Second quantization

Indistinguishable particles → no need to distinguish them! Only thing that matters is how many.
Suppose we can figure out a basis of non-interacting single particle states of some operator $\hat{O}$

$$\hat{O}\,|\psi_i\rangle = k_i\,|\psi_i\rangle \quad \text{for } i\text{-th state}$$

(Example $\{|lm\rangle\}$ states $\hat{L}^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle$)
For multiple particles we can now describe their collective state as

$$|n_1, n_2, \ldots n_i \ldots\rangle$$

$\uparrow$ # of particle in state $|\psi_1\rangle$

$\{n_i\}$ – occupation numbers

This is a description of a state in Fock space (or Fock states)

Special cases: vacuum state

$$|0\rangle = |0, 0 \ldots 0 \ldots\rangle$$

Single-particle state ($n_i = 1$, $n_j = 0$ for $i \neq j$)

$$|0 \ldots 0, n_i = 1, 0 \ldots\rangle = |k_i\rangle \quad (\text{same as } |\psi_i\rangle)$$

We need operators to act in Fock space:

creation operator $\hat{a}_i^+$: $\hat{a}_i^+ |n_1, \ldots n_i, \ldots\rangle \propto |n_1, \ldots n_i+1 \ldots\rangle$

anihilator operator $\hat{a}_i$: $\hat{a}_i |n_1 \ldots n_i \ldots\rangle \propto |n_1 \ldots n_i - 1 \ldots\rangle$

Clearly

$$\hat{a}_i^+ |\emptyset\rangle = |k_i\rangle$$

Thus

$$\langle k_i | k_i \rangle = 1 \quad (\hat{a}_i^+ |\emptyset\rangle)^+ \hat{a}_i^+ |\emptyset\rangle = \langle \emptyset | \hat{a}_i \hat{a}_i^+ |\emptyset\rangle =$$

$$= \langle \emptyset | \underbrace{\hat{a}_i | k_i \rangle}_{= |\emptyset\rangle} = 1$$

$$\hat{a}_i | k_i \rangle = |\emptyset\rangle \qquad \text{vacuum state}$$

and $\hat{a}_i |\emptyset\rangle = 0$

Consequently $\hat{a}_i | k_j \rangle = \delta_{ij} \cdot |\emptyset\rangle$

Two-particle state

Bosons: $\hat{a}_i^+ \hat{a}_j^+ |\emptyset\rangle = \hat{a}_i^+ \hat{a}_j^+ |00\rangle = |11\rangle =$

$= \frac{1}{\sqrt{2}} (|\psi_i\rangle |\psi_j\rangle + |\psi_j\rangle |\psi_i\rangle)$ — must obey the symmetry

$\hat{a}_i^+ \hat{a}_j^+ |\emptyset\rangle = \hat{a}_j^+ \hat{a}_i^+ |\emptyset\rangle$

Fermions: $\hat{a}_i^+ \hat{a}_j^+ |\emptyset\rangle = \hat{a}_i^+ \hat{a}_j^+ |00\rangle = \hat{a}_i^+ |01\rangle = |11\rangle$

but $\hat{a}_j^+ \hat{a}_i^+ = \hat{a}_j^+ |10\rangle = -|11\rangle$

Bosons

use commutators $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$

Fermions

use anticommutators $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

Bosons	Fermions
$0 = \hat{a}_i^+\hat{a}_j^+ - \hat{a}_j^+\hat{a}_i^+ = [\hat{a}_i^+, \hat{a}_j^+]$	$0 = \hat{a}_i^+\hat{a}_j^+ + \hat{a}_j^+\hat{a}_i^+ = \{\hat{a}_i^+, \hat{a}_j^+\}$
$\hat{a}_i\hat{a}_j - \hat{a}_j\hat{a}_i = [\hat{a}_i, \hat{a}_j] = 0$	$\hat{a}_i\hat{a}_j + \hat{a}_j\hat{a}_i = \{\hat{a}_i, \hat{a}_j\} = 0$
$\hat{a}_i\hat{a}_j^+ - \hat{a}_j^+\hat{a}_i = [\hat{a}_i, \hat{a}_j^+] = \delta_{ij}$	$\hat{a}_i\hat{a}_j^+ + \hat{a}_j^+\hat{a}_i = \{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij}$
$\underline{\hat{a}_i\hat{a}_i^+ - \hat{a}_i^+\hat{a}_i = 1}$	$\underline{\hat{a}_i\hat{a}_i^+ + \hat{a}_i^+\hat{a}_i = 1}$

The "only" difference in statistics is in the sign!

