Lecture 0: An introduction to the 2nd quantization method

§1 Harmonic oscillator (warm up)

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2,$$ define characteristic length $l = \sqrt{\frac{\hbar}{m\omega}}$

then $a = \frac{1}{\sqrt{2}}\left[\frac{x}{l} + ilp\right]$, $a^\dagger = \frac{1}{\sqrt{2}}\left[\frac{x}{l} - ipl\right]$

$[a, a^\dagger] = 1$, and $H = \hbar\omega(a^\dagger a + \frac{1}{2})$.

The eigenstate of oscillator can be expressed as $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$

where $|0\rangle$ satisfies $a|0\rangle = 0$.

ex: ① $\langle x|0\rangle = \frac{1}{\sqrt{\pi^{1/2} l}} e^{-\frac{x^2}{2l^2}}$

② $a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$, $a|n\rangle = \sqrt{n}\,|n\rangle$, $a^\dagger a|n\rangle = n|n\rangle$

§2 Bose statistics and Fermi statistics

Suppose we have a set of complete and normalized basis of Singe particle $\underbrace{\text{wavefunctions}}_{\psi_1,\ \psi_2\ \cdots}$, we can use them to construct the N-body wavefunction.

For bosons, we first consider

$$\underbrace{\psi_1(x_1)\cdots\psi_1(x_{n_1})}_{N_1}\ \psi_2(x_{n_1+1})\cdots\psi_2(x_{n_1+n_2})\cdots\{\underbrace{\psi_k()\cdots\psi_k(x_N)}_{N_k}\}$$

and symmetrize it

$$\Psi_{N_1\cdots N_k}(\xi_1\cdots\xi_N) = \left(\frac{N!}{N_1!\cdots N_k!}\right)^{-1/2}\sum_{P_E} P_E\{\underbrace{\psi_1(x_1)\cdots\psi_1(x_{n_1})}_{N_1}\cdots\{\underbrace{\psi_k\cdots\psi_k(\xi_N)}_{N_k}\}\}$$

For fermions, each state can only support one particle

$$\psi_{i_1}(\xi_1)\ \psi_{i_2}(\xi_2)\cdots\psi_{i_N}(\xi_N)$$

$$\rightarrow \Psi_{\{1_{i_1},\cdots 1_{i_N}\}}(\xi_1\cdots\xi_N) = \frac{1}{\sqrt{N!}}\sum_P (-)^P P\, \psi_{i_1}(\xi_1)\psi_{i_2}(\xi_2)\cdots\psi_{i_N}(\xi_N)$$

§3: second quantization for bosons

From the above section, we learn that as long as we have a set of complete and orthogonal single particle basis, and specify the occupation number distribution, we can write down the basis for many body wavefunction. This set of many body wavefunction basis is characterize by the particle numbers in the states of $\psi_1, \psi_2\cdots$ as $N_1, N_2, \cdots$. We define the Fock space as formed by all the eigenstates of particle numbe operator $\hat{n}_1, \hat{n}_2\cdots$. The transformation between different basis is through the creation/annihilation operator of each single particle state.

$$\text{Basis: } \Psi_{N_1N_2\cdots}(\xi_1,\xi_2\cdots\xi_N) = \sqrt{\frac{N_1!\cdots N_k!\cdots}{N!}}\ \sum P_E\{\underbrace{\psi_1(\xi_1)\cdots\psi_1(\xi_{N_1})}_{N_1}\}\{\underbrace{\psi_2(\xi_{N_1+1})\cdots}_{N_2}\}\cdots\}$$

