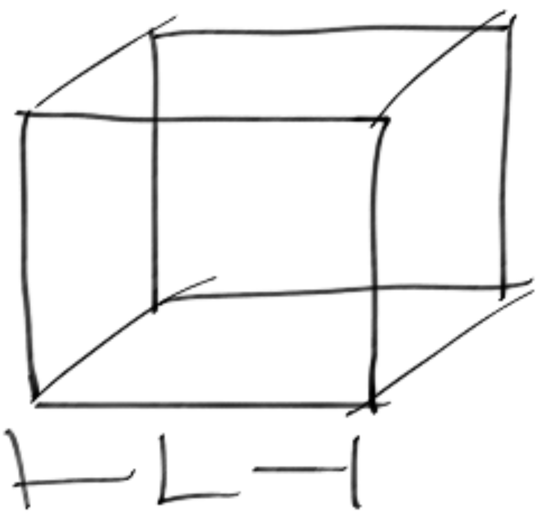
Second Quantisation: The language of Many Body Theory. Jorge Quintanilla

notes taken by H. Irons

Quantum many body problem
- identical particles and coherence of wave functions
- interactions between quantum particles.

→ Particle in a box



Hamiltonian

$$\hat{H}\Psi = E\Psi$$

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\vec{r}}\right)^2$$

$$\Psi(\vec{r}) = \frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}$$

let $L \to \infty$ free electron

momentum $\vec{p} = \hbar\vec{k}$; $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$

two particles

$$\hat{H} = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\vec{r}_1}\right)^2 + \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\vec{r}_2}\right)^2 + \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} V(\vec{r}_i, \vec{r}_j)$$

But doesn't work for identical particles $\rightarrow$ Pauli's exclusion principle.

$$\psi(\vec{r}_1,\vec{r}_2) = \psi_{\vec{k}_1}(\vec{r}_1)\,\psi_{\vec{k}_2}(\vec{r}_2)$$

$$|\psi(\vec{r}_1,\vec{r}_2)|^2 = |\psi(\vec{r}_2,\vec{r}_1)|^2$$

$$\psi(\vec{r}_1,\vec{r}_2) = e^{i\varphi}\psi(\vec{r}_2,\vec{r}_1) = e^{i\varphi}e^{i\varphi}\psi(\vec{r}_1,\vec{r}_2)$$

$$e^{i2\varphi} = 1 \qquad \varphi = \pi n \Rightarrow e^{i\varphi} = +1 \text{ or } -1$$

if $+1 \rightarrow$ bosons   if $-1 \rightarrow$ fermions

$$\psi(\vec{r}_1,\vec{r}_2) = \pm\,\psi(\vec{r}_2,\vec{r}_1)$$

Symmetries

$$\psi_{\vec{k}_1}(\vec{r}_1)\,\psi_{\vec{k}_2}(\vec{r}_2) \pm \psi_{\vec{k}_1}(\vec{r}_2)\,\psi_{\vec{k}_2}(\vec{r}_1)$$

'symmetric'
$\rightarrow$ Bosons $+$
$\rightarrow$ Fermions $-$

consider only fermions from now on.

$$\begin{vmatrix} \psi_{\vec{k}_1}(\vec{r}_1) & \psi_{\vec{k}_1}(\vec{r}_2) & \dots & \psi_{\vec{k}_1}(\vec{r}_N) \\ \psi_{\vec{k}_2}(\vec{r}_1) & \psi_{\vec{k}_2}(\vec{r}_2) & \dots & \psi_{\vec{k}_2}(\vec{r}_N) \\ \vdots & & & \vdots \\ \psi_{\vec{k}_N}(\vec{r}_1) & \psi_{\vec{k}_N}(\vec{r}_2) & \dots & \psi_{\vec{k}_N}(\vec{r}_N) \end{vmatrix}$$

Slater Determinant

1st quantised

normalisation factor $\frac{1}{\sqrt{N!}}$

This is a bit complicated ⇒ dependent on N
system size

Describe the states which have electrons / fermions
→ $|k_1 k_2 \dots k_N\rangle$ occupied states.

side note; De Broglie wavelength

non-interacting gas → turn on interactions

$$\frac{p^2}{2m} \sim k_B T \qquad p = \hbar/\lambda \qquad \Rightarrow \lambda = \frac{\hbar}{\sqrt{2mk_BT}}$$

particles $n = r_s^{-1/3}$ imagine them in boxes

comparison $\sim \lambda = \frac{h}{\sqrt{2mk_BT}} \sim r_s$

to check if the De broglie wave lengths <u>overlap</u>.

i.e - He^4
- BEC

Electrons even on room temperature have a very large λ, i.e are a quantum fluids. consider metals and the fermi sea.

