2.1 Second Quantization (formalism)

Consider $[a, a^\dagger]_\varsigma = 1$ & $[a,a]_\varsigma = [a^\dagger, a^\dagger]_\varsigma = 0$ $\begin{cases} \varsigma = + & \text{Boson.} \\ \varsigma = - & \text{Fermion} \end{cases}$

Suppose $a^\dagger a|n\rangle = n|n\rangle$, with $||n\rangle|^2 = 1$. ($a^\dagger a$ is hermitian).

we have. $\langle n|a^\dagger a|n\rangle = |a|n\rangle|^2 = n \geq 0$

Is $a^\dagger|n\rangle$ an eigenstate of $a^\dagger a \equiv \hat{n}$?

$$a^\dagger \underbrace{a a^\dagger}_{aa^\dagger - \varsigma a^\dagger a = 1}|n\rangle = a^\dagger(1 + \varsigma a^\dagger a)|n\rangle = \begin{cases} a^\dagger|n\rangle + a^\dagger n|n\rangle = (n+1)a^\dagger|n\rangle. & B \\ a^\dagger|n\rangle + 0 & F \end{cases}$$

$$\Rightarrow \begin{cases} a^\dagger|n\rangle = C|n+1\rangle, \ |C|^2 = n \Rightarrow A = \sqrt{n}. & B \\ a^\dagger|n\rangle = C|1\rangle, \ |C|^2 = \langle n|aa^\dagger|n\rangle \end{cases}$$

$a^\dagger|n\rangle$

$aa + aa = 0$

$$a^\dagger a a|n\rangle = \begin{cases} (aa^\dagger - 1)a|n\rangle = (n-1)a|n\rangle. \Rightarrow a|n\rangle = c|n-1\rangle. \\ \quad \langle n|a^\dagger a|n\rangle = n = |c|^2. \Rightarrow c = \sqrt{n} \\ (F)\ 0 = 0|0\rangle = (1 - aa^\dagger)a|n\rangle \Rightarrow (1-n)\,a|n\rangle^{=0} \Rightarrow n = \begin{cases} 0, & a|0\rangle = 0 \\ 1, & a|1\rangle = c|0\rangle \end{cases} \end{cases}$$

$\langle 1|a^\dagger a|1\rangle = 1 = c^2$

must exist $a|0\rangle = 0$. & $a|n\rangle = \sqrt{n}|n-1\rangle$, $n = 0, 1, \ldots$

Similarly: $a^\dagger a \underline{a^\dagger|n\rangle} = a^\dagger(a^\dagger a + 1)|n\rangle = (n+1)a^\dagger|n\rangle \Rightarrow a^\dagger|n\rangle = c|n+1\rangle.$

$\langle n|aa^\dagger|n\rangle = c^2 = 1 + n$

$$\Rightarrow |n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle.$$

Fermi

$a^\dagger(1 - a^\dagger a)|n\rangle = (1-n)a^\dagger|n\rangle. \Rightarrow a^\dagger|n\rangle = c|1-n\rangle. \Rightarrow n = 0, 1$

For $n=0$, $a^\dagger|0\rangle = c|1\rangle \Rightarrow \langle 0|aa^\dagger|0\rangle = c^2 = \langle 0|(1-a^\dagger a)|0\rangle$

$a|0\rangle = 0$. $\qquad = 1$

For $n=1$, $a^\dagger|1\rangle = c|0\rangle \Rightarrow \langle 1|aa^\dagger|1\rangle = \langle 1|(1-a^\dagger a)|1\rangle = 0 = c^2$

$a|1\rangle = |0\rangle$. $\qquad = 0$.

	n	$a^\dagger\|n\rangle$	$a\|n\rangle$	$\|n\rangle$
B	$0,1,2,\dots$	$\sqrt{n}\|n+1\rangle$	$\sqrt{n}\|n-1\rangle$	$\frac{(a^\dagger)^n}{\sqrt{n!}}\|0\rangle$
F	$0,1$	$a^\dagger\|0\rangle=\|1\rangle$ $a^\dagger\|1\rangle=0$	$a\|0\rangle=0$ $a\|1\rangle=\|0\rangle$	

Consider $H|\lambda\rangle = \lambda|\lambda\rangle$, $\sum_\lambda |\lambda\rangle\langle\lambda| = \mathbb{1}$. $\{|\lambda\rangle\}$ = single particle basis

single particle H $\qquad$ $\lambda = \lambda_1, \lambda_2, \dots$ (discrete or continuous).

