Density-Functional Theory for Superconductors (I)
General Formalism

§. System: Electron Liquid

$$K \equiv H - \mu N$$

$$= \sum_\sigma \int d^3r\, \psi_\sigma^+(r) \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_\sigma(r) + \frac{e^2}{2}\sum_{\sigma\sigma'} \int d^3r d^3r' \frac{\psi_\sigma^+(r)\psi_{\sigma'}^+(r')\psi_{\sigma'}(r')\psi_\sigma(r)}{|r - r'|} \quad -(1)$$

We introduce an external potential $\phi(r)$, and anomalous pair potentials $D_{\alpha\beta}(r, r')$, so that

$$\boxed{K_{\phi,D} \equiv K + \int d^3r\, \rho(r)\phi(r) + \sum_{\alpha\beta}\int d^3r d^3r' \left[D^*_{\alpha\beta}(r,r')\psi_\alpha(r)\psi_\beta(r') + \text{H.C.} \right]} \quad -(2)$$

where $\rho(r) = \sum_\sigma \psi_\sigma^+(r)\psi_\sigma(r)$.

§. Minimum Free-Energy Principle

$$\Omega_{H-\mu N}[\rho] \equiv \mathrm{tr}\,\rho\,[H - \mu N + \frac{1}{\beta}\ln\rho]$$

$$= \langle H\rangle - \mu\langle N\rangle - T\langle S\rangle \quad -(3)$$

where $\langle S\rangle = -k_B\,\mathrm{tr}[\rho\ln\rho]$. Then, $\Omega_{H-\mu N}[\rho]$ takes its minimum value

$$\Omega_{H-\mu N}[\rho_{H-\mu N}] = -\frac{1}{\beta}\ln\{\mathrm{tr}[e^{-\beta(H-\mu N)}]\} \quad -(4)$$

when

$$\rho = \rho_{H-\mu N} \equiv e^{-\beta(H-\mu N)}/\mathrm{tr}[e^{-\beta(H-\mu N)}] \quad -(5)$$

under the constraint, $\mathrm{tr}\,\rho = 1$.

□ Proof of Eqs. (3) − (5)

(Lemma)

$$\Omega_{H-\mu N}[\rho_{H'-\mu N}] \geq \Omega_{H-\mu N}[\rho_{H-\mu N}]$$

$\Updownarrow$ equivalent

$$\mathrm{tr}[\rho_{H'-\mu N}\ln\rho_{H'-\mu N}] \geq \mathrm{tr}[\rho_{H'-\mu N}\ln\rho_{H-\mu N}]$$

$$\left(\because\ \mathrm{tr}[\rho'\ln(e^{-\beta(H'-\mu N)}/\mathrm{tr}\,e^{-\beta(H'-\mu N)})] \geq \mathrm{tr}[\rho'\ln\rho]\right.$$

$$\left.-\beta\,\mathrm{tr}[\rho'(H'-\mu N)] - \ln\{\mathrm{tr}\,e^{-\beta(H'-\mu N)}\} \geq -\beta\,\mathrm{tr}[\rho'(H-\mu N)] - \ln\{\mathrm{tr}\,e^{-\beta(H-\mu N)}\}\right)$$

$(\because \mathrm{tr}\,\rho' = 1)$

$$-\mathrm{tr}[\rho'(\cancel{H'-\mu N})] + \underbrace{\Omega_{H'-\mu N}[\rho']}_{\mathrm{tr}\rho'(H'-\mu N+\frac{1}{\beta}\ln\rho')} \geq \cancel{-\mathrm{tr}[\rho'(H-\mu N)]} + \Omega_{H-\mu N}[\rho]$$

$$= \mathrm{tr}\rho'(H'-\mu N+\tfrac{1}{\beta}\rho')$$

$$= \mathrm{tr}\rho'(H-\mu N+\tfrac{1}{\beta}\rho') + \cancel{\mathrm{tr}\rho'(H'-\mu N-H+\mu N)}$$

$$= \Omega_{H-\mu N}[\rho']$$

$$\therefore\ \Omega_{H-\mu N}[\rho'] \geq \Omega_{H-\mu N}[\rho] \qquad //$$

$$a \equiv \mathrm{tr}[\rho'\ln\rho'] - \mathrm{tr}[\rho'\ln\rho]$$

$$= \mathrm{tr}[\rho'\ln\rho'] - \mathrm{tr}[\rho'\ln\rho] + \mathrm{tr}[\rho] - \mathrm{tr}[\rho'] \quad (\because\ \mathrm{tr}[\rho]=1)$$

$$= \sum_j \rho'_j\ln\rho'_j - \sum_j \rho'_j \underbrace{\langle j|\ln\rho|j\rangle}_{\sum_n \langle j|n\rangle \ln\rho_n \langle n|j\rangle} + \sum_n \rho_n - \sum_j \rho'_j$$

Since $\sum_j |\langle j|n\rangle|^2 = \sum_n |\langle j|n\rangle|^2 = 1$,

$$a = \sum_{nj} |\langle j|n\rangle|^2 (\rho'_j\ln\rho'_j - \rho'_j\ln\rho_n + \rho_n - \rho'_j)$$

$$= \sum_{nj} |\langle j|n\rangle|^2 \rho'_j \left(\ln\frac{\rho'_j}{\rho_n} + \frac{\rho_n}{\rho'_j} - 1\right) \geq 0.$$

$$\because\ f(x) = \ln x + \frac{1}{x} - 1$$

$$f'(x) = \frac{1}{x} - \frac{1}{x^2} = \frac{x-1}{x^2}$$

x	0	⋯	1	⋯	∞
f'		$-$		$+$	
f	∞	↘	0	↗	∞

$$\therefore\ f(x) \geq 0 \quad \text{for} \quad 0 \leq x \leq \infty$$

When $\rho'_j = \rho_n$, or $H'-\mu N = H-\mu N$, $a = 0$. //

§. One-to-One Correspondence

We proove that $\{\phi(r)-\mu,\ D_{\alpha\beta}(r,r')\}$ corresponds one-to-one to $\{n(r),\ \Delta_{\alpha\beta}(r,r')\}$, where

$$\boxed{\begin{cases} n(r) = \sum_\sigma \langle \psi_\sigma^\dagger(r)\psi_\sigma(r)\rangle & -(6) \\ \Delta_{\alpha\beta}(r,r') = \langle \psi_\alpha(r)\psi_\beta(r')\rangle & -(7) \end{cases}}$$

the average taken by $\rho_{K_{\phi D}}$.

(Proof : Reductio ad Absurdum)

Assume that $\{\phi(r)-\mu, D_{\alpha\beta}(r,r')\}$ and $\{\phi'(r)-\mu', D'_{\alpha\beta}(r,r')\}$ give the same $\{n(r), \Delta_{\alpha\beta}(r,r')\}$, then

$$\Omega_{\phi'-\mu', D'}[\rho'] = \mathrm{tr}\,\rho'(K_{\phi',D'} + \frac{1}{\beta}\ln\rho')$$

$$= \underbrace{\mathrm{tr}\,\rho'(K_{\phi,D} + \frac{1}{\beta}\rho')}_{\Omega_{\phi D}[\rho']} + \int [(\phi'(r)-\mu') - (\phi(r)-\mu)]\, n(r)\, d^3r$$

$$+ \int [(D'_{\alpha\beta}(rr') - D_{\alpha\beta}(rr'))\Delta_{\alpha\beta}(rr') + \text{c.c.}]\, d^3r d^3r'$$

$$\therefore\ \Omega_{\phi' D'}[\rho'] > \Omega_{\phi D}[\rho] + \int [(\phi'(r)-\mu') - (\phi(r)-\mu)]\, n(r)\, d^3r$$

$$+ \int [(D'_{\alpha\beta}(rr') - D_{\alpha\beta}(rr'))\Delta_{\alpha\beta}(rr') + \text{c.c.}]\, d^3r d^3r' \qquad -(8)$$

In the same way, we can get

$$\Omega_{\phi D}[\rho] > \Omega_{\phi' D'}[\rho'] + \int [(\phi(r)-\mu)-(\phi'(r)-\mu')]\, n(r)\, d^3r$$
$$+ \int [(D_{\alpha\beta}(rr') - D'_{\alpha\beta}(rr'))\Delta_{\alpha\beta}(rr') + c.c.\,]\, d^3r d^3r' \qquad -(9)$$

Adding Eqs. (8) and (9), we obtain

$$\Omega_{\phi D}[\rho] + \Omega_{\phi' D'}[\rho'] > \Omega_{\phi D}[\rho] + \Omega_{\phi' D'}[\rho']$$

which is inconsistent. //

In summary,

$$\Omega_{\phi, D}[n, \Delta] = \int \phi(r)\, n(r)\, d^3r + \int [D^*_{\alpha\beta}(rr')\Delta_{\alpha\beta}(rr') + c.c.\,]\, d^3r d^3r'$$
$$+ F[n, \Delta] \qquad -(10)$$

takes its minimum value when $\{n, \Delta\}$ is the correct densities corresponding to $K_{\phi, D}$, where

$$F[n, \Delta] = \mathrm{tr}\, \rho\, [H - \mu N + \tfrac{1}{\beta} \ln \rho]$$
$$= \langle H \rangle - \mu \langle N \rangle - T \langle S \rangle \qquad -(11)$$

with $\rho = e^{-\beta K_{\phi, D}} / \mathrm{tr}[e^{-\beta K_{\phi, D}}]$.

Density-Functional Theory for Superconductors (II)
Application to the Anisotropic and Inhomogeneous Superconducting Ground State in Electron Liquids

§. Exchange-Correlation Free Energy

We introduce $F_{xc}[n,\Delta]$ by

$$\boxed{\begin{aligned} F[n,\Delta] &= T_s[n,\Delta] - \mu N - T S_s[n,\Delta] \\ &\quad + \frac{e^2}{2}\int \frac{n(r)n(r')}{|r-r'|} d^3r d^3r' \\ &\quad + \frac{1}{V}\sum_{\alpha\beta}\int \Delta^*_{\alpha\beta}(r_1+r/2, r_1-r/2)\, \nu(r)\, \Delta_{\alpha\beta}(r_2+r/2, r_2-r/2)\, d^3r d^3r_1 d^3r_2 \\ &\quad + F_{xc}[n,\Delta] \end{aligned}} \qquad -(1)$$

where T_s and S_s denote the kinetic energy and entropy subject to potentials $\phi_s(r)$ and $D^s_{\alpha\beta}(rr')$ chosen such that $n(r)$ and $\Delta(rr')$ are equal to those of interacting system.

