

PHY 742 Quantum Mechanics II

1-1:50 AM MWF via video link:

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

Extra notes for Lecture 22

Quantization of the Electromagnetic fields

Read XVII. Quantizing Electromagnetic Fields.

1. Classical Hamiltonian for the electromagnetic fields
2. Quantum Hamiltonian for the electromagnetic fields

Historically, the notion of quantized radiation in the form of photons came very early in the development of quantum theory. Our task is to see how this quantization can be derived from the classical equations of Electrodynamics.

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

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

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				
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	<i>Good Friday</i>		
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.

Your questions –

From Surya:

2. In what situation we can use/apply/define coherent states?
3. Do zero-point energy shift and uncontrolled energy shift same?

From Trevor:

1. On slide 9, when you say that we "strategically remove" the uncontrolled energy shift, does that mean that there is some trick we use to get rid of it, or that we're allowed to literally just ignore it for the moment?

From Laxman:

1. What kind of vector potentials do $A(r,t)$ and $A^*(r,t)$ represent?

Question: What kind of vector potentials do $\mathbf{A}(\mathbf{r},t)$ and $\mathbf{A}^*(\mathbf{r},t)$ represent?

Comment: The expression we used was as follows

$$\mathbf{A}(\mathbf{r},t) = \frac{1}{2V} \sum_{\mathbf{k}\sigma} \left(\mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r},t) + \mathbf{A}_{\mathbf{k}\sigma}^*(\mathbf{r},t) \right) = \frac{1}{2V} \sum_{\mathbf{k}\sigma} \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \left(A_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} + A_{\mathbf{k}\sigma}^* e^{-i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} \right)$$

Here we have been a bit less careful in clearly distinguishing Fourier components/transforms in our notation. The right most expression is a superposition of plane wave components with $A_{\mathbf{k}\sigma}$ representing a complex amplitude.

Question: Do zero-point energy shift and uncontrolled energy shift same?

On slide 9, when you say that we "strategically remove" the uncontrolled energy shift, does that mean that there is some trick we use to get rid of it, or that we're allowed to literally just ignore it for the moment?

Comment: This is a tricky point and it does cause problems for some evaluations. For the phonon case which served as our model, the notion of zero point motion makes physical sense. For the electromagnetic Hamiltonian the role of the equivalent concept is not quite clear (at least to me). We need to be careful when we see divergent energies to distinguish physical processes from mathematical issues.

EM Field Hamiltonian acting on eigenstate $|n_{\mathbf{k}\sigma}\rangle$:

$$H_{\text{field}} |n_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}'\sigma'} \hbar\omega_{\mathbf{k}'} \left(a_{\mathbf{k}'\sigma'}^\dagger a_{\mathbf{k}'\sigma'} + \frac{1}{2} \right) |n_{\mathbf{k}\sigma}\rangle = \left(\hbar\omega_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}'\sigma'} \frac{\hbar\omega_{\mathbf{k}'}}{2} \right) |n_{\mathbf{k}\sigma}\rangle$$

$$H_{\text{field}}^{\text{fixed}} |n_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}'\sigma'} (\hbar\omega_{\mathbf{k}'} a_{\mathbf{k}'\sigma'}^\dagger a_{\mathbf{k}'\sigma'}) |n_{\mathbf{k}\sigma}\rangle = \hbar\omega_{\mathbf{k}} n_{\mathbf{k}\sigma} |n_{\mathbf{k}\sigma}\rangle$$

Question: In what situation we can use/apply/define coherent states?

Comments -- Gauber's coherent state: $|c_\alpha\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}} |n\rangle$

Here α represents a complex amplitude

It is possible to prove the following identities for the coherent states:

1. $\langle c_\alpha | c_\alpha \rangle = 1$
2. $\langle c_\alpha | a | c_\alpha \rangle = \alpha$
3. $\langle c_\alpha | a^\dagger | c_\alpha \rangle = \alpha^*$
4. $|\langle c_\alpha | c_\beta \rangle|^2 = e^{-|\alpha - \beta|^2}$

We will investigate these coherent states more next time. What we will generally find is that these states model what happens in an ideal laser.

Related to that question is how to understand/interpret the quantum fields.

What is the expectation value of the E field for a pure eigenstate $|n\rangle$ of the electromagnetic Hamiltonian?

- 1. A complex (non zero) number**
- 2. Zero**
- 3. Infinity**

What is the expectation value of the B field for a pure eigenstate $|n\rangle$ of the electromagnetic Hamiltonian?

- 1. A complex (non zero) number**
- 2. Zero**
- 3. Infinity**

Is your answer consistent with what is observed?

