# PHY 742 Quantum Mechanics II
# 12-12:50 AM MWF Olin 103

## Notes for Lecture 25

## Quantum mechanics of multiple particle systems

## Review Chapter 10. Multiple particles in Professor Carlson's textbook

1. Non-interacting particles
   a. Distinguishable, Fermi, Bose
   b. Second quantized formalisms

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|---|---|---|---|---|---|
| **21** | Fri: 03/25/2022 | Chap. 5 & 17 | Quantization of the Electromagnetic Field | #17 | 03/28/2022 |
| **22** | Mon: 03/28/2022 | Chap. 17 | Quantization of the Electromagnetic Field | #18 | 03/30/2022 |
| **23** | Wed: 03/30/2022 | Chap. 17 | Quantization of the Electromagnetic Field | #19 | 04/01/2022 |
| **24** | Fri: 04/01/2022 | Chap. 18 | Absorption and emission of photons | | |
| **25** | Mon: 04/04/2022 | Chap. 10 (review) | Multiparticle systems and second quantization | #20 | 04/04/2022 |
| **26** | Wed: 04/06/2022 | Chap. 10 (review) | Multiparticle systems and second quantization | | |
| **27** | Fri: 04/08/2022 | Chap. 10 (review) | Multiparticle systems and second quantization | | |

