PHY 742 Quantum Mechanics II

1-1:50 AM MWF via video link:

https://wakeforest-university.zoom.us/my/natalie.holzwarth

Plan for Lecture 26

Quantum mechanics of multiple particle systems

Continue reading Professor Carlson's textbook: Chapter X. Multiple particles (Sec. A&B)

   1. **Non-interacting particles**

   a. **Second quantized formalism for Bose particles**

   b. **Second quantized formalism for Fermi particles**

In this lecture, we will continue our consideration of multiple particle systems which is discussed in Chapter 10 of your textbook.   We continue to consider the ideal situation in which the multiple particles do not interact with each other.

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
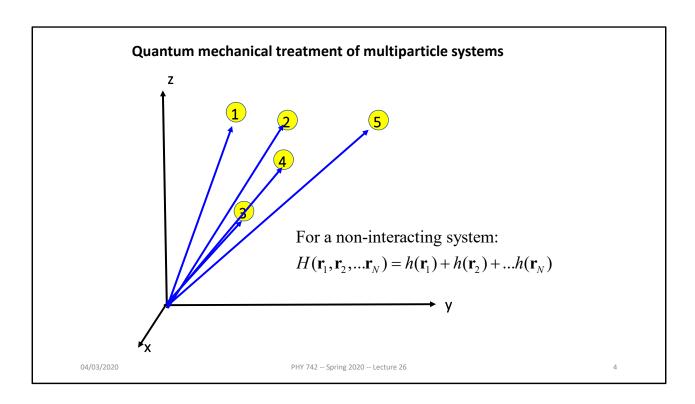
        Density functional approximation

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	Chap. 10	Multiparticle systems	[#21](#)	04/06/2020
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 #21 involves examining the derivations and results of Slide 12 of this lecture.

Quantum mechanical treatment of multiparticle systems

For a non-interacting system:

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

This diagram illustrates a general system to be considered where N particles are described by N different coordinates. The lower case "h" is used to emphasize a single particle Hamiltonian.

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

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

Solution to the many particle problem

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

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

Does not take into account particle symmetry.

Here we summarize the equations from Lecture 25.   The non-interacting total Hamiltonian can be written as a sum of single particle Hamiltonian terms.

Refinement of the results for treatment of distinguishable or indistinguishable particles

For distinguishable particles:

$\mathscr{P}$=permutation operator

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

$$\mathscr{P}(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)) \equiv \varphi_a(\mathbf{r}_2)\varphi_b(\mathbf{r}_1)$$

Two types of indistinguishable particles:

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

$$\Rightarrow \psi_F(\mathbf{r}_1, \mathbf{r}_2, ..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\sum_{\mathscr{P}}(-1)^{\mathscr{P}}\mathscr{P}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)\varphi_c(\mathbf{r}_3)...\varphi_z(\mathbf{r}_N)\right)$$

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

$$\Rightarrow \psi_B(\mathbf{r}_1, \mathbf{r}_2, ..\mathbf{r}_i...\mathbf{r}_j...\mathbf{r}_N) = \frac{1}{\sqrt{N!}}\sum_{\mathscr{P}}\mathscr{P}\left(\varphi_a(\mathbf{r}_1)\varphi_b(\mathbf{r}_2)\varphi_c(\mathbf{r}_3)...\varphi_z(\mathbf{r}_N)\right)$$

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

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

Here we summarize the particle permutation properties of Fermi and Bose particles.
Using the permutation operator.

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.

Eigenstates of the single particle Hamiltonian:

$$h(\mathbf{r})\varphi_a(\mathbf{r}) = \varepsilon_a \varphi_a(\mathbf{r})$$

$$h(\mathbf{r})\varphi_b(\mathbf{r}) = \varepsilon_b \varphi_b(\mathbf{r})$$

$$\vdots$$

$$h(\mathbf{r})\varphi_z(\mathbf{r}) = \varepsilon_z \varphi_z(\mathbf{r})$$

We now assume that the single particle eigenstates $\{\varphi_a(\mathbf{r})\}$

span the function space available to each particle.

Defining the basis eigenstates from the single particle Hamiltonian.

Treating multiparticle systems using "second" quantization formalism -- continued

$$h(\mathbf{r}_1) = \sum_{\alpha} |\varphi_{\alpha}(\mathbf{r}_1)\rangle \varepsilon_{\alpha} \langle \varphi_{\alpha}(\mathbf{r}_1)|$$

$$\langle \varphi_{\alpha}(\mathbf{r}_1) | \psi(\mathbf{r}_1, \mathbf{r}_2, ... \mathbf{r}_N) \rangle = n_{\alpha}$$

=number of times basis function $\varphi_{\alpha}(\mathbf{r}_1)$

appears in the product representation

Second quantization representation:

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

$$H(\mathbf{r}_1, \mathbf{r}_2 .... \mathbf{r}_N) \Rightarrow \sum_{\alpha} \varepsilon_{\alpha} N_{\alpha}$$

where the number operator acts as follows:

$$N_{\alpha} |n_a n_b n_c .... n_z\rangle = n_{\alpha} |n_a n_b n_c .. n_{\alpha} .. n_z\rangle$$

Introducing the notion of "second" quantization.

