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Quantum Mechanics 2

CH. 7 IDENTICAL PARTICLES LECTURE NOTES

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Identical Particles And Groups of Particles

In Quantum mechanics a group of particles with the same intrinsic properties such as mass, spin, etc. are indistinguishable. Since the concept of individual trajectories is meaningless in Quantum Mechanics.

For a given system of n particles, the symmetry of the total wavefunction under permutation of the particles is a fundamental symmetry.

For $j = 1, \ldots n$ particles, a permutation represented by a matrix

$$\sigma \in S_n, \quad \sigma' = \begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \alpha_1 & \alpha_2 & \alpha_3 & \cdots & \alpha_n \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \sigma'_1 & \sigma'_2 & \sigma'_3 & \cdots & \sigma'_n \end{pmatrix}$$

where $\alpha_j = \sigma'(j)$ and $\{\alpha_1, \alpha_2, \ldots \alpha_n\}$ is an arrangement of $j = 1, 2, 3 \ldots n$.

Definition: Cyclic Permutation

A permutation that involves a set of 6 digits that transform in a closed form:

$$\sigma' = \begin{pmatrix} 1 & 2 & \alpha_i & \cdots & \alpha_j & \cdots & \alpha_k & \cdots & n \\ \alpha_1 & \alpha_2 & \cdots & \alpha_j & \cdots & \alpha_k & \cdots & \alpha_n \end{pmatrix}$$

Example

$$\begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 3 & 4 & 5 & 6 & 1 & 2 \end{pmatrix} = (1\,3\,5)(2\,4\,6)$$

Definition: Multiplication of Permutations

For two permutations of the form:

$$\sigma' = \begin{pmatrix} 1 & 2 & \cdots & n \\ \alpha_1 & \alpha_2 & \cdots & \alpha_n \end{pmatrix}, \quad \mu = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_n \\ \beta_1 & \beta_2 & \cdots & \beta_n \end{pmatrix}$$

The product of $\sigma'_\mu \in S_n$ is the permutation

$$\sigma'_\mu = \begin{pmatrix} 1 & 2 & \cdots & n \\ \alpha_1 & \alpha_2 & \cdots & \alpha_n \end{pmatrix}\begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_n \\ \beta_1 & \beta_2 & \cdots & \beta_n \end{pmatrix} = \begin{pmatrix} 1 & 2 & \cdots & n \\ \beta_1 & \beta_2 & \cdots & \beta_n \end{pmatrix}$$

We can define

① Identity:
$$\sigma' = \begin{pmatrix} 1 & 2 & \cdots & n \\ 1 & 2 & \cdots & n \end{pmatrix}$$

② Inverse:
$$\sigma'^{-1} = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_n \\ 1 & 2 & \cdots & n \end{pmatrix} = \begin{pmatrix} 1 & 2 & \cdots & n \\ \sigma_1'^{-1} & \sigma_2'^{-1} & \cdots & \sigma_n'^{-1} \end{pmatrix}$$

Definition: Transposition $\rightarrow$ A cycle of length two

$$Z_{i,j} = \begin{pmatrix} 1, 2, \ldots i \ldots j \ldots n \\ 1, 2, \ldots j \ldots i \ldots n \end{pmatrix} = (i\,j)$$

Theorem: Every permutation is a product of transpositions, where the number of transpositions sets the parity of permutation. (Even or odd).

Definition: Sign of Permutation

For $\sigma \in S_n$, the sign of permutation S_σ is

$$S_\sigma = \begin{Bmatrix} +1 \text{ if } \sigma \text{ is even} \\ -1 \text{ if } \sigma \text{ is odd} \end{Bmatrix}$$

In particular, for a transposition the sign of a transposition : $S_\sigma = -1$. For a general permutation

$$\sigma = \prod_{k=1}^{n_\sigma} z_k \Rightarrow S_\sigma = (-1)^{n_\sigma}$$

Also,

$$S(\sigma\mu) = S_\sigma S_\mu = S(\mu\sigma)$$

$$\Rightarrow S(\sigma\sigma^{-1}) = S_e = \mathbb{1} = S_\sigma S_{\sigma^{-1}}$$

$$\Rightarrow S(\sigma^{-1}) = S_\sigma$$

Symmetrization of A Quantum State

For a system of n particles, every exchange among particles should leave the system invariant. (Wave function can change but observable cannot)

Say we have states, $|\varphi\rangle$ & $|\psi\rangle$, two different states of the system. The basis in the configuration space can be written as

$$|\vec{x}_1, \vec{s}_1, \vec{x}_2, \vec{s}_2, \ldots \vec{x}_n, \vec{s}_n\rangle \equiv \underbrace{|\vec{x}_1, \vec{s}_1\rangle}_{\text{Particle } 1} \underbrace{|\vec{x}_2, \vec{s}_2\rangle}_{2} \ldots \underbrace{|\vec{x}_n, \vec{s}_n\rangle}_{n}$$

Definition: Many Body Wavefunction

We define the many body wavefunction to be

$$\psi_{s_1 \ldots s_n}(\vec{x}_1, \vec{x}_2, \ldots \vec{x}_n) = \langle \vec{x}_1 \vec{s}_1 \ldots \vec{x}_n \vec{s}_n | \psi \rangle$$

If we assume completeness of the basis,

$$\sum_s \int |\vec{x}, \vec{s}\rangle\langle \vec{x}, \vec{s}|\, dx = \mathbb{1}$$

$$\Rightarrow \quad \langle \psi | \varphi \rangle = \sum_{s_1 \ldots s_n} \int d\vec{x}_1 \ldots d\vec{x}_n = \langle \psi | \vec{x}_1 \vec{s}_1 \ldots \vec{x}_n \vec{s}_n \rangle \times \langle \vec{x}_1 \vec{s}_1 \ldots \vec{x}_n \vec{s}_n | \varphi \rangle$$

$$= \sum_{s_1 \ldots s_n} \int d\vec{x}_1 \ldots d\vec{x}_n \times \psi^*_{s_1 \ldots s_n}(\vec{x}_1 \ldots \vec{x}_n) \varphi_{s_1 \ldots s_n}(\vec{x}_1 \ldots \vec{x}_n)$$

For simplicity, we will omit spin indices from now on For a given permutation $\sigma' \in S_n$

$$\sigma' = \begin{pmatrix} 1 & \ldots\ldots & n \\ \alpha_1 & \ldots\ldots & \alpha_n \end{pmatrix}, \quad \sigma' \vec{x}_i = \vec{x}_{\sigma'_i}, \quad i = 1 \ldots n$$

Now, we define the unitary operator $\sigma' \leftrightarrow P_{\sigma'}$

$$P^\dagger_{\sigma'} P_{\sigma'} = P_{\sigma'} P^\dagger_{\sigma'} = \mathbb{1}$$

<u>Definition</u> : <u>Transformed Ket</u>

$$|\psi'\rangle = P_{\sigma'} |\psi\rangle \text{ s.t. } \psi'(\vec{x}) = \psi(\sigma' \cdot \vec{x})$$

or equivalently

$$\langle \vec{x} | \psi' \rangle \equiv \langle \sigma' x | \psi \rangle = \langle \vec{x} | P_{\sigma'} | \psi \rangle$$

In particular

$$\langle \vec{x} | P_{\sigma'} | \vec{x}' \rangle = \langle \sigma'(\vec{x}) | \vec{x}' \rangle = \langle \vec{x}_{\alpha_1} | \vec{x}_1' \rangle \langle \vec{x}_{\alpha_2} | \vec{x}_2' \rangle \ldots \langle \vec{x}_{\alpha_n} | \vec{x}_n' \rangle = \delta(\vec{x}_1' - x_{\alpha_1}) \ldots \delta(\vec{x}_n' - \vec{x}_{\alpha_n})$$