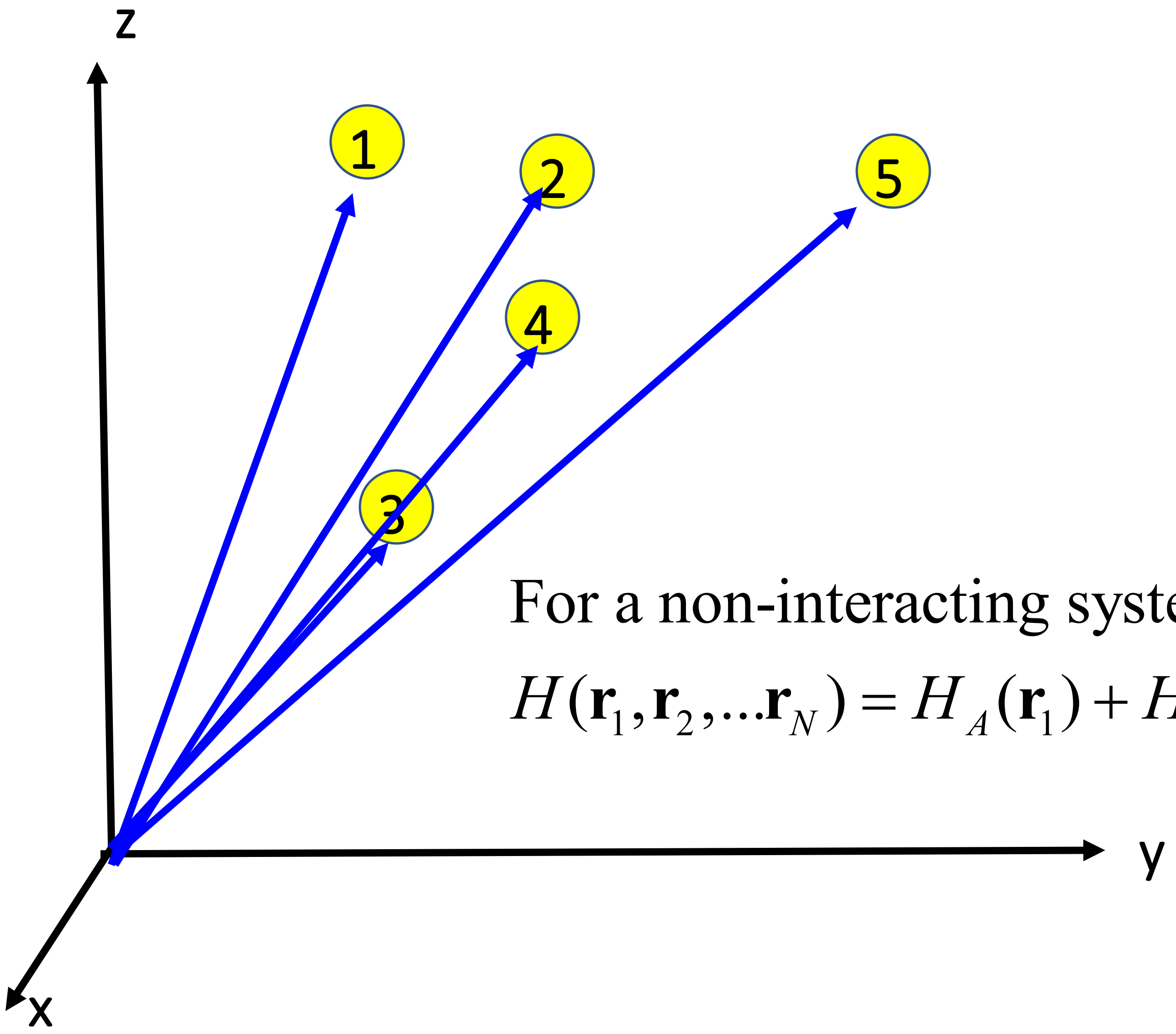
# PHY 742 -- Assignment #20

April 4, 2022

Review Chapter 10 in **Professor Carlson's QM textbook.**.

1. In class, we enumerated all of the distinct states for a system of distinguisable particles, Bose particles, and Fermi particles for the case where there are 2 states *a* and *b* and 2 particles. Perform the same analysis for the case where there are 3 states *a*, *b*, and *c* and 3 particles.

# Quantum mechanical treatment of multiparticle systems




For a non-interacting system:

$$H(\mathbf{r}_1, \mathbf{r}_2, \ldots \mathbf{r}_N) = H_A(\mathbf{r}_1) + H_B(\mathbf{r}_2) + \ldots H_C(\mathbf{r}_N)$$

## Quantum mechanical treatment of multiparticle systems

For a non-interacting system:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = H_A(\mathbf{r}_1) + H_B(\mathbf{r}_2) + ...H_C(\mathbf{r}_N)$$

Energy eigenstates:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N)\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = E\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N)$$

Simplification for separable Hamiltonian

For: $H_A(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a\varphi_a(\mathbf{r}_1)$

$$H_B(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b\varphi_b(\mathbf{r}_2)$$

Solution to the many particle problem

$$\psi(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)...\varphi_z(\mathbf{r}_N)$$

$$E = \varepsilon_a + \varepsilon_b + ....\varepsilon_z$$

**🡸 Turns out to not be generally correct.**

## Quantum mechanical treatment of multiparticle systems – non-interacting particles

**The treatment given on previous slides, assumes that the particles are distinguishable.**

**A more sophisticated treatment is needed for indistinguishable particles.**

Two types of indistinguishable particles:

Fermi particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = -\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Bose particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = +\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

**Consider two particles in a one-dimension labeled with coordinates $x_1$ and $x_2$. Identify each of them as Fermi, Bose, or neither in terms of the functional forms.**

$$1. \quad \psi(x_1, x_2) = e^{-\alpha|x_1 - x_2|}$$

$$2. \quad \psi(x_1, x_2) = (x_1 - x_2)e^{-\alpha|x_1 - x_2|}$$

$$3. \quad \psi(x_1, x_2) = x_1 e^{-\alpha|x_1 - x_2|}$$

## Quantum mechanical treatment of multiparticle systems – non-interacting Fermi particles

Fermi particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = -\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Example for two particles:

$$H(\mathbf{r}_1,\mathbf{r}_2)\psi(\mathbf{r}_1,\mathbf{r}_2) = E\psi(\mathbf{r}_1,\mathbf{r}_2)$$

For: $H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a\varphi_a(\mathbf{r}_1)$

$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b\varphi_b(\mathbf{r}_2)$

Here we assume the Hamiltonian is separable and that the single particle terms are all equal:

$$H_A(\mathbf{r}_1) = H_B(\mathbf{r}_1) \equiv H(\mathbf{r}_1)$$

$$\psi(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) - \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right)$$

$E = \varepsilon_a + \varepsilon_b$

Question: What happens if $\varphi_a(\mathbf{r})$ and $\varphi_b(\mathbf{r})$ have exactly the same functional form?

