Multiparticle States of Fermions and Bosons

Consider first a system of distinguishable particles.

Let $|\psi_1\rangle \cdots |\psi_n\rangle \cdots$ be a set of one-particle states

$\Rightarrow$ $|\Psi\rangle = |\psi_1\rangle|\psi_2\rangle\cdots|\psi_N\rangle$ is a multiparticle state with particle 1 in $|\psi_1\rangle, \ldots, n$ in $|\psi_N\rangle$

Let $|\Phi\rangle = |\varphi_1\rangle \cdots |\varphi_N\rangle$ be another such N-particle state.

Clearly

$$\langle \Phi | \Psi \rangle = \prod_{i=1}^{N} \langle \varphi_i | \psi_i \rangle$$ is the inner product.

e.g. position states

$|\vec{x}_1\rangle \cdot |\vec{x}_2\rangle \cdots |\vec{x}_N\rangle$ is such a state

$$(\langle \vec{x}_1| \cdots \langle \vec{x}_N|)(|\vec{y}_1\rangle \cdots |\vec{y}_N\rangle) = \prod_{i=1}^{N} \langle \vec{x}_i | \vec{y}_i \rangle$$
$$= \prod_{i=1}^{N} \delta(\vec{x}_i - \vec{y}_i)$$

and $$I = \int d^3x_1 \cdots d^3x_N \, (|\vec{x}_1\rangle \cdots |\vec{x}_N\rangle)(\langle \vec{x}_1| \cdots \langle \vec{x}_N|)$$

(completeness)

Indistinguishable particles:

$$|\varphi_1 \cdots \varphi_N\rangle \equiv \frac{1}{\sqrt{N!}} \sum_P \zeta^P |\psi_{P(1)}\rangle \cdots |\psi_{P(N)}\rangle$$

$\uparrow$ all permutations of N objects

$\zeta = \begin{matrix} +1 \\ -1 \end{matrix}$ $\begin{matrix} \text{Bosons} \\ \text{Fermions.} \end{matrix}$

These states have the proper symmetry.

examples: (1) two particles $|a\rangle, |b\rangle$ are single particle states

Bosons: $\Rightarrow |a,b\rangle_{\zeta=1} = \frac{1}{\sqrt{2}}\left(|a\rangle|b\rangle + |b\rangle|a\rangle\right)$

and $|a,a\rangle_{\zeta=1} = \frac{1}{\sqrt{2}} 2 |a\rangle|a\rangle = \sqrt{2}|a\rangle|a\rangle$

Fermions: $\Rightarrow |a,b\rangle_{\zeta=-1} = \frac{1}{\sqrt{2}}\left(|a\rangle|b\rangle - |b\rangle|a\rangle\right)$

$|a,a\rangle_{\zeta=-1} = 0$ (Pauli Pple.)

Inner product:

$$\langle \varphi_1 \cdots \varphi_N | \psi_1 \cdots \psi_N\rangle = \begin{vmatrix} \langle\varphi_1|\psi_1\rangle & \cdots & \langle\varphi_1|\psi_N\rangle \\ \vdots & & \\ \langle\varphi_N|\psi_1\rangle & \cdots & \langle\varphi_N|\psi_N\rangle \end{vmatrix}_\zeta$$

matrix

where $|A|_\zeta = \sum_P \zeta^P A_{1P(1)} \cdots A_{NP(N)}$

For $\zeta = -1 \Rightarrow |A|_{-1} = \det A$ (determinant)

$\zeta = +1 \Rightarrow |A|_{+1} = \operatorname{per} A$ (permanent)

Proof:

$\langle \varphi_1 \cdots \varphi_N | \psi_1 \cdots \psi_N \rangle =$

$$= \frac{1}{N!} \sum_{P,Q} \xi^P \xi^Q \left((\langle \varphi_{P(1)}| \cdots \langle \varphi_{P(N)}|)(|\psi_{Q(1)}\rangle \cdots |\psi_{Q(N)}\rangle) \right)$$

$$= \frac{1}{N!} \sum_{P,Q} \xi^P \xi^Q \langle \varphi_{P(1)} | \psi_{Q(1)} \rangle \cdots \langle \varphi_{P(N)} | \psi_{Q(N)} \rangle$$

reordering the set by permuting factors by P

$$= \frac{1}{N!} \sum_{P,Q} \xi^P \xi^Q \langle \varphi_1 | \psi_{QP^{-1}(1)} \rangle \cdots \langle \varphi_N | \psi_{QP^{-1}(N)} \rangle$$

$$\left(\xi^P = \xi^{P^{-1}} \text{ and } \xi^Q \xi^{P^{-1}} = \xi^{QP^{-1}} \right)$$

$$(R = QP^{-1}) \quad = \frac{1}{N!} \sum_{P,R} \xi^R \langle \varphi_1 | \psi_{R(1)} \rangle \cdots \langle \varphi_N | \psi_{R(N)} \rangle$$

$$= | \langle \varphi_i | \psi_j \rangle |_\xi$$

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Let $\{|1\rangle, |2\rangle \ldots\}$ be a complete set of orthonormal states

$$\langle \alpha | \beta \rangle = \delta_{\alpha\beta} \quad , \quad \sum_\alpha |\alpha\rangle\langle\alpha| = I$$

$\Rightarrow$ $|\alpha_1 \cdots \alpha_N\rangle$ ~~(with $\alpha_1 \le \alpha_2 \le \cdots \le \alpha_N$)~~ are a complete set of N-particle states with $\alpha_1 \le \alpha_2 \le \cdots \le \alpha_N$ for bosons and $\alpha_1 < \alpha_2 < \cdots < \alpha_N$ for fermions.

$\Rightarrow$ Normalization: $\dfrac{|\alpha_1 \cdots \alpha_N\rangle}{\sqrt{n_1! \cdots n_N!}}$ Bosons (n_i = # particles in state i) ($\alpha_1 \le \alpha_2 \le \cdots \le \alpha_N$)

$|\alpha_1 \cdots \alpha_N\rangle$ Fermions ($\alpha_1 < \alpha_2 < \cdots < \alpha_N$)

Completeness:

$$I = \frac{1}{N!} \sum_{\alpha_1 \cdots \alpha_N} |\alpha_1 \cdots \alpha_N\rangle \langle \alpha_1 \cdots \alpha_N|$$

Thus we can define a ~~set of~~ Hilbert space for each N. The case $N=0$ has no particles and we will call it the vacuum state $|0\rangle$

Imagine now that the # of particles ~~may~~ is not fixed. This may happen if they are not conserved (as if the system is in contact with a reservoir) or if the particles are actually excitations of another system (as in the e.m. field). We ~~then~~ have to look at the direct sum of these Hilbert spaces $\mathcal{H}_N$, each with fixed N,

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$$

The space $\mathcal{H}$ is called Fock Space.

A generic state in Fock space is the direct sum

$$|\Psi\rangle = \sum_N |\psi^{(N)}\rangle$$

where $|\psi^{(N)}\rangle \in \mathcal{H}_N$

i.e. $|\psi^{(N)}\rangle = |\psi_1 \cdots \psi_N\rangle$

Clearly states on ≠ Hilbert spaces are orthogonal

$$\langle \phi^{(N)} | \psi^{(M)} \rangle = 0 \qquad N \neq M$$

$$\Rightarrow \quad \langle \phi | \psi \rangle = \sum_{N=0}^{\infty} \langle \phi^{(N)} | \psi^{(N)} \rangle$$

$\Rightarrow$ we have

$$\langle \alpha_1 \cdots \alpha_N | \beta_1 \cdots \beta_M \rangle = \delta_{NM} \begin{vmatrix} \delta_{\alpha_1 \beta_1} & \cdots & \delta_{\alpha_1 \beta_N} \\ \vdots & & \\ \delta_{\alpha_N \beta_1} & \cdots & \delta_{\alpha_N \beta_N} \end{vmatrix}_{\zeta}$$

and

$$\sum_{N=0}^{\infty} \frac{1}{N!} \sum_{\alpha_1 \cdots \alpha_N} | \alpha_1 \cdots \alpha_N \rangle \langle \alpha_1 \cdots \alpha_N | = I$$

(completeness)

e.g.

$$\langle \vec{x}_1 \cdots \vec{x}_N | \vec{y}_1 \cdots \vec{y}_M \rangle = \delta_{N,M} \, | \delta(\vec{x}_i - \vec{y}_j) |_{\zeta}$$

$$\text{and} \quad \sum_{N=0}^{\infty} \frac{1}{N!} \int d^3x_1 \cdots d^3x_N \, | \vec{x}_1 \cdots \vec{x}_N \rangle \langle \vec{x}_1 \cdots \vec{x}_N | = I$$

Let $|\Psi\rangle$ be an arb. state in Fock Space.

$$\rightarrow \quad |\Psi\rangle = \sum_{N=0}^{\infty} \frac{1}{N!} \int d^3x_1 \cdots \int d^3x_N \, | \vec{x}_1 \cdots \vec{x}_N \rangle \underbrace{\psi^{(N)}(\vec{x}_1 \cdots \vec{x}_N)}_{\text{N-particle wave function}}$$

$$\psi^{(N)}(\vec{x}_1 \cdots \vec{x}_N) = \langle \vec{x}_1 \cdots \vec{x}_N | \Psi \rangle$$

Since the (basis) states are properly (anti) symmetrized

$\Rightarrow$ $\psi^{(N)}(\vec{x}_1 \cdots \vec{x}_N)$ also have the proper symmetry.

