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

Plan for Lecture 21

Quantization of the Electromagnetic fields

Review the "raising" and "lowering" operators presented in Professor Carlson's textbook in V. The Harmonic Oscillators. Start reading XVII. Quantizing Electromagnetic Fields.

1. **Review of the harmonic oscillator**
2. **Particle creation and annihilation operator formalism**
3. **Hamiltonian for the electromagnetic fields**

Welcome to the new format of PHY 742. The same motivations and requirements mentioned in the PHY 712 slides apply to PHY 742. In the next few lectures, we will consider the "quantization" of the electromagnetic field, inspired by the detailed results of the analysis of the one dimensional harmonic oscillator.

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**

This is the schedule that we have used from the beginning. Comments/suggestions are welcome.

	Mon: 03/16/2020	No class	*Classes Cancelled*		
	Wed: 03/18/2020	No class	*Classes Cancelled*		
	Fri: 03/20/2020	No class	*Classes Cancelled*		
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		
23	Fri: 03/27/2020				
24	Mon: 03/30/2020				
25	Wed: 04/01/2020				
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		

This is the altered schedule. Note that there is one homework problem which hopefully you will be able to complete before the next lecture.

Review of the harmonic oscillator --

Why?

1. **We like harmonic oscillators?**
2. **All of physics can be mapped into harmonic oscillators?**
3. **Physicists only know how to solve harmonic oscillator problems?**
4. **Harmonic oscillators inspire a new way of thinking about quantum mechanics?**

Do you like harmonic oscillators?

One-dimensional harmonic oscillator

$$H\psi(x) = \left(\frac{P^2}{2m} + \frac{m\omega^2}{2}X^2\right)\psi(x) = E\psi(x)$$

Define:

$$a = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X + i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P$$

$$a^\dagger = \left(\frac{m\omega}{2\hbar}\right)^{1/2} X - i\left(\frac{1}{2m\omega\hbar}\right)^{1/2} P$$

Note that:

$$[a, a^\dagger] = 1$$

It follows that:

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) \qquad \psi \Rightarrow |n\rangle \qquad E \Rightarrow E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

This material is covered in Chapter V of your textbook. Presumably you have previously derived these equations. Are they still true? At this point the operators a and a† seem to be "cute" curiosities?

Representation of the position and momentum operators in terms of the energy eigenstates of the harmonic oscillator:

n= 0 1 2 3 .....

$$X \leftrightarrow \left(\frac{\hbar}{2m\omega}\right)^{1/2} \begin{bmatrix} 0 & 1^{1/2} & 0 & 0 & \cdots \\ 1^{1/2} & 0 & 2^{1/2} & 0 & \\ 0 & 2^{1/2} & 0 & 3^{1/2} & \\ 0 & 0 & 3^{1/2} & 0 & \\ \vdots & & & & \end{bmatrix}$$

$$P \leftrightarrow i\left(\frac{m\omega\hbar}{2}\right)^{1/2} \begin{bmatrix} 0 & -1^{1/2} & 0 & 0 & \cdots \\ 1^{1/2} & 0 & -2^{1/2} & 0 & \\ 0 & 2^{1/2} & 0 & -3^{1/2} & \\ 0 & 0 & 3^{1/2} & 0 & \\ \vdots & & & & \end{bmatrix}$$

It is convenient to evaluate the position and momentum operators in the basis of energy eigenstates of the harmonic oscillator denoted by the integer *n*.

