Review of Wave Phenomenan

Introduction

Description of a wave

Wave equation

Examples

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

$\downarrow$

Schrodinger equation

$V(x) = \frac{1}{2}kx^2$ simple harmonic oscillator

Seperation of variable

Boundary condition.

Superposition Principle

plane wave

Wave Packet

Phase Velocity

Group velocity

Gaussian wavepacket

$\Delta k\,\Delta x \gtrsim 1$

Wave packet

Look at the spatial part
(Look at the wave at $t=0$)

A plane wave

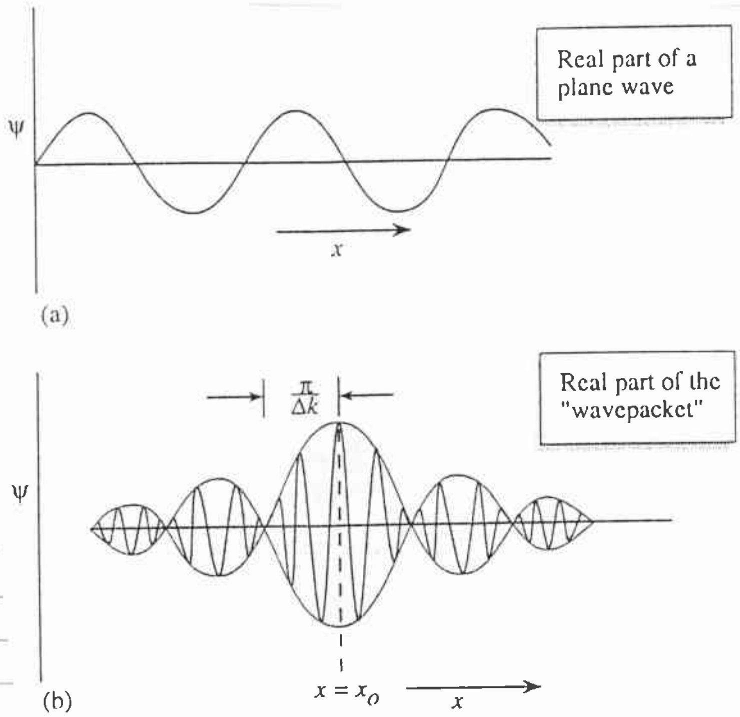
$$\psi_k(x) = e^{ikx}$$ with well defined wavelength

The position of the wave is completely undefined.

To create a wavepacket localized at some point x_0 in space, we have to combine several plane waves

Example $$F(x, x_0) = \int_{k_0-\Delta k}^{k_0+\Delta k} dk\, e^{ik(x-x_0)}$$
$$= \frac{2\sin(\Delta k(x-x_0))}{x-x_0}\, e^{ik(x-x_0)}$$

is centered around the value at x_0 and the probability ($|F|^2$) decays from its maximum value at x_0 to a very small value within a distance $\frac{\pi}{\Delta k}$



(a) A schematic description of a one-dimensional wave $e^{ik\cdot x}$ which is extended over all space; (b) a wavepacket produced by combining several waves produces a packet that is localized in space with a finite spread. The wavepacket is shown centered at x_o and having a spread Δx. The spread is such that $\Delta k \cdot \Delta x \sim 1$. This is an "uncertainty relation" in classical physics for waves. No such uncertainty exists in classical physics for particles.