N-body wavefunction Ψ can be expanded as

$$\Psi(\xi_1,\xi_2\cdots\xi_N) = \sum_{N_1N_2\cdots} \Psi_{N_1N_2\cdots}(\xi_1\xi_2\cdots\xi_N)\, C(N_1N_2\cdots\cdots).$$

$$\text{where } \quad C(N_1N_2\cdots) = \begin{cases} 0 & \text{if } \sum_i N_i \neq N \\ (\Psi_{N_1N_2\cdots}, \Psi) & \text{if } \sum_i N_i = N. \end{cases}$$

we can define inner product of two wave functions as

$$(\Psi_A . \Psi_B) = \sum_{N_1 N_2 \cdots} C_A^*(N_1, N_2, \cdots) C_B(N_1, N_2 \cdots) .$$

Thus all the theory can be represented by using the $\boxed{\text{particle number representation}}$ in which the Wavefunction is written as $C(N_1, N_2 \cdots)$. The many-particle wavefunction basis defined above $\Psi_{N_1' N_2' \cdots N_k'}$ in this representation is

$$\underbrace{C_{N_1' N_2' \cdots N_k' \cdots}}_{\text{indices of basis}} (\underbrace{N_1 N_2 \cdots}) = \delta_{N_1 N_1'} \delta_{N_2 N_2'} \cdots \cdot$$

$\nwarrow$ arguments of variables

More conveniently, we define the ket-space as

$$C_{N_1' N_2' \cdots N_k' \cdots}(N_1 N_2 \cdots) \longleftrightarrow |N_1' N_2' \cdots \rangle$$

$$\alpha C_{N_1' N_2' \cdots}(N_1 N_2) + \beta C_{N_1'' N_2'' \cdots}(N_1 N_2) \longleftrightarrow \alpha |N_1' N_2' \cdots \rangle + \beta |N_1'' N_2'' \cdots \rangle$$

$$\langle N_1' N_2' \cdots | N_1'' N_2'' \cdots \rangle = \sum_{N_1 N_2} (\delta_{N_1 N_1'} \delta_{N_2 N_2'} \cdots)(\delta_{N_1 N_1''} \delta_{N_2 N_2''} \cdots)$$

$$= \delta_{N_1' N_1''} \delta_{N_2' N_2''} \cdots$$

and $$\sum_{N_1 N_2 \cdots} |N_1 N_2 \cdots \rangle \langle N_1 N_2 \cdots | = 1$$

and $$\underset{\psi}{C}(N_1 N_2 \cdots) = \langle N_1 N_2 \cdots | \psi \rangle ,$$ where ψ is an abitary state vector,

☆ Creation/annihilation operators

particle number operators $\hat{n}_i |N_1 N_2 \cdots \rangle = N_i | N_1 N_2 \cdots \rangle$

$\hat{n}_i^\dagger = n_i, \quad [\hat{n}_i, \hat{n}_j] = 0$

we define operators

$$a_i = \sum_{N_1 N_2 \cdots} \sqrt{N_i}\, | N_1 N_2 \cdots (N_i - 1) \cdots \rangle \langle N_1 N_2 \cdots N_i \cdots |,$$

$$a_i^\dagger = \sum_{N_1 N_2 \cdots} \sqrt{N_i + 1}\, | N_1 N_2 \cdots (N_i + 1) \cdots \rangle \langle N_1 N_2 \cdots N_i \cdots |,$$

$$\Rightarrow \quad \begin{aligned} a_i | N_1 N_2 \cdots N_i \cdots \rangle &= \sqrt{N_i}\, | N_1 N_2 \cdots (N_i - 1) \cdots \rangle \\ a_i^\dagger | N_1 N_2 \cdots N_i \cdots \rangle &= \sqrt{N_i + 1}\, | N_1 N_2 \cdots N_i + 1 \cdots \rangle \end{aligned}$$

check $[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i\, a_j] = [a_i^\dagger, a_j^\dagger] = 0$

define that the vaccum $|0\rangle = |0_1\, 0_2 \cdots 0_N \cdots \rangle \Rightarrow$

$$| N_1 N_2 \cdots \rangle = \frac{(a_1^\dagger)^{N_1}}{\sqrt{N_1 !}} \frac{(a_2^\dagger)^{N_2}}{\sqrt{N_2 !}} \cdots |0\rangle .$$