Number operator: measures the occupation numbers

Single-particle state: $\hat{N}_i = \hat{a}_i^+\hat{a}_i$

$\hat{N}_i \, |n_1, n_2 .. \, n_i ...\rangle = n_i \, |n_1, n_2 ... \, n_i ...\rangle$

Total number of particles operator

$\hat{N} = \sum_i \hat{a}_i^+\hat{a}_i = \sum_i \hat{N}_i$

$\hat{N} \, |n_1, n_2 ... \, n_i ..\rangle = (n_1 + n_2 + .. \, n_i + ...) \, |n_1, n_2 ... \, n_i ...\rangle$

One can also show that

$\hat{a}_i \, |... \, n_i ...\rangle = \sqrt{n_i} \, |... \, n_i - 1 .\rangle$

$\hat{a}_i^+ \, |... \, n_i ..\rangle = \sqrt{n_i + 1} \, |... \, n_i + 1 ...\rangle$

(thus $\hat{a}_i^+\hat{a}_i \, |.. \, n_i ...\rangle = \hat{a}_i^+ \, |.. \, n_i - 1 ..\rangle \cdot \sqrt{n_i} =$

$= n_i \, |... \, n_i ...\rangle$

Also, for fermions $n_i = 0$ or 1 only

$(a_i^+)^2 \, |\emptyset\rangle = 0$ Pauli exclusion principle

We now know how to count particles in the states of a particular operator. What if we need to work with a different basis?

$$\hat{O}|\psi_i\rangle = k_i|\psi_i\rangle \quad \text{or} \quad k_i|k_i\rangle$$

and it is more convenient to "recount" the particles in a different basis $\{|\varphi_i\rangle\}$

$$|\psi_i\rangle = \sum_j |\varphi_j\rangle\langle\varphi_j|\psi_i\rangle$$

$\hat{b}_j$ and $\hat{b}_j^+$ are the annihilation and creation operators in the new basis

$$|\varphi_j\rangle = \hat{b}_j^+|\emptyset\rangle$$

Important: vacuum is the same in <u>all</u> bases!

$$|\psi_i\rangle = \hat{a}_i^+|\emptyset\rangle = \sum_j \hat{b}_j^+|\emptyset\rangle\langle\varphi_j|\psi_i\rangle$$

$$\Rightarrow \hat{a}_i^+ = \sum_j \langle\varphi_j|\psi_i\rangle\, \hat{b}_j^+$$

"Additive" single-particle operator

$\hat{\mathcal{K}} |k_i\rangle = k_i |k_i\rangle$

$\hat{\mathcal{K}} |\psi\rangle = \hat{\mathcal{K}} |n_1, n_2, n_3, \ldots\rangle = \sum n_i k_i |\psi\rangle$

Kinetic energy, momentum, any operator with single-particle action

$$\hat{\mathcal{K}} = \sum_i k_i \hat{N}_i = \sum_i k_i \hat{a}_i^+ \hat{a}_i =$$

$$= \sum_i k_i \sum_m \hat{b}_m^+ \langle \varphi_m | \psi_i \rangle \sum_n \hat{b}_n (\langle \varphi_n | \psi_i \rangle)^* =$$

$$= \sum_i k_i \sum_{n,m} \hat{b}_m^+ \langle \varphi_m | \psi_i \rangle \langle \psi_i | \varphi_n \rangle \hat{b}_n =$$

$$= \sum_{n,m} \hat{b}_m^+ \hat{b}_n \langle \varphi_m | \underbrace{\left\{ \sum_i |\psi_i\rangle k_i \langle \psi_i | \right\}}_{= \hat{\mathcal{K}} \sum_i |\psi_i\rangle\langle\psi_i| = \hat{\mathcal{K}}} | \varphi_n \rangle =$$

$$= \sum_{n,m} \hat{b}_m^+ \hat{b}_n \langle \varphi_m | \hat{\mathcal{K}} | \varphi_n \rangle$$

The rule of the second quantization for any non-interacting particles

Can use this trick to calculate the eigenvalues for any additive operator (i.e. for non-interactive particles)

$$|\psi_i\rangle \xleftrightarrow{\hat{V}_{ij}} |\psi_j\rangle$$

Interactions b/w the particles

$$\hat{V}_{int} = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} V_{ij} \hat{N}_i \hat{N}_j + \frac{1}{2} \sum_i V_{ii} (\hat{N}_i^2 - \hat{N}_i) =$$

$$= \frac{1}{2} \sum_{i,j} V_{ij} (\hat{N}_i \hat{N}_j - \hat{N}_i \delta_{ij}) = \frac{1}{2} \sum_{i \neq j} V_{ij} \hat{\Pi}_{ij}$$

$\hat{\Pi}_{ij} = \hat{N}_i \hat{N}_j - \delta_{ij} \hat{N}_i$ pair distribution operator

$$\hat{\Pi}_{ij} = \hat{a}_i^+ \hat{a}_i \hat{a}_j^+ \hat{a}_j - \delta_{ij} \hat{a}_i^+ \hat{a}_i = \hat{a}_i^+ (\delta_{ij} \pm \hat{a}_j^+ a_i) \hat{a}_j - \delta_{ij} \hat{a}_i^+ \hat{a}_i =$$

$$= \pm \hat{a}_i^+ \hat{a}_j^+ \hat{a}_i \hat{a}_j = (\pm)^2 \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i = \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i$$

$$\hat{V}_{int} = \frac{1}{2} \sum V_{ij} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_j \hat{a}_i$$