Representation of the raising and lowering operators in terms of the energy eigenstates of the harmonic oscillator:

$$a^\dagger \leftrightarrow \begin{array}{c} \\ n=0 \\ n=1 \\ n=2 \\ \cdot \\ \cdot \end{array} \begin{array}{c} \begin{array}{cccc} n=0 & n=1 & n=2 & \dots \end{array} \\ \begin{bmatrix} 0 & 0 & 0 & \dots \\ 1^{1/2} & 0 & 0 & \\ 0 & 2^{1/2} & 0 & \\ 0 & 0 & 3^{1/2} & \\ \vdots & & & \end{bmatrix} \end{array}$$

$$a \leftrightarrow \begin{bmatrix} 0 & 1^{1/2} & 0 & 0 & \cdots \\ 0 & 0 & 2^{1/2} & 0 & \\ 0 & 0 & 0 & 3^{1/2} & \\ \vdots & & & & \end{bmatrix}$$

The a and a† operators can also be evaluated in this basis.

Summary of results

$$H|n\rangle = \hbar\omega\left(\frac{1}{2} + a^\dagger a\right)|n\rangle = \hbar\omega\left(\frac{1}{2} + n\right)|n\rangle$$

$$a|n\rangle = \sqrt{n}\,|n-1\rangle$$

$$a^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

These results are derived in detail in Chapter V. Make sure that they make sense to you.

How does this beautiful formalism lead to the notion of creation and annihilation operators?

The phonon number eigenvalues take the values $n = 0, 1, 2, ...$

$a|0\rangle = 0 \quad a|1\rangle = |0\rangle \quad a|2\rangle = \sqrt{2}|1\rangle$ ... interpretation of a as annihilation operator

$a^\dagger|0\rangle = |1\rangle \quad a^\dagger|1\rangle = \sqrt{2}|2\rangle \quad a^\dagger|2\rangle = \sqrt{3}|3\rangle$ ... interpretation of $a^\dagger$ as creation operator

It follows that $|n\rangle = \frac{1}{\sqrt{(n!)}}\left(a^\dagger\right)^n|0\rangle$

➔**We can "create" any phonon state from the ground state with this operator.**

The relations on this slide have no new information, but lead to a different way of thinking of the eigenstates of our system. In particular, the last equation shows that you build up an state with *n* phonons from state with 0 phonons. Ultimately, this leads to mapping the |0> phonon state with "vacuum" and implies that you can create an *n* phonon state out of vacuum.

Extension of these ideas to multiple independent harmonic oscillator modes

$\omega \Rightarrow \{\omega_1, \omega_2, \omega_3 ....\}$

Here *1,2,..i,j…* denotes an arbitrary index referencing distinct modes.

$a \Rightarrow \{a_1, a_2, a_3 ....\}$

Commutation relations: $\left[a_i, a_j \right] = 0$

$a^\dagger \Rightarrow \{a_1^\dagger, a_2^\dagger, a_3^\dagger ....\}$

Commutation relations: $\left[a_i^\dagger, a_j^\dagger \right] = 0$

Commutation relations: $\left[a_i, a_j^\dagger \right] = \delta_{ij}$

This result means that for a multiphonon state $\left| n_1, n_2 .... n_i ... n_j ... n_N \right\rangle$, the action of the creation operator works as follows:

$$a_i^\dagger a_j^\dagger \left| n_1, n_2 .... n_i ... n_j ... n_N \right\rangle = \sqrt{n_i + 1}\sqrt{n_j + 1} \left| n_1, n_2 .... (n_i + 1) ... (n_j + 1) ... n_N \right\rangle$$

Later, we will see how this formalism has the capability of keeping track of symmetry/antisymmetry properties of multi particle systems.

Up to now we have considered an isolated harmonic oscillator. The ideas can be extended to consideration of multiple independent and non-interacting modes at once. The formalism has some very interesting properties that we will use in this chapter and in several other chapters as well.

Maxwell's equations

Microscopic or vacuum form $(\mathbf{P}=0;\ \mathbf{M}=0)$:

Coulomb's law: $\nabla \cdot \mathbf{E} = \rho / \varepsilon_0$

Ampere-Maxwell's law: $\nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = \mu_0 \mathbf{J}$

Faraday's law: $\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$

No magnetic monopoles: $\nabla \cdot \mathbf{B} = 0$

$$\Rightarrow c^2 = \frac{1}{\varepsilon_0 \mu_0}$$

Now – to the matter at hand – we need to consider electromagnetic waves and therefore need to review classical electromagnetic theory.

