

Supplementary material: an introduction to second quantization

§1 Harmonic oscillator (warm up)

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

then $a = \frac{1}{\sqrt{2}} \left[\frac{x}{l} + i \frac{p}{\hbar l} \right], \quad a^\dagger = \frac{1}{\sqrt{2}} \left[\frac{x}{l} - i \frac{p}{\hbar l} \right]$

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

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

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

§2 Bose statistics and Fermi statistics

Suppose we have a set of complete and normalized basis of single particle wavefunctions, we can use them to construct the N -body wavefunction.

$\underbrace{\psi_1, \psi_2, \dots}_{N_1}$

For bosons, we first consider

$$\underbrace{\psi_1(x_1) \cdots \psi_1(x_{n_1})}_{N_1} \quad \underbrace{\psi_2(x_{n_1+1}) \cdots \psi_2(x_{n_1+n_2})}_{N_2} \cdots \quad \underbrace{\{\psi_k(1) \cdots \psi_k(x_N)\}}_{N_k}$$

and symmetrize it

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

For fermions, each state can only support one particle

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

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

S3: 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 many body wavefunction. This set of many body wavefunction basis is characterized by the particle numbers in the states of $\psi_1, \psi_2 \dots$ as N_1, N_2, \dots . We define the Fock space as formed by all the eigenstates of particle number operator $\hat{n}_1, \hat{n}_2, \dots$. The transformation between different basis is through the creation/annihilation operator of each single particle state.

Basis: $\Psi_{N_1 N_2 \dots}(\xi_1, \xi_2 \dots \xi_N) = \sqrt{\frac{N_1! \cdots N_k!}{N!}} \sum_P \underbrace{P \{ \psi_1(\xi_1) \cdots \psi_i(\xi_{N_i}) \}}_{N_1} \underbrace{\{ \psi_2(\xi_{N_i+1}) \cdots \} \cdots}_{N_2} \dots$

N-body wavefunction Ψ can be expanded as

$$\Psi(\xi_1, \xi_2 \dots \xi_N) = \sum_{N_1 N_2 \dots} \Psi_{N_1 N_2 \dots}(\xi_1, \xi_2 \dots \xi_N) C(N_1 N_2 \dots).$$

where $C(N_1 N_2 \dots) = \begin{cases} 0 & \text{if } \sum_i N_i \neq N \\ (\Psi_{N_1 N_2 \dots}, \Psi) & \text{if } \sum_i N_i = N. \end{cases}$

we can define inner product of two wave functions as

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

Thus all the theory can be represented by using the particle number representation in which the Wavefunction is written as $C(N_1, N_2, \dots)$. The many-particle wavefunction basis defined above $\Psi_{N'_1 N'_2 \dots N'_k}$ in this representation is

$$\underbrace{C_{N'_1 N'_2 \dots N'_k}}_{\text{indices of basis}} \underbrace{(N_1, N_2, \dots)}_{\text{arguments of variables}} = \delta_{N_1, N'_1} \delta_{N_2, N'_2} \dots.$$

More conveniently, we define the ket-space as

$$C_{N'_1 N'_2 \dots N'_k} (N_1, N_2, \dots) \longleftrightarrow |N'_1 N'_2 \dots\rangle$$

$$\alpha C_{N'_1 N'_2} (N_1, N_2) + \beta C_{N''_1 N''_2} (N_1, N_2) \leftrightarrow \alpha |N'_1 N'_2 \dots\rangle + \beta |N''_1 N''_2 \dots\rangle$$

$$\begin{aligned} \langle N'_1 N'_2 \dots | N''_1 N''_2 \dots \rangle &= \sum_{N_1, N_2} (\delta_{N_1, N'_1} \delta_{N_2, N'_2} \dots) (\delta_{N_1, N''_1} \delta_{N_2, N''_2} \dots) \\ &= \delta_{N'_1 N''_1} \delta_{N'_2 N''_2} \dots \end{aligned}$$

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

and $C(N_1, N_2, \dots) = \langle N_1, N_2, \dots | \psi \rangle$, where ψ is an arbitrary state vector,

* Creation/annihilation operators

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

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

we define operators

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

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

$$\Rightarrow a_i |N_1 N_2 \dots N_i \dots\rangle = \sqrt{N_i} |N_1 N_2 \dots (N_i-1) \dots\rangle$$

$$a_i^\dagger |N_1 N_2 \dots N_i \dots\rangle = \sqrt{N_i+1} |N_1 N_2 \dots N_i+1 \dots\rangle$$

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

define that the vacuum $|0\rangle = |0, 0_2 \dots 0_N\rangle \Rightarrow$

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

* Field operator

single particle wave function

$$\hat{\psi}(r) = \sum_i \underbrace{\psi_i(r)}_{\text{single particle wave function}} a_i$$

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

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

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

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

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thus $\hat{\psi}(r)$ 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

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

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

* 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 operator is independent of basis, i.e.