* Second Quantisation

Fock space →

$|\bar{k}_1\rangle$

$\frac{1}{\sqrt{2}}(|\bar{k}_1\rangle|\bar{k}_2\rangle - |\bar{k}_2\rangle|\bar{k}_1\rangle)$ like before

or in general i.e $\frac{1}{\sqrt{2}}(|1\rangle|3\rangle - |3\rangle|1\rangle)$

define an operator

$c_1^\dagger$ creation operator

applied to the vacuum $c_n^\dagger|0\rangle = |n\rangle$

explicitly $c_1^\dagger|0\rangle = |1\ 0\ 0\ 0\ 0 \ldots\rangle$

i.e. $|1\rangle \Rightarrow |1\ 0\ 0 \ldots\rangle$

$|2\rangle \Rightarrow |0\ 1\ 0 \ldots\rangle$

$\frac{1}{\sqrt{2}}(|1\rangle|3\rangle - |3\rangle|1\rangle) \Rightarrow |1\ 0\ 1\ 0\ 0 \ldots\rangle$

$c_3^\dagger|1\ 0\ 0 \ldots\rangle = |1\ 0\ 1\ 0 \ldots\rangle \Rightarrow |1,3\rangle$

Want to apply this notation to the Hamiltonian.

note: order of operations matter

example:

$$c_3^\dagger|1\rangle = \tfrac{1}{\sqrt{2}}(|3\rangle|1\rangle - |1\rangle|3\rangle) = |1,3\rangle$$

$$c_5^\dagger|1,3\rangle = (|5\rangle|3\rangle|1\rangle - |5\rangle|1\rangle|3\rangle - |3\rangle|5\rangle|1\rangle + |1\rangle|5\rangle|3\rangle + |3\rangle|1\rangle|5\rangle - |1\rangle|3\rangle|5\rangle)$$

$$= |1,3,5\rangle \Rightarrow |1\ 0\ 1\ 0\ 1\ 0\ 0 \ldots\rangle$$

Order of operations matter

$c_3^\dagger|0\rangle = |3\rangle$

$c_1^\dagger|3\rangle = \frac{1}{\sqrt{2}}(|1\rangle|3\rangle - |3\rangle|1\rangle)$
$= c_1^\dagger c_3^\dagger|0\rangle$
$= -c_3^\dagger c_1^\dagger|0\rangle$ so $\Rightarrow -|1,3\rangle$

They Anti-commute $\boxed{c_\alpha^\dagger c_\beta^\dagger = -c_\beta^\dagger c_\alpha^\dagger}$

so $c_\alpha^\dagger c_\alpha^\dagger = 0$ pauli's exclusion

Annihilation Operator $c_\alpha \rightarrow$ removes a particle from site/state α.

$\boxed{c_\alpha c_\beta = -c_\beta c_\alpha}$ like for the creation operator

$c_\alpha c_\alpha = 0$

note; $c_\alpha|0\rangle = 0$ not $|0\rangle$

Commutation relations

conservation of number of particles so creations = anihilations.

$$c_\alpha^\dagger c_\beta = -c_\beta c_\alpha^\dagger \quad \text{if } \alpha \neq \beta$$

$$= 1 - c_\beta c_\alpha^\dagger \quad \text{if } \alpha = \beta$$

$$\boxed{c_\alpha^\dagger c_\beta = \delta_{\alpha\beta} - c_\beta c_\alpha^\dagger}$$

Krönecker delta function

$$|\alpha,\beta,\gamma\ldots\rangle \equiv |1\,0\,0\ldots\,0\overset{\alpha}{1}0\ldots\,0\overset{\beta}{1}0\ldots\,0\overset{\gamma}{1}0\ldots\rangle$$

Fock space

for this state $c_\alpha^\dagger c_\beta^\dagger c_\gamma^\dagger \ldots |0\rangle = |\alpha\beta\gamma\ldots\rangle$

Writing the Hamiltonian

$\hat{n}_\alpha$ – number of particles in α $= c_\alpha^\dagger c_\alpha$

consider an equal superposition of being on different sites.

$$c_\alpha^\dagger c_\alpha |\ldots \overset{\alpha}{1} \ldots\rangle + |\ldots \overset{\alpha}{0} \ldots\rangle$$

$$c_\alpha^\dagger (|\ldots 0 \ldots\rangle + 0)$$

Consider an observable that can be described by a single particle.