If $|\psi\rangle$ is an N-particle state of the form $|\psi_1 \cdots \psi_N\rangle$

$$\Rightarrow \quad \psi^{(M)}(\vec{x}_1 \cdots \vec{x}_N) = 0 \qquad \text{unless} \quad M = N$$

$$\text{and} \quad \psi^{(N)}(\vec{x}_1 \cdots \vec{x}_N) = \begin{vmatrix} \psi_1(\vec{x}_1) & \cdots & \psi_1(\vec{x}_N) \\ \vdots & & \\ \psi_N(\vec{x}_1) & \cdots & \psi_N(\vec{x}_N) \end{vmatrix}_{\zeta}$$

$$\psi_i(\vec{x}_j) = \langle \vec{x}_j | \psi_i \rangle$$

$\zeta = -1 \Rightarrow$ Slater Determinant.

$\zeta = +1 \Rightarrow$ Permanent.

(L22) Creation and Destruction Operators: We want

to connect different Hilbert spaces in the same Fock space.

Let $|\varphi\rangle$ be a one-particle state and $|\psi_1 \cdots \psi_N\rangle$

an N-particle state $\Rightarrow$ we define the creation operator for the state $|\varphi\rangle$

$$a^+(\varphi)\,|\psi_1 \cdots \psi_N\rangle \equiv |\varphi, \psi_1 \cdots \psi_N\rangle$$

$$\Rightarrow \quad a^+ : \mathcal{H}_N \longmapsto \mathcal{H}_{N+1}$$

Note: $\quad a^+(\varphi)\,|0\rangle = |\varphi\rangle \in \mathcal{H}_1$

Def: Destruction Operator: $\quad a(\varphi) = (a^+(\varphi))^+$

$$a(\varphi) : \mathcal{H}_N \longrightarrow \mathcal{H}_{N-1}$$

Let $|\chi_1 \cdots \chi_{N-1}\rangle \in \mathcal{H}_{N-1}$

$$\Rightarrow \langle \chi_1 \cdots \chi_{N-1} | a(\varphi) | \psi_1 \cdots \psi_N \rangle =$$

$$= \langle \psi_1 \cdots \psi_N | a^\dagger(\varphi) | \chi_1 \cdots \chi_{N-1} \rangle^*$$

$$= \langle \psi_1 \cdots \psi_N | \varphi, \chi_1 \cdots \chi_{N-1} \rangle^*$$

$$= \begin{vmatrix} \langle \psi_1 | \varphi \rangle & \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{N-1} \rangle \\ \vdots & \vdots & & \\ \langle \psi_N | \varphi \rangle & \langle \psi_N | \chi_1 \rangle & \cdots & \langle \psi_N | \chi_{N-1} \rangle \end{vmatrix}_\zeta^*$$

$$= \sum_{k=1}^{N} \zeta^{k-1} \langle \psi_k | \varphi \rangle^* \begin{vmatrix} \langle \psi_1 | \chi_1 \rangle & \cdots & \langle \psi_1 | \chi_{N-1} \rangle \\ & (\text{no } \psi_k) & \\ \langle \psi_N | \chi_1 \rangle & \cdots & \langle \psi_N | \chi_{N-1} \rangle \end{vmatrix}_\zeta^*$$

(expanding in minors)

$$= \sum_{k=1}^{N} \zeta^{k-1} \langle \psi_k | \varphi \rangle^* \langle \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_N | \chi_1 \cdots \chi_{N-1} \rangle^*$$

$$= \sum_{k=1}^{N} \zeta^{k-1} \langle \varphi | \psi_k \rangle \langle \chi_1 \cdots \chi_{N-1} | \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_N \rangle$$

$$\Rightarrow \boxed{a(\varphi) | \psi_1 \cdots \psi_N \rangle = \sum_{k=1}^{N} \zeta^{k-1} \langle \varphi | \psi_k \rangle | \psi_1 \cdots (\text{no } \psi_k) \cdots \psi_N \rangle}$$

$\Rightarrow a(\varphi)$ removes one $|\psi_k\rangle$ at a time leaving an $N-1$ particle state.

From these defs. it follows that

$$a^+(\varphi_1)\, a^+(\varphi_2) = \zeta\, a^+(\varphi_2)\, a^+(\varphi_1)$$

or $$\left[a^+(\varphi_1),\, a^+(\varphi_2)\right]_{-\zeta} = 0$$

$$\Leftrightarrow \quad [A, B]_{-\zeta} = AB - \zeta BA \quad \Rightarrow \quad [A,B]_{-1} = [A,B]$$

commutator

$$[A,B]_{+1} = \{A,B\}$$

anticommutator.

Likewise $$\left[a(\varphi_1),\, a(\varphi_2)\right]_{-\zeta} = 0$$

What about $\left[a(\varphi_1),\, a^+(\varphi_2)\right]_{-\zeta}$?

$$a(\varphi_1)\, a^+(\varphi_2)\, |\psi_1 \cdots \psi_N\rangle =$$

$$= a(\varphi_1)\, |\varphi_2\, \psi_1 \cdots \psi_N\rangle$$

$$= \langle\varphi_1|\varphi_2\rangle\, |\psi_1 \cdots \psi_N\rangle \; +$$

$$+ \sum_{k=1}^{N} \zeta^k \langle\varphi_1|\psi_k\rangle\, |\varphi_2, \psi_1 \ldots (\text{no } \psi_k) \ldots \psi_N\rangle$$

and

$$a^+(\varphi_2)\, a(\varphi_1)\, |\psi_1 \cdots \psi_N\rangle = \sum_{k=1}^{N} \zeta^{k-1} \langle\varphi_1|\psi_k\rangle\, |\varphi_2, \psi_1 \ldots (\text{no } \psi_k) \ldots \psi_N\rangle$$

and also $$\langle\psi_1 \cdots \psi_N|\, a^+(\varphi_2)\, a(\varphi_1)\, |\psi_1 \cdots \psi_N\rangle = \sum_{k=1}^{N} \langle\varphi_1|\psi_k\rangle\langle\varphi|\psi_k\rangle^*$$

Similarly one can prove ~~that~~ $\langle \psi_1 \cdots \psi_N | a^+(\varphi_4)\, a(\varphi_3)\, a^+(\varphi_2)\, a(\varphi_1) | \psi_1 \cdots \psi_N \rangle =$

$$= \sum_{k=1}^{N} \langle \varphi_3 | \varphi_2 \rangle \langle \varphi_1 | \psi_k \rangle \langle \psi_k | \varphi_4 \rangle + \zeta \sum_{k,r=1}^{N} \begin{vmatrix} \langle \psi_r | \varphi_4 \rangle & \langle \psi_r | \varphi_2 \rangle \\ \langle \psi_k | \varphi_4 \rangle & \langle \psi_k | \varphi_2 \rangle \end{vmatrix}_{-\zeta} \langle \varphi_3 | \psi_r \rangle \langle \varphi_1 | \psi_k \rangle$$

$$\Rightarrow \quad [a(\varphi_1), a^+(\varphi_2)]_{-\zeta} = \langle \varphi_1 | \varphi_2 \rangle \cdot I$$