To show that $P_{\sigma'}$ is unitary

$$|\psi'\rangle = P_{\sigma'} |\psi\rangle, \quad |\varphi'\rangle = P_{\sigma'} |\varphi\rangle$$

$$\Rightarrow \langle \psi' | \varphi' \rangle = \int \langle \psi | \vec{x} \rangle \langle \vec{x} | \varphi \rangle \, d\vec{x}$$

$$= \int \psi^{*\prime}(x) \varphi'(x) \, d\vec{x}$$

$$= \int \psi^*[\sigma'(x)] \varphi[\sigma'(x)]$$

After a change of variable

$$\vec{x}' \equiv \sigma'(\vec{x})$$

The Jacobian of the transformation is one. Since we are just rearranging the co-ordinates among the particles

$$d\vec{x} = \left\| \frac{\partial \vec{x}}{\partial \vec{x}'} \right\| d\vec{x}' = d\vec{x}'$$

Therefore we can say

$$\langle \psi' | \varphi' \rangle = \int \psi^*(\vec{x}') \varphi'(\vec{x}') = (\langle \psi | P^\dagger_{\sigma'} P_{\sigma'} | \varphi \rangle) = \langle \psi | \varphi \rangle$$

If Ω is an observable, invariance under the symmetric group means

$$\langle\psi|\Omega|\psi\rangle = \langle\psi|\Omega|\psi'\rangle = \langle\psi|P_\sigma^\dagger \Omega P_\sigma|\psi\rangle$$

we know that for all kets

$$P_\sigma^\dagger \Omega P_\sigma = \Omega \quad \text{or} \quad [\Omega, P_\sigma] = 0$$

<u>Definition</u>: <u>Fully Symmetrized State</u> $|\psi_s\rangle$

For Z_{ij} an arbitrary transposition, then:

$$\langle \vec{x}_1 \dots \vec{x}_n | P_{Z_{ij}} | \psi_S\rangle = \langle \vec{x}_1 \dots \vec{x}_j \dots \vec{x}_i \dots \vec{x}_n | \psi_S\rangle = \langle \vec{x}_1 \dots \vec{x}_i \dots \vec{x}_j \dots \vec{x}_m | \psi_S\rangle$$

Or equivalently

$$\psi_S(Z_{ij}(\vec{x}_1, \dots, \vec{x}_n)) = \psi_S(\vec{x}_1 \dots \vec{x}_j \dots \vec{x}_i \dots \vec{x}_n) = \psi_S(\vec{x}_1 \dots \vec{x}_i \dots \vec{x}_j \dots \vec{x}_n)$$

<u>Definition</u>: <u>Fully Anti-Symmetric State</u> $|\psi_A\rangle$

For Z_{ij} an arbitrary transposition, then:

$$\langle \vec{x}_1 \dots \vec{x}_i \dots \vec{x}_j \dots \vec{x}_m | P_{b_{ij}} | \psi_A\rangle = \langle \vec{x}_1 \dots \vec{x}_j \dots \vec{x}_i \dots \vec{x}_n | \psi_A\rangle = -\langle \vec{x}_1 \dots \vec{x}_i \dots \vec{x}_j \dots \vec{x}_n | \psi_A\rangle$$

we can then say

$$\psi_A(\vec{x}_1 \dots \vec{x}_i \dots \vec{x}_j \dots \vec{x}_n) = -\psi_A(\vec{x}_1 \dots \vec{x}_j \dots \vec{x}_i \dots \vec{x}_m) \Rightarrow P_b|\psi_A\rangle = -|\psi_A\rangle$$

For a generic permutation

1) $\langle \vec{x}_1 \dots \vec{x}_n | P_\sigma | \psi_S\rangle = \langle \vec{x}_{\sigma_1} \dots \vec{x}_{\sigma_n} | \psi_S\rangle = \langle \vec{x}_1 \dots \vec{x}_n | \psi_S\rangle$

2) $\langle \vec{x}_1 \dots \vec{x}_n | P_\sigma | \psi_A\rangle = \langle \vec{x}_{\sigma_1} \dots \vec{x}_{\sigma_2} \dots \vec{x}_{\sigma_n} | \psi_A\rangle = \delta_\sigma \langle \vec{x}_1 \dots \vec{x}_n | \psi_A\rangle$

<u>Implications</u>

A) States with different symmetries are orthogonal to each other if b is a transformation

$$\langle\psi_S|\psi_A\rangle = (\langle\psi_S|P_b^\dagger)(P_b|\psi_A\rangle) = -\langle\psi_S|\psi_A\rangle$$

This then says

$$\langle\psi_S|\psi_A\rangle = 0$$

B) For a given observable Ω, $P_\sigma^\dagger \Omega P_\sigma = \Omega$

$$\langle\psi_S|\Omega|\psi_A\rangle = \langle\psi_S|P_b^\dagger \Omega P_b|\psi_A\rangle = (\langle\psi_S|P_b^\dagger)\Omega(P_b|\psi_A\rangle) = -\langle\psi_S|\Omega|\psi_A\rangle$$

we can conclude

$$\langle \psi_S | \Omega | \psi_A \rangle = 0$$

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Projection Operators

For n particles we may construct Symmetric or Anti-Symmetric states with Symmeterizing or Anti-Symmeterizing projection operators.

Definition: S and A Projection Operators

$$S \equiv \frac{1}{M!} \sum_{\sigma \in S_n} P_\sigma \quad , \quad A \equiv \frac{1}{M!} \sum_{\sigma \in S_n} \delta_j P_j$$

In general

$$\Lambda \equiv \frac{1}{M!} \sum_{\sigma \in S_n} \lambda_\sigma P_\sigma$$

with

$$\lambda_\sigma = \begin{cases} +A & , \text{ for } S \\ \delta_\sigma & , \text{ For } A \end{cases}$$

Those operators have the properties

i) $\Lambda^\dagger = \Lambda$ (Hermitian)

ii) $\Lambda P_\sigma = P_\sigma \Lambda$, For every $\sigma \in S_n$

iii) $\Lambda^2 = \Lambda$, $AS = SA = 0$

Example: Two Particle State

If $\{k'\}$ is a set of Quantum Numbers for n particle states $|k'\rangle$ and $|k''\rangle$ is another set of Quantum numbers in the state $|k''\rangle$. The two particle state is:

$$|k'\rangle |k''\rangle = |k'\rangle \otimes |k''\rangle$$

we may also consider another state:

$$|k''\rangle |k'\rangle$$

Under permutation of the particles. If $k' \neq k''$, the two states are orthogonal

$$(\langle k''| \langle k'|)(|k'\rangle |k''\rangle) = \langle k'|k''\rangle \langle k''|k'\rangle = |\langle k'|k''\rangle|^2 = 0 \quad , \quad \text{for } k' \neq k''$$

Since the particles are indistinguishable, any linear combination

$$c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle$$

corresponds to the same set of eigenvalues of a measurement (Exchange degeneracy).

The group of permutations of two particles has two elements: e, (12).

The permutation operator P_{12} is such that

$$P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle \quad \text{w/} \quad P_{12} = P_{21}, \quad P_{12}^2 = 1$$

For a specific observable A, for each particle,

$$A_1|a'\rangle|a''\rangle = a'|a'\rangle|a''\rangle, \quad A_2|a'\rangle|a''\rangle = a''|a'\rangle|a''\rangle$$

or

$$A_1 \equiv A_1 \otimes \mathbb{1}, \quad A_2 \equiv \mathbb{1} \otimes A_2$$

Applying the permutation operator,

$$P_{12}A_1|a'\rangle|a''\rangle = a' P_{12}|a'\rangle|a''\rangle = a'|a''\rangle|a'\rangle = A_2|a''\rangle|a'\rangle$$

$$= P_{12}A_1P_{12}^{-1}P_{12}|a'\rangle|a''\rangle = P_{12}A_1P_{12}^{-1}|a''\rangle|a'\rangle$$

From this we can say

$$P_{12}A_1P_{12}^{-1} = A_2$$

Therefore the permutation exchanges the label of the observables.