$\nu(r)$ is an effective pairing potential responsible for the formation of pseudomolecules (Cooper pairs).

§. Pairing Potential $w(r)$

We consider states in which Cooper pairs are macroscopically occupied, so that

$$\Psi = \mathcal{N}\left[\varphi(r_1r_2;\sigma_1\sigma_2)\varphi(r_3r_4;\sigma_3\sigma_4)+\cdots - \varphi(r_1r_3;\sigma_1\sigma_3)\varphi(r_2r_4;\sigma_2\sigma_4)\cdots\right] \quad -(2)$$

where $\mathcal{N}$ is the normalization constant and $\varphi(r_1r_2;\sigma_1\sigma_2)$ is the antisymmetrized pseudo-molecule wave function.

We must distinguish two cases: the spin singlet pairing case in which

$$\varphi(rr';\sigma\sigma') = \varphi(rr')\sqrt{2}^{-1}(\uparrow\downarrow - \downarrow\uparrow) \quad -(3)$$

where $\varphi(rr') = \varphi(r'r)$, and spin triplet case in which

$$\varphi(rr';\sigma\sigma') = \varphi_{\uparrow\uparrow}(rr')\,|\uparrow\uparrow\rangle + \varphi_{\uparrow\downarrow}(rr')\sqrt{2}^{-1}(\uparrow\downarrow+\downarrow\uparrow) + \varphi_{\downarrow\downarrow}(rr')\,|\downarrow\downarrow\rangle \quad -(4)$$

where $\varphi_{\alpha\beta}(rr') = -\varphi_{\alpha\beta}(r'r)$.

The pairing potential $w(r)$ is the one working between two particles forming a pseudomolecule, for which we adopt, according to Kukkonen and Overhauser,

$$\boxed{\begin{aligned} w_{kk'} &\equiv \int d^3r\, e^{i(k-k')\cdot r}\, w(r) \\ &= v(q)\left\{ \frac{1 - v(q)G(q,\omega)[1-G(q,\omega)]\chi_L(q,\omega)}{1 - v(q)[1-G(q,\omega)]\chi_L(q,\omega)} + \frac{v(q)G_-(q,\omega)\chi_L(q,\omega)}{1 + v(q)G_-(q)\chi_L(q,\omega)}\,\sigma\cdot\sigma' \right\} \end{aligned}} \quad -(5)$$

Here, $q = k - k'$ and $\omega = \hbar k^2/2m - \hbar k'^2/2m$, $\chi_L(q,\omega)$ is the Lindhard polarizability, $G(q\omega)$ and $G_-(q\omega)$ are defined through $\chi(q\omega) = \chi_L(q\omega)/[1 - v(q)(1-G(q\omega))\chi_L(q\omega)]$ and $\chi_-(q\omega) = \chi_L(q\omega)/[1 + v(q)G_-(q\omega)\chi_L(q\omega)]$ where $\chi(q\omega)$ and $\chi_-(q\omega)$ is the density and spin response functions.

In Eq. (5), σ is the Pauli matrix which we set

$$\boxed{\sigma\cdot\sigma' = \begin{cases} -3 & \text{(spin singlet case)} \\ 1 & \text{(spin triplet case)} \end{cases}} \quad -(6)$$

(☺ of Eq.(6))

$$\sigma = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \quad -(7)$$

$$\sigma_\pm = (\sigma_x \pm i\sigma_y)/2 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad -(8)$$

or

$$\sigma_x = \sigma_+ + \sigma_- \quad , \quad \sigma_y = -i(\sigma_+ - \sigma_-) \quad -(9)$$

) Here,

$$\sigma \cdot \sigma' = 2(\sigma_+\sigma_-' + \sigma_-\sigma_+') + \sigma_z\sigma_z' \quad -(10)$$

then

$$\sigma \cdot \sigma'(\uparrow\downarrow - \downarrow\uparrow) = 2\left(-\uparrow\downarrow + \downarrow\uparrow\right) + (-1)(\uparrow\downarrow - \downarrow\uparrow)$$

$$= -3(\uparrow\downarrow - \downarrow\uparrow)$$

and so on. //

For spin singlet cases, we consider only

$$\boxed{\Delta(rr') = \Delta_{\uparrow\downarrow}(rr') \qquad (\Delta(rr') = \Delta(r'r))} \quad -(11)$$

while for triplet cases, we consider

$$\boxed{\begin{array}{l} \Delta_{\uparrow\uparrow}(rr'),\ \Delta_{\uparrow\downarrow}(rr') = \Delta_{\downarrow\uparrow}(rr'),\ \Delta_{\downarrow\downarrow}(rr') \\ \text{with the condition, } \Delta_{\alpha\beta}(rr') = -\Delta_{\alpha\beta}(r'r) \end{array}} \quad -(12)$$

Density-Functional Theory for Superconductors : Inclusion of Magnetic Fields

(System)

$$K \equiv H - \mu N$$

$$= \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu \right] \psi_\sigma(r) + \frac{e^2}{2}\sum_{\sigma\sigma'} \int d^3r d^3r' \frac{\psi_\sigma^\dagger(r)\psi_{\sigma'}^\dagger(r')\psi_{\sigma'}(r')\psi_\sigma(r)}{|r-r'|}$$

$$- \frac{g}{V}\int d^3r\, \psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r)\psi_\downarrow(r)\psi_\uparrow(r) \qquad -(1)$$

(Electro-Magnetic Field)

$$H = \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left\{ \frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)^2 - e\varphi \right\} \psi_\sigma(r)$$

$$+ \sum_{\sigma\sigma'} \int d^3r\, \psi_\sigma^\dagger(r) \left\{ \underbrace{\frac{e\hbar}{2mc}}_{\mu_B} \sigma \cdot \mathbb{H} \right\} \psi_\sigma(r)$$

$$= \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left\{ -\frac{\hbar^2}{2m}\nabla^2 + \frac{e\hbar}{2mci}(\nabla\cdot A + A\cdot\nabla) + \frac{e^2}{2mc^2}A^2 + e\varphi \right\} \psi_\sigma(r)$$

$$- \int d^3r\, \mathbb{H}(r) \cdot \left\{ -\frac{e\hbar}{2mc}\psi_\sigma^\dagger(r)\sigma_{\sigma\sigma'}\psi_{\sigma'}(r) \right\}$$

Here, we introduce

$$\hat{m}(r) = -\sum_{\sigma\sigma'} \frac{e\hbar}{2mc}\psi_\sigma^\dagger(r)\sigma_{\sigma\sigma'}\psi_{\sigma'}(r) \qquad -(2)$$

then

$$K_{\varphi,A,H,D} = K + \frac{e}{c}\int \hat{j}_p(r)\cdot A(r)\, d^3r + \frac{e^2}{2mc^2}\int \hat{n}(r)\overbrace{}^{A^2(r)} d^3r$$

$$- e\int \hat{n}(r)\,\varphi(r)\, d^3r - \int m(r)\cdot H(r)\, d^3r$$

$$- \int [D^*(rr')\,\psi_\uparrow(r)\psi_\downarrow(r') + H.c.]\, d^3r d^3r' \qquad -(3)$$

where

$$\hat{j}_p(r) = \sum_\sigma \frac{\hbar}{2mi}\{\psi_\sigma^+(r)\nabla\psi_\sigma(r) - (\nabla\psi_\sigma^+(r))\psi_\sigma(r)\} \qquad -(4)$$

$$\hat{n}(r) = \sum_\sigma \psi_\sigma^+(r)\psi_\sigma(r)$$

We introduce $\Delta(rr') = \langle\psi_\uparrow(r)\psi_\downarrow(r')\rangle$, and show

$$\Omega_{\varphi AHD}[n, j_p, m, \Delta] = \frac{e}{c}\int j_p(r)\cdot A(r)\, d^3r + \frac{e^2}{2mc^2}\int n(r)\, A^2(r)\, d^3r$$

$$- e\int n(r)\,\varphi(r)\, d^3r - \int m(r)\cdot H(r)\, d^3r$$

$$- \int [D^*(rr')\,\Delta(rr') + c.c.]\, d^3r d^3r'$$

$$+ F[n, j_p, m, \Delta]$$

takes its minimum value when $\{n, j_p, m, \Delta\}$ take the actual values corresponding to the potentials $\{\varphi, A, H, D\}$; in reality, we adopt $D = 0$ and $H = \nabla\times A$.

where

$$F[n,j_p,m,\Delta] = \mathrm{tr}\, \rho_{\Phi AHD}\,[H - \mu N + \frac{1}{\beta}\rho_{\Phi AHD}]$$

$$= \langle H\rangle_{\Phi AHD} - \mu \langle N\rangle_{\Phi AHD} - T\langle S\rangle_{\Phi AHD} \qquad -(5)$$

with $\rho_{\Phi AHD} = e^{-\beta K_{\Phi AHD}} / \mathrm{tr}\, e^{-\beta K_{\Phi AHD}}$.