Slides from original lecture --

Electromagnetic field energy --

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

In terms of the vector potential, using the Lorenz gauge with $\Phi = 0$:

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

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

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

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

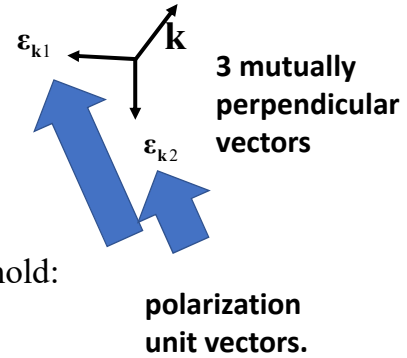
Plane wave solutions to electromagnetic waves in terms of vector potentials

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

A pure plane wave takes the form

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

$$\mathbf{k} \cdot \boldsymbol{\epsilon}_{\mathbf{k}\sigma} = 0 \quad \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \cdot \boldsymbol{\epsilon}_{\mathbf{k}\sigma'} = \delta_{\sigma\sigma'}$$



For the pure plane wave, the following relations hold:

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

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

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 σ .

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

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

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 --

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

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

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

Note that we can use the identity

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

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From the plane wave terms, we can simplify the form of the energy of the electromagnetic field.

Some details, with more care to use real functions --

$$\mathbf{A}(\mathbf{r}, t) = \frac{1}{2V} \sum_{\mathbf{k}\sigma} (\mathbf{A}_{\mathbf{k}\sigma}(\mathbf{r}, t) + \mathbf{A}_{\mathbf{k}\sigma}^*(\mathbf{r}, t)) = \frac{1}{2V} \sum_{\mathbf{k}\sigma} \boldsymbol{\epsilon}_{\mathbf{k}\sigma} (A_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} + A_{\mathbf{k}\sigma}^* e^{-i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t})$$

Electromagnetic field energy --

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

Note that the plane waves are distributed throughout the analysis volume

such that the following orthogonality holds. $\frac{1}{V} \int d^3r e^{i\mathbf{k}\cdot\mathbf{r} - i\mathbf{k}'\cdot\mathbf{r}} = \delta_{\mathbf{k}\mathbf{k}'}$

Also recall that $\omega_{\mathbf{k}} = |\mathbf{k}|c$ and average out all high frequency contributions

to the field energy -- $E_{\text{field}} = \frac{\epsilon_0}{4V} \sum_{\mathbf{k}\sigma} (A_{\mathbf{k}\sigma} A_{\mathbf{k}\sigma}^* + A_{\mathbf{k}\sigma}^* A_{\mathbf{k}\sigma}) (\omega_{\mathbf{k}}^2 + c^2 |\mathbf{k}|^2)$

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

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Here are some details of the derivation.

Electromagnetic field energy expression:

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

Here $A_{\mathbf{k}\sigma}$ represents the amplitude of the vector potential.

Big leap -- Suppose that $A_{\mathbf{k}\sigma} \rightarrow N_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$ $A_{\mathbf{k}\sigma}^* \rightarrow N_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger$

$$E_{\text{field}} = \frac{\epsilon_0}{2V} \sum_{\mathbf{k}\sigma} \omega_{\mathbf{k}}^2 N_{\mathbf{k}\sigma}^2 (a_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger + a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma})$$

More leaping -- $N_{\mathbf{k}\sigma} = \sqrt{\frac{V\hbar}{\epsilon_0 \omega_{\mathbf{k}}}}$

$$E_{\text{field}} = \frac{1}{2} \sum_{\mathbf{k}\sigma} \hbar \omega_{\mathbf{k}} (a_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger + a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}) = \sum_{\mathbf{k}\sigma} \hbar \omega_{\mathbf{k}} \left(a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2} \right)$$

Now consider how the EM field energy can be quantized, thinking in terms of the analogy of these equations to those of the Harmonic oscillator. We introduce a normalization factor and the creation and annihilation operators.

Here $a_{\mathbf{k}\sigma}$ and $a_{\mathbf{k}\sigma}^\dagger$ are "borrowed" from the Harmonic oscillator formalism.

Commutation relations: $[a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\sigma\sigma'}$, $[a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}] = 0$, $[a_{\mathbf{k}\sigma}^\dagger, a_{\mathbf{k}'\sigma'}^\dagger] = 0$

$$H_{\text{field}} = \frac{1}{2} \sum_{\mathbf{k}\sigma} \hbar\omega_{\mathbf{k}} (a_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}^\dagger + a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma}) = \sum_{\mathbf{k}\sigma} \hbar\omega_{\mathbf{k}} \left(a_{\mathbf{k}\sigma}^\dagger a_{\mathbf{k}\sigma} + \frac{1}{2} \right)$$

From the analogy of the Harmonic oscillator, the eigenstates of the EM Field Hamiltonian are integers $n_{\mathbf{k}\sigma}$:

$$H_{\text{field}} |n_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}'\sigma'} \hbar\omega_{\mathbf{k}'} \left(a_{\mathbf{k}'\sigma'}^\dagger a_{\mathbf{k}'\sigma'} + \frac{1}{2} \right) |n_{\mathbf{k}\sigma}\rangle = \left(\hbar\omega_{\mathbf{k}} n_{\mathbf{k}\sigma} + \sum_{\mathbf{k}'\sigma'} \frac{\hbar\omega_{\mathbf{k}'}}{2} \right) |n_{\mathbf{k}\sigma}\rangle$$

$$H_{\text{field}}^{\text{fixed}} |n_{\mathbf{k}\sigma}\rangle = \sum_{\mathbf{k}'\sigma'} (\hbar\omega_{\mathbf{k}'} a_{\mathbf{k}'\sigma'}^\dagger a_{\mathbf{k}'\sigma'}) |n_{\mathbf{k}\sigma}\rangle = \hbar\omega_{\mathbf{k}} n_{\mathbf{k}\sigma} |n_{\mathbf{k}\sigma}\rangle$$

