—Chapter 4—

BdG Equations on a Lattice

4-1 Self-consistent BdG Equations

A. EQUATIONS OF MOTION

(1) The BCS Hamiltonian on lattice

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

Since the Hamiltonian should be a Hermitian operator, i.e.,
$\hat{H}^{\dagger} = \hat{H} \Rightarrow t^{*}_{ij} = t_{ji}$ and $\Delta^{*}_{ij} = \Delta_{ji}$

(2) The equations of motion

Let the imaginary time $\tau = it$

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

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

OS:

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

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

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

B. BOGOLIUBOV TRANSFORMATION

(1) Bogoliubov transformations

$$
\hat{c}_{i\sigma} = \sum_{n} \left(u_i^{n}\hat{\gamma}_{n\sigma} - \sigma v_i^{n*}\hat{\gamma}_{n\bar{\sigma}}^{\dagger}\right)
$$

$$
\hat{c}_{i\sigma}^{\dagger} = \sum_{n} \left(u_i^{n*}\hat{\gamma}_{n\sigma}^{\dagger} - \sigma v_i^{n}\hat{\gamma}_{n\bar{\sigma}}\right)
$$

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

$$
\mathrm{c}_{\uparrow} = \begin{pmatrix} \hat{c}_{1\uparrow} \\ \vdots \\ \hat{c}_{N\uparrow} \end{pmatrix}, \qquad \mathrm{c}_{\downarrow}^{\dagger} = \begin{pmatrix} \hat{c}_{1\downarrow}^{\dagger} \\ \vdots \\ \hat{c}_{N\downarrow}^{\dagger} \end{pmatrix}
$$

$$
\mathrm{u} = \begin{pmatrix} u_1^1 & \cdots & u_1^N \\ \vdots & \ddots & \vdots \\ u_N^1 & \cdots & u_N^N \end{pmatrix}, \qquad \mathrm{v} = \begin{pmatrix} v_1^1 & \cdots & v_1^N \\ \vdots & \ddots & \vdots \\ v_N^1 & \cdots & v_N^N \end{pmatrix}
$$

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

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

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

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

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

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

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

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

(2) Use the Bogoliubov transformation

$$\mathrm{H} = \overbrace{\begin{pmatrix} \gamma_\uparrow^\dagger & \gamma_\downarrow \end{pmatrix} \begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix}^\dagger}^{\begin{pmatrix} \mathrm{c}_\uparrow^\dagger & \mathrm{c}_\downarrow \end{pmatrix}} \cdot \begin{pmatrix} -\mathrm{t} & \Delta \\ \Delta^* & \mathrm{t}^* \end{pmatrix} \cdot \overbrace{\begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix} \begin{pmatrix} \gamma_\uparrow \\ \gamma_\downarrow^\dagger \end{pmatrix}}^{\begin{pmatrix} \mathrm{c}_\uparrow \\ \mathrm{c}_\downarrow^\dagger \end{pmatrix}}$$

$$= \begin{pmatrix} \gamma_\uparrow^\dagger & \gamma_\downarrow \end{pmatrix} \begin{pmatrix} \varepsilon_\uparrow & 0 \\ 0 & -\varepsilon_\downarrow \end{pmatrix} \begin{pmatrix} \gamma_\uparrow \\ \gamma_\downarrow^\dagger \end{pmatrix}$$

$$= \sum_\sigma \mathrm{E}_\sigma \gamma_\sigma^\dagger \gamma_\sigma + \varepsilon_0$$

where

$$\begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix}^\dagger \begin{pmatrix} -\mathrm{t} & \Delta \\ \Delta^* & \mathrm{t}^* \end{pmatrix} \begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix}$$

$$= \begin{pmatrix} -\mathrm{u}^*\mathrm{tu} + \mathrm{u}^*\Delta\mathrm{v} + \mathrm{v}^*\Delta^*\mathrm{u} + \mathrm{v}^*\mathrm{t}^*\mathrm{v} & \mathrm{u}^*\mathrm{tv}^* + \mathrm{u}^*\Delta\mathrm{u}^* - \mathrm{v}^*\Delta^*\mathrm{v}^* + \mathrm{v}^*\mathrm{t}^*\mathrm{u}^* \\ \mathrm{vtu} - \mathrm{v}\Delta\mathrm{v} + \mathrm{u}\Delta^*\mathrm{u} + \mathrm{ut}^*\mathrm{v} & -\mathrm{vtv}^* - \mathrm{v}\Delta\mathrm{u}^* - \mathrm{u}\Delta^*\mathrm{v}^* + \mathrm{ut}^*\mathrm{u}^* \end{pmatrix}$$

and

$$\mathrm{u}^*\mathrm{tv}^* + \mathrm{u}^*\Delta\mathrm{u}^* - \mathrm{v}^*\Delta^*\mathrm{v}^* + \mathrm{v}^*\mathrm{t}^*\mathrm{u}^* = 0$$

$$\mathrm{vtu} - \mathrm{v}\Delta\mathrm{v} + \mathrm{u}\Delta^*\mathrm{u} + \mathrm{ut}^*\mathrm{v} = 0$$

$$\mathrm{E}_\uparrow = -\mathrm{tu}^2 + \Delta\mathrm{u}^*\mathrm{v} + \Delta^*\mathrm{uv}^* + \mathrm{t}^*\mathrm{v}^2 = -\mathrm{tu}^2 + \mathrm{t}^*\mathrm{v}^2 + 2\Re\{\Delta\mathrm{u}^*\mathrm{v}\}$$

$$\mathrm{E}_\downarrow = -\mathrm{t}^*\mathrm{u}^2 + \Delta\mathrm{u}^*\mathrm{v} + \Delta^*\mathrm{uv}^* + \mathrm{tv}^2 = -\mathrm{t}^*\mathrm{u}^2 + \mathrm{tv}^2 + 2\Re\{\Delta\mathrm{u}^*\mathrm{v}\}$$