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

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

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 operators / 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,

$$f\psi_k = f_k \psi_k, \text{ then}$$

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

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

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

$$\Rightarrow \hat{a}_k = \sum_i \langle k | \phi_i \rangle b_i, \quad \hat{a}_k^\dagger = \sum_i \langle \phi_i | k \rangle b_i^\dagger$$

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

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. $\hat{f} = f(r, \nabla_r)$

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

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

$$H_0 = \sum_k \frac{\hbar^2 k^2}{2m} \hat{a}_k^\dagger \hat{a}_k \quad (\text{plane wave})$$

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

* two-body operators

$$G = \frac{1}{2} \sum_{p \neq q}^N g(p, q), \text{ where } g(p, q) = g(q, p) \quad \text{where } p, q \text{ are the indices of two particles.}$$

Let us consider the special case in which

$$g(p, q) \text{ can be written as } g(p, q) = u(p)v(q) + v(p)u(q)$$

factorized into product of single body operator

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

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

$$\Rightarrow \left(\sum_{p=1}^N u(p) \right) \left(\sum_{q=1}^N v(q) \right) = \sum_{i\ell, km} \langle i|u|\ell\rangle \langle k|v|m\rangle a_i^\dagger a_\ell a_k^\dagger a_m$$

$\approx a_{ik} + a_{k\ell}^\dagger a_\ell$

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

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

$$= \sum_{im} \langle i|uv|m\rangle a_i^\dagger a_m + \sum_{il, km} \langle i|u|\ell\rangle \langle k|v|m\rangle a_i^\dagger a_k^\dagger a_\ell a_m$$

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

$$\Rightarrow \hat{G} = \sum_{il, km} \langle i|u|\ell\rangle \langle k|v|m\rangle a_i^\dagger a_k^\dagger a_\ell a_m$$

$$= \sum_{il, km} \langle k|u|m\rangle \langle i|v|\ell\rangle a_i^\dagger a_k^\dagger a_\ell a_m$$

$$= \frac{1}{2} \sum_{il, km} \langle ikl|g|lm\rangle a_i^\dagger a_k^\dagger a_\ell a_m$$

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

$$= \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_i^*(1) \otimes \psi_k^*(2)$$

$$\frac{(u(1)v(2) + v(1)u(2))}{g(i, 2)} \psi_m(2) \psi_l(1)$$

generally, speaking. G can be expanded into a set of U_s and V_s .

the above expression still valid, \Rightarrow

$$\hat{G} = \frac{1}{2} \sum_{ilm} \langle ikl | g | lm \rangle a_i^+ a_k^+ a_m a_l$$

$$\langle ikl | g | lm \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \psi_i^{*(1)} \psi_k^{*(2)} g(1,2) \psi_m^{(2)} \psi_l^{(1)}$$

or in the coordinate Rep: in terms of field operator

$$\hat{G} = \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^t(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) g(\mathbf{r}_1, \mathbf{r}_2) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1)$$

\rightarrow momentum space if $g(\mathbf{r}_1 + \mathbf{r}_2) = g(\mathbf{r}_1 - \mathbf{r}_2)$, we have

$$\hat{G} = \frac{1}{2V} \sum_{k_1 k_2 q} a_{k_1}^+ a_{k_2}^+ a_{k_2-q} a_{k_1+q} g(q), \quad g(q) = \int d\mathbf{r} e^{-iq\mathbf{r}} g(\mathbf{r})$$

\Rightarrow The many-body Hamiltonian \Rightarrow

$$H = \int d\mathbf{r} \hat{\psi}^\dagger(\mathbf{r}) [T + U] \psi(\mathbf{r}) + \frac{1}{2} \int d\mathbf{r}_1 d\mathbf{r}_2 \hat{\psi}^\dagger(\mathbf{r}_1) \hat{\psi}^\dagger(\mathbf{r}_2) (V(1,2)) \psi(\mathbf{r}_2) \psi(\mathbf{r}_1)$$

quantization of $\psi \rightarrow$ second quantization.

