Contents

I Light as Electromagnetic Waves (光是电磁波)

1. Unifying Light and Electromagnetic Waves

1.1 Review

1) Guass's law

$$\nabla \vec{E} = \frac{\rho}{\epsilon_0}$$
$$\nabla \vec{B} = 0$$

2) Faraday

$$\nabla \times \vec{E} + \frac{\partial \vec{B}}{\partial t} = 0$$

3) Ampere-maxwell

$$\nabla \times \vec{B} - \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} = \vec{j}$$

Without change or current (in vacuum (真空))

$$\nabla^2 \vec{E} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2}$$
$$\nabla^2 \vec{B} = \frac{1}{c}\frac{\partial^2 \vec{B}}{\partial t^2}$$

1.2 Plane Wave

Dimension (量纲)

- $[c] = [\frac{[distance]}{[time]}]$
- $[\frac{\partial^2}{\partial t^2}] = \frac{1}{[time]^2}$
- $[\nabla^2] = [\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}] = \frac{1}{[length^2]}$

Dimension (维度)

1) one space dimension (scalar field (标量场))

$$c^2 \frac{\partial^2}{\partial x^2} f(x,t) = \frac{\partial^2}{\partial t^2} f(x,t)$$
$$f(x,t) = f(x - ct)$$
$$f(x,t) = f_0 \cos(kx - \omega t + \phi),\ k = \frac{2\pi}{\lambda},\ \omega = \frac{2\pi}{T}$$

2) three space dimension (vector field (矢量场))

$$\vec{E}(x,t) = \vec{E}_m \cos(\vec{k} \cdot \vec{r} - \omega t + \phi)$$
$$\vec{B}(x,t) = \vec{B}_m \cos(\vec{k} \cdot \vec{r} - \omega t + \phi)$$

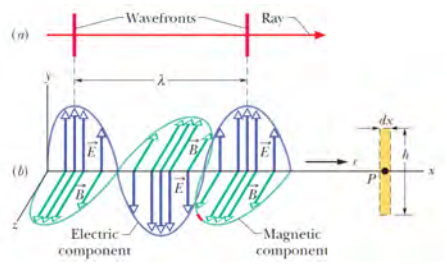

Figure 1: Plane Wave

1.3 Wavefronts

At any instant a wavefront is a surface of constant phase. For the plane wave such a surface is

$$\vec{k} \cdot \vec{r} = constant$$

2. The Propagation of Light Rays (光传播)

Called geometrical optics (几何光学).

2.1 Transmission of Light in Matter

1) the relative permittivity (相对介电常数) also called the dielectric constant k/ϵ_r
2) the relative permeability (相对渗透性) μ_r

A light wave propagating through any substantive medium travels at a speed

$$v = \frac{1}{\sqrt{\epsilon_r \mu_r}} \frac{1}{\sqrt{\epsilon_0 \mu_0}} = \frac{c}{n}$$

where the index of refracton $n = \sqrt{\epsilon_r \mu_r}$.

The dispersion relation (散射率) becomes

$$\omega = vk = \frac{ck}{n}$$

hence $k = nk_0$, where k_0 is the wave number in vacuum.

2.2 Reflection and Refraction

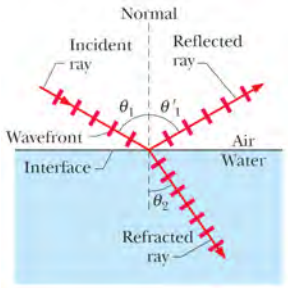

Figure 2: Reflection and Refraction

1) Law of reflection: $\theta_1' = \theta_1$.

2) Law of refraction (or Snell's law): $n_2 \sin\theta_2 = n_1 \sin\theta_1$.

2.3 Total Internal Reflection

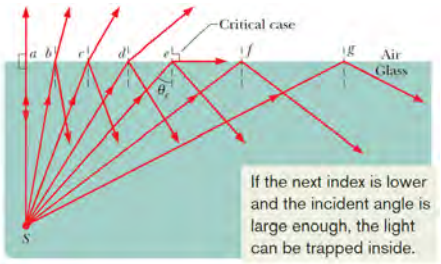

Figure 3: Total Internal Reflection

At a critical (临界) θ_0 , the refracted ray points directly along the interface, i.e.

$$n_{glass} \sin\theta_c = n_{air} \sin\left(\frac{\pi}{2}\right)$$

For larger θ, all the light is reflected.

3. Understanding the Laws of Reflection and Refraction

3.1 Fermat's Principle

The principle of least time: The actual path between two points taken by a beam of light is the one that is traversed in the least time (光路径最短, 走直线).

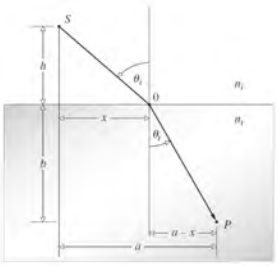

Figure 4: Fermat's Principle

$$t = \frac{\overrightarrow{SO}}{v_i} + \frac{\overrightarrow{OP}}{v_t}, \text{ Let } \frac{dt}{dx} = 0$$
$$\therefore n_i \sin\theta_i = n_t \sin\theta_t$$

The Mirage (海市蜃楼) with Fermat's Principle:

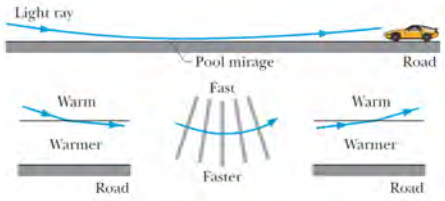

Figure 5: Mirage

3.2 Huygens' Principle

All points on a wavefront serve as point sources of spherical secondary wavelets. After a time t, the new position of the wavefront will be that of a surface tangent to these secondary wavelets.

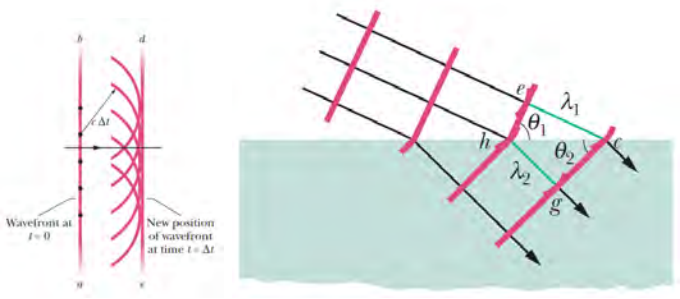

Figure 6: Huygens' Principle

$$\because \frac{\lambda_1}{\lambda_2} = \frac{v_1}{v_2}$$
$$\sin\theta_1 = \frac{\lambda_1}{hc}, \sin\theta_2 = \frac{\lambda_2}{hc}$$
$$\therefore \frac{\sin\theta_1}{\sin\theta_2} = \frac{\lambda_1}{\lambda_2} = \frac{v_1}{v_2} = \frac{\frac{c}{n_1}}{\frac{c}{n_2}} = \frac{n_2}{n_1}$$
$$\text{or } n_2 \sin\theta_2 = n_1 \sin\theta_1$$

3.3 The Electromagnetic Approach

Suppose that the incident, reflected, and transmitted ($\vec{E}_i, \vec{E}_r, \vec{E}_t$, 入射波, 反射波, 透射波) waves can be written as

$$\vec{E}_i = \vec{E}_{0i} \cos\left(\vec{k}_i \cdot \vec{r} - \omega_i t\right)$$
$$\vec{E}_r = \vec{E}_{0r} \cos\left(\vec{k}_r \cdot \vec{r} - \omega_r t + \phi_r\right)$$
$$\vec{E}_t = \vec{E}_{0t} \cos\left(\vec{k}_t \cdot \vec{r} - \omega_t t + \phi_t\right)$$

$\vec{k}$ is space angular velocity.

So we have $\vec{E} = \vec{E}_i + \vec{E}_r$ above the interface and $\vec{E} = \vec{E}_t$ below. For simplicity, we consider the case that $\vec{E}_{0i}, \vec{E}_{0r}, \vec{E}_{0t}$ are constant in time.

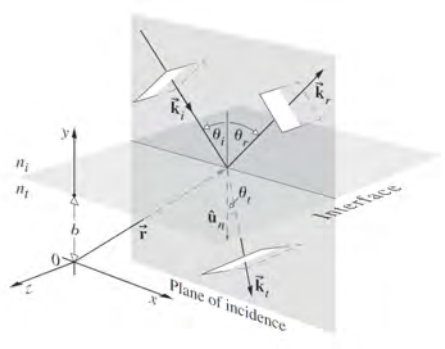

Figure 7: The Electromagnetic Approach

The laws of electromagnetic theory lead to certain requirements that must be met by the fields, and they are referred to as the boundary conditions (边界条件).

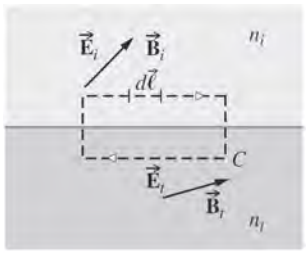

Figure 8: the boundary conditions

For example, we draw a narrow closed path C that runs parallel to the interface inside both media. According to Faraday's induction law

$$\oint \vec{E} \cdot \mathrm{d}\vec{s} = -\frac{\mathrm{d}\Phi_B}{\mathrm{d}t}$$

The loop can be made so narrow such that there is no flux through C . Define $\hat{u}_n$ to be the unit vector normal to the interface. The boundary condition leads to

$$\hat{u}_n \times (\vec{E}_i + \vec{E}_r) - \hat{u}_n \times \vec{E}_t = 0$$

which is satisfied for all values of time and at any point on the interface. That is

$$\begin{aligned} &\hat{u}_n \times \vec{E}_{0i} \cos\left(\vec{k}_i \cdot \vec{r} - \omega_i t\right) \\ +&\hat{u}_n \times \vec{E}_{0r} \cos\left(\vec{k}_r \cdot \vec{r} - \omega_r t + \phi_r\right) \\ =&\hat{u}_n \times \vec{E}_{0t} \cos\left(\vec{k}_t \cdot \vec{r} - \omega_t t + \phi_t\right) \end{aligned}$$

This can only be satisfied if $\omega_i = \omega_r = \omega_t$, which means the charged particles (带电粒子) within the media are undergoing force oscillations (振荡) at the frequency of the incident wave .

Furthermore, for any $\vec{r}$ terminating on the interface

$$\left(\vec{k}_i \cdot \vec{r}\right)\Big|_{y=b} = \left(\vec{k}_r \cdot \vec{r} + \phi_r\right)\Big|_{y=b} = \left(\vec{k}_i \cdot \vec{r} + \phi_t\right)\Big|_{y=b}$$

Thus, we find

$$\begin{aligned} \left[(\vec{k}_i - \vec{k}_r) \cdot \vec{r}\right] &= \phi_r \\ \text{or } (\vec{k}_i - \vec{k}_r) \cdot (\vec{r}_1 - \vec{r}_2) &= 0 \end{aligned}$$

for any pair of $\vec{r}_1$ and $\vec{r}_2$ terminating on the interface.

And we also have $\hat{u}_n \cdot (\vec{r}_1 - \vec{r}_2) = 0$, so $(\vec{k}_i - \vec{k}_r)$ is parallel to $\hat{u}_n$, or $k_i \sin\theta_i = k_r \sin\theta_r$.

Since the incident and reflected waves are in the same medium, $k_i = k_r$, so finally, $\theta_i = \theta_r$.

Similarly, $(\vec{k}_i - \vec{k}_t)$ is also parallel to $\hat{u}_n$,

$$\vec{k}_i \times \hat{u}_n = \vec{k}_t \times \hat{u}_n$$

or (notice $\vec{k} = nk_0\hat{k}$)

$$n_i\left(\hat{k}_i \times \hat{u}_n\right) = n_t\left(\hat{k}_t \times \hat{u}_n\right)$$

which is nothing but the law of refraction.

Note that the law of reflection and the law of refraction only rely on the phase relationship (相位关系) that exists among the phases of $\vec{E}_i$, $\vec{E}_r$ and $\vec{E}_t$ at the boundary.

There is still an interdependence shared by the amplitudes $\vec{E}_{0i}$, $\vec{E}_{0r}$ and $\vec{E}_{0t}$. The additional constraint can be used to calculate the amplitude of the reflected wave and the transmitte wave (the Fresnel equations). This will lead to the phenomenon of polarization by reflection.

3.4 Light in Another Inertial Frame

A light wave looks like a light wave in any inertial frame of reference.

用 Maxwell 导出光速不变, 光速不变又是相对论基础.

II Geometrical Optics

1. Plane Mirrors

1) For a point source of light O (object).

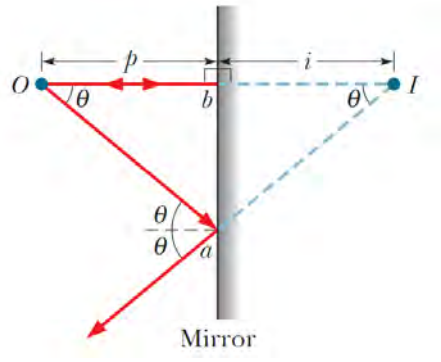

Figure 9: A point source

O represents object , I represents (virtual) image, p represents object distances (positive quantities), i represents image distances (negative quantities).

$$i = -p$$

2) For an extended object O.

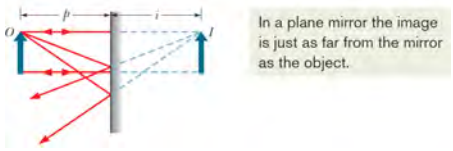

Figure 10: An extended object

2. Spherical Mirrors

2.1 The Concave Mirror (凹面镜) and the Convex Mirror (凸面镜)

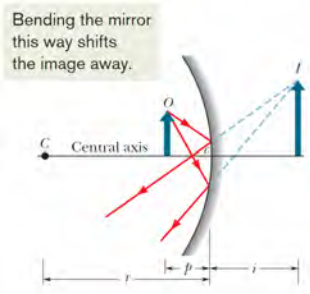

Figure 11: a concave mirror

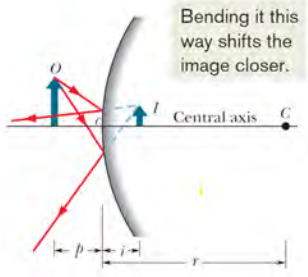

Figure 12: a convex mirror

C represents the center of curvature.

2.2 Focal Points of Spherical Mirrors

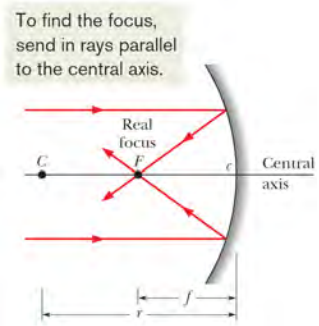

Figure 13: Focal Points of The Concave Mirror

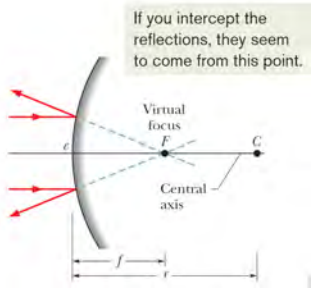

Figure 14: Focal Points of The Convex Mirror

Mirror type	Concave	Convex
F	real	virtual
f	$f > 0$	$f < 0$

Table 1: Mirror types

F represents the focal point, f represents the focal length, r represents the radius of curvature.

$$f = \frac{r}{2}$$

Real images form on the side of a mirror where the object is, and virtual images form on the opposite side.

2.3 Images from Spherical Mirrors

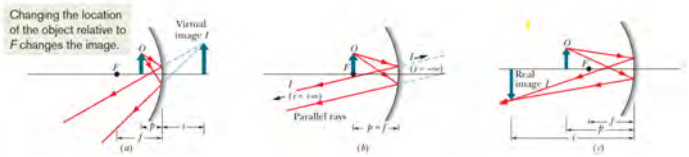

Figure 15: (a) An object O inside the focal point of a concave mirror, and its virtual image I. (b) The object at the focal point F . (c) The object outside the focal point, and its real image I.

$$\frac{1}{p} + \frac{1}{i} = \frac{1}{f}$$

1) The angles should be small.

2) The equation applies to any concave ($f > 0$), convex ($f < 0$), or plane ($f = \infty$) mirror.

3) For a convex or plane mirror, only a virtual image can be formed, regardless of the object' s location on the central axis.

Rules to locate an image:

1) A ray that is initially parallel to the central axis reflects through the focal point F .

2) A ray that reflects from the mirror after passing through the focal point emerges parallel to the central axis.

3) A ray that reflects from the mirror after passing through the center of curvature C returns along itself.

4) A ray that reflects from the mirror at point c is reflected symmetrically about that axis.

