PHY 712 Electrodynamics
10-10:50 AM MWF Olin 103

Notes for Lecture 37:

Some quantum effects in electrodynamics

-- General quantum states of EM fields and related correlations functions

a. Review of eigenstates of EM Hamiltonian and of Glauber's coherent states

b. Squeezed states

c. Correlation measurements on EM signals

24	Mon: 03/13/2023	Chap. 9	Radiation from localized oscillating sources	#17	03/17/2023
25	Wed: 03/15/2023	Chap. 9	Radiation from oscillating sources		
26	Fri: 03/17/2023	Chap. 9 & 10	Radiation and scattering	#18	03/20/2023
27	Mon: 03/20/2023	Chap. 11	Special Theory of Relativity	#19	03/24/2023
28	Wed: 03/22/2023	Chap. 11	Special Theory of Relativity		
29	Fri: 03/24/2023	Chap. 11	Special Theory of Relativity	#20	03/27/2023
30	Mon: 03/27/2023	Chap. 14	Radiation from moving charges	#21	03/29/2023
31	Wed: 03/29/2023	Chap. 14	Radiation from accelerating charged particles	#22	03/31/2023
32	Fri: 03/31/2023	Chap. 14	Synchrotron radiation and Compton scattering	#23	04/3/2023
33	Mon: 04/03/2023	Chap. 15	Radiation from collisions of charged particles		
34	Wed: 04/05/2023	Chap. 13	Cherenkov radiation		
35	Fri: 04/07/2023		Special topic: E & M aspects of superconductivity		
36	Mon: 04/10/2023		Special topic: Quantum Effects in E & M		
37	Wed: 04/12/2023		Special topic: Quantum Effects in E & M		
38	Fri: 04/14/2023		Special topic: Quantum Effects in E & M		
	Mon: 04/17/2023		Presentations I		
	Wed: 04/19/2023		Presentations II		
	Fri: 04/21/2023		Presentations III		
39	Mon: 04/24/2023		Review		
40	Wed: 04/26/2023		Review		

PH.D. DEFENSE

THURSDAY

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APRIL 13, 2023

Modeling Properties of Metal-Organic Frameworks with Density Functional Theory

Metal-organic frameworks (MOFs) have emerged as a new class of highly porous crystalline material and are being used for solving various problems in the field of physics, chemistry, and materials science. Research in the field of MOFs has grown substantially over the last decade, which has enabled them to become viable alternatives for many important industrial and environmental applications. Even though significant developments have been made in order to improve the feasibility of these materials, a more in-depth knowledge about their structure and mechanisms governing the properties of MOFs is necessary. The research presented in this thesis focuses primarily on the modeling and study of functional 3D materials like MOFs and covalent organic frameworks using density functional theory. By combining *ab initio* calculations with experimental results, we have been able to perform extensive studies of the chemical and physical properties of MOFs and answer important fundamental questions. My projects focus both on the

Haardik Pandey
Ph.D. Candidate
WFU Physics

9:00 am - ZSR 404*
Reception to follow - Olin Lobby

Review of what we learned from Lecture 36

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

where $\mathbf{k}$ denotes wavevector and σ denotes polarization direction --

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

Here $n_{\mathbf{k}\sigma} = 0,1,2,3,4.......$

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

$$a^{\dagger}_{\mathbf{k}\sigma}\left|n_{\mathbf{k}\sigma}\right\rangle = \sqrt{n_{\mathbf{k}\sigma}+1}\left|n_{\mathbf{k}\sigma}+1\right\rangle$$

Commutation relations:

$$\left[a_{\mathbf{k}\sigma}, a^{\dagger}_{\mathbf{k}'\sigma'}\right]=\delta_{\mathbf{k}\mathbf{k}'}\delta_{\sigma\sigma'} \quad \left[a_{\mathbf{k}\sigma}, a_{\mathbf{k}'\sigma'}\right]=0 \quad \left[a^{\dagger}_{\mathbf{k}\sigma}, a^{\dagger}_{\mathbf{k}'\sigma'}\right]=0$$

In terms of the same operators and with polarization unit vectors $\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}$ --

Vector potential:

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

Electric field:

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

Magnetic field:

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

While the photon eigenstates $\left|n_{\mathbf{k}'\sigma'}\right\rangle$ form a complete basis for describing quantum electromagnetic fields, they have some troublesome properties such as found in evaluating the field expectation values --

