Lect 3: Applications of the second quantization

§ Exchange energy – a two body problem. Let us conside two particles in momentum eigenstates k_1, k_2. In the first quantization method, we write the two particle wavefunction

$$\psi_{\substack{B\\F}}(r_1 r_2) = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{V}}\right)^2 [e^{ik_1 r_1} e^{ik_2 r_2} \pm e^{ik_1 r_2} e^{ik_2 r_1}]$$

the exchang energy is the part different from the direct energy

$$\langle | V | \rangle := \int dr_1 dr_2 \, \psi^*_{B,F}(r_1 r_2) \, V(r_1 r_2) \, \psi_{B,F}(r_1 r_2)$$

$$= \int dr_1 dr_2 \frac{e^{-ik_1 r_1 - ik_2 r_2}}{V} V(r_1 - r_2) \frac{e^{ik_1 r_1 + ik_2 r_2}}{V} \pm \int dr_1 dr_2 \, e^{-ik_1 r_1 - ik_2 r_2} V(r_1 r_2) \, e^{ik_1 r_2 + k_2 r_1}$$

$$= \frac{1}{V}\int dr \, e^{iqr} v(r) \pm \frac{1}{V}\int dr \, e^{i(k_1 - k_2)\cdot r} V(r_1 - r_2)$$

$(q \to 0)$

$$= \frac{1}{V}[V(q=0) \pm V(k_1 - k_2)]$$

$V(q=0)$: Hartree

$V(k_1-k_2)$: Fock exchange energy

Now let us calculate it in the second quantization

$$|\Psi\rangle = |k_1 k_2\rangle = a^\dagger_{k_1} a^\dagger_{k_2} |0\rangle$$

$$V = \frac{1}{2V}\sum_{kk'q} a^\dagger_k a^\dagger_{k'} a_{k'-q} a_{k+q} v(q)$$

$$\Rightarrow \langle\Psi| V |\Psi\rangle = \frac{1}{2V}\sum_{kk'q} \overbrace{}^{v(q)} \langle 0 | a_{k_2} a_{k_1} a^\dagger_k a^\dagger_{k'} a_{k'-q} a_{k+q} a^\dagger_{k_1} a^\dagger_{k_2} |0\rangle$$

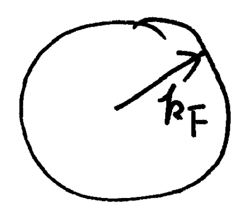
1. $q=0,\ \&\ k=k_1\ \ k'=k_2$; $q=0\ \&\ k=k_2,\ k'=k_1$ $\Big\} \Rightarrow \frac{1}{V} V(q=0) \leftarrow$ Hartree

2. $k=k_2,\ k'=k_1$, $q=k_1-k_2$: $a_{k_2} a_{k_1} a^+_{k_2} a^+_{k_1} a_{k_2} a_{k_1} a^+_{k_1} a^+_{k_2}$

$k=k_1\ \ k'=k_2$, $q=k_2-k_1$: $a_{k_2} a_{k_1} a^+_{k_1} a^+_{k_2} a_{k_1} a_{k_2} a^+_{k_1} a^+_{k_2}$

$\Rightarrow \pm \frac{1}{V} V(k_2-k_1)$ Fock term.

§ Hartree - Fock interaction energy of the state $|G\rangle$ in which the $|k\sigma\rangle$ inside the Fermi sphere (k_F) is occupied.



$$V = \frac{1}{2V} \sum_{k_1 k_2 q} v(q)\, a^+_{k_1+q\,\sigma} a^+_{k_2-q\,\sigma'} a_{k_2\sigma'} a_{k_1\sigma}$$

$$|G\rangle = \prod_{k<k_F} a^+_{k\uparrow} a^+_{-k\downarrow} |0\rangle$$

we need to evaluate $\langle G | V | G\rangle$

Hartree term: $V_H = \frac{1}{2V} \sum_{k_1 k_2 \sigma\sigma'} v(0) \langle G | a^+_{k_1\sigma} a^+_{k_2\sigma'} a_{k_2\sigma'} a_{k_1\sigma} | G\rangle$

$$= \frac{1}{2V} \sum_{\substack{k_1 k_2 \\ \sigma\sigma'}} v(0) \Big\{ \langle G | a^+_{k_1\sigma} a_{k_1\sigma} a^+_{k_2\sigma'} a_{k_2\sigma'} | G\rangle - \langle G | a^+_{k_1\sigma} a_{k_2\sigma'} | G\rangle\, \delta_{k_1 k_2} \delta_{\sigma\sigma'} \Big\}$$

$$= \frac{v(0)}{2V} \Big\{ \Big(\sum_{k\sigma} n_{k\sigma} \Big)^2 - \sum_k (n_{k\sigma}) \Big\} = \frac{1}{2} v(0) \left[\mathrm{Vol} \cdot n^2 - n \right]$$

