量子光学与量子信息-2

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Chapter 1: Classical optics Review

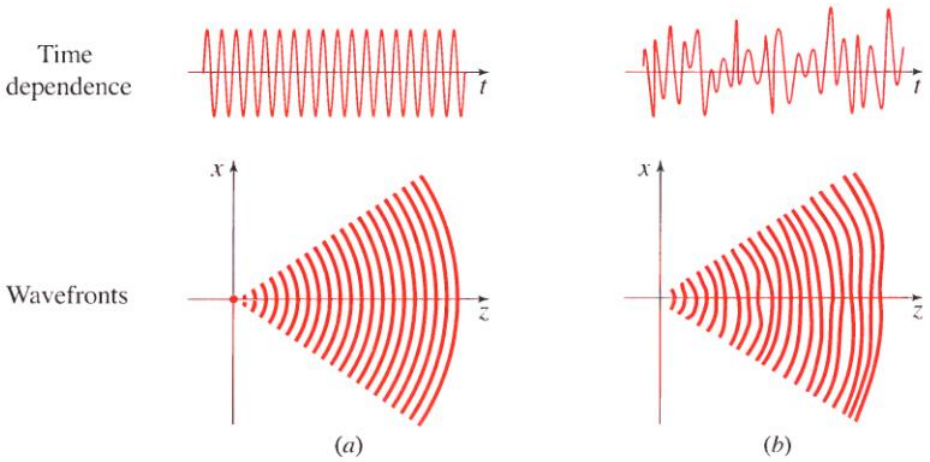
- Classical Models of Light
  - Electromagnetic field
  - Maxwell's equations
  - Electromagnetic waves
  - Polarization
- Diffraction, interference and coherence
  - Diffraction
  - Interference: Michelson interferometer
  - Coherence: First-order correlation function
- Nonlinear optics
  - Nonlinear polarization
  - Fundamental Nonlinear Optical Processes
  - Phase-Matching Condition

Coherence

Coherence is an ideal property of waves that enables stationary (i.e. temporally and spatially constant) interference.

- **Temporal coherence** (longitudinal coherence)
  Related to the bandwidth of the wave.

- **Spatial coherence** (transverse coherence)
  Related to the finite size of the wave source.



Time dependence and wavefronts of
(a) a monochromatic spherical wave; (b) random light.

Temporal coherence

Coherence time τ_c : the time duration over which the phase of the wave remains stable .

Coherence length L_c: $L_c = c\tau_c$

The coherence time is determined by the *spectral width* of the light.

$$\tau_c \approx \frac{1}{\Delta\omega}$$

The temporal coherence of light can be quantified more accurately by the **first-order correlation function**

$$g^{(1)}(\tau) = \frac{\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle}{\langle |\mathcal{E}(t)|^2\rangle}$$

The symbol $\langle \cdots \rangle$ used indicates that we take the average over a long time interval T.

$$\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle = \frac{1}{T}\int_T \mathcal{E}^*(t)\mathcal{E}(t+\tau)\,\mathrm{d}t$$

The first-order correlation function $g^{(1)}(\tau)$ is based on the properties of the first power of the electric field. It is also called the **degree of first-order coherence**.

First-order correlation function

$$g^{(1)}(\tau) = \frac{\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle}{\langle |\mathcal{E}(t)|^2\rangle}$$

Assume that the input field $\mathcal{E}(t)$ is quasi-monochromatic with a center frequency of ω_0

$$\mathcal{E}(t) = \mathcal{E}_0 \mathrm{e}^{-\mathrm{i}\omega_0 t}\mathrm{e}^{\mathrm{i}\phi(t)}$$

So that

$$g^{(1)}(\tau) = \mathrm{e}^{-\mathrm{i}\omega_0\tau}\left\langle \mathrm{e}^{\mathrm{i}[\phi(t+\tau)-\phi(t)]}\right\rangle$$

For $\tau = 0$, $\left|g^{(1)}(\tau)\right| = 1$ for all cases;

For $0 < \tau \ll \tau_c$, $\phi(t+\tau) \approx \phi(t)$, the value of $\left|g^{(1)}(\tau)\right|$ will remain close to unity. As τ increases, $\left|g^{(1)}(\tau)\right|$ decreases due to the increased probability of phase randomness;

For $\tau \gg \tau_c$, $\phi(t+\tau)$ will totally uncorrelated with $\phi(t)$, and $\mathrm{e}^{\mathrm{i}[\phi(t+\tau)-\phi(t)]}$ will average to zero, implying $g^{(1)}(\tau) = 0$.

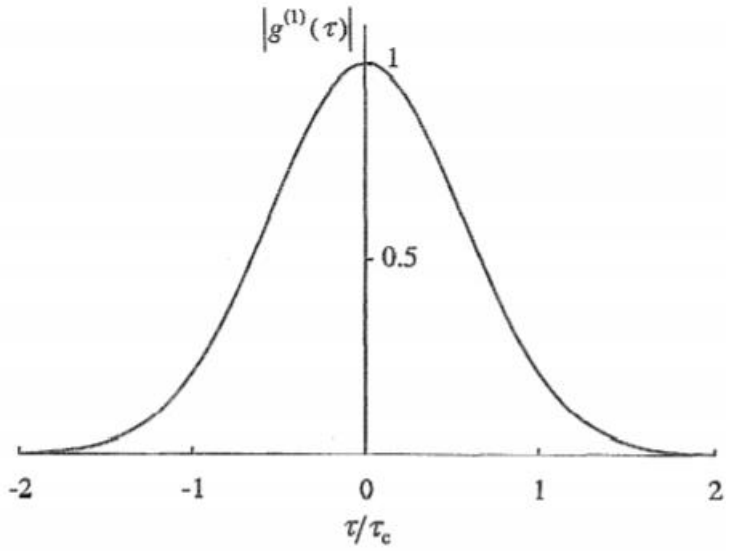
First-order correlation function

The form of $g^{(1)}(\tau)$ for partially coherent light depends on the type of spectral broadening that applies.

For Gaussian lineshape (Doppler-broaden)

$$g^{(1)}(\tau) = \mathrm{e}^{-\mathrm{i}\omega_0\tau} \exp\left[-\frac{\pi}{2}\left(\frac{\tau}{\tau_c}\right)^2\right]$$

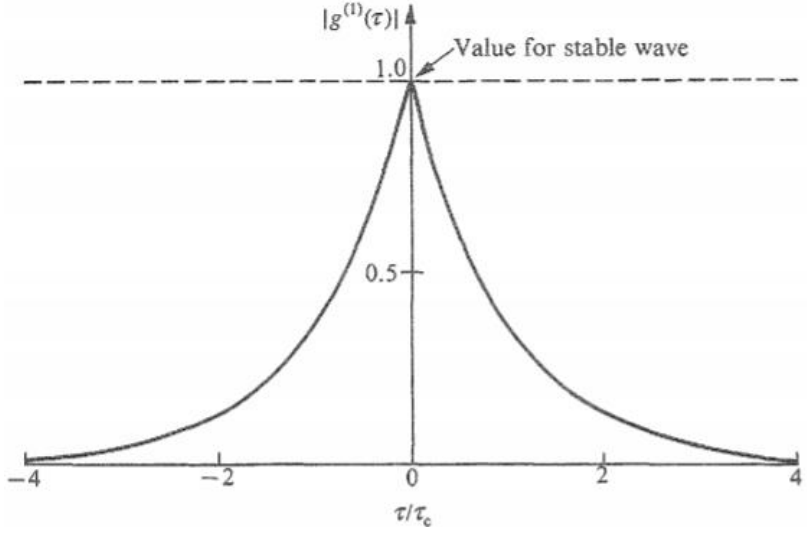
$$\tau_c = (8\pi \ln 2)^{1/2}/\Delta\omega$$



For Lorentzian lineshape (lifetime-broaden)

$$g^{(1)}(\tau) = \mathrm{e}^{-\mathrm{i}\omega_0\tau} \exp(-|\tau|/\tau_c)$$

$$\tau_c = (8\pi \ln 2)^{1/2}/\Delta\omega$$



See details in Ch4 and Loudon (2000, §3.4)

How to measure $g^{(1)}(\tau)$?

