Exercises on second quantization : solutions

1 - Starters

1. $\langle 0 | c_\alpha c_\beta c^+_\alpha c^+_\beta | 0 \rangle$ $\qquad \alpha \neq \beta$

1st method: $\langle 0 | c_\alpha c_\beta c^+_\alpha c^+_\beta | 0 \rangle = \underset{F}{\overset{B}{\pm}} \langle 0 | c_\beta c_\alpha (c^+_\alpha c^+_\beta | 0 \rangle)$

$|\Psi\rangle = c^+_\alpha c^+_\beta |0\rangle$

$$\langle 0 | c_\alpha c_\beta c^+_\alpha c^+_\beta | 0 \rangle = \pm \langle \Psi | \Psi \rangle = \underset{F}{\overset{B}{\pm}} 1 \quad (|\Psi\rangle \text{ is normalized})$$

→ **2nd method:**

F: $\langle 0 | c_\alpha \underbrace{c_\beta c^+_\alpha}_{\leftrightarrow} c^+_\beta | 0 \rangle = - \langle 0 | c_\alpha c^+_\alpha c_\beta c^+_\beta | 0 \rangle$, for $\{c_\beta, c^+_\alpha\} = 0$ if $\alpha \neq \beta$

$$= - \langle 0 | c_\alpha c^+_\alpha (\mathbb{1} - \underbrace{c^+_\beta c_\beta) | 0 \rangle}_{= 0 \text{ (null vector)}}, \text{ for } \{c_\alpha, c^+_\alpha\} = \mathbb{1}$$

$$= - \langle 0 | c_\alpha c^+_\alpha | 0 \rangle$$

$$= - \langle 0 | \mathbb{1} - \underbrace{c^+_\alpha c_\alpha | 0 \rangle}_{= 0} = -1$$

B: same thing with + signs. : +1

2. $\hat{h} = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}} |\vec{k}, \sigma\rangle \langle \vec{k}, \sigma|$, $\quad k_\nu = \frac{2\pi}{L_\nu} n_\nu$, $n_\nu \in \mathbb{Z}$, $\nu = x, y, z$

$\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$, $\langle \vec{r} | \vec{k} \rangle = \frac{e^{i \vec{k} \cdot \vec{r}}}{\sqrt{V}}$ $\qquad \sigma = \uparrow, \downarrow$ (spin)

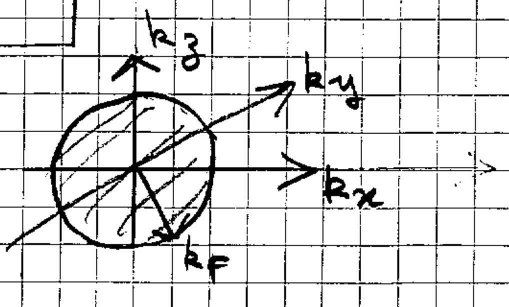
$V = L_x L_y L_z$

Lecture ⇒ $\boxed{\hat{H}_0 = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}} \, c^+_{\vec{k}, \sigma} c_{\vec{k}, \sigma}}$

(a) Fermi Sea (or Fermi Sphere!). Fill all the 1-particle states with increasing 1-particle energy $\varepsilon_{\vec{k}}$:

$$\boxed{|FS\rangle = \prod_{|\vec{k}| < k_F} c^+_{\vec{k}\uparrow} c^+_{\vec{k}\downarrow} | 0 \rangle}$$

The wave-vectors of the occupied 1-part. states lie inside a sphere of radius k_F, the Fermi wave-vector



(b) $\langle \hat{n}_{\vec{k}\sigma} \rangle = \langle FS| c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} |FS\rangle$ ②

1st case: $|\vec{k}| > k_F$; the 1-particle state $|\vec{k},\sigma\rangle$ is unoccupied in $|FS\rangle$, therefore $c_{\vec{k}\sigma}|FS\rangle = 0$ hence $\langle FS| c^+_{\vec{k}\sigma} \underbrace{c_{\vec{k}\sigma}|F\rangle}_{=0} = 0 = \langle \hat{n}_{\vec{k}\sigma} \rangle$

2nd case: $|\vec{k}| < k_F$. We have

$$|FS\rangle = c^+_{\vec{k}_1\uparrow} c^+_{\vec{k}_1\downarrow} \cdots c^+_{\vec{k}_i\uparrow} c^+_{\vec{k}_i\downarrow} \quad c^+_{\vec{k}\uparrow} c^+_{\vec{k}\downarrow} \; c^+_{\vec{k}_{i+1}\uparrow} c^+_{\vec{k}_{i+1}\downarrow} \cdots |0\rangle$$

$\hat{n}_{\vec{k}\uparrow} = c^+_{\vec{k}\uparrow} c_{\vec{k}\uparrow}$ commute with all the first i^{th} pairs (why?), so we have:

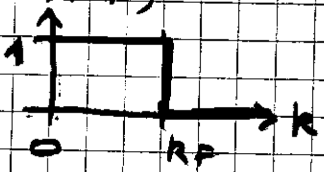
$$\hat{n}_{\vec{k}\uparrow}|FS\rangle = c^+_{\vec{k}_1\uparrow} c^+_{\vec{k}_1\downarrow} \cdots c^+_{\vec{k}_i\uparrow} c^+_{\vec{k}_i\downarrow} \Big(\underbrace{c^+_{\vec{k}\uparrow} c_{\vec{k}\uparrow} c^+_{\vec{k}\uparrow}}_{= c^+_{k\uparrow} - \underbrace{(c^+_{k\uparrow})^2}_{=0} c_{k\uparrow}} \Big) \cdots |0\rangle$$

$$= |FS\rangle$$

Same thing for $\sigma = \downarrow$.