An operator $\hat{O}_1$ $N=1$ $\langle\alpha|\hat{O}_1|\alpha\rangle \equiv O_\alpha$

$\hat{O}$ for $N=1,2,3\ldots\infty$ $\hat{O} = \sum_\alpha O_\alpha \hat{n}_\alpha$

example $\hat{O}_1 = \frac{1}{2m}\left(\frac{\hbar}{i}\nabla_{\vec{r}}\right)^2 \equiv \hat{T}_1$ for wave vector $|k\rangle$

$$\hat{T}_1 |\vec{k}\rangle = \frac{\hbar k^2}{2m}$$

$$\hat{T} = \sum_{\vec{k}} \underbrace{\langle \vec{k} | \hat{T}_1 | \vec{k} \rangle}_{\frac{\hbar^2 k^2}{2m}} \hat{n}_{\vec{k}} = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} \hat{c}^\dagger_{\vec{k}} \hat{c}_{\vec{k}}$$

i.e. Kinetic Energy $\hat{T}$

example for a non-stationary state (not an eigen state)

$\hat{L} = \hat{\vec{r}} \times \hat{\vec{p}}$

$$c^\dagger_\alpha = \sum_n \langle n | \alpha \rangle c^\dagger_n$$

$$c^\dagger_{\vec{k}} = \sum_n \underbrace{\langle \vec{r}_n | \vec{k} \rangle}_{\int d^3\vec{r}\, \varphi^*_n(\vec{r})\, \varphi_k(\vec{r})} c^\dagger_{\vec{r}_n}$$

(superposition of wave packets in a crystal)

changing basis $|\alpha\rangle \to |n\rangle$

$$\hat{O} = \sum_\alpha \langle \alpha | \hat{O} | \alpha \rangle \underbrace{c^\dagger_\alpha}_{\sum_n \langle n|\alpha\rangle c^\dagger_n} \underbrace{c_\alpha}_{\sum_n \langle n|\alpha\rangle^* c_n} =$$

$$= \sum_{nm} \langle n|\alpha\rangle \langle\alpha|O|\alpha\rangle \langle\alpha|m\rangle c_n^{+} c_m$$

$$= \sum_{nm} \langle n|\bar{O}_n|m\rangle c_n^{+} c_m$$

$$\hat{T} = \int d\vec{r} \int d\vec{r}\,' \langle\vec{r}|\, \hat{T}_1 \,|\vec{r}\,'\rangle c_{\vec{r}}^{+} c_{\vec{r}\,'}$$

$$\langle\vec{r}|\hat{T}_1|\vec{r}\,'\rangle = \delta(\vec{r}-\vec{r}\,') \frac{1}{2m} \left(\frac{\hbar}{i} \nabla_{\vec{r}\,'}\right)^2$$

then $\hat{T} = \int d\vec{r}\, c_{\vec{r}}^{+} \frac{1}{2m} \left(\frac{\hbar}{i} \nabla_{\vec{r}}\right)^2 c_{\vec{r}}$

$$\hat{O}^{(2)}_{\alpha\beta} = \langle\alpha|\langle\beta|\, \hat{O}^{(2)} |\alpha\rangle|\beta\rangle$$

$$\hat{V}^{(2)}(\vec{r}_1\vec{r}_2) = \langle\vec{r}_1|\langle r_2|\hat{V}^{(2)}|\vec{r}_1\rangle|\vec{r}_2\rangle$$

example $V^{(2)}(\bar{r}_1\bar{r}_2) = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\bar{r}_1 - \bar{r}_2|}$ Potential energy $\hat{V}$

$$\hat{O} = \frac{1}{2} \sum_{\alpha\beta} O^{(2)}_{\alpha\beta}\, \hat{c}_\alpha^{+} \hat{c}_\beta^{+} \hat{c}_\beta \hat{c}_\alpha$$

$$\hat{V} = \frac{1}{2} \int d^3\vec{r} \int d^3\vec{r}_1\, V^{(2)}(\vec{r}\,\vec{r}\,') \; \hat{c}_{\vec{r}}^{+} \hat{c}_{\vec{r}\,'}^{+} \; \hat{c}_{\vec{r}\,'} \hat{c}_{\vec{r}} \rightarrow$$

$$= \frac{e^2}{8\pi\epsilon_0} \int d^3\vec{r} \int d^3\vec{r}' \frac{1}{|\vec{r}-\vec{r}'|} \underbrace{\hat{c}^{+}_{\vec{r}}}_{\sum_k \underbrace{\langle \vec{r}|\vec{k}\rangle}_{\frac{1}{L^{3/2}} e^{i\vec{k}\cdot\vec{r}}} \hat{c}^{+}_{\vec{k}}} \hat{c}^{+}_{\vec{r}'} \hat{c}_{\vec{r}'} \hat{c}_{\vec{r}}$$

Apply to the Hamiltonian for kinetic and potential energy terms

$$\hat{H} = \hat{T} + \hat{V}$$

to write in Second Quantisation notation.

Reference book;

Quantum Theory of many particle systems.

by Fetter and Walecka

Chapter One.