As t is real,

$$\mathrm{E}_\uparrow = -\mathrm{t}(\mathrm{u}^2 + \mathrm{v}^2) + 2\Re\{\Delta\mathrm{u}^*\mathrm{v}\} = -\mathrm{t} + 2\Re\{\Delta\mathrm{u}^*\mathrm{v}\}$$

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

(3) The equations of motion in terms of c_σ and $c_\sigma^\dagger$

$$\left[\hat{c}_{i\sigma}, \hat{H}\right] = \sum_j -t_{ij}\hat{c}_{j\sigma} + \sigma\Delta_{ij}\hat{c}_{j\bar{\sigma}}^\dagger$$

$$\left[\hat{c}_{i\sigma}^\dagger, \hat{H}\right] = \sum_j t_{ij}^*\hat{c}_{j\sigma}^\dagger - \sigma\Delta_{ij}^*\hat{c}_{j\bar{\sigma}}$$

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

$$\Rightarrow \left[\begin{pmatrix} c_\uparrow \\ c_\downarrow^\dagger \end{pmatrix}, H\right] = \begin{pmatrix} -t & \Delta \\ \Delta^* & t^* \end{pmatrix}\begin{pmatrix} c_\uparrow \\ c_\downarrow^\dagger \end{pmatrix} \cdots\cdots \text{(d)}$$

(4) The equations of motion in terms of γ_σ and $\gamma_\sigma^\dagger$

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

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

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

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

Declare a matrix in code implementation:

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

Diagonalize $\mathbf{H}$ and obtain

eigenvectors:

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

where we define the global indices

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

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

OS:

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

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

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

eigenvalues:

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

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:

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

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

Using global indices, we obtain

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

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

Since

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

$$\langle n_{i\uparrow}\rangle = \sum_{n=1}^{2N} |\mathbf{u}_i^n|^2 \frac{1}{2}\left(1 - \tanh\frac{\beta E_n}{2}\right)$$

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

(2) Superconducting pairing:

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

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

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

Using global indices, we obtain

$$\Delta_{ij} = \frac{V}{2}\sum_{n}\left[u_i^n v_j^{n*} f(-E_{n\uparrow}) - v_i^{n*} u_j^n f(E_{n\downarrow}) - v_j^{n*} u_i^n f(E_{n\uparrow}) + u_j^n v_i^{n*} f(-E_{n\downarrow})\right]$$

$$= \frac{V}{2}\sum_{n=1}^{2N}\left[\mathbf{u}_i^n \mathbf{v}_j^{n*} f(-E_n) - \mathbf{u}_i^n \mathbf{v}_j^{n*} f(E_n)\right]$$

$$= \frac{V}{2}\sum_{n=1}^{2N} \mathbf{u}_i^n \mathbf{v}_j^{n*}\left[1 - 2f(E_n)\right]$$

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

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

EXAMPLES:

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

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

   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

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

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

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

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

$$W_{ij} = W_{ij\uparrow} + W_{ij\downarrow} = V\cdot\Im\left(\left\langle c_{i\uparrow}^\dagger c_{j\uparrow}\right\rangle + \left\langle c_{i\downarrow}^\dagger c_{j\downarrow}\right\rangle\right)$$

$$\left\langle c_{i\uparrow}^{\dagger}c_{j\uparrow}\right\rangle = \sum_{n}\left\langle\left(u_i^{n*}\gamma_{n\uparrow}^{\dagger} - v_i^{n}\gamma_{n\downarrow}\right)\left(u_j^{n}\gamma_{n\uparrow} - v_j^{n*}\gamma_{n\downarrow}^{\dagger}\right)\right\rangle$$

$$= \sum_{n}\left\langle\left(u_i^{n*}\gamma_{n\uparrow}^{\dagger} - v_i^{n}\gamma_{n\downarrow}\right)\left(u_j^{n}\gamma_{n\uparrow} - v_j^{n*}\gamma_{n\downarrow}^{\dagger}\right)\right\rangle$$

$$= \sum_{n}\left[u_i^{n*}u_j^{n}\left\langle\gamma_{n\uparrow}^{\dagger}\gamma_{n\uparrow}\right\rangle + v_i^{n}v_j^{n*}\left\langle\gamma_{n\downarrow}\gamma_{n\downarrow}^{\dagger}\right\rangle\right]$$

$$= \sum_{n}\left[u_i^{n*}u_j^{n}f\left(E_{n\uparrow}\right) + v_i^{n}v_j^{n*}f\left(-E_{n\downarrow}\right)\right]$$

$$\left\langle c_{i\downarrow}^{\dagger}c_{j\downarrow}\right\rangle = \sum_{n}\left\langle\left(u_i^{n*}\gamma_{n\downarrow}^{\dagger} + v_i^{n}\gamma_{n\uparrow}\right)\left(u_j^{n}\gamma_{n\downarrow} + v_j^{n*}\gamma_{n\uparrow}^{\dagger}\right)\right\rangle$$

$$= \sum_{n}\left[u_i^{n*}u_j^{n}\left\langle\gamma_{n\downarrow}^{\dagger}\gamma_{n\downarrow}\right\rangle + v_i^{n}v_j^{n*}\left\langle\gamma_{n\uparrow}\gamma_{n\uparrow}^{\dagger}\right\rangle\right]$$

$$= \sum_{n}\left[u_i^{n*}u_j^{n}f\left(E_{n\downarrow}\right) + v_i^{n}v_j^{n*}f\left(-E_{n\uparrow}\right)\right]$$