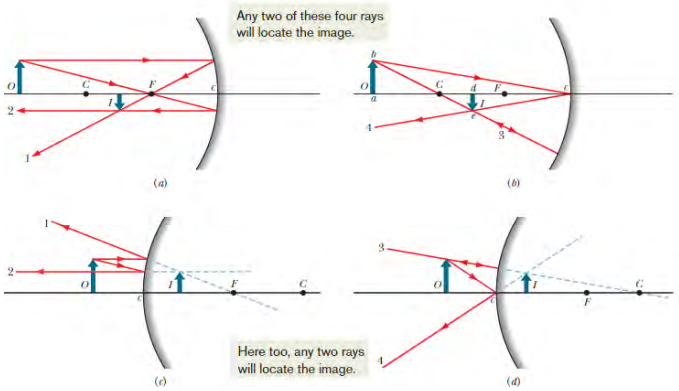

Figure 16: Rules to locate an image

h represents the height of the object, h' represents the height of the image. m is called the lateral magnification (横倍率) produced by the mirror.

$$m \equiv \frac{h'}{h} = -\frac{i}{p}$$

3. Spherical Refraction

For light rays making only small angles with the central axis, so $\sin\theta \sim \theta$.

$$\frac{n_1}{p} + \frac{n_2}{i} = \frac{n_2 - n_1}{2f} = \frac{n_2 - n_1}{r}$$

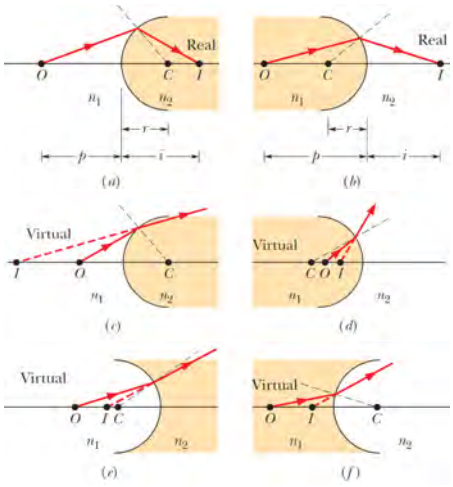

Figure 17: Spherical Refraction

4. Thin Lenses

A lens is a transparent object with two refracting surfaces whose central axes coincide.

A lens that causes light rays initially parallel to the central axis to converge is (reasonably) called a converging lens (汇聚透镜). If, instead, it causes such rays to diverge, the lens is a diverging lens (发散透镜).

We consider a thin lens, i.e., a lens in which the thickest part is thin relative to the object distance p, the image distance i, and the radii of curvature r_1 and r_2 of the two surfaces of the lens.

We also consider only light rays that make small angles with the central axis (again, they are exaggerated in the figures).

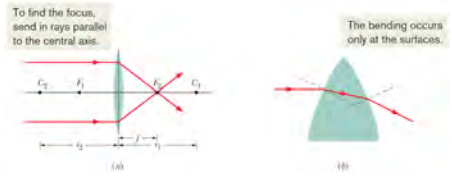

Figure 18: converging lens

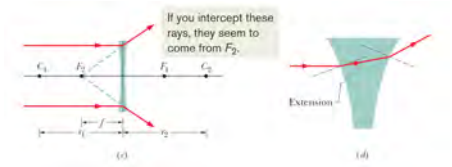

Figure 19: diverging lens

When a thin lens with index of refraction n is sur-

rounded by air, this focal length f is given by the lens maker' s equation:

$$\frac{1}{f} = (n-1)\left(\frac{1}{r_1} - \frac{1}{r_2}\right)$$

If the lens is surrounded by some medium other than air (say, corn oil) with index of refraction n_{medium}, we replace n with $\frac{n}{n_{medium}}$.

For a thin lens with a focal length f , i and p are related to each other by

$$\frac{1}{p} + \frac{1}{i} = \frac{1}{f}$$

1) A ray that is initially parallel to the central axis of the lens will pass through focal point F_2.

2) A ray that initially passes through focal point F_1 will emerge from the lens parallel to the central axis.

3) A ray that is initially directed toward the center of the lens will emerge from the lens with no change in its direction because the ray encounters the two sides of the lens where they are almost parallel.

5. Lens Systems

5.1 Combination of Thin Lenses

We treat the two-lens system with two single-lens calculations, using the normal rules for a single len. The overall (or net) lateral magnification M of a system of lenses (or lenses and a mirror) is the product of the individual lateral magnifications.

5.2 Compound Microscope

A compound microscope consists of an objective (the front lens) of focal length f_{ob} and an eyepiece (the lens near the eye) of focal length f_{ey}. So we generate the virtual image of a real image of the object. We want both images being magnified.

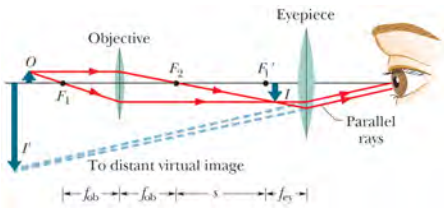

Figure 20: Compound Microscope

For the objective, we want the image to be magnified, so $i_1 \gg p_1$. This can be satisfied by setting $p_1 \gtrsim f_{ob}$.

For the eyepiece, we expect $p_2 \lesssim f_{ey}$.

This leaves the distance between the two lenses $f_{ob} + s + f_{ey}$ the only parameter to tune. The longer the distance, the larger the magnification

$$M = m_1 m_2 \approx -\frac{(f_{ob}+s)}{f_{ob}}\frac{25\text{cm}}{f_{ey}}$$

We can make $s \gg f_{ob}$, so

$$M \approx -\frac{s}{f_{ob}}\frac{25\text{cm}}{f_{ey}}$$

But s is still limited by the practical sizes of the microscope.

III Interference

Optics and Gravitation: Massive galaxies/black holes act like special lenses.

1. The Superposition of Waves

The pheenomena of interference , diffraction and polarization share a commom conceptual basis in that they deal with two or more light waves overlap in some region of space.

Recall that each field component of an electromagnetic wave (E_{xyz}, B_{xyz}) satisfies the scalar 3D differential wave equation

$$\begin{aligned}\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} =& \frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\\ =&\nabla^2\psi\end{aligned}$$

This equation is linear, $\psi(\vec{r},t)$ and its derivatives appear only to the first power. Consequently, if $\psi_i(\vec{r},t)$ are solutions, any linear combination of them

$$\psi(\vec{r},t)=\sum_{i=1}^{n}C_i\psi_i(\vec{r},t)$$

will be a solution as well.

1.1 Examples od Superposition

1) Beats: Two harmonic waves of different frequency traveling in the same direction.

$$\psi=\psi_1+\psi_2=A\cos\omega_1 t+A\cos\omega_2 t,\ \omega_1\approx\omega_2$$

2) Standing waves: Two harmonic waves of the same frequency propagating in opposite directions.

$$\psi=\psi_1+\psi_2=A\cos(kx-\omega t)-A\cos(-kx-\omega t)$$

1.2 The Algbraic Method of Adding Waves

There are several equivalent ways of mathematically adding two or more overlapping waves that have the same frequency and wavelength.

Suppose there are two such waves

$$\begin{aligned}E_1&=E_{01}\cos(\alpha_1-\omega t)\\ E_2&=E_{02}\cos(\alpha_2-\omega t)\end{aligned}$$

where

$$\alpha_i=kx_i+\phi_i$$

with x_i being the distance from the source s_i of the wave to the point of observation.

The linear combination of the waves is

$$E\equiv E_0\cos(\alpha-\omega t)=E_1+E_2$$

where (notice $\cos\omega t$ and $\sin\omega t$ are linearly independent)

$$\begin{aligned}E_0\cos\alpha&=E_{01}\cos\alpha_1+E_{02}\cos\alpha_2\\ E_0\sin\alpha&=E_{01}\sin\alpha_1+E_{02}\sin\alpha_2\end{aligned}$$

and

$$E_0^2=E_{01}^2+E_{02}^2+2E_{01}E_{02}\cos(\alpha_2-\alpha_1)$$

$2E_{01}E_{02}\cos(\alpha_2-\alpha_1)$ is known as the interference term (干涉项).

The crucial factor is the phase difference (相位差) bewteen the two interfering waves E_1 and E_2,

$$\delta\equiv(\alpha_2-\alpha_1)=\frac{2\pi}{\lambda}(x_2-x_1)+(\phi_2-\phi_1)$$

- When $(\alpha_2-\alpha_1)=2m\pi$ for integer m, we have

$$E_0^2=E_{01}^2+E_{02}^2+2E_{01}E_{02}$$

In particular, $E_0=4E_{01}^2$ when $E_{01}=E_{02}$. The two waves interfere constructively.

- When $(\alpha_2-\alpha_1)=(2m+1)\pi$ for integer m, we have

$$E_0^2=E_{01}^2+E_{02}^2-2E_{01}E_{02}$$

In particular, $E_0=0$ when $E_{01}=E_{02}$. The two waves interfere destructively.

1.3 The Complex Method

Above all,

$$\begin{aligned}e^{i\theta}=&\cos\theta+i\sin\theta\\ (e^{i\theta})^*=&e^{-i\theta}\end{aligned}$$

The wave function

$$\begin{aligned}E_1=&E_{01}\cos(\alpha_1-\omega t)\\ =&E_{01}\cos(kx_1-\omega t+\phi_1)\end{aligned}$$

can be written as

$$\begin{aligned}\tilde{E}_1=&E_{01}e^{i(\alpha_1-\omega_1 t)}\\ =&E_{01}e^{i\alpha_1}e^{-i\omega_1 t}\end{aligned}$$

if we are interseted only in the real part.

Suppose that there are two such overlapping waves having the same frequency and traveling in the positive x-direction. The resultant wave is given by

$$\tilde{E} = E_0 e^{i\alpha} e^{-i\omega t} = \left[E_{01} e^{i\alpha_1} + E_{02} e^{i\alpha_2}\right] e^{-i\omega t}$$

where $E_0 e^{i\alpha}$ is known as the complex amplitude of the composite wave.

Since $E_0^2 = (E_0 e^{i\alpha})^* (E_0 e^{i\alpha})$, we find

$$\begin{aligned} E_0^2 =& \left[E_{01} e^{-i\alpha_1} + E_{02} e^{-i\alpha_2}\right] \left[E_{01} e^{i\alpha_1} + E_{02} e^{i\alpha_2}\right] \\ =& E_{01}^2 + E_{02}^2 + E_{01} E_{02} \left[e^{i(\alpha_2 - \alpha_1)} + e^{-i(\alpha_2 - \alpha_1)}\right] \\ =& E_{01}^2 + E_{02}^2 + 2E_{01} E_{02} \cos(\alpha_2 - \alpha_1) \end{aligned}$$

1.4 Phasor Addition

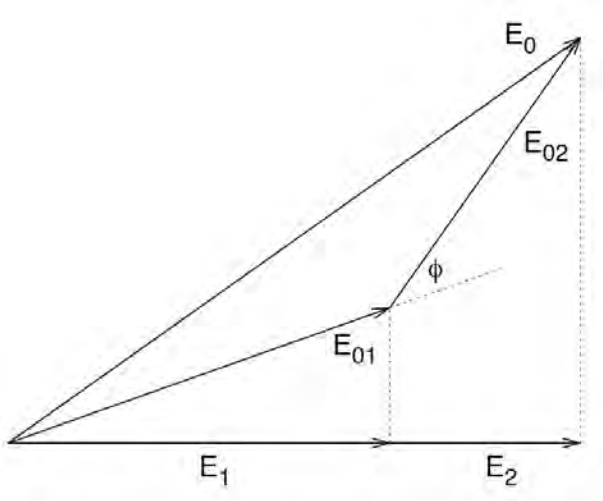

Figure 21: Phasor Addition

We represent a wave, which has an amplitude and a phase, to a vector, know as a phasor, in a two-dimensional plane, such that

$$\begin{aligned} E_i =& E_{0i} \cos(\alpha_i - \omega t) \\ =& (E_{0i} \cos\alpha_i) \cos\omega t + (E_{0i} \sin\alpha_i) \sin\omega t \\ \Longrightarrow \vec{E}_i =& (E_{0i} \cos\alpha_i)\, \hat{x} + (E_{0i} \sin\alpha_i)\, \hat{y} \end{aligned}$$

The algebraic sum, $E = E_1 + E_2$ is the projection on the x axis of the corresponding phasor sum.

If we denote the phase delay $\phi = \alpha_2 - \alpha_1$ as shown in the phasor diagram, the law of cosines applied to the triangle of sides $\vec{E}_{01}$, $\vec{E}_{02}$ and $\vec{E}_0$ yields

$$E_0^2 = E_{01}^2 + E_{02}^2 + E_{01} E_{02} \cos(\alpha_2 - \alpha_1)$$

2. Young's Double-Slit Interference Experiment

2.1 Natural Light

The light from two fine incandescent wires wouldn't interfere, because the light is emitted by vast numbers of atoms in the wires, acting randomly and independently for extremely short times — of the order of nanoseconds. The light is said to be incoherent (不相干, 离散). As a result, at any given point on the viewing screen, the interference between the waves from the two sources varies rapidly and randomly between fully constructive and fully destructive. The screen is seen as being uniformly illuminated (over the time scale of our observation).

Conditions for Interference:

1) Two beams must have (nearly) the same frequency ω. therwise, the phase difference is time-dependent. During the detection interval, the interference pattern will be averaged away.

2) The clearest pattern (with maximum contrast) exists when interfering waves have (nearly) equal amplitude.

3) Initial phase difference can exist between sources, as long as it remains constant; the two sources are said to be coherent (相干, 一致).

2.2 Huygen's Principle

lf waves strike a barrier with a small opening, the waves may be seen to expand from the opening Notice the wavelength is larger than the opening in this case.

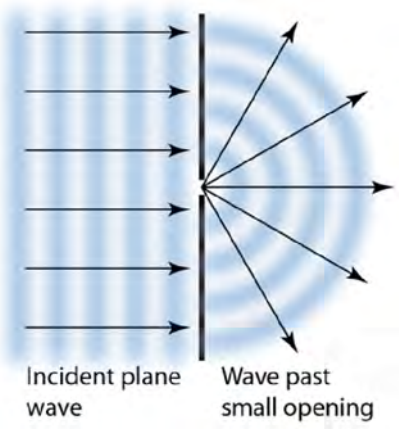

Figure 22: Huygen's Principle

2.3 *Young's Interference Experiment*

Here is the ingenious arrangement of Thomas Young's double-slit experiment.

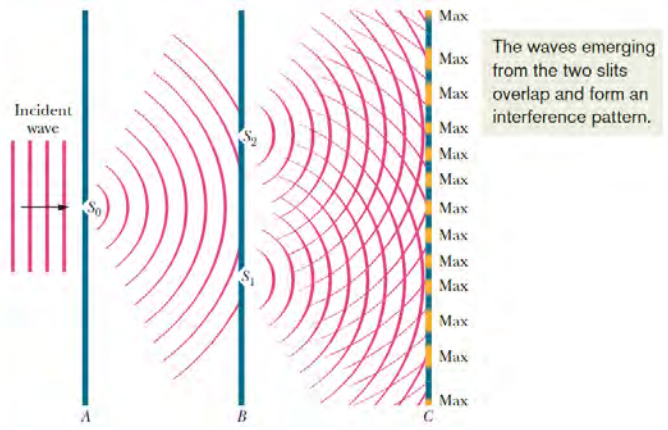

Figure 23: Young's Interference Experiment

The slit S_0 in screen A creats a spatially coherent beam that could identically illuminate slits S_1 and S_2 in screen B. Nowdays, plane waves from a laser can provide the spatial coherence the experiment needs. Finally, light waves produce fringes in a Young's double-slit interference experiment.

The waves are in phase (相同) when they pass through the two slits because there they are just portions of the same incident wave. However, once they have passed the slits, the two waves must travel different distances to reach point P on screen C. The path length difference is, when $d \ll D$,

$$\Delta L = d \sin\theta$$

However, the electric field components of these waves at point P are not in phase and vary with time as

$$E_1 = E_0 \cos(kr_1 - \omega t) = E_0 \cos(kL + \beta - \omega t)$$
$$E_2 = E_0 \cos(kr_2 - \omega t) = E_0 \cos(kL - \beta - \omega t)$$

where the phase difference $\left[L = \frac{r_1+r_2}{2} = \sqrt{D^2+y^2}\right]$

$$\delta_2 = 2\beta = k\Delta L = \frac{2\pi d}{\lambda}\sin\theta$$

The total intensity is thus given by

$$I = 2E_0^2\,[1 + \cos(2\beta)] = I_{max}\cos^2\beta$$

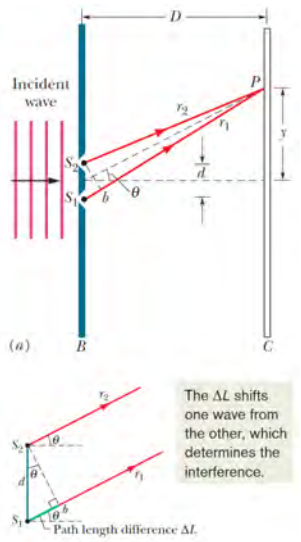

Figure 24: The waves pass through the two slits

Therefore, a bright fringe appears when

$$\Delta L = d \sin\theta = m\lambda$$

when m is an integer.

On the other hand, a dark fringe appears when

$$\Delta L = d \sin\theta = \left(m + \frac{1}{2}\right)\lambda$$

where m is an integer.

We can then find the angle θ to any fringe and thus use the values of m to label the fringes.

3. Interference from Thin Films

Consider a thin transparent film of uniform thickness L and index of refraction n_2, illuminated by bright light of wavelength λ from a distant point source. We assume $n_1 = n_3 = n_{air}$. For simplicity, we also assume that the light rays are almost perpendicular to the film ($\theta \approx 0$).