**Uncontrolled
energy shift**

Reviewing the commutation relations for the creation and annihilation operators. At the end, we do arrive at an expression that is very much like that of the Harmonic oscillator. However, in this case, the constant term causes trouble because it represents an uncontrolled energy. No problem. If it is unphysical it is strategically removed. Unfortunately, it will come back to bother us on occasion...

Creation and annihilation operators:

$$a_{\mathbf{k}\sigma} |n_{\mathbf{k}\sigma}\rangle = \sqrt{n_{\mathbf{k}\sigma}} |n_{\mathbf{k}\sigma} - 1\rangle$$

$$a_{\mathbf{k}\sigma}^\dagger |n_{\mathbf{k}\sigma}\rangle = \sqrt{n_{\mathbf{k}\sigma} + 1} |n_{\mathbf{k}\sigma} + 1\rangle$$

Quantum mechanical form of vector potential --

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}} \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \left(a_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} + a_{\mathbf{k}\sigma}^\dagger e^{-i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} \right)$$

Note: We are assuming that the polarization vector is real.

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With these definitions of the vector potential amplitudes, we can now write an expression for the quantum mechanical form of the vector potential.

Quantum mechanical form of vector potential --

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}} \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \left(a_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t} + a_{\mathbf{k}\sigma}^\dagger e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)} \right)$$

Electric field:

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} \Rightarrow \mathbf{E}(\mathbf{r}, t) = i \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}} \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \left(a_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t} - a_{\mathbf{k}\sigma}^\dagger e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)} \right)$$

Magnetic field:

$$\mathbf{B} = \nabla \times \mathbf{A} \Rightarrow \mathbf{B}(\mathbf{r}, t) = i \sum_{\mathbf{k}\sigma} \sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}} \mathbf{k} \times \boldsymbol{\epsilon}_{\mathbf{k}\sigma} \left(a_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t} - a_{\mathbf{k}\sigma}^\dagger e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)} \right)$$

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From the vector potential, we can also write expressions for the electric and magnetic fields.

What is the expectation value of the E field for a pure eigenstate $|n\rangle$ of the electromagnetic Hamiltonian?

- 1. A complex (non zero) number**
- 2. Zero**
- 3. Infinity**

What is the expectation value of the B field for a pure eigenstate $|n\rangle$ of the electromagnetic Hamiltonian?

- 1. A complex (non zero) number**
- 2. Zero**
- 3. Infinity**

What do you think is going to happen?

How does a quantum mechanical E or B field exist? Consider a linear combination of pure photon states --

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PHYSICAL REVIEW LETTERS

1 FEBRUARY 1963

PHOTON CORRELATIONS*

Roy J. Glauber

Lyman Laboratory, Harvard University, Cambridge, Massachusetts

(Received 27 December 1962)

In 1956 Hanbury Brown and Twiss¹ reported that the photons of a light beam of narrow spectral width have a tendency to arrive in correlated pairs. We have developed general quantum mechanical methods for the investigation of such correlation effects and shall present here results for the distribution of the number of photons counted in an incoherent beam. The fact that photon correlations are enhanced by narrowing the spectral bandwidth has led to a prediction² of large-scale correlations to be observed in the beam of an optical maser. We shall indicate that this prediction is misleading and follows from an inappropriate model of the maser beam. In considering these problems we shall outline

a method of describing the photon field which appears particularly well suited to the discussion of experiments performed with light beams, whether coherent or incoherent.

The correlations observed in the photoionization processes induced by a light beam were given a simple semiclassical explanation by Purcell,³ who made use of the methods of microwave noise theory. More recently, a number of papers have been written examining the correlations in considerably greater detail. These papers^{2,4-6} retain the assumption that the electric field in a light beam can be described as a classical Gaussian stochastic process. In actuality, the behavior of the photon field is considerably more

In this paper, the notion of a "coherent" state was introduced. As we will see, the expectation values of the electric and magnetic fields are non-zero for a system in a coherent state.

Gauber's coherent state: $|c_\alpha\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}} |n\rangle$

Here α represents a complex amplitude

It is possible to prove the following identities for the coherent states:

1. $\langle c_\alpha | c_\alpha \rangle = 1$
2. $\langle c_\alpha | a | c_\alpha \rangle = \alpha$
3. $\langle c_\alpha | a^\dagger | c_\alpha \rangle = \alpha^*$
4. $|\langle c_\alpha | c_\beta \rangle|^2 = e^{-|\alpha-\beta|^2}$

It is possible to prove these identities (for HW #18).