Using global indices, we obtain

$$W_{ij} = V\cdot\Im\sum_{n}\Big[u_i^{n*}u_j^{n}f\left(E_{n\uparrow}\right) + v_i^{n}v_j^{n*}f\left(-E_{n\downarrow}\right)$$

$$+ u_i^{n*}u_j^{n}f\left(E_{n\downarrow}\right) + v_i^{n}v_j^{n*}f\left(-E_{n\uparrow}\right)\Big]$$

$$= V\cdot\Im\sum_{n=1}^{2N}\left[\mathbf{u}_i^{n*}\mathbf{u}_j^{n}f\left(E_n\right) + \mathbf{v}_i^{n*}\mathbf{v}_j^{n}\left[1 - f\left(E_n\right)\right]\right]$$

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

$$\hat{\mathcal{H}}_B = \frac{1}{2m}\left(\hat{p} + \frac{e}{c}\vec{A}\right)^2 + V(\vec{r})$$

$$\tilde{\psi}_k(\vec{r}) = \frac{1}{\sqrt{N}}\sum_R e^{i\vec{k}\cdot\vec{R}}\,\tilde{w}\left(\vec{r} - \vec{R}\right)$$

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

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

The Schrödinger equation gives

$$\hat{\mathcal{H}}_B\tilde{\psi}_k(\vec{r}) = \frac{1}{\sqrt{N}}\sum_R e^{i\vec{k}\cdot\vec{R}}\,\hat{\mathcal{H}}\tilde{w}\left(\vec{r} - \vec{R}\right)$$

$$= \frac{1}{\sqrt{N}}\sum_R e^{i\vec{k}\cdot\vec{R}}\left[\frac{1}{2m}\left(\hat{p} + \frac{e}{c}\vec{A}\right)^2 + V(\vec{r})\right]\tilde{w}\left(\vec{r} - \vec{R}\right)$$

Since

$$\hat{p}e^{i\phi}w\left(\vec{r} - \vec{R}\right) = -i\hbar\nabla e^{i\phi}w\left(\vec{r} - \vec{R}\right)$$

$$= -i\hbar\left[e^{i\phi}\nabla w\left(\vec{r} - \vec{R}\right) + ie^{i\phi}\nabla\phi w\left(\vec{r} - \vec{R}\right)\right]$$

$$= e^{i\phi}(\hat{p} + \hbar\nabla\phi)w\left(\vec{r} - \vec{R}\right)$$

$$\left(\hat{p} + \frac{e}{c}\vec{A}\right)^2\tilde{w}\left(\vec{r} - \vec{R}\right) = \left(\hat{p} + \frac{e}{c}\vec{A}\right)\cdot\left(\hat{p} + \frac{e}{c}\vec{A}\right)e^{i\phi}w\left(\vec{r} - \vec{R}\right)$$

$$= \left(\hat{p} + \frac{e}{c}\vec{A}\right)\cdot e^{i\phi}\left(\hat{p} + \frac{e}{c}\vec{A} + \hbar\nabla\phi\right)w\left(\vec{r} - \vec{R}\right)$$

$$= e^{i\phi}\left(\hat{p} + \frac{e}{c}\vec{A} + \hbar\nabla\phi\right)^2 w\left(\vec{r} - \vec{R}\right)$$

Thus, we obtain

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

Since

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

We need to set

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

Thus, we obtain

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

⇒ 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

$$\tilde{t}_{ij} = -\int \widetilde{w}^*\left(\vec{r}-\vec{R}_i\right)\widehat{\mathcal{H}}_B\widetilde{w}\left(\vec{r}-\vec{R}_j\right)d^3r$$

$$= -\int e^{-i\phi_i}w^*\left(\vec{r}-\vec{R}_i\right)e^{i\phi_j}\widehat{\mathcal{H}}w\left(\vec{r}-\vec{R}_j\right)d^3r$$

$$= -\int e^{-i\left(\phi_i-\phi_j\right)}w^*\left(\vec{r}-\vec{R}_i\right)\widehat{\mathcal{H}}w\left(\vec{r}-\vec{R}_j\right)d^3r$$

$$= -e^{-i\left(\phi_i-\phi_j\right)}t_{ij}$$

Since

$$\phi_i - \phi_j = -\frac{e}{\hbar c}\left(\int_{R_i}^r \vec{A}(\vec{r}')\cdot d\vec{r}' + \int_{R_j}^r \vec{A}(\vec{r}')\cdot d\vec{r}'\right)$$

$$= -\frac{e}{\hbar c}\int_{R_i\to r\to R_j}\vec{A}(\vec{r}')\cdot d\vec{r}'$$

$$= -\frac{e}{\hbar c}\oint_{\vec{R}_i\to\vec{r}\to\vec{R}_j\to\vec{R}_i}\vec{A}(\vec{r}')\cdot d\vec{r}' - \frac{e}{\hbar c}\int_{R_i}^{R_j}\vec{A}(\vec{r}')\cdot d\vec{r}'$$

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,

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

Let

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

where Φ_0 is the single-particle flux quantum,

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

Thus, we obtain

$$\phi_i - \phi_j \approx -\phi_{ij}$$

which is yielding the desired result,

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

⇒ 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

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

Now, we can solve the BdG equations as follows:

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

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

$$\sum_j \left[-t_{ij} e^{-i\left(\phi_i - \phi_j\right)} \tilde{u}_j^n + \tilde{\Delta}_{ij} \tilde{v}_j^n \right] = E_{n\uparrow} \tilde{u}_i^n$$

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

$$\sum_j \left[-t_{ij} e^{i\phi_j} \tilde{u}_j^n + \tilde{\Delta}_{ij} \tilde{v}_j^n e^{i\phi_i} \right] = E_{n\uparrow} \tilde{u}_i^n e^{i\phi_i}$$

To make the equations covariant, let

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

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

$$\widetilde{\Delta}_{ij} = \Delta_{ij} e^{-i\left(\phi_i - \phi_j\right)}$$

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

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

EXAMPLES:

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

presence of a magnetic field,

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

We then obtain the pairing using

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

Since the d-wave superconductivity is

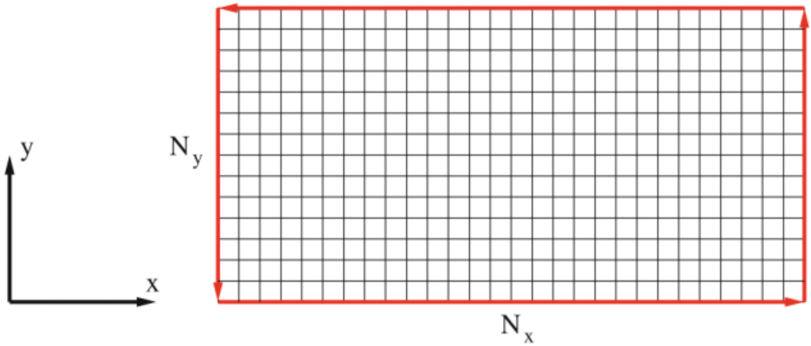
$$\Delta_i = \frac{1}{4}\left(\Delta_{i+x} + \Delta_{i-x} - \Delta_{i+y} - \Delta_{i-y}\right)$$

We need calculate each pairing as

$$\Delta_{ij} = \widetilde{\Delta}_{ij} e^{i(\phi_i - \phi_j)} = \tilde{\Delta}_{ij} e^{-i\phi_{ij}}$$

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

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

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

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

where $\square$ implies a closed loop

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

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

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

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

$$\sum_{\square} \phi_{ij} = \frac{2\pi}{\Phi_0} BN_xN_ya^2 = 2\pi$$

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

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

we should let

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

(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

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

Thus, we have

$$\vec{A}(\hat{T}_{m0}\vec{r}) = (-B\hat{T}_{m0}y, 0,0) = (-By, 0,0) = \vec{A}(\vec{r}) = \vec{A}(\vec{r}) + \nabla\chi\left(\vec{R}\right)$$

$$\Rightarrow \nabla\chi\left(\vec{R}\right) = 0$$

and

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

Thus, we obtain

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

From 1-4-C, we have

$$\begin{aligned}u_i' &= e^{i\frac{e}{\hbar c}\chi(R)}u_i = e^{i2\pi\chi(R)/\Phi_0}u_i\\ v_i' &= e^{-i\frac{e}{\hbar c}\chi(R)}v_i = e^{-i2\pi\chi(R)/\Phi_0}v_i\\ \Delta_{ij}' &= e^{i2\frac{e}{\hbar c}\chi(R)}\Delta_{ij} = e^{i4\pi\chi(R)/\Phi_0}\Delta_{ij}\end{aligned}$$

where

$$\chi\left(\vec{R}\right) = -BnN_y amN_x a = -mn\Phi_0$$

By considering a closed path around the rectangular lattice,

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

the acquired flux of the superconducting pairing is

$$\sum_{\square}\phi = -\frac{4\pi}{\Phi_0}(-\phi_0) = 4\pi$$

⇒ The flux enclosed by a unit cell has two superconducting flux quanta. Each vortex carrys the flux quantum $hc/2e$.

C. PERIODIC BOUNDARY CONDITIONS

(1) Since a magnetic unit cell contains two vortexes, 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

$$\sum_{\square}\phi_{ij} = \sum_{\square}\frac{2\pi}{\Phi_0}\int_{R_i}^{R_j}\vec{A}(\vec{r})\cdot d\vec{r} = \phi_{①} + \phi_{②} + \phi_{③} + \phi_{④}$$

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

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

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

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

$$\sum_{\square}\phi_{ij} = \frac{2\pi}{\Phi_0}Ba^2 = \frac{2\pi}{\Phi_0}\frac{\Phi_0}{N_xN_ya^2}a^2 = \underbrace{\frac{2\pi}{N_xN_y}}_{=\varphi_0} = \varphi_0$$

The Peierls phase factors are

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

at the boundaries

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

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

$$\sum_{\square}\phi_{ij} = \sum_{\square}\frac{2\pi}{\Phi_0}\int_{R_i}^{R_j}\vec{A}(\vec{r})\cdot d\vec{r} = \phi_{①} + \phi_{②} + \phi_{③}$$

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

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

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

$$\sum_{\square}\phi_{ij} = \frac{2\pi}{\Phi_0}B\frac{a^2}{2} = \frac{2\pi}{\Phi_0}\frac{\Phi_0}{N_xN_ya^2}\frac{a^2}{2} = \frac{1}{2}\underbrace{\frac{2\pi}{N_xN_y}}_{=\varphi_0} = \frac{\varphi_0}{2}$$

The Peierls phase factors are

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

at the boundaries

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

OS:

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

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

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

$$\sum_{\square} \phi_{ij} = \sum_{\square} \frac{2\pi}{\Phi_0} \int_{R_i}^{R_j} \vec{A}(\vec{r}) \cdot d\vec{r} = \phi_{①} + \phi_{②} + \phi_{③} + \phi_{④}$$

$$\phi_{①} = \frac{2\pi}{\Phi_0} \int_{x,y}^{x+2,y} \vec{A}(\vec{r}) \cdot d\vec{r} = -\frac{2\pi}{\Phi_0} B2ya^2$$

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

$$\phi_{③} = \frac{2\pi}{\Phi_0} \int_{x+2,y+2}^{x,y+2} \vec{A}(\vec{r}) \cdot d\vec{r} = \frac{2\pi}{\Phi_0} B2(y+1)a^2$$

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

$$\sum_{\square} \phi_{ij} = \frac{2\pi}{\Phi_0} B2a^2 = \frac{2\pi}{\Phi_0} \frac{2\Phi_0}{N_x N_y a^2} a^2 = 2 \underbrace{\frac{2\pi}{N_x N_y}}_{=\varphi_0} = 2\varphi_0$$