The visibility of interference fringes $\quad \text{visibility} = \dfrac{I_{\max} - I_{min}}{I_{\max} + I_{min}}$

Assume we have a light source with a constant average intensity.

The output field (50: 50 BS, $\Delta\phi = \pi$, $\tau = 2\Delta L/c$)

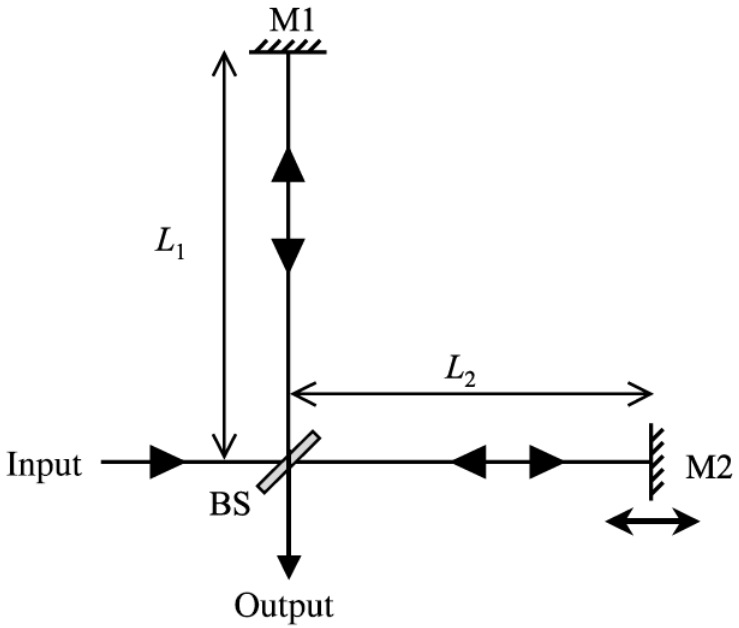
$$\mathcal{E}^{\text{out}}(t) = \frac{1}{\sqrt{2}}\big(\mathcal{E}(t) - \mathcal{E}(t+\tau)\big)$$

The time-averaged intensity

$$I(\tau) \propto \left\langle \mathcal{E}^{\text{out}^*}(t)\mathcal{E}^{\text{out}}(t)\right\rangle$$

$$\propto (\langle \mathcal{E}^*(t)\mathcal{E}(t)\rangle + \langle \mathcal{E}^*(t+\tau)\mathcal{E}(t+\tau)\rangle$$

$$-\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle - \langle \mathcal{E}^*(t+\tau)\mathcal{E}(t)\rangle)/2$$



The Michelson interferometer

$$\langle \mathcal{E}^*(t)\mathcal{E}(t)\rangle = \langle \mathcal{E}^*(t+\tau)\mathcal{E}(t+\tau)\rangle \qquad \big(\mathcal{E}^*(t)\mathcal{E}(t+\tau)\big)^* = \big(\mathcal{E}^*(t+\tau)\mathcal{E}(t)\big)$$

$$\Rightarrow I(\tau) \propto \langle \mathcal{E}^*(t)\mathcal{E}(t)\rangle - \text{Re}[\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle]$$

Relation between $g^{(1)}(\tau)$ and visibility

$$g^{(1)}(\tau) = \frac{\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle}{\langle |\mathcal{E}(t)|^2\rangle}$$

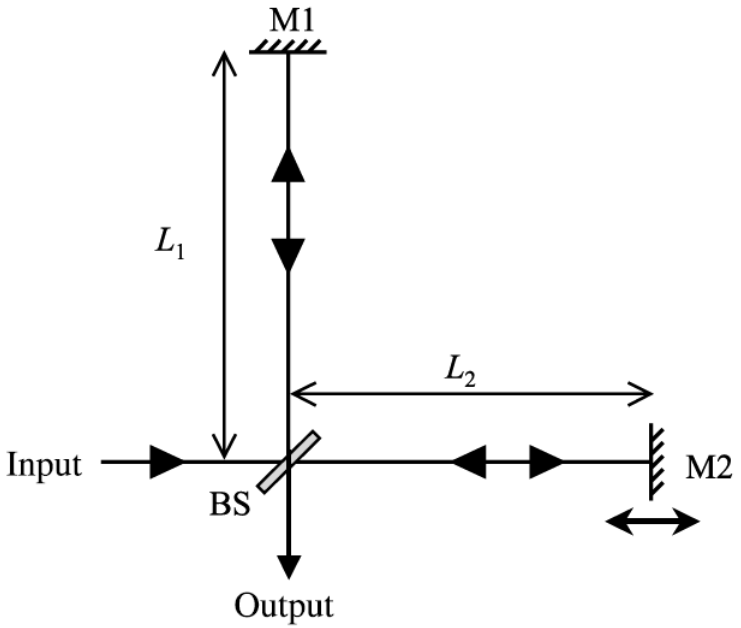
$$I(\tau) \propto \langle \mathcal{E}^*(t)\mathcal{E}(t)\rangle - \mathrm{Re}[\langle \mathcal{E}^*(t)\mathcal{E}(t+\tau)\rangle]$$

$$I(\tau) \propto \langle \mathcal{E}^*(t)\mathcal{E}(t)\rangle\left(1 - \mathrm{Re}\left[g^{(1)}(\tau)\right]\right)$$

$$= I_0\left(1 - \mathrm{Re}\left[g^{(1)}(\tau)\right]\right)$$

$$I_{\max/\min} = I_0\left(1 \pm \left|g^{(1)}(\tau)\right|\right)$$

$$\text{Visibility} = \frac{I_{\max} - I_{min}}{I_{\max} + I_{min}} = \left|g^{(1)}(\tau)\right|$$



The Michelson interferometer

Description of light	Spectral width	Coherence	Coherence time	$\lvert g^{(1)}(\tau)\rvert$
Perfectly monochromatic	0	Perfect	Infinite	1
Chaotic	$\Delta\omega$	Partial	$\sim 1/\Delta\omega$	$1 > \lvert g^{(1)}(\tau)\rvert > 0$
Incoherent	Effectively infinite	None	Effectively zero	0

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  - Nonlinear polarization
  - Fundamental Nonlinear Optical Processes
  - Phase-Matching Condition

Nonlinear optics

The linear relationship between the electric polarization of a dielectric medium and the electric field of a light wave:

$$\boldsymbol{P} = \epsilon_0 \chi \boldsymbol{\mathcal{E}}$$

Here $\boldsymbol{P}$ is the induced dipole moment per unit volume and $\boldsymbol{\mathcal{E}}$ is the electric field.