Consider the Hamiltonian for a pair of identical particles

$$\mathcal{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + V_{Int}(|\vec{x}_1 - \vec{x}_2|) + V_{EXT}(\vec{x}_1) + V_{EXT}(\vec{x}_2)$$

Clearly this Hamiltonian is invariant under the exchange of particles

$$P_{12}\mathcal{H}P_{12}^{-1} = \mathcal{H} \Rightarrow [P_{12}, \mathcal{H}] = 0$$

Therefore P_{12} has the same eigenstates as the Hamiltonian.

If p' is the eigenvalue of P_{12}

$$P_{12}^2 = \mathbb{1} \Rightarrow p'^2 = \mathbb{1} \quad (p' = \pm 1)$$

Also, in the basis

$$\{ |k'\rangle|k''\rangle, |k''\rangle|k'\rangle \}$$

Since

$$P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle \quad , \quad P_{12}|k''\rangle|k'\rangle = |k'\rangle|k''\rangle$$

Where

$$P_{12}|k'k''\rangle_{\pm} = \pm|k'k''\rangle$$

Those two states correspond to the action of Symmetrizing or Anti-Symmetrizing operators over an arbitrary state,

$$S \equiv \frac{1}{2}(1+P_{12}) \quad , \quad A \equiv \frac{1}{2}(1-P_{12})$$

Where

$$\left.\begin{matrix} S \\ \\ A \end{matrix}\right\} (c_1|k'k''\rangle + c_2|k''k'\rangle) = \frac{(c_1+c_2)}{2}(|k'k''\rangle \pm |k''\rangle|k'\rangle)$$

Since $[\mathcal{H}, P_{12}] = 0 \Rightarrow$ the eigenstates of the Hamiltonian or any observable must be symmetrized or Anti-Symmetrized states in the $\{|k'\rangle|k''\rangle\}$ basis.

For an arbitrary permutation,

$$\langle \vec{x}|P_{\sigma}|\psi\rangle = \langle \sigma\vec{x}|\psi\rangle = \langle \vec{x}_{\sigma_1} \dots \vec{x}_{\sigma_m}|(|k_1\rangle \dots |k_m\rangle) = \langle \vec{x}_1 \dots \vec{x}_m|k_{\sigma_1^{-1}} \dots k_{\sigma_m^{-1}}\rangle$$

$$\Rightarrow \qquad P_{\sigma}|k_1\rangle \dots |k_m\rangle = |k_{\sigma_1^{-1}}\rangle \dots |k_{\sigma_m^{-1}}\rangle$$

operates the reverse permutation in the space of the kets.

Symmetrization Postulates

The example of two particles has only Symmetric or Anti-Symmetric states. In the more general case, there are states that are linear combinations of S and A kets.

For three particles take the state $|k'\rangle|k''\rangle|k'''\rangle$

$$|k'k''k'''\rangle_{A,S} = (|k'k''k'''\rangle + |k''k'''k'\rangle + |k'''k'k''\rangle$$
$$\pm |k'k'''k''\rangle \pm |k'''k''k'\rangle \pm |k''k'k'''\rangle)$$

With $+ \rightarrow S$ and $- \rightarrow A$. But the total degeneracy is $\underline{6}$, so there must be other 4 states with mixed symmetry which are linearly independent.

<u>Postulate</u>: In nature, there are only two types of Symmetry for a system of identical particles.

A) <u>Bosons</u>: which satisfy the Bose Einstein Statistics, have a completely Symmetric ket.

$$P_{ij}|N\rangle_{bosons} = +|N\rangle_{bosons}$$

B) <u>Fermions</u>: Satisfy the Fermi Dirac Statistics, with a completely Anti-Symmetric ket

$$P_{ij}|N\rangle_{Fermions} = -|N\rangle_{Fermions}$$

for any permutation of two particles.

The statistics comes from the spin,

i) Fermions have semi integer spin

ii) Bosons have integer spin

<u>Pauli Exclusion Principle</u>

Two Fermions cannot occupy the same quantum state (since they are Anti-Symmetric under exchange)

<u>Example</u>: $N=2$, $(k', k'') \Rightarrow k' \neq k''$

a.) Fermions: only one possibility

$$\frac{1}{2}\left(|k'\rangle|k''\rangle - |k''\rangle|k'\rangle\right)$$

b.) Bosons: Three possibilities with symmetric kets

$$\frac{1}{\sqrt{2}}\left(|k'\rangle|k''\rangle + |k''\rangle|k'\rangle\right),\ |k'\rangle|k'\rangle,\ |k''\rangle|k''\rangle$$

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We examine the <u>Two Electron system</u>

Determining the ket

$$|\vec{x}_1, \vec{s}_1; \vec{x}_2, \vec{s}_2\rangle$$

to a two particle state, the wave function is the linear combination

$$\psi_\alpha(\vec{x}_1, \vec{x}_2) = \sum_{s_1 s_2} C(s_1, s_2)\langle \vec{x}_1, \vec{s}_1; \vec{x}_2, \vec{s}_2|\alpha\rangle$$

with a given set of quantum numbers. For a closed system, the total spin is conserved

$$[\mathcal{H}, \tilde{S}^2] = 0$$

$\therefore$ the eigenstates of $\mathcal{H}$ are the same eigenstates of S^2. If ψ is separable in the spin and orbital parts

$$\Psi_\alpha = \varphi(\vec{x}_1, \vec{x}_2)\, \chi(s_1, s_2)$$

where the spin part is either a singlet or a triplet,

$$D^{(1/2)} \otimes D^{(1/2)} = D^{(0)} \otimes D^{(1)}$$

$D^{(0)}$: Singlet $\Rightarrow$ $\displaystyle \chi(s_1, s_2) = \frac{1}{\sqrt{2}}\Big[\underbrace{\chi(+-) - \chi(-+)}_{\text{Anti-Symmetric}}\Big]$

$D^{(1)}$: Triplet $\Rightarrow$ $\begin{cases} \chi(++) \\ \chi(--) \\ \dfrac{1}{\sqrt{2}}\left[\chi(+-) + \chi(-+)\right] \end{cases}$

The permutation operator can be separated in a spin part and a spatial part,

$$P_{12} = P_{12}^{ab} \otimes P_{12}^{(spin)}$$

where

$$[P_{12}^{(spin)}, P_{12}^{ab}] = 0$$

Determining the exchange operator

$$T = \vec{S}_1 \cdot \vec{S}_2 = \frac{1}{2}(S^2 - S_1^2 - S_2^2) = \frac{\hbar^2}{2}\left[s(s+1) - s_1(s_1+1) - s_2(s_2+1)\right] \times \mathbb{I}$$

where $s_1 = s_2 = \frac{1}{2}$ for electrons

$$\frac{T}{\hbar^2} = \frac{1}{2}\left[s(s+1) - 3/2\right]\mathbb{1}$$

For special values

$$\frac{1}{\hbar^2} T|s,m\rangle = \begin{cases} -3/4\, |s,m\rangle, & \text{for } s=0 \\ 1/4\, |s,m\rangle, & \text{for } s=1 \end{cases}$$

Hence the operator

$$\Omega \equiv \frac{1}{2}\left(1+\frac{4}{\hbar^2}\vec{S}_1\cdot\vec{S}_2\right)$$