Vector potential:

$$\left\langle n_{\mathbf{k}'\sigma'}\right|\mathbf{A}(\mathbf{r},t)\left|n_{\mathbf{k}'\sigma'}\right\rangle = \sum_{\mathbf{k}\sigma}\sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}\left\langle n_{\mathbf{k}'\sigma'}\right|\left(a_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}+a^{\dagger}_{\mathbf{k}\sigma}e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)}\right)\left|n_{\mathbf{k}'\sigma'}\right\rangle = 0$$

Electric field:

$$\left\langle n_{\mathbf{k}'\sigma'}\right|\mathbf{E}(\mathbf{r},t)\left|n_{\mathbf{k}'\sigma'}\right\rangle = i\sum_{\mathbf{k}\sigma}\sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}}\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}\left\langle n_{\mathbf{k}'\sigma'}\right|\left(a_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}-a^{\dagger}_{\mathbf{k}\sigma}e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)}\right)\left|n_{\mathbf{k}'\sigma'}\right\rangle = 0$$

Magnetic field:

$$\left\langle n_{\mathbf{k}'\sigma'}\right|\mathbf{B}(\mathbf{r},t)\left|n_{\mathbf{k}'\sigma'}\right\rangle = i\sum_{\mathbf{k}\sigma}\sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}}\mathbf{k}\times\boldsymbol{\varepsilon}_{\mathbf{k}\sigma}\left\langle n_{\mathbf{k}'\sigma'}\right|\left(a_{\mathbf{k}\sigma}e^{i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t}-a^{\dagger}_{\mathbf{k}\sigma}e^{-(i\mathbf{k}\cdot\mathbf{r}-i\omega_{\mathbf{k}}t)}\right)\left|n_{\mathbf{k}'\sigma'}\right\rangle = 0$$

A convenient superposition thanks to R. Glauber, PR 131, 2766 (1963)

$$\left|c_\alpha\right\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}} \left|n\right\rangle \quad \text{based on a single mode } n \rightarrow n_{\mathbf{k}\sigma}$$

Electric field: $\left\langle c_\alpha \right| \mathbf{E}(\mathbf{r},t) \left| c_\alpha \right\rangle = i\sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}} \boldsymbol{\varepsilon}_{\mathbf{k}\sigma} \left(\alpha_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} - \alpha^*_{\mathbf{k}\sigma} e^{-(i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t)} \right)$

Magnetic field: $\left\langle c_\alpha \right| \mathbf{B}(\mathbf{r},t) \left| c_\alpha \right\rangle = i\sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}} \mathbf{k} \times \boldsymbol{\varepsilon}_{\mathbf{k}\sigma} \left(\alpha_{\mathbf{k}\sigma} e^{i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t} - \alpha^*_{\mathbf{k}\sigma} e^{-(i\mathbf{k}\cdot\mathbf{r} - i\omega_{\mathbf{k}}t)} \right)$

Let $\alpha = \Lambda e^{i\Psi}$ where both Λ and Ψ are unitless parameters.

$$\left\langle c_\alpha \right| \mathbf{E}(\mathbf{r},t) \left| c_\alpha \right\rangle = -2\sqrt{\frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}} \boldsymbol{\varepsilon}_{\mathbf{k}\sigma} \Lambda \sin\left(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t + \psi\right)$$

$$\left\langle c_\alpha \right| \mathbf{B}(\mathbf{r},t) \left| c_\alpha \right\rangle = -2\sqrt{\frac{\hbar}{2V\epsilon_0\omega_{\mathbf{k}}}} \mathbf{k} \times \boldsymbol{\varepsilon}_{\mathbf{k}\sigma} \Lambda \sin\left(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t + \psi\right)$$

Single mode coherent state continued

It can also be shown that

$$\left\langle c_\alpha \left| \left|\mathbf{E}(\mathbf{r},t)\right|^2 \right| c_\alpha \right\rangle = \frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}\left(4\Lambda^2 \sin^2\left(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}}t + \psi\right) + 1\right)$$

Therefore

$$\left\langle c_\alpha \left| \left|\mathbf{E}(\mathbf{r},t)\right|^2 \right| c_\alpha \right\rangle - \left|\left\langle c_\alpha \left| \mathbf{E}(\mathbf{r},t) \right| c_\alpha \right\rangle\right|^2 = \frac{\hbar\omega_{\mathbf{k}}}{2V\epsilon_0}$$

This means that variance of the E field for the coherent state is independent of the amplitude Λ. Therefore, for large Λ the variance is small in comparison.