Many-particle state:

$$|n_{\lambda_1}, n_{\lambda_2}, \dots\rangle = \frac{(a^\dagger_{\lambda_1})^{n_{\lambda_1}}}{\sqrt{n_{\lambda_1}!}} \frac{(a^\dagger_{\lambda_2})^{n_{\lambda_2}}}{\sqrt{n_{\lambda_2}!}} \cdots |0\rangle \quad \begin{cases} n_\lambda = 0,1,2,\dots & \text{(B)} \\ n_\lambda = 0,1 & \text{(F)} \end{cases}$$

form a basis

e.g. $a^\dagger_{\lambda_1} a^\dagger_{\lambda_3} a^\dagger_{\lambda_4}|0\rangle =$
$= -a^\dagger_{\lambda_1} a^\dagger_{\lambda_4} a^\dagger_{\lambda_3}|0\rangle$ $\left(\text{exchange particle} \rightarrow -1\right)$

Many-body operators

$$\text{one-body}: \quad \hat{O}_1 = \sum_{n=1}^{N} \hat{O}_n = \sum_{\lambda} O_\lambda \hat{n}_\lambda = \sum O_\lambda a_\lambda^\dagger a_\lambda$$

single particle operator eg. $\frac{\hat{p}_n^2}{2m}$

one particle basis

eigenvalue: $\hat{O}_n |\lambda\rangle = O_\lambda |\lambda\rangle$

same for diff. n.

in a different one-particle basis $\{|\mu\rangle\}$

$$\boxed{a_\lambda^\dagger}|0\rangle = |\lambda\rangle = \sum_\mu |\mu\rangle\langle\mu|\lambda\rangle = \boxed{\sum_\mu \langle\mu|\lambda\rangle a_\mu^\dagger}|0\rangle$$

also $\boxed{a_\lambda = \sum_\mu \langle\lambda|\mu\rangle a_\mu}$

$$\text{So } \hat{O}_1 = \sum_\lambda O_\lambda \left(\sum_\mu \langle\mu|\lambda\rangle a_\mu^\dagger\right)\left(\sum_\nu \langle\lambda|\nu\rangle a_\nu\right)$$

$$= \sum_{\mu\nu} \langle\mu| \underbrace{\left(\sum_\lambda |\lambda\rangle O_\lambda \langle\lambda|\right)}_{\hat{o}} |\nu\rangle a_\mu^\dagger a_\nu$$

$$\boxed{\hat{O}_1 = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu} \quad (1)$$

Note that: $\hat{O}_1 = \sum_{n=1}^{N} \sum_{\mu,\nu} |\mu\rangle_n \underbrace{\langle\mu|\hat{O}_n|\nu\rangle_n}_{\text{same for diff. } n. \to \langle\mu|\hat{O}|\nu\rangle} \langle\nu|_n$

$$= \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle \left(\sum_n |\mu\rangle_n \langle\nu|_n\right) \quad (2)$$

Compare (1) & (2),

$$\boxed{\sum_n |\mu\rangle_n \langle\nu|_n = a_\mu^\dagger a_\nu} \quad (3)$$

$\to$ will be used to derive 2-body operator.

Two-body Operators

eg. $V(\vec{r}_m, \vec{r}_n) = \frac{e^2}{|\vec{r}_m - \vec{r}_n|}$

$$\hat{O}_2 = \frac{1}{2} \sum_{m \neq n} \hat{O}_{m,n}$$

$$= \frac{1}{2} \sum_{m\neq n} \sum_{\mu\mu'\nu\nu'} |\mu\rangle_m |\mu'\rangle_n \underbrace{{}_m\langle\mu| {}_n\langle\mu'| \hat{O}_{m,n} |\nu\rangle_m |\nu'\rangle_n}_{\langle \mu,\mu'|\hat{O}|\nu,\nu'\rangle} \langle\nu|_m \langle\nu'|_n$$

$$= \frac{1}{2} \sum_{\mu\mu'\nu'\nu'} \langle\mu,\mu'|\hat{O}|\nu,\nu'\rangle \left(\sum_{mn} |\mu\rangle_m \langle\nu|_m \, |\mu'\rangle_n \langle\nu'|_n - \sum_n |\mu\rangle_n \delta_{\nu\mu'} \langle\nu'|_n \right)$$