Recall the electromagnetic field energy --

$$E_{\text{field}} = \frac{\epsilon_0}{2}\int d^3r \left(\left|\mathbf{E}(\mathbf{r},t)\right|^2 + c^2 \left|\mathbf{B}(\mathbf{r},t)\right|^2 \right)$$

It will be convenient to express Maxwell's equations and the electromagnetic field energy in terms of scalar and vector potentials:

$$\nabla \cdot \mathbf{B} = 0 \qquad \Rightarrow \quad \mathbf{B} = \nabla \times \mathbf{A}$$

$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \quad \Rightarrow \nabla \times \left(\mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} \right) = 0 \quad \Rightarrow \mathbf{E} + \frac{\partial \mathbf{A}}{\partial t} = -\nabla\Phi \quad \Rightarrow \mathbf{E} = -\nabla\Phi - \frac{\partial \mathbf{A}}{\partial t}$$

Far from sources, the remaining equations become:

$$\nabla \cdot \mathbf{E} = 0 \qquad \Rightarrow \nabla^2\Phi + \frac{\partial \nabla \cdot \mathbf{A}}{\partial t} = 0$$

$$\nabla \times \mathbf{B} - \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} = 0 \quad \Rightarrow \nabla \times \left(\nabla \times \mathbf{A} \right) + \frac{1}{c^2}\left(\frac{\partial \nabla\Phi}{\partial t} + \frac{\partial^2 \mathbf{A}}{\partial t^2} \right) = 0$$

Ultimately, we will need the Hamiltonian for electromagnetic phenomena, and this will come for the electromagnetic field energy. It is convenient to express this in terms of the vector potential.

Further manipulations of Maxwell's equations in terms of scalar and vector potentials --

$$\nabla\cdot\mathbf{E}=0 \qquad \Rightarrow\ \nabla^2\Phi+\frac{\partial\nabla\cdot\mathbf{A}}{\partial t}=0$$

$$\nabla\times\mathbf{B}-\frac{1}{c^2}\frac{\partial\mathbf{E}}{\partial t}=0 \quad \Rightarrow\nabla\times\left(\nabla\times\mathbf{A}\right)+\frac{1}{c^2}\left(\frac{\partial\nabla\Phi}{\partial t}+\frac{\partial^2\mathbf{A}}{\partial t^2}\right)=0$$

$$\Rightarrow\nabla\left(\nabla\cdot\mathbf{A}\right)-\nabla^2\mathbf{A}+\frac{1}{c^2}\left(\frac{\partial\nabla\Phi}{\partial t}+\frac{\partial^2\mathbf{A}}{\partial t^2}\right)=0$$

$$\Rightarrow\left(\nabla^2\mathbf{A}-\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2}\right)-\nabla\underbrace{\left(\nabla\cdot\mathbf{A}+\frac{1}{c^2}\frac{\partial\Phi}{\partial t}\right)}_{\text{zero in Lorenz gauge}}=0$$

zero in Lorenz gauge

$$\nabla^2\Phi-\frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2}=0 \qquad \nabla^2\mathbf{A}-\frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2}=0$$

Here we are interested in the electromagnetic waves far from their sources.