When the electric field is large, the nonlinear terms cannot be ignored and we enter the realm of nonlinear optics.

$$\boldsymbol{P} = \epsilon_0 \chi^{(1)} \boldsymbol{\mathcal{E}} + \epsilon_0 \chi^{(2)} \boldsymbol{\mathcal{E}}^2 + \epsilon_0 \chi^{(3)} \boldsymbol{\mathcal{E}}^3 + \cdots$$

$\boldsymbol{P^{(1)}} = \epsilon_0 \chi^{(1)} \boldsymbol{\mathcal{E}}$

$\chi^{(1)}$ describes linear optics, e.g., how lenses work

$\boldsymbol{P^{(2)}} = \epsilon_0 \chi^{(2)} \boldsymbol{\mathcal{E}}^2$

$\chi^{(2)}$ describes second-order effects, e.g.,

- Second-Harmonic Generation (SHG)

SHG

$\boldsymbol{P^{(3)}} = \epsilon_0 \chi^{(3)} \boldsymbol{\mathcal{E}}^3$

$\chi^{(3)}$ describes third-order effects, e.g.,

- Third-Harmonic Generation (THG)
- Four-wave mixing (FWM)
- Intensity-Dependent Refractive Index

FWM

NL index

Fundamental Nonlinear Optical Processes

The second-order nonlinear polarization

$$P^{(2)} = \epsilon_0 \chi^{(2)} \mathcal{E}^2$$

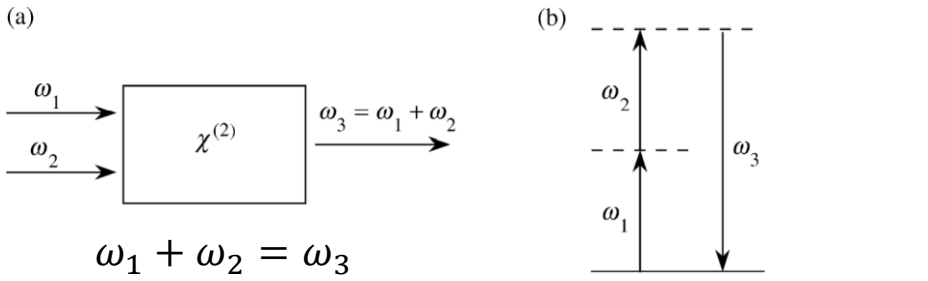
$$\begin{aligned} P^{(2)}(t) &= \epsilon_0 \chi^{(2)} \times \mathcal{E}_1 \cos\omega_1 t \times \mathcal{E}_2 \cos\omega_2 t \\ &= \epsilon_0 \chi^{(2)} \mathcal{E}_1 \mathcal{E}_2 \frac{1}{2} [\cos(\omega_1 + \omega_2)t + \cos(\omega_1 - \omega_2)t] \end{aligned}$$

The second-order nonlinear response generates an oscillating polarization at the sum and difference frequencies of the input fields according to:

$$\omega_{\text{sum}} = \omega_1 + \omega_2$$
$$\omega_{\text{diff}} = |\omega_1 - \omega_2|$$

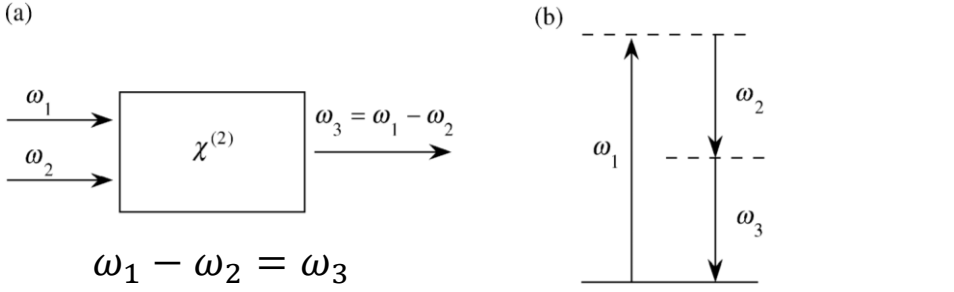
The medium then reradiates at ω_{sum} and ω_{diff} , thereby emitting light at frequencies $(\omega_1 + \omega_2)$ and $|\omega_1 - \omega_2|$. (**Sum-Frequency Generation (SFG)** and **Difference-Frequency Generation (DFG)**, respectively)

- Sum-Frequency Generation (SFG)



$\omega_1 + \omega_2 = \omega_3$

- Difference-Frequency Generation (DFG)

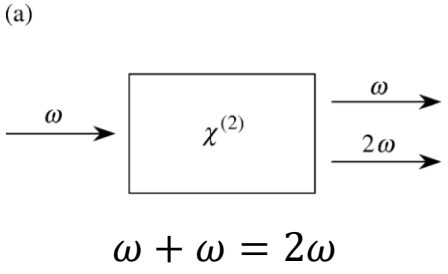


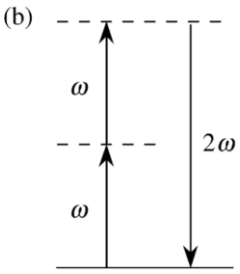
$\omega_1 - \omega_2 = \omega_3$

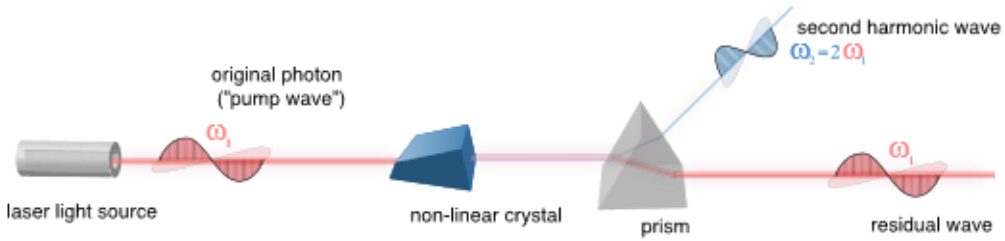
Fundamental Nonlinear Optical Processes

If $\omega_1 = \omega_2$, the effect is called **frequency doubling** or **second harmonic generation**.

- Second-Harmonic Generation (SHG)

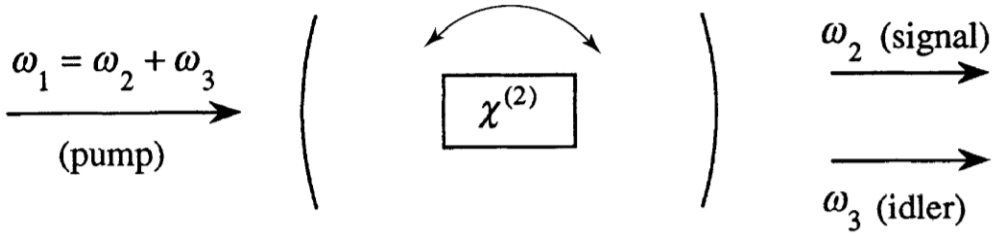


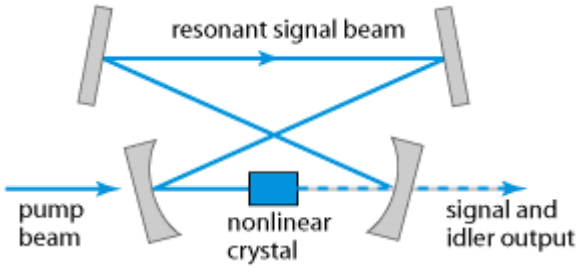




If the nonlinear crystal used in SFG process is placed inside an optical resonator, the ω_2 and/or ω_3 fields can build up to large values.

