

PHY 741 Quantum Mechanics
12-12:50 PM MWF Olin 103

Plan for Lecture 12:
Read Chapter #10 in Shankar
Quantum mechanics of
multiparticle systems

- 1. Non-interacting particles**
 - a. Distinguishable, Fermi, Bose**
 - b. Second quantized formalism**
- 2. Interacting particles**

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Course schedule
(Preliminary schedule – subject to frequent adjustment)

Date	F&W Reading	Topic	Assignment	Due
1 Mon, 8/28/2017	Chap. 1	Review of basic principles	#1	9/6/2017
2 Wed, 8/30/2017	Chap. 1	Linear vector spaces	#2	9/6/2017
3 Fri, 9/01/2017	Chap. 1	Linear vector spaces	#3	9/6/2017
4 Mon, 9/04/2017	Chap. 4	Principles of Quantum Mechanics	#4	9/8/2017
5 Wed, 9/06/2017	Chap. 5	Examples in 1 dimension		
6 Fri, 9/08/2017	Chap. 5	Schrödinger equation in one-dimension	#5	9/13/2017
7 Mon, 9/11/2017	Chap. 5	Schrödinger equation in one-dimension		
8 Wed, 9/13/2017	Chap. 7	Schrödinger equation in one-dimension	#6	9/15/2017
9 Fri, 9/15/2017	Chap. 7	Schrödinger equation in one-dimension	#7	9/20/2017
10 Mon, 9/18/2017	Chap. 5 and 7	Schrödinger equation in one-dimension		
11 Wed, 9/20/2017	Chap. 9	Commutator formalism	#8	9/22/2017
12 Fri, 9/22/2017	Chap. 10	Quantum mechanics of multiparticle systems	#9	9/25/2017
13 Mon, 9/25/2017				
14 Wed, 9/27/2017				
15 Fri, 9/29/2017				
Mon, 10/02/2017		Take-home exam – No class		
Wed, 10/04/2017		Take-home exam – No class		

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Quantum mechanical treatment of multiparticle systems

For a non-interacting system:
 $H(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = H(\mathbf{r}_1) + H(\mathbf{r}_2) + \dots H(\mathbf{r}_N)$

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Quantum mechanical treatment of multiparticle systems

For a non-interacting system:

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

Energy eigenstates:

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

Simplification for separable Hamiltonian
 For: $H(\mathbf{r}_1)\phi_a(\mathbf{r}_1) = \varepsilon_a\phi_a(\mathbf{r}_1)$
 $H(\mathbf{r}_2)\phi_b(\mathbf{r}_2) = \varepsilon_b\phi_b(\mathbf{r}_2)$

Solution to the many particle problem

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2)\dots\phi_z(\mathbf{r}_N)$$

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

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

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

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

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: $H(\mathbf{r}_1)\phi_a(\mathbf{r}_1) = \varepsilon_a\phi_a(\mathbf{r}_1)$
 $H(\mathbf{r}_2)\phi_b(\mathbf{r}_2) = \varepsilon_b\phi_b(\mathbf{r}_2)$

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(\phi_a(\mathbf{r}_1)\phi_b(\mathbf{r}_2) - \phi_a(\mathbf{r}_2)\phi_b(\mathbf{r}_1))$$

$$E = \varepsilon_a + \varepsilon_b$$

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

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

Example for N particles using Slater determinant:

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

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

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

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

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

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

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

$E = \varepsilon_a + \varepsilon_b$

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

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

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

Possible states for distinguishable particles:

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

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

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

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

Possible states for Fermi particles:

$$\psi_I(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) - \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)) \quad E_I = \varepsilon_a + \varepsilon_b$$

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

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

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

Possible states for Bose particles:

$$\psi_I(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2}}(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2) + \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)) \quad E_I = \varepsilon_a + \varepsilon_b$$

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

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

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Treating multiparticle systems using “second” quantization formalism

Consider a non-interacting system:

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

For a system of non-interacting identical particles, the single particle Hamiltonians $H(\mathbf{r}_i)$ are also identical. Suppose we have a complete basis set that describes each single-particle state;

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

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

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Example for Fermi particles

Slater determinant for N particles:

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

Second quantization representation:

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

For Fermi particles, the occupation eigenvalues can be $n_\alpha = 0$ or 1

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Operators for Fermi system

Creation operator:

$$a_\alpha^\dagger |0\rangle = |1_\alpha\rangle$$

Destruction operator:

$$a_\alpha |1_\alpha\rangle = |0_\alpha\rangle$$

$$a_\alpha^\dagger a_\beta^\dagger = -a_\beta^\dagger a_\alpha^\dagger$$

$$a_\alpha a_\beta = -a_\beta a_\alpha$$

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Second quantization creation and annihilation operators

$$a_\alpha |n_\alpha\rangle = \sqrt{n_\alpha} |n_\alpha - 1\rangle$$

$$a_\alpha^\dagger |n_\alpha\rangle = \sqrt{n_\alpha + 1} |n_\alpha + 1\rangle$$

$$a_\alpha^\dagger a_\alpha |n_\alpha\rangle = n_\alpha |n_\alpha\rangle$$

$$a_\alpha a_\alpha^\dagger |n_\alpha\rangle = (n_\alpha + 1) |n_\alpha\rangle$$

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