Further, $F_{xc}[n,j_p,m,\Delta]$ is defined by

$$F[n,j_p,m,\Delta] = T_S - \mu N - T S_S[n,\Delta]$$

$$+ \frac{e^2}{2}\int \frac{n(r)n(r')}{|r-r'|} d^3r d^3r'$$

$$- \frac{g}{V}\int \overset{*}{\Delta}(rr')\Delta(rr')\, d^3r d^3r'$$

$$+ F_{xc}[n,j_p,m,\Delta] \qquad -(6)$$

(Bogoliubov Equation)

$$\left[\frac{1}{2m}\left\{\frac{\hbar}{i}\nabla+\frac{e}{c}[A(r)+A_{xc}(r)]\right\}^2+\frac{e^2}{2mc^2}\left\{A^2(r)-[A(r)+A_{xc}(r)]^2\right\}\right.$$
$$\left.+\left\{v(r)+e^2\int\frac{n(r')}{|r-r'|}d^3r'+v_{xc}(r)\right\}\right]\delta_{\sigma\tau}-\mu_B\left\{\mathbb{H}(r)+\mathbb{H}_{xc}(r)\right\}\cdot\sigma_{\sigma\tau}$$
$$\equiv \quad h_{\sigma\tau}(r) \qquad -(7)$$

where

$$\begin{cases} v_{xc}(r) = \delta F_{xc}/\delta n(r) \\ \frac{e}{c}A_{xc}(r) = \delta F_{xc}/\delta j_p(r) \\ -\mu_B \mathbb{H}_{xc}(r) = \delta F_{xc}/\delta \mathbb{m}(r) \end{cases}$$

then

$$\begin{cases} \sum_\tau \left\{h_{\sigma\tau}(r)-\epsilon_m\delta_{\sigma\tau}\right\}u_m(r\tau) = -\sum_\tau\int D_s(rr')\rho_{\sigma\tau}\, v_m(r'\tau)\, d^3r' & -(8) \\ \sum_\tau \left\{h^*_{\sigma\tau}(r)+\epsilon_m\delta_{\sigma\tau}\right\}v_m(r\tau) = \sum_\tau\int D^*_s(rr')\,\rho_{\sigma\tau}\, u_m(r'\tau)\, d^3r' & -(9) \end{cases}$$

where

$$D_s(rr') = D(rr') + \int w(r'r\,r_1r_1')\,\Delta(r_1r_1')\,d^3r_1 d^3r_1' \underbrace{-\,\delta F_{xc}/\delta\Delta^*(rr')}_{D_{xc}(rr')} \qquad -(10)$$

$$\rho_{\sigma\tau} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_z$$

(Gap Equation)

$$\Delta(r,r') = \sum_m \left[v_m^*(r'\downarrow)\, u_m(r\uparrow)\,(1-f_m(T)) - v_m^*(r\uparrow)\, u_m(r'\downarrow)\, f_m(T) \right]$$

$$\langle \psi_\uparrow(r)\,\psi_\downarrow(r') \rangle \qquad -(11)$$

Derivation of Bogoliubov-de Gennes Equation

§. Mean-Field Hamiltonian

(Grand Hamiltonian : Gor'kov Form)

$$\boxed{\begin{aligned} K &= H - \mu N \\ &= \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A(r)\right)^2 - \mu\right] \psi_\sigma(r) \\ &\quad + \sum_{\sigma\tau} \int d^3r\, \psi_\sigma^\dagger(r)\, v_{\sigma\tau}(r)\, \psi_\tau(r) - w \int d^3r\, \psi_\downarrow^\dagger(r)\psi_\uparrow^\dagger(r)\psi_\uparrow(r)\psi_\downarrow(r) \\ &= \sum_{\sigma\tau} \int d^3r\, \psi_\sigma^\dagger(r)\, K_{\sigma\tau}(r)\, \psi_\tau(r) - w \int d^3r\, \psi_\downarrow^\dagger(r)\psi_\uparrow^\dagger(r)\psi_\uparrow(r)\psi_\downarrow(r) \end{aligned}} \qquad -(1)$$

where

$$\boxed{K_{\sigma\tau}(r) = \left[\frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A(r)\right)^2 - \mu\right]\delta_{\sigma\tau} + v_{\sigma\tau}(r) .} \qquad -(2)$$

(Lemma)

$$\boxed{\int d^3r\, \psi_\sigma^\dagger(r)\, K_{\sigma\tau}(r)\, \psi_\tau(r) = \int d^3r \left(K^*_{\tau\sigma}(r)\, \psi_\sigma^\dagger(r)\right) \psi_\tau(r)} \qquad -(3)$$

∵ 1°) $\displaystyle\int d^3r\, \psi_\sigma^\dagger(r) \left(\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)\left(\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)\psi_\sigma(r)\right)$

$$= \int d^3r \left[\left(-\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)\psi_\sigma^\dagger(r)\right]\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)\psi_\sigma(r)$$

$$= \int d^3r \left[\underbrace{\left(-\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)^2}_{\left[\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A\right)^2\right]^*,\ \text{if } A(r) \text{ is real.}} \psi_\sigma^\dagger(r)\right] \psi_\sigma(r)$$

2) Note that, $V_{\sigma\tau}(r) = v(r)\delta_{\sigma\tau} + h(r)\cdot \sigma_{\sigma\tau}$. Then,

$$V^{*}_{\tau\sigma}(r) = v(r)\underbrace{\delta_{\tau\sigma}}_{\delta_{\sigma\tau}} + h(r)\cdot \underbrace{\left(\begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}0&i\\-i&0\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}\right)_{\tau\sigma}}_{\left(\begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}0&-i\\i&0\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}\right)_{\sigma\tau} = \sigma_{\sigma\tau}}$$

$= V_{\sigma\tau}(r)$, if v(r) and h(r) is real. //

※ (Scalar Potential and Spin-Magnetic-Field Couplings)

$$\underbrace{\rho(r)}_{\sum_\sigma \psi^{+}_{\sigma}(r)\psi_{\sigma}(r)} v(r) - \underbrace{m(r)}_{-\frac{e\hbar}{2mc}\sum_{\sigma\tau}\psi^{+}_{\sigma}(r)\sigma_{\sigma\tau}\psi_{\tau}(r)}\cdot H(r)$$

$$= \sum_{\sigma\tau} \psi^{+}_{\sigma}(r) \left[v(r)\delta_{\sigma\tau} + \frac{e\hbar}{2mc} H(r)\cdot\sigma_{\sigma\tau} \right] \psi_{\tau}(r)$$

$$\boxed{\begin{array}{l} V_{\sigma\tau}(r) = v(r)\delta_{\sigma\tau} + \mu_B H(r)\cdot \sigma_{\sigma\tau} \\ \text{where} \quad \mu_B = e\hbar/2mc. \end{array}} \quad \text{— (4)}$$

(Mean-Field Hamiltonian)

The mean-field Hamiltonian is defined as

$$K_m = \sum_{\sigma\tau} \int d^3r\, \psi_\sigma^\dagger(r) K_{\sigma\tau}(r) \psi_\tau(r)$$
$$+ \int d^3r \left[w^{-1} |\Delta(r)|^2 - \Delta^*(r) \psi_\uparrow(r) \psi_\downarrow(r) - \Delta(r) \psi_\downarrow^\dagger(r) \psi_\uparrow^\dagger(r) \right] \quad -(5)$$

where

$$\boxed{\Delta(r) = w \langle \psi_\uparrow(r) \psi_\downarrow(r) \rangle} \quad -(6)$$

is the anormalous pair field.

Here,

- $\psi_\uparrow(r)\psi_\downarrow(r) = -\psi_\downarrow(r)\psi_\uparrow(r) = \frac{1}{2}\left(\psi_\uparrow(r)\psi_\downarrow(r) - \psi_\downarrow(r)\psi_\uparrow(r)\right)$

$$= \frac{1}{2} (\psi_\uparrow\ \psi_\downarrow) \underbrace{\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}}_{\equiv \rho} \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix}$$

$$= \frac{1}{2} \sum_{\sigma\tau} \psi_\sigma(r) \rho_{\sigma\tau} \psi_\tau(r) = -\frac{1}{2} \sum_{\sigma\tau} \psi_\tau(r) \rho_{\sigma\tau} \psi_\sigma(r)$$

- $\psi_\downarrow^\dagger(r)\psi_\uparrow^\dagger(r) = \frac{1}{2}\left(-\psi_\uparrow^\dagger(r)\psi_\downarrow^\dagger(r) + \psi_\downarrow^\dagger(r)\psi_\uparrow^\dagger(r)\right) = -\frac{1}{2}\sum_{\sigma\tau} \psi_\sigma^\dagger(r) \rho_{\sigma\tau} \psi_\tau^\dagger(r)$

$$\therefore \quad K_m = \int d^3r \Big[v^{-1} |\Delta(r)|^2 + \frac{1}{2}\sum_{\sigma\tau} \psi^\dagger_\sigma(r) \{ \kappa_{\sigma\tau}(r)\psi_\tau(r) + \Delta(r)\rho_{\sigma\tau}\psi^\dagger_\tau(r)\}$$

$$+ \frac{1}{2}\sum_{\sigma\tau} \{ \kappa^*_{\sigma\tau}(r)\psi^\dagger_\tau(r) + \Delta^*(r)\rho_{\sigma\tau}\psi_\tau(r)\} \psi_\sigma(r) \Big] \quad -(7)$$

where

$$\rho = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = i\,\sigma_2 \quad -(8)$$

(☺ of Eq.(7))

$$\int d^3r\, \psi^\dagger_\tau(r)\kappa_{\tau\sigma}(r)\psi_\sigma(r) = \int d^3r\, (\kappa^*_{\sigma\tau}(r)\psi^\dagger_\tau(r))\psi_\sigma(r)$$ (☺ from Lemma) //

§. Bogoliubov Equation

$$\boxed{\begin{cases} \sum_{\tau} \{ K_{\sigma\tau}(r) u_\nu(r\tau) + \Delta(r) \rho_{\sigma\tau} v_\nu(r\tau) \} = E_\nu u_\nu(r\sigma) \\ \sum_{\tau} \{ K^*_{\sigma\tau}(r) v_\nu(r\tau) + \Delta^*(r) \rho_{\sigma\tau} u_\nu(r\tau) \} = -E_\nu v_\nu(r\sigma) \end{cases}} \qquad -(9)$$

We denote an eigen state, $w_\nu(rs) = (u_\nu(r\uparrow), u_\nu(r\downarrow), v_\nu(r\uparrow), v_\nu(r\downarrow))$,

where we restrict to positive solutions, $E_\nu > 0$.