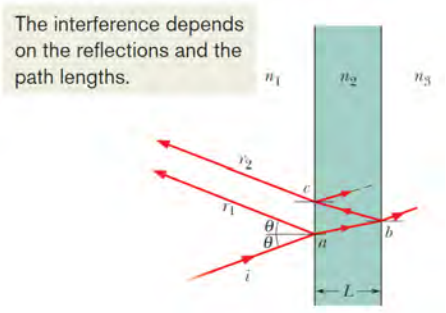

Figure 25: Interference from Thin Films

Reflection at an interface can cause a phase change (相变), depending on the indexes of refraction on the two sides of the interface. There is no phase change for refraction. The results for light reflecting off a medium can be summarized as

Reflection	Reflection phase shift
Off lower index	0
Off higher index	0.5 wavelength

Table 2: light reflecting off a medium

So reflecting off higher index, ray r_1 has an additional reflection phase shift 0.5 wavelength. There is no such shift for r_2. In addition, the light waves of rays r_1 and r_2 has a path difference $2L$, which occurs in index n_2. Notice the wavelength in the medium (r_2) is

$$\lambda_2 = \frac{v_2}{f} = \frac{c}{n_2 f} = \frac{\lambda}{n_2}$$

the r_1 and r_2 are ($k_2 = \frac{2\pi}{\lambda_2}$)

$$\begin{aligned}
\vec{E}_1 =& E_0 \cos\left(k\left(x + \frac{1}{2}\lambda\right) - \omega t\right) \\
=& E_0 \cos(\pi + kx - \omega t) \\
\vec{E}_2 =& E_0 \cos(k_2 2L + kx - wt) \\
\therefore \vec{E}^2 =& \left(\vec{E}_1 + \vec{E}_2\right)^2 = 2E_0^2\left(1 + \cos(k_2 2L - \pi)\right)
\end{aligned}$$

Therefore, rays are in phase if

$$\begin{aligned}
(k_2 2L - \pi) &= 2m\pi \\
2L = \left(m + \frac{1}{2}\right)\lambda_2 &= \left(m + \frac{1}{2}\right)\frac{\lambda}{n_2}
\end{aligned}$$

for integer m. They produce an interference maximum and the nearby region on the film is bright to observers.

Similarly, if they are exactly out of phase (不同相位)

$$\begin{aligned}
(k_2 2L - \pi) &= (2m+1)\pi \\
2L = m\lambda_2 &= m\frac{\lambda}{n_2}
\end{aligned}$$

for integer m. They produce an interference minimum and the nearby region is dark, even though it is illuminated.

3.1 Negligible Film Thickness

A special situation arises when a film is so thin that L is much less than λ, say $L < 0.1\lambda$. Then the path length difference $2L$ can be neglected, and the phase difference between r_1 and r_2 is due only to reflection phase shifts. Thus r_1 and r_2 are exactly out of phase, and thus the film is dark, regardless of the wavelength and intensity of the light.

IV Diffraction

1. Single-Slit Diffraction

We considedr the diffraction parrern of plane waves of light of wavelength λ that are diffracted by a single long , narrow slit of width a (aperture) in an otherwise opaque screen B. Waves from different points within the slit undergo interference and produce a diffraction pattern of bright and dark fringes on screen C.

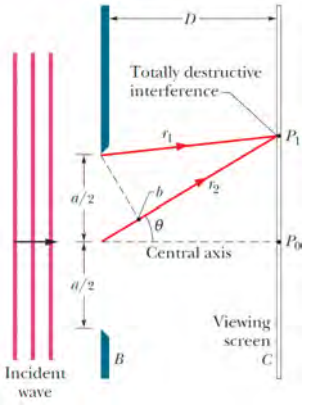

Figure 26: Single-Slit Diffraction

1.1 Fraunhofer vs Fresnel Diffraction

At large screen distance ($D > \frac{a^2}{\lambda}$), the shape of the projected pattern is independent of D. This is Fraunhofer or far-field diffraction (远场衍射).

At small D, however, both the size and shape of the diffraction pattern changes with distance. This phenomenon is known as Fresnel or near-field diffraction (近场衍射).

1.2 Locations of the Dark Fringes

First, we mentally divide the slit into two zones of equal widths $\frac{a}{2}$. We extend r_1 and r_2 to P_1. The wavelets of the pair of rays r_1 and r_2 are in phase within the slit because they originate from the same wavefront passing through the slit, along the width of the slit. To find the dark fringes, we want the wavelets along these two rays to cancel rech other when they arrive at P_1. So they should be out of phase by $\frac{\lambda}{2}$ when they reach P_1. Then any similar pairing of rays from the two zones will give cancellation at the same point P_1, because $D \gg a$.Thus we have approximately

$$\frac{a}{2}\sin\theta = \frac{\lambda}{2}$$

The angle θ of the first dark fringe above and (by symmetry) below the central axis is, therefore, determined by

$$\sin\theta = \frac{\lambda}{a}$$

If we narrow the slit such that $a = \lambda$, the angle θ at which the first dark fringes appear increases to 90°. This means that bright fringe must then cover the entire viewing screen.

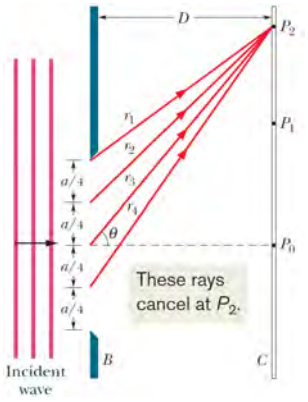

Figure 27: divide the slit into four zones

To find the second dark fringes above and below the central axis, we now divide the slit into four zones of equal width $\frac{a}{4}$. To produce the second dark fringe at P_2, the path length difference between r_1 and r_2, that between r_2 and r_3, and that between r_3 and r_4 must all be equal to $\frac{\lambda}{2}$. For $D \gg a$, we can approximately these four rays as being parallel, at angle θ to the central axis. The path length difference for any two rays that originate at corresponding points in two adjacent zones is $\frac{a}{4}\sin\theta$. Thus we have

$$\frac{a}{4}\sin\theta = \frac{\lambda}{2}$$

We could now continue to locate dark fringes in the diffraction pattern by splitting up the slit into more zones of equal width. We would find that the dark fringes above and below the central axis can be located with the general equation

$$\frac{a}{2m}\sin\theta = \frac{\lambda}{2}$$
$$a\sin\theta = m\lambda$$

for $m = 1, 2, 3, \dots$.

In ohter words, in a single-slit diffraction experiment, dark fringes are produced where the path length differences $(a \sin\theta)$ between the top and bottom rays are equal to $\lambda, 2\lambda, 3\lambda, \dots$.

2. Electric Field and Intensity

To find an expression for the intensity at an arbitrary point P on the viewing screen, corresponding to a particular small angle θ, we need to divide the slit into N zones of equal widths $\Delta x = \frac{a}{N}$ small enough that we can assume each zone acts as a source of Huygens wavelets. We then add the phasors for the wavelets, which form a geometric series (notice $r_{i+1} - r_i = \Delta x \sin\theta$)

$$\begin{aligned}\tilde{E}_\theta =& \frac{E_0}{N} e^{-i\omega t} \sum_{i=1}^{N} e^{ikr_i} \\ =& \frac{E_0}{N} e^{-i\omega t} e^{ikr_1} \times \left[1 + e^{ik(r_2 - r_1)} + \cdots + e^{ik(r_N - r_1)}\right]\end{aligned}$$

The arc of phasors represents the wavelets that reach an arbitrary point P on the viewing screen, corresponding to a small angle θ. The amplitude E_θ of the resultant wave at P is the vector sum of these phasors. In the limit of $N \longrightarrow \infty$, the arc of phasors approaches the arc of a circle.

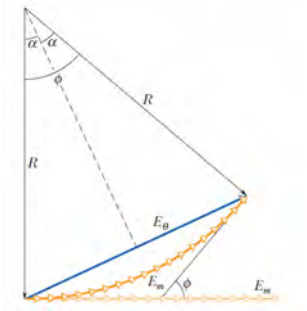

Figure 28: the arc of phasors

We use a graphic construction

$$\frac{I(\theta)}{I_{max}} = \frac{E_\theta^2}{E_m^2} = \left[\frac{(2R\sin\alpha)^2}{(2R\alpha)^2}\right] = \left[\frac{\sin\alpha}{\alpha}\right]^2$$

where $\alpha = \frac{\pi}{\lambda} a \sin\theta$. Noitce $\phi = 2\alpha$ is the phase difference bewteen the rays from the top and bottom of the entire slit.

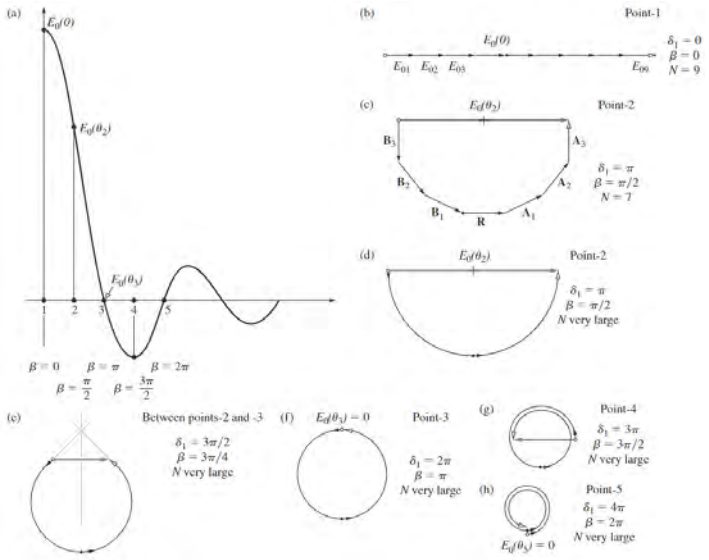

Figure 29: Electric field for single-slit Fraunhofer diffraction. Notice the notation changes $\beta \equiv \alpha$ and $\delta_1 \equiv \phi = 2\alpha$.

As the slit width increases (relative to the wavelength), the width of the central diffraction maximum increases, the relative height o fthe secondary maxima increases, but the width of the secondary maxima decreases.

Finally, the geometric serise of phasors is

$$\begin{aligned}\tilde{E}_\theta =& \frac{E_0}{N} e^{-i\omega t} \sum_{i=1}^{N} e^{ikr_i} \\ =& \frac{E_0 \Delta x}{a} e^{-i\omega t} \sum_{i=1}^{N} e^{ikr_i} \\ =& \lim_{N\to\infty} E_0 e^{-i\omega t} \frac{1}{a} \int_0^a e^{ik(r_1 + x\sin\theta)}\, \mathrm{d}x \\ \sim& \int_0^a e^{ik_x x}\, \mathrm{d}x \sim \int_{-\frac{a}{2}}^{\frac{a}{2}} e^{ik_x x}\, \mathrm{d}x\end{aligned}$$

where $k_x = k \sin\theta$

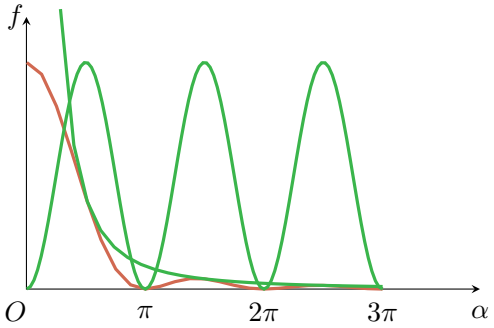

Figure 30: $f(\alpha) = \left(\frac{\sin\alpha}{\alpha}\right)^2$, $\sin\theta_{min} = \frac{m\lambda}{a}$

3. Fourier Methods in Diffraction Theory

3.1 Fourier Transform

The Fourier transform of a one-dimensional function $f(x)$ is defined as

$$F(k_x) = \int_{\infty}^{\infty} f(x) e^{-ik_x x}\,\mathrm{d}x$$

whose inverse transform is

$$f(x) = \frac{1}{2\pi}\int_{\infty}^{\infty} F(k_x) e^{ik_x x}\,\mathrm{d}k_x$$

3.2 The Fourier Method for the Single Slit

Consider the long slit in the y-direction, illuminated by a plane wave. Assuming that there are no phase or amplitude variations across the aperture, the one-dimensional aperture function has the form of a square pulse

$$E_{sq}(x) = \begin{cases} E_0 & |x| \le \frac{a}{2} \\ 0 & |x| > \frac{a}{2} \end{cases}$$

The Fourier transform of $E_{sq}(x)$ is

$$\begin{aligned}
\tilde{E}_{sq}(k_x) =& \frac{1}{a}\int_{-\infty}^{\infty} E_{sq}(x) e^{-ik_x x}\,\mathrm{d}x \\
=& \frac{E_0}{a}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{-ik_x x}\,\mathrm{d}x \\
=& -\frac{E_0}{a}\frac{1}{ik_x}\int_{-\frac{a}{2}}^{\frac{a}{2}} e^{-ik_x x}\,\mathrm{d} - ik_x x \\
=& -\frac{E_0}{a}\frac{1}{ik_x} e^{-ik_x x}\Big|_{-\frac{a}{2}}^{\frac{a}{2}} \\
=& -\frac{E_0}{a}\frac{1}{ik_x}\left(e^{-ik_x\frac{a}{2}} - e^{ik_x\frac{a}{2}}\right) \\
\underline{\underline{\alpha=\frac{a}{2}k_x}}& \frac{E_0}{a}\frac{a}{2}\frac{2i\sin\alpha}{i\alpha} \\
=& E_0\frac{\sin\alpha}{\alpha}
\end{aligned}$$

where $\alpha = \frac{a}{2}k_x = \frac{a}{2}k\sin\theta$.

This leads to the result we have derived

$$I_{sq}(\theta) = I_{max}\left[\frac{\sin\alpha}{\alpha}\right]^2$$

The key message is that the field distribution in the Fraunhofer diffraction pattern is the Fourier transform of the field distribution across the aperture (打到屏幕的光分布是过小孔的光分布的傅里叶变换).

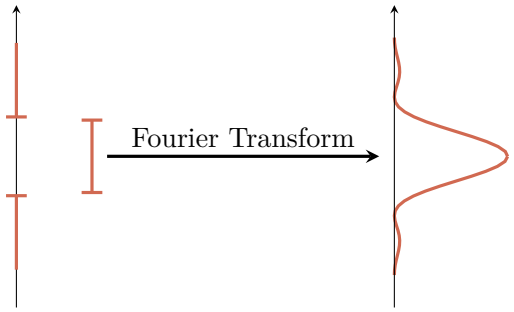

Figure 31: The Fourier Method for the Single Slit

3.3 The Fourier Method for the Double Silt

Consider the double slit with its long side in the y -direction, illuminated by a plane wave. Assuming the one-dimensional aperture function along the x direction has the following form

$$E_{ds}(x) = \begin{cases} 0 & |x| < \frac{d-a}{2} \\ E_0 & \frac{d-a}{2} \le |x| \le \frac{d+a}{2} \\ 0 & |x| > \frac{d+a}{2} \end{cases}$$

The Fourier transform of $E_{ds}(x)$ is

$$\begin{aligned}
\tilde{E}_{ds}(k_x) =& \int_{\infty}^{\infty} E_{ds}(x) e^{-ik_x x}\,\mathrm{d}x \\
=& \int_{-\frac{d+a}{2}}^{-\frac{d-a}{2}} E_0 e^{-ik_x x}\,\mathrm{d}x + \int_{\frac{d-a}{2}}^{\frac{d+a}{2}} E_0 e^{-ik_x x}\,\mathrm{d}x \\
\underline{\underline{x'=x+\frac{d}{2}, x''=x-\frac{d}{2}}}& \int_{-\frac{a}{2}}^{\frac{a}{2}} E_0 e^{-ik_x(-\frac{d}{2}+x')}\,\mathrm{d}x' \\
&+ \int_{-\frac{a}{2}}^{\frac{a}{2}} E_0 e^{-ik_x(\frac{d}{2}+x'')}\,\mathrm{d}x'' \\
=& \left(e^{ik_x\frac{d}{2}} + e^{-ik_x\frac{d}{2}}\right)\int_{-\frac{a}{2}}^{\frac{a}{2}} E_0 e^{-ik_x x'}\,\mathrm{d}x'
\end{aligned}$$

$\left(e^{ik_x\frac{d}{2}} + e^{-ik_x\frac{d}{2}}\right)$ is double-slit interference

$\int_{-\frac{a}{2}}^{\frac{a}{2}} E_0 e^{-ik_x x'}\,\mathrm{d}x'$ is single-slit diffraction

The interference pattern can be understood by a convolution theorem for Fourier transformation: The transform of the convolution of two function is the product of their transforms. ($\mathcal{F}[f\circ g] = \mathcal{F}[f]\times\mathcal{F}[g]$)

The Young's double-slit interference result (with negligible slit width) as the Fourier transform of an aperture

function

$$h(x) = \delta\left(x + \frac{d}{2}\right) + \delta\left(x - \frac{d}{2}\right)$$

$$\begin{aligned}\mathcal{F}[h(x)] =& \int_{-\infty}^{\infty} h(x)e^{-ikx}\,\mathrm{d}x \\ =& e^{ik\frac{d}{2}} + e^{-ik\frac{d}{2}} \\ =& 2\cos\left(k\frac{d}{2}\right)\end{aligned}$$

