First quantization

$$\Psi(\vec{r}) \longrightarrow \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$$

$$|\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)|^2 \prod_{j=1}^{N} d\vec{r}_j =: $$ Probability of finding N particles in $\prod_{j=1}^{N} d\vec{r}_j$ around $(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$

Permutation symmetry and indistinguishability.

$$\Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N) = \lambda \Psi(\vec{r}_1, \dots, \vec{r}_k, \dots, \vec{r}_j, \dots, \vec{r}_N)$$
$$= \lambda^2 \Psi(\vec{r}_1, \dots, \vec{r}_j, \dots, \vec{r}_k, \dots, \vec{r}_N)$$

then,
$$\lambda^2 = 1 \longrightarrow \lambda = \pm 1$$

+ Bossons - Fermions

Anions $\rightarrow$ 2D and $e^{i\phi}$ (Berry phase)

if $\vec{r}_j = \vec{r}_K \rightarrow \Psi = 0$ exclusion principle

there no exist Ψ and under interchange of particles $\Psi = -\Psi$.

States of a particle like a basis:

$$\}\Psi_\nu(\vec{r}_N)\{$$

$$\sum_\nu \Psi_\nu^*(\vec{r}\,')\Psi_\nu(\vec{r}) = \delta(\vec{r} - \vec{r}\,')$$

$$\int d\vec{r}\, \Psi_{\nu'}^*(\vec{r})\Psi_\nu(\vec{r}) = \delta_{\nu,\nu'}$$

let
$$A_{\nu_1}(\vec{r}_2, \dots, \vec{r}_N) := \int d\vec{r}_1\, \Psi_{\nu_1}^*(\vec{r}_1)\Psi(\vec{r}_1, \dots, \vec{r}_N)$$

we may invert

$$\sum_{\nu_1} \Psi_{\nu_1}(\tilde{\vec{r}}_1) A_{\nu_1}(\vec{r}_2, \dots, \vec{r}_N) = \sum_{\nu_1} \int d\vec{r}_1\, \Psi_{\nu_1}(\tilde{\vec{r}}_1)\Psi_{\nu_1}^*(\vec{r}_1)\Psi(\vec{r}_1, \dots, \vec{r}_N)$$

then

$$\Psi(\tilde{\vec{r}}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{\nu_1} \psi_{\nu_1}(\tilde{\vec{r}}_1) A_{\nu_1}(\vec{r}_2, \ldots, \vec{r}_N)$$

Analogously

$$A_{\nu_1,\nu_2}(\vec{r}_3, \ldots, \vec{r}_N) := \int d\vec{r}_2 \, \psi^*_{\nu_2}(\vec{r}_2) A_{\nu_1}(\vec{r}_2, \ldots, \vec{r}_N)$$

Also

$$\Psi(\tilde{\vec{r}}_1, \tilde{\vec{r}}_2, \vec{r}_3, \ldots, \vec{r}_N) = \sum_{\nu_1,\nu_2} \psi_{\nu_1}(\tilde{\vec{r}}_1) \psi_{\nu_2}(\tilde{\vec{r}}_2) A_{\nu_1,\nu_2}(\vec{r}_3, \ldots, \vec{r}_N)$$

Continuing,

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N) = \sum_{\nu_1,\ldots,\nu_N} A_{\nu_1,\ldots,\nu_N} \psi_{\nu_1}(\vec{r}_1) \psi_{\nu_2}(\vec{r}_2) \ldots \psi_{\nu_N}(\vec{r}_N)$$

$$\hat{S}_{\pm} \prod_{j=1}^{N} \psi_{\nu_j}(\vec{r}_j) = \begin{vmatrix} \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \\ \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \end{vmatrix}_{\pm}$$

$\pm :=$ Skew-symmetrization
Symmetrization
operator

The skew-symmetric information is in the determinant.

$n_{\nu'} :=$ Number of times that state $|\nu'\rangle$ appear in $\{|\nu_1\rangle, \ldots, |\nu_N\rangle\}$

$$n_{\nu'} = \begin{cases} 0 \text{ or } 1 & \text{for fermions.} \\ 0, 1, \ldots, N & \text{for Bossons.} \end{cases}$$

$$\begin{vmatrix} \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \\ \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_\nu(\vec{r}) & \psi_\nu(\vec{r}) & \cdots & \psi_\nu(\vec{r}) \end{vmatrix}_{\pm} = \begin{cases} \sum_{p \in S_N} \left(\prod_{j=1}^{N} \psi_{\nu_j}(\vec{r}_{p(j)}) \right) \\ \sum_{p \in S_N} \left(\prod_{j=1}^{N} \psi_{\nu_j}(\vec{r}_{p(j)}) \right) \mathrm{Sign}(p) \end{cases}$$

S_N Group of $N!$ permutations p

$\mathrm{Sign}(p)$ Sign of the permutation.

$$\Psi(\vec{r}_1,\vec{r}_2,\dots,\vec{r}_N) = \sum_{\nu_1,\dots,\nu_N} B_{\nu_1,\nu_2,\dots,\nu_N} \hat{S}_{\pm} \varphi_{\nu_1}(\vec{r}_1)\varphi_{\nu_2}(\vec{r}_2)\cdots\varphi_{\nu_N}(\vec{r}_N)$$

B is completely symmetric.

$$\varphi_{\nu_m}(\vec{r}_n) \longrightarrow |\nu_m\rangle_n \qquad \text{Quantum state.}$$