Negative eigen states are obtained by taking the complex conjugate of Eq. (9),

$$\begin{cases} \sum_{\tau} \{ K_{\sigma\tau}(r) v^*_\nu(r\tau) + \Delta(r) \rho_{\sigma\tau} u^*_\nu(r\tau) \} = -E_\nu v^*_\nu(r\sigma) \\ \sum_{\tau} \{ K^*_{\sigma\tau}(r) u^*_\nu(r\tau) + \Delta^*(r) \rho_{\sigma\tau} v^*_\nu(r\tau) \} = E_\nu u^*_\nu(r\sigma) \end{cases} \qquad -(9^*)$$

thus we denote a negative eigen state as $\bar{w}_\nu(rs) \equiv (v^*_\nu(r\uparrow), v^*_\nu(r\downarrow), u^*_\nu(r\uparrow), u^*_\nu(r\downarrow))$.

(Orthonomality of the Eigenstate Set)

$$\boxed{\begin{aligned} \langle \mu | \nu \rangle &= \sum_{S=1}^{4} \int d^3r \, \langle \mu | rS \rangle \langle rS | \nu \rangle \\ &= \sum_{S=1}^{4} \int d^3r \, w_\mu^*(rS)\, w_\nu(rS) = \delta_{\mu\nu} \end{aligned}} \qquad -(10)$$

(Completeness)

$$\boxed{\begin{aligned} \sum_{\nu=-\infty}^{\infty} \langle rS | \nu \rangle \langle \nu | r'S' \rangle &= \sum_{\nu>0} \left\{ w_\nu(rS)\, w_\nu^*(r'S') + w_{-\nu}(rS)\, w_{-\nu}^*(r'S') \right\} \\ &= \delta_{SS'}\, \delta^3(r-r') \end{aligned}} \qquad -(11)$$

§. Bogoliubov Transformation

We define $\underline{\psi(rs) \equiv (\psi_\uparrow(r), \psi_\downarrow(r), \psi_\uparrow^\dagger(r), \psi_\downarrow^\dagger(r))}$. Using this quantity, the Bogoliubov transformation is given by

$$\boxed{\psi(rs) = \sum_{\nu>0} \alpha_\nu w_\nu(rs) + \sum_{\nu>0} \alpha_\nu^\dagger w_{-\nu}(rs)} \quad -(12)$$

(Inverse Transformation)

○ $\sum_s \int d^3r\, w_\nu^*(rs)\psi(rs)$

$$= \sum_{\mu>0} \alpha_\mu \underbrace{\sum_s \int d^3r\, w_\nu^*(rs) w_\mu(rs)}_{\delta_{\mu\nu}} = \alpha_\nu$$

○ $\sum_s \int d^3r\, w_{-\nu}^*(rs)\psi(rs)$

$$= \sum_{\mu>0} \alpha_\mu^\dagger \underbrace{\sum_s \int d^3r\, w_{-\nu}^*(rs) w_{-\mu}(rs)}_{\delta_{\mu\nu}} = \alpha_\nu^\dagger$$

$$\boxed{\begin{cases} \alpha_\nu = \sum_s \int d^3r\, w_\nu^*(rs)\psi(rs) \\ \alpha_\nu^\dagger = \sum_s \int d^3r\, w_{-\nu}^*(rs)\psi(rs) \end{cases}} \quad -(13)$$

or,

$$\boxed{\begin{cases} \alpha_\nu = \sum_\sigma \int d^3r \, [\, u_\nu^*(r\sigma)\psi_\sigma(r) + v_\nu^*(r\sigma)\psi_\sigma^\dagger(r) \,] \\ \alpha_\nu^\dagger = \sum_\sigma \int d^3r \, [\, v_\nu(r\sigma)\psi_\sigma(r) + u_\nu(r\sigma)\psi_\sigma^\dagger(r) \,] \end{cases} \text{ O.K.}} \quad -(14)$$

§. Anticommutation Relations

① $$\{\alpha_\mu, \alpha_\nu^\dagger\} = \sum_{\sigma\sigma'} \int d^3r d^3r' \{ u_\mu^*(r\sigma)\psi_\sigma(r) + v_\mu^*(r\sigma)\psi_\sigma^\dagger(r), v_\nu(r'\sigma')\psi_{\sigma'}(r') + u_\nu(r'\sigma')\psi_{\sigma'}^\dagger(r') \}$$

$$u_\mu^*(r\sigma)u_\nu(r\sigma)\delta_{\sigma\sigma'}\delta(r-r') + v_\mu^*(r\sigma)v_\nu(r\sigma)\delta_{\sigma\sigma'}\delta(r-r')$$

$$= \sum_\sigma \int d^3r \, \{ u_\mu^*(r\sigma)u_\nu(r\sigma) + v_\mu^*(r\sigma)v_\nu(r\sigma) \}.$$

$$= \sum_s \int d^3r \, w_\mu^*(rs) w_\nu(rs) = \delta_{\mu\nu}$$

② $$\{\alpha_\mu, \alpha_\nu\} = \sum_{\sigma\sigma'} \int d^3r d^3r' \{ u_\mu^*(r\sigma)\psi_\sigma(r) + v_\mu^*(r\sigma)\psi_\sigma^\dagger(r), u_\nu^*(r'\sigma')\psi_{\sigma'}(r') + v_\nu^*(r'\sigma')\psi_{\sigma'}^\dagger(r') \}$$

$$(u_\mu^*(r\sigma)v_\nu^*(r\sigma) + v_\mu^*(r\sigma)u_\nu^*(r\sigma))\, \delta_{\sigma\sigma'}\delta(r-r')$$

$$= \sum_\sigma \int d^3r \, \{ u_\mu^*(r\sigma)v_\nu^*(r\sigma) + v_\mu^*(r\sigma)u_\nu^*(r\sigma) \}$$

$$= \sum_s \int d^3r \, w_\mu^*(rs) w_{-\nu}(r\sigma) = 0$$

$$\therefore\ \boxed{\{\alpha_\mu, \alpha_\nu^\dagger\} = \delta_{\mu\nu}, \quad \{\alpha_\mu, \alpha_\nu\} = \{\alpha_\mu^\dagger, \alpha_\nu^\dagger\} = 0} \qquad -(15)$$

§. Diagonalization of K_m

We rewrite Eq. (12) as,

$$\boxed{\begin{cases} \psi(r\,1,2) = \sum_\nu [\alpha_\nu u_\nu(r\uparrow\downarrow) + \alpha_\nu^\dagger v_\nu^*(r\uparrow\downarrow)] = \psi_{\uparrow\downarrow}(r) \\ \psi(r\,3,4) = \sum_\nu [\alpha_\nu v_\nu(r\uparrow\downarrow) + \alpha_\nu^\dagger u_\nu^*(r\uparrow\downarrow)] = \psi_{\uparrow\downarrow}^\dagger(r) \end{cases}} \qquad -(16)$$

① $\frac{1}{2}\sum_{\sigma\tau}\int d^3r\, \psi_\sigma^\dagger(r)\,[K_{\sigma\tau}(r)\psi_\tau(r) + \Delta(r)\rho_{\sigma\tau}\psi_\tau^\dagger(r)]$

$$= \frac{1}{2}\sum_\sigma\int d^3r\, \psi_\sigma^\dagger(r) \sum_\tau \Big\{ K_{\sigma\tau}(r)\sum_\nu [\alpha_\nu u_\nu(r\tau) + \alpha_\nu^\dagger v_\nu^*(r\tau)].$$

$$+ \Delta(r)\rho_{\sigma\tau}\sum_\nu [\alpha_\nu v_\nu(r\tau) + \alpha_\nu^\dagger u_\nu^*(r\tau)] \Big\}$$

$$= \frac{1}{2}\sum_\sigma\int d^3r\, \psi_\sigma^\dagger(r)\sum_\nu \Big\{ \alpha_\nu \underbrace{\sum_\tau [K_{\sigma\tau}(r)u_\nu(r\tau) + \Delta(r)\rho_{\sigma\tau}v_\nu(r\tau)]}_{E_\nu u_\nu(r\sigma)}$$

$$+ \alpha_\nu^\dagger \underbrace{\sum_\tau [K_{\sigma\tau}(r)v_\nu^*(r\tau) + \Delta(r)\rho_{\sigma\tau}u_\nu^*(r\tau)]}_{-E_\nu v_\nu^*(r\sigma)} \Big\}$$

$$= \frac{1}{2}\sum_{\mu\nu} \overbrace{\Big[\sum_\sigma}^{(E_\nu)} \int d^3r\, (\alpha_\mu v_\mu(r\sigma) + \alpha_\mu^\dagger u_\mu^*(r\sigma)) \times (\alpha_\nu u_\nu(r\sigma) - \alpha_\nu^\dagger v_\nu^*(r\sigma)) \quad \cdots (\#)$$