- Optical Parametric Oscillation



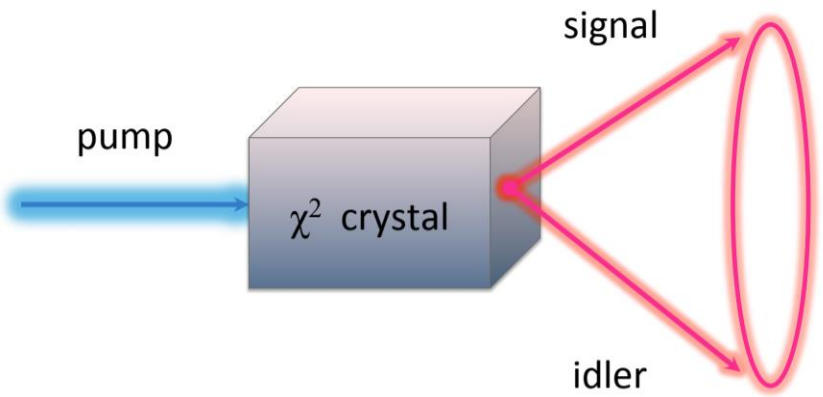


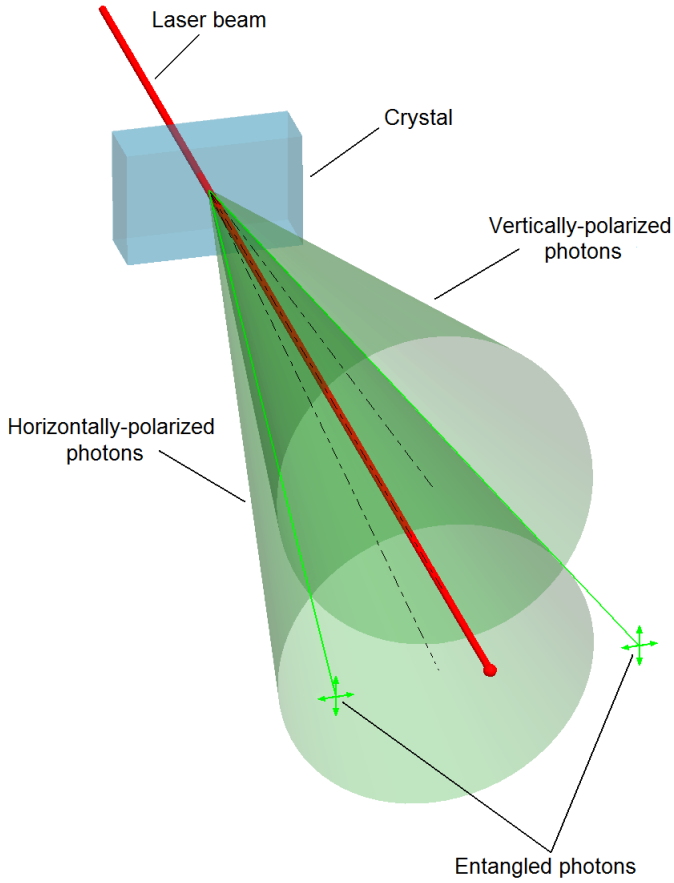
Spontaneous Parametric Down-Conversion

Spontaneous parametric down-conversion (also known as **SPDC**): converts one photon of higher energy **pump**, into a pair of photons (**signal** and **idler**) of lower energy under *conservation of energy and momentum*.

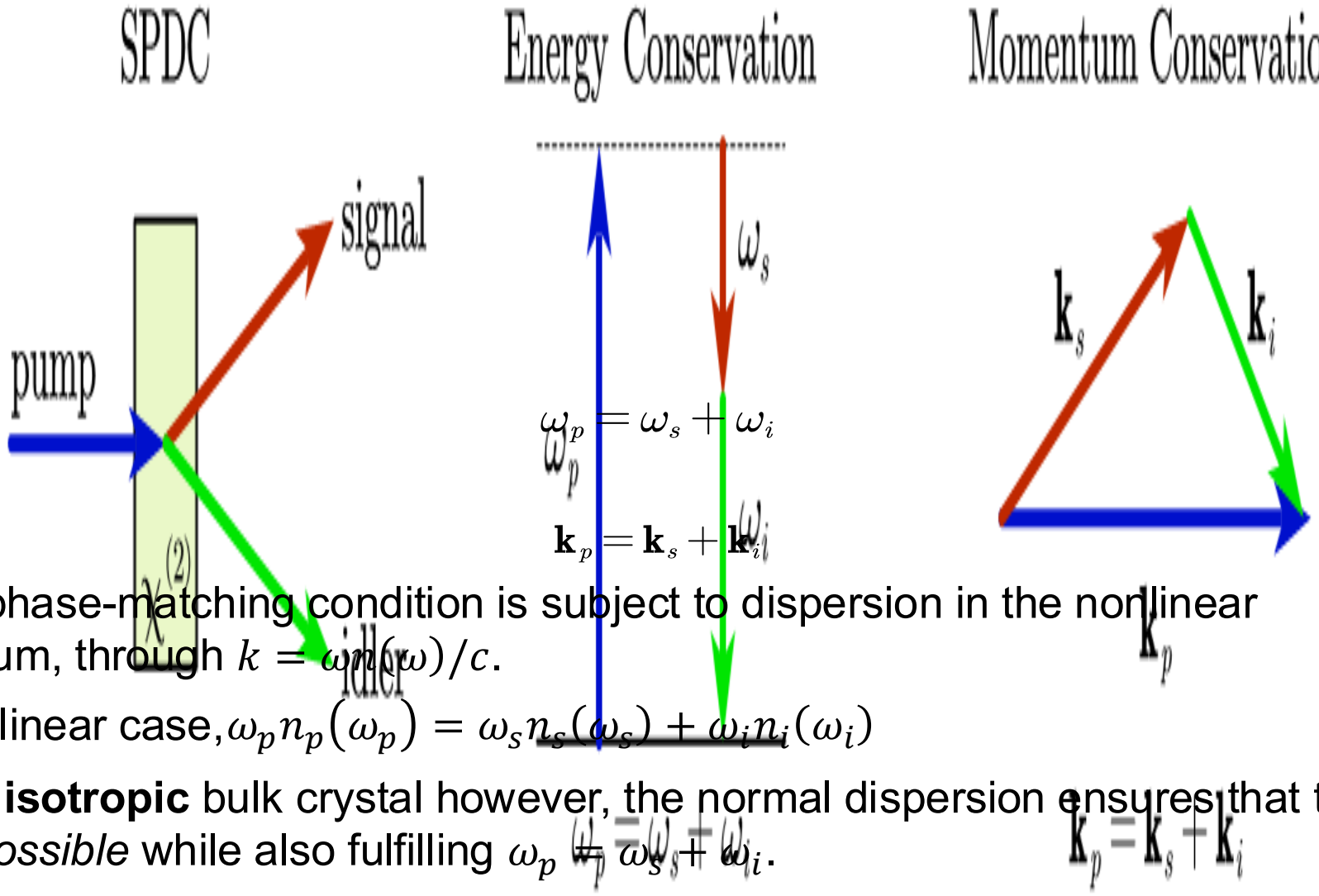
Applications

- single photon as well as photon pairs source
- entangled photon source





Phase-Matching Condition



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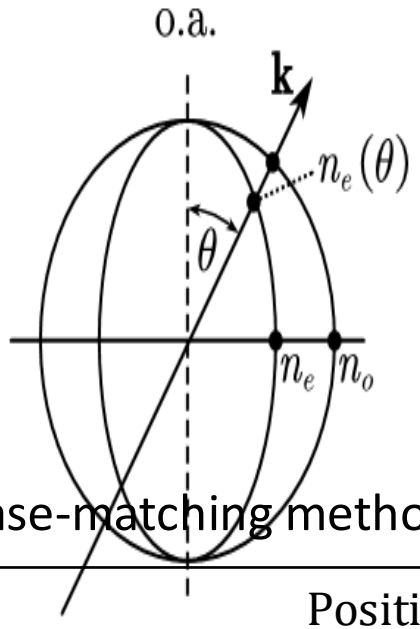
The phase-matching condition is subject to dispersion in the nonlinear medium, through $k = \omega n(\omega)/c$.