☆ Field opearator

$$\hat{\psi}(r) = \sum_i \overbrace{\psi_i(r)}^{\text{single particle wavefunction}} a_i$$

$$\hat{\psi}^\dagger(r) = \sum_i \psi_i^*(r)\, a_i^\dagger \rightarrow \text{a parameter}$$

Let's check the physical meaning of $\hat{\psi}^\dagger(r)$, Define $|r'\rangle$ the single particle position eigenstate

$$\langle r' | \hat{\psi}^\dagger(r) | 0 \rangle = \sum_i \langle r' | a_i^\dagger | 0 \rangle \psi_i^*(r)$$

$$= \sum_i \psi_i(r) \psi_i^*(r') = \delta(r' - r)$$ which doesn't depend on the basis.

thus $\psi^\dagger(r)$ means the creation of one particle at the location r, it's the creation operator in the coordinate representation.

$\hat{\psi}^\dagger(r)\hat{\psi}(r)$ is the density operator at location r, and

$$[\hat{\psi}(r)\ \hat{\psi}^\dagger(r')] = \sum_{ij} \psi_i(r)\psi_j^*(r')\,[a_i, a_j^\dagger] = \sum_i \psi_i(r)\psi_i^*(r') = \delta(r-r')$$

$$[\psi(r)\ \psi(r')] = [\psi^\dagger(r), \psi^\dagger(r')] = 0$$

★ transformation of creation / annihilation operators in different basis.

suppose that we define a set of operators $a_i, a_i^\dagger$ associated with basis ψ_i, and a set of operators $b_i, b_i^\dagger$ associated with basis of ϕ_i,

Because the field opearator is independent of basis, i.e.

$$\hat{\psi}(r) = \sum_i \psi_i(r)\, a_i = \sum \phi_i(r)\, b_i$$

$$\Rightarrow a_i = \sum_j \langle \psi_i | \phi_j \rangle b_j , \qquad a_i^\dagger = \sum_j \langle \phi_j | \psi_i \rangle b_j^\dagger$$

for example $\hat{\psi}(r) = \sum_k \frac{1}{\sqrt{V}} e^{ikr} a_k$,

$$a_k = \int dr\, \frac{e^{-ikr}}{\sqrt{V}} \psi(r)$$

★ expression of opearaters / Schrödinger equation

1) Single body operator

$F = \sum_{p=1}^{N} f(p)$ in the first quantization, where f(p) only depends on the variable of the p-th particle.

let us begin with a representation in which f is diagonal,

$f\psi_k = f_k \psi_k$, then

$$\hat{F}\,|N_1 N_2 \cdots\rangle = (N_1 f_1 + N_2 f_2 + \cdots)\,|N_1 N_2 \cdots\rangle = \sum_k f_k \hat{n}_k \,|N_1 N_2 \cdots\rangle$$

$$\Rightarrow \quad \hat{F} = \sum_k f_k \overset{a^\dagger}{a_k} a_k = \sum_k \langle k|f|k\rangle a_k^\dagger a_k$$ in the diagonal basis.

Let us change to a general basis $|\phi_i\rangle$ with associated operators $b_i^\dagger$

$$\Rightarrow a_k = \sum_i \langle k|\phi_i\rangle b_i, \qquad a_k^\dagger = \sum_i \langle \phi_i|k\rangle b_i^\dagger$$

$$\Rightarrow \hat{F} = \sum_{k,i,j} \langle\phi_j|k\rangle\langle k|f|k\rangle\langle k|\phi_i\rangle\, b_j^\dagger b_i = \sum_{ij} \langle\phi_j|f|\phi_i\rangle\, b_j^\dagger b_i$$