Satisfies

$$\Omega|00\rangle = \frac{1}{2}\left[1+\frac{4}{\hbar^2}\left(-\frac{3}{4}\hbar^2\right)\right]|00\rangle = -|00\rangle \Rightarrow \text{(Singlet)}$$

and

$$\Omega|S=1,m\rangle = \frac{1}{2}\left[1+\frac{4}{\hbar^2}\frac{\hbar^2}{4}\right]|S=1,m\rangle = |S=1,m\rangle \Rightarrow \text{(Triplet)}$$

Therefore Ω is the Spin permutation operator

$$P_{1,2}^{(spin)} = \frac{1}{2}\left(1+\frac{4}{\hbar^2}\vec{S}_1\cdot\vec{S}_2\right)$$

The transformation

$$|\alpha\rangle \rightarrow P_{12}|\alpha\rangle$$

implies that

$$\phi(\vec{x}_1,\vec{x}_2) \longrightarrow \phi(\vec{x}_2,\vec{x}_1)$$
$$\chi(S_1,S_2) \longrightarrow \chi(S_2,S_1)$$

For two particles, φ and χ are either symmetric or Anti-Symmetric (S or A). Since the product $\varphi\chi$ must be Anti-Symmetric <u>always</u> for Fermions, then

$$\psi = \begin{cases} \varphi_S\cdot\chi_A \\ \varphi_A\cdot\chi_S \end{cases}$$

If the particles do not interact with each other, then the Hamiltonian is in the form:

$$\mathcal{H}(\vec{p}_1,\vec{p}_2;\vec{x}_1,\vec{x}_2) = \frac{\vec{p}_1^{\,2}}{2m}+\frac{\vec{p}_2^{\,2}}{2m}+V_{ext}(\vec{x}_1)+V_{ext}(\vec{x}_2) = H_0(\vec{p}_1,\vec{x}_1)+H_0(\vec{p}_2,\vec{x}_2)$$

Since $\mathcal{H}$ is spin independent, the Ψ is separable

$$\Psi(\vec{x}_1,S_1;\vec{x}_2,S_2) = \varphi(\vec{x}_1,\vec{x}_2)\chi(S_1,S_2)$$

Where χ is a singlet or a triplet. Since $\mathcal{H}$ is also separable among the particles

$$\varphi(\vec{x}_1, \vec{x}_2) \longrightarrow w_A(\vec{x}_1) w_B(\vec{x}_2)$$

Since the total wave function is anti-symmetric under the exchange of the particles,

$$\varphi_\pm(\vec{x}_1, \vec{x}_2) = \frac{1}{\sqrt{2}}\left[w_A(\vec{x}_1) w_B(\vec{x}_2) \pm w_A(\vec{x}_2) w_B(\vec{x}_1)\right]$$

Where φ_+ is the orbital part for a singlet χ^0 and φ_- for a triplet $\chi^{(1)}$.

The probability of finding an electron between $(\vec{x}_1, d^3\vec{x}_1)$ and $2(\vec{x}_2, d^3\vec{x}_2)$ is:

$$|\varphi_\pm(\vec{x}_1, \vec{x}_2)|^2 d^3x_1 d^3x_2 = \frac{1}{2}\Big[|w_A(\vec{x}_1)|^2 |w_B(\vec{x}_2)|^2 + |w_A(\vec{x}_2)|^2 |w_B(\vec{x}_1)|^2 \pm$$
$$w_A(\vec{x}_1) w_B(\vec{x}_2) w_A^*(\vec{x}_2) w_B^*(\vec{x}_1) + w_A^*(\vec{x}_1) w_B^*(\vec{x}_2) w_A(\vec{x}_2) w_B(\vec{x}_1)\Big] \pm$$
$$2\,\mathrm{Re}\left[w_A(\vec{x}_1) w_B(\vec{x}_2) w_A^*(\vec{x}_2) w_B^*(\vec{x}_1)\right] d^3x_1 d^3x_2$$

The last term accounts for interference effects and is called the exchange density.

Including interactions as a perturbation,

$$\hat{V}(\vec{x}_1, \vec{x}_2) = \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}$$

the expectation value for S or A orbital states,

$$\left\langle \frac{e^2}{|\vec{x}_1 - \vec{x}_2|} \right\rangle_\pm = \langle \varphi_\pm | \hat{V} | \varphi_\pm \rangle \int d^3x_1 d^3x_2 \, \frac{1}{2}$$

$$= \langle \varphi_\pm | \hat{V} | \varphi_\pm \rangle \int d^3x_1 d^3x_2 \, \frac{1}{2}\left[w_A^*(\vec{x}_1) w_B^*(\vec{x}_2) \pm w_A^*(\vec{x}_2) w_B^*(\vec{x}_1)\right] \Rightarrow$$

$$\Rightarrow \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}\left[w_A(\vec{x}_1) w_B(\vec{x}_2) \pm w_A(\vec{x}_2) w_B(\vec{x}_1)\right]$$

<u>Definition</u>: Direct Term

$$I \equiv \int d^3x_1 d^3x_2 \; e^2 \frac{|w_A(\vec{x}_1)|^2 |w_B(\vec{x}_2)|^2}{|\vec{x}_1 - \vec{x}_2|}$$

Which is a classical term proportional to the product of the charge densities

$$\rho_A(\vec{x}_1) \equiv e|w_A(\vec{x}_1)|^2$$

$$\rho_B(\vec{x}_2) \equiv e|w_B(\vec{x}_2)|^2$$

<u>Definition</u>: Exchange Term

$$J \equiv \int d^3x_1 d^3x_2 \frac{w^*_A(\vec{x}_1) w^*_B(\vec{x}_2) w_A(\vec{x}_2) w_B(\vec{x}_1)}{|\vec{x}_1 - \vec{x}_2|}$$

has no classical analog and follows from the statistics

$$\left\langle \frac{e^2}{|\vec{x}_1 - \vec{x}_2|} \right\rangle_\pm = I \pm J = \begin{cases} I + J, & \text{Singlet} \\ I - J, & \text{Triplet} \end{cases}$$

Where I and J are to be determined.

The Hamiltonian is:

$$\mathcal{H} = H_0(\vec{p}_1, \vec{x}_1) + H_0(\vec{p}_2, \vec{x}_2) + \frac{e^2}{|\vec{x}_1 - \vec{x}_2|}$$

The kinetic term is

$$E_0^\pm = \int d^3x_1\, w^*_A(\vec{x}_1) H_0(\vec{p}_1, \vec{x}_1) w_A(\vec{x}_1) \times \int d^3x_2\, |w_B(\vec{x}_2)|^2$$
$$+ \int d^3x_1\, |w_A(\vec{x}_1)|^2 + \int d^3x_2\, w^*_B(\vec{x}_2) H_0(\vec{p}_2, \vec{x}_2) w_B(\vec{x}_2) = E_A + E_B$$

Which do not depend on the symmetry of the state $\therefore$

$$E_\pm = E_A + E_B + I \pm J, \quad \begin{cases} +, & \text{for } S=0 \\ -, & \text{for } S=1 \end{cases}$$

These two energies can be found from a spin dependent Hamiltonian

$$\mathcal{H}(1,2) = E_A + E_B + I - \frac{2}{\hbar^2} J\left(\vec{S}_1 \cdot \vec{S}_2 \cdot \frac{\hbar^2}{4}\right)$$

Indeed, for the singlet,

$$\mathcal{H}(1,2)|0\rangle = \left[E_A + E_B + I - \frac{2}{\hbar^2} J\left(-\frac{3}{4}\hbar^2 + \frac{\hbar^2}{4}\right)\right]|0\rangle = \left[E_A + E_B + I + J\right]|0\rangle = E_+|0\rangle$$

