mathbf{u}_j^n f(E_n) + \mathbf{v}_i^n \mathbf{v}_j^{n*} [1 - f(E_n)] + \text{H.c.}]$$

$$\begin{aligned}
\langle \hat{K}_x(i, j) \rangle &= - \sum_{\sigma} \left\langle t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H. c.} \right\rangle \\
&= - \left\langle t_{ij} c_{i\uparrow}^{\dagger} c_{j\uparrow} + t_{ij} c_{i\downarrow}^{\dagger} c_{j\downarrow} + t_{ji}^* c_{j\uparrow}^{\dagger} c_{i\uparrow} + t_{ji}^* c_{j\downarrow}^{\dagger} c_{i\downarrow} \right\rangle \\
&= - \sum_n \left[t_{ij} u_i^{n*} u_j^n \langle \gamma_{n\uparrow}^{\dagger} \gamma_{n\uparrow} \rangle + t_{ij} v_i^n v_j^{n*} \langle \gamma_{n\downarrow} \gamma_{n\downarrow}^{\dagger} \rangle + t_{ij} u_i^{n*} u_j^n \langle \gamma_{n\downarrow}^{\dagger} \gamma_{n\downarrow} \rangle \right. \\
&\quad + t_{ij} v_i^n v_j^{n*} \langle \gamma_{n\uparrow} \gamma_{n\uparrow}^{\dagger} \rangle + t_{ji}^* u_j^{n*} u_i^n \langle \gamma_{n\uparrow}^{\dagger} \gamma_{n\uparrow} \rangle + t_{ji}^* v_j^n v_i^{n*} \langle \gamma_{n\downarrow} \gamma_{n\downarrow}^{\dagger} \rangle \\
&\quad \left. + t_{ji}^* u_j^{n*} u_i^n \langle \gamma_{n\downarrow}^{\dagger} \gamma_{n\downarrow} \rangle + t_{ji}^* v_j^n v_i^{n*} \langle \gamma_{n\uparrow} \gamma_{n\uparrow}^{\dagger} \rangle \right] \\
&= -2 \sum_n \text{Im } t_{ij} \left[\mathbf{u}_j^n \mathbf{u}_i^{n*} f(E_n) + \mathbf{v}_i^n \mathbf{v}_j^{n*} (1 - f(E_n)) \right]
\end{aligned}$$

where $t_{ij} = t_{ji}^*$

- (2) Paramagnetic response given by the transverse current-current correlation function

$$\Lambda_{xx}(r, i\Omega) = \int_0^{\beta} d\tau e^{-i\Omega\tau} \langle T_{\tau} \hat{J}_x^P(r, \tau) \hat{J}_x^P(r', 0) \rangle$$

Paramagnetic current density

$$\begin{aligned}
\hat{J}_x^P(r) &= -i \sum_{\sigma} \left(t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - t_{ij}^* c_{j\sigma}^{\dagger} c_{i\sigma} \right) \\
\langle T_{\tau} \hat{J}_x^P(r, \tau) \hat{J}_x^P(r', 0) \rangle &= - \sum_{\sigma\sigma'} \left\langle T_{\tau} \left(t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} - t_{ji}^* c_{j\sigma}^{\dagger} c_{i\sigma} \right) \left(t_{i'j'} c_{i'\sigma'}^{\dagger} c_{j'\sigma'} - t_{j'i'}^* c_{j'\sigma'}^{\dagger} c_{i'\sigma'} \right) \right\rangle \\
&= - \sum_{\sigma\sigma'} t_{ij} t_{i'j'} \left(\left\langle T_{\tau} c_{i\sigma}^{\dagger} c_{j\sigma} c_{i'\sigma'}^{\dagger} c_{j'\sigma'} \right\rangle + \left\langle T_{\tau} c_{j\sigma}^{\dagger} c_{i\sigma} c_{j'\sigma'}^{\dagger} c_{i'\sigma'} \right\rangle \right. \\
&\quad \left. - \left\langle T_{\tau} c_{i\sigma}^{\dagger} c_{j\sigma} c_{j'\sigma'}^{\dagger} c_{i'\sigma'} \right\rangle - \left\langle T_{\tau} c_{j\sigma}^{\dagger} c_{i\sigma} c_{i'\sigma'}^{\dagger} c_{j'\sigma'} \right\rangle \right)
\end{aligned}$$