③ $\hookrightarrow a^\dagger_\mu a_\nu a^\dagger_{\mu'} a_{\nu'} - a^\dagger_\mu \begin{pmatrix} a_\nu a^\dagger_{\mu'} - a^\dagger_{\mu'} a_\nu \\ a_\nu a^\dagger_{\mu'} + a^\dagger_{\mu'} a_\nu \end{pmatrix} a_{\nu'}$

$$= \begin{cases} a^\dagger_\mu a^\dagger_{\mu'} a_\nu a_{\nu'} \\ - a^\dagger_\mu a^\dagger_{\mu'} a_\nu a_{\nu'} \end{cases} = a^\dagger_\mu a^\dagger_{\mu'} a_{\nu'} a_\nu$$

$$\Rightarrow \boxed{\hat{O}_2 = \frac{1}{2} \sum_{\mu\mu'\nu\nu'} \langle\mu\mu'|\hat{O}|\nu\nu'\rangle \, a^\dagger_\mu a^\dagger_{\mu'} \underline{a_{\nu'} a_\nu}}$$

+ Spin

$S_{\sigma\sigma'} \otimes \mathbb{1}_\lambda$

$$\hat{S} = \sum_{\lambda,\sigma\sigma'} a^\dagger_{\lambda\sigma} S_{\sigma\sigma'} a_{\lambda\sigma'}$$

$\cdots \otimes \mathbb{1}_\sigma$

$$\hat{H}_0 = \int d^d\vec{r} \sum_\sigma a^\dagger_\sigma(\vec{r}) \left[\frac{\hat{P}^2}{2m} + V(\vec{r}) \right] a_\sigma(\vec{r})$$

$$\hat{V}_{ee} = \frac{1}{2} \int d^d\vec{r} \, d^d\vec{r}' \sum_{\sigma\sigma'} V_{ee}(\vec{r}-\vec{r}') \overset{k_1}{a^\dagger_\sigma(\vec{r})} \overset{k_1'}{a^\dagger_{\sigma'}(\vec{r}')} \overset{k_2'}{a_{\sigma'}(\vec{r}')} \overset{k_2}{a_\sigma(\vec{r})}$$

2.2 Applications

Momentum Space: For nearly free electrons. $(V(\vec r) \approx 0)$

F.T. $\begin{cases} a^\dagger(\vec r) = \frac{1}{L^d}\sum_{\vec k} e^{i\vec k\cdot\vec r}\, a^\dagger(\vec k) = \frac{1}{\cancel{L^d}}\frac{\cancel{L^d}}{(2\pi)^d}\int d^d\vec k\, e^{i\vec k\vec r}\, a^\dagger(\vec k) \\ a^\dagger(\vec k) = \int d^d\vec r\, e^{-i\vec k\cdot\vec r}\, a^\dagger(\vec r)\,, \end{cases}$

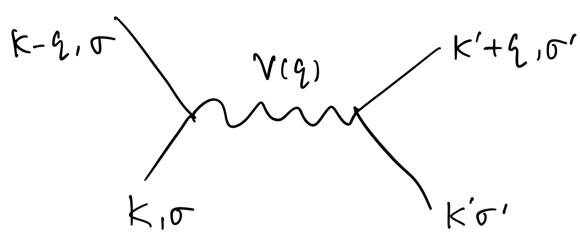
$$\begin{cases} \int d^d\vec r\, e^{i(\vec k-\vec k')\cdot\vec r} = L^d\,\delta_{k,k'} = (2\pi)^d\,\delta^{(d)}(\vec k-k') \\ \int \frac{d^d\vec k}{(2\pi)^d}\, e^{-i\vec k(\vec r-\vec r')} = \delta^{(d)}(\vec r-\vec r') \end{cases}$$