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

Here α represents a complex amplitude

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

1. $\left\langle c_\alpha \middle| c_\alpha \right\rangle = 1$

2. $\left\langle c_\alpha \middle| a \middle| c_\alpha \right\rangle = \alpha$

3. $\left\langle c_\alpha \middle| a^\dagger \middle| c_\alpha \right\rangle = \alpha^*$

4. $\left|\left\langle c_\alpha \middle| c_\beta \right\rangle\right|^2 = e^{-|\alpha-\beta|^2}$

Visualization of coherent state electric fields for various amplitudes

Source:
R. Loudon, "The Quantum Theory of Light"

The quantized radiation field **151**

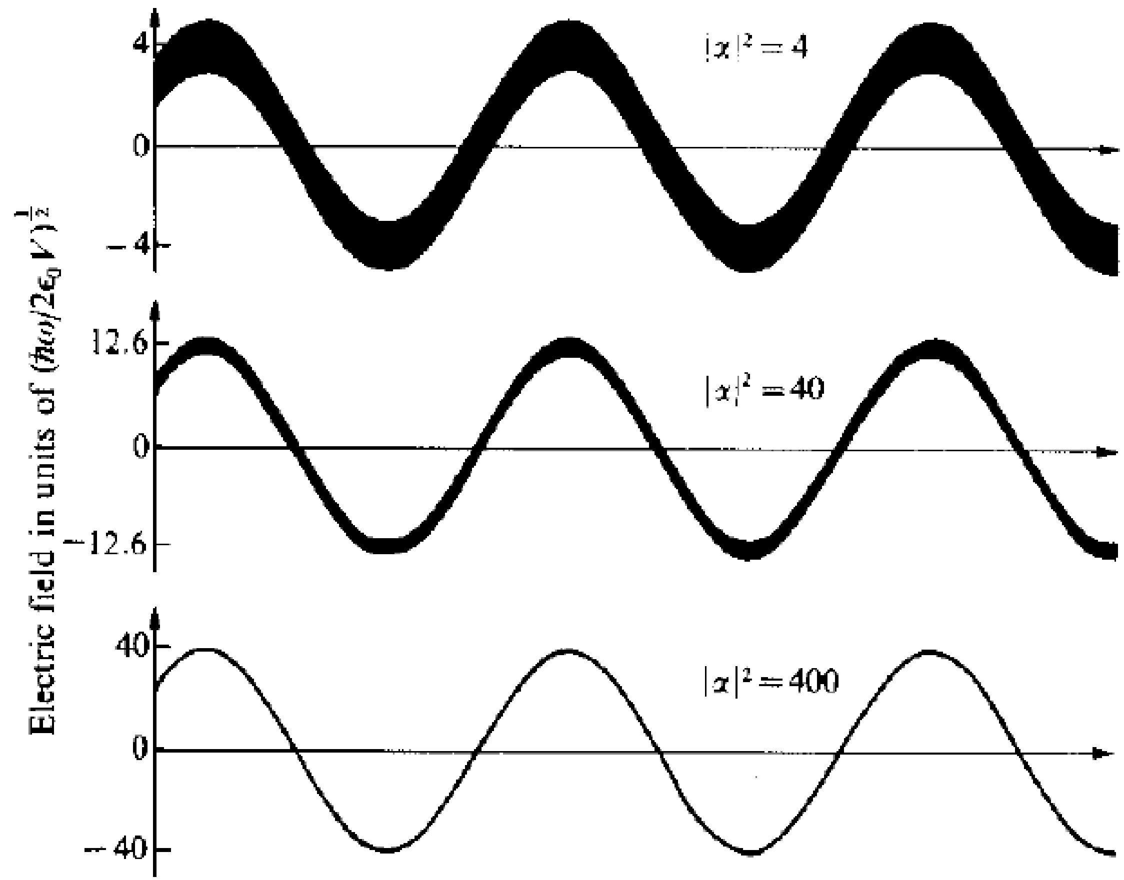


FIG. 4.3. Pictorial representation of the electric-field variation in a cavity mode excited to state $|\alpha\rangle$. Three different values of the mean photon number $|\alpha|^2$ are shown, the vertical scales being different for the three cases. The uncertainties in field values are indicated by the vertical widths $2\Delta E$ of the sine waves. These widths can also be regarded as combinations of the amplitude uncertainty associated with Δn and the phase uncertainty associated with $\Delta \cos\phi$.