According to Wick's theorem

$$\begin{aligned}
\left\langle T_{\tau} c_{i\uparrow}^{\dagger} c_{j\uparrow} c_{i'\uparrow}^{\dagger} c_{j'\uparrow} \right\rangle &= \left\langle T_{\tau} c_{j\uparrow} c_{i\uparrow}^{\dagger} \right\rangle \left\langle T_{\tau} c_{j'\uparrow} c_{i'\uparrow}^{\dagger} \right\rangle - \left\langle T_{\tau} c_{j'\uparrow} c_{i\uparrow}^{\dagger} \right\rangle \left\langle T_{\tau} c_{j\uparrow} c_{i'\uparrow}^{\dagger} \right\rangle \\
&= G_{ji}^{\uparrow} G_{j'i'}^{\uparrow} - G_{j'i}^{\uparrow} G_{ji'}^{\uparrow} \\
\left\langle T_{\tau} c_{i\downarrow}^{\dagger} c_{j\downarrow} c_{i'\downarrow}^{\dagger} c_{j'\downarrow} \right\rangle &= \left\langle T_{\tau} c_{i\downarrow}^{\dagger} c_{j\downarrow} \right\rangle \left\langle T_{\tau} c_{i'\downarrow}^{\dagger} c_{j'\downarrow} \right\rangle - \left\langle T_{\tau} c_{i\downarrow}^{\dagger} c_{j'\downarrow} \right\rangle \left\langle T_{\tau} c_{i'\downarrow}^{\dagger} c_{j\downarrow} \right\rangle \\
&= G_{ij}^{\downarrow} G_{i'j'}^{\downarrow} - G_{ij'}^{\downarrow} G_{i'j}^{\downarrow}
\end{aligned}$$

$$\begin{aligned}
\langle T_\tau c_{i\uparrow}^\dagger c_{j\uparrow} c_{i'\downarrow}^\dagger c_{j'\downarrow} \rangle &= -\langle T_\tau c_{j\uparrow} c_{i\uparrow}^\dagger \rangle \langle T_\tau c_{i'\downarrow}^\dagger c_{j'\downarrow} \rangle + \langle T_\tau c_{i'\downarrow}^\dagger c_{i\uparrow}^\dagger \rangle \langle T_\tau c_{j\uparrow} c_{j'\downarrow} \rangle \\
&= -G_{ji}^\uparrow G_{i'j'}^\downarrow + F_{i'i}^* F_{jj'} \\
\langle T_\tau c_{i\downarrow}^\dagger c_{j\downarrow} c_{i'\uparrow}^\dagger c_{j'\uparrow} \rangle &= -\langle T_\tau c_{i\downarrow}^\dagger c_{j\downarrow} \rangle \langle T_\tau c_{j'\uparrow} c_{i'\uparrow}^\dagger \rangle + \langle T_\tau c_{i\downarrow}^\dagger c_{i'\uparrow}^\dagger \rangle \langle T_\tau c_{j'\uparrow} c_{j\downarrow} \rangle \\
&= -G_{ij}^\downarrow G_{j'i'}^\uparrow + F_{ii'}^* F_{j'j} \\
\sum_{\sigma\sigma'} \langle T_\tau c_{i\sigma}^\dagger c_{j\sigma} c_{i'\sigma'}^\dagger c_{j'\sigma'} \rangle &= G_{ji}^\uparrow G_{j'i'}^\uparrow - G_{j'i}^\uparrow G_{ji'}^\uparrow + G_{ij}^\downarrow G_{i'j'}^\downarrow - G_{ij'}^\downarrow G_{i'i}^\downarrow \\
&\quad - G_{ji}^\uparrow G_{i'j'}^\downarrow + F_{i'i}^* F_{jj'} - G_{ij}^\downarrow G_{j'i'}^\uparrow + F_{ii'}^* F_{j'j} \\
\sum_{\sigma\sigma'} \langle T_\tau c_{j\sigma}^\dagger c_{i\sigma} c_{j'\sigma'}^\dagger c_{i'\sigma'} \rangle &= G_{ij}^\uparrow G_{i'j'}^\uparrow - G_{i'j}^\uparrow G_{ij'}^\uparrow + G_{ji}^\downarrow G_{j'i'}^\downarrow - G_{ji'}^\downarrow G_{j'i}^\downarrow \\
&\quad - G_{ij}^\uparrow G_{j'i'}^\downarrow + F_{j'j}^* F_{ii'} - G_{ji}^\downarrow G_{i'j'}^\uparrow + F_{jj'}^* F_{i'i} \\
\sum_{\sigma\sigma'} \langle T_\tau c_{i\sigma}^\dagger c_{j\sigma} c_{j'\sigma'}^\dagger c_{i'\sigma'} \rangle &= G_{ji}^\uparrow G_{i'j'}^\uparrow - G_{i'i}^\uparrow G_{jj'}^\uparrow + G_{ij}^\downarrow G_{j'i'}^\downarrow - G_{ii'}^\downarrow G_{j'j}^\downarrow \\
&\quad - G_{ji}^\uparrow G_{j'i'}^\downarrow + F_{j'i}^* F_{ji'} - G_{ij}^\downarrow G_{i'j'}^\uparrow + F_{ij'}^* F_{i'j} \\
\sum_{\sigma\sigma'} \langle T_\tau c_{j\sigma}^\dagger c_{i\sigma} c_{i'\sigma'}^\dagger c_{j'\sigma'} \rangle &= G_{ij}^\uparrow G_{j'i'}^\uparrow - G_{j'j}^\uparrow G_{ii'}^\uparrow + G_{ji}^\downarrow G_{i'j'}^\downarrow - G_{jj'}^\downarrow G_{i'i}^\downarrow \\
&\quad - G_{ij}^\uparrow G_{i'j'}^\downarrow + F_{i'j}^* F_{ij'} - G_{ji}^\downarrow G_{j'i'}^\uparrow + F_{ji'}^* F_{j'i}
\end{aligned}$$