thus for a general basis

$$\boxed{\hat{F} = \sum_{ij} \langle i|f|j\rangle\, b_i^\dagger b_j}$$

example: in the coordinate basis

$$\hat{F} = \int dr\, dr'\, \langle r|f|r'\rangle\, \hat{\psi}^\dagger(r)\, \hat{\psi}(r')$$

if the coordinate rep. $\hat{f} = f(r, \nabla_r)$

$$\langle r|f|r'\rangle = \int dx\, \delta(x-r)\, f(x, \nabla_x)\, \delta(x-r') = f(r, \nabla_r)\,\delta(r-r')$$

$$\boxed{\hat{F} = \int dr\, dr' \{f(r, \nabla_r)\,\delta(r-r')\}\, \hat{\psi}^\dagger(r)\, \hat{\psi}(r') = \int dr\, \psi^\dagger(r)\, f(r, \nabla_r)\, \psi(r)}$$

$$H_0 = \sum_k \frac{\hbar^2 k^2}{2m} a_k^\dagger a_k$$ (plane wave)

$$H = \cancel{-t} \sum_{\langle ij\rangle} c_i^\dagger c_j \langle i|h|j\rangle$$ (tight-binding model)

☆ two-body opearaters.

$$G = \frac{1}{2}\sum_{p\neq q}^{N} g(p,q)\,, \quad \text{where } g(p,q) = g(q,p)$$

where p, q are the indices of two particles.

let us consider the special case in which

$g(p,q)$ $\underbrace{\text{can be written as}}_{\text{factorized into product of single body operater}}$ $g(p,q) = u(p)v(q) + v(p)u(q)$

$$\Rightarrow G = \frac{1}{2}\sum_{p\neq q}^{N} g(p,q) = \frac{1}{2}\Big(\sum_{p\neq q}^{N}\big(u(p)v(q)+v(p)u(q)\big)\Big) = \Big(\sum_{p=1}^{N} u\Big)\Big(\sum_{q=1}^{N} v\Big) - \sum_{q=1}^{N}\big(u(q)\cdot v(q)\big)$$

$$\sum_{p=1}^{N} u(p) = \sum_{il} \langle i|u|l\rangle\, a_i^{\dagger} a_l\,, \quad \sum_{q=1}^{N} v(q) = \sum_{km}\langle k|v|m\rangle\, a_k^{\dagger} a_m$$

$$\Rightarrow \Big(\sum_{p=1}^{N} u(p)\Big)\Big(\sum_{q=1}^{N} v(q)\Big) = \sum_{il,km} \langle i|u|l\rangle\langle k|v|m\rangle\, a_i^{\dagger}\underbrace{a_l a_k^{\dagger}}_{\delta_{lk}+a_k^{\dagger}a_l} a_m$$

$$= \sum_{im}\sum_{l}\langle i|u|l\rangle\langle l|v|m\rangle\, a_i^{\dagger} a_m$$

$$+ \sum_{il,km}\langle i|u|l\rangle\langle k|v|m\rangle\, a_i^{\dagger} a_k^{\dagger} a_l a_m$$

$$= \sum_{im}\langle i|uv|m\rangle\, a_i^{\dagger} a_m + \sum_{ilkm} \langle i|u|l\rangle\langle k|v|m\rangle\, a_i^{\dagger} a_k^{\dagger} a_l a_m$$

The first term is just $\sum_{q=1}^{N}(u(q)v(q))$

$$\Rightarrow \hat{G} = \sum_{ilkm}\langle i|u|l\rangle\langle k|v|m\rangle\, a_i^{\dagger} a_k^{\dagger} a_l a_m$$

$$= \sum_{ilkm}\langle k|u|m\rangle\langle i|v|l\rangle\, a_i^{\dagger} a_k^{\dagger} a_l a_m$$

$$= \frac{1}{2}\sum_{ilkm}\langle ik|g|lm\rangle\, a_i^{\dagger} a_k^{\dagger} a_l a_m$$

where $\langle ik|g|lm\rangle$

$$= \int dr_1 dr_2\, \psi_i^{*}(1)\, \psi_k^{*}(2)\, \underbrace{\big(u(1)v(2)+v(1)u(2)\big)}_{g(1,2)}\, \psi_m(2)\,\psi_l(1)$$

generally, speaking. G can be expanded into a set of Us and Vs.