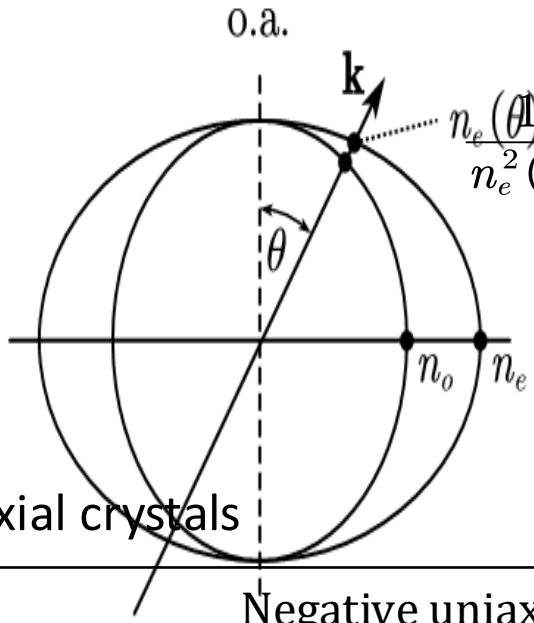
In collinear case, $\omega_p n_p(\omega_p) = \omega_s n_s(\omega_s) + \omega_i n_i(\omega_i)$

In an **isotropic** bulk crystal however, the normal dispersion ensures that this is *not possible* while also fulfilling $\omega_p = \omega_s + \omega_i$.

Phase-Matching Condition

It is possible to satisfy both in a dispersive medium by making use of the **birefringence** of the nonlinear crystal.





$$\frac{1}{n_e^2(\theta)} = \frac{\cos^2\theta}{n_o^2} + \frac{\sin^2\theta}{n_e^2}$$

Phase-matching methods for uniaxial crystals

	Positive uniaxial Negative uniaxial crystal ($n_e > n_o$)	Negative uniaxial Positive uniaxial crystal ($n_e < n_o$)
Type I	$\omega_p n_p^o = \omega_s n_s^e + \omega_i n_i^e$	$\omega_p n_p^e = \omega_s n_s^o + \omega_i n_i^o$
Type II	$\omega_p n_p^o = \omega_s n_s^o + \omega_i n_i^e$	$\omega_p n_p^e = \omega_s n_s^e + \omega_i n_i^o$

Fundamental Nonlinear Optical Processes

The third-order nonlinear polarization

$$P^{(3)} = \epsilon_0 \chi^{(3)} \mathcal{E}^3$$

Consider the simple case

$$\mathcal{E}(t) = \mathcal{E}_0 \cos \omega t$$

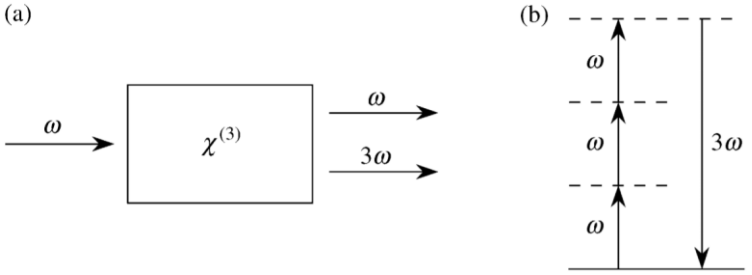
Then,

$$\cos^3 \omega t = \frac{1}{4} \cos 3\omega t + \frac{3}{4} \cos \omega t$$

$$P^{(3)}(t) = \frac{1}{4} \epsilon_0 \chi^{(3)} \mathcal{E}^3 \cos 3\omega t + \frac{3}{4} \epsilon_0 \chi^{(3)} \mathcal{E}^3 \cos \omega t$$

The first term in the above equation describes a response at frequency 3ω that is created by an applied field at frequency ω.

- Third-Harmonic Generation (THG) or Frequency Tripling



Fundamental Nonlinear Optical Processes

$$P^{(3)}(t) = \frac{1}{4}\epsilon_0\chi^{(3)}\mathcal{E}^3\cos 3\omega t + \frac{3}{4}\epsilon_0\chi^{(3)}\mathcal{E}^3\cos\omega t$$

The second term describes a nonlinear contribution to the polarization at the frequency of the incident field; this term hence leads to a nonlinear contribution to the refractive index experienced by a wave at frequency ω.

- Intensity-Dependent Refractive Index

$$n = n_0 + n_2 I$$

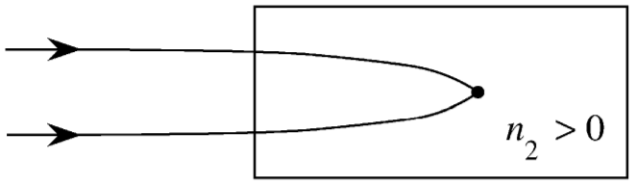
$$I = \frac{1}{2}c\epsilon_0 n\mathcal{E}_0^2$$

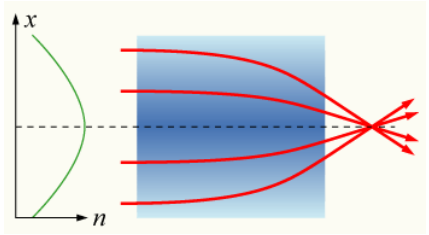
n_0 is the usual (i.e., linear or low-intensity) refractive index
n_2 is an optical constant that characterizes the strength of the optical nonlinearity

$$n_2 = \frac{3}{2n_0^2\epsilon_0 c}\chi^{(3)}$$

➢ Self-Focusing

When a beam of light having a nonuniform transverse intensity distribution propagates through a material for which n_2 is positive.





gradient-index lens

Fundamental Nonlinear Optical Processes

The third-order nonlinear polarization

$$P^{(3)} = \epsilon_0 \chi^{(3)} \mathcal{E}^3$$

An applied field that consists of three frequency components

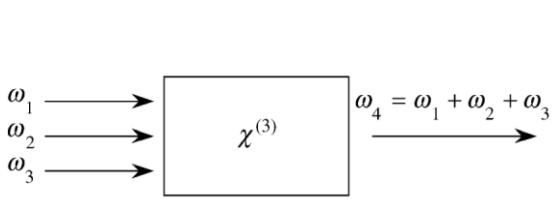
$$\mathcal{E}(t) = \mathcal{E}_1 \mathrm{e}^{-\mathrm{i}\omega_1 t} + \mathcal{E}_2 \mathrm{e}^{\mathrm{i}\omega_2 t} + \mathcal{E}_3 \mathrm{e}^{\mathrm{i}\omega_3 t} + c.c.$$

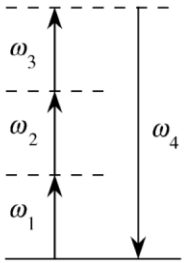
The resulting expression contains 44 different frequency components (consider positive and negative frequencies to be distinct)

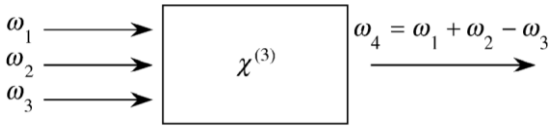
$$\omega_1, \omega_2, \omega_3, 3\omega_1, 3\omega_2, 3\omega_3, (\omega_1 + \omega_2 + \omega_3), (\omega_1 + \omega_2 - \omega_3),$$
$$(\omega_1 + \omega_3 - \omega_2), (\omega_2 + \omega_3 - \omega_1), (2\omega_1 \pm \omega_2), (2\omega_1 \pm \omega_3), (2\omega_2 \pm \omega_1),$$
$$(2\omega_2 \pm \omega_3), (2\omega_3 \pm \omega_1), (2\omega_3 \pm \omega_2),$$

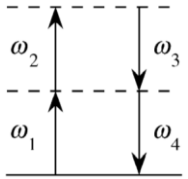
and the negative of each.

Two of the possible mixing processes:









Chapter 2: Quantum mechanics

Quantum Mechanics

- QM is a linear theory
- A physical state is a vector in a Hilbert space- $\mathcal{H}$
- Physical properties (position, momentum) are operators acting in the states

Contents

- Formalism of quantum mechanics
  - The Schrödinger equation
  - Properties of wave functions
  - Measurements and expectation values
  - Commutators and the uncertainty principle
  - Angular momentum
  - Dirac notation
- Quantized states in atoms
  - The gross structure
  - Fine and hyperfine structure
  - The Zeeman effect
- Classical/quantum harmonic oscillators
  - Classical/quantum harmonic oscillators
  - Operator solution of the harmonic oscillator
- The Stern–Gerlach experiment

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The Schrödinger equation

The physical state of a particle within a quantum system is completely described by its **wave function** Ψ, which is the Prob_Amp of finding a particle at ($\boldsymbol{r}$, t).