Since $G_{ji}^\sigma G_{j'i'}^\sigma$ are disconnected part which will form a bubble, we can ignore the contribution from the bubble.

$$G_{ji}^\sigma = G_{ij}^\sigma$$

$$\begin{aligned}
\langle T_\tau \hat{J}_x^P(r, \tau) \hat{J}_x^P(r', 0) \rangle &= -t_{ij} t_{i'j'} \left(-G_{j'i}^\uparrow G_{ji'}^\uparrow - G_{ij'}^\downarrow G_{i'j}^\downarrow + F_{i'i}^* F_{jj'} + F_{ii'}^* F_{j'j} \right) \\
&= -t_{ij} t_{i'j'} \left(-G_{i'j}^\uparrow G_{ij'}^\uparrow - G_{ji'}^\downarrow G_{j'i}^\downarrow + F_{j'j}^* F_{ii'} + F_{jj'}^* F_{i'i} \right) \\
&\quad + t_{ij} t_{i'j'} \left(-G_{i'i}^\uparrow G_{jj'}^\uparrow - G_{ii'}^\downarrow G_{j'j}^\downarrow + F_{j'i}^* F_{ji'} + F_{ij'}^* F_{i'j} \right) \\
&\quad + t_{ij} t_{i'j'} \left(-G_{j'j}^\uparrow G_{ii'}^\uparrow - G_{jj'}^\downarrow G_{i'i}^\downarrow + F_{i'j}^* F_{ij'} + F_{ji'}^* F_{j'i} \right)
\end{aligned}$$

Since

1. $G_{i'i}^\uparrow$ does not contribute to the current
2. $F_{i'i} = 0$ in d -wave superconductivity

$$\begin{aligned}
\langle T_\tau \hat{J}_x^P(r, \tau) \hat{J}_x^P(r', 0) \rangle &= -t_{ij} t_{i'j'} \left(-G_{j'i}^\uparrow G_{ji'}^\uparrow - G_{ij'}^\downarrow G_{i'j}^\downarrow - G_{i'j}^\uparrow G_{ij'}^\uparrow - G_{ji'}^\downarrow G_{j'i}^\downarrow \right. \\
&\quad \left. + F_{j'i}^* F_{ji'} + F_{i'j}^* F_{ij'} + F_{ji'}^* F_{j'i} + F_{ij'}^* F_{i'j} \right) \\
&= -2t_{ij} t_{i'j'} \left(-G_{i'j}^\uparrow G_{ij'}^\uparrow - G_{jj'}^\downarrow G_{i'i}^\downarrow + F_{ij'}^* F_{i'j} + F_{i'j}^* F_{ij'} \right)
\end{aligned}$$