the above expression still valid, ⇒

$$\boxed{\begin{aligned} \hat{G} &= \frac{1}{2} \sum_{ilkm} \langle ik | g | lm \rangle \, a_i^{+} a_k^{+} a_m a_l \\ \langle ik | g | lm \rangle &= \int dr_1 dr_2 \, \psi_i^{*}(1) \psi_k^{*}(2) \, g(1,2) \, \psi_m(2) \psi_l(1) \end{aligned}}$$

or in the coordinate Rep: in terms of field operater

$$\hat{G} = \frac{1}{2} \int dr_1 dr_2 \, \hat{\psi}^{+}(r_1) \hat{\psi}^{+}(r_2) \, g(r_1, r_2) \, \psi(r_2) \psi(r_1)$$

→ momentum space if $g(r_1, r_2) = g(r_1 - r_2)$, we have

$$\underline{\hat{G} = \frac{1}{2V} \sum_{k_1 k_2 q} a_{k_1}^{+} a_{k_2}^{+} a_{k_2 - q} a_{k_1 + q} \; g(q)}, \quad \boxed{g(q) = \int dr \, e^{-iqr} g(r)}$$

⇒ The many-body Hamiltinian ⇒

$$H = \int dr \, \hat{\psi}^{+}(r) \, [T + U] \, \psi(r) + \frac{1}{2} \int dr_1 dr_2 \, \hat{\psi}^{+}(r_1) \psi^{+}(r_2) \, (V(1,2)) \, \psi(r_2) \psi(r_1)$$

quantization of ψ → second quantization.

or $$H = \sum_{ii'} \langle i | T + U | i' \rangle a_i^{+} a_{i'} + \frac{1}{2} \sum_{\substack{ik \\ i'k'}} \langle ik | V | i'k' \rangle a_i^{+} a_k^{+} a_{k'} a_{i'}$$

tight-binding

$$\underline{\langle ik | V | i'k' \rangle = \int dr_1 dr_2 \, \phi_i(1) \phi_k(2) \, V(12) \, \phi_{k'}(2) \phi_{i'}(1)}$$

§4. Second quantization for fermions

Again we define the many-body wavefunction basis with occupation numbers. We give the sequence $\{\psi_i\}$ $i=1,2,3\cdots$, with particle number distribution $N_1, N_2, N_3 \cdots$; N_i can only be 0 or 1.

index of single particle wavefunctions

Pauli-exclusion / Fermi statistics, exchange one pair of particle $\Psi \to -\Psi$

$$\Psi_{N_1 N_2 N_3 \cdots}(\xi_1 \cdots \xi_N) = (-)^{N_\ell N_{\ell-1}} \Psi_{N_1 N_2 \cdots N_\ell N_{\ell-1} N_{\ell+1} \cdots}(\xi_1 \cdots \xi_N)$$

$$= (-)^{N_\ell \sum_{j=1}^{\ell-1} N_j} \Psi_{N_\ell N_1 N_2 \cdots}(\xi_1 \cdots \xi_N)$$ (~~many~~ N-body basis)