Equations within the Lorenz gauge --

$$\nabla^2\Phi - \frac{1}{c^2}\frac{\partial^2\Phi}{\partial t^2} = 0 \qquad \nabla^2\mathbf{A} - \frac{1}{c^2}\frac{\partial^2\mathbf{A}}{\partial t^2} = 0$$

It is further convenient to seek solutions with $\Phi \equiv 0 \quad \Rightarrow \nabla\cdot\mathbf{A} = 0$

$$\mathbf{E} = -\frac{\partial\mathbf{A}}{\partial t} \qquad \mathbf{B}=\nabla\times\mathbf{A}$$

Electromagnetic field energy --

$$E_{\text{field}} = \frac{\epsilon_0}{2}\int d^3r\left(\left|\mathbf{E}(\mathbf{r},t)\right|^2 + c^2\left|\mathbf{B}(\mathbf{r},t)\right|^2\right)$$

$$= \frac{\epsilon_0}{2}\int d^3r\left(\left|\frac{\partial\mathbf{A}(\mathbf{r},t)}{\partial t}\right|^2 + c^2\left|\nabla\times\mathbf{A}(\mathbf{r},t)\right|^2\right)$$

The final equation here is expressed purely in terms of the vector potential.

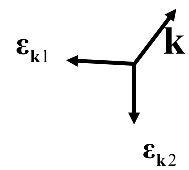
Plane wave solutions to electromagnetic waves in terms of vector potentials

$$\nabla^2 \mathbf{A} - \frac{1}{c^2}\frac{\partial^2 \mathbf{A}}{\partial t^2} = 0 \qquad \nabla \cdot \mathbf{A} = 0$$

A pure plane wave takes the form

$$\mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r},t) = A_{\mathbf{k}\sigma}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t} \qquad \omega_{\mathbf{k}} = |\mathbf{k}|c$$

$$\mathbf{k}\cdot\boldsymbol{\varepsilon}_{\mathbf{k}\sigma} = 0 \qquad \boldsymbol{\varepsilon}_{\mathbf{k}\sigma}\cdot\boldsymbol{\varepsilon}_{\mathbf{k}\sigma'} = \delta_{\sigma\sigma'}$$



3 mutually perpendicular vectors

For the pure plane wave, the following relations hold:

$$\frac{\partial \mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r},t)}{\partial t} = -i\omega_{\mathbf{k}} A_{\mathbf{k}\sigma}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}$$

$$\nabla \times \mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r},t) = i\mathbf{k}\times A_{\mathbf{k}\sigma}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}$$

From the equations for the vector potential, we find that there are two plane wave solutions with two different polarizations as indicated by the index σιγμα.

General form of vector potential as a superposition of plane waves:

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{V}\sum_{\mathbf{k}\sigma} \mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r},t) = \frac{1}{V}\sum_{\mathbf{k}\sigma} A_{\mathbf{k}\sigma}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}$$

Here V denotes the volume of the analysis system; different treatments put this factor in different ways.

Now we must evaluate the electromagnetic field energy --

$$E_{\text{field}} = \frac{\epsilon_0}{2}\int d^3r \left(\left| \frac{\partial \mathbf{A}(\mathbf{r},t)}{\partial t} \right|^2 + c^2 \left| \nabla \times \mathbf{A}(\mathbf{r},t) \right|^2 \right)$$

Because of the orthogonality of the plane waves, the result can be expressed as a sum over distinct plane wave modes:

$$E_{\text{field}} = \frac{\epsilon_0}{2V}\sum_{\mathbf{k}\sigma} \left| A_{\mathbf{k}\sigma} \right|^2 \left(\omega_{\mathbf{k}}^2 + c^2 \left|\mathbf{k}\right|^2 \right)$$

Note that we can use the identity

$$(\mathbf{a}\times\mathbf{b})\cdot(\mathbf{c}\times\mathbf{d}) = (\mathbf{a}\cdot\mathbf{c})(\mathbf{b}\cdot\mathbf{d}) - (\mathbf{a}\cdot\mathbf{d})(\mathbf{b}\cdot\mathbf{c})$$

You should make sure that you are in agreement with the derivation of these equations.

Up to now, we have treated classical electromagnetic waves.
Next time, we will consider the quantum treatment of the electromagnetic field energy ⇔ electromagnetic Hamiltonian

Next time we will consider the experimental evidence that motivated consider of a quantized field and use the analogy with the Harmonic oscillator formalism to deduce the form of the quantization.