Example : Add plane wave with a Gaussian weighting factor

$$f(k-k_0) = e^{-\frac{(k-k_0)^2}{2(\Delta k)^2}}$$

$\downarrow$

Gaussian distribution with width Δk

$$\psi(x, x_0) = \int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2(\Delta k)^2}} e^{ik(x-x_0)} dk$$

$$= e^{ik_0(x-x_0) - \frac{(x-x_0)^2}{2}(\Delta k)^2}$$
$$\times \int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2(\Delta k)^2} + i(k-k_0)(x-x_0) + \frac{(x-x_0)^2}{2}(\Delta k)^2}$$
$$= \sqrt{2\pi \Delta k}\; e^{ik_0(x-x_0) - \frac{1}{2}(x-x_0)^2(\Delta k)^2}$$

$\Rightarrow$ represent a Gaussian wavepacket in space around x_0 with width $\frac{1}{(\Delta k)^2} \sim (\Delta x)^2$

$\Rightarrow \quad \Delta k \, \Delta x \simeq 1$

Intuitive argument

$-\frac{\Delta x}{2}$ 0 $\frac{\Delta x}{2}$ wave packet is localized in Δx

Two plane wave with wave number k_1 , k_2 is in phase at $x = 0$

Wave packet is localized in Δx

The waves (plane) will have to interfere destructively outside Δx

$$(k_1 - k_2)\frac{\Delta x}{2} \sim \pi$$

$\Rightarrow \quad \Delta k \, \Delta x \simeq 1$

分類：	
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總號：	

Wave equation is linear

$\Rightarrow$ Physically, this leads to the principle of superposition i.e., if two or more waves are traveling in the same medium, the resultant disturbance will be equal to the sum of the individual disturbance.

Simplest example: two waves with different wavelengths travelling at the same speed in the same direction

$$y_1 = A \sin[k_1(x - vt)]$$
$$y_2 = A \sin[k_2(x - vt)]$$

$$\Rightarrow \quad y = y_1 + y_2$$

$$\Rightarrow \quad y = 2A \sin[k'(x-vt)] \cos[k''(x-vt)]$$

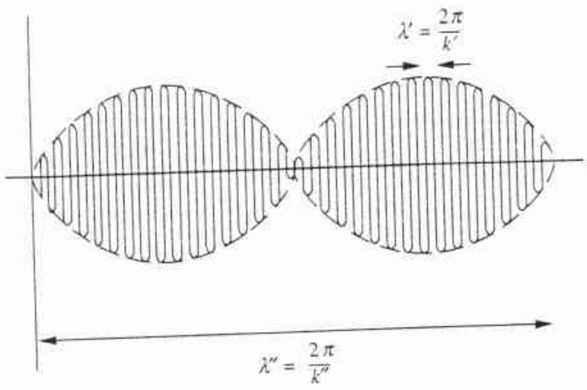
where $k' = \frac{1}{2}(k_1 + k_2) \sim k_1$

$k_1'' = \frac{1}{2}(k_1 - k_2) = \frac{1}{2}\Delta k$

$$\Rightarrow \quad y = 2A \sin[k_1(x-vt)] \cos[\frac{\Delta k}{2}(x-vt)]$$

At $t = 0$ $\quad y = 2A \sin k_1 x \cos \frac{\Delta k}{2} x$

The superposition of two waves with different wavelengths. The wavenumbers k' and k'' are defined in the text.



$$\Rightarrow \quad y = 2A \cos[(\Delta k)x - (\Delta\omega)t] \sin(k_1 x - \omega t)$$

$v_p = \frac{\omega_1}{k_1}$ = phase velocity $\Rightarrow$ the speed of the wave with the average wave number k_1

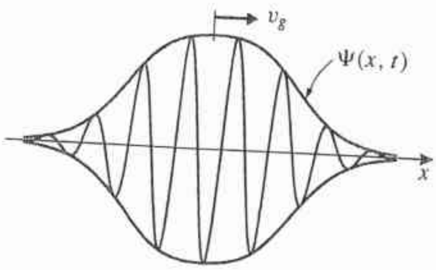
The other velocity is associated with the amplitude, i.e., the overall shape of wave $\Rightarrow$ $v_g = \frac{\Delta\omega}{\Delta k} \rightarrow \frac{d\omega}{dk}$

The wave within the group has an avarge velocity v_p

the group of waves has a velocity v_g

Since the energy of a wave depend on the amplitude, it must travel at the group velocity.