Again we can expand any N-body wavefunction

$$\Psi(\xi_1 \cdots \xi_N) = \sum_{N_1 N_2 \cdots} \Psi_{N_1 N_2 \cdots}(\xi_1 \cdots \xi_N) \underline{C(N_1 N_2 \cdots)}$$

wavefunction in the particle number Rep

Aagain we introduce Ket-vector

$$C_{N_1' N_2' \cdots}(N_1, N_2 \cdots) \longleftrightarrow |N_1' N_2' \cdots\rangle$$

index of basis   variable

$$\alpha C_{N_1' N_2'}(N_1 N_2 \cdots) + \beta C_{N_1'' N_2''}(N_1 N_2 \cdots) \longleftrightarrow \alpha |N_1' N_2' \cdots\rangle + \beta |N_1'' N_2'' \cdots\rangle$$

$$|N_1 N_2 \cdot N_{\ell-1} N_\ell \cdots\rangle = (-)^{N_\ell N_{\ell-1}} |N_1 N_2 \cdots N_\ell N_{\ell-1} \cdots\rangle$$

$$= (-)^{N_\ell \sum_{j=1}^{\ell-1} N_j} |N_\ell N_1 N_2 \cdots\rangle$$

$$\sum_{N_1 N_2 \cdots} |N_1 N_2 \cdots\rangle\langle N_1 N_2 \cdots| = 1 \ , \quad C(N_1 N_2 \cdots) = \langle N_1 N_2 \cdots | \Psi \rangle$$

Again, we define particle number operater

$$\hat{n}_i |N_1 \cdots N_i \cdots\rangle = N_i |N_1 \cdots N_i \cdots\rangle$$

and $$\hat{n}_i = \sum_{N_1 N_2 \cdots} N_i |N_1 \cdot N_2 \cdots\rangle\langle N_1 N_2 \cdots| ,$$

$$\hat{n}_i^{\dagger} = n_i, \quad [\hat{n}_i, \hat{n}_{i'}] = 0$$

annihilation / Creation: $$a_i^{\dagger} |N_1 \cdots N_{i-1}\, 0_i\, N_{i+1} \cdots\rangle = (-)^{\sum_{l=1}^{i-1} N_l} |N_1 \cdots N_2\, 1_i\, N_{i+1} \cdots\rangle$$

$$a_i^{\dagger} |N_1 \cdots\cdots 1_i \cdots\rangle = 0$$

$$\Rightarrow a_i^{\dagger} = \sum_{N_1 N_2 \cdots} (-)^{\sum_{l=1}^{i-1} N_l} |N_1 N_2 \cdots 1_i \cdots\rangle\langle N_1 N_2 \cdots 0_i \cdots|$$

$$a_i = \sum_{N_1 N_2 \cdots} (-)^{\sum_{l=1}^{i-1} N_l} |N_1 N_2 \cdots 0_i \cdots\rangle\langle N_1 N_2 \cdots 1_i \cdots|$$

Then $\{a_i, a_j^{\dagger}\} = \delta_{ij}$, $\{a_i, a_i\} = \{a_i^{\dagger}\, a_i^{\dagger}\} = 0$

$$|N_1 N_2 \cdots\rangle = (a_1^{\dagger})^{N_1} (a_2^{\dagger})^{N_2} \cdots |0\rangle$$

$$|N_2 N_1 \cdots\rangle = (a_2^{\dagger})^{N_2} (a_1^{\dagger})^{N_1} \cdots |0\rangle = (-)^{N_1 N_2} |N_1 N_2 \cdots\rangle$$

again we define field operators which are annihilation/creation operators in the coordinate Rep

$$\hat{\psi}(r) = \sum_i \psi(r)\, a_i ; \quad \hat{\psi}^{\dagger}(r) = \sum_i \psi_i^*(r)\, a_i^{\dagger}$$

which satisfy $\{\hat{\psi}(r), \hat{\psi}^{\dagger}(r')\} = \delta(r-r')$, $\{\psi(r), \psi(r')\} = 0$