$$\begin{aligned}
\Lambda_{xx}(r, i\Omega) &= \int_0^\beta d\tau e^{-i\Omega\tau} \langle T_\tau \hat{f}_x^P(r, \tau) \hat{f}_x^P(r', 0) \rangle \\
&= \frac{1}{\beta} \sum_\omega \sum_{nn'} \langle T_\tau \hat{f}_x^P(r, \omega) \hat{f}_x^P(r', \Omega + \omega) \rangle \\
\frac{1}{\beta} \sum_\omega \sum_{nn'} G_{i'j}^\uparrow G_{ij'}^\uparrow &= \frac{1}{\beta} \sum_\omega \sum_{n=1} \sum_{n'=1} \frac{\mathbf{u}_i^n \mathbf{u}_j^{n*}}{i\omega - E_n} \frac{\mathbf{u}_i^{n'} \mathbf{u}_{j'}^{n'*}}{i(\Omega + \omega) - E_{n'}} \\
&= \sum_{n=1} \sum_{n'=1} \mathbf{u}_i^n \mathbf{u}_j^{n*} \mathbf{u}_i^{n'} \mathbf{u}_{j'}^{n'*} \frac{f(E_n) - f(i\Omega + E_{n'})}{i\Omega + E_n - E_{n'}}
\end{aligned}$$

The Meissner effect is the current response to a static ($\Omega = 0$) and transverse gauge potential

$$\begin{aligned}
\frac{1}{\beta} \sum_\omega \sum_{nn'} G_{i'j\uparrow\uparrow} G_{ij'\uparrow\uparrow} &= \sum_{n=1} \sum_{n'=1} \mathbf{u}_i^n \mathbf{u}_j^{n*} \mathbf{u}_i^{n'} \mathbf{u}_{j'}^{n'*} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}} \\
\Lambda_{xx}(i, j, \Omega = 0) &= -2t_{ij}t_{i'j'} \sum_{n=1} \sum_{n'=1} \left(-\mathbf{u}_i^n \mathbf{u}_j^{n*} \mathbf{u}_i^{n'} \mathbf{u}_{j'}^{n'*} - \mathbf{v}_i^n \mathbf{v}_{j'}^{n*} \mathbf{v}_i^{n'} \mathbf{v}_{j'}^{n'*} \right. \\
&\quad \left. - \mathbf{v}_i^n \mathbf{u}_{j'}^{n*} \mathbf{u}_i^{n'} \mathbf{v}_j^{n'*} - \mathbf{v}_i^{n'} \mathbf{u}_j^{n*} \mathbf{u}_i^n \mathbf{v}_{j'}^{n'*} \right) \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}}
\end{aligned}$$

Let

$$\begin{aligned}
\mathbf{\Gamma}_{ij}^{nn'} &= t_{ij} \left(\mathbf{u}_j^{n*} \mathbf{u}_i^{n'} - \mathbf{v}_i^n \mathbf{v}_j^{n'*} \right) \\
\Lambda_{xx}(i, j, \Omega = 0) &= -2t_{ij}t_{i'j'} \sum_{n=1} \sum_{n'=1} \mathbf{\Gamma}_{ij}^{nn'} \mathbf{\Gamma}_{i'j'}^{nn'} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}}
\end{aligned}$$

We obtain

$$\begin{aligned}
\rho_s(i, j) &= \langle -K_x(i, j) \rangle - \Lambda_{xx}(i, j, \Omega = 0) \\
&= - \sum_{n=1} \sum_{n'=1} \mathbf{\Gamma}_{ij}^{nn'} \mathbf{\Gamma}_{i'j'}^{nn'} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}} \\
&\quad - \sum_n t_{ij} \left[\mathbf{u}_j^n \mathbf{u}_i^{n*} f(E_n) + \mathbf{v}_i^n \mathbf{v}_j^{n*} (1 - f(E_n)) \right]
\end{aligned}$$