Because exponent



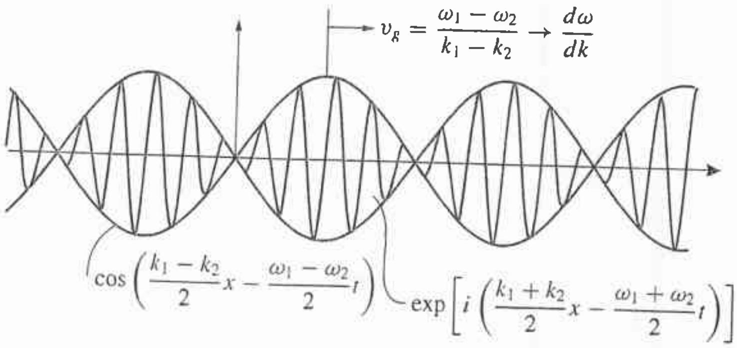
A wave packet results from overlaying many waves $\psi(x,t) = \int c(k) e^{i(kx-\omega t)} dk$ (see volume 1: *Mechanics*).

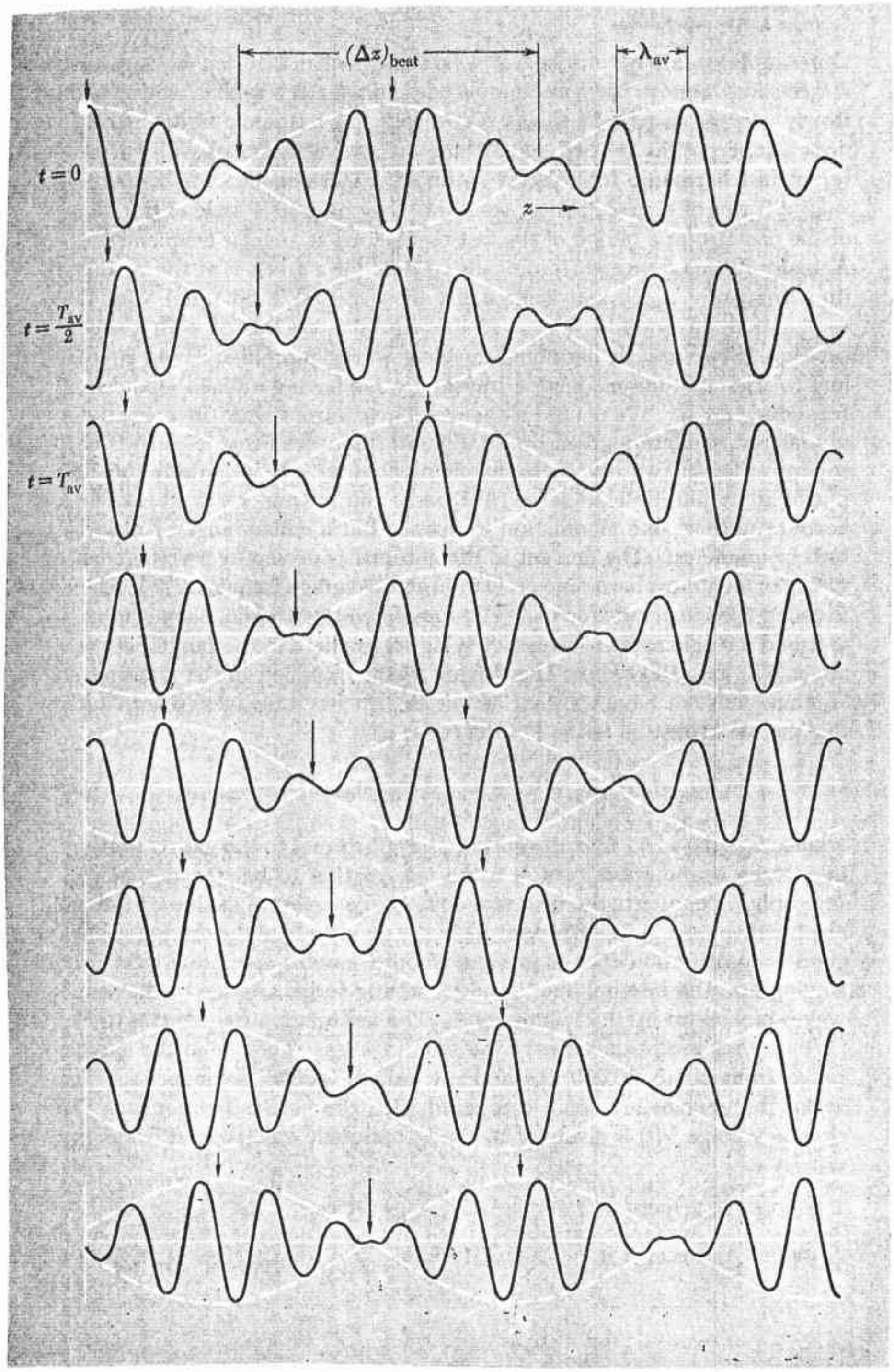
$$\psi(x,t) = \int c(k)\, e^{i(kx-\omega t} dk$$