And for a triplet

$$\mathcal{H}(1,2)|1\rangle = \left[E_A + E_B + I - \frac{2}{\hbar^2} J\left(\frac{\hbar^2}{4} + \frac{\hbar^2}{4}\right)\right]|1\rangle = \left[E_A + E_B + I - J\right]|1\rangle = E_-|1\rangle$$

<u>Definition</u>:

$$\mathcal{J} \equiv \frac{2}{\hbar^2} J$$

The effective spin Hamiltonian has the form

$$\mathcal{H} = -\mathcal{J}\,\vec{S}_1\cdot\vec{S}_2 + \text{Const}$$

(Spin exchange interaction) where the exchange coupling follows from the exchange part of the Coulomb interaction. Since $\mathcal{J} > 0$, the ground state is Ferromagnetic

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<u>Fock space</u>: (occupation space)

The wave functions that describe physical states of many identical particles are:

$$\psi^{\wedge}_{k_1,k_2,\dots k_N}(\vec{x}_1,\vec{x}_2,\dots,\vec{x}_N) = N^{\wedge}\langle\vec{x}_1,\vec{x}_2,\dots\vec{x}_N|\Lambda|k_1,\dots k_N\rangle$$

$$= \frac{N^{\wedge}}{N!}\sum_{\sigma\in S_n}\lambda_c\langle\vec{x}_1\dots\vec{x}_N|k_{\sigma(1)},\dots k_{\sigma(N)}\rangle$$

Where $N^{\wedge}$ is some normalization constant and

$$\Lambda \equiv \frac{1}{N!}\sum_{\sigma\in S_n}\lambda_{\sigma}P_{\sigma}$$

is symmetrizing ($\lambda_{\sigma}=1$) or anti-symmetrizing operator.

Since the particles are indistinguishable there is no physical meaning in knowing the state occupied by a given particle, but in how many particles occupy a given state. In the occupation basis, instead of labeling the quantum numbers, we label the occupation of that quantum number

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

Definition:

$$\langle\vec{x}_1\dots\vec{x}_N|n_1,\dots n_N\rangle \equiv N^{\wedge}\langle\vec{x}_1\dots\vec{x}_N|\Lambda|k_1\dots k_N\rangle$$

In this representation, the exchange degeneracy is taken care of automatically.

i) <u>Bosons</u>: $|n_1\dots n_N\rangle$ is symmetrized

$$n_i = 0,1,2\dots N \quad w/ \quad N = \sum_i n_i$$

ii) <u>Fermions</u>: $|n_1\dots n_N\rangle$ is anti-symmetrized $\Rightarrow$ a given 1 particle state cannot have occupancy higher (otherwise the wave function is zero)

<u>Second Quantization</u>: (Bosons)

The Fock space satisfies:

$$\sum_{|\mu\rangle} |\mu_0 \dots \mu_i\rangle\langle \mu_0 \dots \mu_i| = \mathbb{1}$$

with

$$\langle \mu_0 \dots \mu_i | \mu_0' \dots \mu_i'\rangle = \delta_{\mu_0\mu_0'}\delta_{\mu_1\mu_1'}\delta_{\mu_i\mu_i'}$$

<u>Definition</u> : <u>Annihilation</u> <u>operator</u>

$$a_i|\mu_0 \dots \mu_i\rangle \equiv \sqrt{\mu_i}\,|\mu_0 \dots \mu_i - 1\rangle$$

which destroys one particle in the single particle state $\{\lambda_i\}$

<u>For</u> <u>$i<j$</u>

$$\begin{aligned} a_i a_j |\mu_1 \dots \mu_i \dots \mu_j\rangle &= \sqrt{\mu_j}\, a_i|\mu_1 \dots \mu_i \dots \mu_j - 1\rangle \\ &= \sqrt{\mu_i \mu_j}\,|\mu_1 \dots \mu_i - 1 \dots \mu_j - 1\rangle \\ &= a_j a_i |\mu_0 \dots \mu_1 \dots \mu_j \dots\rangle \end{aligned}$$

This then implies

$$a_i a_j = a_j a_i \quad \therefore \quad [a_i, a_j] = 0 \quad , \quad \text{For all } i,j$$

<u>Definition</u> : <u>Creation</u> <u>Operator</u>

$$\Rightarrow \qquad a_i^\dagger |\mu_0 \dots \mu_i\rangle \equiv \sqrt{\mu_i + 1}\,|\mu_0 \dots \mu_1 + 1\rangle$$

where $a^\dagger$ is the Hermitian conjugate

$$\Rightarrow \qquad [a_i^\dagger, a_j^\dagger] = 0 \quad , \quad \text{For all } i,j$$

<u>For</u> <u>$i<j$</u>

$$\begin{aligned} a_i a_j^\dagger |\mu_0 \dots \mu \dots \mu_j\rangle &= \sqrt{\mu_j + 1}\, a_1|\mu_0 \dots \mu_1 \dots \mu_j + 1\rangle \\ &= \sqrt{(\mu_j + 1)\mu_i}\,|\mu_0 \dots \mu_{i-1} \dots \mu_j + 1\rangle \\ &= a_j^\dagger a|\mu_0 \dots \mu_1 \dots \mu_j\rangle \end{aligned}$$

Where we have

$$[a_i, a_j^\dagger] = 0 \quad \text{for } i \neq j$$

<u>For</u> <u>$i=j$</u>

$$a_i a_i^\dagger |\mu_0 \dots \mu_1 \dots\rangle = \sqrt{\mu_i + 1}\, a_1|\mu_0 \dots \mu_1 + 1\rangle$$

At the same time,

$$a_1^\dagger a_1 | \mu_0 \dots \mu_1 \rangle = \sqrt{\mu_1}\, a_1^\dagger | \mu_0 \dots \mu_i - 1 \rangle = \mu_1 | \mu_0 \dots \mu_1 \rangle$$

we then say

$$\Rightarrow \qquad a_i a_i^\dagger = a_i^\dagger a_i + 1 \quad \therefore \quad [a_i, a_j] = \mathbb{1}$$

<u>Summary</u>

$$[a_i, a_j] = [a_i^\dagger, a_j^\dagger] = 0 \Rightarrow [a_i, a_j^\dagger] = \delta_{ij}$$

<u>Definition</u>: <u>Number of particles operator</u>

$$N_i \equiv a_i^\dagger a_i$$

The eigenvalues of N_i are occupation numbers,

$$N_i | \mu_0 \dots \mu_i \rangle = \mu_i | \mu_0 \dots \mu_1 \rangle$$

<u>Definition</u>: <u>Total number of Particles Operator</u>

$$\hat{N} \equiv \sum_i N_i = \sum_i a_i^\dagger a_i$$

we have

$$\hat{N} | \mu_0 \dots \mu_N \rangle = \sum_i \mu_1 | \mu_0 \dots \mu_i \rangle = N | \mu_0 \dots \mu_i \rangle$$

where $N = \sum_i \mu_i$

<u>Properties</u>:

i) $$[N_i, a_j] = [a_i^\dagger a_i, a_j] = [a_i^\dagger, a_j] a_i = -a_i \delta_{ij}$$

Also,

$$[N_i, a_j^\dagger] = [a_i^\dagger a_i, a_j^\dagger] = a_i^\dagger [a_i, a_j^\dagger] = a_i^\dagger \delta_{ij}$$

Finally,

$$N_1 (a_1^\dagger | \mu_0 \dots \mu_i \rangle) = (a_i^\dagger N_i + a_i^\dagger) | \mu_0 \dots \mu_i \rangle = (\mu_i + 1)(a_i^\dagger | \mu_0 \dots \mu_i \rangle)$$

$\therefore$ $a_1^\dagger | \mu_0 \dots \mu_i \rangle$ is an eigenstate of N_i with eigenvalue $\mu_i + 1$

ii) <u>Theorem</u>: The eigenvalues of N_i are non-negative

$$\langle \mu_0 \dots \mu_i | N_i | \mu_0 \dots \mu_i \rangle = \mu_i = \Big(\langle \mu_0 \dots \mu_i | a_i^\dagger \Big) \Big(a_1 | \mu_0 \dots \mu_i \rangle \Big) > 0$$

This then implies

$\Rightarrow$ $\mu_i > 0$ Since $\mathcal{N}_i$ is Hermitian

$\therefore$ one can apply the annihilation operator only a Finite number of times,

$$(a_i)^{\mu} |\mu_0 \dots \mu_i\rangle = \sqrt{\mu_i(\mu_i - 1)\dots(\mu_i - \mu + 1)}\, |\mu_0 \dots \mu_i\rangle$$

Such that $\mu_i - \mu \geq 0$, for all μ.