Following the same procedure as for a single-particle second quantization, but for two particles

$$\hat{V}_{int} = \frac{1}{2} \sum_{\substack{mn \\ qp}} \langle mn | \hat{V}_{int} | qp \rangle \hat{b}_m^+ \hat{b}_n^+ \hat{b}_q \hat{b}_p$$

with $\langle mn | \hat{V}_{int} | qp \rangle = \sum_{ij} V_{ij} \langle \varphi_m | \psi_i \rangle \times$

$$\times \langle \varphi_n | \psi_j \rangle \langle \psi_i | \varphi_q \rangle \langle \psi_j | \varphi_p \rangle$$

Electron - electron interactions

$$\hat{V}_{int} = \frac{e^2}{|\vec{r}-\vec{r}'|} \quad \text{— two particles}$$

For the system

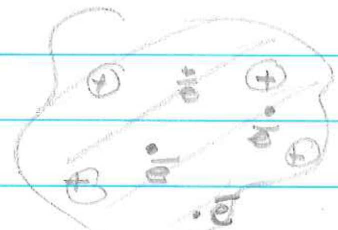
$$\sum_{i,j} \longrightarrow \int d^3\vec{r}\, d^3\vec{r}'$$

(know electron density)

However, it is more convenient to work in the momentum representation for energy calculations

$$|\vec{p} = \hbar k\rangle \propto e^{-ikr}$$

Degenerate electron gas in the presence of the uniform background + charge $\rho = eN/V$ (N – number of electrons)



$$\hat{H} = \hat{H}_{el} + \hat{H}_{bg} + \hat{H}_{el-bg}$$

$$\hat{H}_{el} = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j} \frac{e^{-\mu|\vec{r}_i-\vec{r}_j|}}{|\vec{r}_i-\vec{r}_j|}$$

(screened Coulumb potential)

$$\hat{H}_{bg} = \frac{1}{2}\int d^3\vec{r}\, d^3\vec{r}'\, \rho(\vec{r})\rho(\vec{r}') \frac{e^{-\mu|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} = \frac{2\pi e^2 N^2}{V\mu^2}$$

$$\hat{H}_{el-bg} = -e\sum_{i=1}^{N}\int d^3\vec{r}'\, \rho(\vec{r}) \frac{e^{-\mu|\vec{r}-\vec{r}_i|}}{|\vec{r}-\vec{r}_i|} = -\frac{4\pi e^2 N^2}{V\mu^2}$$

$$\hat{H} = -\frac{2\pi e^2 N^2}{V\mu^2} + \underbrace{\sum_i \frac{\hat{p}_i^2}{2m}}_{\text{"additive" operator}} + \underbrace{\boxed{\frac{1}{2} e^2 \sum_{i \neq j} \frac{e^{-\mu|\bar{r}_i - \bar{r}_j|}}{|\bar{r}_i - \bar{r}_j|}}}_{\hat{V}_{ee}}$$

$$\sum_i \frac{\hat{p}_i^2}{2m} \longrightarrow \sum_{\bar{k},\lambda} \frac{\hbar^2 k^2}{2m} \hat{a}^{+}_{k\lambda} \hat{a}_{k\lambda}$$

λ - spin of an $\bar{e}$

$$\hat{V}_{ee} = \frac{1}{2} \sum_{\substack{k_1, k_2 \\ k_3 k_4}} \langle k_1 \lambda_1; k_2 \lambda_2 | \hat{V}_{ee} | k_3 \lambda_3; k_4 \lambda_4 \rangle \times$$

$$\times \hat{a}^{+}_{k_1\lambda_1} \hat{a}^{+}_{k_2\lambda_2} \hat{a}_{k_3\lambda_3} \hat{a}_{k_4\lambda_4}$$

$$\langle .. | \hat{V}_{ee} | .. \rangle = \frac{e^2}{V} \frac{4\pi}{|\bar{k}_1 - \bar{k}_3|^2 + \mu^2} \underbrace{\delta_{\lambda_1\lambda_4} \delta_{\lambda_2\lambda_3}}_{\text{no change in spins}} \overbrace{\delta_{k_1+k_2,\, k_3+k_4}}^{\text{momentum conservation}}$$

After some careful manipulations (see Sacurai 7.5) we can set $\mu \to 0$

$$\hat{H} = \sum_{k\lambda} \frac{\hbar^2 k^2}{2m} \hat{a}_k^{+} \hat{a}_k + \frac{e^2}{2V} \sum_{kpq} \sum_{\lambda_1,\lambda_2} \frac{4\pi}{q^2} \times$$

$$\times \hat{a}^{+}_{\bar{k}+\bar{q},\lambda_1} \hat{a}^{+}_{\bar{p}-\bar{q},\lambda_2} \hat{a}_{\bar{p},\lambda_2} \hat{a}_{\bar{k},\lambda_1}$$

Can solve with the second term as perturbation