Therefore: $\langle FS| \hat{n}_{\vec{k}\sigma} |FS\rangle = 1$ if $|\vec{k}| < k_F$

Conclusion: $\langle FS| \hat{n}_{\vec{k}\sigma} |FS\rangle = \Theta(k_F - |\vec{k}|)$



$$E_0 = \langle FS| \hat{H}_0 |FS\rangle = \sum_{k\sigma} \varepsilon_k \langle FS| \hat{n}_{k\sigma} |FS\rangle$$

$$= \sum_{k\sigma} \varepsilon_k \, \Theta(k_F - |\vec{k}|)$$

$V \to \infty$: $\sum_k \to V \int \frac{d^3\vec{k}}{(2\pi)^3}$ (3D)

$$\frac{E_0}{V} = \underset{\text{spin}}{2} \int_{|\vec{k}|<k_F} \frac{d^3\vec{k}}{(2\pi)^3} \frac{\hbar^2 k^2}{2m}$$

$$= 2 \, \frac{\overset{\text{angles}}{(4\pi)}}{(2\pi)^3} \frac{\hbar^2}{2m} \int_0^{k_F} dk \, k^4$$

$$\boxed{\frac{E_0}{V} = \frac{1}{10\pi^2} \frac{\hbar^2}{m} k_F^5}$$

③

$$N = \sum_{|\vec{k}| < k_F} 1 \underset{V \to \infty}{\overset{\uparrow}{=}} \overset{\swarrow \text{spin}}{2}\, V \int_{k<k_F} \frac{d^3\vec{k}}{(2\pi)^3}$$

$$= 2\, V \frac{(4\pi)^{\swarrow \text{angles}}}{(2\pi)^3} \int_0^{k_F} dk\, k^2$$

$$\boxed{\frac{N}{V} = \frac{k_F^3}{3\pi^2}}$$

3. $c^+_\alpha |\{n_\beta\}\rangle = c^+_\alpha |n_1\, n_2 - - - - n_\alpha - - - n_N\rangle$

$n_\beta = 0$ or 1

By convention, we order the creation operators in the definition of a Fock state $|n_1\, n_2 - - n_\alpha - n_N\rangle$, from left to right. For example if the 1-part states $|1\rangle$ and $|2\rangle$ are occupied, we write $|\overset{1}{1}\ \overset{2}{1}\rangle \equiv c^+_1\, c^+_2\, |0\rangle$.

If by definition, we write $(c^+)^0 \equiv 1$, we can write:

$$|n_1 n_2 - - n_N\rangle = (\underset{\uparrow \text{operator}}{c^+_1})^{n_1 \leftarrow \text{occupation number}} (c^+_2)^{n_2} - - \quad (c^+_N)^{n_N} |0\rangle$$

Hence we have:

$$c^+_\alpha |\{n_\beta\}\rangle = c^+_\alpha \ (c^+_1)^{n_1} (c^+_2)^{n_2} \cdots (c^+_\alpha)^{n_\alpha} - (c^+_N)^{n_N} |0\rangle$$

It is easy to see that c^+_α anticommute with $(c^+_\beta)^{n_\beta}$ if $n_\beta = 1$ and commute ($(c^+_\beta)^{n_\beta} = 1\!\!1$!) if $n_\beta = 0$

Therefore $c^+_\alpha\, (c^+_\beta)^{n_\beta} = (-1)^{n_\beta} (c^+_\beta)^{n_\beta}\, c^+_\alpha$

Thus we have:

$$c^+_\alpha |\{n_\beta\}\rangle = (-1)^{n_1 + n_2 - - n_{\alpha-1}} (c^+_1)^{n_1} - - - c^+_\alpha (c^+_\alpha)^{n_\alpha} - - - |0\rangle$$

if $n_\alpha = 1$: $c^+_\alpha\, c^+_\alpha = 0$

if $n_\alpha = 0$: we recover the Fock state with $n_\alpha = 1$

$$\boxed{\underline{\text{Conclusion}}: c^+_\alpha |\{n_\beta\}\rangle = \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta} |n_1 - - \overset{\alpha}{1} \ n_N\rangle, & n_\alpha = 0 \\ 0 & , n_\alpha = 1 \end{cases}}$$

In the same way, we find:

$$\boxed{c_\alpha|\{n_\beta\}\rangle = \begin{cases} 0 & \text{if } n_\alpha = 0 \\ (-1)^{(\sum_{\beta<\alpha} n_\beta)} |n_1 n_2 \cdots \overset{\alpha}{0} \cdots n_N\rangle, & \text{if } n_\alpha = 1 \end{cases}}$$

4. $c^+_\beta = \sum_\alpha U_{\beta\alpha} c^+_\alpha$, hence $c_\beta = \sum_\alpha (U_{\beta\alpha})^* c_\alpha$

F: $\{c_\beta, c_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} U_{\beta'\alpha'} \{c_\alpha, c_{\alpha'}\}$ (1)

or $\{c_\beta, c^+_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \{c_\alpha, c^+_{\alpha'}\}$ (2)

- If $\{c_\beta, c^+_{\beta'}\} = \delta_{\beta\beta'}$ and $\{c_\alpha, c^+_{\alpha'}\} = \delta_{\alpha\alpha'}$,

from (2):

$$\delta_{\beta\beta'} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \delta_{\alpha\alpha'}$$
$$= \sum_\alpha U_{\beta\alpha} \underbrace{(U_{\beta'\alpha})^*}_{\equiv U^+_{\alpha\beta'}} = \sum_\alpha U_{\beta\alpha} U^+_{\alpha\beta'}$$
$$= (UU^+)_{\beta\beta'}$$

Therefore $UU^+ = \mathbb{1}$.

- If U is unitary and $\{c_\alpha, c_{\alpha'}\} = 0$, $\{c_\alpha, c^+_{\alpha'}\} = \delta_{\alpha\alpha'}$

From (1): $\{c_\beta, c_{\beta'}\} = \sum_{\alpha\alpha'} U\,U \times 0 = 0$

From (2): $\{c_\beta, c^+_{\beta'}\} = \sum_{\alpha\alpha'} U_{\beta\alpha} (U_{\beta'\alpha'})^* \delta_{\alpha\alpha'}$

$$= \sum_\alpha U_{\beta\alpha} \underbrace{(U_{\beta'\alpha})^*}_{\equiv U^+_{\alpha\beta'}} = (UU^+)_{\beta\beta'}$$
$$= \delta_{\beta\beta'}$$

Therefore we recover the canonical commutation relation for the operators in the new basis.