Superposition of two waves of equal amplitude and distinct, but neighboring frequenies ω_1, k_1 and ω_2, k_2

$$\psi(x,t) = A\left(e^{i(k_1 x - \omega_1 t)} + e^{i(k_2 x - \omega_2 t)} \right)$$

$$= 2A \cos\left(\frac{k_1-k_2}{2} x - \frac{\omega_1-\omega_2}{2} t \right) e^{i \frac{(k_1+k_2)}{2} x - i(\omega_1+\omega_2) t}$$





The group velocity

The arrow follow the beats, which travel at the group velocity v_g

The open circles follow individual wave crest which travel at the average phase velocity v_p

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Wave Packet

The phase velocity is the traveling velocity of the phase of a propagrating wave.

Example $\psi = A \sin(kx - \omega t)$
plane harmonic wave

$A \rightarrow$ amplitude

$kx - \omega t \rightarrow$ argument (the phase)

The maximum of ψ is reached when $kx - \omega t = \frac{\pi}{2}, \frac{5\pi}{2}$ ...

Obviously it moves with the velocity $v_{ph} = \frac{\omega}{k}$

It is important to understand that such a plane wave extending from $-\infty$ to ∞ cannot transfer information. (the uniformity and "monotony" of the wave must be destroyed, i.e., one must create a wave peak and see how it propagates only this perturbation is visible (recordable)

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Add two harmonic plane wave

$$y_1 = A \sin(k_1 x - \omega_1 t)$$

$$y_2 = A \sin(k_2 x - \omega_2 t)$$

Superposition of the two waves

$$y = y_1 + y_2$$

$$= A \sin(k_1 x - \omega_1 t) + A \sin(k_2 x - \omega_2 t)$$

$$= 2A \sin\left[\tfrac{1}{2}((k_1+k_2)x - (\omega_1+\omega_2)t\right]$$

$$\cdot \cos\left[\tfrac{1}{2}((k_1-k_2)x - (\omega_1-\omega_2)t\right]$$

With $k_1 \sim k_2$, $\omega_1 \sim \omega_2$

$k_1 - k_2 = \Delta k$, $\omega_1 - \omega_2 = \Delta\omega$

$$\Rightarrow \quad y = 2A \cos\left[\tfrac{1}{2}\Delta k \cdot x - \Delta\omega \cdot t\right] \sin(\bar{k} x - \bar{\omega} t)$$

$v_{ph} = \dfrac{\bar{\omega}}{\bar{k}}$ = phase velocity

$v_g = \dfrac{\Delta\omega}{\Delta k}$ = group velocity

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$$\psi(x,t) = \int_{-\infty}^{\infty} c(k)\, e^{i(\omega t - kx)}\, dk$$

$\psi(x,t) \downarrow$ wave packet

superposition of plane harmonic wave with a weighing factor (spectra) $c(k)$

Here and in the following discussion, what is really used is only the real part of function $e^{i(\omega t - kx)}$

The imaginary part of the function is simply taken along, but not used.