Additional properties of single mode coherent state --

Consider the expectation values of the number operator and its square:

$$\mathbf{N}_{\mathbf{k}\sigma} \equiv a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma}$$

$$\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle = |\alpha|^2 \qquad \left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma}\mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle = |\alpha|^4 + |\alpha|^2$$

Square of the variance: $\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma}\mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle - \left|\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle\right|^2 = |\alpha|^2$

Fractional uncertainty in the number of photons for the coherent state:

$$\frac{\sqrt{\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma}\mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle - \left|\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle\right|^2}}{\left\langle c_\alpha \middle| \mathbf{N}_{\mathbf{k}\sigma} \middle| c_\alpha \right\rangle} = \frac{\sqrt{|\alpha|^4 + |\alpha|^2 - |\alpha|^4}}{|\alpha|^2} = \frac{1}{|\alpha|} = \frac{1}{\Lambda}$$

when $\alpha = \Lambda e^{i\Psi}$

Interpretation of a single mode coherent state

$$\left|c_\alpha\right\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}}\left|n\right\rangle \quad \text{based on a single mode } n \to n_{\mathbf{k}\sigma}$$

The probability of finding n photons in this state is given by:

$$\left|\left\langle n \middle| c_\alpha \right\rangle\right|^2 = \frac{|\alpha|^{2n} e^{-|\alpha|^2}}{n!}$$

This is the form of a Poisson distribution

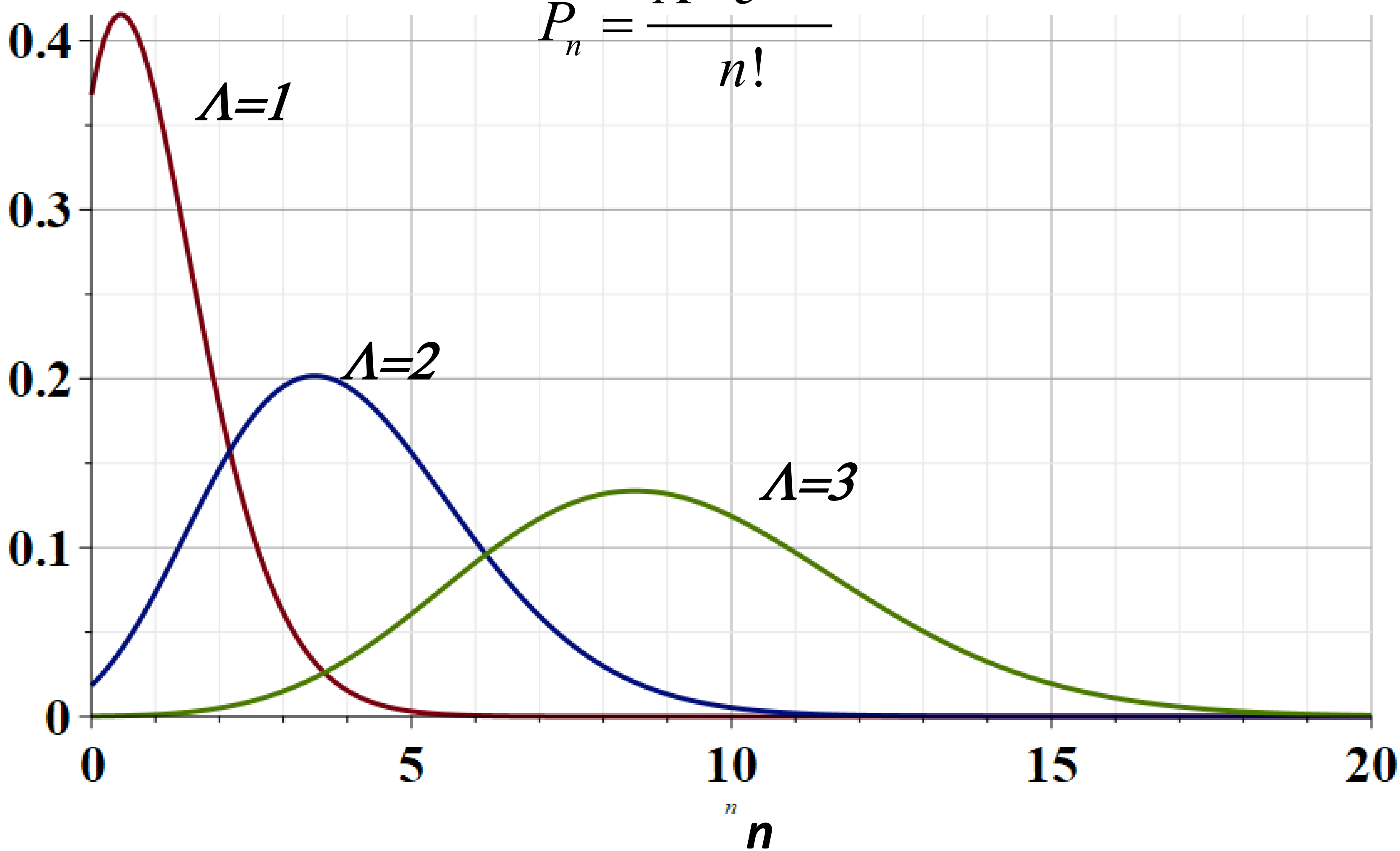
for a mean value of $|\alpha|^2$.