The probability of finding the particle within a volume increment dV

$$\mathcal{P}(\boldsymbol{r},t)\,\mathrm{d}V = |\Psi(\boldsymbol{r},t)|^2\,\mathrm{d}V$$ probability density

The equation of motion of the wave function is given by the **Schrödinger equation**:

$$\hat{H}\Psi(\boldsymbol{r},t) = \mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\boldsymbol{r},t)$$

$\hat{H}$ is the **Hamiltonian operator**: $\hat{H} = \hat{T} + \hat{V}$

$\hat{T} = \dfrac{\hat{\boldsymbol{p}}^2}{2m}$ is the kinetic energy operators,

$\hat{V}$ is the potential energy operators.

Position operator: $\hat{\boldsymbol{r}} = \boldsymbol{r}$ Momentum operator: $\hat{\boldsymbol{p}} = -\mathrm{i}\hbar\nabla$

$$\hat{H} = \frac{\hat{\boldsymbol{p}}^2}{2m} + \hat{V}(\boldsymbol{r}) = -\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\boldsymbol{r})$$

The Schrödinger equation

Schrödinger equation $\hat{H}\Psi(\boldsymbol{r},t) = \mathrm{i}\hbar\dfrac{\partial}{\partial t}\Psi(\boldsymbol{r},t)$

Hamiltonian operator $\hat{H} = \dfrac{\hat{p}^2}{2m} + \hat{V}(\boldsymbol{r}) = -\dfrac{\hbar^2}{2m}\nabla^2 + \hat{V}(\boldsymbol{r})$

Solution: $\Psi(\boldsymbol{r},t) = \psi(r)\Theta(t)$ Separate time and spatial parts

We find: $\Theta(t) = \exp(-\mathrm{i}Et/\hbar)$ E: total energy of the system

The spatial part of the wave function satisfies the **time-independent Schrödinger equation**:

$$\hat{H}\psi(\boldsymbol{r}) \equiv -\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r}) + \hat{V}(\boldsymbol{r})\psi(\boldsymbol{r}) = E\psi(\boldsymbol{r})$$

$$\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})\exp(-\mathrm{i}Et/\hbar)$$

Schrödinger picture: state change with t
Heisenberg picture: operator change with t

The Schrödinger equation—spatial part

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\boldsymbol{r})+\hat{V}(\boldsymbol{r})\psi(\boldsymbol{r})=E\psi(\boldsymbol{r})$$

In one-dimensional systems

$$\hat{x}=x,$$

$$\hat{p}_x=-\mathrm{i}\hbar\frac{\partial}{\partial x},$$

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\hat{V}(x).$$

the **one-dimensional time-independent Schrödinger equation** becomes:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2}+\hat{V}(x)\psi(x)=E\psi(x)$$

The wave functions that satisfy the time-independent Schrödinger equation are called the **eigenfunctions** of the Hamiltonian.

$$\hat{H}\psi_n(\boldsymbol{r})=E_n\psi_n(\boldsymbol{r})$$

E_n is the energy of the nth state.

Contents

- Formalism of quantum mechanics
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  - Properties of wave functions
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  - Classical/quantum harmonic oscillators
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Properties of wave functions

Normalization

$$\mathcal{P}(\boldsymbol{r},t)\,\mathrm{d}V = |\Psi(\boldsymbol{r},t)|^2\,\mathrm{d}V \longrightarrow \int |\Psi(\boldsymbol{r},t)|^2\,\mathrm{d}^3\boldsymbol{r} = 1$$

probability density

$$\Psi(\boldsymbol{r},t) = \psi(\boldsymbol{r})\exp(-\mathrm{i}Et/\hbar) \longrightarrow \int |\psi(\boldsymbol{r})|^2\,\mathrm{d}^3\boldsymbol{r} = 1 \qquad \text{three-dimensional}$$

$$\int_{-\infty}^{+\infty} |\psi(x)|^2\,\mathrm{d}x = 1 \qquad \text{one-dimensional}$$

Orthogonality

Two wave functions $\psi(\boldsymbol{r})$ and $\varphi(\boldsymbol{r})$ are said to be **orthogonal** if:

$$\int \psi^*(\boldsymbol{r})\varphi(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r} = 0$$

Superposition state

A wave function is said to be in a **superposition state** if it can be written as a non-factorizable linear combination of two or more orthogonal wave functions:

$$\Psi(\boldsymbol{r},t) = c_1\Psi_1(\boldsymbol{r},t) + c_2\Psi_2(\boldsymbol{r},t) + \cdots.$$

Properties of WFs—Orthonormality

Kronecker delta function

$$\delta_{nn'} = \begin{cases} 1 & \text{if } n = n', \\ 0 & \text{if } n \neq n'. \end{cases}$$

Dirac delta function

$$\delta(x) = \begin{cases} +\infty & \text{if } x = 0, \\ 0 & \text{if } x \neq 0. \end{cases} \qquad \int_{-\infty}^{+\infty} \delta(x)\,\mathrm{d}x = 1$$

The eigenfunctions of the Hamiltonian are *orthogonal* to each other and are *normalized* so that:

Orthonormality

$$\int \psi_n^* \psi_{n'}\,\mathrm{d}^3\boldsymbol{r} = \delta_{nn'}$$

The eigenfunctions of the Hamiltonian form a *complete basis*. At a given time, an arbitrary wave function can always be written in the form:

$$\Psi(\boldsymbol{r}, 0) = \sum_n c_n \psi_n(\boldsymbol{r}) \qquad \sum_n |c_n|^2 = 1$$

The wave function evolves according to

$$\Psi(\boldsymbol{r}, t) = \sum c_n \psi_n(\boldsymbol{r}) \exp(-\mathrm{i}E_n t/\hbar)$$

Properties of wave functions

Geometric interpretation

Make an analogy between the *eigenfunctions* and the *basis vectors* $\{a_1, a_2, \ldots, a_N\}$ of an N-dimensional vector space.

arbitrary wave function

$$\Psi(\boldsymbol{r}, 0) = \sum_n c_n \psi_n(\boldsymbol{r})$$

$$\int \psi_n^* \psi_{n'} \, \mathrm{d}^3\boldsymbol{r} = \delta_{nn'}$$

$$\sum_n |c_n|^2 = 1$$

arbitrary unit vector

$$\boldsymbol{\alpha} = \sum_i c_i \boldsymbol{a}_i$$

$$\boldsymbol{a}_i \cdot \boldsymbol{a}_j = \delta_{ij}$$

$$\sum_i |c_i|^2 = 1$$

The vector space that the *eigenfunctions* span is called **Hilbert space**.

The Hilbert space of a particular system has the **same** number of dimensions as the number of eigenfunctions of the Hamiltonian for this system.

Measurements, operators and expectation values

Physically measurable quantities are represented by *operators* in QM.
Each operator has its own set of eigenfunctions and eigenvalues.

Eigenvalue equation $\hat{O}\varphi_i = O_i\varphi_i$

The eigenfunctions form a complete orthonormal basis.

$$\psi = \sum_i c_i \varphi_i \qquad \{c_i\} \text{ are complex numbers}$$

If the experiment is repeated many times on an ensemble of particles each prepared in the same state ψ, the average of the results will be equal to

expectation value $$\left\langle \hat{O} \right\rangle = \int \psi^* \hat{O} \psi \, \mathrm{d}^3 \boldsymbol{r}$$

mean square variation (the **variance,方差**)

$$(\Delta O)^2 = \int \psi^* \left(\hat{O} - \left\langle \hat{O} \right\rangle \right)^2 \psi \, \mathrm{d}^3 \boldsymbol{r}$$

$$= \left\langle \hat{O}^2 \right\rangle - \left\langle \hat{O} \right\rangle^2$$

Commutators

The **commutator** of two quantum mechanical operators $\hat{A}$ and $\hat{B}$ is defined by

$$\left[\hat{A},\hat{B}\right] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$$

The operators are said to **commute** if $\left[\hat{A},\hat{B}\right] = 0$

If the two operators do not commute, it will not be possible to measure their values with arbitrary accuracy at the same time.