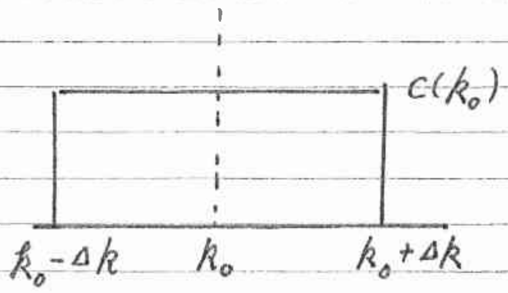
This makes the calculation easier. (Fourier transform)

In general ω is a function of k.

↓ for example, as in dispersive medium.

Example $\quad c(k) = c(k_0) \quad$ for $k_0 - \Delta k < k < k_0 + \Delta k$

$\qquad\qquad\quad\; 0 \quad$ otherwise



$$\frac{\Delta k}{k_0} \ll 1$$

$$\omega = \omega_0 + \left(\frac{d\omega}{dk}\right)_0 (k - k_0)$$

$$k = k_0 + \underbrace{(k - k_0)}_{\xi}$$

$$\Rightarrow \quad \psi(x,t) = c(k_0)\, e^{i\omega_0 t - k_0(t)} \int_{-\Delta k}^{\Delta k} e^{i\left(\left(\frac{d\omega}{dk}\right)_0 t - x\right)\xi}\, d\xi$$

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Performing the simple integration with respect to ξ

$$\psi(x,t) = 2c(k_0)\,\frac{\sin\{[(\frac{d\omega}{dk})_0 t - x)}{[(\frac{d\omega}{dk})_0 t - x]}\, e^{i(\omega_0 t - k_0 x)}$$

$$= c(x,t)\; e^{i(\omega_0 t - k_0 x)}$$

$c(x,t)$ can be considered as the amplitude of an almost monochromatic wave.

$c(x,t)$ is of the form $f(vt - x)$ with $v = (\frac{d\omega}{dk})_0$

$\downarrow$

the maximum will move with group velocity

$v_g = (\frac{d\omega}{dk})_0$

Finally, we shall take the example of a Gaussian wave packet

$$c(k) = c(k') \quad \text{with} \quad k' = k - k_0$$

$$= e^{-k'^2/2(\Delta k)^2}$$

Gaussian distribution in k with width Δk

With $\omega(k) = \omega(k_0) + \left(\frac{\partial\omega}{\partial k}\right)_0 (k-k_0) + \cdots$

$$\psi(x,t) = \sqrt{2\pi(\Delta k)^2}$$

$$\cdot\ e^{i(k_0 x - \omega_0 t)} \leftarrow \text{phase factor}$$

$$\cdot\ e^{-\frac{(\Delta k)^2}{2}(x - v_g t)^2} \leftarrow \text{amplitude}$$

$$v_g = \left(\frac{\partial\omega}{\partial k}\right)_0$$

Remarks.

- It is Gaussian wavepack
- The wideth of the wave packet in real with width $(\Delta k)^{-1}$
- The result can be readily obtained by setting $x_0 = 0, \ \alpha = 0$ (See 147 - 148)
- With $\alpha \neq 0$, the wave packet with spread, i.e., the width in real space is

$$\Delta x = \Delta x(t=0)\sqrt{1 + \frac{\alpha^2 t^2}{[\Delta x(t=0)]^4}}$$

1.6 WAVES, WAVEPACKETS, AND UNCERTAINTY

In classical physics when we deal with wave phenomena we are aware of a little "fuzziness" in the description of certain features of the wave. For example, let us imagine a child creating a wave on the surface of a pond by throwing a stone into the pond. We know from experience that a "wavepacket" or wave "pulse" intially localized around the point where the stone hit the water surface is produced. This wave then propagates toward the edges of the pond. Can we, at any time, *precisely* define the location of the wave and its wavelength? We know from experience and from classical physics that this is not possible. If we try to create a wavepacket highly localized in space we lose the knowledge of the wave's wavelength. On the other hand, if we try to create a "plane wave" with a well-defined wavelength, we lose the knowledge regarding the spatial position of the wave.