For $\alpha = \Lambda e^{i\Psi}$, the probability of finding the eigenstate with eigenstate $|n\rangle$ is given by

$$P_n = \frac{\Lambda^{2n} e^{-\Lambda^2}}{n!}$$

Poisson distributions

$$P_n = \frac{\Lambda^{2n} e^{-\Lambda^2}}{n!}$$



Further analysis and modifications of the "coherent state"

Recall that we can write the EM Hamiltonian for a single mode $\omega_{\mathbf{k}} \equiv \omega$ --

$$H = \frac{1}{2}\hbar\omega\left(a^\dagger a + a a^\dagger\right) \quad \text{where } \left[a, a^\dagger\right] = 1$$

Define convenient unitless operators

$$\hat{X} \equiv \frac{1}{2}\left(a^\dagger + a\right) \quad \text{and} \quad \hat{Y} \equiv \frac{i}{2}\left(a^\dagger - a\right) \quad \Rightarrow \left[\hat{X}, \hat{Y}\right] = \frac{i}{2}$$

$$H = \hbar\omega\left(\hat{X}^2 + \hat{Y}^2\right)$$

From the Heisenberg uncertainty ideas applied to the standard deviations:

$$\Delta\hat{X}\Delta\hat{Y} \geq \frac{1}{4}$$

In terms of the eigenstates of the EM Hamiltonian:

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

$$\Delta\hat{X} = \sqrt{\left\langle n\right|\hat{X}^2\left|n\right\rangle - \left|\left\langle n\right|\hat{X}\left|n\right\rangle\right|^2} = \sqrt{\frac{1}{2}\left(n+\frac{1}{2}\right)} = \Delta\hat{Y}$$

$$\Rightarrow \Delta\hat{X}\Delta\hat{Y} = \frac{1}{2}\left(n+\frac{1}{2}\right)$$

For the coherent state:

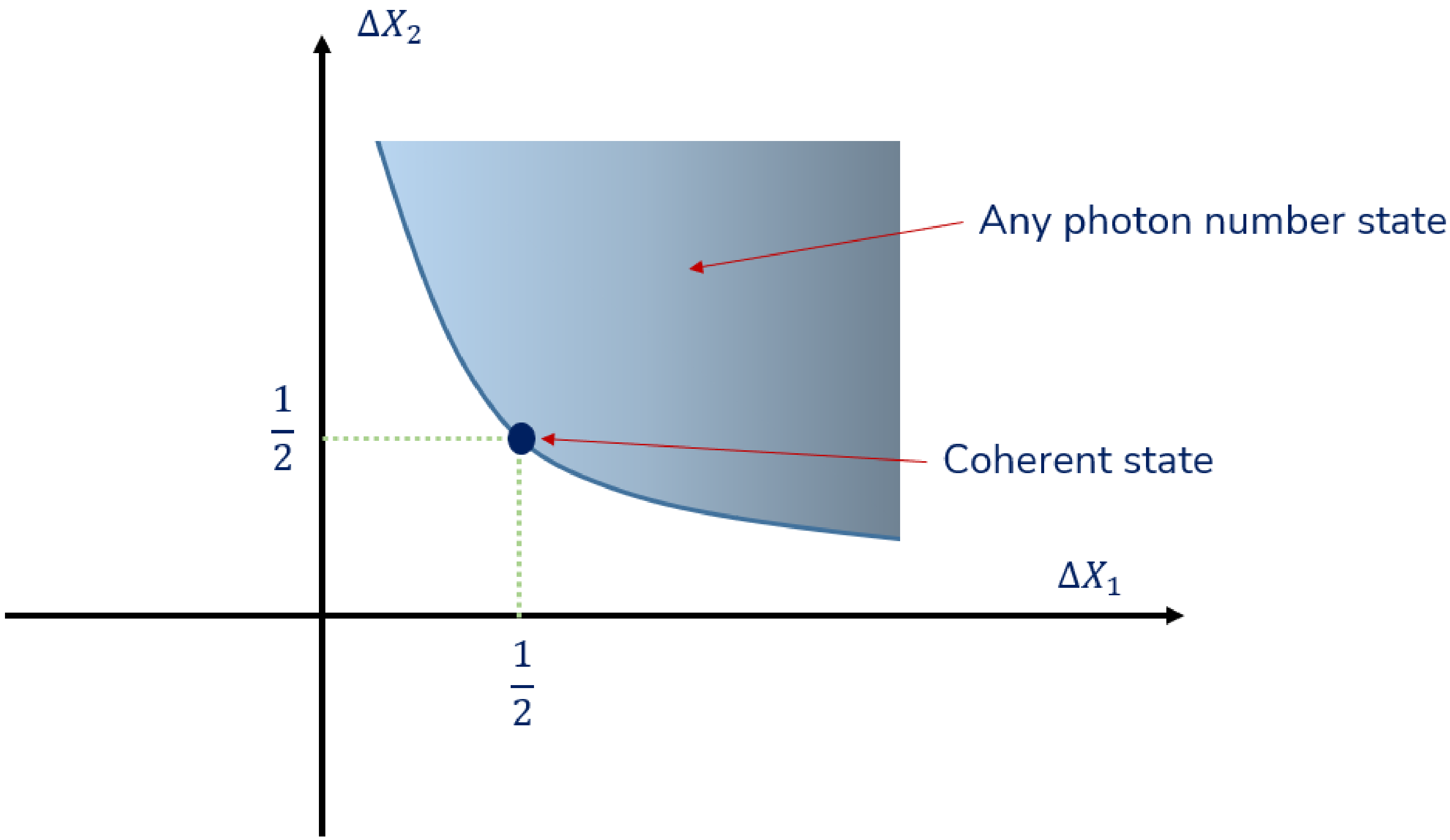
$$\left|c_\alpha\right\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}} \left|n\right\rangle$$

$$\Delta\hat{X} = \sqrt{\left\langle c_\alpha \left| \hat{X}^2 \right| c_\alpha \right\rangle - \left| \left\langle c_\alpha \left| \hat{X} \right| c_\alpha \right\rangle \right|^2} = \frac{1}{2} = \Delta\hat{Y}$$

$$\Rightarrow \Delta\hat{X}\Delta\hat{Y} = \frac{1}{4}$$

In this sense, the coherent state represents the minimum uncertainty process.

Plot of possible standard deviations (Figure from Prof. A. Kandada)



It is possible to modify the coherent state to produce fields with other properties within the blue region of the plot

Next time, we will introduce the notion of a "squeezed" state

First, note that the pure coherent state can be written:

$$\left|c_\alpha\right\rangle \equiv \sum_{n=0}^{\infty} \frac{\alpha^n e^{-|\alpha|^2/2}}{\sqrt{n!}}\left|n\right\rangle = e^{\alpha a^\dagger - \frac{1}{2}|\alpha|^2}\left|0\right\rangle \qquad \text{where } \left|0\right\rangle \text{ denotes the vacuum state}$$

To form a "squeezed" state we introduce a multiplicative operator

$$S(\zeta) \equiv e^{\frac{1}{2}\zeta^* a^2 - \frac{1}{2}\zeta a^{\dagger 2}}$$