For $\mu = \mu_i$

$$a_i |\mu_0 \dots 0_{(i)}\rangle = 0$$

otherwise μ_i would be negative

Definition: Vacuum of Bosonic Operators, $|0\rangle$

$|0\rangle$ is the state where

$$a_i|0\rangle = 0 \Rightarrow \mathcal{N}_i|0\rangle = 0, \text{ for all } i$$

There are no particles in this state

Some arbitrary state $|\mu_0 \dots \mu_i\rangle$ can be constructed from the vacuum. For one state

$$a^{+}|0\rangle = \sqrt{1}\,|1\rangle, \quad a^{+}|1\rangle = \sqrt{2}\,|2\rangle \quad \therefore \quad a^{+}|\mu - 1\rangle = \sqrt{\mu}\,|\mu\rangle$$

With our state $|\mu\rangle$ as

$$|\mu\rangle = \frac{(a^{+})^{\mu}}{\sqrt{\mu!}}|0\rangle$$

Generalizing for several states,

$$|\mu_0 \dots \mu_i\rangle = \frac{(a_0^{+})^{\mu_0} \dots (a_i^{+})^{\mu_i} \dots |0\rangle}{\sqrt{\mu_0! \dots \mu_i!}}$$

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Second Quantization (Fermions)

Definition: Destruction, a_1

$$a_1 |\mu_0 \dots \mu_1 \dots \mu_i\rangle = (-1)^{\delta_1} \mu_i |\mu_0 \dots \mu_1 \dots \mu_{i-1}\rangle$$

Where we have the factor

$$\delta_1 = \sum_{k<i} \mu_k$$

is a phase that depends on the occupation of the states on the left of λ_i.

If $i<j$

$$a_i a_j |\mu_0 \ldots \mu_i \ldots \mu_j\rangle = (-1)^{S_j} \mu_j (a_i | \mu_0 \ldots \mu_i \ldots \mu_{i-1}\rangle)$$
$$= (-1)^{S_i+S_j} \mu_j \mu_i | \mu_0 \ldots \mu_{i-1} \ldots \mu_{j-1}\rangle$$

In the reverse and on,

$$a_j a_i |\mu_0 \ldots \mu_i \ldots \mu_j\rangle = (-1)^{S_i} \mu_1 a_j | \mu_0 \ldots \mu_{i-1} \ldots \mu_j\rangle$$
$$= (-1)^{S_i+S_j-1} \mu_1 \mu_0 | \mu_0 \ldots \mu_{i-1} \ldots \mu_{j-1}\rangle$$

$\Rightarrow$
$$a_i a_j = -a_j a_i$$

<u>Definition</u>: <u>Anti-commutator</u>

we have the following relationships

$$\{a_i, a_j\} = 0$$

In particular, for $i=j$

$$a_1^2 = 0 \qquad \Rightarrow \qquad \text{Pauli Exclusion Principle}$$

In the same way,

$$\{a_i, a_j\} = 0 \quad , \quad (a^+_1)^2 = 0$$

<u>Definition</u>: <u>Creation Operator</u>, a_1^+

$$a_1^+ |\mu_0 \ldots \mu_1 \ldots\rangle = (-1)^{S_i} (1-\mu) | \mu_0 \ldots \mu_1 \ldots\rangle$$

Where the factor $(1-\mu)$ enforces $(a^+_1)^2 = 0$ explicitly. Indeed,

$$(a^+_1)^2 |\mu_0 \ldots \mu_1 \ldots\rangle = (-1)^{2S_i} (-1) \mu_1 (1-\mu_1) | \mu_0 \ldots \mu+2\rangle = 0$$

$\Rightarrow$
$$\mu_1(1-\mu_1) = \mu_1 - \mu_1^2 = 0 \quad \therefore \quad \mu_1 = c_1 \wedge_1$$

Again, for $i<j$

$$a_i a_j^+ |\mu_0 \ldots \mu_1 \ldots \mu_j\rangle = (-1)^{S_j} (1-\mu_j) a_1 | \mu_0 \ldots \mu_1 \ldots \mu_{j+1}\rangle$$
$$= (-1)^{S_i+S_j} (1-\mu_j) \mu_1 | \mu_0 \ldots \mu_{i-1} \ldots \mu_{j+1}\rangle$$

Also, Finally
$$a_j^+ a_i |\mu_0 \ldots \mu_i \ldots \mu_j\rangle = (-1)^{S_1} \mu_1 a_j^+ | \mu_0 \ldots \mu_{i-1} \ldots \mu_j\rangle$$

$$= (-1)^{S_i+S_j-1} \mu_i (1-\mu_j) | \mu_0 \dots \mu_{i-1} \dots \mu_{j+1} \rangle$$

From this we can say

$$\{a_i, a_j^\dagger\} = 0 \quad \text{For } i \neq j$$

<u>For $i=j$</u>

$$a_1 a_1^\dagger | \mu_0 \dots \mu_1 \dots \rangle = (-1)^{S_1} (1-\mu_1) a_1 | \mu_0 \dots \mu_{i+1} \rangle = (-1)^{2S_1} (1-\mu_1)(\mu_1+1) | \mu_0 \dots \mu_1 \rangle$$

At the same time,

$$a_1^\dagger a_1 | \mu_0 \dots \mu_1 \dots \rangle = (-1)^{S_i} \mu_1 a_1^\dagger | \mu_0 \dots \mu_{i-1} \rangle = (-1)^{2S_i} \mu_j (1-\mu_{i+1}) | \mu_0 \dots \mu_i \rangle$$

Since

$$\mu_i^2 = \mu_i$$

Then

$$A = (1-\mu_i)(1+\mu_i) = 1-\mu_i^2 = 1-\mu_i \quad , \quad B = \mu_1(2-\mu_1) = 2\mu_1 - \mu_1^2 = \mu_1$$

Now,

$$a_1^\dagger a_1 | \mu_0 \dots \mu_i \rangle = (1-\mu_i) | \mu_0 \dots \mu_i \dots \rangle$$

and

$$a_1 a_1^\dagger | \mu_0 \dots \mu_1 \rangle = \mu_1 | \mu_0 \dots \mu_1 \dots \rangle$$

$\Rightarrow$ $$a_1^\dagger a_1 + a_1^\dagger a_1 = \{a_1, a_1^\dagger\} = \mathbb{I}$$

Hence,

$$\{a_i, a_j^\dagger\} = \delta_{ij}$$

Where we now have

$$N_1 | \mu_0 \dots \mu_1 \dots \rangle = \mu_1 | \mu_0 \dots \mu_1 \dots \rangle$$

Hence,

$$N_1^2 = a_1^\dagger a_1 a_1^\dagger a_1 = a_1^\dagger (1 - a_1^\dagger a_1) a_1 = a_1^\dagger a_1 - (a_1^\dagger)^2 a_1^2 = a_1^\dagger a_1 = N_1$$

$\Rightarrow$ $$N_1(N_1 - 1) = 0 \Rightarrow \mu_1 = 0$$

$N_1 = a_1^\dagger a_1$ is a positive defined operation

$$\mu_1 \geq 0$$

implying in the existence of the vacuum $|0\rangle$,

$$a_1|0\rangle = 0 \quad , \quad N_1|0\rangle = 0$$

Every ket can be written in terms of the vacuum,

$$|\mu_0 \dots \mu_1 \dots \mu_i\rangle = (a_0^+)^{\mu_0}(a_1^+)^{\mu_1}(a_1^+)^{\mu_2}|0\rangle$$

Where the order of the operations matters since they anti-commute (anti-symmetric state).