Q: $\quad [\hat{x},\hat{p}_x] = ?$

Operate on an arbitrary wave function

$$[\hat{x},\hat{p}_x]\psi = \left(\hat{x}\hat{p}_x - \hat{p}_x\hat{x}\right)\psi$$

$$[\hat{x},\hat{p}_x]\psi = -\mathrm{i}\hbar\left(x\frac{\partial\psi}{\partial x} - \frac{\partial(x\psi)}{\partial x}\right)$$

$$= \mathrm{i}\hbar\psi$$

$$\hat{x} = x,$$

$$\hat{p}_x = -\mathrm{i}\hbar\frac{\partial}{\partial x}.$$

Hence we conclude that:

$$[\hat{x},\hat{p}_x] = \mathrm{i}\hbar$$

The uncertainty principle

Uncertainty principle

$$(\Delta A)^2(\Delta B)^2 \geqslant \left|\left[\hat{A},\hat{B}\right]\right|^2/4 \qquad (\Delta O)^2 = \left\langle \hat{O}^2 \right\rangle - \left\langle \hat{O} \right\rangle^2$$

This sets a minimum limit to the error with which the two properties can be measured, and shows that a very precise measurement of one variable increases the uncertainty of the other, and vice versa.

$$\left[\hat{x},\hat{p}_x\right] = \mathrm{i}\hbar$$

$$(\Delta x)^2(\Delta p_x)^2 \geqslant |\mathrm{i}\hbar|^2/4$$

$$\Delta x\,\Delta p_x \geqslant \hbar/2$$

This result is called the **Heisenberg uncertainty principle**.

The uncertainty principle—Orbital angular momentum

Orbital angular momentum $\hat{l} = \hat{\boldsymbol{r}} \times \hat{\boldsymbol{p}}$

$\hat{l}_x, \hat{l}_y$ and $\hat{l}_z$: components along the three Cartesian axes.

$\hat{\boldsymbol{l}}^2$: the squared angular momentum.

$$\left[\hat{\boldsymbol{l}}^2, \hat{l}_x\right] = 0,$$

$$\left[\hat{\boldsymbol{l}}^2, \hat{l}_y\right] = 0,$$

$$\left[\hat{\boldsymbol{l}}^2, \hat{l}_z\right] = 0.$$

$$\left[\hat{l}_x, \hat{l}_y\right] = \mathrm{i}\hbar\hat{l}_z,$$

$$\left[\hat{l}_y, \hat{l}_z\right] = \mathrm{i}\hbar\hat{l}_x,$$

$$\left[\hat{l}_z, \hat{l}_x\right] = \mathrm{i}\hbar\hat{l}_y.$$

We can simultaneously know the precise values of the square of the orbital angular momentum and one of its components, but not the other two, except in isolated cases, e.g. when $l = 0$.

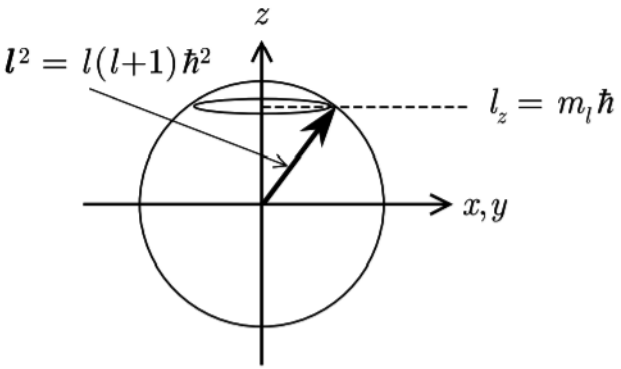
The uncertainty principle—Orbital angular momentum

$$\left[\hat{\boldsymbol{l}}^2, \hat{l}_z\right] = 0$$

Simultaneous eigenfunctions of both $\hat{\boldsymbol{l}}^2$ and $\hat{l}_z$:

$$\hat{\boldsymbol{l}}^2 Y_l^{m_l} = l(l+1)\hbar^2 Y_l^{m_l}$$

$$\hat{l}_z Y_l^{m_l} = m_l \hbar Y_l^{m_l}$$



Spherical harmonics: $Y_l^{m_l}(\theta,\varphi) = C_l^{m_l} P_l^{m_l}(\cos\theta)\mathrm{e}^{\mathrm{i}m_l\varphi}$

$C_l^{m_l}$ is a normalization constant, $P_l^{m_l}$ is the Legendre function.

l is the **orbital quantum number**, m_l is the **magnetic quantum number**.

$l=0,\ m_l=0.$

$$Y_0^0(\theta,\varphi) = \sqrt{\frac{1}{4\pi}}$$

$l=1,\ m_l=\pm1, 0.$

$$Y_1^{-1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}}\sin\theta\mathrm{e}^{-\mathrm{i}\varphi}$$

$$Y_1^0(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\mathrm{e}^{\mathrm{i}\varphi}$$

$l=2,\ m_l=\pm2, \pm1, 0.$

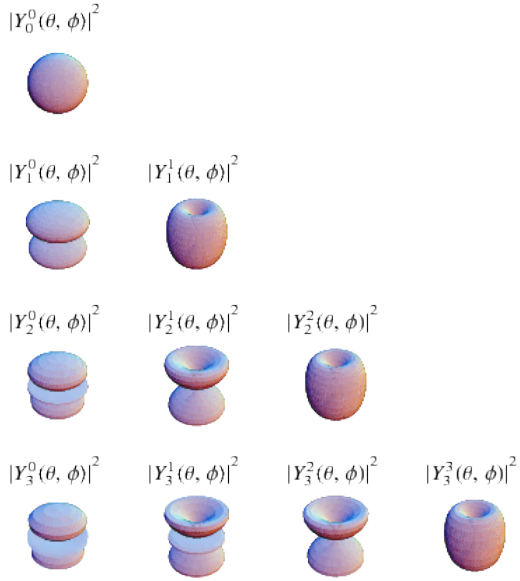
$$Y_2^{-2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\mathrm{e}^{-2\mathrm{i}\varphi}$$

$$Y_2^{-1}(\theta,\varphi) = \sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\mathrm{e}^{-\mathrm{i}\varphi}$$

$$Y_2^0(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_2^1(\theta,\varphi) = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\mathrm{e}^{\mathrm{i}\varphi}$$

$$Y_2^2(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}\sin^2\theta\mathrm{e}^{2\mathrm{i}\varphi}$$



The uncertainty principle—Spin angular momentum

Spin angular momentum

$$[\hat{\boldsymbol{s}}^2, \hat{s}_x] = 0, \qquad [\hat{s}_x, \hat{s}_y] = \mathrm{i}\hbar \hat{s}_z,$$
$$[\hat{\boldsymbol{s}}^2, \hat{s}_y] = 0, \qquad [\hat{s}_y, \hat{s}_z] = \mathrm{i}\hbar \hat{s}_x,$$
$$[\hat{\boldsymbol{s}}^2, \hat{s}_z] = 0. \qquad [\hat{s}_z, \hat{s}_x] = \mathrm{i}\hbar \hat{s}_y.$$