$\Rightarrow$ For the orthonormal one-particle states $\{|\alpha\rangle\}$ we can define $a_\alpha = a(\alpha)$ and $a_\alpha^+ = a(\alpha)^+$

$$\Rightarrow \quad \langle \alpha | \beta \rangle = \delta_{\alpha\beta} \Rightarrow$$

$$[a_\alpha, a_\beta^+]_{-\zeta} = \delta_{\alpha\beta}$$

Bose Case:

Let
$$| n_1\, n_2 \cdots \rangle = \frac{|\overbrace{1 \ldots 1}^{n_1}, \overbrace{2 \ldots 2}^{n_2}, \overbrace{\cdots\cdots}^{n_3} \rangle}{\sqrt{n_1!\, n_2!\, n_3! \cdots}}$$

$$\Rightarrow \quad a_\alpha^+ | n_1\, n_2 \cdots n_\alpha \cdots \rangle = \sqrt{n_\alpha + 1}\; | n_1\, n_2 \cdots n_\alpha + 1 \cdots \rangle$$

$$a_\alpha | n_1\, n_2 \cdots n_\alpha \cdots \rangle = \sqrt{n_\alpha}\; | n_1\, n_2 \cdots n_\alpha - 1 \cdots \rangle$$

and
$$[a_\alpha, a_\beta]_{-\zeta} = [a_\alpha^+, a_\beta^+]_{-\zeta} = 0$$

$$[a_\alpha, a_\beta^+]_{-\zeta} = \delta_{\alpha\beta}$$

The operator which counts the # of particles in the state $|\alpha\rangle$ is $N_\alpha = a_\alpha^+ a_\alpha$

and the total # of particles is

$$N = \sum_\alpha N_\alpha = \sum_\alpha a_\alpha^+ a_\alpha$$

Fermi case $|\alpha_1 \cdots \alpha_N\rangle$ is an N-particle state of fermions.

$$\Rightarrow \quad a^\dagger_\alpha |\alpha_1 \cdots \alpha_N\rangle = |\alpha, \alpha_1 \cdots \alpha_N\rangle \in \mathcal{H}_{N+1}$$

$$a_\alpha |\alpha_1 \cdots \alpha_N\rangle = \sum_{k=1}^{N} (-1)^{k-1} \delta_{\alpha\alpha_k} |\alpha_1 \cdots \alpha_{k-1}, \alpha_{k+1} \cdots \alpha_N\rangle$$

Since $\alpha_1 < \alpha_2 \cdots < \alpha_N$

$\Rightarrow$ we can also use the notation

$$|n_1 n_2 \cdots\rangle = |\alpha_1 \alpha_2 \cdots\rangle$$

state $|\alpha_1\rangle \cdots$ appears n_1 times

$$\Rightarrow \quad (a(\varphi))^2 = (a^\dagger(\varphi))^2 = 0 \qquad \forall |\varphi\rangle$$

(for fermions) (i.e. we can't have two fermions ~~in~~ in the same state).

Clearly:
$$[a_\alpha, a_\beta]_+ = \{a_\alpha, a_\beta\} = 0$$
$$[a^\dagger_\alpha, a^\dagger_\beta]_+ = \{a^\dagger_\alpha, a^\dagger_\beta\} = 0$$

and
$$[a_\alpha, a^\dagger_\beta]_+ = \{a_\alpha, a^\dagger_\beta\} = \delta_{\alpha\beta}$$

are the commutation relations for fermions.

Also
$$|\alpha_1 \cdots \alpha_N\rangle \equiv \prod_{i=1}^{N} a^\dagger_{\alpha_i} |0\rangle$$

$$\Rightarrow \quad \langle \vec{x}_1 \cdots \vec{x}_N | \alpha_1 \cdots \alpha_N\rangle = \langle \vec{x}_1 \cdots \vec{x}_N | \prod_{i=1}^{N} a^\dagger_{\alpha_i} |0\rangle = \det\left[\varphi_{\alpha_i}(\vec{x}_j)\right]$$

Slater Determinant

Consider the one-particle <u>momentum</u> basis $|\vec{p}\rangle$

Since $\langle \vec{p} | \vec{p}\,' \rangle = (2\pi)^3 \delta^3(\vec{p} - \vec{p}\,')$

$$\Rightarrow \left[a(\vec{p}),\ a^{+}(\vec{p}\,') \right]_{-\zeta} = (2\pi)^3 \delta^3(\vec{p} - \vec{p}\,')$$

$$\left[a(\vec{p}),\ a(\vec{p}\,') \right]_{-\zeta} = \left[a^{+}(\vec{p}),\ a^{+}(\vec{p}\,') \right]_{-\zeta} = 0$$

$$\Rightarrow |\vec{p}_1 \cdots \vec{p}_N \rangle = a^{+}(\vec{p}_1) \cdots a(\vec{p}_N) |0\rangle$$

while for the position states $|\vec{x}\rangle$ we get

$$\langle \vec{x} | \vec{x}\,' \rangle = \delta^3(\vec{x} - \vec{x}\,')$$

$$\Rightarrow \left[a(\vec{x}),\ a^{+}(\vec{x}\,') \right]_{-\zeta} = \delta^3(\vec{x} - \vec{x}\,')$$

and $|\vec{x}_1 \cdots \vec{x}_N \rangle = a^{+}(\vec{x}_1) \cdots a^{+}(\vec{x}_N) |0\rangle$

<u>Change of basis:</u>

Let $|\chi\rangle = \alpha |\psi\rangle + \beta |\varphi\rangle$

$$\Rightarrow a^{+}(\chi) = \alpha\, a^{+}(\psi) + \beta\, a^{+}(\varphi)$$

$$a(\chi) = \alpha^{*} a(\psi) + \beta^{*} a(\varphi)$$

a^{+} transforms like kets

a " " bras.

$$|\vec{p}\rangle = \int d^3x \quad |\vec{x}\rangle \langle \vec{x}|\vec{p}\rangle = \int d^3x \; |\vec{x}\rangle \, e^{i\vec{p}\cdot\vec{x}}$$

$$|\vec{x}\rangle = \int \frac{d^3p}{(2\pi)^3} \; |\vec{p}\rangle \langle \vec{p}|\vec{x}\rangle = \int \frac{d^3p}{(2\pi)^3} \; |\vec{p}\rangle \quad e^{-i\vec{p}\cdot\vec{x}}$$

$$\Rightarrow \quad a^+(\vec{p}) = \int d^3x \quad a^+(\vec{x}) \quad e^{i\vec{p}\cdot\vec{x}}$$

$$a^+(\vec{x}) = \int \frac{d^3p}{(2\pi)^3} \quad a^+(\vec{p}) \; e^{-i\vec{p}\cdot\vec{x}}$$

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Operators:

Let $A^{(1)}$ be an operator acting on single particle states, i.e. $\langle \varphi | A^{(1)} | \psi \rangle$ are its matrix elements.

$\Rightarrow$ we want to define an operator A that acts on $|\psi\rangle = |\psi_1 \cdots \psi_N\rangle = |\psi_1\rangle \times \cdots \times |\psi_N\rangle$ as follows

$$A|\psi\rangle = A^{(1)}|\psi_1\rangle \times \cdots \times |\psi_N\rangle + |\psi_1\rangle \times A^{(1)}|\psi_2\rangle \times \cdots \times |\psi_N\rangle +$$
$$+ \cdots + |\psi_1\rangle \times |\psi_2\rangle \times \cdots \times A^{(1)}|\psi_N\rangle$$

For instance, if each $|\psi_i\rangle$ is an eigenstate of $A^{(1)}$,

$A^{(1)}|\psi_i\rangle = a_i |\psi_i\rangle \Rightarrow$

$$A|\psi\rangle = (a_1 + \cdots + a_N)|\psi\rangle$$

In particular, if $A^{(1)} = I^{(1)} \Rightarrow I^{(1)}|\psi_i\rangle = |\psi_i\rangle$

$\Rightarrow A|\psi\rangle = (1 + \cdots + 1)|\psi\rangle = N|\psi\rangle$

$\Rightarrow A = \hat{N}$ the # operator.

We will construct the operator A as follows.