B: same thing

- $U_{\beta\alpha} = \langle\beta|\alpha\rangle$, $(U^+)_{\alpha\beta} \equiv (U_{\beta\alpha})^* = (\langle\beta|\alpha\rangle)^* = \langle\alpha|\beta\rangle$

$(U^+U)_{\alpha\alpha'} = \sum_\beta (U^+)_{\alpha\beta} U_{\beta\alpha'}$

$$= \sum_\beta \langle \alpha | \beta \rangle \langle \beta | \alpha' \rangle = \langle \alpha | \underbrace{\left(\sum_\beta | \beta \rangle \langle \beta | \right)}_{= \mathbb{1}} | \alpha' \rangle$$

$$= \langle \alpha | \alpha' \rangle = \delta_{\alpha \alpha'}$$

Therefore U is unitary.

$$\sum_\beta c^+_\beta c_\beta = \sum_\beta \left(\sum_{\alpha_1} U_{\beta \alpha_1} c^+_{\alpha_1} \right) \left(\sum_{\alpha_2} (U_{\beta \alpha_2})^* c_{\alpha_2} \right)$$

$$= \sum_{\alpha_1 \alpha_2} c^+_{\alpha_1} \left(\sum_\beta U_{\beta \alpha_1} \underbrace{(U_{\beta \alpha_2})^*}_{U^+_{\alpha_2 \beta}} \right) c_{\alpha_2}$$

$$= \sum_{\alpha_1 \alpha_2} c^+_{\alpha_1} \underbrace{\left(\sum_\beta U^+_{\alpha_2 \beta} U_{\beta \alpha_1} \right)}_{(U^+ U)_{\alpha_2 \alpha_1} = \delta_{\alpha_1 \alpha_2}} c_{\alpha_2}$$

$$= \sum_{\alpha_1} c^+_{\alpha_1} c_{\alpha_1} .$$

$\hat{N}$ has the same expression in the two basis.

5. We check that, if $|n_1 n_2 \dots \rangle = \prod_i \frac{(b^+_i)^{n_i}}{\sqrt{n_i!}} |0\rangle$, we have:

i) $b^+_i | \dots n_i \dots \rangle = \sqrt{n_i + 1} \, | \dots n_i + 1 \dots \rangle$

ii) $b_i | \dots n_i \dots \rangle = \sqrt{n_i} \, | \quad n_i - 1 \dots \rangle$

<u>i)</u> $b^+_i | n_1 n_2 \dots \rangle$: b^+_i <u>commutes</u> with the $(b^+_j)^{n_j}$. Hence:

$$b^+_i | n_1 n_2 \dots \rangle = \frac{(b^+_1)^{n_1}}{\sqrt{n_1!}} \dots \underbrace{b^+_i \frac{(b^+_i)^{n_i}}{\sqrt{n_i!}}} \frac{(b^+_{i+1})^{n_{i+1}}}{\sqrt{}} \dots |0\rangle$$

$$= \frac{(b^+_i)^{n_i+1}}{\sqrt{(n_i+1)!}} \times \sqrt{n_i + 1}$$

$$= \sqrt{n_i+1} \, | n_1 n_2 \dots \rangle$$

ii) b_i <u>commutes</u> with all the $(b^+_j)^{n_j}$ if $j \neq i$.
Moreover, all the $(b^+_j)^{n_j}$'s commute, and we place $(b^+_i)^{n_i}$ at the rightmost place.

$$b_i | n_1 n_2 \dots \rangle = \frac{(b^+_1)^{n_1}}{\sqrt{n_1!}} \dots b_i \frac{(b^+_i)^{n_i}}{\sqrt{n_i!}} |0\rangle$$

using : $bb^+ = 1 + b^+b$, we easily find :

$$b(b^+)^n = \underbrace{bb^+}_{1+b^+b}(b^+)^{n-1} = (b^+)^{n-1} + b^+\underbrace{b(b^+)^{n-1}}_{(b^+)^{n-2}+b^+b(b^+)^{n}}$$

$$= 2(b^+)^{n-1} + (b^+)^2\, b(b^+)^{n-2}$$

$$\vdots$$

$$= n(b^+)^{n-1} + (b^+)^n\, b$$

Therefore: $b_i|n_1 n_2 \dots\rangle = \frac{(b^+_1)^{n_1}}{\sqrt{n_1!}} \dots \frac{1}{\sqrt{n_i!}}\left(n_i(b^+_i)^{n_i-1} + (b^+_i)^{n_i}\underbrace{b_i)|0\rangle}_{=0}\right.$

$$= \sqrt{n_i}\,\frac{(b^+_1)^{n_1}}{\sqrt{n_1!}} \dots \frac{(b^+_i)^{n_i-1}}{\sqrt{(n_i-1)!}}|0\rangle$$

$$= \sqrt{n_i}\,|n_1 \dots n_i - 1 \dots\rangle$$

6. $[\hat{H}_0, \hat{N}] = \sum_{\substack{k_1 k_2\\ \sigma_1 \sigma_2}} \varepsilon_{k_1} [c^+_{k_1\sigma_1}c_{k_1\sigma_1}, c^+_{k_2\sigma_2}c_{k_2\sigma_2}]$

- if $(\underbrace{k_1\sigma_1}_{\equiv 1}) \neq (\underbrace{k_2\sigma_2}_{\equiv 2})$, $[c^+_1c_1, c^+_2c_2] = c^+_1[c_1, c^+_2c_2] + [c^+_1, c^+_2c_2]c_1$

  $[c_1, c^+_2c_2] = \underbrace{c_1c^+_2}_{-c^+_2c_1}c_2 - c^+_2c_2c_1 = (-1)^2c^+_2c_2c_1 - c^+_2c_2c_1$ $= 0$

  and in the same way $[c^+_1, c^+_2c_2] = 0$

  Therefore $[c^+_1c_1, c^+_2c_2] = 0$

- if $(k_1\sigma_1) = (k_2\sigma_2)$, we have obviously $[\hat{n}_1, \hat{n}_1] = 0$

Therefore $[\hat{H}_0, \hat{N}] = 0$

From Quantum Mechanics, if a system of hamiltonian $\hat{H}_0$ commutes with an observable $\hat{O}$, this means $\hat{O}$ <u>is conserved</u>. Here, we find that for a system of free fermions (hamiltonian H_0), the total particle number is conserved, which is obvious!