The uncertainty described above is not of concern in classical physics when we deal with particles. For example, we have no problem defining *precisely* any combinations of physical observables of a particle. However, a wave description will inevitably bring in an uncertainty in the precision with which we can simultaneously define certain physical observables. To see how this occurs, we examine the uncertainty arising in the wavelength or, for convenience, the wavevector k ($k = 2\pi/\lambda$), and the position of waves.

To describe the wavepacket, let us begin from a plane wave given by

$$\psi_k(x) = e^{ikx} \tag{1.26}$$

The position of the wave is completely undefined (as shown in Fig. 1.7a). To create a wavepacket localized at some point x_0 in space, we have to combine several plane waves. One example is to use an equal amplitude combination of waves centered around k_0 with a spread $\pm\Delta k$. The resulting function, say k_0, but from a spread $\pm\Delta k$, then the function

$$F(x, x_0) = \int_{k_0-\Delta k}^{k_0+\Delta k} dk \; e^{ik(x-x_0)}$$

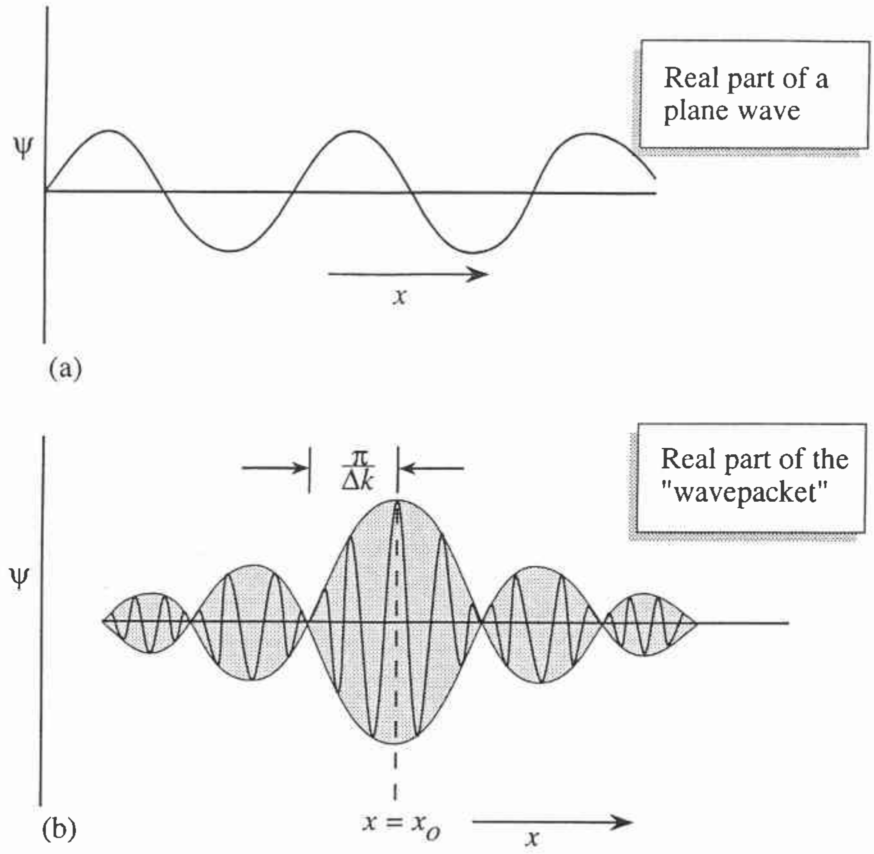

Figure 1.7: (a) A schematic description of a one-dimensional wave $e^{ik\cdot x}$ which is extended over all space; (b) a wavepacket produced by combining several waves produces a packet that is localized in space with a finite spread. The wavepacket is shown centered at x_o and having a spread Δx. The spread is such that $\Delta k \cdot \Delta x \sim 1$. This is an "uncertainty relation" in classical physics for waves. No such uncertainty exists in classical physics for particles.