First, we look at $A^{(1)} = |\alpha\rangle\langle\beta|$ where $|\alpha\rangle, |\beta\rangle$ are two one-particle states.

$$\Rightarrow \quad A|\psi\rangle = \langle\beta|\psi_1\rangle |\alpha\, \psi_2 \dots \psi_N\rangle + \langle\beta|\psi_2\rangle |\psi_1\, \alpha\, \psi_3 \dots \psi_N\rangle + \dots + \langle\beta|\psi_N\rangle |\psi_1 \dots \psi_{N-1}\, \alpha\rangle$$

Let us look at the action of $a^+(\alpha)\, a(\beta)$ on $|\psi\rangle$

$$a^+(\alpha)\, a(\beta)|\psi\rangle = \sum_{k=1}^{N} \zeta^{k-1} \langle\beta|\psi_k\rangle |\alpha\, \psi_1 \dots (\text{no } \psi_k) \dots \psi_N\rangle$$

$$= \sum_{k=1}^{N} \langle\beta|\psi_k\rangle |\psi_1 \dots \psi_{k-1}\, \alpha\, \psi_{k+1} \dots \psi_N\rangle$$

$$\Rightarrow \quad A^{(1)} = |\alpha\rangle\langle\beta| \Rightarrow A = a^+(\alpha)\, a(\beta)$$

Similarly

$$A^{(1)} = \sum_{\alpha\beta} A_{\alpha\beta} |\alpha\rangle\langle\beta| \Rightarrow A = \sum_{\alpha,\beta} A_{\alpha\beta}\, a^+(\alpha)\, a(\beta)$$

where $A_{\alpha\beta} = \langle\alpha| A^{(1)} |\beta\rangle$

$$\Rightarrow \quad I^{(1)} = \sum_\alpha |\alpha\rangle\langle\alpha|$$
$$= \int d^3x\, |\vec{x}\rangle\langle\vec{x}|$$
$$= \int \frac{d^3p}{(2\pi)^3} |\vec{p}\rangle\langle\vec{p}|$$

$\Rightarrow$

$$N = \sum_\alpha a^+_\alpha a_\alpha$$
$$= \int d^3x \; a^+(\vec{x}) \, a(\vec{x})$$
$$= \int \frac{d^3p}{(2\pi)^3} \, a^+(\vec{p}) \, a(\vec{p})$$

Momentum: $\vec{p}^{(1)} = \int \frac{d^3p}{(2\pi\hbar)^3} \, \vec{p} \, |\vec{p}\rangle \langle \vec{p}|$

$$= \int d^3x \; |\vec{x}\rangle \, \frac{\hbar}{i} \vec{\nabla} \langle \vec{x}|$$

$$\langle \vec{x} | \vec{p}^{(1)} | \vec{y} \rangle = \frac{\hbar}{i} \vec{\nabla}_x \, \delta(\vec{x}-\vec{y})$$

$\Rightarrow$ total momentum:

$$\vec{P} = \int \frac{d^3p}{(2\pi\hbar)^3} \; \vec{p} \; a^+(\vec{p}) \; a(\vec{p})$$
$$= \int d^3x \quad a^+(\vec{x}) \, \frac{\hbar}{i} \vec{\nabla} a(\vec{x})$$

Hamiltonian

$$H^{(1)} = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x})$$

$$\langle \vec{x} | H^{(1)} | \vec{x}' \rangle = -\frac{\hbar^2}{2m} \nabla_x^2 \, \delta^3(\vec{x}-\vec{x}') + V(\vec{x}) \, \delta^3(x-x')$$

$$\Rightarrow H = \int d^3x \int d^3x' \left[-\frac{\hbar^2}{2m} \nabla_x^2 \, \delta^3(\vec{x}-\vec{x}') + V(\vec{x}) \, \delta^3(x-x') \right] a^+(\vec{x}) \, a(\vec{x}')$$

$$= \int d^3x \quad a^+(x) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] a(\vec{x})$$
$$= \int d^3x \left[\frac{\hbar^2}{2m} (\vec{\nabla} a^+) \cdot (\vec{\nabla} a) + V(\vec{x}) \; a^+(\vec{x}) \, a(\vec{x}) \right]$$

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momentum representation:

$$\langle \vec{p}\,|\,H^{(1)}|\vec{p}\,'\rangle = \frac{\vec{p}^{\,2}}{2m}(2\pi\hbar)^3\,\delta^3(\vec{p}-\vec{p}\,') + \int d^3x\; e^{-i\frac{\vec{p}\cdot\vec{x}}{\hbar}}\,V(\vec{x})\,e^{i\frac{\vec{p}\,'\cdot\vec{x}}{\hbar}}$$

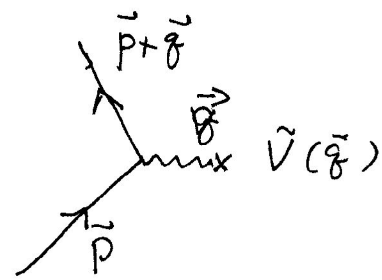
$$= \frac{\vec{p}^{\,2}}{2m}(2\pi\hbar)^3\,\delta^3(\vec{p}-\vec{p}\,') + \tilde{V}(\vec{p}-\vec{p}\,')$$

$$\tilde{V}(\vec{q}) = \int d^3x\; V(\vec{x})\,e^{-\frac{i}{\hbar}\vec{q}\cdot\vec{x}}$$

$$\Rightarrow\quad H = \int\frac{d^3p}{(2\pi\hbar)^3}\,\frac{\vec{p}^{\,2}}{2m}\,a^\dagger(\vec{p})\,a(\vec{p}) + \int\frac{d^3p}{(2\pi\hbar)^3}\int\frac{d^3p'}{(2\pi\hbar)^3}\,\tilde{V}(\vec{p}-\vec{p}\,')\,a^\dagger(\vec{p})\,a(\vec{p}\,')$$

$$= \int\frac{d^3p}{(2\pi\hbar)^3}\,\frac{p^2}{2m}\,a^\dagger(p)\,a(p) + \int\frac{d^3p}{(2\pi\hbar)^3}\int\frac{d^3q}{(2\pi\hbar)^2}\,\tilde{V}(\vec{q})\,a^\dagger(\vec{p}+\vec{q})\,a(\vec{p})$$

the last term destroys a particle of momentum $\vec{p}$ and creates another with momentum $\vec{p}+\vec{q}$ and the amplitude for this process is $\tilde{V}(\vec{q})$



Feynman Diagram

Particle Density $\equiv$ $\rho(\vec{x}) = a^\dagger(\vec{x})\;a(\vec{x})$

$$N = \int d^3x\;\rho(\vec{x}) = \int d^3x\;a^\dagger(\vec{x})\;a(\vec{x})$$

Pot. energy $= \int d^3x\;V(\vec{x})\,\rho(\vec{x})$

<u>Interacting Particles:</u> we need two-particle operators.

such as

$$V^{(2)} = \frac{1}{2} \int d^3x \int d^3y \quad |\vec{x}, \vec{y}\rangle \; V^{(2)}(\vec{x}, \vec{y}) \; \langle \vec{x}, \vec{y}|$$

where $V^{(2)}(\vec{x}, \vec{y})$ is a two-body ~~force~~ potential.

i.e. we want an operator V s.t.

$$V|x_1 \cdots x_N\rangle = \sum_{i<j} V^{(2)}(\vec{x}_i, \vec{x}_j)\, |\vec{x}_1 \cdots \vec{x}_N\rangle$$

$$= \frac{1}{2} \sum_{i \neq j} V^{(2)}(x_i, x_j)\, |\vec{x}_1 \cdots \vec{x}_N\rangle$$

Since $a^+(\vec{x})\, a^+(\vec{y})$ creates the state $|\vec{x}, \vec{y}\rangle$

and $a(\vec{y})\, a(\vec{x})$ destroys the state $|\vec{x}, \vec{y}\rangle$

$$\Rightarrow V = \frac{1}{2} \int d^3x \int d^3y \;\; a^+(\vec{x})\, a^+(\vec{y})\, V^{(2)}(\vec{x}, \vec{y})\, a(\vec{y})\, a(\vec{x})$$

$$\cancel{= \frac{1}{2} \int d^3x \int d^3y \; a^+(x)\, a^+(y)}$$

Can we write V in terms of ρ ?

$$\rho(x)\, \rho(y) = a^+(x)\, a(x)\, a^+(y)\, a(y) =$$

$$= \cancel{\zeta}\; a^+(x)\, a(y)\, \delta(x-y) + \zeta\, a^+(x)\, a^+(y)\, a(x)\, a(y)$$

normal ordering] $\rightarrow$ $= a^+(x)\, a(x)\, \delta(x-y) + \zeta^2\, a^+(x)\, a^+(y)\, a(y)\, a(x)$

since $\zeta^2 = 1$

$$\Rightarrow a^+(x)\, a^+(y)\, a(y)\, a(x) = \rho(x)\, \rho(y) - \rho(x)\, \delta(x-y)$$

$$V = \frac{1}{2}\int d^3x \int d^3y \; V^{(2)}(x,y)\; a^{+}(x)\, a^{+}(y)\, a(y)\, a(x)$$

$$= \frac{1}{2}\int d^3x \int d^3y \; V^{(2)}(x,y)\; \rho(x)\,\rho(y)$$

$$- \frac{1}{2}\int d^3x \int d^3y \; V^{(2)}(x,y)\; \rho(x)\,\delta(x-y)$$

$$\Rightarrow V = \frac{1}{2}\int d^3x \int d^3y \; V^{(2)}(x,y)\; \rho(x)\,\rho(y)$$

$$- \frac{1}{2}\int d^3x \; \rho(x)\; V^{(2)}(x,x)$$

$$\equiv V' - \frac{1}{2}\int d^3x \; \rho(x)\; V^{(2)}(x,x)$$

diagonal term.