The Peierls phase factors are

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

at the boundaries

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

4-3 Local Density of States

A. GREEN'S FUNCTIONS ON LATTICE

(1) Matsubara Green's function

$$G_{ij\uparrow}(\tau) = -\left\langle \hat{\mathrm{T}}\left[\hat{c}_{i\uparrow}(\tau)\hat{c}_{j\uparrow}^{\dagger}(0)\right]\right\rangle = -\Theta(\tau)\left\langle \hat{c}_{i\uparrow}(\tau)\hat{c}_{j\uparrow}^{\dagger}(0)\right\rangle + \Theta(-\tau)\left\langle \hat{c}_{j\uparrow}^{\dagger}(0)\hat{c}_{i\uparrow}(\tau)\right\rangle$$

$$G_{ij\downarrow}^{*}(\tau) = -\left\langle \hat{\mathrm{T}}\left[\hat{c}_{i\downarrow}^{\dagger}(\tau)\hat{c}_{j\downarrow}(0)\right]\right\rangle$$

$$= -\Theta(\tau)\left\langle c_{i\downarrow}^{\dagger}(\tau)c_{j\downarrow}(0)\right\rangle + \Theta(-\tau)\left\langle c_{j\downarrow}(0)c_{i\downarrow}^{\dagger}(\tau)\right\rangle$$

$$F_{ij}(\tau) = -\left\langle \hat{\mathrm{T}}\left[\hat{c}_{i\uparrow}(\tau)\hat{c}_{j\downarrow}(0)\right]\right\rangle = -\Theta(\tau)\left\langle c_{i\uparrow}(\tau)c_{j\downarrow}(0)\right\rangle + \Theta(-\tau)\left\langle c_{j\downarrow}(0)c_{i\uparrow}(\tau)\right\rangle$$

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

The equations of motion of Green's function

$$\frac{\partial}{\partial\tau}G_{ij\uparrow}(\tau) = -\frac{\partial}{\partial\tau}\Theta(\tau)\left\langle c_{i\uparrow}(\tau)c_{j\uparrow}^{\dagger}(0)\right\rangle + \frac{\partial}{\partial\tau}\Theta(-\tau)\left\langle c_{j\uparrow}^{\dagger}(0)c_{i\uparrow}(\tau)\right\rangle$$
$$-\Theta(\tau)\left\langle \frac{\partial}{\partial\tau}c_{i\uparrow}(\tau)c_{j\uparrow}^{\dagger}(0)\right\rangle + \Theta(-\tau)\left\langle c_{j\uparrow}^{\dagger}(0)\frac{\partial}{\partial\tau}c_{i\uparrow}(\tau)\right\rangle$$

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

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

Use

$$-\frac{\partial}{\partial\tau}\hat{c}_{i\sigma}^{\dagger}(\tau) = \left[c_{i\sigma}^{\dagger}(\tau), \hat{H}\right] = \sum_{j} t_{ij}^{*}\hat{c}_{j\sigma}^{\dagger} - \sigma\Delta_{ij}^{*}c_{v\bar{\sigma}}$$

$$-\frac{\partial}{\partial\tau}c_{i\sigma}(\tau) = \left[c_{i\sigma}(\tau), \hat{H}\right] = \sum_{l} -t_{il}\hat{c}_{l\sigma}(\tau) + \sigma\Delta_{il}\hat{c}_{l\bar{\sigma}}^{\dagger}(\tau)$$

We obtain

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

$$\frac{\partial}{\partial\tau}G^*_{ij\downarrow}(\tau) = -\delta(\tau)\left\langle\left\{c^\dagger_{i\downarrow}(\tau), c_{j\downarrow}(0)\right\}\right\rangle - \left\langle\hat{\mathrm{T}}\left[\frac{\partial}{\partial\tau}c^\dagger_{i\downarrow}(\tau)c_{j\downarrow}(0)\right]\right\rangle$$

$$= \delta(\tau)\delta_{ij} + \sum_l\left(-t^*_{il}G^*_{lj\downarrow}(\tau) - \Delta^*_{il}F_{lj}(\tau)\right)$$

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

$$= \sum_l\left(t_{il}F_{lj}(\tau) - \Delta_{il}G^*_{lj\downarrow}(\tau)\right)$$

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

$$= \sum_l\left(-\Delta^*_{il}G_{lj\uparrow}(\tau) - t^*_{il}F^*_{lj}(\tau)\right)$$

These equations are rearranged

$$-\frac{\partial}{\partial\tau}G_{ij\uparrow}(\tau) - \sum_l\left(-t_{il}G_{lj\uparrow}(\tau) + \Delta_{il}F^*_{lj}(\tau)\right) = \delta(\tau)\delta_{ij}$$

$$-\frac{\partial}{\partial\tau}F_{ij}(\tau) - \sum_l\left(-t_{il}F_{lj}(\tau) + \Delta_{il}G^*_{lj\downarrow}(\tau)\right) = 0$$

$$-\frac{\partial}{\partial\tau}F^*_{ij}(\tau) - \sum_l\left(\Delta^*_{il}G_{lj\uparrow}(\tau) + t^*_{il}F^*_{lj}(\tau)\right) = 0$$

$$-\frac{\partial}{\partial\tau}G^*_{ij\downarrow}(\tau) - \sum_l\left(t^*_{il}G^*_{lj\downarrow}(\tau) + \Delta^*_{il}F_{lj}(\tau)\right) = \delta(\tau)\delta_{ij}$$