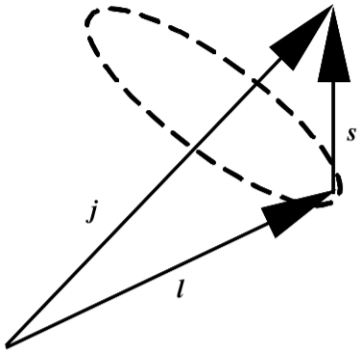
The fact that $\hat{\boldsymbol{s}}^2$ and $\hat{s}_z$ commute means that simultaneous eigenfunctions can exist.

$$\hat{\boldsymbol{s}}^2 \chi = s(s+1)\hbar^2 \chi,$$
$$\hat{s}_z \chi = m_s \hbar \chi. \qquad -s \leqslant m_s \leqslant s \text{ in integer steps}$$

s and m_s are the quantum numbers for the spin magnitude and its z component.

spin-$\frac{1}{2}$ particle: electrons, protons, and neutrons… $s = \frac{1}{2}$ $m_s = -\frac{1}{2}, +\frac{1}{2}$

spin up and spin down



Total angular momentum Multi-particle system

$$\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s} \qquad \boldsymbol{J} = \boldsymbol{J}_1 + \boldsymbol{J}_2$$
$$|l - s| \leqslant j \leqslant (l + s) \qquad |J_1 - J_2| \leqslant J \leqslant (J_1 + J_2)$$
$$-j \leqslant m_j \leqslant j \qquad -J \leqslant m_J \leqslant J$$

Quantum Mechanics-Dirac notation

Quantum Mechanics-Math

Dirac notations

kets: $|\varphi\rangle$ *bra*: $\langle\psi|$

Addition: if $|\varphi\rangle$ and $|\psi\rangle$ are in $\mathcal{H}$, then $|\varphi\rangle$ + $|\psi\rangle$ are in $\mathcal{H}$

Multiplication: if $|\varphi\rangle$ is in $\mathcal{H}$, then $\alpha|\varphi\rangle$ is in $\mathcal{H}$ (α, complex)

Linear independence (LI) : if $\{|\varphi_i\rangle\}$ are LI sets, then $\sum_i c_i|\varphi_i\rangle =$

0 iff $c_i = 0 \; \forall \; i$.

The dimensions of $\mathcal{H}$ is the maximum # of LI vectors.

Quantum Mechanics-Math

Basis of space:

A maximal set of LI vectors in the space is called a basis.

Any vector in the space can be written as a linear superposition of the basis vector

$$|\psi\rangle = \sum_k a_k |\phi_k\rangle$$

Quantum Mechanics-Math

Inner product:

A map from two vectors to a complex number.

$$c = \langle \psi | \varphi \rangle$$

Positivity: $\langle \psi | \psi \rangle \geq 0$

Linearity: $\langle \psi | (c_1 \varphi_1 \rangle + c_2 | \varphi_2 \rangle) = c_1 \langle \psi | \varphi_1 \rangle + c_2 \langle \psi | \varphi_2 \rangle$

Skew symmetry: $\langle \psi | \varphi \rangle = \langle \varphi | \psi \rangle^*$

Orthonormal set $\{|\varphi_k\rangle\}$: $\langle \varphi_k | \varphi_j \rangle = \delta_{k,j}$

Quantum Mechanics-Math

Phase of a state: global phase and relative phase

$$|\psi\rangle = e^{i\vartheta}|\psi\rangle \qquad |\psi\rangle + e^{i\vartheta}|\phi\rangle \neq |\psi\rangle + |\phi\rangle$$

Norm: $\|\psi\| = \sqrt{\langle\psi|\psi\rangle}$

Schwartz inequality: $|\langle\psi|\varphi\rangle|^2 \leq \langle\psi|\psi\rangle\langle\varphi|\varphi\rangle$

Triangular inequality: $\|(\psi + \varphi)\| \leq \|\varphi\| + \|\psi\|$

Quantum Mechanics-Operator

Operator: mapping between two vectors/states

$$A|\psi\rangle = |\phi\rangle$$

Linear operator: $A(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1 A|\psi_1\rangle + c_2 A|\psi_2\rangle$

Decompose the operators on orthonormal sets: $A_{k,j} = \langle v_k | A | v_j \rangle$

Acting on arbitrary state: $A|\psi\rangle = |\varphi\rangle \rightarrow \sum_{i=1}^{N} A a_i |v_i\rangle = \sum_{i=1}^{N} b_i |v_i\rangle$

Obtain the new eigenvalues:

$$\sum_{i=1}^{N} \langle v_k | A a_i | v_i \rangle = b_k \rightarrow \sum_i A_{ki} a_i = b_k$$

Quantum Mechanics-Operator

Operator's properties:

Sum: $(A+B)|\psi\rangle = A|\psi\rangle + B|\psi\rangle)$

Multiplication: $(AB)|\psi\rangle = A(B|\psi\rangle)$

Association: $A(BC)|\psi\rangle = (AB)C|\psi\rangle$

Commutation: $AB|\psi\rangle \neq BA|\psi\rangle$ Generally not

Commutator: $[A,B] = AB - BA$

Quantum Mechanics-Operator

Adjoint operator :

the adjoint of an operator is the conjugate transpose of that operator

$$A^\dagger_{k,j} = \langle k| A^\dagger |j\rangle = \langle j| A |k\rangle^* = A^*_{j,k}$$

Self-adjoint:

$$A^\dagger = A$$

$$A_{ki} = A^*_{ik}$$

Q: Prove that $(cA)^\dagger = c^* A^\dagger$

$$\langle (cA)^\dagger \phi | \psi \rangle = \langle \phi | cA\psi \rangle = c\langle \phi | A\psi \rangle = c\langle A^\dagger \phi | \psi \rangle = \langle c^* A^\dagger \phi | \psi \rangle$$

Quantum Mechanics-Operator

Hermitian operator: self-adjoint operator (in discrete H-S)

Properties:

The eigenvalues of a Hermitian operator are real;

Distinct eigenvectors are orthogonal;

Distinct eigenvalues correspond orthogonal eigenvectors.

1. if A, B are both Hermitian, then $A + B$ is Hermitian

2. if A, B are both Hermitian but do not commute, then at least $AB + BA$ is Hermitian.

Q: Prove 2

$$(AB + BA)^\dagger = B^\dagger A^\dagger + A^\dagger B^\dagger = BA + AB$$

Quantum Mechanics-Operator

Projective operator (Projector): $P_i = |v_i\rangle\langle v_i|$

$$P_j|\psi\rangle = P_j \sum_k c_k |v_k\rangle = c_j |v_j\rangle$$

Closure relation: $\sum_i |v_i\rangle\langle v_i| = \mathbb{1}$

Orthogonal relation: $P_j P_k = \delta_{ik} P_j$

Trace: $\mathrm{Tr}\{A\} = \sum_{j=1}^{N} A_{jj}$ Basis independent

Spectral decomposition of a Hermitian operator: $A|v_j\rangle = a_j |v_j\rangle$

$$A = \sum_j a_j |v_j\rangle\langle v_j|$$

Quantum Mechanics-Operator

Unitary operator：

$$U^\dagger U = \mathbb{1}$$

E.g. evolution of a closed quantum system.

Functions of operators:

$$f(A) = f(0)\mathbb{1} + f'(0)A + \cdots + \tfrac{1}{n!}f^{(n)}(0)A^n + \ldots$$

Taylor expansion

Q: if $A = \sum_a \lambda_a |a\rangle \langle a|$, show $f(A) = \sum_a f(\lambda_a) |a\rangle \langle a|$

Hint:

$$A^2 = (\sum_a \lambda_a |a\rangle \langle a|)(\sum_a \lambda_a |a\rangle \langle a|) = \sum_{a,b} \lambda_a \lambda_b (|a\rangle \langle a|)(|b\rangle \langle b|) = \sum_a \lambda_a^2 |a\rangle \langle a|$$