n is the density

Fock term: $\sigma = \sigma'$ & $k_2 - q = k_1$, $k_1 \neq k_2$

$$V_{Fock} = \frac{1}{2V} \sum_{k_1 \neq k_2} \langle G | a^\dagger_{k_2\sigma} a^\dagger_{k_1\sigma} a_{k_2\sigma} a_{k_1\sigma} | G \rangle \, v(k_1 - k_2)$$

$$= \frac{-1}{2V} \sum_{k_1 \neq k_2} V(k_1 - k_2) \langle G | a^\dagger_{k_2\sigma} a_{k_2\sigma} a^\dagger_{k_1\sigma} a_{k_1\sigma} | G \rangle$$

$$\xrightarrow[\text{over spin}]{\text{sum}} = \frac{-1}{2V} \sum_{k_1 \neq k_2} V(k_1 - k_2) \, 2 n_{k_1} n_{k_2} = \frac{-1}{Vol} \cdot Vol^2 \left[\int \frac{dk_1}{(2\pi)^3} \frac{dk_2}{(2\pi)^3} V(k_1 - k_2) \, n(k_1) n(k_2) \right)$$

keep leading order

$$\boxed{V_{Fock}/Vol = \int \frac{d\vec{k}_1}{(2\pi)^3} \int \frac{d\vec{k}_2}{(2\pi)^3} n(k_1) n(k_2) V(k_1 - k_2)}$$

§3. Cooper pairing problem

Consider that we have a full-filled Fermi sphere with Fermi wave vector k_F. We add two extra electrons with $(k\uparrow)$ and $(-k\downarrow)$ outside the sphere. Neglect that electrons inside the Fermi sphere can be scattered outside the Fermi surface. Assume that the attrative interactions between two electrons as

$$H = \sum_k \epsilon_k C^\dagger_{k\sigma} C_{k\sigma} - \frac{U}{V} \sum_{kk'} C^\dagger_{k\uparrow} C^\dagger_{-k\downarrow} C_{-k\downarrow} C_{k\uparrow}$$

Solve the bound state energy.

Let us assume that the eigenstate is a linear superposition of $(k\uparrow, -k\downarrow)$ as $|\psi\rangle = \sum_{k>k_F} \alpha(k)\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow} |F\rangle$ ↖ full filled Fermi sea

$$H|\psi\rangle = (H_0 + H_{int})\,|\psi\rangle$$

$$= \sum_{k>k_F} \alpha(k)\,(H_0 + H_{int})\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow} |F\rangle$$

$$H_0\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow} |F\rangle = (C^{+}_{k\uparrow} C^{+}_{-k\downarrow})\{2\mathcal{E}_k + H_0\}|F\rangle = (2\mathcal{E}_k + E_0)\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle$$

$$H_{int}\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle = -\frac{U}{V}\sum_{k'k''}\left[C^{+}_{k'\uparrow} C^{+}_{-k'\downarrow} C_{-k''\downarrow} C_{k''\uparrow}\right] C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle$$

$$= -\frac{U}{V}\sum_{k'k''} \delta(k\,k'')\, C^{+}_{k'\uparrow} C^{+}_{-k'\downarrow}|F\rangle = -\frac{U}{V}\sum_{k'} C^{+}_{k'\uparrow} C^{+}_{-k'\downarrow}|F\rangle$$

$$\Rightarrow H|\psi\rangle = \sum_{k} \alpha(k)\,[2\mathcal{E}_k + E_0]\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle$$

$$- \sum_{k} \alpha(k)\,\frac{U}{V}\sum_{k'} C^{+}_{k'\uparrow} C^{+}_{-k'\downarrow}|F\rangle$$

$$= E|\psi\rangle$$

$$\Rightarrow \sum_{k}\left[(2\mathcal{E}_k + E_0)\,\alpha(k) - \frac{U}{V}\sum_{k'}\alpha(k')\right] C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle$$

$$= E\sum_{k}\alpha(k)\, C^{+}_{k\uparrow} C^{+}_{-k\downarrow}|F\rangle$$

$$\Rightarrow \quad (2\mathcal{E}_k + E_0)\,\alpha(k) - \frac{U}{V}\sum_{k'}\alpha(k') = E\,\alpha(k)$$

$$\alpha(k) = \frac{U}{E_0 - E + 2\mathcal{E}_k}\frac{1}{V}\sum_{k'}\alpha(k')$$

$$\Rightarrow \quad \frac{1}{U} = \frac{1}{V}\sum_{k>k_F}\frac{1}{2\mathcal{E}_k - (E-E_0)} \quad \text{or} \quad \frac{1}{U} = \frac{1}{V}\sum_{k>k_F}\frac{1}{2\mathcal{E}_k - \Delta E}$$

$$\frac{1}{U} = N(0)\int_0^{\hbar\omega_D} d\epsilon\,\frac{1}{2\epsilon - \Delta E} = \frac{N(0)}{2}\ln\frac{2\hbar\omega_D + |\Delta E|}{|\Delta E|}$$

$$\frac{2}{N(0)U} \approx \ln\frac{2\hbar\omega_D}{|\Delta E|} \quad \Rightarrow \quad \Delta E = -2\hbar\omega_D\, e^{-\frac{2}{N(0)U}}$$

gap energy