We now write these equations in a matrix form

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

$$-\begin{pmatrix} -t_{11} & \cdots & -t_{1N} & \Delta_{11} & \cdots & \Delta_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ -t_{N1} & \cdots & -t_{NN} & \Delta_{N1} & \cdots & \Delta_{NN} \\ \Delta^*_{11} & \cdots & \Delta^*_{11} & t^*_{11} & \cdots & t^*_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \Delta^*_{11} & \cdots & \Delta^*_{11} & t^*_{N1} & \cdots & t^*_{NN} \end{pmatrix}\begin{pmatrix} G_{11\uparrow} & \cdots & G_{1N\uparrow} & F_{11} & \cdots & F_{1N} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ G_{N1\uparrow} & \cdots & G_{NN\uparrow} & F_{N1} & \cdots & F_{NN} \\ F^*_{11} & \cdots & F^*_{1N} & G^*_{11\downarrow} & \cdots & G^*_{1N\downarrow} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ F^*_{N1} & \cdots & F^*_{NN} & G^*_{N1\downarrow} & \cdots & G^*_{NN\downarrow} \end{pmatrix}$$

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

Let

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

The equations can be rewritten as

$$-\frac{\partial}{\partial\tau}\begin{pmatrix} \mathrm{G}_\uparrow & \mathrm{F} \\ \mathrm{F}^* & \mathrm{G}_\downarrow^* \end{pmatrix}(\tau) - \begin{pmatrix} -\mathrm{t} & \Delta \\ \Delta^* & \mathrm{t}^* \end{pmatrix}\begin{pmatrix} \mathrm{G}_\uparrow & \mathrm{F} \\ \mathrm{F}^* & \mathrm{G}_\downarrow^* \end{pmatrix}(\tau) = \delta(\tau)\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

This equation is known as Gor'kov equations.

(2) Fourier transform of the Green's functions

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

$$\delta(\tau) = \frac{1}{\beta}\sum_\omega e^{-i\omega\tau}$$

Substituting into Gor'kov equations, we obtain

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

$$\Rightarrow \left[\begin{pmatrix} i\omega & 0 \\ 0 & i\omega \end{pmatrix} - \begin{pmatrix} -\mathrm{t} & \Delta \\ \Delta^* & \mathrm{t}^* \end{pmatrix}\right]\begin{pmatrix} \mathrm{G}_\uparrow & \mathrm{F} \\ \mathrm{F}^* & \mathrm{G}_\downarrow^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Insert Bogoliubov unitary transformation matrix

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

The solutions of BdG equations give us

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

$$\Rightarrow \begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix}\begin{pmatrix} i\omega - \mathrm{E}_\uparrow & 0 \\ 0 & i\omega + \mathrm{E}_\downarrow \end{pmatrix}\begin{pmatrix} \mathrm{u} & -\mathrm{v}^* \\ \mathrm{v} & \mathrm{u}^* \end{pmatrix}^\dagger\begin{pmatrix} \mathrm{G}_\uparrow & \mathrm{F} \\ \mathrm{F}^* & \mathrm{G}_\downarrow^* \end{pmatrix}(i\omega) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

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

$$= \begin{pmatrix} u & -v^* \\ v & u^* \end{pmatrix}\begin{pmatrix} \frac{1}{i\omega - E_\uparrow} & 0 \\ 0 & \frac{1}{i\omega + E_\downarrow} \end{pmatrix}\begin{pmatrix} u^* & v^* \\ -v & u \end{pmatrix}$$

$$= \begin{pmatrix} \frac{uu^*}{i\omega - E_\uparrow} + \frac{v^*v}{i\omega + E_\downarrow} & \frac{uv^*}{i\omega - E_\uparrow} - \frac{v^*u}{i\omega + E_\downarrow} \\ \frac{vu^*}{i\omega - E_\uparrow} - \frac{u^*v}{i\omega + E_\downarrow} & \frac{v^*v}{i\omega - E_\uparrow} + \frac{uu^*}{i\omega + E_\downarrow} \end{pmatrix}$$

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

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

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

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

Thus, we obtain

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

B. LOCAL DENSITY OF STATES

(1) The local density of states at zero temperature

$$\rho_i(\omega) = -\frac{1}{\pi}\Im\left(G_{ii\uparrow} + G_{ii\downarrow}\right)$$

$$-\frac{1}{\pi}\Im\left(G_{ii\uparrow}\right) = -\frac{1}{\pi}\sum_n \Im\left(\frac{\mathbf{u}_i^n \mathbf{u}_i^{n*}}{i\omega - E_n}\right) = -\sum_n \left|\mathbf{u}_i^n\right|^2 \delta(E_n - \omega)$$

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

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

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

$$\delta(E_n - \omega) = -f'(E_n - \omega) = -\frac{df(\omega)}{d\omega}$$

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

Since

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

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

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

C. SUPERCELL

(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

$$\mathrm{u}_k\left(\vec{r}+M\vec{L}\right)=e^{i\vec{k}\cdot M\vec{L}}\mathrm{u}_k(\vec{r})=\mathrm{u}_k(\vec{r})$$

$$\Rightarrow e^{ik_iM_iN_ia_i}=1$$

$$\Rightarrow k_i=\frac{2\pi\ell_i}{M_iN_ia_i}\text{ where }\ell_i=0,\cdots,M_iN_i-1$$

The Bloch wavefunctions for each supercell are

$$\mathrm{u}_k(\vec{r})=e^{i\frac{\ell_i}{M_iN_i}\frac{2\pi}{a_i}\cdot r_i}\mathrm{u}(\vec{r})$$

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

$$\mathrm{u}_k=e^{i\vec{k}\cdot\vec{r}}\mathrm{u}$$

$$\mathrm{v}_k=e^{i\vec{k}\cdot\vec{r}}\mathrm{v}$$

(2) BdG equations are

$$\begin{pmatrix}-\mathrm{t}_k & \Delta_k\\ \Delta_k^* & \mathrm{t}_k^*\end{pmatrix}\begin{pmatrix}\mathrm{u}_k & -\mathrm{v}_k^*\\ \mathrm{v}_k & \mathrm{u}_k^*\end{pmatrix}=\begin{pmatrix}\mathrm{u}_k & -\mathrm{v}_k^*\\ \mathrm{v}_k & \mathrm{u}_k^*\end{pmatrix}\begin{pmatrix}\mathrm{E}_{k\uparrow} & 0\\ 0 & -\mathrm{E}_{k\downarrow}\end{pmatrix}$$