② $\frac{1}{2}\sum_{\sigma\tau}\int d^3r \left[\kappa^*_{\sigma\tau}(r)\, \psi^\dagger_\tau(r) + \Delta^*(r)\, \rho_{\sigma\tau}\, \psi_\tau(r) \right] \psi_\sigma(r)$

$$= \frac{1}{2}\sum_{\sigma}\int d^3r \sum_\tau \Big\{ \kappa^*_{\sigma\tau}(r) \sum_\nu \left[\alpha_\nu v_\nu(r\tau) + \alpha^\dagger_\nu u^*_\nu(r\tau) \right] + \Delta^*(r)\rho_{\sigma\tau} \sum_\nu \left[\alpha_\nu u_\nu(r\tau) + \alpha^\dagger_\nu v^*_\nu(r\tau) \right] \Big\} \psi_\sigma(r)$$

$$= \frac{1}{2}\sum_{\sigma}\int d^3r \sum_\nu \Big\{ \alpha_\nu \underbrace{\sum_\tau \left[\kappa^*_{\sigma\tau}(r) v_\nu(r\tau) + \Delta^*(r)\rho_{\sigma\tau} u_\nu(r\tau) \right]}_{-E_\nu v_\nu(r\sigma)} + \alpha^\dagger_\nu \underbrace{\sum_\tau \left[\kappa^*_{\sigma\tau}(r) u^*_\nu(r\tau) + \Delta^*(r)\rho_{\sigma\tau} v^*_\nu(r\tau) \right]}_{E_\nu u^*_\nu(r\sigma)} \Big\} \psi_\sigma(r)$$

$$= \frac{1}{2}\sum_{\mu\nu} E_\nu \sum_\sigma \int d^3r \left(-\alpha_\nu v_\nu(r\sigma) + \alpha^\dagger_\nu u^*_\nu(r\sigma) \right) \times \left(\alpha_\mu u_\mu(r\sigma) + \alpha^\dagger_\mu v^*_\mu(r\sigma) \right) \qquad -(b)$$

$$(\#)+(b) = \frac{1}{2}\sum_{\mu\nu} E_\nu \sum_\sigma \int d^3r$$

$$\Big\{ \alpha_\mu\alpha_\nu \left(v_\mu(r\sigma) u_\nu(r\sigma) + u_\mu(r\sigma) v_\nu(r\sigma) \right)$$
$$+ \alpha^\dagger_\mu\alpha^\dagger_\nu \left(-u^*_\mu(r\sigma) v^*_\nu(r\sigma) - v^*_\mu(r\sigma) u^*_\nu(r\sigma) \right)$$
$$+ \alpha^\dagger_\mu\alpha_\nu \left(u^*_\mu(r\sigma) u_\nu(r\sigma) + v^*_\mu(r\sigma) v_\nu(r\sigma) \right) - \delta_{\mu\nu} |v_\nu(r\sigma)|^2$$
$$+ \alpha^\dagger_\nu\alpha_\mu \left(v^*_\nu(r\sigma) v_\mu(r\sigma) + u^*_\nu(r\sigma) u_\mu(r\sigma) \right) - \delta_{\mu\nu} |v_\nu(r\sigma)|^2 \Big\}$$

$$= \frac{1}{2}\sum_{\mu\nu} E_\nu \left\{ \begin{aligned} & \cancel{\alpha_\mu \alpha_\nu \sum_s \int d^3r\, w^*_{-\nu}(rs)\, w_\mu(rs)} \\ & \cancel{-\alpha^\dagger_\mu \alpha^\dagger_\nu \sum_s \int d^3r\, w^*_\nu(rs)\, w_{-\mu}(rs)} \\ & + \alpha^\dagger_\mu \alpha_\nu \underbrace{\sum_s \int d^3r\, w^*_\mu(rs)\, w_\nu(rs)}_{\delta_{\mu\nu}} \\ & + \alpha^\dagger_\nu \alpha_\mu \underbrace{\sum_s \int d^3r\, w^*_\nu(rs)\, w_\mu(rs)}_{\delta_{\mu\nu}} \end{aligned} \right\}$$

$$- \frac{1}{2}\sum_\nu \sum_\sigma \int d^3r\, E_\nu |v_\nu(r\sigma)|^2 - \frac{1}{2}\sum_\nu \sum_\sigma \int d^3r\, E_\nu |v_\nu(r\sigma)|^2$$

$$= \sum_\nu E_\nu \alpha^\dagger_\nu \alpha_\nu - \sum_\nu \sum_\sigma \int d^3r\, E_\nu |v_\nu(r\sigma)|^2$$

$$\boxed{\begin{aligned} K_m = & \int d^3r \left[w^{-1} |\Delta(r)|^2 - \sum_\nu \sum_\sigma E_\nu |v_\nu(r\sigma)|^2 \right] \\ & + \sum_\nu E_\nu \alpha^\dagger_\nu \alpha_\nu \end{aligned}} \quad -(17)$$

§. Gap and Density

$$\text{①}\ \Delta(r) = w \langle \psi_\uparrow(r)\psi_\downarrow(r) \rangle$$

$$= \frac{w}{2} \langle \psi_\uparrow(r)\psi_\downarrow(r) - \psi_\downarrow(r)\psi_\uparrow(r) \rangle$$

$$= \frac{w}{2} \sum_{\sigma\tau} \langle \psi_\sigma(r) \rho_{\sigma\tau} \psi_\tau(r) \rangle$$

$$= \frac{w}{2} \sum_{\sigma\tau} \sum_{\mu\nu} \langle (\alpha_\mu u_\mu(r\sigma) + \alpha_\mu^\dagger v_\mu^*(r\sigma)) \rho_{\sigma\tau} (\alpha_\nu u_\nu(r\tau) + \alpha_\nu^\dagger v_\nu^*(r\tau)) \rangle$$

$$= \frac{w}{2} \sum_{\sigma\tau} \sum_{\mu\nu} \Big\{ \underbrace{\langle \alpha_\mu^\dagger \alpha_\nu \rangle}_{\delta_{\mu\nu} f(E_\nu)} v_\mu^*(r\sigma) \rho_{\sigma\tau} u_\nu(r\tau)$$

$$+ \underbrace{\langle \alpha_\mu \alpha_\nu^\dagger \rangle}_{\delta_{\mu\nu}(1-f(E_\nu))} u_\mu(r\sigma) \rho_{\sigma\tau} v_\nu^*(r\tau) \Big\}$$

$$= \frac{w}{2} \sum_{\sigma\tau} \sum_{\nu} \Big\{ u_\nu(r\sigma) \underbrace{\rho_{\tau\sigma}}_{-\rho_{\sigma\tau}} v_\nu^*(r\tau) f(E_\nu) + u_\nu(r\sigma) \rho_{\sigma\tau} v_\nu^*(r\tau) (1-f(E_\nu)) \Big\}$$

$$\boxed{\Delta(r) = \frac{w}{2} \sum_{\nu} \sum_{\sigma\tau} u_\nu(r\sigma) \rho_{\sigma\tau} v_\nu^*(r\tau) \left[1 - 2f(E_\nu) \right]} \qquad -(18)$$

where we have used

$$\boxed{\langle \alpha_\nu^\dagger \alpha_\nu \rangle = f(E_\nu) \quad , \quad f(E_\nu) = \left[\exp(\beta E_\nu) + 1 \right]^{-1}} \qquad -(19)$$

② $$n(r) = \sum_{\sigma} \langle \psi^{\dagger}_{\sigma}(r) \psi_{\sigma}(r) \rangle$$

$$= \sum_{\sigma} \sum_{\mu\nu} \langle (\alpha_{\mu} v_{\mu}(r\sigma) + \alpha^{\dagger}_{\mu} u^{*}_{\mu}(r\sigma)) (\alpha_{\nu} u_{\nu}(r\sigma) + \alpha^{\dagger}_{\nu} v^{*}_{\nu}(r\sigma)) \rangle$$

$$= \sum_{\sigma} \sum_{\nu} \left[f(E_{\nu}) u^{*}_{\nu}(r\sigma) u_{\nu}(r\sigma) + (1 - f(E_{\nu})) \cdot v^{*}_{\nu}(r\sigma) v_{\nu}(r\sigma) \right]$$

$$\boxed{n(r) = \sum_{\nu} \sum_{\sigma} \left[f(E_{\nu}) |u_{\nu}(r\sigma)|^2 + (1 - f(E_{\nu})) |v_{\nu}(r\sigma)|^2 \right]} \qquad -(20)$$

③ $$m(r) = -\mu_B \sum_{\sigma\tau} \langle \psi^{\dagger}_{\sigma}(r) \sigma_{\sigma\tau} \psi_{\tau}(r) \rangle$$

$$\boxed{\begin{aligned} m(r) = -\mu_B \sum_{\nu} \sum_{\sigma\tau} \Big[& u^{*}_{\nu}(r\sigma) \sigma_{\sigma\tau} u_{\nu}(r\tau) f(E_{\nu}) \\ & + v_{\nu}(r\sigma) \sigma_{\sigma\tau} v^{*}_{\nu}(r\tau) (1 - f(E_{\nu})) \Big] \end{aligned}}$$

| |

Density-Functional Theory for Superconductors

§. Grand-Canonical Hamiltonian

$$\mathcal{K} = \mathcal{H} - \mu N$$

$$= \sum_\sigma \int d^3r\, \psi^\dagger_\sigma(r)\left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\psi_\sigma(r) + \frac{e^2}{2}\sum_{\sigma\sigma'}\int d^3r d^3r' \frac{\psi^\dagger_\sigma(r)\psi^\dagger_{\sigma'}(r')\psi_{\sigma'}(r')\psi_\sigma(r)}{|r - r'|}$$

$$- w\int d^3r\, \psi^\dagger_\downarrow(r)\psi^\dagger_\uparrow(r)\psi_\uparrow(r)\psi_\downarrow(r) \qquad -(1)$$

$$\mathcal{K}_{vAHD} = \mathcal{K} + \frac{e}{c}\int d^3r\, \hat{j}_p(r)\cdot A(r) + \frac{e^2}{2mc^2}\int d^3r\, \hat{n}(r) A^2(r)$$

$$+ \int d^3r\, \hat{n}(r) v(r) - \int d^3r\, \hat{m}(r)\cdot H(r)$$

$$- \int d^3r\, [D^*(r)\hat{\Delta}(r) + \text{H.C.}] \qquad -(2)$$

where $\hat{j}_p(r) = (\hbar/2mi)\sum_\sigma [\psi^\dagger_\sigma(r)\nabla\psi_\sigma(r) - (\nabla\psi^\dagger_\sigma(r))\psi_\sigma(r)]$; $\hat{n}(r) = \sum_\sigma \psi^\dagger_\sigma(r)\psi_\sigma(r)$, $\hat{m}(r) = -\mu_B\sum_{\sigma\tau}\psi^\dagger_\sigma(r)\sigma_{\sigma\tau}\psi_\tau(r)$ $(\mu_B = e\hbar/2mc)$, and $\hat{\Delta}(r) = \psi_\uparrow(r)\psi_\downarrow(r)$.