Interactions do not change the total particle number therefore we also have $[\hat{H}_{int}, \hat{N}] = 0$

7. Lecture: field operator

$$\psi(\vec r) = \sum_\alpha \underbrace{\varphi_\alpha(\vec r)}_{\langle \vec r | \alpha \rangle} c_\alpha$$ for $\{|\alpha\rangle\}$ orthonorml 1-part.-ba

e.g.: $$\psi(\vec r) = \sum_{\vec k} \frac{e^{i\vec k\cdot\vec r}}{\sqrt V} c_{\vec k}$$

Inverse: $$c_\alpha = \int d\vec r \, (\varphi_\alpha(\vec r))^* \psi(\vec r)$$

e.g.: $$c_{\vec k} = \int d\vec r \, \frac{e^{-i\vec k\cdot\vec r}}{\sqrt V} \psi(\vec r)$$

(a)

$$\hat H_0 = -\frac{\hbar^2}{2m}\int d\vec r \, \psi^+(\vec r) \, \nabla^2 \underbrace{\psi(\vec r)}_{=\sum_{\vec k} \frac{1}{\sqrt V} e^{i\vec k\cdot\vec r} c_{\vec k}}$$

$$= \left(-\frac{\hbar^2}{2m}\right)\sum_{\vec k}\left[\int d\vec r \, \psi^+(\vec r) \, \underbrace{\nabla^2\left(\frac{e^{i\vec k\cdot\vec r}}{\sqrt V}\right)}_{-k^2\frac{e^{i()}}{\sqrt V}}\right] c_{\vec k}$$

$$= \sum_{\vec k} \frac{\hbar^2 k^2}{2m} \underbrace{\left[\int d\vec r \, \frac{e^{i\vec k\cdot\vec r}}{\sqrt V} \psi^+(\vec r)\right]}_{c^+_k} c_k$$

$$\hat H_0 = \sum_{\vec k} \frac{\hbar^2 k^2}{2m} c^+_k c_k$$

(b) $$\hat V_{\text{Coulomb}} = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int dr_1 dr_2 \, V(r_1-r_2) \, \psi^+_{\sigma_1}(r_1)\psi^+_{\sigma_2}(r_2)\psi_{\sigma_2}(r_2)\psi_{\sigma_1}(r_1)$$

$$= \frac{1}{2}\sum_{\sigma_1\sigma_2}\sum_{k_{1,2,3,4}}\left[\int dr_1 dr_2 \, V(r_1-r_2)\frac{e^{i(-k_4\cdot r_1 - k_3\cdot r_2 + k_2\cdot r_2 + k_1\cdot r_1)}}{(\sqrt V)^4}\right]$$

$$c^+_{k_4\sigma_1} c^+_{k_3\sigma_2} c_{k_2\sigma_2} c_{k_4\sigma_1}$$

change of variables: $$\begin{cases}\rho = r_1 - r_2 \\ R = \frac{1}{2}(r_1+r_2)\end{cases}, \quad dr_1 dr_2 = d\rho \, dR \quad (J=1)$$

$$\Leftrightarrow \begin{cases} r_1 = R + \rho/2 \\ r_2 = R - \rho/2 \end{cases}$$

$$-k_4 r_1 - k_3 r_2 + k_2 r_2 + k_1 r_1 = (-k_4+k_1)(R+\frac{\rho}{2}) + (-k_3+k_2)(R-\frac{\rho}{2})$$

$$= (-(k_1+k_2)-(k_3+k_4)) \cdot R$$

$$+ (+k_1 - k_4 - k_2 + k_3) \cdot \frac{\rho}{2}$$

- $\int dR\ \bar{e}^{i(+(k_1+k_2)-(k_3+k_4))\cdot R} = V\,\delta_{k_1+k_2,\,k_3+k_4}$

$k_3+k_4 = k_1+k_2$ $\Rightarrow$ 3 indep. vectors k_1, k_4

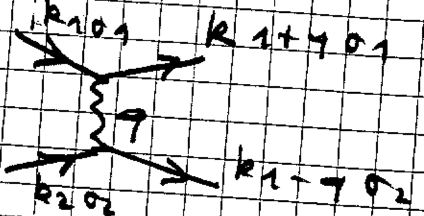
Define $q \equiv k_4 - k_1$; 3 new variables

$= -(k_3-k_2)$

- $+k_1-k_4-k_2+k_3 = -2q$

$\int d\rho$ $\int d\rho\ \bar{e}^{iq\cdot\rho}\ V(\rho) = \tilde{V}(q)$ (FT of V

el $\hat{V}_{Coulomb} = \frac{1}{2}\sum_{\sigma_1\sigma_2} \frac{1}{V} \sum_{k_1 k_2 q} \tilde{V}(q)\, c^+_{k_1+q\sigma_1}\, c^+_{k_2-q\sigma_2}\, c_{k_2\sigma_2}\, c_{k_1\sigma}$



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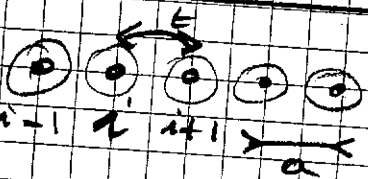


Atomic orbital (s, p, d ...) located around $\vec{R}_i$. State $|i\rangle$

$i = 1, N_S$

Tight-binding hamiltonian :

$\hat{H} = -t \sum_i c^+_i c_{i+1} + h.c.$; periodic boundary condition

Define $\boxed{c_k = \sum_{n=1}^{N_s} \frac{1}{\sqrt{N_s}}\, \bar{e}^{ikna}\, c_n}$

Unitary transform $\langle n|k\rangle = \frac{\bar{e}^{ikna}}{\sqrt{N_s}}$ $\Rightarrow$ c_k is a fermion annihilation operator.