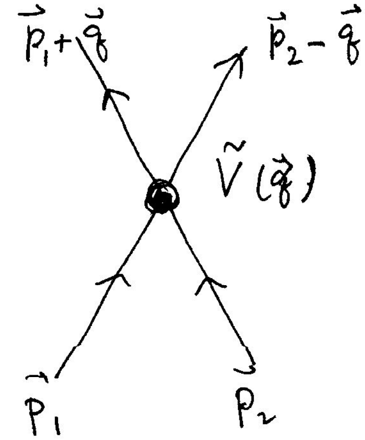
~~Effect of V: it destroys~~

momentum space: $\quad V^{(2)}(x,y) = V(x-y) = \int \frac{d^3p}{(2\pi\hbar)^3}\, \tilde{V}(p)\, e^{\frac{i}{\hbar}\vec{p}\cdot(\vec{x}-\vec{y})}$

$$\Rightarrow V = \frac{1}{2}\int \frac{d^3q}{(2\pi\hbar)^3}\int \frac{d^3p}{(2\pi\hbar)^3}\int \frac{d^3p'}{(2\pi\hbar)^3}\; \tilde{V}(\vec{q})\; a^{+}(\vec{p}+\vec{q})\, a^{+}(\vec{p}\,'-\vec{q})\, a(\vec{p}\,')$$

$a(\vec{p})$

Effect of V:



L42

Ground State of a Free Fermion System:

$\zeta = -1$

Suppose we know the eigenstates of a one-particle Hamiltonian

$H^{(1)}|\alpha\rangle = E_\alpha|\alpha\rangle$ $\qquad \alpha = 1, 2, 3, \ldots$ (labels the states)

$\Rightarrow \quad H = \sum_{\alpha=1}^{\infty} E_\alpha\, a_\alpha^\dagger a_\alpha \quad , \quad E_1 \le E_2 \le E_3 \le \ldots$

$\Rightarrow \quad |\alpha_1 \cdots \alpha_N\rangle = a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_N}|0\rangle$

Notice that $\quad N = \sum_{\alpha=1}^{\infty} a^\dagger_\alpha a_\alpha \quad$ commutes with H

$$[N, H] = 0$$

(i.e. H conserves the # of particles)

$\Rightarrow$ we can specify the # of particles. Suppose we want to understand the behavior of a system with $N = G$ particles. What is the gnd. state of this system?

Clearly $|0\rangle$ is not the gnd state since

$$N|0\rangle = 0 \neq G \,!$$

If the levels are ordered $E_1 \le E_2 \le \ldots \Rightarrow$

the state $|1, \ldots, G\rangle = a_1^\dagger \cdots a_G^\dagger |0\rangle$ has the correct # of particles, i.e.

$$N\, a_1^\dagger \cdots a_G^\dagger|0\rangle = G\, a_1^\dagger \cdots a_G^\dagger |0\rangle$$

[this follows ~~that~~ from that fermions satisfy

$$a^+_\alpha a_\alpha a^+_\beta = \begin{cases} a^+_\beta \; a^+_\alpha a_\alpha & \alpha \neq \beta \\ a^+_\alpha & \alpha = \beta \end{cases} \quad]$$

or $[N, a^+_\beta] = a^+_\beta$

and $\quad H|1\dots G\rangle = \left(\sum_{\beta=1}^{\infty} E_\beta a^+_\beta a_\beta\right) a^+_1 \dots a^+_G |0\rangle$

$$= \left(\sum_{\alpha=1}^{G} E_\alpha\right) a^+_1 \dots a^+_G |0\rangle$$

$\Rightarrow$ the e.v. is $E = \sum_{\alpha=1}^{G} E_\alpha = E_{gnd}$

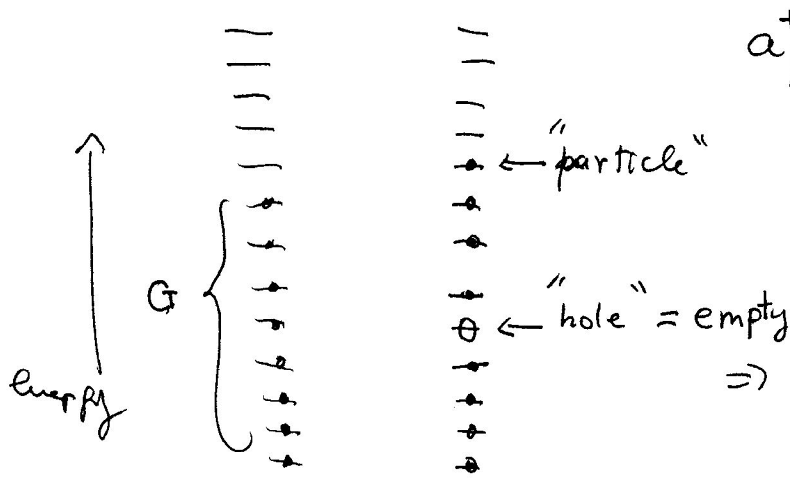
since $E_1 \leq E_2 \leq \dots \Rightarrow E$ has the lowest possible value for this fun (notice that each single particle state is occupied just once).

$\det[\varphi_i(\vec{x}_j)]$

$\Rightarrow$ Gnd state $\quad |gnd\rangle = |1 \dots G\rangle$

$\Rightarrow$ Gnd. state wave function is the Slater Determinant $\langle x_1 \dots x_N | gnd\rangle = \det[\varphi_i(\vec{x}_j)]_{1\leq i\leq G}$

Exitations :



$$a^+_{\alpha_1} a_{\alpha_2} |gnd\rangle \equiv |\alpha_1 \, \alpha_2\rangle$$

$$H \, a^+_{\alpha_1} a_{\alpha_2} |gnd\rangle = (E_{\alpha_1} - E_{\alpha_2} + E_{gnd}) \, a^+_{\alpha_1} a_{\alpha_2} |gnd\rangle$$

$$\Rightarrow E(\alpha_1, \alpha_2) - E_{gnd} = \underbrace{E_{\alpha_1}}_{\text{positive energy}} - \underbrace{E_{\alpha_2}}_{\text{negative energy}} \geq 0$$

$\Rightarrow$ relative to E_{gnd} the particle state $|\alpha_1\rangle$ has positive energy and the "hole" state has negative energy. The excitation energy of the particle-hole pair is ≥ 0

Normal Ordering: Define $b_\beta = a^+_\beta \quad \beta \le G$ as a hole destruction operator.

and $a_\alpha \quad (\alpha > G)$ as a particle destruction operator.

$$\Rightarrow \quad [a_\alpha, a_{\alpha'}]_+ = [a_\alpha, b_\beta]_+ = [b_\beta, b_{\beta'}]_+ = 0$$

$$[a_\alpha, a^+_{\alpha'}]_+ = \delta_{\alpha\alpha'} \qquad [b_\beta, b^+_{\beta'}]_+ = \delta_{\beta\beta'}$$

$$[a_\alpha, b^+_\beta]_+ = 0$$

$\Rightarrow$ $a_\alpha^+ \quad (\alpha > G)$ and $b_\beta^+ \quad (\beta \le G)$ are creation ops.