§. Density-Functional Theory

$$\Omega_{vAHD}[n\, j_p\, m\, \Delta] = \frac{e}{c}\int d^3r\, j_p(r)\cdot A(r) + \frac{e^2}{2mc^2}\int d^3r\, n(r) A^2(r)$$
$$+ \int d^3r\, n(r)\, v(r) - \int d^3r\, m(r)\cdot H(r)$$
$$- \int d^3r [D^*(r)\,\Delta(r) + c.c.]$$
$$+ F[n\, j_p\, m\, \Delta] \qquad -(3)$$

takes its minimum value when $\{n, j_p, m, \Delta\}$ are the equilibrium densities corresponding to the external fields $\{v, A, H, D\}$. In Eq. (3),

$$F[n, j_p, m, \Delta] = \mathrm{tr}\, \rho_{vAHD}[\mathcal{H} - \mu\mathcal{N} + \frac{1}{\beta}\rho_{vAHD}]$$
$$= \langle\mathcal{H}\rangle - \mu\langle\mathcal{N}\rangle - \theta\langle S\rangle \qquad -(4)$$

where $\rho_{vAHD} = e^{-\beta\mathcal{K}_{vAHD}} / \mathrm{tr}[e^{-\beta\mathcal{K}_{vAHD}}]$.

The exchange-correlation free energy $F_{xc}[n, j_p, m, \Delta]$ is defined by

$$F[n, j_p, m, \Delta] = F_s[n\, j_p\, m\, \Delta]$$
$$+ \frac{e^2}{2}\int d^3r\, d^3r' \frac{n(r)\, n(r')}{|r-r'|} - w\int d^3r\, \Delta^*(r)\,\Delta(r),$$
$$+ F_{xc}[n, j_p, m, \Delta] \qquad -(5)$$

where

$$F_s[n, j_p, m, \Delta] = T_s[n, j_p, m, \Delta] - \mu N - \theta S_s[n, j_p, m, \Delta] \qquad -(6)$$

§. Self-Consistent Equations

We minimize Eq. (3) with respect to $\{n, j_p, m, \Delta\}$.

① $$\frac{\delta F_s}{\delta n(r)} + \frac{e^2}{2mc^2} A(r) + v_s(r) = 0 \qquad -(7)$$

where

$$\begin{cases} v_s(r) = v(r) + e^2 \int d^3r' \frac{n(r')}{|r-r'|} + v_{xc}(r) & -(8) \\ v_{xc}(r) = \delta F_{xc} / \delta n(r) & -(9) \end{cases}$$

② $$\frac{\delta F_s}{\delta j_p(r)} + \frac{e}{c} A_s(r) = 0 \qquad -(10)$$

where

$$\begin{cases} A_s(r) = A(r) + A_{xc}(r) & -(11) \\ A_{xc}(r) = (c/e)\, \delta F_{xc} / \delta j_p(r) & -(12) \end{cases}$$

③ $$\frac{\delta F_s}{\delta m(r)} - H_s(r) = 0 \qquad -(13)$$

where

$$\begin{cases} H_s(r) = H(r) + H_{xc}(r) & -(14) \\ H_{xc}(r) = -\delta F_{xc} / \delta m(r) & -(15) \end{cases}$$

④ $$\frac{\delta F_S}{\delta \Delta^*(r)} - D_S(r) = 0 \qquad -(16)$$

where

$$\begin{cases} D_S(r) = D(r) + w\Delta(r) + D_{xc}(r) & -(17) \\ D_{xc}(r) = -\delta F_{xc}/\delta\Delta^*(r) & -(18) \end{cases}$$

We must solve the following noninteracting Hamiltonian,

$$\left.\begin{aligned} \mathcal{H}_S = &\sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\psi_\sigma(r) \\ &+ \frac{e}{c}\int d^3r\, \hat{j}_p(r)\cdot A_S(r) + \frac{e^2}{2mc^2}\int d^3r\, \hat{n}(r) A^2(r) \\ &+ \int d^3r\, \hat{n}(r)\, v_S(r) - \int d^3r\, \hat{m}(r)\cdot H_S(r) \end{aligned}\right\} \mathcal{K}$$

$$- \int d^3r\, [D_S^*(r)\hat{\Delta}(r) + \text{H.c.}] \qquad -(19)$$

① $$\mathcal{K} = \sum_{\sigma\tau}\int d^3r\, \psi_\sigma^\dagger(r) \Big[\underbrace{\Big\{\Big[\frac{1}{2m}\Big(\frac{\hbar}{i}\nabla + \frac{e}{c}A_S(r)\Big)^2 - \mu\Big] + \frac{e^2}{2mc^2}[A^2(r) - A_S^2(r)] + v_S(r)\Big\}\delta_{\sigma\tau} + \mu_B \sigma_{\sigma\tau}\cdot H_S(r)}_{\equiv\, K_{\sigma\tau}(r)} \Big] \psi_\tau(r)$$

$$= \sum_{\sigma\tau}\int d^3r\, \big(K_{\tau\sigma}^*(r)\,\psi_\sigma^\dagger(r)\big)\,\psi_\tau(r)$$

$$\left(\begin{aligned} &∵ (1)\ \int d^3r\, \psi_\sigma^\dagger(r) \Big(\frac{\hbar}{i}\nabla + \frac{e}{c}A\Big)^2 \psi_\sigma(r) = \int d^3r \Big[\Big(-\frac{\hbar}{i}\nabla + \frac{e}{c}A\Big)^2 \psi_\sigma^\dagger(r)\Big]\psi_\sigma(r) \\ &(2)\ (\sigma_{\tau\sigma})^* = \left(\begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}0&i\\-i&0\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}\right)_{\tau\sigma} = \left(\begin{pmatrix}0&1\\1&0\end{pmatrix}, \begin{pmatrix}0&-i\\i&0\end{pmatrix}, \begin{pmatrix}1&0\\0&-1\end{pmatrix}\right)_{\sigma\tau} = \sigma_{\sigma\tau} \ // \end{aligned} \right)$$

② $- \int d^3r\, D_s^*(r)\, \psi_\uparrow(r)\psi_\downarrow(r)$

$$= -\frac{1}{2}\int d^3r\, D_s^*(r)\, \left(\psi_\uparrow(r)\psi_\downarrow(r) - \psi_\downarrow(r)\psi_\uparrow(r)\right)$$

$$= -\frac{1}{2}\int d^3r\, D_s^*(r)\, (\psi_\uparrow(r)\ \psi_\downarrow(r)) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \psi_\uparrow(r) \\ \psi_\downarrow(r) \end{pmatrix}$$

$$= -\frac{1}{2}\sum_{\sigma\tau}\int d^3r\ \psi_\sigma(r)\, D_s^*(r)\, \rho_{\sigma\tau}\, \psi_\tau(r)$$

$$= \frac{1}{2}\sum_{\sigma\tau}\int d^3r\, \psi_\tau(r)\, D_s^*(r)\, \rho_{\sigma\tau}\ \psi_\sigma(r)$$

③ $- \int d^3r\, D_s(r)\, \psi_\downarrow^+(r)\psi_\uparrow^+(r)$

$$= \frac{1}{2}\sum_{\sigma\tau}\int d^3r\, \psi_\sigma^+(r)\, D_s(r)\, \rho_{\sigma\tau}\, \psi_\tau^+(r)$$

$$\mathcal{H}_s = \frac{1}{2}\sum_{\sigma\tau}\int d^3r \Big[\ \psi_\sigma^+(r)\left\{ \kappa_{\sigma\tau}(r)\psi_\tau(r) + D_s(r)\rho_{\sigma\tau}\psi_\tau^+(r)\right\}$$
$$+ \left\{ \kappa_{\sigma\tau}^*(r)\psi_\tau^+(r) + D_s^*(r)\rho_{\sigma\tau}\psi_\tau(r)\right\}\psi_\sigma(r)\Big] \qquad -(20)$$

where

$$\kappa_{\sigma\tau}(r) = \left\{ \frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A_s(r)\right)^2 - \mu + \frac{e^2}{2mc^2}[A^2(r) - A_s^2(r)] + v_s(r)\right\}\delta_{\sigma\tau}$$
$$+ \mu_B\, \sigma_{\sigma\tau}\cdot H_s(r) \qquad -(21)$$

and $\rho = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

§. Gap etc. (cf. "Derivation of deGennes-Bogoliubov Eq.", 7/11)

(1) $\Delta(r) = \frac{1}{2}\sum_{\nu}\sum_{\sigma\tau} u_\nu(r\sigma)\rho_{\sigma\tau} v_\nu^*(r\tau)[1-2f(E_\nu)]$ — (22)

(2) $n(r) = \sum_{\nu}\sum_{\sigma} [\,|u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2(1-f(E_\nu))\,]$ — (23)

(3) $m(r) = -\mu_B \sum_{\nu}\sum_{\sigma\tau}[u_\nu^*(r\sigma)\sigma_{\sigma\tau}u_\nu(r\tau)\, f(E_\nu)$
$+ v_\nu(r\sigma)\sigma_{\sigma\tau}v_\nu^*(r\tau)(1-f(E_\nu))\,]$ — (24)

(4) $j_p(r) = \frac{\hbar}{2mi}\sum_{\sigma}\sum_{\nu}\langle(\alpha_\nu v_\nu(r\sigma)+\alpha_\nu^+ u_\nu^*(r\sigma))\nabla(\alpha_\nu u_\nu(r\sigma)+\alpha_\nu^+ v_\nu^*(r\sigma))\rangle$

$-[\nabla(\alpha_\nu v_\nu + \alpha_\nu^+ u_\nu^*)](\alpha_\nu u_\nu + \alpha_\nu^+ v_\nu^*)\rangle$

$= \frac{\hbar}{2mi}\sum_{\sigma}\sum_{\nu}[u_\nu^*\nabla u_\nu f + v_\nu\nabla v_\nu^*(1-f)$