$c_{k+\frac{2\pi}{a}} = \sum \bar{e}^{i2\pi n}\ (\ )\ = c_k \Rightarrow k \in 1BZ = [-\frac{\pi}{a}, \frac{\pi}{a}]$

$\underline{k}$? $|k\rangle = \sum_{n=1}^{N_s} \frac{\bar{e}^{ikna}}{\sqrt{N_s}}\ |n\rangle$

$|k\rangle$: eigenvector of translation operator $\hat{T}_a$: $\hat{T}_a|n\rangle = |n+1\rangle$

$\hat{T}_a|k\rangle = \sum_{n=1}^{NS} \frac{\bar{e}^{ikna}}{\sqrt{\ }}\ |n+1\rangle = \frac{e^{-ika}}{\sqrt{\ }}\Big[\ \bar{e}^{2ika}|2\rangle + ..\ \bar{e}^{ikN_sa}|N_s\rangle + \bar{e}^{ikN_sa}\bar{e}^{ika}\underbrace{|N_s+1\rangle}_{=1}\Big]$

$|k\rangle$ eigenvector with eigenvalue $\bar{e}^{ika}$

iff $\boxed{\bar{e}^{ikN_sa} = 1}$ $\boxed{k = \frac{2\pi}{N_s a} m,\ m \in \mathbb{Z} \text{ and } k \in [-\pi/a, \pi/a]}$ (periodic b.c.)

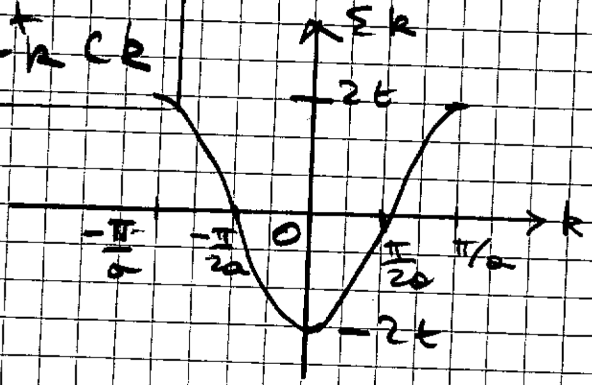
check : $c_n = \sum_{k\in 1BZ} \frac{1}{\sqrt{N_s}} e^{-ikna} c_k$

$$\hat{H} = -t \sum_n \left(\sum_{k_1} \frac{1}{\sqrt{}} e^{ik_1na} c^+_{k_1}\right)\left(\sum_{k_2} e^{-ik_2(n+1)a} c_{k_2}\right)$$
$+ h.c.$

$$= \sum_{k_1k_2} \frac{1}{(\sqrt{N_s})^2}(-t)\underbrace{\left(\sum_n e^{ina(k_1-k_2)}\right)}_{N_s\delta_{k_1,k_2}} e^{-ik_2a} c^+_{k_1} c_{k_2} + h.c.$$

$$= \sum_{k_1} -t(e^{-ik_1a} + e^{+ik_1a}) c^+_{k_1} c_{k_1}$$

$$\boxed{\hat{H} = \sum_k -2t\cos ka \ c^+_k c_k}$$



9. 1part operator:

$\hat{\rho}^{(1)}(\vec r) = |\vec r\rangle\langle \vec r|$

2nd quant^{on}:

$$\hat\rho(\vec r) = \sum_{\lambda_1\lambda_2} \langle\lambda_1|\hat\rho^{(1)}(\vec r)|\lambda_2\rangle c^+_{\lambda_1} c_{\lambda_2}$$

$$= \sum_{\lambda_1\lambda_2} \underbrace{\langle\lambda_1|\vec r\rangle}_{(\varphi_{\lambda_1}(\vec r))^*}\underbrace{\langle\vec r|\lambda_2\rangle}_{\varphi_{\lambda_2}(\vec r)} c^+_{\lambda_1} c_{\lambda_2} = \sum_{\lambda_1\lambda_2} (\varphi_{\lambda_1}(\vec r))^*\varphi_{\lambda_2}(\vec r)\, c^+_{\lambda_2} c_{\lambda_2}$$

- $|\lambda_1\rangle = |\vec r_1\rangle$: $\varphi_{\lambda_1}(\vec r) = \langle \vec r_1|\vec r\rangle = \delta(\vec r_1 - \vec r)$

$c_{\lambda_1} = \Psi(\vec r_1)$

$$\hat\rho(\vec r) = \int dr_1 dr_2\, \delta(\vec r_1-\vec r)\,\delta(\vec r_2 - \vec r)\,\Psi^+(\vec r_1)\Psi(\vec r_2)$$

$$\boxed{\hat\rho(\vec r) = \Psi^+(\vec r)\,\Psi(\vec r)}$$

- $|\lambda_1\rangle = |k_1\rangle$ $\varphi_{\lambda_1}(\vec r) = \frac{1}{\sqrt V} e^{i\vec k_1\cdot\vec r}$

$$\hat\rho(\vec r) = \sum_{k_1k_2} \frac{1}{V} e^{-i(k_1-k_2)\cdot\vec r} c^+_{k_1}c_{k_2}$$

$$\int d\vec r\, e^{-i\vec q\cdot\vec r}\hat\rho(\vec r) = \sum_{k_1k_2}\frac{1}{V}\left[\int d\vec r\, e^{-i\vec r(q+k_1-k_2)}\right] c^+_{k_1}c_{k_2}$$

$[\ ] = V\delta_{k_2-k_1,q}$: $k_1 = k_2 - q$

$$\boxed{\hat{\rho}(\vec{q}) = \sum_{k} c^{+}_{\vec{k}-\vec{q}}\, c_{\vec{k}}}$$

2- Spin operator:

$$\vec{S} = \sum_\lambda c^+_{\lambda\alpha'} \frac{\sigma_{\alpha'\alpha}}{2} c_{\lambda\alpha}$$

$$\sigma_x = \begin{array}{c|cc} & |\uparrow\rangle & |\downarrow\rangle \\ \hline \langle\uparrow| & 0 & 1 \\ \langle\downarrow| & 1 & 0 \end{array} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Summation on α and α'. Einstein notation (repeated indices).