$$|\underbrace{\alpha_1 \cdots \alpha_m}_{\substack{m\\ \text{particles}}} \underbrace{\beta_1 \cdots \beta_n}_{\substack{n \\ \text{holes}}}, \text{gnd}\rangle = a^+_{\alpha_1} \cdots a^+_{\alpha_m} b^+_{\beta_1} \cdots b^+_{\beta_n} |\text{gnd}\rangle$$

$$\alpha_i > G$$

$$\beta_i \le G$$

$$a_\alpha |\text{gnd}\rangle = b_\beta |\text{gnd}\rangle = 0 \qquad (|\text{gnd}\rangle \text{ is a new vacuum})$$

$$H = \sum_{\alpha=1}^{\infty} E_\alpha a^+_\alpha a_\alpha = \sum_{\alpha=1}^{G} E_\alpha a^+_\alpha a_\alpha + \sum_{\alpha=G+1}^{\infty} E_\alpha a^+_\alpha a_\alpha$$

$$= \sum_{\beta=1}^{G} E_\beta b_\beta b^+_\beta + \sum_{\alpha=G+1}^{\infty} E_\alpha a^+_\alpha a_\alpha$$

$$= \underbrace{\left(\sum_{\beta=1}^{G} E_\beta\right)}_{E_{\text{gnd}}} - \underbrace{\sum_{\beta=1}^{G} E_\beta b^+_\beta b_\beta}_{\text{holes}} + \underbrace{\sum_{\alpha=G+1}^{\infty} E_\alpha a^+_\alpha a_\alpha}_{\text{particles}}$$

$$H = E_{\text{gnd}} + \sum_{\alpha > G} E_\alpha a^+_\alpha a_\alpha - \sum_{\alpha \le G} E_\alpha b^+_\alpha b_\alpha$$

$$N = \sum_{\alpha=1}^{\infty} a_\alpha^+ a_\alpha = \sum_{\alpha=1}^{G} a_\alpha^+ a_\alpha + \sum_{\alpha > G} a_\alpha^+ a_\alpha$$

$$= \sum_{\alpha \le G} b_\alpha b_\alpha^+ + \sum_{\alpha > G} a_\alpha^+ a_\alpha$$

$$\Rightarrow N = G + \underbrace{\sum_{\alpha > G} a_\alpha^+ a_\alpha}_{\text{particles}} - \underbrace{\sum_{\alpha \le G} b_\alpha^+ b_\alpha}_{\text{holes.}} =$$

Similarly:

$$U = \sum_{\alpha, \beta} U^{(1)}_{\alpha\beta} a_\alpha^+ a_\beta$$

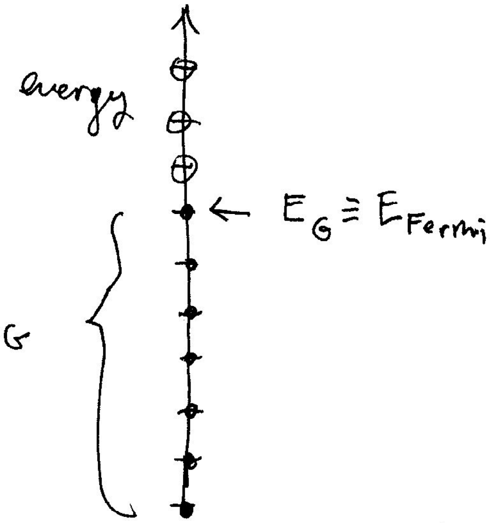
$$= \sum_{\substack{\alpha > G \\ \beta > G}} U^{(1)}_{\alpha\beta} a_\alpha^+ a_\alpha + \underbrace{\sum_{\substack{\alpha > G \\ \beta \le G}} U^{(1)}_{\alpha\beta} a_\alpha^+ b_\beta^+}_{\text{creates a particle hole pair}}$$

$$+ \underbrace{\sum_{\substack{\alpha \le G \\ \beta > G}} U^{(1)}_{\alpha\beta} b_\alpha a_\beta}_{\text{destroys a particle hole pair.}} - \sum_{\substack{\alpha \le G \\ \beta \le G}} U^{(1)}_{\alpha\beta} b_\beta^+ b_\alpha + \underbrace{\sum_{\alpha \le G} U^{(1)}_{\alpha\alpha}}_{\text{energy shift.}}$$

Notice that N is still conserved ($[N, U] = 0$)

but $N' = \sum_{\alpha > G} a_\alpha^+ a_\alpha + \sum_{\alpha \le G} b_\alpha^+ b_\alpha$ is <u>not</u> conserved

Back to the spectrum



Since all the action takes place near $E_\phi = E_F$, we will shift the zero of the energy to E_F and define

$$E_\alpha = \mathcal{E}_\alpha + E_F \qquad (E_F = E_G)$$

$$\Rightarrow \mathcal{E}_{gnd} = \sum_{\alpha=1}^{G} \mathcal{E}_\alpha = \sum_{\alpha=1}^{G} (E_\alpha - E_F)$$

$$\Rightarrow \quad \mathcal{E}_{gnd} = E_{gnd} - G\,E_G$$

Now we have

$$H = \mathcal{E}_{gnd} + \sum_{\alpha > G} \mathcal{E}_\alpha\, a^+_\alpha a_\alpha - \sum_{\alpha \le G} \mathcal{E}_\alpha\, b^+_\alpha b_\alpha$$

but since $\quad \mathcal{E}_\alpha = E_\alpha - E_G$

$$\Rightarrow \alpha > G \quad , \mathcal{E}_\alpha > 0$$

$$\alpha < G \quad , \mathcal{E}_\alpha < 0 \quad \Rightarrow \quad -\mathcal{E}_\alpha > 0$$

$\Rightarrow$ the excitations created by a^+_α have ~~energy~~ energy $\mathcal{E}_\alpha > 0$ $(\alpha > G)$ while the excitation created by b^+_α have energy $-\mathcal{E}_\alpha > 0 \qquad (\alpha \le G)$

i.e. $\quad H\, a^+_\alpha |gnd\rangle = \mathcal{E}_\alpha\, a^+_\alpha |gnd\rangle$ + gnd state energy

$\quad H\, b^+_\alpha |gnd\rangle = -\mathcal{E}_\alpha\, b^+_\alpha |gnd\rangle$ + gnd. state energy

and $\quad -\mathcal{E}_\alpha = -(E_\alpha - E_F) = E_F - E_\alpha \geq 0$ for $\alpha \le G$

Likewise the charge (relative to the gnd state) is

$$Q = -e\left(\sum_{\alpha=1}^{\infty} a_\alpha^+ a_\alpha - G\right)$$

$$Q = -e\left(\sum_{\alpha>G} a_\alpha^+ a_\alpha - \sum_{\alpha\le G} b_\alpha^+ b_\alpha\right)$$

$$\Rightarrow \quad Q\, a_\alpha^+|\text{gnd}\rangle = -e\, a_\alpha^+|\text{gnd}\rangle \qquad (\alpha > G)$$

$$Q\, b_\alpha^+|\text{gnd}\rangle = +e\, b_\alpha^+|\text{gnd}\rangle$$

$\Rightarrow$ We have two types of excitations, with opposite charges, called <u>particles</u> and <u>holes</u> (or <u>particles</u> and <u>antiparticles</u> in relativistic theories).