* operators represented by second quantization

$$F = \sum_{p=1}^{N} f(p) \rightarrow \hat{F} = \sum_{ik} \langle i|f|k\rangle\, a_i^{\dagger} a_k = \int dr\, \hat{\psi}^{\dagger}(r)\, f\, \psi(r)$$

$$G = \sum_{p<q}^{N} g(p,q) \rightarrow \hat{G} = \frac{1}{2} \sum_{iklm} \langle ik|g|lm\rangle\, a_i^{\dagger} a_k^{\dagger}\, a_m\, a_l$$

where $\langle ik|g|lm\rangle = \int d\xi_1 d\xi_2 \; \psi_i^*(\xi_1)\, \psi_j^*(\xi_2)\; g(1,2)\; \psi_l(\xi_1)\, \psi_m(\xi_2)$

$$\rightarrow \hat{G} = \int dr_1 dr_2 \; \psi^\dagger(r_1)\, \psi^\dagger(r_2)\; g(1,2)\; \psi(r_2)\, \psi(r_1)$$

if we have spin $\Rightarrow$ $\hat{G} = \int dr_1 dr_2 \; \psi^\dagger_\sigma(r_1)\, \psi^\dagger_{\sigma'}(r_2)\; g(1,2)\; \psi_{\sigma'}(r_2)\, \psi_\sigma(r_1)$

The many body hamiltonian

$$H = \int dr \; \hat{\psi}^\dagger_\sigma(r)\,(T+U)\,\psi_\sigma(r) + \frac{1}{2}\int dr_1 dr_2 \; \hat{\psi}^\dagger_\sigma(r_1)\hat{\psi}^\dagger_{\sigma'}(r_2)\; V(1,2)\; \hat{\psi}_{\sigma'}(r_2)\hat{\psi}_\sigma(r_1)$$

$$= \sum_{ii'} \langle i|T+U|i'\rangle a_i^\dagger a_{i'} + \frac{1}{2}\sum_{iki'k'} \langle ik|V|i'k'\rangle \, a^\dagger_{i\sigma} a^\dagger_{k\sigma'} a_{k'\sigma'} a_{i'\sigma}$$

§ Examples :

① Evaluation of the Hartree - Fock interaction energy of the state $|G\rangle$ in which the $|k\sigma\rangle$ inside the Fermi sphere (k_F) is occupied.

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

$$|G\rangle = \prod_{k<k_F} a^\dagger_{k\uparrow}\, a^\dagger_{k\downarrow}\, |0\rangle$$

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

Hartree term:
$q=0$

$$V_H = \frac{1}{2V}\sum_{k_1,k_2} V(0) \; \langle G|\, a^\dagger_{k_1\sigma}\, a^\dagger_{k_2\sigma'}\, a_{k_2\sigma'}\, a_{k_1\sigma}\, |G\rangle$$

$$= \frac{1}{2V} \sum_{k_1 k_2} V(0) \langle G | a^{+}_{k_1\sigma} a_{k_1\sigma} a^{+}_{k_2\sigma'} a_{k\sigma'} \mp a^{+}_{k_1\sigma} a_{k_2\sigma'} \delta_{k_1 k_2} \delta_{\sigma\sigma'} | G \rangle$$

$$= \frac{V(0)}{2V}\left[\left(\sum_{k_1} n_{k\sigma}\right)^2 - \sum_{k} (n_{k\sigma})\right] = \frac{1}{2} v(0) \left[Vn^2 - n\right]$$

(This energy in the interacting electron system can be canceled by the positive background charge)

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

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

$$= \frac{-1}{2V} \sum_{k_1 k_2} V(k_1-k_2) \langle G | a^{+}_{k_2\sigma} a_{k_2\sigma} a^{+}_{k_1\sigma} a_{k_1\sigma} | G \rangle = \frac{-1}{2V} \sum_{k_1 k_2} V(k_1-k_2) n_{k_2} n_{k_1} \cdot 2$$

$$= -\frac{1}{V} \cdot V^2 \int \frac{dk_1}{(2\pi)^3} \int \frac{dk_2}{(2\pi)^3} V(k_1-k_2) n_{k_1} n_{k_2} = - V \int \frac{d\vec{k}_1 d\vec{k}_2}{(2\pi)^3} n_{k_1} n_{k_2} V(k_1-k_2)$$

② Cooper pair problem!