In such a plane wave the probability density of the the wave, $\psi\psi^*$, is the same in all regions of space. Such a description is not useful if one wants to discuss transport of an optical pulse or of a particle from one point to another. For example, in describing electron transport we wish to describe an electron which moves from one point to another. Thus the wavefunction must be peaked at a particular place in space for such a description. This physical picture is realized by constructing a wavepacket picture.

Construction of a Wavepacket

Let us examine a one-dimensional plane wave state with a wave vector k_0

$$\psi_{k_0}(x) = e^{ik_0 x} \tag{1.32}$$

We note that if a state was constructed not from a single k_0 component, but from a spread $\pm\Delta k$, then the function

$$\begin{aligned} F(x, x_0) &= \int_{k_0-\Delta k}^{k_0+\Delta k} dk\ e^{ik(x-x_0)} \\ &= \frac{2\sin(\Delta k\ (x-x_0))}{(x-x_0)}\ e^{ik_0(x-x_0)} \end{aligned} \tag{1.33}$$

is centered around the point x_0 and the probability ($|F|^2$) decays from its maximum value at x_0 to a very small value within a distance $\pi/\Delta k$.

If Δk is small, this new "wavepacket" has essentially the same properties as ψ at k_0, but is localized in space and is thus very useful to describe motion of the particle. A more useful wavepacket is constructed by multiplying the integrand in the wavepacket by a Gaussian weighting factor

$$f(k-k_0) = \exp\left[-\frac{(k-k_0)^2}{2(\Delta k)^2}\right] \tag{1.34}$$

$$\begin{aligned} \psi(x, x_0) &= \int_{-\infty}^{\infty} \exp\left[-\frac{(k-k_0)^2}{2(\Delta k)^2} + ik(x-x_0)\right] dk \\ &= \exp\left[ik_0(x-x_0) - \frac{(x-x_0)^2}{2}(\Delta k)^2\right] \\ &\times \int_{-\infty}^{\infty} \exp\left[-\frac{(k-k_0)^2}{2(\Delta k)^2} + i(k-k_0)(x-x_0) + \frac{(x-x_0)^2}{2}(\Delta k)^2\right] \\ &= \sqrt{2\pi\Delta k}\ \exp\left[ik_0(x-x_0) - \frac{1}{2}(x-x_0)^2(\Delta k)^2\right] \end{aligned} \tag{1.35}$$

$\psi(x, x_0)$ represents a Gaussian wavepacket in space which decays rapidly away from x_0. We note that when we considered the original state $\exp(ik_0 x)$, the wave was spread infinitely in space, but has a precise k-value. By constructing a wavepacket, we sacrificed its precision in k-space by Δk and gained a precision Δx in real space. In general, the width of the wavepacket in real and k-space can be seen to have the relation

$$\Delta k\ \Delta x \approx 1 \tag{1.36}$$

We can repeat this procedure for a wave of the form

$$\psi \sim e^{i\omega t} \tag{1.37}$$

and also obtain a wavepacket which is localized in time and frequency, the widths again being related by

$$\Delta\omega\ \Delta t \approx 1 \tag{1.38}$$

Let us now consider how a wavepacket moves through space and time. For this we need to bring in the time dependence of the wavefunction, i.e., the term $\exp(-iEt/\hbar)$ or $\exp(-i\omega t)$.