$-(\nabla u_\nu^*)u_\nu f - (\nabla v_\nu)v_\nu^*(1-f)]$

$j_p(r) = \frac{\hbar}{2mi}\sum_{\nu}\sum_{\sigma}\{[u_\nu^*(r\sigma)\nabla u_\nu(r\sigma) - (\nabla u_\nu^*(r\sigma))u_\nu(r\sigma)]\, f(E_\nu)$

$+[v_\nu(r\sigma)\nabla v_\nu^*(r\sigma) - (\nabla v_\nu(r\sigma))v_\nu^*(r\sigma)][1-f(E_\nu)]\}$ — (25)

§. Simplified Spin

We set $A(r) = 0$, and assume $\vec{H}(r)$ and $\vec{m}(r)$ have only z components. Then, in Eq. (21),

$$K_{\sigma\tau}(r) = \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_S(r) + \mu_B \sigma H_S(r)\right]\delta_{\sigma\tau} \quad -(26)$$

The Bogoliubov equation becomes

$$\begin{cases} \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_S(r) + \mu_B \sigma H_S(r)\right] u_\nu(r\sigma) + D_S(r) \sum_\tau \rho_{\sigma\tau} v_\nu(r\tau) = E_\nu u_\nu(r\sigma) \\ \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_S(r) + \mu_B \sigma H_S(r)\right] v_\nu(r\sigma) + D_S^*(r) \sum_\tau \rho_{\sigma\tau} u_\nu(r\tau) = -E_\nu v_\nu(r\sigma) \end{cases}$$

$$-(27)$$

$$\begin{cases} n(r) = \sum_\nu \sum_\sigma \left[|u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2 (1 - f(E_\nu))\right] \\ m(r) = \sum_\nu \sum_\sigma \sigma \left[|u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2 (1 - f(E_\nu))\right] \end{cases} \quad -(28)$$

Density-Functional Theory for Superconductors: Inclusion of Spins

We apply the density-functional theory to superconductors in magnetic fields.[1,2]

§. System

The grand-canonical Hamiltonian is written as

$$\mathcal{H} = \mathcal{H} - \mu N$$

$$= \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right) \psi_\sigma(r) + \frac{e^2}{2}\sum_{\sigma\sigma'} \int d^3r d^3r' \frac{\psi_\sigma^\dagger(r)\psi_{\sigma'}^\dagger(r')\psi_{\sigma'}(r')\psi_\sigma(r)}{|r-r'|}$$

$$- w \int d^3r\, \psi_\downarrow^\dagger(r)\psi_\uparrow^\dagger(r)\psi_\uparrow(r)\psi_\downarrow(r) \qquad -(1)$$

Next, we introduce an external potential $v(r)$, a vector potential $A(r)$, a magnetic field $H(r) = \nabla \times A(r)$, and a pair potential $D(r)$.

Then, the Hamiltonian becomes

$$\mathcal{H}_{vAHD} = \mathcal{H} + \frac{e}{c}\int d^3r\, \hat{j}_p(r)\cdot A(r) + \frac{e^2}{2mc^2}\int d^3r\, \hat{n}(r) A^2(r)$$

$$+ \int d^3r\, \hat{n}(r)\, v(r) - \int d^3r\, \hat{m}(r)\cdot H(r)$$

$$- \int d^3r\, [D^*(r)\hat{\Delta}(r) + \text{H.c.}] \qquad -(2)$$

where $\hat{j}_p(r) = (\hbar/2mi)\sum_\sigma [\psi_\sigma^\dagger(r)\nabla\psi_\sigma(r) - (\nabla\psi_\sigma^\dagger(r))\psi_\sigma(r)]$, $\hat{n}(r) = \sum_\sigma \psi_\sigma^\dagger(r)\psi_\sigma(r)$, $\hat{m}(r) = -\mu_B \sum_{\sigma\tau} \psi_\sigma^\dagger(r)\,\boldsymbol{\sigma}_{\sigma\tau}\psi_\tau(r)$ [$\mu_B = e\hbar/2mc$ and $\boldsymbol{\sigma}$ is the Pauli matrix], and $\hat{\Delta}(r) = \psi_\uparrow(r)\psi_\downarrow(r)$.

§. Variational Formulation

The thermodynamic potential is written as a functional of $\{n, j_p, m, \Delta\} = \{\langle n\rangle, \langle j_p\rangle, \langle m\rangle, \langle\Delta\rangle\}$ as

$$\Omega_{vAHD}[n, j_p, m, \Delta] = \frac{e}{c}\int d^3r\,\hat{j}_p(r)\cdot A(r) + \frac{e^2}{2mc^2}\int d^3r\,n(r)\cdot A^2(r) + \int d^3r\,n(r)v(r) - \int d^3r\,m(r)\cdot H(r) - \int d^3r\,[D^*(r)\Delta(r) + \text{c.c.}] + F[n, j_p, m, \Delta] \qquad -(3)$$

In Eq. (3),

$$F[n, j_p, m, \Delta] = \mathrm{tr}\,\rho_{vAHD}[\mathcal{H} - \mu\mathcal{N} + \frac{1}{\beta}\rho_{vAHD}]$$

$$= \langle\mathcal{H}\rangle - \mu\langle\mathcal{N}\rangle - \theta\langle S\rangle \qquad -(4)$$

where $\rho_{vAHD} = \exp(-\beta\mathcal{H}_{vAHD})/\mathrm{tr}[\exp(-\beta\mathcal{H}_{vAHD})]$, and θ is the temperature.

It is prooved that Eq.(3) takes minimum value when densities $\{n, j_p, m, \Delta\}$ are the equillibrium value corresponding to the external potentials $\{v, A, H, D\}$.

§. Self-Consistent Equations

First, the exchange-correlation free energy $F_{xc}[n, j_p, m, \Delta]$ is defined by the equality

$$F[n,j_p,m,\Delta] = F_s[n,j_p,m,\Delta] + \frac{e^2}{2}\int d^3r d^3r' \frac{n(r)n(r')}{|r-r'|} - \nu\int d^3r\, \Delta^*(r)\Delta(r) + F_{xc}[n,j_p,m,\Delta] \quad -(5)$$

where

$$F_s[n,j_p,m,\Delta] = T_s[n,j_p,m,\Delta] - \mu N - \theta S_s[n,j_p,m,\Delta] \quad -(6)$$

is the free energy of a noninteracting system whose densities are equal to those of the interacting system.

Minimization of Eq.(3) with respect to $\{n, j_p, m, \Delta\}$ leads to the following equations.

① $$\frac{\delta F_s}{\delta n(r)} + \frac{e^2}{2mc^2} A^2(r) + v_s(r) = 0 \qquad -(7)$$

where

$$v_s(r) = v(r) + e^2 \int d^3r' \frac{n(r')}{|r-r'|} + v_{xc}(r) \qquad -(8)$$

and $v_{xc}(r) = \delta F_{xc} / \delta n(r)$.

② $$\frac{\delta F_s}{\delta j_p(r)} + \frac{e}{c} A_s(r) = 0 \qquad -(9)$$

where $A_s(r) = A(r) + A_{xc}(r)$, and $A_{xc}(r) = (c/e)\,\delta F_{xc}/\delta j_p(r)$.

③ $$\frac{\delta F_s}{\delta m(r)} - H_s(r) = 0 \qquad -(10)$$

where $H_s(r) = H(r) + H_{xc}(r)$, and $H_{xc}(r) = -\delta F_{xc}/\delta m(r)$.

④ $$\frac{\delta F_s}{\delta \Delta^*(r)} - D_s(r) = 0 \qquad -(11)$$

where

$$D_s(r) = D(r) + w\Delta(r) + D_{xc}(r) \qquad -(12)$$

and $D_{xc}(r) = -\delta F_{xc}/\delta \Delta^*(r)$.

∴ Equations (7), (9), (10) and (11) are equivalent to solving the following noninteracting Hamiltonian.

$$\mathcal{H}_S = \sum_\sigma \int d^3r\, \psi_\sigma^\dagger(r) \left(-\frac{\hbar^2}{2m} - \mu\right) \psi_\sigma(r)$$

$$+ \frac{e}{c}\int d^3r\, \hat{j}_p(r)\cdot A_S(r) + \frac{e^2}{2mc^2}\int d^3r\, \hat{n}(r) A^2(r)$$

$$+ \int d^3r\, \hat{n}(r) v_S(r) - \int d^3r\, \hat{m}(r)\cdot H_S(r)$$

$$- \int d^3r\, [D_S^*(r)\hat{\Delta}(r) + \text{H.C.}] \qquad -(13)$$

Equation (13) may be rewritten as[3]

$$\mathcal{H}_S = \frac{1}{2}\sum_{\sigma\tau}\int d^3r \left\{ \psi_\sigma^\dagger(r)\left[K_{\sigma\tau}(r)\psi_\tau(r) + D_S(r)\rho_{\sigma\tau}\psi_\tau^\dagger(r)\right] + \left[K_{\sigma\tau}^*(r)\psi_\tau^\dagger(r) + D_S^*(r)\rho_{\sigma\tau}\psi_\tau(r)\right]\psi_\sigma(r)\right\} \qquad -(14)$$

where

$$K_{\sigma\tau}(r) = \left\{\frac{1}{2m}\left(\frac{\hbar}{i}\nabla + \frac{e}{c}A_S(r)\right)^2 - \mu + \frac{e^2}{2mc^2}\left(A^2(r) - A_S^2(r)\right) + v_S(r)\right\}\delta_{\sigma\tau} + \mu_B \sigma_{\sigma\tau}\cdot H_S(r) \qquad -(15)$$

and $\rho = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

(※ To derive Eq. (14), we have used the following relation,

$$\int d^3r\, \psi_\sigma^\dagger(r) K_{\sigma\tau}(r)\psi_\tau(r) = \int d^3r\, [K_{\sigma\tau}^*(r)\psi_\sigma^\dagger(r)]\,\psi_\tau(r)\ )$$

(Bogoliubov Transformation)