<u>Example</u>: Free fermions in a large box of volume $V = L^3$

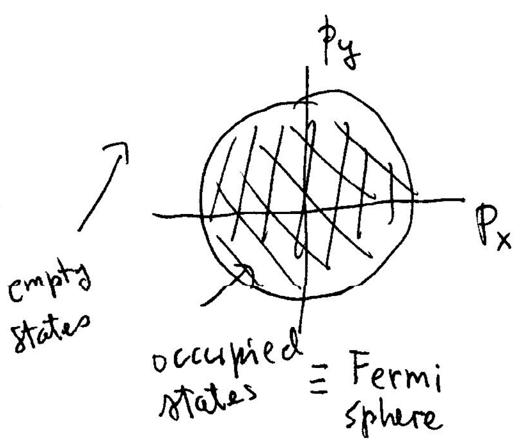
states: plane waves $\langle \vec{x}|\vec{k}\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{x}}$

$$E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$$

If we have N fermions

$$N = \sum_{\text{spin}} \sum_{\substack{\text{occupied}\\ \text{states}}} 1 = (2s+1) V \int \frac{d^3 k}{(2\pi\hbar)^3}\, \theta(p_F - |p|)$$

Fermi momentum.



$$N = (2s+1)\frac{V}{(2\pi\hbar)^3}\int_0^{p_F} dp\, p^2\, 4\pi = \frac{4\pi}{3} V \frac{p_F^3}{(2\pi\hbar)^3}$$

$$\frac{N}{V} = \bar{\rho} = \underset{(2s+1)}{\uparrow}\frac{4\pi}{3}\frac{p_F^3}{(2\pi\hbar)^3} \Rightarrow p_F = 2\pi\hbar\left(\frac{3\bar{\rho}}{4\pi \underset{2s+1}{\uparrow}}\right)^{1/3}$$

Fermi Energy: $E_F = \dfrac{P_F^2}{2m}$ where $P_F = 2\pi\hbar \left(\dfrac{3\rho}{8\pi}\right)^{1/2}$

($2S+1 = 2$ for $S=1/2$)

$\Rightarrow$ $\sigma = \uparrow, \downarrow$

$$a_\sigma^\dagger(\vec{x}) = \int \frac{d^3p}{(2\pi\hbar)^3}\, a_\sigma^\dagger(\vec{p})\, e^{-i\vec{p}\cdot\vec{x}}$$

$$\equiv \int_{|\vec{p}|>P_F} \frac{d^3p}{(2\pi\hbar)^3}\, a_\sigma^\dagger(\vec{p})\, e^{-i\vec{p}\cdot\vec{x}}$$

$$+ \int_{|\vec{p}|<P_F} \frac{d^3p}{(2\pi\hbar)^3}\, b_\sigma(\vec{p})\, e^{-i\vec{p}\cdot\vec{x}}$$

Gnd. state: $|gnd\rangle = \prod_{|\vec{p}|<P_F} \prod_{\sigma} a_\sigma^\dagger(\vec{p})\, |0\rangle$ $\equiv$ "Filled Fermi Sea"

empty state

Excitations: $|-e, \vec{p}, \sigma\rangle \equiv a_\sigma^\dagger(\vec{p})\, |gnd\rangle$
$|\vec{p}| > P_F$

This state has energy $\dfrac{\vec{p}^{\,2}}{2m} - E_F$, spin $\sigma = \pm\frac{1}{2}$, momentum $\vec{p}$ and charge $-e$. It is an <u>electron</u>.

$|+e, \vec{p}, \sigma\rangle \equiv b_\sigma^\dagger(\vec{p})\, |gnd\rangle$ $\quad$ ($|\vec{p}| < P_F$)

it has energy $E_F - \dfrac{\vec{p}^{\,2}}{2m}$, momentum $\vec{p}$, spin $\sigma = \pm\frac{1}{2}$ and charge $+e$. It is a <u>hole</u>.

Interacting Systems

In general it is very hard to deal with interacting systems. Examples of exactly solvable interacting systems are very rare and very special. Thus, in general it becomes necessary to resort to approximate methods to solve a general problem. The most common approach is perturbation theory. It is a useful way to gain intuition but in many cases is either not very accurate or just plain wrong (although this happens mostly for systems with $N \to \infty$).

I will describe a variational approach which has many generalizations in the form of mean field theories. These are not a panacea either but are much better than straightforward perturbation theory.

A typical variational approach goes as follows. Let H be a Hamiltonian and let Ψ be a ("trial") wave function. The wave function will be required to be normalized

$\Rightarrow \int d\sigma\ \psi^* \psi = 1$

$\uparrow$ integral over all degrees of freedom.

Let us consider the average energy

$$\langle \psi | H | \psi \rangle = \int dv\ \psi^* H\ \psi$$

We want to find ψ subject to the condition that $\langle \psi | H | \psi \rangle$ is a minimum and ψ is normalized $\Rightarrow$ use Lagrange multipliers. Form the quantity

$$F = \int dv\ \psi^* H\ \psi - E\left(\int dv \psi^* \psi - 1\right)$$

$E \in \mathbb{R}$

Extremum $\Rightarrow$ $\dfrac{\delta F}{\delta E} = 0 \Longrightarrow \int dv\ |\psi|^2 = 1$

and $\int dv\ \left[\delta\psi^* (H-E)\psi + \psi^*(H-E)\delta\psi\right] = 0$

$\Rightarrow \int dv \left[\delta\psi^* (H-E)\psi + ((H-E)\psi)^* \delta\psi\right] = 0$

$\Rightarrow$ variations over $\delta\psi$ and $\delta\psi^*$ are indep. $\Rightarrow$

$(H-E)\psi = 0$

$\Rightarrow H\psi = E\psi \Rightarrow$ E must be an eigenvalue.

Let u_n be a complete set of eigenstates of H

$\Rightarrow \quad \psi = \sum_n a_n u_n$

$$\Rightarrow \quad \langle \psi | \psi \rangle = 1 \Rightarrow \sum_n |a_n|^2 = 1$$

and $\quad H u_n = E_n u_n$

$$H\,\psi = E\,\psi = \sum_n a_n E_n u_n$$

$$\Rightarrow \quad \langle \psi | H | \psi \rangle = \sum_n |a_n|^2 E_n \geqslant E_0 \sum_n |a_n|^2 = E_0$$

$$(E_n \geqslant E_0)$$

$\Rightarrow \quad \langle \psi | H | \psi \rangle \geqslant E_0 \Rightarrow$ i.e. $\langle \psi | H | \psi \rangle$ is an upper bound of the ground state energy.

We will now look at a many particle (electron) system from this point of view.

<u>Hartree - Fock Theory</u>

Consider a system such as a multi-electron atom (or, for this matter, it would also be a system of electrons in a solid). ~~Define~~ We define some so far unknown one-particle states (spin included) $u_i(r,\sigma) \equiv u_i(r)\,\chi_i(m)$

orbital ↑ spin ↑

and form the N-electron antisymmetric (Slater) state

$$|\Psi\rangle = \prod_{j=1}^{N} a_j^{+}[u_i] \; |0\rangle$$

$$\Rightarrow \langle \vec{x}_1 m_1; \cdots ; \vec{x}_N m_N | \Psi \rangle = \psi^{(N)}(\vec{r}_1 m_1, \cdots, r_N m_N)$$

$$\psi^{(N)}(\vec{r}_1 m_1, \cdots, \vec{r}_N m_N) = \frac{1}{\sqrt{N!}} \; \det \left[u_i(\vec{r}_j) \, \chi_i[m_j] \right]$$

Slater determinant.

The Hamiltonian is

$$H = \int d^3r \sum_m a_m^{+}(\vec{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right] a_m(\vec{r})$$

$$+ \frac{1}{2} \int d^3r \int d^3r' \sum_{m,m'} a_m^{+}(\vec{r}) \; a_m(\vec{r}) \; a_{m'}^{+}(\vec{r}') \; a_{m'}(\vec{r}') \, U(\vec{r}-\vec{r}')$$

$$V(\vec{r}) = - \frac{Ze^2}{|\vec{r}|}$$ (attractive) interaction with nucleus.

$$U(\vec{r}-\vec{r}') = + \frac{e^2}{|\vec{r}-\vec{r}'|}$$ electron-electron Coulomb repulsion.

(L25)

$u_i(\vec{r}_j, m_j)$ ← spin projection.

$u_i(j) \equiv$ ~~[illegible]~~ ; $r_{ij} = |\vec{r}_i - \vec{r}_j|$

$$\Rightarrow \langle H \rangle = \sum_i \int d^3r\, u_i^*(\vec{r}) \left[-\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r} \right] u_i(\vec{r})$$

↑ including sum over spin projections

$$+ \sum_{i<j} \left[\int d^3r_1 \int d^3r' \frac{e^2}{|\vec{r}-\vec{r}'|} |u_i(\vec{r})|^2 |u_j(\vec{r}')|^2 \right.$$

$V(r) = -\frac{Ze^2}{r}$

$$\left. - \delta_{m_i m_j} \int d^3r \int d^3r' \frac{e^2}{|\vec{r}-\vec{r}'|} u_i^*(\vec{r}) u_j^*(\vec{r}') u_j(\vec{r}) u_i(\vec{r}') \right]$$

We will minimize $\langle H \rangle$ subject to the condition that the wavefunctions $u_i(\vec{r})$ are orthonormal.