Consider that we have a full-filled Fermi sphere with Fermi wavevector k_F. We add two electrons with $(k\uparrow)$ and $(-k\downarrow)$. Neglect that electrons inside the Fermi sphere can be scattered outside the Fermi surface. Aassum attractive interaction betwee these two electrons.

$$H = \sum_{k} \varepsilon_k C^{+}_{k\sigma} C_{k\sigma} - V \sum_{kk'} C^{+}_{k\uparrow} C^{+}_{-k\downarrow} C_{-k\downarrow} C_{k\uparrow} .$$

Solve the spectrum for these two electrons.

interactions cause scattering $(k\uparrow ; -k\downarrow) \longrightarrow (k'\uparrow ; -k\downarrow)$.

the eigenstate should be a linear superposition of these states.

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

where $\alpha(k)$ is the coefficent

$|F\rangle$ the Full-filled Fermi sphere.

$$H|\psi\rangle = \sum_k \alpha(k) \left(\underset{+\,\mathcal{U})}{H_0}\, C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle \right.$$

$$H_0 C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle = \left(\underbrace{C^+_{k\uparrow} C^+_{-k\downarrow} H_0 |F\rangle}_{+\,2\varepsilon_k)} \right. = (2\varepsilon_k + E_0)\, C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle$$

$$\mathcal{U}\, C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle = \mathcal{U} \sum_{k'k''} C^+_{k'\uparrow} C^+_{-k'\downarrow} C^-_{-k''\downarrow} C_{k''\uparrow} C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle$$

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

$$\Rightarrow H|\psi\rangle = \sum_k \alpha(k) \left[2\varepsilon_k + E_0 \right] C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle - \sum_k \overset{\alpha(k)}{\vee}\, \mathcal{U} \sum_{k'} C^+_{k'\uparrow} C^+_{-k'\downarrow} |F\rangle$$

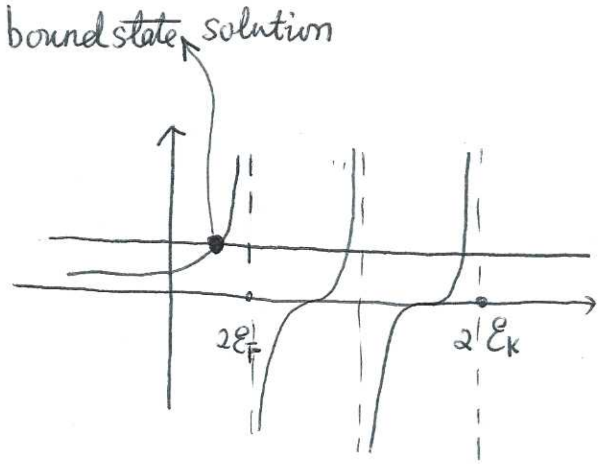
$$= E \sum_k \alpha(k)\, C^+_{k\uparrow} C^+_{-k\downarrow} |F\rangle$$

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

i.e. $(2\varepsilon_k + E_0)\,\alpha(k) - \mathcal{U} \sum_{k'} \alpha(k') = E\,\alpha(k)$

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

$$\Rightarrow \frac{1}{\mathcal{U}} = \sum_k \frac{1}{2\varepsilon_k - (E - E_0)} \Rightarrow +\frac{1}{\mathcal{U}} = \sum_k \frac{1}{-\Delta E + 2\varepsilon_k}$$



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

$$= \frac{N(0)}{2} \ln \frac{2\hbar\omega_D - \Delta E}{-\Delta E}$$

$$\Rightarrow \frac{2}{N(0)U} \simeq \ln \frac{2\hbar\omega_D}{|\Delta E|}$$

$$\boxed{\Delta E = 2\hbar\omega_D \, e^{-\frac{2}{N(0)U}}}$$

Cooper pair binding energy!