Notice that

$$\delta(x) = \begin{cases} 1 & x = 0 \\ 0 & otherwise \end{cases}$$

$$f(a) = \int_{-\infty}^{\infty} f(x)\delta(x-a)\,\mathrm{d}x$$

Therefore, we can express the double-slit aperture function and its Fourier transform as

$$\begin{aligned}E_{ds}(x) =& \int_{-\infty}^{\infty} E_{sq}(x')h(x-x')\,\mathrm{d}x' \\ \mathcal{F}\left[E_{ds}(x)\right] =& \mathcal{F}\left[E_{sq}(x)\right]\mathcal{F}\left[h(x)\right]\end{aligned}$$

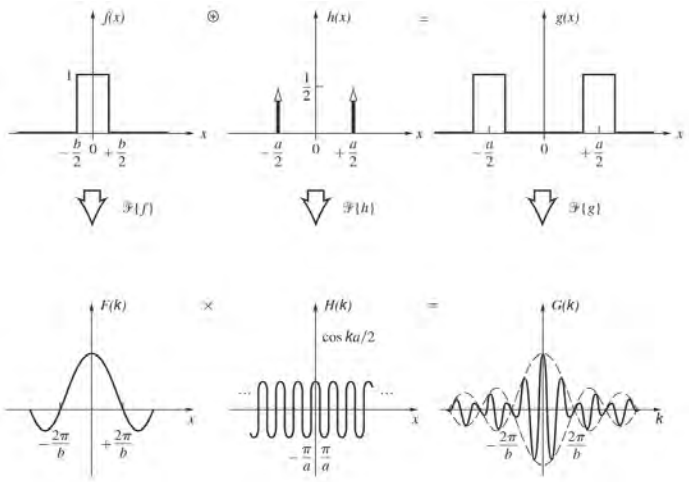

Figure 32: The Fourier Method for the Double Silt

Formally, with diffraction effects taken into account, the intensity of a double-slit interference pattern is

$$\begin{aligned}I(\theta) =& I_0\left(\frac{\sin\alpha}{\alpha}\right)^2\cos^2\beta \\ \beta =& \frac{\delta_2}{2} = \frac{\pi}{\lambda}d\sin\theta \\ \alpha =& \frac{\pi}{\lambda}a\sin\theta\end{aligned}$$

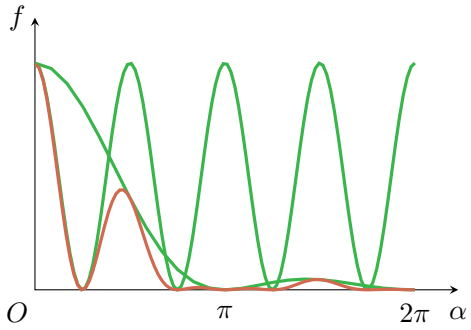

Figure 33: The Fourier Method for the Double Silt

The first minimum occurs where the phase difference between the two slits ($N = 2$) is

$$\delta_2 = \frac{2\pi}{\lambda}d\sin\theta = \pi$$

The first minimum of the envelope occurs where the phase difference between one edge and the center of a single slit is

$$\alpha = \frac{2\pi}{\lambda}\sin\theta = \pi$$

Therefore, one can determine $\frac{d}{a}$ by counting firnges. In both cases, the larger the length (d or a) is, the smaller the θ ($k_x = k \in \theta$) is.

4. Diffraction by a Circular Aperture

Consider diffraction by a circular aperture of diameter d — that is, a circular opening, such as acircular lens, through which light can pass. Theimage is nota point, as geometrical optics would suggest, but a circular disk surrounded by several progressively fainter secondary rings.

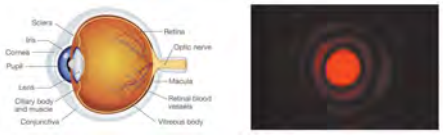

Figure 34: Diffraction by a Circular Aperture

We are essentially collecting only a fraction of the incident wavefront and therefore can't hope to form a perfect image. The image is related to the Fourier transform of a disk and is known as the Airy pattern. The analysis of such patterns shows that the first minimum for the diffraction pattern of a circular aperture of diameter a is located

by

$$\sin\theta = 1.22\frac{\lambda}{a}$$

in contrast to $\sin\theta = \frac{\lambda}{a}$ in the slit case.

The fact that lens images are diffraction patterns is important when we wish to resolve (distinguish) two distant point objects whose angular separation is small. Two objects cannot be distinguished from a single point object, if their diffraction patterns (mainly their central maxima) overlap.

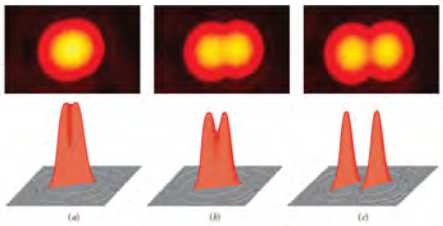

Figure 35: two distant point objects whose angular separation is small

Rayleighs criterion for resolvability states that the two point objects are barely resolved if their angular separation is such that the central maximum of the diffraction pattern of one source is centered on the first minimum of the diffraction pattern of the other, i.e,

$$\theta_R = \sin^{-1}\frac{1.22\lambda}{a} \approx 1.22\frac{\lambda}{a}$$

V Grating and Spectra (光栅与光谱)

1. Diffraction by a Double Slit

1.1 interference vs Diffraction

1) Let $a \to 0$, then $\alpha \to 0$ and $\frac{\sin\alpha}{\alpha} \to 1$, the equation just describes the interference pattern.

2) Let $d \to 0$, then $\beta \to 0$ and $\cos^2\beta \to 1$, the equation just describes the diffraction pattern.

If the combining waves originate from a small number of elementary coherent sources (as in a double-slit experiment with $\alpha \ll \lambda$), we call the process interference.

If the combining waves originate in a single wavefront (as in a single-slit experiment), we call the process diffraction.

2. Diffraction Gratings

in doble-slit interference with $a \ll \lambda$

$$I(\theta) = I_{max}\cos^2\left[\frac{\pi d}{\lambda}\sin\theta\right]$$

The bright fringes due to different wavelengths overlap too much to be distinguished.

A useful tool in the study of light and of objects that emit and absorb light is the diffraction grating, which has a much greater number N of slits, often called rulings (裁定), perhaps as many as several thousand per millimeter.

2.1 Mutiple Slits with Monochromatic Light

With monochromatic light incident on $N = 2 \sim 6$ long narrow slits with slit-separation d, the normalized intensity (irradiance) evolves with sharper and sharper peaks. The phase difference between adjacent slits is

$$\delta_N = \frac{2\pi}{\lambda}\sin\theta$$

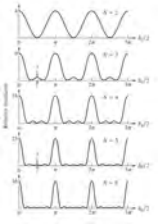

Figure 36: with monochromatic light incident on N = 2 to 6

This case is for $N = 4$

$$\tilde{E}_\theta = E_0 \left(e^{-3i\frac{\delta_4}{2}} + e^{-i\frac{\delta_4}{2}} + e^{i\frac{\delta_4}{2}} + e^{3i\frac{\delta_4}{2}} \right)$$

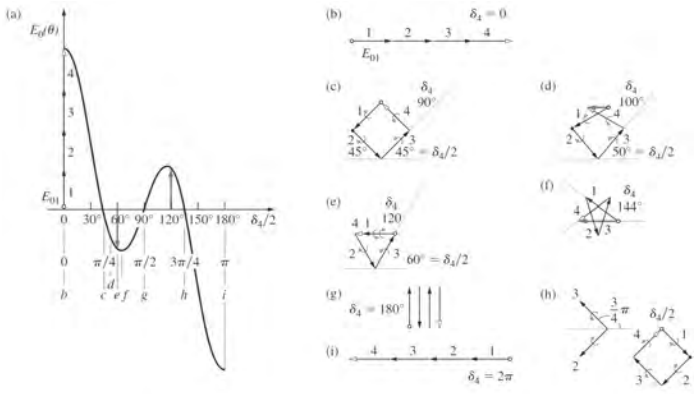

Figure 37: with monochromatic light incident on N = 4

With monochromatic (red) light incident on a diffraction grating (with a large number N), we can see on a viewing screen very narrow (and so are called lines). These lines correspond to

$$\delta_N = \frac{2\pi}{\lambda} \sin\theta = 2\pi m$$
$$\text{or } d\sin\theta = m\lambda$$

They are separated by relatively wide dark regions.

2.2 *Width of the Lines*

A grating's ability to resolve (separate) lines of different wavelengths depends on the linewidth. The half-width of the central line $\Delta\theta_{hw}$ is determined by the first minimum in intensity, at which the N rays from the N slits of the grating cancel one another. The first minimum occurs where the phase difference bewteen the adjacent slits is

$$\delta_N = \frac{2\pi}{\lambda} \sin\Delta\theta_{hw} = \frac{2\pi}{N}$$
$$\text{or } \Delta\theta_{hw} = \frac{\lambda}{Nd}$$

Note that for light of a given wavelength λ and a given ruling separation d, the linewidths decrease with increasing N and so reduce overlap. Therefore, light of several unknown wavelengths can be distinguished and identified by a grating. For example, the light emitted by a hydrogen lamp, which contains hydrogen gas, has four discrete wavelengths in the visble range

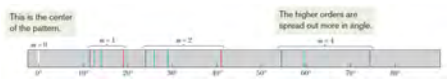

Figure 38: Hydrogen Spectra

2.3 *Atomic Grating*

A crystalline solid, which consists of a regular array of atoms, resembles a diffraction grating with separation d on the atomic scale ($\sim 10^{-10}m$). Waves can be diffracted as if they were reflected by a family of parallel planes, with angles measured relative to the planes (not to a normal as in optics).

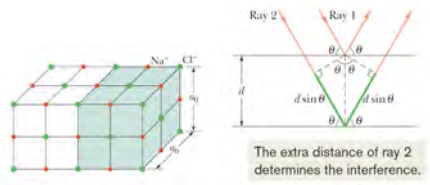

Figure 39: Atomic Grating

Suppose we would like to use the visble light ($\lambda \simeq 5.5 \times 10^{-7}m$) to study the diffraction. The first-order mximum ($m = 1$) would occur at

$$\sin\theta = \frac{m\lambda}{2d} = 2750 \gg 1$$

This means that we wouldn't observe the first-order maxima. Therefore, we need waves with much shorter wavelength ($\lambda \approx d$), that is, X rays.

3. X-Ray Diffraction

X rays are electromagnetic radiation whose wavelengths are of the order of $10^{-10}m$.

When an X-rays beam enters a crystal such as NaCl, X rays are scattered in all directions by the crystal structure. In some directions teh scattered waves unergos destructive interference, resulting in intensity minima; in other directions the interference is constructive, resulting in intensity maxima.

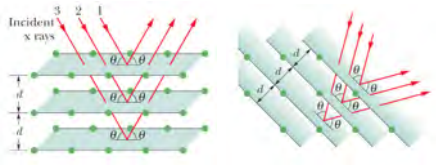

Figure 40: X-Ray Diffraction

The maxima turn out to be in directions as if the X rays were reflected by a family of crystal planes that extend through the atoms within the crystal and that contain regular arrays of the atoms. Bragg's law states that the intensity maxima for X-ray diffraction is

$$2d \sin\theta = m\lambda$$

where $m = 1, 2, 3, ...$ is the order number of an intensity maximum. A monochromatic X-ray beam can be used to determine the geometrical structure of a crystal.

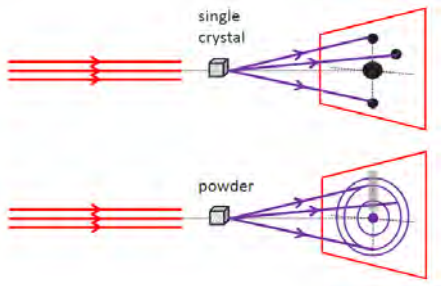

Figure 41: A powder sample contains tens of thousands of randomly oriented crystallites.

VI Polarization

Recall the general solution of electromagnectic waves progating in the z-direction. The oscillating electric field components are generally given by

$$\begin{aligned}\vec{E}: \; E_x(z,t) =& E_{0x}\cos(kz - \omega t + \phi_x)\\ E_y(z,t) =& E_{0y}\cos(kz - \omega t + \phi_y)\\ E_z =& 0\end{aligned}$$

1. Polarization and Mathematical Description

1.1 Polarization

Light is a transverse electromagnectic wave. Tus far we have considered only light for which the orientation of the electric field is constant, although its magnitude and sign vary in time. In general, we can condiser two such harmonic lightwaves of the same frequency, moving through the same region of space, in the same direction $\hat{z}$

$$\begin{aligned}\vec{E}_x(z,t) =& \hat{i}E_{0x}\cos(kz - \omega t)\\ \vec{E}_y(z,t) =& \hat{j}E_{0y}\cos(kz - \omega t + \epsilon)\end{aligned}$$

Linear polarization: If *epsilon* is zero or an integral multiple of $\pm 2\pi$, the resultant wave is

$$\begin{aligned}\vec{E} =& \vec{E}_x + \vec{E}_y\\ =& \left(\hat{i}E_{0x} + \hat{j}E_{0y}\right)\cos(kz - \omega t)\end{aligned}$$

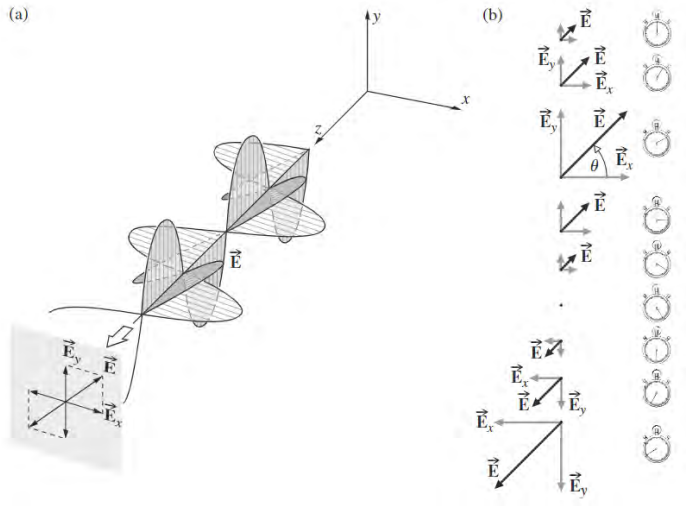

Figure 42: Linear polarization

Circular polarization:

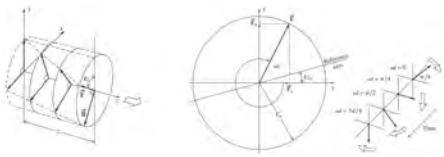

Figure 43: Circular polarization

1) When both constituent waves have equal amplitudes ($E_{0x} = E_{0y} = E_0$) and their relative phase difference $\epsilon = -\frac{\pi}{2} + 2m\pi$, where m is an integer, the resultant wave is

$$\begin{aligned}\vec{E} =& \hat{i}E_0\cos(kz-\omega t) + \hat{j}E_0\cos(kz-\omega t-\frac{\pi}{2})\\ =& E_0\left[\hat{i}\cos(kz-\omega t) + \hat{j}\sin(kz-\omega t)\right]\end{aligned}$$

The resultant $\vec{E}$ is rotating clockwise at an angular frequency of ω, as seen by an observer toward whom the light is moving. This is referred to as right-circular polarized. The $\vec{E}$-vector makes one complete rotation as the wave advances through one wavelength.

2) When their relative phase difference $\epsilon = \frac{\pi}{2} + 2m\pi$, where m is an integer, the resultant wave is

$$\begin{aligned}\vec{E} =& \hat{i}E_0\cos(kz-\omega t) + \hat{j}E_0\cos(kz-\omega t+\frac{\pi}{2})\\ =& E_0\left[\hat{i}\cos(kz-\omega t) - \hat{j}\sin(kz-\omega t)\right]\end{aligned}$$

The amplitudes is unaffected, but $\vec{E}$ now rotates counterclockwise, and the wave is left-circular polarized.

A linearly polarized wave can be synthesized from two oppositely polarized circular waves of equal amplitude.

1.2 A Math Description of Polarization

Written in column and complex form, this Jones vector is

$$\begin{aligned}\vec{E} =& \begin{bmatrix}E_x(t)\\ E_y(t)\end{bmatrix}\\ =& \begin{bmatrix}E_{0x}e^{i(kz-\omega t+\phi_x)}\\ E_{0y}e^{i(kz-\omega t+\phi_y)}\end{bmatrix}\end{aligned}$$

In many applications it is not necessary to know the exact amplitudes and phases. We can rewrite the Jones vector by

$$\tilde{E} = \begin{bmatrix}E_{0x}e^{i\phi_x}\\ E_{0y}e^{i\phi_y}\end{bmatrix}$$

Horizontal and vertical linearly polarized are thus given by

$$|H\rangle = \begin{pmatrix}1\\0\end{pmatrix}$$
$$|V\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

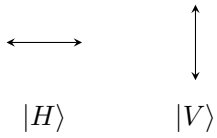

Figure 44: Horizontal and vertical linearly polarized

Linearly polarized at $+45at^\circ$ from the x-axis (diagonal) and at $-45at^\circ$ from the x-axis (anti-diagonal) are given by

$$\begin{aligned}|D\rangle =& \frac{1}{\sqrt{2}}\left(|H\rangle + |V\rangle\right)\\ =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\\ |A\rangle =& \frac{1}{\sqrt{2}}\left(|H\rangle - |V\rangle\right)\\ =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}\end{aligned}$$

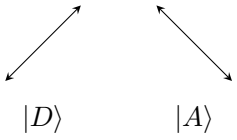

Figure 45: Diagonal and anti-diagonal linearly polarized

Note that we are only interested in polarization, so the vectors are normalized, or in one unit length.

