Second Quantization

First quantization : Crudely, particles are waves.

Second quantization - Crudely, waves are particles.

First quantization deals with wavefunctions &

Second quantization deals with operators that create or destroy particles in states described by (single particle) wavefunctions.

Particles that are created are identical.

Two particles wavefunction

$\psi(x_1, x_2)$

Identical particles $\Rightarrow$ $\psi(x_2, x_1) = e^{i\theta}\psi(x_1, x_2)$

Interchange can only produce a phase.

Second interchange brings $\psi(x_1, x_2)$ back to itself (not true in 2D)

so $\psi(x_1, x_2) = e^{i\theta}\psi(x_2, x_1) = e^{i2\theta}\psi(x_1, x_2)$

$\Rightarrow e^{i2\theta} = 1$ or $e^{i\theta} = 1$ or -1

Bosons

$\psi_B(x_1, x_2) = \psi_B(x_2, x_1)$

Fermions

$\psi_F(x_1, x_2) = -\psi_F(x_2, x_1)$

With more particles.

For bosons $\psi_B(x_1, x_2, \dots x_i, \dots x_j, \dots x_N)$
$= \psi_B(x_1, x_2, \dots x_j, \dots x_i, \dots x_N)$

for any pair of particles i and j

For fermions, $\psi_F(x_1, x_2, \dots x_i, \dots x_j, \dots x_N)$
$= -\psi_F(x_1, x_2, \dots x_j, \dots x_i, \dots x_N)$

for any pair of particles i and j

Multiparticle system Hilbert space
$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathcal{H}_3 \otimes \dots \mathcal{H}_i \otimes \dots \mathcal{H}_j \otimes \dots \mathcal{H}_N$

Thus $\psi(x_1, x_2, \dots x_i, \dots x_j, \dots x_N)$
$= \sum_{\{P\}} a_P \, \varphi_{\alpha_1}(x_1)\, \varphi_{\alpha_2}(x_2) \dots \varphi_{\alpha_i}(x_i) \dots \varphi_{\alpha_j}(x_j) \dots \varphi_{\alpha_N}(x_N)$

P denotes the permutations of $\alpha_1, \alpha_2, \dots \alpha_N$.
Here, it is assumed that $\alpha_1, \alpha_2, \dots$ are a set of single particle states and each permutation is counted only once

For bosons, $a_P = \dfrac{1}{\sqrt{\dfrac{N!}{\prod_\lambda n_\lambda!}}}$

N - total number of particles, n_λ - # of particles in the state λ; $\sum_\lambda n_\lambda = N$

For fermions, $a_P = \dfrac{1}{\sqrt{N!}}(-1)^P$

P - # of transpositions that brings $(\alpha_1, \alpha_2 \dots \alpha_N)$ to $(1, 2, \dots N)$.

$$\varphi_F(x_1, x_2 \dots x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \cdots & \varphi_N(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \cdots & \varphi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(x_N) & \varphi_2(x_N) & \cdots & \varphi_N(x_N) \end{vmatrix}$$

Slater determinant.

Fock space

$F = \bigoplus_{N=0}^{\infty} F^N$; F^N - Hilbert space of N particles

F^0 contains only the vacuum state

Occupation number representation

1) Choose a basis of single particle states $(\lambda_1, \lambda_2, \dots)$.

2) Specify occupancy of each state $|n_1, n_2 \dots\rangle \Rightarrow n_1$ particles in λ_1, n_2 in $\lambda_2, \dots$

3) Eg. for bosons

$$|1,1,0,0 \dots\rangle \equiv \frac{1}{\sqrt{2}}\left[\varphi_1(x_1)\varphi_2(x_2) + \varphi_2(x_1)\varphi_1(x_2)\right]$$

$$|2,0,0,0,\dots\rangle \equiv \varphi_1(x_1)\varphi_1(x_2)$$

$$|2,1,0\,0,\dots\rangle \equiv \frac{1}{\sqrt{3}}\left[\varphi_1(x_1)\varphi_1(x_2)\varphi_2(x_3) + \varphi_1(x_1)\varphi_1(x_3)\varphi_2(x_2) + \varphi_1(x_2)\varphi_1(x_3)\varphi_2(x_1)\right]$$

$$|1,1,1,0,0,0 \dots\rangle \equiv \frac{1}{\sqrt{3!}}\Big[\varphi_1(x_1)\varphi_2(x_2)\varphi_3(x_3) + \varphi_1(x_2)\varphi_2(x_1)\varphi_3(x_3) + \varphi_1(x_3)\varphi_2(x_2)\varphi_3(x_1) + \varphi_1(x_1)\varphi_2(x_3)\varphi_3(x_2) + \varphi_1(x_2)\varphi_2(x_3)\varphi_3(x_1) + \varphi_1(x_3)\varphi_2(x_1)\varphi_3(x_2)\Big]$$