## Quantum mechanical treatment of multiparticle systems – non-interacting Fermi particles

Fermi particles: $\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = -\psi(\mathbf{r}_1,\mathbf{r}_2,..\mathbf{r}_j...\mathbf{r}_i...\mathbf{r}_N)$

Example for $N$ particles using Slater determinant:

$$\psi(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_a(\mathbf{r}_1) & \varphi_a(\mathbf{r}_2) & \varphi_a(\mathbf{r}_3) & \cdots & \varphi_a(\mathbf{r}_N) \\ \varphi_b(\mathbf{r}_1) & \varphi_b(\mathbf{r}_2) & \varphi_b(\mathbf{r}_3) & \cdots & \varphi_b(\mathbf{r}_N) \\ \varphi_c(\mathbf{r}_1) & \varphi_c(\mathbf{r}_2) & \varphi_c(\mathbf{r}_3) & \cdots & \varphi_c(\mathbf{r}_N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \varphi_z(\mathbf{r}_1) & \varphi_z(\mathbf{r}_2) & \varphi_z(\mathbf{r}_3) & \cdots & \varphi_z(\mathbf{r}_N) \end{vmatrix}$$

$$E = \varepsilon_a + \varepsilon_b + ....\varepsilon_z$$

For $N$=2: $\psi(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) - \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right)$

## Quantum mechanical treatment of multiparticle systems – non-interacting Bose particles

Bose particles: $\psi(\mathbf{r}_1, \mathbf{r}_2, ..\mathbf{r}_i ... \mathbf{r}_j ... \mathbf{r}_N) = \psi(\mathbf{r}_1, \mathbf{r}_2, ..\mathbf{r}_j ... \mathbf{r}_i ... \mathbf{r}_N)$

Example for two particles:

$$H(\mathbf{r}_1, \mathbf{r}_2)\psi(\mathbf{r}_1, \mathbf{r}_2) = E\psi(\mathbf{r}_1, \mathbf{r}_2)$$

For: $H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a \varphi_a(\mathbf{r}_1)$

$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b \varphi_b(\mathbf{r}_2)$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) + \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right)$$

$$E = \varepsilon_a + \varepsilon_b$$

**It is possible to extend these ideas using a modified determinant function --**

Example for two Bose particles:

$$\psi(\mathbf{r}_1,\mathbf{r}_2)=\frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)+\varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right)$$

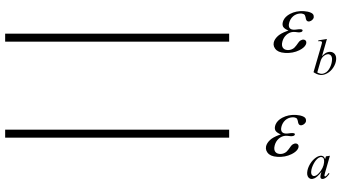
For three Bose particles:

$$\psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=\frac{1}{\sqrt{3!}}\begin{vmatrix}\varphi_a(\mathbf{r}_1) & \varphi_a(\mathbf{r}_2) & \varphi_a(\mathbf{r}_3)\\ \varphi_b(\mathbf{r}_1) & \varphi_b(\mathbf{r}_2) & \varphi_b(\mathbf{r}_3)\\ \varphi_c(\mathbf{r}_1) & \varphi_c(\mathbf{r}_2) & \varphi_c(\mathbf{r}_3)\end{vmatrix}_+$$

**Determinant but without minus signs.**

## Quantum mechanical treatment of multiparticle systems – non-interacting particles; multiplicity of eigenstates

**Consider a system with two independent particle states and two particles:**



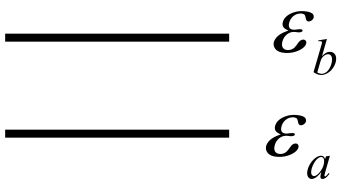

$$H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a\varphi_a(\mathbf{r}_1)$$
$$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b\varphi_b(\mathbf{r}_2)$$