Operators in First Quantization

$$T_j = T(\vec{r}_j, \nabla_{\vec{r}_j}) \qquad \text{Operator of a particle}$$

Examples:

$$-\frac{\hbar^2}{2m}\nabla^2_{\vec{r}_j} \qquad \text{Kinetic energy.}$$

$$V(\vec{r}) \qquad \text{External potential.}$$

Proposition:

$$\hat{T}_j = \sum_{\nu_a,\nu_b} T_{\nu_b\nu_a} |\nu_b\rangle_j \, {}_j\langle \nu_a|$$

where

$$T_{\nu_b\nu_a} = \int d\vec{r}_j \, \varphi^*_{\nu_b}(\vec{r}_j) T(\vec{r}_j, \nabla_{\vec{r}_j}) \varphi_{\nu_a}(\vec{r}_j)$$

Proof:

$$\hat{T}_j = \left(\sum_{\nu_b} |\nu_b\rangle_j \, {}_j\langle \nu_b|\right)\left(\int d\vec{r}_j \, |\vec{r}_j\rangle\langle\vec{r}_j|\right) \times$$

$$\times \; \hat{T}_j \left(\int d\vec{r}_j{}' \, |\vec{r}_j{}'\rangle\langle\vec{r}_j{}'|\right)\left(\sum_{\nu_a} |\nu_a\rangle_j \, {}_j\langle \nu_b|\right)$$

$$= \sum_{\nu_b,\nu_a} |\nu_b\rangle_j \iint d\vec{r}_j \, d\vec{r}_j{}' \, {}_j\langle \nu_b|\vec{r}_j\rangle\langle\vec{r}_j|\hat{T}_j|\vec{r}_j{}'\rangle\langle\vec{r}_j{}'|\nu_a\rangle_j \, {}_j\langle b|$$

$$= \sum_{\nu_b,\nu_a} |\nu_b\rangle_j \iint d\vec{r}_j \, d\vec{r}_j{}' \, \varphi^*_{\nu_b}(\vec{r}_j) T(\vec{r}_j, \nabla_j) \delta(\vec{r}_j - \vec{r}_j{}') \varphi_{\nu_a}(\vec{r}_j{}') \, {}_j\langle \nu_b|$$

$$= \sum_{\nu_b,\nu_a} |\nu_b\rangle_j \int d\vec{r}_j \, \varphi^*_{\nu_b}(\vec{r}_j) T(\vec{r}_j, \nabla_j) \varphi_{\nu_a}(\vec{r}_j{}') \, {}_j\langle \nu_b|$$

$$= \sum_{\nu_a,\nu_b} T_{\nu_b,\nu_a} |\nu_b\rangle_j \, {}_j\langle \nu_a|$$

$$\hat{T}_{tot} = \sum_{j=1}^{N} \hat{T}_j$$ System of N particles

$$\hat{T}_{tot} |\nu_1\rangle_1 |\nu_2\rangle_2 \cdots |\nu_N\rangle_N$$

$$= \sum_{j=1}^{N} \sum_{\nu_a,\nu_b} T_{\nu_b\nu_a} |\nu_b\rangle_j \, {}_j\langle \nu_a| \left(|\nu_1\rangle_1 |\nu_2\rangle_2 \cdots |\nu_N\rangle_N \right)$$

$$= \sum_{j=1}^{N} \sum_{\nu_a,\nu_b} T_{\nu_b\nu_a} |\nu_b\rangle_j \, |\nu_1\rangle_1 |\nu_2\rangle_2 \cdots \delta_{\nu_a,\nu_j} \cdots |\nu_N\rangle_N$$

$$= \sum_{j=1}^{N} \sum_{\nu_a,\nu_b} T_{\nu_b\nu_a} \, \delta_{\nu_a,\nu_j} |\nu_1\rangle_1 \cdots |\nu_b\rangle_j \cdots |\nu_N\rangle_N$$

Operator of two particles V_{jk}

Example: $V(\vec{r}_j - \vec{r}_k) = \dfrac{e^2}{4\pi\varepsilon_0} \dfrac{1}{|\vec{r}_j - \vec{r}_k|}$ Coulombian interaction

$$\hat{V}_{jk} = \sum_{\substack{\nu_a \nu_b \\ \nu_c \nu_d}} V_{\nu_c\nu_d,\nu_a\nu_b} |\nu_c\rangle_j \, |\nu_d\rangle_k \, {}_j\langle \nu_a| \, {}_k\langle \nu_b|$$

$$V_{\nu_c\nu_d,\nu_a\nu_b} = \int d\vec{r}_j \, d\vec{r}_k \, \varphi^*_{\nu_c}(\vec{r}_j) \varphi^*_{\nu_d}(\vec{r}_k) V(\vec{r}_j - \vec{r}_k) \varphi_{\nu_a}(\vec{r}_j) \varphi_{\nu_b}(\vec{r}_k)$$

$$\hat{V}_{tot} = \sum_{j>k}^{N} V_{jk} = \frac{1}{2} \sum_{\substack{j \\ k \neq j}} V_{jk}$$

$$\hat{V}_{tot} |\nu_1\rangle_1 |\nu_2\rangle_2 \cdots |\nu_N\rangle_N$$

$$= \frac{1}{2} \sum_{j \neq k}^{N} \sum_{\substack{\nu_a \nu_b \\ \nu_c \nu_d}} V_{\nu_c\nu_d\nu_a\nu_b} \, \delta_{\nu_a,\nu_{n_j}} \, \delta_{\nu_b\nu_{n_k}} |\nu_1\rangle_1 \cdots |\nu_c\rangle_j \cdots |\nu_d\rangle_k \cdots |\nu_N\rangle_N$$

$$\hat{H} = \hat{T}_{tot} + \hat{V}_{tot} = \sum_{j=1}^{N} \hat{T}_j + \frac{1}{2} \sum_{j \neq k}^{N} \hat{V}_{jk}$$