<u>Example</u>:

a) <u>1 Particle state</u>

$$\langle \vec{x}|a_1^+|0\rangle = \langle \vec{x}|\Lambda_i\rangle = \psi_1(\vec{x})$$

b) <u>Two Particle State</u>

$$\langle \vec{x}_1\vec{x}_2|a_i^+a_j^+|0\rangle = \langle \vec{x}_1\vec{x}_2|\Lambda_i\Lambda_j\rangle = \frac{1}{\sqrt{2}}\left[\psi_i(\vec{x}_1)\psi_j(\vec{x}_2) - \psi_i(\vec{x}_2)\psi_j(\vec{x}_1)\right]$$

$$= -\langle \vec{x}_1\vec{x}_2|\Lambda_j\Lambda_i\rangle = -\langle \vec{x}_2\vec{x}_1|\Lambda_j\Lambda_i\rangle$$

<u>Field Operators</u>

To introduce the co-ordinate representation in many body states, it is convenient to define <u>Field operators</u>

<u>Definition</u> : <u>Field Operators</u>

If $\varphi_1(\vec{x}) = \langle \vec{x}|\lambda_i\rangle$ is the wavefunction associated to the eigenvalue λ_1 of some 1 particle observable, we define the field operator

$$\tilde{\varphi}(\vec{x}) = \sum_i \langle \vec{x}|\lambda_i\rangle a_i = \sum_i \varphi_1(\vec{x})a_i$$

Where a_i is the destruction operator associated with the state $|\lambda_i\rangle$. The Hamiltonian conjugate (creation operator) is

$$\tilde{\varphi}^+(\vec{x}) = \sum_i \langle \vec{x}|\lambda_1\rangle^* a_1^+ = \sum_i \varphi_1^*(\vec{x})a_1^+$$

For <u>both</u> Bosons and Fermions.

Defining

$$[\tilde{A},\tilde{B}]_\pm = AB \pm BA$$

Where "+" For Fermions and "-" For Bosons, we have

$$[\tilde{\varphi}(\vec{x}), \tilde{\varphi}^{+}(\vec{x}')]_{\pm} = \sum_i \sum_j \langle \vec{x} | \lambda_i \rangle \langle \vec{x}' | \lambda_j \rangle^* [a_i, a_j^{+}]_{\pm}$$
$$= \sum_i \sum_j \delta_{ij} \langle \vec{x} | \lambda_i \rangle \langle \lambda_j | \vec{x}' \rangle = \delta^{(1)}(\vec{x} - \vec{x}')$$

Also,

$$[\tilde{\varphi}(\vec{x}), \hat{\varphi}(\vec{x}')]_{\pm} = [\tilde{\varphi}^{+}(\vec{x}), \tilde{\varphi}^{+}(\vec{x}')] = 0$$

Indeed,

$$\int \hat{\varphi}^{+}(\vec{x}) \hat{\varphi}(\vec{x})\, d\vec{x} = \sum_i \sum_j a_i^{+} a_j \rightsquigarrow \int \langle \vec{x} | \lambda_i \rangle^* \langle \vec{x} | \lambda_j \rangle\, d\vec{x} = \sum_i \sum_j a_i^{+} a_j \langle \lambda_i | \lambda_j \rangle$$
$$= \sum_i a_i^{+} a_i = \sum_i N_i = \hat{N}$$

<u>Physical Interpretation of $\varphi^* \varphi$ Operators</u>

i) $\varphi^*(\vec{x})|0\rangle \rightarrow$ Single particle state

We First compute the commutator

$$[\hat{N}, \varphi^{+}(\vec{x})]_{\pm} = \int [\hat{\varphi}^{+}(\vec{x}') \hat{\varphi}(\vec{x}), \hat{\varphi}^{+}(\vec{x})]_{\pm}\, d\vec{x}' = \int \hat{\varphi}^{+}(\vec{x}') [\hat{\varphi}(\vec{x}'), \hat{\varphi}(\vec{x})]\, d\vec{x}'$$
$$= \int \hat{\varphi}^{+}(\vec{x}') \delta(\vec{x}' - \vec{x})\, d\vec{x}' = \hat{\varphi}^{+}(\vec{x})$$

Now,

$$\hat{N}(\hat{\varphi}^{+}|0\rangle) = (\mp \hat{\varphi}^{+} \hat{N} + \hat{\varphi}^{+})|0\rangle = \hat{\varphi}^{+}|0\rangle$$

$\therefore$ $\hat{\varphi}^{+}(\vec{x})|0\rangle$ is an eigenstate of $\hat{N}$ with eigenvalue 1. A 1 particle state.

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$$\varphi^{+}(\vec{x})|0\rangle = |\vec{x}\rangle$$

Is a 1 particle state with co-ordinate $\vec{x}$.

For two particles,

$$\varphi^{+}(\vec{x}_1) \varphi^{+}(\vec{x}_2)|0\rangle = \sum_i \sum_j \langle \vec{x}_1 | \lambda_i \rangle^* \langle \vec{x}_2 | \lambda_j \rangle^* a_i^{+} a_j^{+} |0\rangle$$

This can be written as

$$= \sum_i \sum_j \frac{1}{2} (|\lambda_i\rangle |\lambda_j\rangle \pm |\lambda_j\rangle |\lambda_i\rangle) \langle \lambda_i | \vec{x}_1 \rangle \langle \lambda_j | \vec{x}_2 \rangle$$

Where $\pm$ for bosons or fermions

Using the completeness relation,

$$\sum_i |\lambda_i\rangle\langle\lambda_i| = \mathbb{1}$$

we get:

$$\varphi^+(\vec{x}_1)\varphi^+(\vec{x}_2)|0\rangle = \frac{1}{2}\left(|\vec{x}_1\rangle|\vec{x}_2\rangle \pm |\vec{x}_2\rangle|\vec{x}_1\rangle\right) = \begin{cases} S|\vec{x}_1,\vec{x}_2\rangle & \text{(Bosons)} \\ A|\vec{x}_1,\vec{x}_2\rangle & \text{(Fermions)} \end{cases}$$

In general,

$$S = \frac{1}{N!}\sum_{\sigma \in S_N} P_\sigma, \quad A = \frac{1}{N!}\sum_{\sigma \in S_N} \delta_\sigma P_\sigma$$

<u>Representation</u> <u>of</u> <u>Some</u> <u>Observables</u>

$$\tilde{\mathcal{H}} = \sum_{\alpha=1}^{N} \frac{P_\alpha^2}{2m} + \sum_{i=1}^{N} V_{ext}(\vec{x}_\alpha) + \sum_{\alpha\neq\beta}^{N} V_{INT}(|\vec{x}_\alpha - \vec{x}_\beta|)$$

Is an N particle Hamiltonian, one can separate it into two parts:

$$\tilde{\mathcal{H}}^{(1)} = \sum_\alpha \left\{ \frac{P_\alpha^2}{2m} + V_{ext}(\vec{x}_\alpha) \right\} \quad (1)$$

$$\tilde{\mathcal{H}}^{(2)} = \sum_{\alpha\neq\beta} V_{INT}(|\vec{x}_\alpha - \vec{x}_\beta|) \quad (2)$$

Where (1) is a 1 particle term and (2) is a two particle term. If

$$F = \sum_\alpha f(\vec{x}_\alpha, \vec{p}_\alpha)$$

is the sum of 1 particle operators, written in just quantized language.