Possible states for distinguishable particles:

$$\psi_I(\mathbf{r}_1,\mathbf{r}_2) = \varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) \qquad E_I = \varepsilon_a + \varepsilon_b$$
$$\psi_{II}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1) \qquad E_{II} = \varepsilon_a + \varepsilon_b$$
$$\psi_{III}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_a(\mathbf{r}_1)\varphi_a(\mathbf{r}_2) \qquad E_{III} = 2\varepsilon_a$$
$$\psi_{IV}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_b(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) \qquad E_{IV} = 2\varepsilon_b$$

## Quantum mechanical treatment of multiparticle systems – non-interacting particles; multiplicity of eigenstates

**Consider a system with two independent particle states and two particles:**




$$H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a\varphi_a(\mathbf{r}_1)$$
$$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b\varphi_b(\mathbf{r}_2)$$

Possible states for Fermi particles:

$$\psi_{I+II}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) - \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right) \qquad E_{I+II} = \varepsilon_a + \varepsilon_b$$

**Quantum mechanical treatment of multiparticle systems – non-interacting particles; multiplicity of eigenstates**

**Consider a system with two independent particle states and two particles:**

$\varepsilon_b$

$\varepsilon_a$

$$H(\mathbf{r}_1)\varphi_a(\mathbf{r}_1) = \varepsilon_a \varphi_a(\mathbf{r}_1)$$
$$H(\mathbf{r}_2)\varphi_b(\mathbf{r}_2) = \varepsilon_b \varphi_b(\mathbf{r}_2)$$

Possible states for Bose particles:

$$\psi_{I+II}(\mathbf{r}_1,\mathbf{r}_2) = \frac{1}{\sqrt{2}}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) + \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)\right) \qquad E_{I+II} = \varepsilon_a + \varepsilon_b$$

$$\psi_{III}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_a(\mathbf{r}_1)\varphi_a(\mathbf{r}_2) \qquad E_{III} = 2\varepsilon_a$$

$$\psi_{IV}(\mathbf{r}_1,\mathbf{r}_2) = \varphi_b(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) \qquad E_{IV} = 2\varepsilon_b$$

## Treating multiparticle systems using "second" quantization formalism

Consider a non-interacting system:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = H(\mathbf{r}_1) + H(\mathbf{r}_2) + ...H(\mathbf{r}_N)$$

For a system of non-interacting identical particles,

the single particle Hamiltonians $H(\mathbf{r}_1)$ are also identical.

Suppose we have a complete basis set that describes

each single-particle state;

$$\Phi(\mathbf{r},t) = \sum_\alpha C_\alpha \varphi_\alpha(\mathbf{r}) e^{-i\varepsilon_\alpha t/\hbar}$$

For convenience, we assume orthonormality:

$$\langle \varphi_\alpha | \varphi_\beta \rangle = \delta_{\alpha\beta}$$

These basis functions can be used to represent

the many particle wavefunctions.

## Operators for Bose system

Creation operator: $b_\alpha^\dagger|0\rangle = |1_\alpha\rangle \quad b_\alpha^\dagger|n_\alpha\rangle = \sqrt{n_\alpha + 1_\alpha}\,|n_\alpha + 1_\alpha\rangle$

Destruction operator: $b_\alpha|1_\alpha\rangle = |0_\alpha\rangle \quad b_\alpha|n_\alpha\rangle = \sqrt{n_\alpha}\,|n_\alpha - 1_\alpha\rangle$

## Commutator notation

$$b_\alpha^\dagger b_\beta^\dagger = b_\beta^\dagger b_\alpha^\dagger \qquad \left[b_\alpha^\dagger, b_\beta^\dagger\right] = 0$$

$$b_\alpha b_\beta = b_\beta b_\alpha \qquad \left[b_\alpha, b_\beta\right] = 0$$

$$\left[b_\alpha, b_\beta^\dagger\right] = \delta_{\alpha\beta}$$

**Some details --**

$$\text{Single particle:} \quad b_\alpha^\dagger \left|0\right\rangle = \left|1_\alpha\right\rangle \quad \Rightarrow \quad \left|\varphi_\alpha\right\rangle$$

$$\text{Two particles:} \quad b_\alpha^\dagger b_\beta^\dagger \left|0\right\rangle \equiv b_\alpha^\dagger b_\beta^\dagger \left|00\right\rangle = \left|1_\alpha 1_\beta\right\rangle \quad \Rightarrow \quad \left|\varphi_\alpha \varphi_\beta\right\rangle$$