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

$$\sum_j\left[-t_{ij}(k)e^{i\vec{k}\cdot\vec{r}_j}u_j^n+\Delta_{ij}(k)e^{i\vec{k}\cdot\vec{r}_j}v_j^n\right]=E_{n,k\uparrow}e^{i\vec{k}\cdot\vec{r}_i}u_i^n$$

$$\sum_j\left[-t_{ij}(k)e^{-i\vec{k}\cdot\left(\vec{r}_i-\vec{r}_j\right)}u_j^n+\Delta_{ij}(k)e^{-i\vec{k}\cdot\left(\vec{r}_i-\vec{r}_j\right)}v_j^n\right]=E_{n,k\uparrow}u_i^n$$

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

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

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

$$\rho_i(\omega)=\frac{\beta}{4}\frac{1}{M_xM_y}\sum_{n,k}\left\{\left|\mathbf{u}_i^{n,k}\right|^2\left[1-\tanh^2\left(\frac{\beta\left(E_{n,k}-\omega\right)}{2}\right)\right]+\left|\mathbf{v}_i^{n,k}\right|^2\left[1-\tanh^2\left(\frac{\beta\left(E_{n,k}+\omega\right)}{2}\right)\right]\right\}$$

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.

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

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

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

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

$$\hat{J}^P_x(\vec{r}_i) = -i\sum_\sigma\left(t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} - t^*_{ij}c^{\dagger}_{j\sigma}c_{i\sigma}\right)$$

and the kinetic energy operator is defined as

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

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

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

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

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

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

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

B. KUBO FORMULA

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

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

The expectation of a physical variable is found to be

$$\langle\hat{O}\rangle = \mathrm{Tr}\left[\hat{\rho}(-\infty)\hat{O}\right] - \frac{i}{\hbar}\int_{-\infty}^{t}\mathrm{Tr}\left\{\hat{\rho}(-\infty)\left[\hat{O}(t'), \hat{H}'(t')\right]\right\}dt'$$
$$= \langle\hat{O}\rangle_0 - \frac{i}{\hbar}\int_{-\infty}^{t}\langle\left[\hat{O}(t'), \hat{H}'(t')\right]\rangle dt'$$

where

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

(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

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

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

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

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

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

Thus, we obtain

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

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

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

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

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

According to Wick's theorem

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

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

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

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

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

Since

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

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

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

$$=\frac{1}{\beta}\sum_\omega\sum_{nn'}\langle T_\tau \hat{J}_x^P(r,\omega)\hat{J}_x^P(r',\Omega+\omega)\rangle$$

$$\frac{1}{\beta}\sum_\omega\sum_{nn'}G_{i'j}^{\uparrow}G_{ij'}^{\uparrow}=\frac{1}{\beta}\sum_\omega\sum_{n=1}\sum_{n'=1}\frac{\mathbf{u}_{i'}^{n}\mathbf{u}_{j}^{n*}}{i\omega\ -E_n}\frac{\mathbf{u}_{i}^{n'}\mathbf{u}_{j'}^{n'*}}{i(\Omega+\omega)\ -E_{n'}}$$

$$=\sum_{n=1}\sum_{n'=1}\mathbf{u}_{i'}^{n}\mathbf{u}_{j}^{n*}\mathbf{u}_{i}^{n'}\mathbf{u}_{j'}^{n'*}\frac{f(E_n)-f(i\Omega+E_{n'})}{i\Omega+E_n-E_{n'}}$$

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

$$\frac{1}{\beta}\sum_\omega\sum_{nn'}G_{i'j\uparrow\uparrow}G_{ij'\uparrow\uparrow}=\sum_{n=1}\sum_{n'=1}\mathbf{u}_{i'}^{n}\mathbf{u}_{j}^{n*}\mathbf{u}_{i}^{n'}\mathbf{u}_{j'}^{n'*}\frac{f(E_n)-f(E_{n'})}{E_n-E_{n'}}$$

$$\Lambda_{xx}(i,j,\Omega=0)=-2t_{ij}t_{i'j'}\sum_{n=1}\sum_{n'=1}\Big(-\mathbf{u}_{i'}^{n}\mathbf{u}_{j}^{n*}\mathbf{u}_{i}^{n'}\mathbf{u}_{j'}^{n'*}-\mathbf{v}_{i}^{n}\mathbf{v}_{j'}^{n*}\mathbf{v}_{i'}^{n'}\mathbf{v}_{j}^{n'*}$$

$$-\mathbf{v}_{i}^{n}\mathbf{u}_{j'}^{n*}\mathbf{u}_{i'}^{n'}\mathbf{v}_{j}^{n'*}-\mathbf{v}_{i'}^{n}\mathbf{u}_{j}^{n*}\mathbf{u}_{i}^{n'}\mathbf{v}_{j'}^{n'*}\Big)\frac{f(E_n)-f(E_{n'})}{E_n-E_{n'}}$$