In the Fock space representation

$$F = \int \varphi^+(\vec{x}) f(\vec{x},\vec{p}) \varphi(\vec{x})\, d\vec{x}$$

Since,

$$\varphi(\vec{x}) = \sum_i \langle\vec{x}|\lambda_i\rangle a_i, \quad \varphi^+(\vec{x}) = \sum_i \langle\vec{x}|\lambda_i\rangle^* a_i^+$$

Hence,

$$F = \sum_i\sum_j a_j^+ a_i \int \langle\vec{x}|\lambda_j\rangle^* f(\vec{x},\vec{p}) \langle\vec{x}|\lambda_i\rangle = \sum_i\sum_j a_j^+ a_i f_{ij}$$

where,

$$F_{ij} = \int \langle\lambda_j|\vec{x}\rangle \hat{f}(\vec{x},\vec{p}) \langle\vec{x}|\lambda_i\rangle = \langle\lambda_j|\hat{f}|\lambda_i\rangle$$

For two particle operators,

$$G = \frac{1}{2} \sum_{\alpha \neq \beta} g(\vec{x}_\alpha, \vec{x}_\beta)$$

The representation in Fock space is:

$$G = \frac{1}{2} \int \varphi^\dagger(\vec{x}) \varphi^\dagger(\vec{x}') g(\vec{x}, \vec{x}') \varphi(\vec{x}') \varphi(\vec{x}) \, d\vec{x} \, d\vec{x}'$$

In a similar way,

$$G = \frac{1}{2} \sum_{ii'} \sum_{jj'} \langle \lambda_j \lambda_{j'} | \hat{g} | \lambda_{i'} \lambda_i \rangle a_j^\dagger a_{j'}^\dagger a_{i'} a_i$$

where,

$$\langle \lambda_j \lambda_{j'} | \hat{g} | \lambda_{i'} \lambda_i \rangle = \int \varphi_j^*(\vec{x}) \varphi_{j'}^*(\vec{x}') \, g(\vec{x}, \vec{x}') \, \varphi_{i'}(\vec{x}') \varphi_i(\vec{x}) \, d\vec{x} \, d\vec{x}'$$

<u>Example 1</u> : <u>Kinetic Energy</u>

The first quantized version is

$$K \equiv \sum_\alpha \frac{p_\alpha^2}{2m} = \sum_\alpha f(\vec{p}_\alpha)$$

In the co-ordinate representation,

$$f(\vec{p}) = \frac{p^2}{2m} = \frac{-\hbar^2}{2m} \nabla^2$$

The matrix element of f,

$$\langle \lambda_i | \hat{f} | \lambda_j \rangle = \int \varphi_i^*(\vec{x}) \left(\frac{-\hbar^2}{2m} \nabla^2 \right) \varphi_j(\vec{x}) \, d\vec{x} = \frac{-\hbar^2}{2m} \int \varphi_i^*(\vec{x}) \nabla^2 \varphi_j(\vec{x}) \, d\vec{x}$$

using the identity

$$f \nabla^2 g = \vec{\nabla} \cdot (f \vec{\nabla} g) - \vec{\nabla} f \cdot \vec{\nabla} g$$

we now have

$$= \frac{-\hbar^2}{2m} \int \overset{(i)}{\vec{\nabla}(\varphi_i^*(\vec{x}) \vec{\nabla} \varphi_j(\vec{x}))} \, d\vec{x} + \frac{\hbar^2}{2m} \int \overset{(ii)}{\vec{\nabla}(\varphi_i^*(\vec{x}) \vec{\nabla} \varphi_j(\vec{x}))} \, d\vec{x}$$

The first term (i)

$$\int_V \vec{\nabla} \cdot (\varphi_i^* \vec{\nabla} \varphi_j) \, d\vec{x} = \int_{S(V)} (\varphi_i^* \vec{\nabla} \varphi_j) \cdot d\vec{a} = 0$$

using the Gauss theorem (surface term) assuming that the wavefunctions are integrable at $\vec{x} \to \infty$ ($\varphi \to 0$)

Therefore,

$$f_{ij} = \frac{\hbar^2}{2m} \int \vec{\nabla} \varphi_i(\vec{x}) \circ \vec{\nabla} \varphi_j(\vec{x}) \quad \Rightarrow \quad K = \sum_i \sum_j f_{ij} a^\dagger_i a_j$$

Which is Hermitian, since $F_{ij}^* = F_{ji}$

<u>Example 2</u>: <u>Ideal Quantum Gas</u>

we have a Hamiltonian of a free particle

$$\tilde{\mathcal{H}} = \frac{-\hbar^2}{2m} \int \varphi^\dagger(\vec{x}) \nabla^2 \varphi(\vec{x})$$

Since momentum $\vec{k}$ is a good Quantum number a convenient 1 particle state wave Function are plane waves,

$$\langle \vec{x} | \vec{k} \rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}\cdot\vec{x}} \equiv \varphi_{\vec{k}}(\vec{x})$$

where the volume V normalizes the wave function. The spin of the particles enters as a degeneracy factor of $2S+1$.

For periodic boundary conditions,

$$K_i = \frac{2\pi}{L} \nu_i \,, \quad \nu_i = \pm 1, \pm 2 \quad , \quad i = x, y, z$$

now

$$\varphi(\vec{x}) = \sum_{\vec{k}} \varphi_{\vec{k}}(\vec{x}) a_{\vec{k}} = \frac{1}{\sqrt{\nu}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{x}} a_{\vec{k}}$$

$\hookrightarrow \doteq \Psi(\vec{x})$

we then have,

$$\varphi^\dagger(\vec{x}) = \sum_{\vec{k}} \varphi^*_{\vec{k}}(\vec{x}) a^\dagger_{\vec{k}} = \frac{1}{\sqrt{\nu}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{x}} a^\dagger_{\vec{k}}$$

The functions $\varphi_k(\vec{x})$ are orthogonal,

$$\langle \vec{k} | \vec{k}' \rangle = \int \langle \vec{k} | \vec{x} \rangle \langle \vec{x} | \vec{k}' \rangle \, d\vec{x} = \int \frac{1}{\nu} e^{i(\vec{k}'-\vec{k})\cdot\vec{x}} = \delta_{\vec{k},\vec{k}'}$$

Since,

$$\nabla^2 \varphi(\vec{x}) = \frac{-1}{\sqrt{\nu}} \sum_{\vec{k}'} (\vec{k}')^2 e^{i\vec{k}'\cdot\vec{x}} a_{\vec{k}'}$$

Then we have,

$$\mathcal{H} = \sum_{\vec{k}} \sum_{\vec{k}'} \frac{\hbar^2}{2m} (\vec{k}')^2 a^\dagger_k a_k \times \frac{1}{V} \int e^{-i(\vec{k}-\vec{k}')\cdot\vec{x}} d\vec{x} = \sum_{\vec{k}} \frac{\hbar^2 k^2}{2m} a^\dagger_k a_k$$

Which is diagonal in $\vec{k}$, where

$$\varepsilon_{\vec{k}} \equiv \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

Is the dispersion (energy spectrum). Other observables can be found in the same way,

$$\vec{P} = \int \varphi^\dagger(\vec{x}) (-i\vec{\nabla}) \varphi(\vec{x})\, d\vec{x} = \sum_{K} \hbar K\, a^\dagger_k a_k$$