## Example for Fermi particles

Slater determinant for $N$ particles:

$$|\psi(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N)\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} \varphi_a(\mathbf{r}_1) & \varphi_a(\mathbf{r}_2) & \varphi_a(\mathbf{r}_3) & \cdots & \varphi_a(\mathbf{r}_N) \\ \varphi_b(\mathbf{r}_1) & \varphi_b(\mathbf{r}_2) & \varphi_b(\mathbf{r}_3) & \cdots & \varphi_b(\mathbf{r}_N) \\ \varphi_c(\mathbf{r}_1) & \varphi_c(\mathbf{r}_2) & \varphi_c(\mathbf{r}_3) & \cdots & \varphi_c(\mathbf{r}_N) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \varphi_z(\mathbf{r}_1) & \varphi_z(\mathbf{r}_2) & \varphi_z(\mathbf{r}_3) & \cdots & \varphi_z(\mathbf{r}_N) \end{vmatrix}$$

Second quantization representation:

$$|\psi(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N)\rangle \Rightarrow |n_a n_b n_c ....n_z\rangle$$

**For Fermi particles, the occupation eigenvalues can be $n_a=0$ or $1$**

**Operators for Fermi system**

Creation operator: $f_\alpha^\dagger \left|0\right\rangle = \left|1_\alpha\right\rangle$

Destruction operator: $f_\alpha \left|1_\alpha\right\rangle = \left|0_\alpha\right\rangle$

**Anti commutator notation**

$$f_\alpha^\dagger f_\beta^\dagger = -f_\beta^\dagger f_\alpha^\dagger \qquad \left\{ f_\alpha^\dagger, f_\beta^\dagger \right\} = 0$$

$$f_\alpha f_\beta = -f_\beta f_\alpha \qquad \left\{ f_\alpha, f_\beta \right\} = 0$$

$$\left\{ f_\alpha, f_\beta^\dagger \right\} = \delta_{\alpha\beta}$$

**Beginnings of a systematic treatment**

- **Non-interacting particles**
  - **Complete set of basis functions**
  - **Representation of the Hamiltonian in terms of matrix elements in the basis**
  - **Second-quantized representation of the Hamiltonian**
- **Representation of interaction terms**

## Complete set of basis functions

Consider a non-interacting system:

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = H(\mathbf{r}_1) + H(\mathbf{r}_2) + ...H(\mathbf{r}_N)$$

For a system of non-interacting identical particles,

the single particle Hamiltonians $H(\mathbf{r}_1)$ are also identical.

Suppose we have a complete basis set that describes each single-particle state;

$$\Phi(\mathbf{r},t) = \sum_\alpha C_\alpha \varphi_\alpha(\mathbf{r}) e^{-i\varepsilon_\alpha t/\hbar}$$

where $H(\mathbf{r})\varphi_\alpha(\mathbf{r}) = \varepsilon_\alpha \varphi_\alpha(\mathbf{r})$

For convenience, we assume orthonormality:

$$\langle \varphi_\alpha | \varphi_\beta \rangle = \delta_{\alpha\beta}$$

These basis functions can be used to represent the many particle wavefunctions.

**Example for Bose particles**

$$H(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N) = E\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N)$$

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\ldots\mathbf{r}_N) = \frac{1}{\sqrt{N!}} \prod_{\text{Permutations } i,j} \varphi_i(\mathbf{r}_j)$$

$$i = a,b,c.....\qquad j = 1,2,3....N$$

Matrix elements: $\langle \varphi_a | H | \varphi_b \rangle = \varepsilon_a \delta_{a,b}$