4) Eg for fermions

$$|1,1,0,0\ldots\rangle \equiv \frac{1}{\sqrt{2}}\left[\varphi_1(x_1)\varphi_2(x_2) - \varphi_1(x_2)\varphi_2(x_1)\right]$$

$$\begin{aligned} |1,1,1,0,0\ldots\rangle \equiv \frac{1}{\sqrt{3!}}\Big[& \varphi_1(x_1)\varphi_2(x_2)\varphi_3(x_3) \\ & - \varphi_2(x_1)\varphi_1(x_2)\varphi_3(x_3) \\ & - \varphi_3(x_1)\varphi_2(x_2)\varphi_3(x_1) \\ & - \varphi_1(x_1)\varphi_3(x_2)\varphi_2(x_3) \\ & + \varphi_2(x_1)\varphi_3(x_2)\varphi_1(x_3) \\ & + \varphi_3(x_1)\varphi_1(x_2)\varphi_2(x_3)\Big] \end{aligned}$$

\# of filled states
= \# of particles. $n_\lambda = 0$ or 1

Fock space states can consist of superpositions with different \#s of particles

Eg $\frac{1}{\sqrt{2}}\left(|1,0,\ldots\rangle + |1,1,\ldots\rangle\right)$ etc.

$$\langle \ldots\ldots m_2, m_1 | n_1, n_2, \ldots\ldots \rangle = \delta_{n_1 m_1}\delta_{n_2 m_2}\ldots$$

Creation operators

$$a_i^\dagger |n_1, n_2, \ldots n_i, \ldots\ldots\rangle = \left(\underline{n_i+1}\right)^{1/2} \rho^{S_i} |n_1, n_2, \ldots \underline{n_i+1}, \ldots\rangle$$

$$S_i = \sum_{j=1}^{i-1} n_j$$

For bosons
$\rho = 1$, $\underline{n_i+1} = n_i + 1$

For fermions
$\rho = -1$, $\underline{n_i+1} = (n_i+1) \bmod 2$

Annihilation operator

$$a_i|n_1,n_2,\dots n_i,\dots\rangle = n_i^{1/2}\rho^{s_i}|n_1,n_2,\dots \underline{n_i-1},\dots\rangle$$

Note that $n_i=0 \Rightarrow a_i|n_1,n_2,\dots n_i,\dots\rangle = 0$

$0 \neq |0\rangle$

$(a_i^\dagger)^\dagger = a_i$

From the definition of the creation operator

$a_i^\dagger a_j^\dagger - \rho a_j^\dagger a_i^\dagger |n_1,n_2,\dots\rangle = 0$

$\Rightarrow [a_i^\dagger, a_j^\dagger]_\rho = 0$

$[A,B]_\rho = AB - \rho BA$

$[\ ,\ ]_1 = [\ ,\ ]$ - commutator

$[\ ,\ ]_{-1} = \{\ ,\ \}$ - anticommutator

IIIly for the annihilation operator

$[a_i,a_j]_\rho = 0$

Also $[a_i,a_j^\dagger]_\rho = \delta_{ij}$

Note $[A,B] = -[B,A]$

$\{A,B\} = \{B,A\}$

$$|n_1, n_2, \dots\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} (a_i^+)^{n_i} |0\rangle$$

$$|0\rangle = |0, 0, \dots\rangle$$

Change of basis

$$\sum_\lambda |\lambda\rangle\langle\lambda| = \mathbb{1}$$

$$|\tilde{\lambda}\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde{\lambda}\rangle$$

$$|\lambda\rangle = a_\lambda^+ |0\rangle ; |\tilde{\lambda}\rangle = a_{\tilde{\lambda}}^+ |0\rangle$$

$$\Rightarrow a_{\tilde{\lambda}}^+ = \sum_\lambda \langle\lambda|\tilde{\lambda}\rangle a_\lambda^+ \text{ and}$$

$$a_{\tilde{\lambda}} = \sum_\lambda \langle\tilde{\lambda}|\lambda\rangle a_\lambda$$

$$\tilde{\lambda} = x$$

$$a(x) = \sum_\lambda \langle x|\lambda\rangle a_\lambda = \sum_\lambda \varphi_\lambda(x) a_\lambda$$

Fourier space

$$a_k = \int_0^L dx \langle k|x\rangle a(x) = \frac{1}{\sqrt{L}} \int_0^L e^{-ikx} a(x)$$

Number operator

$$a_i^\dagger a_i |n_1, n_2, \cdots n_i, \cdots\rangle = n_i |n_1, n_2, \cdots n_i, \cdots\rangle$$

$\hat{n}_\lambda = a_\lambda^\dagger a_\lambda$ - number operator

One body operator

$O_1 = O(x_1) + O(x_2) + \cdots\cdots$; $\hat{O}_1 |x_1, x_2, \cdots\rangle = O(x_1)|x_1, x_2, \cdots\rangle + O(x_2)|x_1, x_2, \cdots\rangle + \cdots$