(3) The local or site-specific superfluid density is then given by

Let $j = i$

$$\begin{aligned}
\rho_s(i) &= \langle -\hat{K}_x(i) \rangle - \Lambda_{xx}(i, \Omega = 0) \\
&= - \sum_{n=1} \sum_{n'=1} \mathbf{\Gamma}_i^{nn'} \mathbf{\Gamma}_{i+x}^{nn'} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}} \\
&\quad - \sum_i t_{ii+x} [\mathbf{u}_{i+x}^n \mathbf{u}_i^{n*} f(E_n) + \mathbf{v}_i^n \mathbf{v}_{i+x}^{n*} (1 - f(E_n))] \\
\mathbf{\Gamma}_i^{nn'} &= t_{ii+x} (\mathbf{u}_{i+x}^{n*} \mathbf{u}_i^{n'} - \mathbf{v}_i^n \mathbf{v}_{i+x}^{n'*})
\end{aligned}$$

(4) The superfluid density is evaluated as

$$\frac{\rho_s(T)}{4} = \langle -\hat{K}_x \rangle - \Lambda_{xx}(q_x = 0, q_y = 0, \Omega = 0)$$

where $\langle -\hat{K}_x \rangle$ is average kinetic energy along $\hat{x}$ direction, and $\Lambda_{xx}(q, \Omega)$ is a diagonal element of the current-current correlation.

$$\begin{aligned}
\langle \hat{K}_x \rangle &= \frac{1}{N} \sum_i \sum_{\sigma} \left\langle [t_{i,i+x} c_{i\sigma}^{\dagger} c_{i+x\sigma} + \text{H. c.}] \right\rangle \\
\Lambda_{xx}(q, i\Omega_n) &= \frac{1}{N} \int_0^{1/T} d\tau e^{-i\Omega_n \tau} \langle T_{\tau} \hat{j}_x^P(q, \tau) \hat{j}_x^P(-q, 0) \rangle
\end{aligned}$$

The retarded current-current correlation function is obtained by analytically continuing $i\Omega_n \rightarrow \Omega + i\delta$

$$\Lambda_{xx}(q, \Omega) = \frac{-i}{N} \int_{-\infty}^t dt' e^{-i\Omega(t-t')} \langle T_{\tau} \hat{j}_x^P(q, t) \hat{j}_x^P(-q, t') \rangle$$

4-5 Spin Relaxation Time

A. SPIN-SPIN CORRELATION

(1) Spin-spin correlation

$$\chi_{ij}^{+-}(\tau) = \left\langle \hat{T} \left[\hat{S}_i^+(\tau) \hat{S}_j^-(0) \right] \right\rangle$$

Let

$$\hat{S}_i^+ = \hat{c}_{i\uparrow}^\dagger \hat{c}_{i\downarrow} \cdots \cdots \text{Spin raise operator}$$

$$\hat{S}_i^- = \hat{c}_{i\downarrow}^\dagger \hat{c}_{i\uparrow} \cdots \cdots \text{Spin lower operator}$$

We obtain

$$\chi_{ij}^{+-}(\tau) = \left\langle \hat{T} \left[c_{i\uparrow}^\dagger(\tau) c_{i\downarrow}(\tau) c_{j\downarrow}^\dagger(0) c_{j\uparrow}(0) \right] \right\rangle$$

Use Wick's theorem, the product of four operators can be factorized into sums of products of pairs,

$$\begin{aligned} \chi_{ij}^{+-}(\tau) = & \left\langle \hat{T} \left[c_{j\uparrow}(0) c_{i\uparrow}^\dagger(\tau) \right] \right\rangle \left\langle \hat{T} \left[c_{j\downarrow}^\dagger(0) c_{i\downarrow}(\tau) \right] \right\rangle \\ & - \left\langle \hat{T} \left[c_{j\uparrow}(0) c_{i\downarrow}(\tau) \right] \right\rangle \left\langle \hat{T} \left[c_{j\downarrow}^\dagger(0) c_{i\uparrow}^\dagger(\tau) \right] \right\rangle \end{aligned}$$