1. $c^+ = (c_1^+ \, - - - \, c_N^+)$ $\quad c = \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}$

$$[c^+ A c, c^+ B c] = \overset{\text{or } [c_1^+ A_{12} c_2, c_3^+ A_{34} c_4]}{[c^+_{\alpha_1} A_{\alpha_1\alpha_2} c_{\alpha_2}, c^+_{\alpha_3} B_{\alpha_3\alpha_4} c_{\alpha_4}]}$$

$$= A_{\alpha_1\alpha_2} B_{\alpha_3\alpha_4} [c^+_{\alpha_1} c_{\alpha_2}, c^+_{\alpha_3} c_{\alpha_4}]$$

$$[c_1^+ c_2, c_3^+ c_4] = c_1^+ [c_2, c_3^+ c_4] + [c_1^+, c_3^+ c_4] c_2$$

$$= \delta_{2,3} c_1^+ c_4 - \delta_{1,4} c_3^+ c_2$$

$$[\ \ ,\ \ ] = A_{\alpha_1\alpha_2} B_{\alpha_3\alpha_4} (\delta_{\alpha_2,\alpha_3} c^+_{\alpha_1} c_{\alpha_4} - \delta_{\alpha_1,\alpha_4} c^+_{\alpha_3} c_{\alpha_2})$$

$$= c^+_{\alpha_1} A_{\alpha_1\alpha_2} B_{\alpha_2\alpha_4} c_{\alpha_4}$$

$$- c^+_{\alpha_3} B_{\alpha_3\alpha_4} A_{\alpha_1\alpha_2} c_{\alpha_2}$$

$$= c^+ A B c - c^+ B A c$$

$$= c^+ \underbrace{[A, B]}_{N \times N \text{ matrix}} c$$

2. $\nu = x, y, z$

$$\hat{S}_\nu = \sum_\lambda c^+_{\lambda\alpha'} \left(\tfrac{1}{2}\sigma_\nu\right)_{\alpha'\alpha} c_{\lambda\alpha}$$

$$[\hat{S}_\nu, \hat{S}_{\nu'}] = \sum_{\lambda,\lambda'} [\ \ \lambda\ \ ,\ \ \lambda'\ ]$$

$[\ ] = 0$ if $\lambda' \neq \lambda$

2×2 matrices

$$= \sum_\lambda [c^+_\lambda \overbrace{\left(\tfrac{1}{2}\sigma_\nu\right)} c_\lambda, c^+_\lambda \overbrace{\left(\tfrac{1}{2}\sigma_{\nu'}\right)} c_\lambda]$$

$$c^+_\lambda = (c^+_{\lambda\uparrow} \ c^+_{\lambda\downarrow})$$

$$= \sum_\lambda c^+_\lambda \underbrace{\left[\tfrac{1}{2}\sigma_\nu, \tfrac{1}{2}\sigma_\nu\right]}_{i \varepsilon_{\nu\nu'\nu''} \frac{\sigma_{\nu''}}{2}} c_\lambda$$

$$= i\,\varepsilon_{\nu\nu'\nu''}\ \hat{S}_{\nu''} \qquad (``\hbar = 1") \qquad ⑫$$

These ~~are~~ the Commutation relations of angular momentum operators (Liegroup "SU(2)").

3. 1st quantization:

$$\hat{\vec{S}} = \sum_{i=1}^{N} \hat{\vec{s}}^{(i)}\ ; \quad \text{Addition of } N \text{ spins } 1/2.$$

$$\text{Total spin } \begin{cases} 0 & N \text{ even} \\ \frac{1}{2} & N \text{ odd} \end{cases} \leq S \leq \frac{N}{2}$$

$$\vec{S}^2 : \hbar^2 S(S+1).$$

4.
$$\hat{S}^{+} = S_x + i S_y$$
$$= \frac{1}{2}\sum_{\lambda} c^{+}_{\lambda\alpha'} (\sigma_x + i\sigma_y)_{\alpha'\alpha}\, c_{\lambda\alpha}$$

$$\frac{1}{2}(\sigma_x + i\sigma_y) = \begin{pmatrix} 0 & \frac{1}{2}(1-i^2) \\ \frac{1}{2}(1+i^2) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$ only terms ≠ 0: $\alpha' = \uparrow, \alpha = \downarrow$

$$\boxed{\hat{S}^{+} = \sum_{\lambda} c^{+}_{\lambda\uparrow}\, c_{\lambda\downarrow}} \qquad \hat{S}_z = \frac{1}{2}\sum_{\lambda} c^{+}_{\lambda\uparrow} c_{\lambda\uparrow} - c^{+}_{\lambda\downarrow} c_{\lambda\downarrow}$$

$$\hat{S}^{-} = \sum_{\lambda} c^{+}_{\lambda\downarrow}\, c_{\lambda\uparrow}$$

5. Single site. Hilbert space: $\{|0\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}$

Dimension: **4**. $|\sigma\rangle = d^{+}_{\sigma}|0\rangle$
$|\uparrow\downarrow\rangle = d^{+}_{\uparrow} d^{+}_{\downarrow}|0\rangle$

6. $\hat{H}|0\rangle = 0$, $\hat{H}|\uparrow\rangle = \varepsilon_d|\uparrow\rangle$, $\hat{H}|\downarrow\rangle = \varepsilon_d|\downarrow\rangle$

$\hat{H}|\uparrow\downarrow\rangle = (2\varepsilon_d + U)|\uparrow\downarrow\rangle$

Matrix
$$\hat{H} = \begin{array}{cccc} |0\rangle & |\uparrow\rangle & |\downarrow\rangle & |\uparrow\downarrow\rangle \\ \end{array}$$
$$\begin{pmatrix} 0 & & & \\ & \varepsilon_d & & 0 \\ & & \varepsilon_d & \\ 0 & & & 2\varepsilon_d + U \end{pmatrix}$$