Right-circular light and left-circular light is given by

$$\begin{aligned}|R\rangle =& \frac{1}{\sqrt{2}}\left(|H\rangle - i\,|V\rangle\right)\\ =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}\\ |L\rangle =& \frac{1}{\sqrt{2}}\left(|H\rangle + i\,|V\rangle\right)\\ =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}\end{aligned}$$

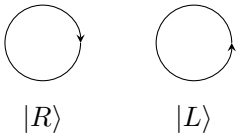

Figure 46: Right-circular light and left-circular light

Note that on interference, we discussed the addition in a two-dimensional real space $\mathbb{R}^2$. The space is also equivalent to a one-dimensional complex space $\mathbb{C}^1$, or a two-component real vector space. Now with polarization, we have generalized the one-dimensional complex space $\mathbb{C}^1$ to a two-dimensional complex space $\mathbb{C}^2 = \mathbb{C}^1 \otimes \mathbb{C}^1$, or a two-component complex vector space (in Jones' vector representation). The additional $\mathbb{C}^1$ space is spanned by the two orthogonal (正交), linearly polarized states $|H\rangle$ and $|V\rangle$.

Two vectors $\vec{A}$ and $\vec{B}$ are said to be orthogonal when $\vec{A} \cdot \vec{B} = 0$, similarly two complex vectors $\vec{A}$ and $\vec{B}$ are said to b orthogonal when $\langle A|\,|B\rangle \equiv \tilde{A}^\dagger \cdot \tilde{B} = 0$. Note that

$$\begin{aligned} |A\rangle =& \tilde{A} \\ \langle A| =& \tilde{A}^\dagger \end{aligned}$$

† means transposed complex conjugation (转置复共轭).

Any polarization state will have a corresponding orthogonal state. Notice that

$$\langle H|\,|V\rangle = \langle D|\,|A\rangle = \langle L|\,|R\rangle = 0$$

As we have seen, any polarization state can be described by a linear combination of the vectors in either one of the orthogonal sets. These same ideas are of considerable importance in quantum mechanics, where deals with orthogonal wave functions.

2. Monochromatic Light and Natural Light

2.1 Monochromatic Light

An idealized monochromatic plane wave must be depicted as an infinite wavetrain. If this disturbance is resolved into two orthogonal components perpendicular to the direction of propagation, they, in turn, must have the same frequency, be infinite in extentm, and therefore be mutually coherent (i.e. $\epsilon = constant$)

$$\begin{aligned} \vec{E}_x(z,t) =& \hat{i} E_{0x} \cos(kz - \omega t) \\ \vec{E}_y(z,t) =& \hat{j} E_{0y} \cos(kz - \omega t + \epsilon) \end{aligned}$$

A perfectly monochromatic plane wave is always polarized.

The most spectacular of all present-day sources is the laser. Under optimum conditions, with temperature variations and vibrations meticulously suppressed, a laser was actually operated at quite close to its theoretical limit of frequency constancy.

2.2 Natural Light

Natural light is composed of a rapidly varying succession ($\sim 10^{-8} s$) of the different polarization states. It is also known as unpolarized or randomly polarized light. We can mathematical represent natural light in terms of two arbitrary, incoherent, orthogonal, linearly polarized waves of equal amplitude (i.e. waves for which the relative phase difference varies rapidly and randomly).

Coherence (相干) is a measure of the correlation bewteen the phases measured at different (temporal and spatial) points on a wave.

1) Temporal coherence is a measure of the correlation of light wave's phase at different points along the direction of propagation — it tells us how monochromatic a source is.

2) Spatial coherence is a measure of the correlation of light wave's phase at different points transverse to the direction of propagation — it tells us how uniform the phase of the wavefront is.

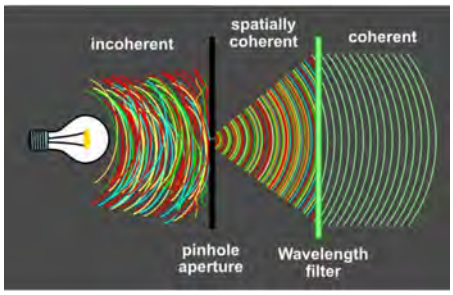

Figure 47: how to prepare a monochromatic wave that is both temporally and spatially coherent from incoherent natural light

In reality, light is generally neither completely polarized nor completely unpolarized. More often, the electric-field vector varies in a way that is neither totally regular nor totally irregular, and such an optical disturbance is

partially polarized. One useful way of describing this behavior is to envision it as the result of the superposition of specific amounts of natural and polarized light.

3. Polarizing Sheets

unpolarized visible light can be transformed into polarized light by sending it through a polarizing sheet, or a polaroid sheet. A polarizing sheet consists of certain long molecules embedded in plastic. When light is then sent through the sheet, the electric field component parallel to the polarizing direction is passed (transmitted); the component perpendicular to it is absorbed.

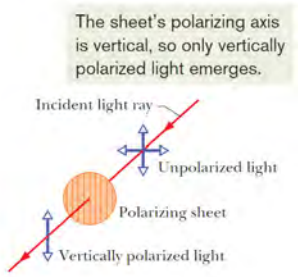

Figure 48: Polarizing Sheets

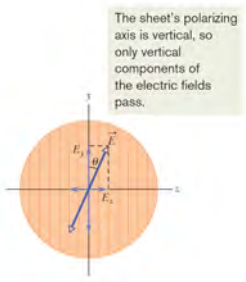

Figure 49: The polarized light emerging from a polarizing sheet

Electric field oscillations of unpolarized light can resolve into two components with equal intensity. Therefore, the intensity I of the polarized light emerging from a polarizing sheet is then half the intensity I_0 of the original light, i.e.

$$I = \frac{I_0}{2}$$

For polarized light, only the component parallel to the polarizing direction of the sheet ($E_y = E\cos\theta$) can be transmitted. Therefore, the intensity of the emerging wave is

$$I = I_0 \cos^2\theta$$

If the polarizing directions are parallel, all the light can pass the sheet. If the polarizing directions are perpendicular, no light can pass the sheet.

4. Polarization by Reflection

One of the most common sources of polarized light is the ubiquitous process of reflection from dielectric media. Consider a ray of unpolarized light incident on a glass surface. The field $\vec{E}$ of the incident light can be decomposed into two components of equal magnitude, one perpendicular and another parallel to the plane of incidence. In general, the reflected light is partially polarized.

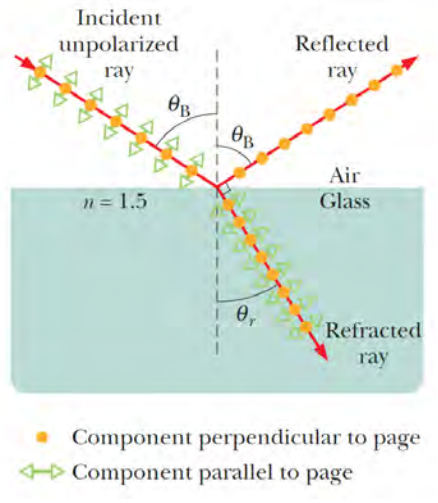

Figure 50: Polarization by Reflection

When the light is incident at a particular incident angle, caleld the Brewster angle θ_B, the reflected light is fully polarized. One finds experimentally that at the incident angle θ_B the reflected and refracted rays are perpendicular to each other:

$$\theta_B + \theta_r = 90^\circ$$

According to Snell's law

$$\begin{aligned} n_i \sin\theta_B &= n_r \sin\theta_r \\ &= n_r \sin(90^\circ - \theta_B) \\ &= n_r \cos\theta_B \end{aligned}$$

or

$$\frac{n_r}{n_i} = \tan\theta_B$$

If the incident and reflected rays travel in air, we can approximate n_i as unity, so

$$n_r = \tan\theta_B$$

VII The Quantum Nature of Light

1. The Photoelectric Effect

Light of frequency f is directed onto target T and ejects electrons from it. A potential difference V is maintained bewteen target T and collector cup C to sweep up these electrons, said to be photoelectrons. This collection produces a photoelectric current i that is measured with meter A.

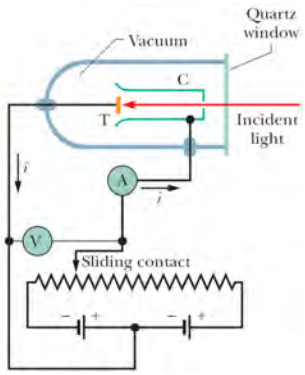

Figure 51: The Photoelectric Effect

Experiments show that if you direct a beam of light of short enough wavelength onto a clean metal surface, the light will eject the electrons from the surface. We adjust the potential difference V by moving the sliding contact so collector C is slightly negative with respect to target T. At the stopping potential $V = V_{stop}$, the readin of meter A has just dropped to zero, the most energetic ejected electrons are turned back just before reaching the collector. Then K_{max}, the kinetic energy of these most energetic electrons, is $k_{max} = eV_{stop}$.

Einstein proposed that electromagnetic radiation or simply light is quantized and exists in elementary amounts (quanta) that we now call photons. According to his proposal, the quantum of a light wave of frequency f has the energy

$$E = hf = \hbar\omega$$

where $h = 2\pi\hbar = 6.63 \times 10^{-34} J \cdot s$ is the Planck constant, and ω is the angular frequency. The total energy of a light wave of frequency f must be an integer multiple of hf, with the smallest amount being hf, the energy of a single photon.

2. Photon, the Quantum of Light

Einstein further proposed that when light is absorbed or emitted by an object (matter), the absorption or emission event occurs in the atoms of the object. In the absorption event, the energy hf of one photon is transferred from the light to the atom; the photon vanishes and the atom is said to absorb it. For an object consisting of many atoms, there can be many photon absorptions (such as with sunglasses) or photon emissions (such as with lamps). In classical physics, such events involve so much light that we had no need of quantum physics.

The electrons within the target are held by electric forces. To just escape from the target, an electron must pick up a certain minimum energy W, where W is a property of the target material called its work function. The energy that can be transferred from the incident light to an electron in the target is that of a single photon hf. According the conservation of energy, the kinetic energy K acquired by the electron satisfies

$$hf = K + W$$

In the most favorable circumstance, the electron can escape through the surface without losing any of this kinetic energy in the process, i.e. $K_{max} = hf - W$. Increasing the light intensity increases the number of photons in the light, not the photon energy, so the energy transferred to the kinetic energy of an electron is also unchanged. If the energy hf transferred to an electron by a photon exceeds the work function of the material (if $hf > W$), the electron can esacpe the target. If the energy transferred doesn't exceed the work function (if $hf < W$), the electron can't escape.

3. Photon Momentum and Compton Scattering

3.1 Photons Have Momentum

A photon, or a light quantum, is a particle with energy $E = hf$. It has a velocity of the speed of light c, but no mass ($m = 0$). Einstein proposed that a quantum of light has linear momentum. According to the theory of relativity

$$
\begin{aligned}
m =& \frac{m_0}{\sqrt{1-\frac{v^2}{c^2}}} \\
E =& mc^2 = \frac{m_0 c^2}{\sqrt{1-\frac{v^2}{c^2}}} \\
p =& mv = \frac{m_0 v}{\sqrt{1-\frac{v^2}{c^2}}} \\
\therefore p =& E\frac{v}{c^2} \\
\therefore E^2 =& \frac{m_0^2 c^4}{1-\frac{p^2c^2}{E^2}} \\
\therefore E^2 - p^2c^2 =& m_0^2 c^4
\end{aligned}
$$

$$\text{Let } E^2 - p^2c^2 = m_0^2c^4 = 0$$

so the magnitude of the photon momentum is

$$
\begin{aligned}
p =& \frac{E}{c} = \frac{hf}{c} \\
=& \frac{h}{\lambda} \\
=& \hbar k
\end{aligned}
$$

3.2 *Compton Scattering*

When a photon interacts with matter, energy and momentum are transferred, as if there were a collision bewteen the photon and matter in the classical sense. To demonstrate, Compton measured the wavelength and intensities of a beam of X rays that were scattered in various directions from a carbon target.

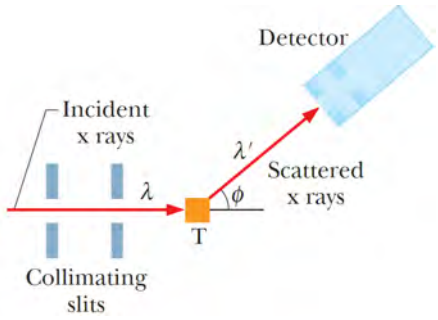

Figure 52: Compton Scattering

Compton found that although there is only a single wavelength ($\lambda = 71.1pm$) in the incident X-ray beam, the scattered X rays contain a range of wavelength with two prominent intensity peaks. One peak is centered about the incident wavelength λ. The other is centered about a wavelength λ' that is longer than λ by an amount $\Delta\lambda$, the Compton shift. The value of the Compton shift varies with the angle at which the scattered X rays are detected and is greater for a greater angle.

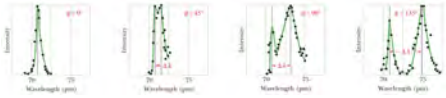

Figure 53: X-ray

In classical physics, an electron in the carbon target undergoes forced oscillations in the sinusoidally oscillating electromagnetic wave. Hence, the electron should send out scattered waves at the same frequency.

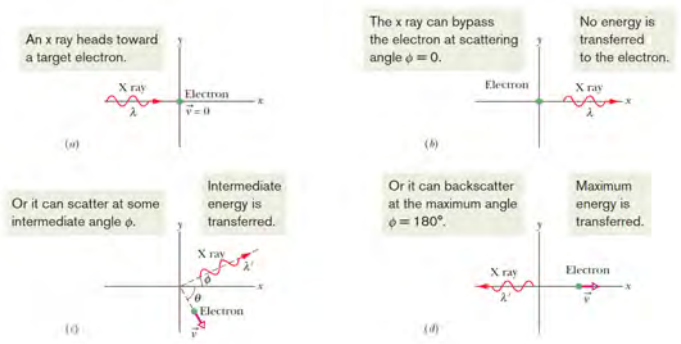

Figure 54: With quantum physics and relativity

With quantum physics and relativity, the energy and momentum conservation becomes

$$\text{Energy: } \frac{hc}{\lambda} + mc^2 = \frac{hc}{\lambda'} + \gamma mc^2$$

$$\text{Momentum: } \begin{cases} \frac{h}{\lambda} = \frac{h}{\lambda'}\cos\phi + \gamma mv\cos\theta & \text{in x} \\ 0 = \frac{h}{\lambda'}\sin\phi + \gamma mv\sin\theta & \text{in y} \end{cases}$$

To solve for $\Delta\lambda$, we rearrange the equations into

$$
\begin{aligned}
\frac{h}{\lambda} - \frac{h}{\lambda'} + mc =& \gamma mc \\
\frac{h}{\lambda} - \frac{h}{\lambda'}\cos\phi =& \gamma mv\cos\theta \\
\frac{h}{\lambda'}\sin\phi =& \gamma mv\sin\theta
\end{aligned}
$$

Take the square of the first equation, subtracting the

squares of the ohter two, we find, after some algebra

$$\begin{aligned}\Delta\lambda =& \frac{h}{mc}(1-\cos\phi)\\ =& \frac{2h}{mc}\sin^2\frac{\phi}{2}\end{aligned}$$

The quantity $\frac{h}{mc}$ is a constant called the Compton wavelength. Its value depends on the mass m of the particle from which the X rays scatter. Strictly speaking, the particle can be a loosely bound electron, or a carbon atom (with tightly bound electrons).

- For an electron, the Compton wavelength is

$$\frac{h}{mc} = \frac{hc}{mc^2} = \frac{12400\,eV\cdot\text{Å}}{511,00\,eV} = 2.426\,pm$$

- For a carbon atom, the Compton wavelength is $12\times 1836 \approx 22,000$ tiems samlled and, hence, can be neglected. Therefore, there is a peak at the incident wavelength at any angle.

4. Angular Momentum of Photons and Polarization

According to the quantum-mechanical description, a photon also has an intrinsic spin angular momentum, which is either $-\hbar$ or $+\hbar$, where the signs indicate right- or left-handedness, respectively. Whenever a charged particle emits or absorbs electromagnetic radiation, along with changes in its energy and linear momentum, it will undergo a change of $\pm\hbar$ in its angular momentum. The energy transferred to a target by an incident monocromatic electromagnetic wave can be envisaged as being transported in the form of a stream of identical photons. A purely left-circularly (right-circularly) polarized plane wave will impart angular momentum to the target as if all the constituent photons in the bem had their spins aligned in (opposite) the direction of propagation.