To diagonalize Eq.(14), we must first solve the deGennes–Bogoliubov like equations,

$$\boxed{\begin{cases} \sum_\tau [K_{\sigma\tau}(r)\, u_\nu(r\tau) + D_S(r)\rho_{\sigma\tau}\, v_\nu(r\tau)] = E_\nu\, u_\nu(r\sigma) \\ \sum_\tau [K^*_{\sigma\tau}(r)\, v_\nu(r\tau) + D^*_S(r)\rho_{\sigma\tau}\, u_\nu(r\tau)] = -E_\nu\, v_\nu(r\sigma) \end{cases}} \quad -(16)$$

with the constraint $E_\nu > 0$. Denoting a positive-energy solution as $w_\nu(rs) = (u_\nu(r\uparrow), u_\nu(r\downarrow), v_\nu(r\uparrow), v_\nu(r\downarrow))$, the coresponding negative-energy solution is given by $w_{-\nu}(rs) = (v^*_\nu(r\uparrow), v^*_\nu(r\downarrow), u^*_\nu(r\uparrow), u^*_\nu(r\downarrow))$. The orthonomality and completeness of the set of the eigenstates are written as

$$\begin{cases} \langle\mu|\nu\rangle = \sum_{S=1}^{4}\int d^3r\, w^*_\mu(rs)\, w_\nu(rs) = \delta_{\mu\nu} & -(17) \\ \sum_\nu \langle rs|\nu\rangle\langle\nu|r's'\rangle = \sum_{\nu>0}[w_\nu(rs)w^*_\nu(r's') + w_{-\nu}(rs)w^*_{-\nu}(r's')] = \delta_{ss'}\delta^3(r-r') & -(18) \end{cases}$$

Defining $\psi(rs) = (\psi_\uparrow(r), \psi_\downarrow(r), \psi^\dagger_\uparrow(r), \psi^\dagger_\downarrow(r))$, Eq.(14) is diagonalized by the Bogoliubov transformation

$$\psi(rs) = \sum_{\nu>0}[\alpha_\nu\, w_\nu(rs) + \alpha^\dagger_\nu\, w_{-\nu}(rs)] \quad -(19)$$

α_ν and $\alpha_\nu^\dagger$ are proved to satisfy ordinary anticommutation relations, and Eq.(14) is diagonalized as

$$\boxed{\mathcal{H}_S = \sum_\nu E_\nu \alpha_\nu^\dagger \alpha_\nu - \sum_\nu \sum_\sigma E_\nu \int d^3r \, |v_\nu(r\sigma)|^2} \quad -(20)$$

Using u_ν's and v_ν's, the densities are expressed as

① $$\Delta(r) = \frac{1}{2} \sum_\nu \sum_{\sigma\tau} u_\nu(r\sigma) \rho_{\sigma\tau} v_\nu^*(r\tau) [1 - 2f(E_\nu)] \quad -(21)$$

② $$n(r) = \sum_\nu \sum_\sigma [\, |u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2 (1 - f(E_\nu))\,] \quad -(22)$$

③ $$m(r) = -\mu_B \sum_\nu \sum_{\sigma\tau} [\, u_\nu^*(r\sigma) \sigma_{\sigma\tau} u_\nu(r\tau) f(E_\nu) + v_\nu(r\sigma) \sigma_{\sigma\tau} v_\nu^*(r\tau) (1 - f(E_\nu))\,] \quad -(23)$$

④ $$j_p(r) = (\hbar/2mi) \sum_\nu \sum_\sigma \Big\{ [\, u_\nu^*(r\sigma) \nabla u_\nu(r\sigma) - (\nabla u_\nu^*(r\sigma)) u_\nu(r\sigma) \,] f(E_\nu) + [\, v_\nu(r\sigma) \nabla v_\nu^*(r\sigma) - (\nabla v_\nu(r\sigma)) \nabla v_\nu^*(r\sigma) \,] (1 - f(E_\nu)) \Big\} \quad -(24)$$

where $f(E_\nu) = [\exp(\beta E_\nu) + 1]^{-1}$.

After solving the self-consistent equations, Eq. (3) is calucul‍ated, using Eqs. (4), (8), (12), (13) etc., as

$$\boxed{\begin{aligned}\Omega_{vAHD}[n, j_p, m, \Delta] = &-\theta\, \mathrm{tr}[e^{-\beta\mathcal{H}_s}] - \frac{e}{c}\int d^3r\, j_p(r)\cdot A_{xc}(r) \\ &- \frac{e^2}{2}\int d^3r d^3r' \frac{n(r)n(r')}{|r-r'|} - \int d^3r\, n(r)\, v_{xc}(r) \\ &+ \int d^3r\, m(r)\cdot H_{xc}(r) + w\int d^3r\, \Delta^*(r)\Delta(r) \\ &+ \int d^3r\, [D_{xc}^*(r)\Delta(r) + c.c.] + F_{xc}[n, j_p, m, \Delta]\end{aligned}} \quad -(25)$$

§. Simplified Treatment of Spins

We set $A(r) = 0$, and assume $\vec{H}(r)$ and $\vec{m}(r)$ have only z component $H(r)$ and $m(r)$. Then, the deGennes-Bogoliubov like equations becomes

$$\boxed{\begin{cases} [-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_S(r) + \mu_B\sigma H_S(r)]\, u_\nu(r\sigma) + D_S(r)\sum_\tau \rho_{\sigma\tau} v_\nu(r\tau) = E_\nu u_\nu(r\sigma) \\ [-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_S(r) + \mu_B\sigma H_S(r)]\, v_\nu(r\sigma) + D_S^*(r)\sum_\tau \rho_{\sigma\tau} u_\nu(r\tau) = -E_\nu v_\nu(r\sigma) \end{cases}}$$

$-(26)$

where $\sigma = \pm 1$.

The densities are given by

$$
\boxed{
\begin{cases}
\Delta(r) = \frac{1}{2}\sum_{\nu}\sum_{\sigma\tau} u_\nu(r\sigma)\, \rho_{\sigma\tau}\, v_\nu^*(r\tau)\,[1-2f(E_\nu)] \\
n(r) = \sum_{\nu}\sum_{\sigma} [\,|u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2 (1-f(E_\nu))\,] \\
m(r) = \sum_{\nu}\sum_{\sigma} \sigma\,[\,|u_\nu(r\sigma)|^2 f(E_\nu) + |v_\nu(r\sigma)|^2 (1-f(E_\nu))\,]
\end{cases}
}
$$

—(21)

—(22)

—(27)

and the single-particle potentials are

$$
\boxed{
\begin{cases}
D_s(r) = D(r) + w\Delta(r) + D_{xc}(r) \\
v_s(r) = v(r) + e^2\int d^3r' \frac{n(r')}{|r-r'|} + v_{xc}(r) \\
H_s(r) = H(r) + H_{xc}(r)
\end{cases}
}
$$

—(12)

—(8)

—(28)

where $D_{xc}(r) = -\delta F_{xc}/\delta\Delta^*(r)$, $v_{xc}(r) = \delta F_{xc}(r)/\delta n(r)$, $H_{xc}(r) = -\delta F_{xc}/\delta m(r)$.

§. Gap Equation near Transition Point

We consider a non-magnetic case, $H(r) = 0$, then the eigenstates of Eq.(26) can be classified into $w_{\nu 1}(rs) = (u_\nu(r), 0, 0, v_\nu(r))$ and $w_{\nu 2}(rs) = (0, u_\nu(r), -v_\nu(r), 0)$, where $u_\nu(r)$ and $v_\nu(r)$ satisfy

$$\begin{cases} \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_s(r)\right] u_\nu(r) + D_s(r) v_\nu(r) = E_\nu u_\nu(r) \\ \left[-\frac{\hbar^2}{2m}\nabla^2 - \mu + v_s(r)\right] v_\nu(r) - D_s^*(r) u_\nu(r) = -E_\nu v_\nu(r) \end{cases} \quad -(29)$$

In Eq.(29), if we set $D(r) = 0$,

$$\begin{cases} D_s(r) = w\,\Delta(r) + \boxed{D_{xc}(r)} & -(30) \\ \Delta(r) = \sum_\nu u_\nu(r) v_\nu^*(r)\left[1 - 2f(E_\nu)\right] & -(31) \end{cases}$$

Near the transition point, where $D_s(r)$ is small, the solution of Eq.(20) can be expanded in terms of $D_s(r)$. When this expansion is substituted in Eq.(31), it becomes

$$\boxed{\Delta(r) = \int d^3r_1\, K(r, r_1) D_s(r_1) + \int d^3r_1 d^3r_2 d^3r_3\, K^{(4)}(r, r_1, r_2, r_3)\, D_s^*(r_1) D_s(r_2) D_s(r_3) + \cdots} \quad -(32)$$

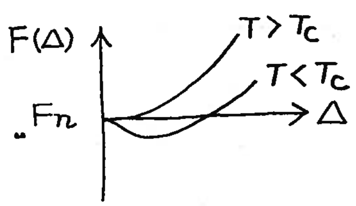
where the kernel $K(r, r')$ is given by[4)]

$$\boxed{K(r,r') = \sum_{\nu\mu}[1-2f(E_\nu)]\left[\frac{\theta(\xi_\nu)}{|\xi_\nu|+\xi_\mu}+\frac{\theta(-\xi_\nu)}{|\xi_\nu|-\xi_\mu}\right] \times \phi_\nu^*(r)\phi_\nu(r')\phi_\mu^*(r)\phi_\mu(r')} \quad -(33)$$

where $\phi_\nu(r)$ and ξ_ν satisfy

$$\left[-\frac{\hbar^2}{2m}\nabla^2-\mu+v_s(r)\right]\phi_\nu(r) = \xi_\nu\phi_\nu(r), \quad -(34)$$

i.e., the normal-state eigen solutions. Equation (32) is the Ginzburg-Landau equation, which can be used for determining a gap function $\Delta(r)$ near a transition temperature. To determine the transition point, the non-linear term including $K^{(4)}(r_1 r_2 r_3 r_4)$ is essential. Further, to discuss inhomogeneous superconducting states, non-locality in $K^{(4)}$ is important.



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