Spin of each eigenstate:

$|0\rangle$: $S=0$

$|\uparrow\rangle$: $S=\frac{1}{2}$, $|\downarrow\rangle$: $S=\frac{1}{2}$

$|\uparrow\downarrow\rangle$: $S=0$

Proof:

$$\hat{S}^+ |\uparrow\downarrow\rangle = d^+_\uparrow d_\downarrow \, d^+_\uparrow d^+_\downarrow |0\rangle$$

$$= -\underbrace{d^+_\uparrow d^+_\uparrow}_{=0} d_\downarrow d^+_\downarrow |0\rangle = 0$$

$$\hat{S}^- |\uparrow\downarrow\rangle = \underbrace{d^+_\downarrow d_\uparrow}_{-1} \underbrace{d^+_\uparrow d^+_\downarrow}_{-1} |0\rangle$$

$$= (-1)^2 d_\uparrow d^+_\uparrow \underbrace{(d^+_\downarrow)^2}_{=0} |0\rangle = 0$$

$$\hat{S}_z |\uparrow\downarrow\rangle = \frac{1}{2}(d^+_\uparrow d_\uparrow - d^+_\downarrow d_\downarrow) d^+_\uparrow d^+_\downarrow |0\rangle$$

$$= \left(\frac{1}{2} - \frac{1}{2}\right) d^+_\uparrow d^+_\downarrow |0\rangle = 0$$

3. Hartree-Fock: $H = \hat{T} + \hat{V}$

1. Ground state of the non-interacting system.

Fermi-Sea

$$|FS\rangle = \prod_{|\vec{k}|<k_F} c^+_{\vec{k}\uparrow} c^+_{\vec{k}\downarrow} |0\rangle$$

2. Perturbation theory 1st order in $\hat{V}$.

$$\delta E = \langle FS| \hat{V} |FS\rangle$$

$$= \frac{1}{2V} \sum_{\substack{\sigma_1\sigma_2 \\ q k_1 k_2}} \frac{e^2}{\varepsilon_0 q^2} \langle FS| c^+_{k_1+q,\sigma_1} c^+_{k_2-q,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |F$$

$$\langle FS| \underbrace{c^+_{k_1+q,\sigma_1} c^+_{k_2-q,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |FS\rangle}_{\text{This state must be } |FS\rangle \text{ (with a prefactor)}}$$

Therefore the annihilated particles must be created "later".

2 cases:

$i)$ $(k_1+q, \sigma_1) = (k_1, \sigma_1)$ "Hartree"
$(k_2-q, \sigma_2) = (k_2, \sigma_2)$

$ii)$ $(k_1+q, \sigma_1) = (k_2, \sigma_2)$ "Fock"
$(k_2-q, \sigma_2) = (k_1, \sigma_1)$

$i)$ $q=0$, $\langle\ \rangle = \langle FS| c^+_{k_1,\sigma_1} c^+_{k_2,\sigma_2} c_{k_2,\sigma_2} c_{k_1,\sigma_1} |FS\rangle$

$\neq 0$ iff $|k_1| < k_F$, $|k_2| < k_F$ $(k_1,\sigma_1) \neq (k_2,\sigma_2)$

$$\langle\ \rangle = (-1)^2 \langle FS| c^+_{k_2,\sigma_2} c_{k_2,\sigma_2} \underbrace{c^+_{k_1,\sigma_1} c_{k_1,\sigma_1} |FS\rangle}_{\theta(k_F-|k_1|)|FS\rangle}$$

$$= \theta(k_F-|k_1|)\,\theta(k_F-|k_2|)$$

NB: $(k_1\sigma_1) = (k_2\sigma_2)$ gives 0, but negligible weight.

Hartree contribution: $\frac{1}{2V} \frac{e^2}{\varepsilon_0 (0)^2} \left(\sum_{k_1} \theta(k_F-|k_1|)\right)\left(\sum_{k_2} \theta(k_F-|k_2|)\right)$

DIVERGENT!

→ needs a background of positive ions (cf. jellium model)

①

ii) $\sigma_2 = \sigma_1 \qquad k_2 = k_1 + q$

$$\langle FS | c^{+}_{k_1+q,\sigma_1} \, c^{+}_{k_1,\sigma_1} \, c_{k_1+q,\sigma_1} \, c_{k_1,\sigma_1} | FS \rangle$$

· If $q \neq 0$, $\langle \; \rangle = \ominus \langle FS | c^{+}_{k_1+q,\sigma_1} c_{k_1+q,\sigma_1} \, c^{+}_{k_1,\sigma_1} c_{k_1,\sigma_1} | FS \rangle$

$$= \ominus\, \theta(k_F - |k_1|)\, \theta(k_F - |k_1+q|)$$

· If $q = 0$, $\langle (c^{+}_{k_1+q,\sigma_1})^2 \, (c_{k_1,\sigma_1})^2 \rangle = 0$

Fock contribution:

$$\ominus \frac{1}{2V} 2 \sum^{\text{spin}}_{q \neq 0} \frac{e^2}{\varepsilon_0 q^2} \left[\sum_{k_1} \theta(k_F - |k_1|)\, \theta(k_F - |k_1+q|) \right]$$

cf text: $[\;] \equiv V_q = \frac{V}{(2\pi)^3} \frac{4\pi k_F^3}{3} \left[1 - \frac{3}{4} \frac{q}{k_F} + \frac{1}{16} \left(\frac{q}{k_F}\right)^3 \right]$

$$\theta(|q| - 2k_F)$$

$$\delta E_{\text{Fock}} = -\frac{1}{2\cancel{V}} 2 \frac{V}{(2\pi)^3} \frac{4\pi k_F^3}{3} \frac{e^2}{\varepsilon_0} \frac{\cancel{V}}{(2\pi)^3} \int_{|q|<2k_F} d^3\vec{q} \, \frac{1}{q^2} \left[1 - \frac{3}{4} \frac{q}{k_F} + \frac{1}{16} \left(\frac{q}{k_F}\right)^3 \right]$$