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

tight-binding

$$\langle ikl | V | i'k' \rangle = \int d\mathbf{r}_1 d\mathbf{r}_2 \phi_i^{(1)} \phi_k^{(2)} V(1,2) \phi_{k'}^{(2)} \phi_{i'}^{(1)}$$

§4. Second quantization for fermions

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

$\downarrow \swarrow$
index of single particle wavefunctions

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

$$\begin{aligned}\Psi_{N_1 N_2 N_3 \dots} (\xi_1 \dots \xi_N) &= (-)^{N_e N_{e+1}} \bar{\Psi}_{N_1 N_2 \dots N_e N_{e+1} N_{e+2} \dots} (\xi_1 \dots \xi_N) \\ &= (-)^{N_e} \sum_{j=1}^{e-1} N_j \bar{\Psi}_{N_e N_1 N_2 \dots} (\xi_1 \dots \xi_N) \quad (\text{only } N\text{-body basis})\end{aligned}$$

Again we can expand any ~~an~~ N -body wavefunction

$$\Psi (\xi_1 \dots \xi_N) = \sum_{N_1 N_2 \dots} \bar{\Psi}_{N_1 N_2 \dots} (\xi_1 \dots \xi_N) C(N_1 N_2 \dots)$$

wavefunction in the
particle number Rep

Again we introduce Ket-vector

$$C_{N'_1 N'_2 \dots} (N_1 N_2 \dots) \longleftrightarrow |N'_1 N'_2 \dots\rangle$$

\downarrow
index of basis variable

$$\alpha C_{N'_1 N'_2} (N_1 N_2 \dots) + \beta C_{N''_1 N''_2} (N_1 N_2 \dots) \leftrightarrow \alpha |N'_1 N'_2 \dots\rangle + \beta |N''_1 N''_2 \dots\rangle$$

$$|N_1 N_2 \dots N_{e-1} N_e \dots\rangle = (-)^{N_e N_{e+1}} |N_1 N_2 \dots N_e N_{e+1} \dots\rangle$$

$$= (-)^{N_e} \sum_{j=1}^{e-1} N_j |N_e N_1 N_2 \dots \dots\rangle$$

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

Again, we define particle number operator

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

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

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

annihilation / creation : $a_i^\dagger |N_1 \dots N_{i-1} 0_i N_{i+1} \dots\rangle = (-)^{\sum_{\ell=1}^{i-1} N_\ell} |N_1 \dots N_2 \dots l_i N_{i+1} \dots\rangle$

$$a_i^\dagger |N_1 \dots \dots l_i \dots\rangle = 0$$

$$\Rightarrow a_i^\dagger = \sum_{N_1 N_2 \dots} (-)^{\sum_{\ell=1}^{i-1} N_\ell} |N_1 N_2 \dots l_i \dots\rangle \langle N_1 N_2 \dots 0_i \dots|$$

$$a_i = \sum_{N_1 N_2 \dots} (-)^{\sum_{\ell=1}^{i-1} N_\ell} |N_1 N_2 \dots 0_i \dots\rangle \langle N_1 N_2 \dots l_i \dots|$$

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

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

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

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

* operators represented by second quantization

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

$$G = \sum_{p < q} g(p, q) \rightarrow \hat{G} = \frac{1}{2} \sum_{i \neq k \neq m} \langle i k | g | l m \rangle a_i^\dagger a_k^\dagger a_{m \neq l} a_l$$

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where $\langle ik|g|lm\rangle = \int d\zeta_1 d\zeta_2 \psi_i^*(\zeta_1) \psi_j^*(\zeta_2) g(1,2) \psi_l(\zeta_1) \psi_m(\zeta_2)$

$$\rightarrow \hat{G} = \int dr_1 dr_2 \psi_{\sigma}^*(r_1) \psi_{\sigma'}^*(r_2) g(1,2) \psi_{\sigma'}(r_2) \psi_{\sigma}(r_1)$$

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

The many body hamiltonian

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

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

§ 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.

$$V = \frac{1}{2V} \sum_{k_1 k_2 q} V(q) a_{k_1 q \sigma}^{\dagger} a_{k_2 q \sigma}^{\dagger} a_{k_2 \sigma} a_{k_1 \sigma}$$

$$|G\rangle = \prod_{k < k_F} a_{k\uparrow}^{\dagger} a_{k\downarrow}^{\dagger} |0\rangle$$