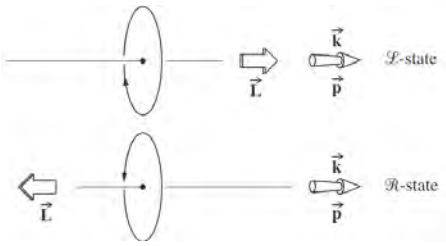

Figure 55: Angular Momentum of Photons

A beam of linearly polarized light will interact with matter as if it were composed, at that instant, of equal numbers of right- and left-handed photons. There is a subtle point. Strictly speaking, we can't say that th beam is actually made up of precisely equal amounts of well-defined right- and left-handed photons; the photons are all identical. Rather, each individual photon exists in either spin state with equal likelihood.

$$|H\rangle = \frac{|R\rangle + |L\rangle}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} + \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}\right]$$

This probabilistic interpretation also applies to diagonally polarized light

$$\begin{aligned}|D\rangle =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{|H\rangle + |V\rangle}{\sqrt{2}}\\ |A\rangle =& \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{|H\rangle - |V\rangle}{\sqrt{2}}\end{aligned}$$

Or inversely,

$$\begin{aligned}|H\rangle =& \frac{|D\rangle + |A\rangle}{\sqrt{2}}\\ |V\rangle =& \frac{|D\rangle - |A\rangle}{\sqrt{2}}\end{aligned}$$

VIII Matter Waves

1. Mystery of the Light Wave

1.1 A Fundamental Mystery

How light can be a wave (which spreads out over a region) in classical physics but be emitted and absorbed as photons (which originate and vanish at points) in quantum physics?

1.2 Light as a Probability Wave

Double-slit experiments tell us

1) Light is generated in the source as photons,
2) absorbed in the detector as photons, and
3) travels bewteen source and detector as a probability wave.

The probability density of detecting a photon at some point P in space depends on the irradiance $I \propto E_0^2$ at that point. Thus, the net E_0 at P can be interpreted as the probability amplitude. To go further, one will need quantum electrodynamics(QED), the quantum theory of the interaction of light and matter.

2. Electrons and Matter Waves

2.1 De Broglie Hypothesis

A beam of light is a wave, but it transfers energy and momentum to matter only at points, via photons. Electron is a particle with energy and momentum. We can think of a beam of moving electron — or any other particle — as a matter wave. De Broglie proposed that one could assign a wavelength λ to a particle with momentum of magnitude p. Like that of photons, we define

$$\begin{aligned}\lambda =& \frac{h}{p} \\ =& \frac{h}{mv} = \frac{h}{m_0 v}\sqrt{1-\frac{v^2}{c^2}}\end{aligned}$$

When $v \ll c$, $\lambda = \dfrac{h}{m_0 v}$

which is known as the de Broglie wavelength of the moving particle.

2.2 Electron Diffraction

Both X rays and electrons are waves.

2.3 The Interference of Electrons

In a more recent experiment, an interference pattern was built up when electrons were sent, one by one, through a double-slit apparatus. When an electron hit the viewing screen, it caused a flash of light whose position was recorded. Repeat the experiment at such low intensity that at any given time there is just one particle in the interference region.

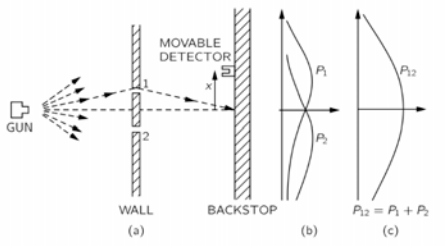

Figure 56: Newtonian Physics

In Newtonian physics, a particle is only aware of the slit through which it goes, it has no idea how many other slits are open or closed or even exist. Therefore, when both slits are open, $P_{12} = P_1 + P_2$.

2.4 Matter Wave

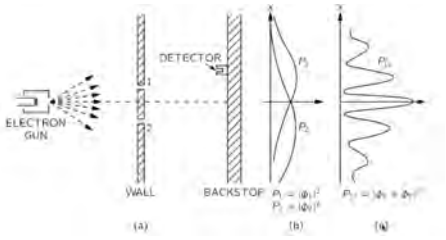

Figure 57: Matter Wave

The electrons arrive in lumps, like particles, and the probability of arrival of these lumps is distributed like the distribution of intensity of a wave.

It is in this sense that an electron behaves sometimes like a particle and sometimes like a wave. Our rescue, of course, come from optics, where light or photons also interfere. There, we need to add amplitude A, rather than intensity $|A|^2$. Similarly here, the experimental observation forces us to introduce the probability amplitude ψ which is a complex number. The probability of an event in an ideal experiment is then given by $|\psi|^2 = \psi * \psi$.

When an event can occur in several alternative ways, the probability amplitude for the event is the sum of the probability amplitudes for each way considered separately.

$$\psi = \psi_1 + \psi_2 + \cdots$$

The probability for the event is,

$$P = |\psi|^2 = |\psi_1|^2 + |\psi_2|^2 + 2\Re(\psi_1^\dagger \psi_2) + \cdots$$

The interference term $2\Re(\psi_1^\dagger \psi_2)$ is responsible for the rapid oscillations in the experiment.

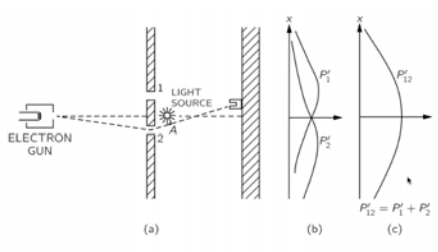

Figure 58: The Which-Way Experiment

Not weird enough? Now, if an experiment is performed which is capable of determining whether one or another alternative is actually taken, the interference is lost. The experiment tells us that the probability of the event in the which-way experiment is the sum of the probabilities for each alternative,

$$P = |\psi|^2 = |\psi_1|^2 + |\psi_2|^2$$

just as what happens in the classical case. Thus an electron acts like it went through one particular slit if we see it doing that and acts like it did not have a specific path (through a specific slit) when it is not seen.

To see an electron with a resolution comparable to slit separation d, (so we know which slit it took) requires light with $\lambda < d$, this is just standard wave theory. But, the light is made of photons each with momentum $p > \frac{h}{d}$. So measuring the position of the electron has made us disturb its momentum. The amount of momentum transferred to the electron in the act of observation is indefinite.This is a manifestation of Heisenberg's uncertainty principle, which says you cannot measure the momentum and coordinate of a particle simultaneously to arbitrary accuracy.

3. Heisenberg's Uncertainty Principle

The probabilistic nature of quantum physics places an important limitation on detecting a particle's position and momentum. That is, it is not possible to measure the position $\vec{r}$ and the momentum $\vec{p}$ of a particle simultaneously with unlimited precision. The uncertainties in the components of these quantities are given by

$$\Delta x \cdot \Delta p_x \geq \hbar$$
$$\Delta y \cdot \Delta p_y \geq \hbar$$
$$\Delta z \cdot \Delta p_z \geq \hbar$$

They are due to the fact that electrons and other particles are matter waves and that repeated measurements of their positions and momenta involve probabilities, not certainties. In the statistics of such measurements, we can view, say, Δx and Δp_x as the spread (actually, the standard deviations) in the measurements. Couldn't we very precisely measure p_x and then next very precisely measure x wherever the electron happens to show up? Doesn't that mean that we have measured both p_x and x simultaneously and very precisely? No, the flaw is that although the first measurement can give us a precise value for p_x , the second measurement necessarily alters that value.

What form does the electron wave function have? The naive guess could be sin kx , or cos kx . But they have spatial variance that is inconsistent with our intuition. To represent the electron by a wave, we need a function, which is called wave function, with a wavelength $\lambda = \frac{2\pi}{k}$, but its square should not show any variation in x, i.e.

$$\psi(x) = e^{i(kx - \omega t)}$$

If we measure p_x now, we obtain $p_x = \hbar k$ without uncertainty, but the particle exists anywhere with the same probability, $\Delta x = \infty$.

If we measure x then, we will find the electron somewhere at x_0. Once we find it, it can't be elsewhere. So the wave function suddenly collapses to

$$\psi(x) = \delta(x - x_0)$$

Now, the Fourier transform of the δ-function tells us

$$\bar{\psi}(p) = \mathcal{F}(\psi(x)) = constant$$

In this case, $\Delta x = 0$ but $\Delta p = \infty$.

The major significance of the wave-particle duality is that all behavior of light and matter can be explained through the use of a complex wave function $\psi(x, y, z, t)$. The probability of finding a particle somewhere at a particular time is proportional to

$$P(x, y, z, t) = \psi^\dagger(x, y, z, t)\psi(x, y, z, t)$$

It turns out that the wave function satisfies a differential equation, known as Schroedinger's equation.

IX Schroedinger' s Equation

A classical wave $\psi(x, y, z, t)$ satisfies the wave equation

$$\frac{1}{v^2}\frac{\partial^2\psi}{\partial t^2} = \nabla^2\psi$$

In the quantum theroy, a microscopic particle i described by a probability amplitude $\psi(x, y, z, t)$, and the probability of finding it is proportional to

$$P(x, y, z, t) = |\psi(x, y, z, t)|^2$$

1. Schroedinger' s Equation

1.1 Classical Particle

Let us start with a pedagogical discussion on how to write down an equation that governs the quantum behavior of a free particle of mass m represented by a wave

$$\psi(x, t) = e^{i(kx-\omega t)}$$

For a free classical one-dimensional particle, on the other hand, the energy is

$$E = \frac{p^2}{2m}$$

According to the de Broglie's hypothesis, we expect

$$\begin{aligned} p =& \frac{h}{\lambda} = \hbar k = -i\hbar\frac{1}{\psi(x,t)}\frac{\partial\psi(x,t)}{\partial x} \\ p^2 =& -\hbar^2\frac{1}{\psi(x,t)}\frac{\partial^2\psi(x,t)}{\partial x^2} \end{aligned}$$

Similarly, we expect

$$E = h\nu = \hbar\omega = i\hbar\frac{1}{\psi(x,t)}\frac{\partial\psi(x,t)}{\partial x}$$

So using wave function, the energy-momentum relation is

$$i\hbar\frac{1}{\psi(x,t)}\frac{\partial\psi(x,t)}{\partial x} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x,t)}\frac{\partial^2\psi(x,t)}{\partial x^2}$$

In the presence of potential, e.g. a harmonic potential $U(x) = \frac{ax^2}{2}$, the classical relation is modified to

$$E = \frac{p^2}{2m} + U(x)$$

where E is a constant of motion, but p is not. In the other words, a plane wave is not a solution any more.

1.2 Schroedinger' s Equation

Schroedinger proposedthat the wave function $\psi(x,t)$ of a single particle moving around in 1D satisfies

$$i\hbar\frac{\partial\psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + U(x,t)\psi(x,t)$$

where $U(x,t)$ is the potential energy of the particle and m is the mass of the particle.

We can easily generalize it to higher dimensions. Note that Schroedinger' s equation is a postulate of quantum mechanics, not derived from classical physics.

In most cases we discuss, the potential energy $U = U(x)$ is independent of time.

We can solve the Schroedinger equation by an ansatz $\psi(x,t) = \phi(x)e^{-iEt/\hbar}$. The wave function $\phi(x)$ satisfies

$$\frac{\partial^2\phi(x)}{\partial x^2} + \frac{2m}{\hbar^2}[E - U(x)]\phi(x) = 0$$

The particular solutions are e^{ikx} and e^{-ikx}, the general solution is the linear combination of two particular solutions. In free space, $U(x) = 0$. The general solution is

$$\phi(x) = Ae^{ikx} + B^{-ikx}$$

where A and B are constants and $k = \sqrt{2mE}/\hbar$.

The complete time-dependent wave function is

$$\psi(x,t) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

where $\omega = E/\hbar$. The two terms correspond to right- and left-moving waves, respectively.

Consider the right-moving wave $\psi(x,t) = Ae^{i(kx-\omega t)}$, the probability density is

$$|\psi(x,t)|^2 = \psi^\dagger(x,t)\psi(x,t) = |A|^2$$

That means that if we make a measurement to locate the particle, the location could turn out t be at any x value.

2. Reflection from a Potential Step

Consider a beam of nonrelativistic electrons, each o ftotal energy E, along an x axis through a narrow tube. They experience a negative electric potential step of height $V_b < 0$ at $x = 0$.

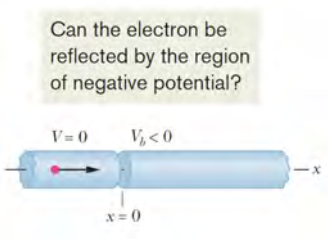

Figure 59: a beam of nonrelativistic electrons through a narrow tube

We consider the situation where $E > qV_b$. Classically, electrons should all pass through the boundary. Their total energy should be conserved, so their kinetic energy, hence speed, decreases when their potential energy increases.

But in quantum mechanically, we apply Schroedinger's equation to the two regions separately. The wave function should be consistent with each other at $x = 0$, both in value and in slope (boundary conditions).

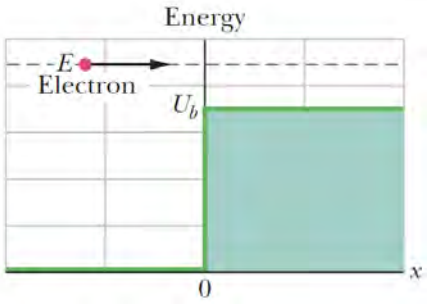

Figure 60: the two regions

- Region 1 ($x < 0$): $k = \sqrt{2mE}/\hbar$

$$\psi_1 = Ae^{ikx} + Be^{-ikx}$$

- Region 2 ($x > 0$): $k_b = \sqrt{2m(E - qV_b)}/\hbar$

$$\psi_2 = Ce^{ik_bx} + De^{-ik_bx}$$

We can first set $D = 0$, because there is no electron source off to the right, and there can be no electrons moving to the left in region 2. We now consider boundary conditions at $x = 0$:

$$A + B = C \text{ (matching of values)}$$
$$Ak - Bk = Ck_b \text{ (matching of slopes)}$$

We should be able to solve B/A and C/A, but not A, B and C. Note that the absolute values are not important for our purpose (it can be related to the beam intensities, though).

2.1 Reflection and Transmission Coefficients

Indeed, to find the probability that electrons reflect from the step, we need to relate the probability density of the reflected wave (Be^{-ikx}) to that of the incident wave (Ae^{ikx}). We thus define a reflection coefficient R:

$$R = \frac{|B|^2}{|A|^2} = \left|\frac{k-k_b}{k+k_b}\right|^2$$

Quantum mechanically, electrons are reflected from the boundary, but only with a probability.

Similarly, the transmission coefficient (the probability of transmission) is

$$T = 1 - R = \frac{4kk_b}{|k+k_b|^2}$$

What inspires us to define T in this way? Well, one can consider an alternative quantity

$$\frac{|C|^2}{|A|^2} = \frac{4k^2}{|k+k_b|^2} = T\frac{k}{k_b}$$

Recall current density $J = nqv$. Not surprisingly, one finds

$$T = \frac{|C|^2 k_b}{|A|^2 k} = \frac{|C|^2 q(\hbar k_b/m)}{|A|^2 q(\hbar k/m)} = \frac{J_{transmitted}}{J_{incident}}$$

One can also write

$$R = \frac{J_{reflected}}{J_{incident}}$$

Therefore, $T = 1 - R$ is nothing but the conservation of current

$$J_{transmitted} = J_{incident} - J_{reflected}$$

3. Tunneling through a Potential Barrier

Now consider a potential energy barrier, which is a region of thickness L where the electric potential is $V_b(< 0)$ and the height is $U_b(= qV_b)$.

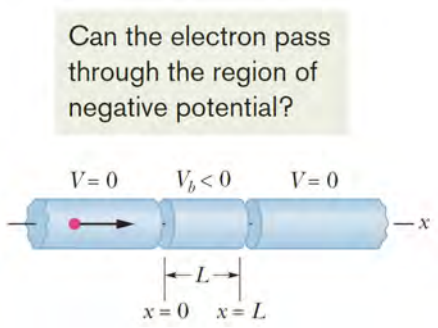

Figure 61: Tunneling through a Potential Barrier

We consider the situtaion where $E < qV_b$. Classically, electrons are forbidden in the barrier region, hence all reflected. However, a matter wave, has a finite probability of leaking (or, better, tunneling) through the barrier and materializing on the other side.

We are interested in the probability of the electron appearing on the other side of the barrier. Thus, we want the transmission coefficient T. The general procedure is the following.

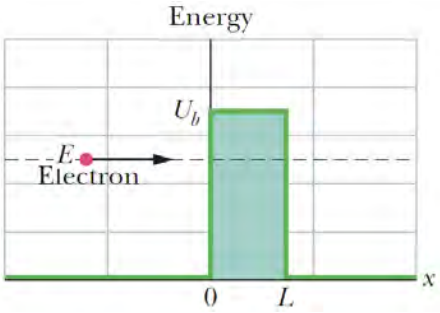

Figure 62: three regions

1) Separate the space into three regions and solve Schroedinger's equation in each region ($3 \times 2 - 1 = 5$ unknowns).