Actually, for a Slater det. state it is sufficient to require that each u_i / $\int d^3r\, |u_i(\vec{r})|^2 = 1$ and orthogonality follows (Bethe & Jackiw).

$\Rightarrow$ We extremize the expression

$$F = \langle H \rangle - \sum_i \varepsilon_i \left[\int d^3r\, |u_i(r)|^2 - 1 \right]$$

(sum over sp states included)

We will vary u_i and u_i^* arbitrarily

$$\Rightarrow \int dr\, \delta u_i^*(r) \Big[-\varepsilon_i u_i(r) + \left(-\frac{\hbar^2}{2m} \nabla^2 + V(r) \right) u_i(r) +$$

$$+ \sum_j \int dr'\, u_j^*(r') \frac{e^2}{|r-r'|} \Big(u_i(r) u_j(r') -$$

$$- \delta_{m_i m_j} u_i(r') u_j(r) \Big) + \text{c.c.} \Big] = 0$$

$\Rightarrow$

$$-\frac{\hbar^2}{2m}\nabla^2 u_i(\vec r) - \frac{Ze^2}{r} u_i(r) +$$

$$+ \left[\sum_j \int d^3r' \frac{e^2}{|r-r'|} |u_j(r')|^2\right] u_i(r)$$

$$- \sum_j \delta_{m_i m_j} \left[\int d^3r' \frac{e^2}{|r-r'|} u_j^*(r') u_i(r')\right] u_j(r) =$$

$$= \varepsilon_i u_i(r)$$

This ~~are~~ is the Hartree-Fock equation.

We recognize

$$\int d^3r' \frac{e^2}{|r-r'|} \sum_j |u_j(r')|^2 \quad \text{as the Coulomb Integral}$$

and the exchange integral

$$\int d^3r' \frac{e^2}{|r-r'|} u_j^*(r') u_i(r')$$

We see that we can define an <u>effective potential</u> <u>$V_{eff}(\vec r)$</u>

$$V_{eff}(\vec r) = -\frac{Ze^2}{r} + \sum_j \int d^3r' \frac{e^2}{|r-r'|} |u_j(r')|^2$$

$$- \sum_j \delta_{m_i m_j} \int d^3r' \frac{e^2}{|r-r'|} u_j^*(r') u_i(r')$$

which ~~is~~ a ~~[illegible]~~ function(al) of the $u_i(r)$'s which satisfy

$$-\frac{\hbar^2}{2m}\nabla^2 u_i + V_{eff}(\vec r) u_i = \varepsilon_i u_i$$

This is an example of a self-~~[illegible]~~ consistent approximation.

what is the energy of the state?

$$E = \sum_i \varepsilon_i - \sum_{i<j} \int d^3r \int d^3r' \frac{e^2}{|r-r'|} u_i^*(r)\, u_j^*(r') \Big[\underbrace{u_i(r)\, u_j(r')}_{\text{direct}} - \underbrace{u_i(r')\, u_j(r)}_{\text{exchange}} \Big]$$

[please recall that $u_i(r) \equiv \underbrace{u_i(r)}_{\text{orbital}} \underbrace{\chi_i(m)}_{\text{spin}}$]

[$\int d^3r \to \int d^3r \sum_m$ etc.]

<u>Hartree and Thomas-Fermi:</u>

If the exchange terms are neglected $\Rightarrow$ we can identify $\underbrace{\sum_j}_{\text{including spin}} |u_j(\vec{r})|^2 = \rho(\vec{r})$ $\leftarrow$ density

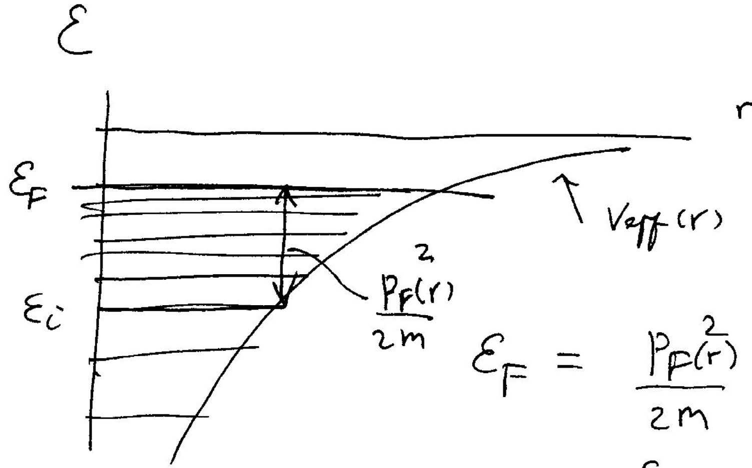
$$\Rightarrow \quad V_{eff}(\vec{r}) = \int d^3r' \frac{e^2}{|\vec{r}-\vec{r}'|} \rho(\vec{r}') - \frac{Ze^2}{r} \qquad \text{(Hartree)}$$

Thomas-Fermi: $V_{eff}(r)$ varies slowly in the region where most electrons are present $\Rightarrow$ semiclassical approx. (WKB)

$$\Rightarrow u_i(\vec{r}) \sim e^{\frac{i}{\hbar} \vec{p}_i(\vec{r}) \cdot \vec{r}} \times \text{spin factor.}$$

$$\Rightarrow \quad \varepsilon_i = \frac{\vec{p}_i^{\,2}}{2m} + V_{eff}(\vec{r})$$

OK if $\varepsilon_i \gg V_{eff}(\vec{r})$



$$\mathcal{E}_F = \frac{p_F^2(r)}{2m} + V_{eff}(r)$$

$$\Rightarrow \quad p_F(r) = \left[2m\left(\mathcal{E}_F - V_{eff}(r)\right)\right]^{1/2}$$

since $V_{eff} \simeq$ const $\Rightarrow$ (to a first approx.) $\rho(r)$ is determined by p_F

(as in a free Fermi gas)

$$\rho(\vec{r}) = \frac{p_F^3(r)}{3\pi^2\hbar^3} \Rightarrow \quad p_F(r) = \hbar\left(3\pi^2\rho(r)\right)^{1/3}$$

$$\hbar\left(3\pi^2\rho(r)\right)^{1/3} = \left(2m\left(\mathcal{E}_F - V_{eff}(r)\right)\right)^{1/2}$$

$$\boxed{\rho(r) = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\left(\mathcal{E}_F - V_{eff}(r)\right)\right)^{3/2}}$$

But

$$V_{eff}(r) = \int d^3r' \, \frac{e^2}{|r-r'|}\rho(r') - \frac{Ze^2}{r}$$

and $\displaystyle -\nabla_r^2 \frac{1}{|r-r'|} = 4\pi\delta(r-r')$

$$\Rightarrow \quad -\nabla^2 V_{eff}(r) = \int d^3r' \, e^2\rho(r') \, 4\pi\delta(r-r') - Ze^2 4\pi\delta(r)$$

nucleus.

$$\boxed{-\nabla^2 V_{eff}(r) = 4\pi e^2\rho(r) - 4\pi Z e^2\delta(r)}$$

For $r \to 0$ $\quad V_{eff} \sim -\frac{Ze^2}{r}$

and for $r \to \infty$ $\quad V_{eff} \to 0$ (screening). (for a neutral atom)

I will look for isotropic solutions

$$\Rightarrow \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}\left(-V_{eff}(r)\right) = \frac{4e^2}{3\pi}\left[\frac{2m}{\hbar^2}\left(\varepsilon_F - V_{eff}(r)\right)\right]^{3/2}$$

$$V_{eff}(r) = -\frac{Ze^2}{r}\,\Phi(r) \quad , \quad r = \frac{bx}{Z^{1/3}}$$

$$b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{2/3} a_0 = 0.8853\, a_0$$

$$\Rightarrow \sqrt{x}\,\frac{d^2\Phi}{dx^2} = \Phi^{3/2}$$

with the b.c.'s $\quad \Phi(0) = 1 \quad$ and $\quad \Phi(\infty) = 0$

$$\Rightarrow \Phi(x) \approx \begin{cases} 1 - 1.59\,x + \cdots & \text{as } x \to 0 \\ \frac{144}{x^3}, & \text{as } x \to \infty \end{cases}$$

$$\Rightarrow V_{eff}(r) = -\frac{Ze^2}{r} + 1.80\, Z^{4/3}\frac{e^2}{a_0} + \cdots \quad (\text{small } r)$$