Assume

$$G_{ji\uparrow}(-\tau) = G_{ji\uparrow}(0, \tau) = \left\langle \hat{T} \left[c_{j\uparrow}(0) c_{i\uparrow}^\dagger(\tau) \right] \right\rangle$$

$$G_{ji\downarrow}(\tau) = G_{ji\downarrow}(\tau, 0) = \left\langle \hat{T} \left[c_{j\downarrow}^\dagger(0) c_{i\downarrow}(\tau) \right] \right\rangle$$

$$F_{ji}(-\tau) = F_{ji}(0, \tau) = \left\langle \hat{T} \left[c_{j\uparrow}(0) c_{i\downarrow}(\tau) \right] \right\rangle$$

$$F_{ji}^*(\tau) = F_{ji}^*(\tau, 0) = \left\langle \hat{T} \left[c_{j\downarrow}^\dagger(0) c_{i\uparrow}^\dagger(\tau) \right] \right\rangle$$

We have

$$\chi_{ij}^{+-}(\tau) = G_{ji\uparrow}(-\tau) G_{ji\downarrow}(\tau) - F_{ji}(-\tau) F_{ji}^*(\tau)$$

(2) The Fourier transformation of χ

$$\begin{aligned} \chi_{ij}^{+-}(i\Omega_l) &= \int_0^\beta e^{i\Omega_l \tau} \chi_{ij}^{+-}(\tau) d\tau \\ &= \int_0^\beta e^{i\Omega_l \tau} \frac{1}{\beta^2} \sum_{\omega_l \omega'_l} e^{i\omega_l \tau} e^{-i\omega'_l \tau} \\ &\quad \times \left[G_{ji\uparrow}(i\omega_n) G_{ji\downarrow}(i\omega'_n) - F_{ji}(i\omega_n) F_{ji}^*(i\omega'_n) \right] d\tau \end{aligned}$$

Since

$$\int_0^\beta e^{i(\Omega_n + \omega_n - \omega'_n)\tau} d\tau = \beta \delta(\Omega_n + \omega_n - \omega'_n)$$

we obtain

$$\begin{aligned} \chi_{ij}^{+-}(i\Omega_n) &= \frac{1}{\beta^2} \sum_{\omega_n \omega'_n} \beta \delta(\Omega_n + \omega_n - \omega'_n) \\ &\quad \times \left[G_{ji\uparrow}(i\omega_n) G_{ji\downarrow}(i\omega'_n) - F_{ji}(i\omega_n) F_{ji}^*(i\omega'_n) \right] \\ &= \frac{1}{\beta} \sum_{\omega'_n} \left[G_{ji\uparrow}(i\omega_n) G_{ji\downarrow}(i\Omega_n + i\omega_n) - F_{ji}(i\omega_n) F_{ji}^*(i\Omega_n + i\omega_n) \right] \\ &= \frac{1}{\beta} \sum_{\omega_n, n, m} \left[\frac{\mathbf{u}_j^n \mathbf{u}_i^{n*}}{i\omega_n - E_n} \cdot \frac{\mathbf{v}_j^m \mathbf{v}_i^{m*}}{i\Omega_n + i\omega_n - E_m} \right. \\ &\quad \left. - \frac{\mathbf{u}_j^n \mathbf{v}_i^{n*}}{i\omega_n - E_n} \cdot \frac{\mathbf{v}_j^m \mathbf{u}_i^{m*}}{i\Omega_n + i\omega_n - E_m} \right] \end{aligned}$$

where we have used global indices $\mathbf{u}_i^n$, $\mathbf{v}_i^n$, and E_n , i.e.,

$$\begin{aligned} \mathbf{u}_i &= (\underbrace{u_i^1}_{\mathbf{u}_i^1} \dots \underbrace{u_i^N}_{\mathbf{u}_i^N} \underbrace{-v_i^{1*}}_{\mathbf{u}_i^{N+1}} \dots \underbrace{-v_i^{N*}}_{\mathbf{u}_i^{2N}}) \\ \mathbf{v}_i &= (\underbrace{v_i^1}_{\mathbf{v}_i^1} \dots \underbrace{v_i^N}_{\mathbf{v}_i^N} \underbrace{u_i^{1*}}_{\mathbf{v}_i^{N+1}} \dots \underbrace{u_i^{N*}}_{\mathbf{v}_i^{2N}}) \\ \begin{pmatrix} E_1 \\ \vdots \\ E_N \\ E_{N+1} \\ \vdots \\ E_{2N} \end{pmatrix} &= \begin{pmatrix} E_{1\uparrow} \\ \vdots \\ E_{N\uparrow} \\ -E_{1\downarrow} \\ \vdots \\ -E_{N\downarrow} \end{pmatrix} \end{aligned}$$