Let

$$\mathbf{\Gamma}_{ij}^{nn'}=t_{ij}\left(\mathbf{u}_{j}^{n*}\mathbf{u}_{i}^{n'}-\mathbf{v}_{i}^{n}\mathbf{v}_{j}^{n'*}\right)$$

$$\Lambda_{xx}(i,j,\Omega=0)=-2t_{ij}t_{i'j'}\sum_{n=1}\sum_{n'=1}\mathbf{\Gamma}_{ij}^{nn'}\mathbf{\Gamma}_{i'j'}^{nn'}\frac{f(E_n)-f(E_{n'})}{E_n-E_{n'}}$$

$$\rho_s(i,j)=\langle -K_x(i,j)\rangle-\Lambda_{xx}(i,j,\Omega=0)$$

$$=-\sum_{n=1}\sum_{n'=1}\mathbf{\Gamma}_{ij}^{nn'}\mathbf{\Gamma}_{i'j'}^{nn'}\frac{f(E_n)-f(E_{n'})}{E_n-E_{n'}}$$

$$-\sum_n t_{ij}\left[\mathbf{u}_{j}^{n}\mathbf{u}_{i}^{n*}f(E_n)+\mathbf{v}_{i}^{n}\mathbf{v}_{j}^{n*}(1-f(E_n)\right]$$

(3) The local or site-specific superfluid density is then given by
Let $j=i$

$$\rho_s(i) = \langle -\hat{K}_x(i) \rangle - \Lambda_{xx}(i, \Omega = 0)$$

$$= -\sum_{n=1}\sum_{n'=1} \mathbf{\Gamma}_i^{nn'} \mathbf{\Gamma}_{i+x}^{nn'} \frac{f(E_n) - f(E_{n'})}{E_n - E_{n'}}$$

$$- \sum_{n} t_{ii+x} \left[\mathbf{u}_{i+x}^{n} \mathbf{u}_i^{n*} f(E_n) + \mathbf{v}_i^{n} \mathbf{v}_{i+x}^{n*} (1 - f(E_n)) \right]$$

$$\mathbf{\Gamma}_i^{nn'} = t_{ii+x} \left(\mathbf{u}_{i+x}^{n*} \mathbf{u}_i^{n'} - \mathbf{v}_i^{n} \mathbf{v}_{i+x}^{n'*} \right)$$

(4) The superfluid density is evaluated as

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

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.

$$\langle \hat{K}_x \rangle = \frac{1}{N} \sum_i \sum_\sigma \left\langle \left[t_{i,i+x} c_{i\sigma}^{\dagger} c_{i+x\sigma} + \text{H.c.} \right] \right\rangle$$

$$\Lambda_{xx}(q, i\Omega_n) = \frac{1}{N} \int_0^{1/T} d\tau \, e^{-i\Omega_n \tau} \langle T_\tau \hat{J}_x^P(q,\tau) \hat{J}_x^P(-q, 0) \rangle$$

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

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

4-5 Spin Relaxation Time

A. SPIN-SPIN CORRELATION

(1) Spin-spin correlation

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

Let

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

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

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

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

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

Assume

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

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

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

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

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

(2) The Fourier transformation of χ

$$\chi_{ij}^{+-}(i\Omega_l) = \int_0^{\beta} e^{i\Omega_l \tau} \chi_{ij}^{+-}(\tau)\, d\tau$$

$$= \int_0^{\beta} e^{i\Omega_l \tau} \frac{1}{\beta^2} \sum_{\omega_l \omega_l'} e^{i\omega_l \tau} e^{-i\omega_l' \tau} \times \left[G_{ji\uparrow}(i\omega_n) G_{ji\downarrow}(i\omega_n') - F_{ji}(i\omega_n) F_{ji}^{*}(i\omega_n') \right] d\tau$$

Since

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

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

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

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

Since

$$\frac{1}{\beta}\sum_{\omega_n'}\left[\frac{1}{i\omega_n - E_n}\cdot\frac{1}{i\Omega_n + i\omega_n - E_m}\right]$$
$$= \frac{1}{\beta}\sum_{\omega_n'}\left[\frac{1}{i\omega_n - E_n} - \frac{1}{i\Omega_n + i\omega_n - E_m}\right]\frac{1}{i\Omega_n + E_n - E_m}$$
$$= \frac{f(E_n) - f(E_m - i\Omega_n)}{i\Omega_n + E_n - E_m}$$
$$\chi_{ij}^{+-}(i\Omega_n) = \sum_{n,m}\left(\mathbf{u}_j^n\mathbf{u}_i^{n*}\mathbf{v}_j^m\mathbf{v}_i^{m*} - \mathbf{u}_j^n\mathbf{v}_i^{n*}\mathbf{v}_j^m\mathbf{u}_i^{m*}\right)\frac{f(E_n) - f(E_m - i\Omega_n)}{i\Omega_n + E_n - E_m}$$

(3) Analytic continuation

$$i\Omega \to \Omega + i\eta$$

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

B. SPIN RELAXATION TIME (T_1)

(1) The spin-lattice relaxation time is

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

where

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

(2) Since

$$\mathbf{u}_i^n \mathbf{u}_i^{n*} \mathbf{v}_i^m \mathbf{v}_i^{m*} - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} = |\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*}$$

$$\Im\left(\frac{1}{\Omega_n + i\eta + E_n - E_m} \right) = (-\pi)\delta(\Omega_n + E_n - E_m)$$

Thus, we obtain

$$\Im\left(\chi_{ii}^{+-}(\Omega_n + i\eta) \right) = \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \times [f(E_n) - f(E_m - \Omega_n - i\eta)](-\pi)\delta(\Omega_n + E_n - E_m)$$

$$\left.\frac{1}{T_1 T}\right|_{\Omega_n \to 0} = \lim_{\Omega_n \to 0} \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \times \frac{f(E_n) - f(E_m - \Omega_n - i\eta)}{\Omega_n} (-\pi)\delta(\Omega_n + E_n - E_m)$$

$$= \sum_{n,n'} \left(|\mathbf{u}_i^n|^2 |\mathbf{v}_i^m|^2 - \mathbf{u}_i^n \mathbf{v}_i^{n*} \mathbf{v}_i^m \mathbf{u}_i^{m*} \right) \left[-f'(E_n)\pi\delta(E_n - E_m) \right]$$