$$\hat H_0 = \sum_{\vec k\sigma}\frac{k^2}{2m}\, a^\dagger_{k\sigma}a_{k\sigma} \qquad \left(\frac{k^2}{2m} \text{ is diagonal in both } k \,\&\, \sigma\right)$$

$$\hat V_{ee} = \frac12\int d^d\vec r\, d^d\vec r' \sum_{\sigma\sigma'}\frac{1}{L^d}\sum_{\vec q} V(q)\, e^{i\vec q\cdot(\vec r-\vec r')}\,\frac{1}{L^{2d}}\sum_{k,k'} e^{i(\vec k_1-\vec k_2)\cdot\vec r + i(\vec k_1'-\vec k_2')\cdot\vec r'} \cdot a^\dagger_{k_1\sigma}a^\dagger_{k_1'\sigma'}a_{k_2'\sigma'}a_{k_2\sigma}$$

$$= \frac{1}{2L^{3d}}\sum_{\sigma\sigma' q k k'} L^{2d}\,\underbrace{\delta_{k_1-k_2+q,0}}_{k_1=k_2-q}\,\underbrace{\delta_{k_1'-k_2'-q,0}}_{k_1'=k_2'+q}\, a_{k_1\sigma}a_{k_1'\sigma'}a_{k_2'\sigma'}a_{k_2\sigma}$$

$$\xrightarrow{k_2\to k} \frac{1}{2L^d}\sum_{kk'q\sigma\sigma'}\boxed{V(q)}\, a^\dagger_{k-q,\sigma}a^\dagger_{k'+q,\sigma'}a_{k'\sigma'}a_{k\sigma}$$



$$V(q) = \lim_{\mu\to 0}\int d^d\vec r\, e^{-i\vec q\cdot\vec r}\,\frac{e^2}{|\vec r|}\cdot e^{-\mu r} = \boxed{\frac{4\pi e^2}{q^2}}$$

Jellium model (Homogenious background charges + $Q_{tot}=0 \to \vec{q}\neq 0$) + $N \gg 1$

density of iron $\equiv n_0 = \frac{N}{L^d}$

(ignore spin)

$$V_{ii} = \frac{1}{2}\int d^dr\, d^dr' \frac{e^2 n_0^2}{|r-r'|} = \frac{n_0^2}{2}\cdot L^d \cdot V(q=0) = \boxed{\frac{1}{2}\frac{N^2}{L^d} V(q=0)}$$

$$V_{ei} = N\cdot\left(-\int d^dr' \frac{n_0 e^2}{|r-r'|}\right) = \boxed{-\frac{N^2}{L^d}V(q=0)}$$

$$V_{ee}(q=0) = \frac{1}{2L^d}\sum_{kk'q} V(q=0)\, a_k^\dagger \underbrace{a_{k'}^\dagger a_{k'} a_k}_{-a_{k'}^\dagger a_k a_{k'} = (a_k a_{k'}^\dagger - \delta_{kk'})a_{k'}}$$

$$= \frac{1}{2L^d}\sum_{kk'q} V(q=0)\left(a_k^\dagger a_k a_{k'}^\dagger a_{k'} - \delta_{kk'} a_k^\dagger a_{k'}\right)$$

$$= \frac{1}{2L^d} V(q=0)\cdot\left(\hat{N}^2 - \hat{N}\right) \approx \boxed{\frac{N^2}{2L^d}V(q=0)}$$ cancel

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Bloch Theorem

For periodic potention $V(r+a) = V(r)$

$$T(a)V(r)T^{-1}(a) = V(r+a) = V(r) \quad \text{or} \quad [T(a), V] = 0$$

and $[T(a), H] = 0. \Rightarrow$ $T(a)$ must be unitary with eigenvalue e^{ika}.

