**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.

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|---|---|---|---|---|---|
| **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.

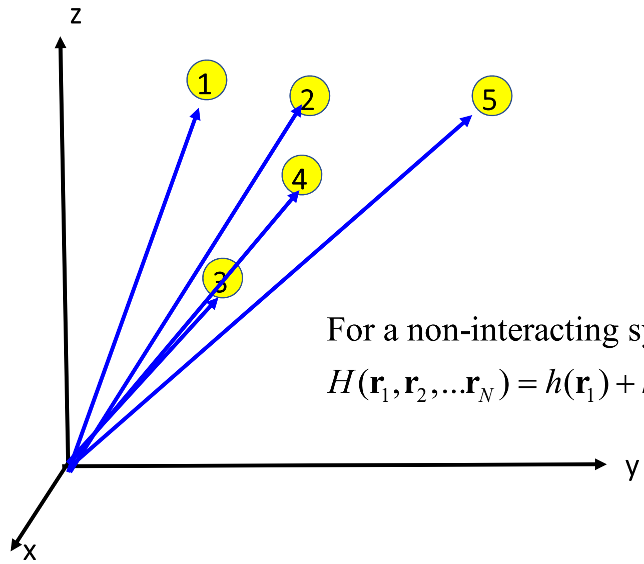
**Your questions:**

**From Trevor:** 1. At the top of slide 13, should the relations not be b*b|0> = bb*|0> and f*f|0> = -ff*|0>?

**Comment:** I think the equations on slide 13 are correct. We will discuss this further, as we go systematically through the slides.

## Slides from original lecture

**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. The lower case “h” is used to emphasize a single particle Hamiltonian.

**Quantum mechanical treatment of multiparticle systems**

For a non-interacting system:

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

Energy eigenstates:

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

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

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

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

**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**

$\mathscr{P}$=**permutation operator**

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

For distinguishable particles:

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

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**

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

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

=number of times basis function $\varphi_\alpha(\mathbf{r}_1)$ appears in the product representation

Second quantization representation:

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

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

Here the notation $N_\alpha$ indicates an operator

where the number operator acts as follows:

$$N_\alpha \left| n_a n_b n_c \ldots n_z \right\rangle = n_\alpha \left| n_a n_b n_c .. n_\alpha .. n_z \right\rangle$$



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**

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

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

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

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

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

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

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

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



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

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

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

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

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

Non-trivial operations:

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

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

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

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



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**

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

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

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

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

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

interparticle interaction

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

In this case, the second quantized forms can be written

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

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

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.

**Pros and Cons for using second quantization –**

**Pros –**

1. **Beautiful, compact, ….**
2. **Worthy of physicists …**

**Cons –**

1. **Does not really introduce new physics**
2. **Slater determinants and symmetrization/antisymmetrization operators are good enough**

**Historical paper and its use of second quantization --**

PHYSICAL REVIEW VOLUME 108, NUMBER 5 DECEMBER 1, 1957

# Theory of Superconductivity*

J. Bardeen, L. N. Cooper,† and J. R. Schrieffer‡
*Department of Physics, University of Illinois, Urbana, Illinois*

(Received July 8, 1957)

A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar\omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $(\hbar\omega)^2$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5kT_c$ at $T=0°K$ to zero at $T_c$. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.

**Model Hamiltonian for Cooper pairs (weakly paired electrons described by $b_k$ which interact via the potential term --**

$$H_{\rm red}=2\sum_{k>k_F}\epsilon_{\bf k}b_{\bf k}{}^*b_{\bf k}+2\sum_{k<k_F}|\epsilon_{\bf k}|b_{\bf k}b_{\bf k}{}^* - \sum_{\bf kk'}V_{\bf kk'}b_{\bf k'}{}^*b_{\bf k}. \quad (2.14)$$

$$b_{\bf k}=c_{-{\bf k}\downarrow}c_{{\bf k}\uparrow}, \quad (2.9)$$

$$b_{\bf k}{}^*=c_{{\bf k}\uparrow}{}^*c_{-{\bf k}\downarrow}{}^*. \quad (2.10)$$

These operators satisfy the commutation relations

$$[b_{\bf k},b_{\bf k'}{}^*]_-=(1-n_{{\bf k}\uparrow}-n_{-{\bf k}\downarrow})\delta_{\bf kk'}, \quad (2.11)$$

$$[b_{\bf k},b_{\bf k'}]_-=0, \quad (2.12)$$

$$[b_{\bf k},b_{\bf k'}]_+=2b_{\bf k}b_{\bf k'}(1-\delta_{\bf kk'}), \quad (2.13)$$