2) Apply boundary conditions at the two boundaries ($2 \times 2 = 4$ equations).

3) Calculate the tunneling coefficient.

We shall just examine the general results.

1) The oscillating curve to the left of the barrier (for $x < 0$) is a combination of the incident matter wave and the reflected matter wave (which has a smaller amplitude than the incident wave). The oscillation occur because these two waves, traveling in opposite di-

rections, interfere with each other, setting up a standing wave pattern.

2) Within the barrier (for $0 < x < L$) the probability density decreases exponentially with x. However, if L is small, the probability density is not quite zero at $x = L$.

3) To the right of the barrier (for $x > L$), the probability density plot describes a transmitted wave (through the barrier) with low but constant amplitude.

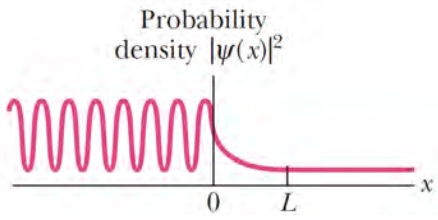

Figure 63: the general results

We can assign a transmission coefficient T to the incident matter wave and the barrier. The transmission coefficient T is approximately

$$T \approx e^{-2kL}$$

$$\text{where } k = \frac{\sqrt{2m(qV_b - E)}}{\hbar}$$

The exact result can be obtained for any $U_b (= qV_b)$ and L.

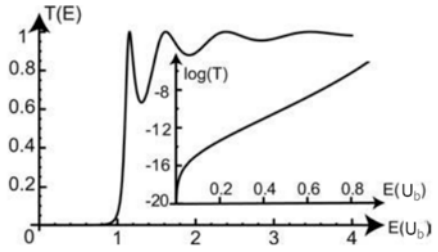

Figure 64: T and U_b

In general, we speak of tunneling if $E < U_b$. In this regime, $T(E)$ increases approximately exponentially with energy, as shown in the inset. For $E \gg U_b$, $T(E) = 1$ as expected classically.

4. Scanning Tunneling Microscope (STM)

The size of details that can be seen in an optical microscope is limited by the wavelength of the light the microscope uses (about 300 nm for ultraviolet light). We use electron matter waves (tunneling through potential barriers) to create images on the atomic scale. A fine metallic tip, mounted on quartz rods, is placed close to the surface to be examined. The space between the surface and the tip forms a potential energy barrier.

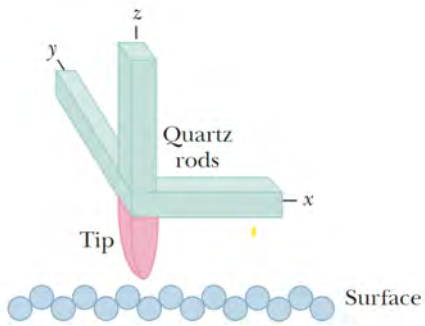

Figure 65: Scanning Tunneling Microscope

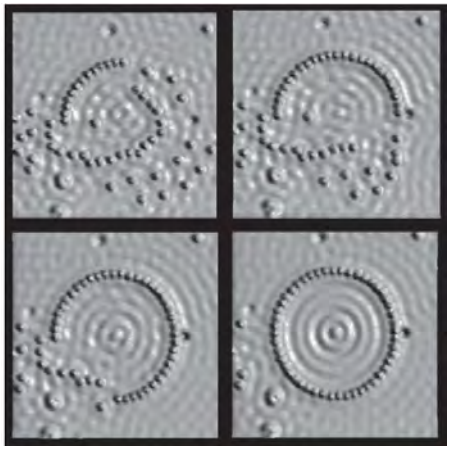

Figure 66: An STM not only can provide an image of a static surface, it can also be used to manipulate atoms and molecules on a surface.

5. Wave Packets

What is the speed of a free quantum mechanical particle? The general solution of the particle is

$$\psi(x) = Ae^{ikx} + Be^{-ikx},\ k = \sqrt{2mE}/\hbar$$

or with standard time dependence, $e^{-i\omega t}$, $\omega = E/\hbar$

$$\psi(x,t) = Ae^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}$$

The formula represents a right- and a left-moving wave with speed (of the wavefront)

$$v_{qh} = \frac{\omega}{k} = \frac{E}{k\hbar} = \sqrt{\frac{E}{2m}}$$

On the other hand, the classical speed of a free particle with energy E is given by

$$v_{cl} = \sqrt{\frac{2E}{m}} = 2v_{qh}$$

There are some Problems:

1) The quantum mechanical wave function travels at half the speed of the particle it is sipposed to represent.

2) How to normalize the wave function of the free particle, say, represented by Ae^{ikx}?

$$\int_{\infty}^{\infty} |\psi(x)|^2 \, \mathrm{d}x = |A|^2 \int_{\infty}^{\infty} 1 \, \mathrm{d}x = |A|^2 \infty$$

This wave function is not normalizable.

Apparently, the stationary (separable) solution don't represent physically realizable states; there is no such thing as a free particle with a definite energy.

In quantum theory, a localized particle is modeled by a linear superposition of these stationary free-particle (or plane-wave) states.

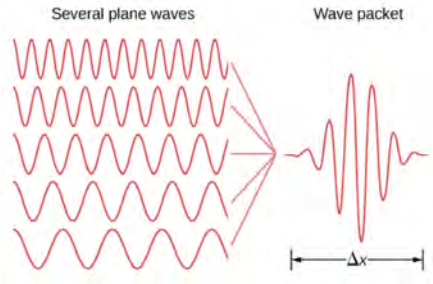

Figure 67: a localized particle

In general, we can construct a linear combination (integral over continuous k)

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{\infty}^{\infty} \phi(k) e^{i(kx-\omega t)} \, \mathrm{d}k$$

This wave function can be normalized for appropriate $\phi(k)$. We call it a wave packet, which carries a range of k and, hence, a range of energies and speeds. In a general quantum problem, we are given $\Psi(x,0)$ and needed to find $\Psi(x,0)$. The particle can be better localized (Δx can be decreased) if more plane-wave states of different wavelengths or momenta are added together in the right way (Δp is increased). According to Heisenberg, these uncertainties obey

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

It turns out that the group velocity of the wave packet, not the phase velocity of the stationary states, matches the classical particle velocity.

X Quantum Wells

Traveling Waves vs Standing Waves

On a stretched string we can set up both traveling waves and standing waves.

- A traveling wave, on a long string, can have any frequency.
- A standing wave, set up on a string with a finite length, can have only discrete frequencies.

In other words, confining the wave to a finite region of space leads to quantization of the motion — to the existence of discrete states for the wave, each state with a sharply defined frequency.

This observation appllies to waves of all kinds, including matter waves. For matter waves, however, it is more convenient to deal with the energy E of the associated particle than the frequency f of the wave.

Consider the matter wave associated with an electron moving in the positive x direction and subject to no net force — a so-called free particle. The energe of such an electron can have any reasonable value, just as a wave traveling along a stretched string of infinite length can have any reasonable frequency.

Consider next the matter wave associated with an atomic electron, perhaps the valence (least tightly bound) electron. The electron — held within the atom by the attractive Coulomb force bewteen it and the positively charger nucleus — is a bound particle. It can exist only in a set of discrete states, each having a discrete energy E. This sounds much like the discrete states and quantized frequencies that apply to a stretched string of finite length.

For matter waves, then, as for all other kinds of waves, wa may state a confinement principle: Confinement of a wave leads to quantization — that is, to the existence of discrete states with discrete energies.

1. An Electron in an Infinite Potential Well

1.1 One-Dimensional Infinite Potential Well

Consider a nonrelativistic electron confined to a one-dimensional electron trap (or a limited region of space).

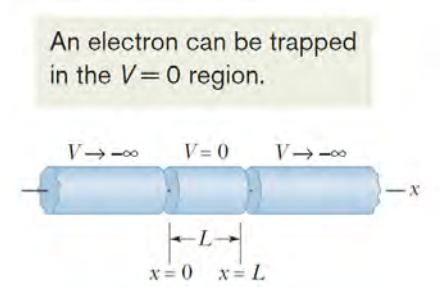

Figure 68: One-Dimensional Infinite Potential Well

The trap consists of two semi-infinitely long cylinders, each of which has an electric potential approaching $-\infty$; bewteen them is a hollow cylinders of length L, which has an electric potential of zero. We put a single electron into this central cylinder to trap it.

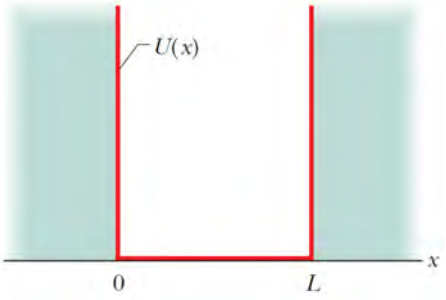

Figure 69: 1D Trap

When the electron is in the central cylinder, its potential energy $U = -eV$ is zero. If the electron couldn't get out of this region, its potential energy would be positively infinite outside. It is a potential "well" because an electron placed in the central cylinder cann't escape from it.

1.2 Standing Waves in a 1D Trap

We examine by analogy with standing waves on a string of finite length, stretched along an x axis and confined bewteen rigid supports. Because the supports are rigid, the two ends of the string are nodes, or points at which the string is always at rest. The states, or discrete standing wave patterns in which the string can oscillate, are those for which the length L of the string is equal to an integer number of half-wavelengths; that is, the string can occupy only states for which

$$L = \frac{n\lambda}{2} \text{ for } n = 1, 2, 3, ...$$

Each value of the integer n identifies a state of the oscillating string.

For a given n, the transverse displacement of the string at any position x along the string is given by

$$y_n(x) = A \sin\left(\frac{n\pi}{L}x\right)$$

where A is the amplitude of the standing wave. For the electron in the trap, we promote the transverse displacement to wave function $\psi_n(x)$.

1.3 Probability of Detection

Classically, we expect to detect the electron anywhere in the infinite well with a constant probability density. Quantum mechanically, we find the probability density

$$P_n(x) = |\psi_n(x)|^2 = |A|^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

for a given n. The constant A (up to a phase) can be determined by the normalization condition

$$\int_{-\infty}^{\infty} |\psi_n(x)|^2 \, \mathrm{d}x = \int_0^L |\psi_n(x)|^2 \, \mathrm{d}x = 1$$

so $A = \sqrt{\frac{2}{L}}$

1.4 Energies of the Trapped Electron

The de Broglie wavelength λ of the electron is defined as

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mK}} = \frac{2L}{n}$$

where $K = \frac{p^2}{2m}$ is the kinetic energy of the nonrelativistic electron.

For an electron moving within the central cylinder, where $U = 0$, the total (mechanical) energy E is equal to the kinetic energy K. Thereforce, the tota energy for an electron moving in the central cylinder is

$$E_n = \frac{h^2}{8mL^2}n^2$$

for $n = 1, 2, 3, \ldots$.

The positive integer n here is the quantum number of the electron quantum state in the trap. The quantum state with the lowest possible energy level E_1 with quantum number $n = 1$ is called the ground state of the electron.

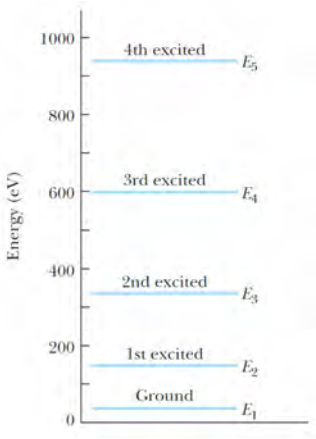

Figure 70: the total energy for an electron moving in the central cylinder

Why is $n = 0$ not allowed? Choosing $n = 0$ would indeed yield a lower energy of zero. However, as we will see below the corresponding probability density is $|\psi| = 0$, which we can interpret only to mean that there is no electron in the well; so $n = 0$ is not a possible quantum number. It is an important conclusion of quantum physics that confined systems must always have a certain minimum energy called the zero-point energy.

Electrons can be excited or de-excited by the absorption or emission of a photon with energy

$$\hbar\omega = \frac{hc}{\lambda} = \Delta E = E_{high} - E_{low}$$

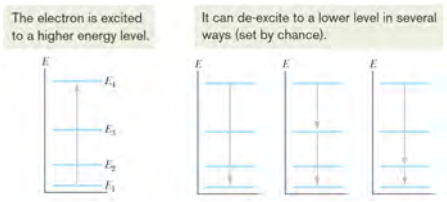

Figure 71: excited and de-excited

1.5 Wave Function of the Trapped Electron

If we solve Schroedinger's equation, for an electron trapped in the 1D infinite well of width L, we could write the solutions as

$$\psi_n(x) = e^{ikx}$$
$$\text{or } \psi_n(x) = e^{-ikx}$$
$$k = \frac{2\pi}{\lambda} = \frac{n\pi}{L}$$

However, the traveling waves don't satisfy the boundary conditions

$$\psi_n(0) = \psi_n(L) = 0$$

The appropriated solutions can only be certain linear combinations of the traveling wave functions, given by

$$\psi_n(x) = A\sin(kx)$$

for $0 \leq x \leq L$. The constant A is to be determined. Note that the wave functions $\psi_n(x)$ have the same form as the displacement functions $y_n(x)$ for a standing wave on a string stretched bewteen rigid supports.

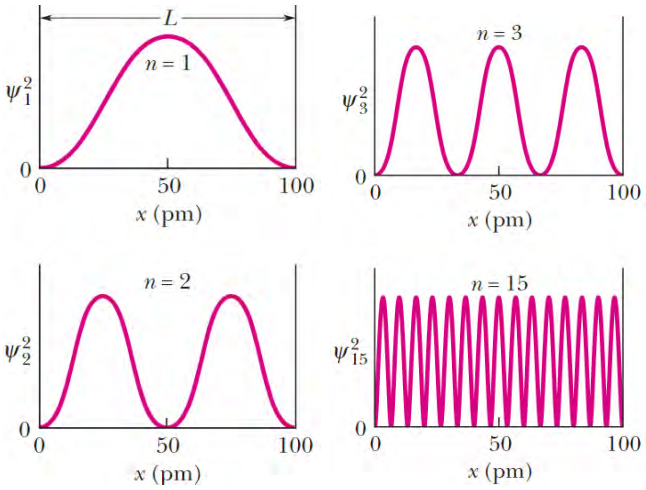

Figure 72: The probability density for n=1,2,3,15

For sufficiently large n, the probability of detection becomes more and more uniform across the well. This result is an instance of a general principle called the correspondence principle: At large enough quantum numbers, the predictions quantum physics merge smoothly with those of classical physics.

2. An Electron in a Finite Potential Well

We can picture an electron trapped in a one-dimensional well between infinite-potential walls as being a standing matter wave. The solutions must be zero at the infinite walls. For finite walls, however, the analogy bewteen waves on a stretched string and matter waves fails. Matter wave nodes no longer exist at $x = 0$ and at $x = L$; wave function can penetrate the walls into classically forbidden regions.

To find the wave function describing the quantum states of an electron in a finite well, we must resort to the time-independent Schroedinger's equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x)$$

Rather than solving this equation for the finite well, much alike what we did in the case of a potential barrier, we proceed with a qualitative discussions.

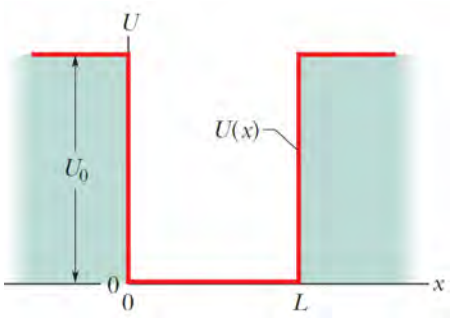

Figure 73: An Electron in a Finite Potential Well

2.1 Wave Functions of the Trapped Electron

As in the tunneling problem, the matter wave "leaks" into the walls of a finite potential energy well; the leakage is greater for greater value of quantum number n. As a result, the wavelength λ for any given quantum state is greater when teh electron is trapped in a finite well than when it is trapped in an infinite well of the same length L.

2.2 Energies of the Trapped Electron

Thus, the corresponding energy $E = \frac{\frac{h}{\lambda}^2}{2m}$ for an electron in any given state is less in the finite well than in the infinite well. An electrons with an energy greater than the well depth has too much energy to be trapped in the finite well. Thus, there is a continuum of energies beyond the top of the well; a high-energy electron is not confined, and its energy isn't quantized.

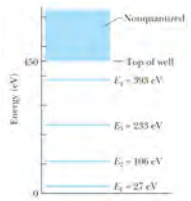

Figure 74: an electron in the finite well

3. High Dimensional Electron Traps

3.1 Schroedinger's Equation in High Dimensions

Assuming $U = 0$. We can generalize Schroedinger's equation to 2D (and similarly to 3D) as

$$E\Psi(x,y) = -\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\Psi(x,y)$$

We are interested in a family of wave functions $\Psi(x,y) = X(x)Y(y)$, whose Schroedinger's equation is equivalent to

$$E = -\frac{\hbar^2}{2m}\frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} - \frac{\hbar^2}{2m}\frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2}$$

This has the form $E = F(x) + G(y)$, which can only be satisfied when $F(x) = E_1$ and $G(y) = E - E_1$, i.e. each function must separately be a constant. As a consequence, separation of variables breaks the multivariate partial differential equation into a set of independent ordinary differential equations (ODEs). We can solve the ODEs for $X(x)$ and $Y(y)$. The wave function for the original equation is simply their product $X(x)Y(y)$. Success requires choice of an appropriate coordinate system and may not be attainable at all depending on the equation.