Eigenstates of O are $\varphi_\lambda(x)$ with eigenvalue O_λ

$$\hat{O} = \sum_i O_{\lambda_i} |\lambda_i\rangle\langle\lambda_i|$$

$$O_{\lambda_i} = \langle\lambda_i|\hat{O}|\lambda_i\rangle$$

$$\langle \cdots, n'_{\lambda_2}, n'_{\lambda_1}|\hat{O}_1|n_{\lambda_1}, n_{\lambda_2}\cdots\rangle = \sum_i O_{\lambda_i} n_{\lambda_i} \langle\cdots n'_{\lambda_2}, n'_{\lambda_1}|n_{\lambda_1}, n_{\lambda_2}\cdots\rangle$$

$$= \langle\cdots\cdots, n'_{\lambda_2}, n'_{\lambda_1}|\sum_i O_{\lambda_i}\hat{n}_{\lambda_i}|n_{\lambda_1}, n_{\lambda_2}\cdots\rangle$$

$$\hat{O}_1 = \sum_\lambda O_\lambda \hat{n}_\lambda = \sum_\lambda \langle\lambda|\hat{o}|\lambda\rangle a_\lambda^\dagger a_\lambda$$

In a general basis

$$\hat{O}_1 = \sum_{\mu\nu} \langle\mu|\hat{o}|\nu\rangle a_\mu^\dagger a_\nu$$

Local density operator

$\hat{\rho}(\vec{r}) = a^\dagger(\vec{r}) a(\vec{r})$. Total number operator

$$\hat{N} = \int d^d r\, \hat{\rho}(\vec{r})$$

$\hat{V} = \int d^d\vec{r}\, V(\vec{r}) a^\dagger(\vec{r}) a(\vec{r})$

$V(\vec{r})\hat{\rho}(\vec{r})$

Two body operators

$V(\vec{r}_m, \vec{r}_n) \equiv V(\vec{r}_n, \vec{r}_m)$ (symmetric potential)

$$\hat{V} | \vec{r}_1, \vec{r}_2, \ldots \vec{r}_N \rangle = \sum_{n<m}^{N} V(\vec{r}_n, \vec{r}_m) | \vec{r}_1, \vec{r}_2, \ldots \vec{r}_N \rangle$$

$$= \frac{1}{2} \sum_{n \neq m}^{N} V(\vec{r}_n, \vec{r}_m) | \vec{r}_1, \vec{r}_2, \ldots \vec{r}_N \rangle$$

$$\hat{V} = \frac{1}{2} \int d^d \vec{r} \int d^d \vec{r}\,' \; a^\dagger(\vec{r}) a^\dagger(\vec{r}\,') V(\vec{r}, \vec{r}\,') a(\vec{r}\,') a(\vec{r})$$

$$\neq \frac{1}{2} \int d^d \vec{r} \int d^d \vec{r}\,' \; V(\vec{r}, \vec{r}\,') \hat{\rho}(\vec{r}\,') \hat{\rho}(\vec{r})$$

More generally

$$\hat{O}_2 = \sum_{\lambda \lambda' \mu \mu'} \langle \mu, \mu' | \hat{O}_2 | \lambda, \lambda' \rangle a^\dagger_\mu a^\dagger_{\mu'} a_\lambda a_{\lambda'}$$

Examples

One body Hamiltonian for a free particle

$$\hat{H} = \int d^d \vec{r} \, a^\dagger(\vec{r}) \left[\frac{\hat{p}^2}{2m} + V(\vec{r}) \right] a(\vec{r})$$

$\hat{p} = -i\hbar\partial$

Spin operator $\hat{S} = \sum_{\lambda} a^{+}_{\lambda\alpha'} \vec{S}_{\alpha'\alpha} a_{\lambda\alpha}$

State ket $|\lambda, \alpha\rangle$, α - spin index

$\vec{S}_{\alpha\alpha'}$ - spin - matrix

For spin $1/2$; $\vec{S}_{\alpha\alpha'} = \frac{1}{2} \vec{\sigma}_{\alpha\alpha'}$

$\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices

Spin - Spin interaction

$$\hat{V} = \frac{1}{2} \int d^d\vec{r} \int d^d\vec{r}\,' \sum_{\alpha\alpha'\beta\beta'} J(\vec{r}, \vec{r}\,') \vec{S}_{\alpha\beta} \vec{S}_{\alpha'\beta'} \; a^{+}_{\alpha}(\vec{r}) a^{+}_{\alpha'}(\vec{r}\,') a_{\beta'}(\vec{r}\,') a_{\beta}(\vec{r})$$

$J(\vec{r}, \vec{r}\,')$ denotes exchange interaction