In general, the number operator can be expressed in terms of a product of two operators. For the case of Bose particles, these operators are very similar to the raising and lowering operators of the harmonic oscillator.

$$N_\alpha = b_\alpha^\dagger b_\alpha$$

Bose particle commutation relations:

$$[b_\alpha, b_\beta] \equiv b_\alpha b_\beta - b_\beta b_\alpha = 0$$

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

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

Considering first the case of Bose particles.

Second quantization for Bose particles, continued

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

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

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

For example: $b_\alpha^\dagger |0_\alpha\rangle = |1_\alpha\rangle$

$$b_\alpha^\dagger |1_\alpha\rangle = \sqrt{2}\,|2_\alpha\rangle$$

$$\left(b_\alpha^\dagger\right)^n |0_\alpha\rangle = \sqrt{n!}\,|n_\alpha\rangle$$

$$\Rightarrow n_\alpha = 0, 1, 2, \ldots\infty$$

To represent 3 states: $|n_1 n_2 n_3\rangle = \dfrac{\left(b_3^\dagger\right)^{n_3}}{\sqrt{n_3!}}\dfrac{\left(b_2^\dagger\right)^{n_2}}{\sqrt{n_2!}}\dfrac{\left(b_1^\dagger\right)^{n_1}}{\sqrt{n_1!}}|0\rangle$

For Bose particles, we can use the same relationships found for harmonic oscillators and for the quantized electromagnetic fields.

Second quantization for Fermi particles

$$N_\alpha = f_\alpha^\dagger f_\alpha$$

Fermi particle anticommutation relations:

$$\left\{ f_\alpha, f_\beta \right\} \equiv f_\alpha f_\beta + f_\beta f_\alpha = 0$$

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

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

Now consider the case for Fermi particles.

Second quantized creation and annhilation Fermi operators

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

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

$$f^\dagger{}_\alpha |n_\alpha\rangle = \sqrt{1 - n_\alpha} |1 - n_\alpha\rangle$$

These results follow from the anti commutator relations of the operators.

Non-trivial operations:

$$f_\alpha |0_\alpha\rangle = 0 \qquad f_\alpha |1_\alpha\rangle = |0_\alpha\rangle$$

$$f_\alpha^\dagger |0_\alpha\rangle = |1_\alpha\rangle \quad f_\alpha^\dagger |1_\alpha\rangle = 0$$

$$\Rightarrow n_\alpha = 0 \text{ or } 1$$

To represent 3 states: $|n_a n_b n_c\rangle = \left(f_c^\dagger\right)^{n_c} \left(f_b^\dagger\right)^{n_b} \left(f_a^\dagger\right)^{n_a} |0\rangle$

These results follow from the anti-commutation relations.   Your homework for this lecture is to verify these relationships.

Note that the symmetry of the wavefunction is built into the formalism for Bose particles

$$b_a^\dagger b_b^\dagger |0\rangle = b_b^\dagger b_a^\dagger |0\rangle$$

Note that the antisymmetry of the wavefunction is built into the formalism for Fermi particles

$$f_a^\dagger f_b^\dagger |0\rangle = -f_b^\dagger f_a^\dagger |0\rangle$$

In this case, the second quantized forms for the non-interacting system can be written:

$$H(\mathbf{r}_1, \mathbf{r}_2 .... \mathbf{r}_N) \Rightarrow \sum_\alpha \varepsilon_\alpha b_\alpha^\dagger b_\alpha \quad \text{for Bose particles}$$

$$H(\mathbf{r}_1, \mathbf{r}_2 .... \mathbf{r}_N) \Rightarrow \sum_\alpha \varepsilon_\alpha f_\alpha^\dagger f_\alpha \quad \text{for Fermi particles}$$

What do you think are the advantages/disadvantages of this second quantized formalism?

More general treatment of multiparticle system

$$H(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \sum_{i=1}^{N} h(\mathbf{r}_i) + V(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N)$$

interparticle
interaction

Often: $V(\mathbf{r}_1,\mathbf{r}_2,...\mathbf{r}_N) = \sum_{i=1\,(i>j)}^{N} \sum_{j=1}^{N} v(\mathbf{r}_i - \mathbf{r}_j)$

In this case, the second quantized forms can be written

$$H(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N) \Rightarrow \sum_{\alpha} \varepsilon_\alpha b_\alpha^\dagger b_\alpha + \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} b_\alpha^\dagger b_\beta^\dagger b_\gamma b_\delta \quad \text{for Bose particles}$$

$$H(\mathbf{r}_1,\mathbf{r}_2....\mathbf{r}_N) \Rightarrow \sum_{\alpha} \varepsilon_\alpha f_\alpha^\dagger f_\alpha + \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} f_\alpha^\dagger f_\beta^\dagger f_\gamma f_\delta \quad \text{for Fermi particles}$$

Here $v_{\alpha\beta\gamma\delta}$ denotes matrix elements such as

$$v_{\alpha\beta\gamma\delta} = \int d^3 r_1 \int d^3 r_2 \; \varphi_\alpha^*(\mathbf{r}_1)\varphi_\beta^*(\mathbf{r}_2) v(\mathbf{r}_1 - \mathbf{r}_2)\varphi_\gamma(\mathbf{r}_1)\varphi_\delta(\mathbf{r}_2)$$

Next time, we will start to think about what happens when the particles interact.