Since

$$\begin{aligned} &\frac{1}{\beta} \sum_{\omega'_n} \left[\frac{1}{i\omega_n - E_n} \cdot \frac{1}{i\Omega_n + i\omega_n - E_m} \right] \\ &= \frac{1}{\beta} \sum_{\omega_n} \left[\frac{1}{i\omega_n - E_n} - \frac{1}{i\Omega_n + i\omega_n - E_m} \right] \frac{1}{i\Omega_n + E_n - E_m} \\ &= \frac{f(E_n) - f(E_m - i\Omega_n)}{i\Omega_n + E_n - E_m} \end{aligned}$$

we obtain

$$\chi_{ij}^{+-}(i\Omega_n) = \sum_{n, m} \left(\mathbf{u}_j^n \mathbf{u}_i^{n*} \mathbf{v}_j^m \mathbf{v}_i^{m*} - \mathbf{u}_j^n \mathbf{v}_i^{n*} \mathbf{v}_j^m \mathbf{u}_i^{m*} \right) \frac{f(E_n) - f(E_m - i\Omega_n)}{i\Omega_n + E_n - E_m}$$

(3) Analytic continuation

$$i\Omega \rightarrow \Omega + i\eta$$

$$\begin{aligned} \chi_{ij}^{+-}(\Omega + i\eta) &= \sum_{n,m} \left(\mathbf{u}_j^n \mathbf{u}_i^{n*} \mathbf{v}_j^m \mathbf{v}_i^{m*} - \mathbf{u}_j^n \mathbf{v}_i^{n*} \mathbf{v}_j^m \mathbf{u}_i^{m*} \right) \\ &\quad \times \frac{f(E_n) - f(E_m - \Omega_n - i\eta)}{\Omega_n + i\eta + E_n - E_m} \end{aligned}$$

B. SPIN RELAXATION TIME (T_1)

(1) The spin-lattice relaxation time is

$$\frac{1}{T_1 T} \Big|_{\Omega_n \rightarrow 0} = \lim_{\Omega_n \rightarrow 0} \frac{1}{\Omega_n} \Im \left(\chi_{ii}^{+-}(i\Omega_n \rightarrow \Omega_n + i\eta) \right)$$

where

$$\begin{aligned} \Im \left(\chi_{ii}^{+-}(i\Omega_n \rightarrow \Omega_n + i\eta) \right) &= \sum_{n,m} \left(\mathbf{u}_i^n \mathbf{u}_i^{n*} \mathbf{v}_i^m \mathbf{v}_i^{m*} - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \\ &\quad \times \Im \left(\frac{f(E_n) - f(E_m - \Omega_n - i\eta)}{\Omega_n + i\eta + E_n - E_m} \right) \end{aligned}$$

(2) Since

$$\begin{aligned} \mathbf{u}_i^n \mathbf{u}_i^{n*} \mathbf{v}_i^m \mathbf{v}_i^{m*} - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} &= |\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \\ \Im \left(\frac{1}{\Omega_n + i\eta + E_n - E_m} \right) &= (-\pi) \delta(\Omega_n + E_n - E_m) \end{aligned}$$

Thus, we obtain

$$\begin{aligned} \Im \left(\chi_{ii}^{+-}(\Omega_n + i\eta) \right) &= \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \\ &\quad \times [f(E_n) - f(E_m - \Omega_n - i\eta)] (-\pi) \delta(\Omega_n + E_n - E_m) \\ \frac{1}{T_1 T} \Big|_{\Omega_n \rightarrow 0} &= \lim_{\Omega_n \rightarrow 0} \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \\ &\quad \times \frac{f(E_n) - f(E_m - \Omega_n - i\eta)}{\Omega_n} (-\pi) \delta(\Omega_n + E_n - E_m) \\ &= \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \left[-f'(E_n) \pi \delta(E_n - E_m) \right] \end{aligned}$$