PHY 742 Quantum Mechanics II
1-1:50 AM MWF via video link:
https://wakeforest-university.zoom.us/my/natalie.holzwarth

Plan for Lecture 25

Quantum mechanics of multiple particle systems

Read Professor Carlson's textbook: Chapter X. Multiple particles

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

In this lecture, we will begin our consideration of multiple particle systems which is discussed in Chapter 10 of your textbook. First we consider the ideal situation that the multiple particles do not interact with eachother.

Topics for Quantum Mechanics II

Single particle analysis

- **Single particle interacting with electromagnetic fields – EC Chap. 9**
- **Scattering of a particle from a spherical potential – EC Chap. 14**
- **More time independent perturbation methods – EC Chap. 12, 13**
- **Single electron states of a multi-well potential ➔ molecules and solids – EC Chap. 2,6**
- **Time dependent perturbation methods – EC Chap. 15**
- **Relativistic effects and the Dirac Equation – EC Chap. 16**
- **Path integral formalism (Feynman) – EC Chap. 11.C**

Multiple particle analysis

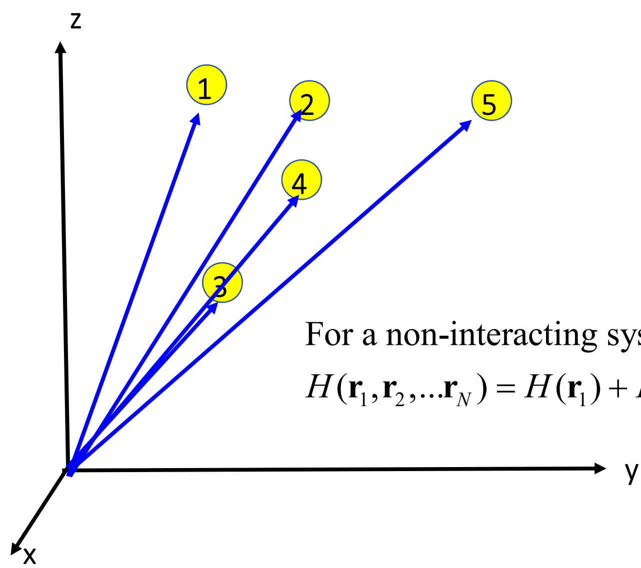
- **Quantization of the electromagnetic fields – EC Chap. 17**
- **Photons and atoms – EC Chap. 18**
- **Multi particle systems; Bose and Fermi particles – EC Chap. 10**
- **Multi electron atoms and materials**
  - **Hartree-Fock approximation**
  - **Density functional approximation**

Here is the course outline that we have been following.

21	Mon: 03/23/2020	Chap. 17	Quantization of the Electromagnetic Field	#17	03/25/2020
22	Wed: 03/25/2020	Chap. 17	Quantization of the Electromagnetic Field	#18	03/27/2020
23	Fri: 03/27/2020	Chap. 17	Quantization of the Electromagnetic Field	#19	03/30/2020
24	Mon: 03/30/2020	Chap. 18	Photons and atoms		
25	Wed: 04/01/2020	Chap. 10	Multiparticle systems	#20	04/03/2020
26	Fri: 04/03/2020				
27	Mon: 04/06/2020				
28	Wed: 04/08/2020				
	Fri: 04/10/2020	No class	*Good Friday*		
29	Mon: 04/13/2020				
30	Wed: 04/15/2020				
31	Fri: 04/17/2020				
32	Mon: 04/20/2020				
33	Wed: 04/22/2020				
34	Fri: 04/24/2020				
35	Mon: 04/27/2020				
36	Wed: 04/29/2020		Review		

Homework #20 asks you to do a problem from the end of Chapter 10 of Professor Carlson's textbook.

Quantum mechanical treatment of multiparticle systems



For a non-interacting system:

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

This diagram illustrates a general system to be considered where N particles are described by N different coordinates. For the moment, we will be considering systems which do not vary in time. This can be generalized later.

Quantum mechanical treatment of multiparticle systems

For a non-interacting system:

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

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

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

Solution to the many particle problem

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

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

In order to describe our system we need to account for the coordinates of our N particles in the probability amplitude psi. Since the particles do not interact with each other, we can analyze the individual particle states by solving each single particle Schrodinger equation in terms of their probability amplitudes phi. The many particle probability amplitude is then simply the product of the single particle functions and the eigenstate energy is the sum of the single particle energies.

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

However the product of single particle states is missing some of the know properties of indistinguishable multiparticle systems. In particular, it is known that there are two types of particles, named Fermi particles and Bose particles which behave differently. The difference between the two is represented in terms of how their probability amplitudes are affected by the exchange of two particles in the function.

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

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

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

$$E = \varepsilon_a + \varepsilon_b$$

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Returning to the non-interacting particles. By construction, this form of psi satisfies the Fermi particle exchange equation. What do you think happens of the two functions phia and phib have exactly the same shape?

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:

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

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

The antisymmetrization of single particle states can be conveniently be written in terms of a so-called Slater determinant.

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

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

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

$$E = \varepsilon_a + \varepsilon_b$$

Returning to the non-interacting particles. By construction, this form of psi satisfies the Bose particle exchange equation. What do you think happens of the two functions phia and phib have exactly the same shape?

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

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

ε_b

ε_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 distinguishable particles:

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

Here we can find 4 different 2-particle states for the distinguishable particle case.

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

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

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

Possible states for Fermi particles:

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

Is there really only one possibility here?

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

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

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

Possible states for Bose particles:

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

How could it be that there are more possibilities here?

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;

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

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

It turns out that the creation and annihilation operators can be used to help us with a convenient formalism to take the particle symmetry into account. We need to start with a complete set of single particle basis functions.

Operators for Bose system

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

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

Commutator notation

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

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

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

From our experience with creation and annihilation operators we can deduce the following relationships .

Example for Fermi particles

Slater determinant for N particles:

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

Second quantization representation:

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

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

Now, consider the case for Fermi particles. Why are the occupation eigenvalues restricted as stated for Fermi particles?

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

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

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

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

We will show next time, that we construct creation and annihilation operators for Fermi particles as well. These ideas will be elaborated next time.