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

Hartree term:

$$q=0 \quad V_H = \frac{1}{2V} \sum_{k_1 k_2} V(0) \langle G | a_{k_1 \sigma}^{\dagger} a_{k_2 \sigma}^{\dagger} a_{k_2 \sigma} a_{k_1 \sigma} | G \rangle$$

$$\begin{aligned}
 &= \frac{1}{2V} \sum_{k_1, k_2} V(0) \langle G | a_{k_1\sigma}^+ a_{k_1\sigma} a_{k_2\sigma}^+ a_{k_2\sigma} | a_{k_1\sigma}^+ a_{k_2\sigma} \delta_{k_1 k_2} \delta_{\sigma\sigma'} | G \rangle \\
 &= \frac{V(0)}{2V} \left[\left(\sum_k n_{k\sigma} \right)^2 - \sum_k (n_{k\sigma}) \right] = \frac{-1}{2} V(0) [Vn^2 - n]
 \end{aligned}$$

(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 $k_1 \neq k_2$

$$\begin{aligned}
 V_{\text{Fock}} &= \frac{1}{2V} \sum_{k_1 k_2} V(k_1 - k_2) \langle G | a_{k_2\sigma}^+ a_{k_1\sigma}^+ a_{k_2\sigma} a_{k_1\sigma} | G \rangle \\
 &= \frac{-1}{2V} \sum_{k_1 k_2} V(k_1 - k_2) \langle G | a_{k_2\sigma}^+ a_{k_2\sigma} a_{k_1\sigma}^+ a_{k_1\sigma} | G \rangle = \frac{-1}{2V} \sum_{k_1 k_2} V(k_1 - k_2) n_{k_2} n_{k_1} \omega \\
 &= -\frac{1}{V} \cdot V^2 \int \frac{dk_1}{(2\pi)^3} \int \frac{dk_2}{(2\pi)^3} V(k_1 - k_2) n_{k_1} n_{k_2} = -V \int \frac{d\vec{k}_1 d\vec{k}_2}{(2\pi)^3} n_{\vec{k}_1} n_{\vec{k}_2} V(\vec{k}_1 - \vec{k}_2)
 \end{aligned}$$

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.
Assume attractive interaction between these two electrons.

$$H = \sum_k E_k C_{k\sigma}^+ C_{k\sigma} - V \sum_{kk'} C_{k\uparrow}^+ C_{k\downarrow}^+ C_{k'\downarrow} C_{k'\uparrow}$$

Solve the spectrum for these two electrons.

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

the eigenstate should be a linear superposition of these states.

$$|\psi\rangle = \sum_k \alpha(k) C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle \quad \text{where } \alpha(k) \text{ is the coefficient}$$

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

$$H|\psi\rangle = \sum_k \alpha(k) (H_0 C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle + U)$$

$$H_0 C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle = (C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger H_0 |F\rangle - (2\epsilon_k + E_0) C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle)$$

$$U C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle = U \sum_{k''} C_{k'\uparrow}^\dagger C_{k''\downarrow}^\dagger C_{k''\downarrow}^\dagger C_{k'\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle$$

$$= U \sum_{k'k''} \delta(k, k'') C_{k'\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle = U \sum_{k'} C_{k'\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle$$

$$\Rightarrow H|\psi\rangle = \sum_k \alpha(k) [2\epsilon_k + E_0] C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle - \sum_k U \sum_{k'} \underbrace{\alpha(k)}_{\alpha(k')} C_{k'\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle$$

$$= E \sum_k \alpha(k) C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle$$

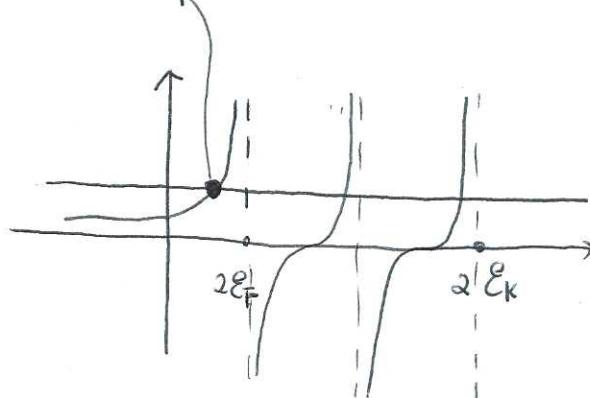
$$\Rightarrow \sum_k \left[(2\epsilon_k + E_0) - U \sum_{k'} \alpha(k') \right] C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle = E \sum_k \alpha(k) C_{k\uparrow}^\dagger C_{-k\downarrow}^\dagger |F\rangle$$

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

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

$$\Rightarrow \frac{1}{U} = \sum_k \frac{1}{2\epsilon_k - (E - E_0)} \Rightarrow \frac{1}{U} = \sum_k \frac{1}{-4E + 2\epsilon_k}$$

bound state solution



Cooper pair binding
energy!

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

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

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

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