$\underline{\int d^3\vec{q}}$: $\int d\Omega \rightarrow 4\pi$ (angles)

$$\rightarrow 4\pi \int_0^{2k_F} dq \, \cancel{q^2} \frac{1}{\cancel{q^2}} [1 - - -] \qquad x = q/k_F$$

$$= 4\pi k_F \int_0^2 dx \left[1 - \frac{3}{4} x + \frac{1}{16} x^3 \right] = 4\pi k_F \left[x - \frac{3}{8} x^2 + \frac{1}{64} x^4 \right]_0^2$$

$$= 4\pi k_F \left[2 - \frac{3}{2} + \frac{1}{4} \right] = 3\pi k_F$$

$$\underline{\frac{\delta E_{\text{Fock}}}{V}} = -\frac{\cancel{2}}{2} \frac{4\pi \cdot 3\pi}{(2\pi)^3 \cdot \cancel{3} \cdot (2\pi)^3} \frac{e^2}{\varepsilon_0} k_F^4$$

$$= -\frac{1}{16\pi^4} \frac{e^2}{\varepsilon_0} k_F^4$$

$$\boxed{\frac{\delta E_{\text{Fock}}}{V} = -\frac{k_F^4}{4\pi^3} \frac{e^2}{4\pi\varepsilon_0}}$$

4. Finite temperature and thermodynamics:

1. $$Z = \mathrm{Tr}\left[e^{-\beta \left(\sum_\lambda (\varepsilon_\lambda - \mu) \hat{n}_\lambda \right)} \right]$$

Basis of Fock states:

$$| \overset{\lambda_1}{n_{\lambda_1}} \quad \overset{\lambda_2}{n_{\lambda_2}} \quad \ldots \quad \rangle$$

$F : n_\lambda = 0, 1$

$B : n_\lambda = 0, 1, 2 \ldots \infty$

$$Z = \sum_{n_{\lambda_1} = 0, 1 \ldots} \sum_{n_{\lambda_2} = 0, 1} \ldots \langle n_{\lambda_1} n_{\lambda_2} \ldots | e^{-\beta \sum_\lambda (\varepsilon_\lambda - \mu) \hat{n}_\lambda} | n_{\lambda_1} n_{\lambda_2} \ldots \rangle$$

$$= \qquad e^{-\beta \sum_\lambda (\varepsilon_\lambda - \mu) \underset{\uparrow \, n_b !}{n_\lambda}}$$

$$= \left(\sum_{n_{\lambda_1} = 0, 1 \ldots} e^{-\beta (\varepsilon_{\lambda_1} - \mu) n_{\lambda_1}} \right) \left(\sum_{n_{\lambda_2} = } \qquad \right) \left(\qquad \right)$$

$$Z = Z_{\lambda_1} \cdot Z_{\lambda_2} \ldots = \prod_\lambda Z_\lambda$$

2. $$Z_\lambda = \sum_{\substack{n_\lambda = 0, 1 \quad F \\ \{0, 1, \ldots \infty \quad B}} e^{-\beta (\varepsilon_\lambda - \mu) n_\lambda}$$

F : $$\boxed{Z_\lambda = 1 + e^{-\beta (\varepsilon_\lambda - \mu)}}$$

B : $$Z_\lambda = 1 + e^{-\beta (\varepsilon_\lambda - \mu)} + e^{-2\beta (\varepsilon_\lambda - \mu)} + \ldots e^{-n\beta (\varepsilon_\lambda - \mu)}$$

$$\boxed{Z_\lambda = \frac{1}{\left[1 - e^{-\beta (\varepsilon_\lambda - \mu)} \right]}} \qquad (\varepsilon_\lambda - \mu > 0 \, !)$$

3. $$\langle \hat{n}_\lambda \rangle = \frac{1}{Z} \sum_{n_{\lambda_1} = 0, 1 \ldots} \sum_{n_{\lambda_2} = 0, 1 \ldots} \ldots \sum_{n_\lambda = 0, 1 \ldots} n_\lambda e^{-\beta (\varepsilon_\lambda - \mu) n_\lambda}$$

$$= \frac{\prod_{\lambda_1 \neq \lambda} Z_{\lambda_1} \left[\sum_{n_\lambda = \ldots} n_\lambda e^{-\beta (\varepsilon_\lambda - \mu) n_\lambda} \right]}{\prod_{\lambda_1 \neq \lambda} Z_{\lambda_1} \left[\sum_{n_\lambda = \ldots} e^{-\beta (\varepsilon_\lambda - \mu) n_\lambda} \right]}$$

$$\langle \hat{n}_\lambda \rangle = \frac{1}{\beta} \frac{\frac{\partial}{\partial \mu} (Z_\lambda)_T}{Z_\lambda} = \frac{1}{\beta} \frac{\partial}{\partial \mu} (\log Z_\lambda)_T$$

$$\underline{F}: \langle \hat{n}_\lambda \rangle = \frac{1}{\cancel{\beta}} \frac{\cancel{\beta} e^{-\beta(\varepsilon_\lambda - \mu)}}{1 + e^{-\beta(\varepsilon_\lambda - \mu)}}$$

$$\boxed{\langle \hat{n}_\lambda \rangle = \frac{1}{\left[1 + e^{\beta(\varepsilon_\lambda - \mu)}\right]}}$$

"Fermi – Dirac"

$$B: \langle \hat{n}_\lambda \rangle = -\frac{1}{\beta} \frac{\partial}{\partial \mu} \left(\log \frac{1}{Z_\lambda}\right) = -\frac{1}{\cancel{\beta}} \left(\frac{-\cancel{\beta} e^{-\beta(\varepsilon_\lambda - \mu)}}{\left(1 - e^{-\beta(\varepsilon_\lambda - \mu)}\right)}\right.$$

$$\boxed{\langle \hat{n}_\lambda \rangle = \frac{1}{\left[e^{\beta(\varepsilon_\lambda - \mu)} - 1\right]}}$$

"Bose – Einstein"