3.2 2D & 3D Infinite Potential Wells

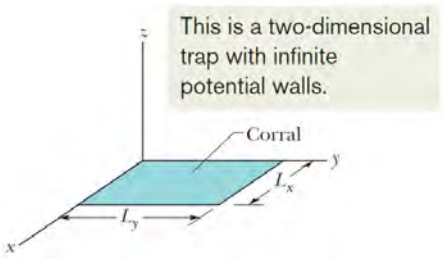

Figure 75: 2D infinite potential well

Consider a 2D infinite potential well of widths L_x and L_y (e.g. for an electron on a surface). The normalized wave function are

$$\begin{aligned}\psi_n(x,y) =& \frac{2}{\sqrt{L_x L_y}}\sin(k_x x)\sin(k_y y)\\ k_x =& \frac{2\pi}{\lambda_x} = \frac{n_x\pi}{L_x}\\ k_y =& \frac{2\pi}{\lambda_y} = \frac{n_y\pi}{L_y}\end{aligned}$$

with two quantum numbers n_x and n_y, and the corresponding energies are

$$E_{n_x,n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right)$$

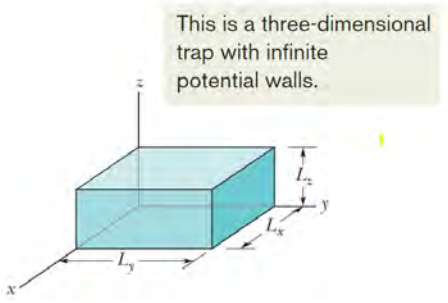

Figure 76: a 3D infinite potential well

An electrons can also be trapped in a 3D infinite potential well with a volume $V = L_x L_y L_z$. Now a trapped electron has three quantum numbers n_x, n_y abd n_z. The normalized wave function and their energies are

$$\begin{aligned}\psi_n(x,y,z) =& \sqrt{\frac{8}{V}}\sin(k_x x)\sin(k_z z)\sin(k_z z)\\ k_x =& \frac{n_x\pi}{L_x},\ k_y = \frac{n_y\pi}{L_y},\ k_z = \frac{n_z\pi}{L_z}\\ E_{n_x,n_y,n_z} =& \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)\end{aligned}$$

XI The Hydrogen Atom

1. Mystery of the Hydrogen Atom

By the early 1900s, scientists understood that matter came in tiny pieces called atoms and that an atom of hydrogen contained charge $+e$ proton at its center and charge $-e$ electron outside that center.

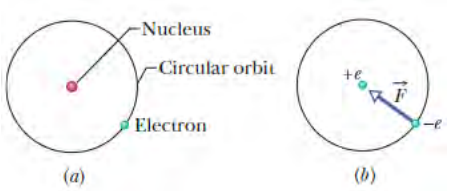

Figure 77: Bohr' s model for hydrogen resembles the orbital model of a planet around a star.

Because the proton's mass is much greater than the electron's mass, we shall assume that the proton is fixed in place. So, the atom is a fixed potential trap with the electron moving around inside it. A hydrogen atom contains an electron that is trapped by the Coulomb force it experiences from the proton, which is the nucleus of the atom. Under Newtonian laws, the electron would move around the proton, like planets around the Sun, i.e.,

$$\frac{1}{4\pi\epsilon_0}\frac{e^2}{r^2} = m\frac{v^2}{r}$$

Multiplying by $-r$, we obtain

$$E_C = -\frac{e^2}{4\pi\epsilon_0 r} = -mv^2 = -2E_K$$

Alternatively, the total energy of the electron is

$$E = E_K + E_C = \frac{E_C}{2} = -E_K$$

However, any charged particle which moves in a curved path will emit electromagnetic radiation, hence losing energy continuously. Why doesn' t the electrical attraction between the electron and the positive charge simply cause the two to collapse together?

One clue lay in the experimental fact that a hydrogen atom can emit and absorb only four wavelengths in the visible spectrum (656 nm, 486 nm, 434 nm, and 410 nm).

2. The Bohr Model

Bohr made two bold (and completely unjustified) assumptions:

1) The electron in a hydrogen atom orbits the nucleus in a circle much like Earth orbits the Sun.

2) The magnitude of the angular momentum $\vec{L}$ of the electron in its orbit is restricted (quantized) to the values

$$L = n\hbar$$

for $n = 1, 2, 3, ...$

However, as successful as his theory was on the four visible wavelengths and on why the atom did not simply collapse, it turned out to be quite wrong in almost every other aspect of the atom. We follow Bohr to quantize the electron orbit:

$$L = rmv = n\hbar$$

from which we find $v = \frac{n\hbar}{mr}$.

Combining with the Newtonian result, we find

$$r_n = n^2 a_B$$

where the characteristic length

$$a_B = \frac{\hbar^2}{\frac{me^2}{4\pi\epsilon_0}} = 0.529\text{Å}$$

In the Bohr model of the hydrogen atom, the electron' s orbital radius r is quantized and the smallest possible orbital radius (for $n = 1$) is a_B , which is called the Bohr radius. According to the Bohr model, the electron cannot get any closer to the nucleus than orbital radius a_B , and that is why the attraction between electron and nucleus does not simply collapse them together.

The energy of the hydrogen atom, according to the Bohr model, is then

$$E_n = \frac{1}{2}mv^2 - \frac{1}{4\pi\epsilon_0}\frac{e^2}{r} = -\frac{E_R}{n^2}$$

where the characteristic energy (known as the Rydberg)

$$E_R = \frac{\frac{me^4}{(4\pi\epsilon_0)^2}}{2\hbar^2} = 13.6\,\text{eV}$$

Note that we still have, for each orbit

$$E = E_K + E_C = \frac{E_C}{2} = -E_K$$

2.1 The Hydrogen Spectrum

The energy of a hydrogen atom (or, equivalently, of its electron) changes when the atom emits or absorbs light. Emission and absorption involve a quantum of light according to

$$\hbar\omega_{nm} = E_R\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

for integers $m > n$. The wavelengths of the emitted or absorbed light are given by

$$\frac{1}{\lambda} = \frac{E_R}{hc}\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

The collection of such lines (or wavelengths), such as in those in the visible range, is called a spectrum of the hydrogen atom. For convenience, we often quote the value of the combination $hc = 12400\text{eVÅ}$. Hence, we have

$$\frac{hc}{E_R} = 912\text{Å}$$

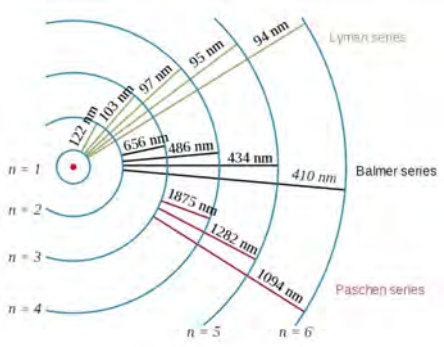

Figure 78: The Hydrogen Spectrum

2.2 Combinations of Physical Constants

As a side remark, it is often convenient to remember and use combinations of physical constants. Some examples are

$$\begin{aligned} hc &= 12400\text{eV}\cdot\text{Å} \\ \hbar c &= hc/(2\pi) = 1973\text{eV}\cdot\text{Å} \\ e^2/(4\pi\epsilon_0) &= 14.4\text{eV}\cdot\text{Å} \\ k_B T_{\text{room}} &= 1/40\text{eV} \\ m_e c^2 &= 511000\text{eV} = 0.511\text{MeV} \\ m_p/m_e &= 1836 \end{aligned}$$

3. Ground-State Energy from Uncertainty Principle

The ground-state energy is the lowest energy allowed by Heisenberg's uncertainty principle. For a hydrogen atom, the size of the wave function, Δr , is the uncertainty in position. The uncertainty in momentum is, roughly speaking, $\Delta p \sim \hbar/\Delta r$, by the uncertainty principle. The energy of the electron can be estimated to be

$$E \sim \frac{(\Delta p)^2}{2m} - \frac{e^2}{4\pi\epsilon_0\Delta_r} = \frac{\hbar^2}{2m(\Delta r)^2} - \frac{e^2}{4\pi\epsilon_0\Delta_r}$$

To find the minimal energy, we solve, for Δr

$$\frac{\mathrm{d}E}{\mathrm{d}(\Delta r)} = 0$$

After some algebra, we find

$$\begin{aligned} \Delta r &= \frac{\hbar^2}{\frac{me^2}{4\pi\epsilon_0}} \equiv a_B \\ E &= -\frac{\frac{me^2}{4\pi\epsilon_0}}{2\hbar^2} \equiv -E_R \end{aligned}$$

The energy of the ground state (or any stationary state) is uniquely determined. This is because of the energy-time uncertainty principle,

$$\Delta t \cdot \Delta E \geq \hbar/2$$

In the extreme case of a stationary state, $\Delta t = \infty$, so we have $\Delta E = 0$. Note, however, both kinetic energy and potential energy have uncertainties, due to the uncertainties of position and momentum.

4. Solutions of Schroedinger's Equation

In Schroedinger's model of the hydrogen atom, the electron (charge $-e$) is in a potential energy trap due to its electrical attraction to the proton (charge $+e$) at the center of the atom.

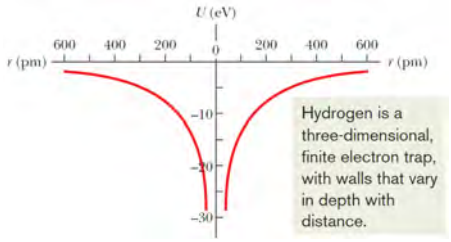

Figure 79: Schroedinger's Equation for the H-Atom

With the central potential, we can use separation of variables and assume

$$\Psi(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)$$

which breaks the equation into three separate differential equations for $R(r)$, $\Theta(\theta)$ and $\Phi(\phi)$.

The Φ function is found to have the quantum number m where

$$\Phi_{m_l}(\phi) \sim e^{im_l\phi},\ m_l = 0, \pm 1, \pm 2, ...$$

The Θ function is known as Legendre polynomials, which have quantum number m_l and l. When Θ and Φ are multiplied together, the product is known as spherical harmonics

$$Y_l^{m_l}(\theta,\phi) = \Theta_l^{m_l}(\theta)\Phi_{m_l}(\phi)$$

The radial wave function $R_{n,l}(r)$ has quantum number n and l.

4.1 Hydrogen Wave Functions

The solution for the energy levels is exactly what Bohr found by using the incorrect planetary model of the atom. The corresponding wave function of a particular quantum state of the hydrogen atom can be labeled by a set of quantum numbers (n, l, m_l)

1) The corresponding energy only depends on the principal quantum number $n = 1, 2, 3, ...$

2) The orbital quantum number $l = 1, 2, 3, ...\ , n-1$ is a measure of the magnitude of the angular momentum of the quantum state. States with $l = 0, 1, 2, 3$ are called s, p, d, f .

3) The orbital magnetic quantum number $m_l = -l, -l+1, ..., l-1, l$ is related to the space orientation of this angular momentum vector.

4.2 Ground State Wave Function

The wave function for the ground state of the hydrogen atom, as obtained by solving the three-dimensional Schroedinger equation and normalizing the result, is

$$\psi_{100}(\vec{r}) = R_{10}(r) = \frac{1}{\sqrt{\pi}a_B^{3/2}}e^{-r/a_B}$$

Note that the hydrogen atom in its ground state has zero angular momentum, which is not predicted in the Bohr model.

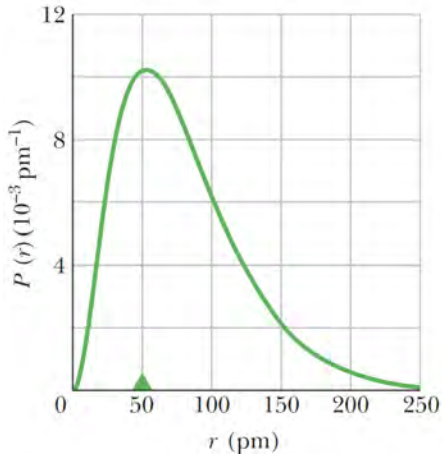

Figure 80: The radial probability density $P(r)$

The probability that the electron can be detected in any given (infinitesimal) volume element $\mathrm{d}V$ located at radius r from the center of the atom is $|\psi_{100}(\vec{r})|^2\,\mathrm{d}V$. With spherical symmetry, we have $\mathrm{d}V = 4\pi r^2\,\mathrm{d}r$. We define radial probability density $P(r)$ such that

$$P(r)\,\mathrm{d}r = |\psi_{100}(\vec{r})|^2\,\mathrm{d}V$$

The popular view that electrons in atoms follow well-defined orbits like planets smoving around the Sun is incorrect. All that we can ever know about the location of the electron in the ground state of the hydrogen atom is the radial probability density. We can show the probabilistic nature of the wave function by a dot plot: The density of dots represents the probability density of detection of the electron with the hydrogen atom in its ground state.

4.3 Bohr' s Correspondence Principle

The probability density for a hydrogen atom state with a relatively high n and the highest $l = n - 1$ forms a ring that indeed look like a de Broglie wave. The resemblance of the probability density to the electron orbit of classical physics is another illustration of Bohr' s correspondence principle —namely, that at large quantum numbers the predictions of quantum mechanics merge smoothly with those of classical physics

5. The Pauli Exclusion Principle

For multiple electrons in the same trap, we must consider the Pauli exclusion principle, named after Wolfgang Pauli. The Pauli principle states that no two electrons confined to the same trap can have the same set of values

for their quantum numbers. In other words, there can be two electrons at most at any energy level; they have opposite spins. This principle applies not only to electrons but also to protons and neutrons, all of which have $s = 1/2$; they are known as Fermions.

Consider electrons in an infinite square well with side length L (with $E_{n_1,n_2} = n_1^2 + n_2^2$, in units of $\frac{h^2}{8mL^2}$).

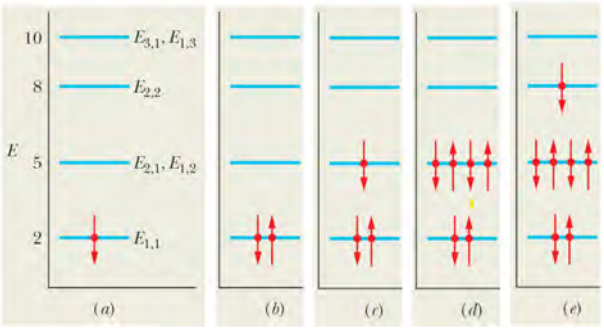

Figure 81: The Pauli Exclusion Principle

5.1 Carbon

A carbon atom has a nucleus of 6 protons and 6 neutrons with a total charge of $6e$. The lowest level ($1s$) contains 2 electrons, one spin up and one spin down. There are 4 electrons on the outer shell [$2s$ (lower in energy) and $2p$].

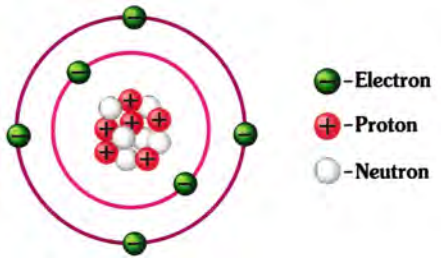

Figure 82: Carbon

6. Wave Function Hybridization

Hybridization is the idea that atomic orbitals fuse to form newly hybridized orbitals, which in turn, influences molecular geometry and bonding properties.

6.1 sp^3 Hybridization

In menthane, the carbon 2s and 2p orbitals are hybridized.

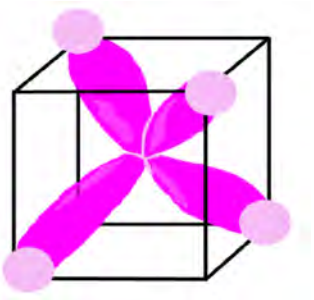

Figure 83: sp^3 Hybridization

6.2 sp^2 Hybridization

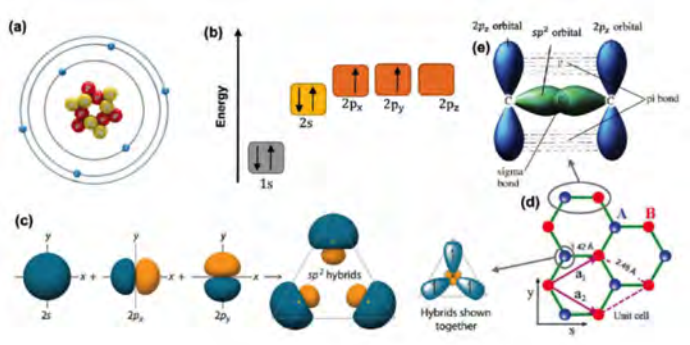

Figure 84: sp^2 Hybridization