$k \in (-\pi,\pi)/a$ the label of rep. or crystal mom.

also denote the simutanuous eigenstates of $T(a)$ & H by $\psi_k(r)$

i.e. $T(a)\psi_k(r) = \psi_k(r+a) = e^{ika}\psi_k(r)$ & $H\psi_k(r) = \mathcal{E}(k)\psi_k(r)$

Now, rewrite

$$\psi_k(r) = e^{ik\cdot r} u_k(r) \qquad \text{(nothing illegal)}$$

we have

$$T(a)\,\psi_k(r) = e^{ika+ikr} u_k(r+a) \qquad \text{(traslation)}$$

$$= e^{ika}\psi_k(r) = e^{ika} e^{ikr} u_k(r) \qquad \text{(eigen)}$$

$$\Rightarrow \boxed{u_k(r+a) = u_k(r) \qquad \text{periodic!}}$$

Consequence: band structure

$$H\psi_k(r) = \mathcal{E}(k)\,\psi_k(r)$$

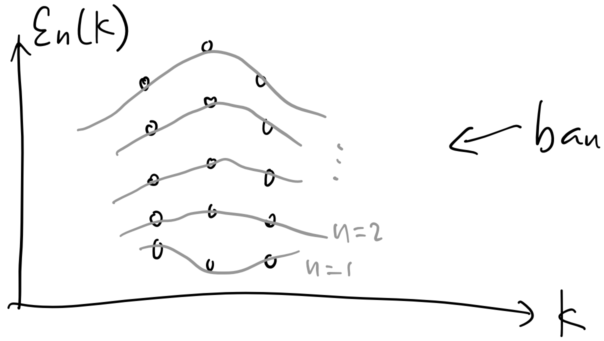
$$\to \left[\frac{p^2}{2m} + V(r)\right] e^{ikr} u_k(r)$$

$$= \cancel{e^{ikr}}\left[\frac{(p+\overset{\hbar=1}{k})^2}{2m} + V(r)\right] u_k(r) = \cancel{e^{ikr}}\,\mathcal{E}(r)\,u_k(r)$$

$$\to \quad H(p+k)\,u_k(r) = \mathcal{E}_n(k)\,u_k(r)$$

since $u_k(r)$ is periodic

For each k, $\mathcal{E}(k)$ has many solutions labeled by n.



← band structure.

Wannier States (Fourier transfrom of the lattice mom.)

a lable.

Now go back to $\psi_k(r) \xrightarrow{\text{Bloch Thm.}} \psi_{kn}(r)$ (periodic)

(Bloch states)

lattice mom. band label.

of $H_0 = \frac{p^2}{2m} + V(r)$ with energy $\varepsilon_n(k)$

More abstractly, $|\psi_{kn}\rangle$ form a basis. $\left(\psi_{kn}(r) = \langle r|\psi_{kn}\rangle\right)$

Let us Fourier transform the $\vec{k}$ to $\vec{R}_i$, the lattice sites. (discrete)

discrete

$$|\psi_{R_i n}\rangle = \frac{1}{\sqrt{N}} \sum_{k,n'}^{B.Z.} e^{-ik\cdot R_i} |\psi_{kn'}\rangle$$

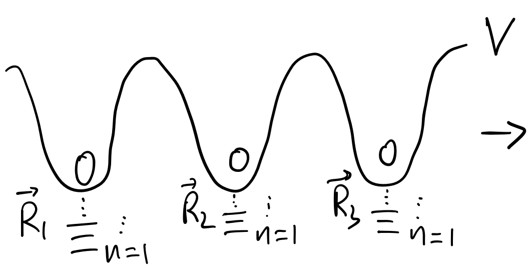
Wannier States (Not a basis)

Let $a_{in}^\dagger |0\rangle = |\psi_{R_i n}\rangle$

In Wannier basis:

$$H_0 = \sum_{n,ij} \underbrace{\langle \psi_{R_i n}| H_0 |\psi_{R_j n}\rangle}_{} a_{in}^\dagger a_{jn}$$

$$\langle \psi_{R_i n}| \left(\sum_{kn'} \varepsilon_{n'}(k) |\psi_{kn'}\rangle\langle\psi_{kn'}| \right) |\psi_{R_j n}\rangle \propto \sum_k e^{ik(R_i - R_j)} \varepsilon(k)$$



→ gives good motivation for the wannier basis.