$$\psi(x, t) = \int_{-\infty}^{\infty} f(k-k_0)\ \exp\{i[k(x-x_0) - \omega t]\}\ dk \tag{1.39}$$

If ω has a simple dependence on k

$$\omega = ck \tag{1.40}$$

we can write

$$\psi(x,t) = \int_{-\infty}^{\infty} f(k-k_0)\ \exp\left[ik(x-x_0-ct)\right]\ dk \tag{1.41}$$

which means that the wavepacket simply moves with its center at

$$x - x_0 = ct \tag{1.42}$$

and its shape is unchanged with time. If, however, we have a dispersive media and the ω vs. k relation is more complex, we can, in general, write

$$\omega(k) = \omega(k_0) + \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0} \cdot (k-k_0) + \frac{1}{2}\left.\frac{\partial^2\omega}{\partial k^2}\right|_{k=k_0} (k-k_0)^2 + \cdots \tag{1.43}$$

Setting

$$\begin{aligned} \omega(k_0) &= \omega_0 \\ \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0} &= v_g \\ \left.\frac{\partial^2\omega}{\partial k^2}\right|_{k=k_0} &= \alpha \end{aligned} \tag{1.44}$$

we get

$$\begin{aligned} \psi(x,t) &= \exp\left[i(k_0(x-x_0)-\omega_0 t)\right]\int_{-\infty}^{\infty} f(k-k_0) \\ &\times \exp\left[i(k-k_0)(x-x_0-v_g t) - \frac{i\alpha}{2}(k-k_0)^2 t\right]\ dk \end{aligned} \tag{1.45}$$

If α were zero, the wavepacket would move with its peak centered at

$$x - x_0 = v_g t \tag{1.46}$$

i.e., with a velocity

$$v_g = \left.\frac{\partial\omega}{\partial k}\right|_{k=k_0} \tag{1.47}$$

However, for nonzero α, we show that the shape of the wavepacket also changes. To see this, let us again assume that

$$\begin{aligned} f(k-k_0) &= f(k') \\ &= \exp\left(\frac{-k'^2}{2\Delta k^2}\right) \end{aligned} \tag{1.48}$$

Then

$$\psi(x,t) = \exp\{i[k_0(x-x_0)-\omega_0 t]\} \times \int_{-\infty}^{\infty} \exp\left[ik'(x-x_0-v_g t) - \frac{k'^2}{2}\left(i\alpha t + \frac{1}{(\Delta k)^2}\right)\right] dk' \tag{1.49}$$

To evaluate this integral we complete the square in the integrand by adding and subtracting terms

$$\psi(x,t) = \exp\left\{i[k_0(x-x_0)-\omega_0 t] - \frac{(x-x_0-v_g t)^2(\Delta k)^2}{2[1+i\alpha t(\Delta k)^2]}\right\} \times \int_{-\infty}^{\infty} \exp\left\{\frac{-1}{2}\left[\frac{1+i\alpha t\,(\Delta k)^2}{(\Delta k)^2}\right] \times \left[k' - i\frac{(x-x_0-v_g t)\,(\Delta k)^2}{1+i\alpha t\,(\Delta k)^2}\right]^2\right\} dk' \tag{1.50}$$

The integral has a value

$$\sqrt{\frac{2\pi\,(\Delta k)^2}{1+i\alpha t\,(\Delta k)^2}}$$

Further multiplying and dividing the right-hand side exponent by $(1-i\alpha t\,(\Delta k)^2)$ we get

$$\psi(x,t) = \exp\{i[k_0(x-x_0)-\omega_0 t]\}\sqrt{\frac{2\pi\,(\Delta k)^2}{1+i\alpha t\,(\Delta k)^2}} \times \exp\left[-\frac{(\Delta k)^2}{2}\frac{(x-x_0-v_g t)^2}{1+t^2\,(\Delta k)^4\alpha^2}\right] \times \exp\left[\frac{i\alpha t}{2}\frac{(\Delta k)^4\,(x-x_0-v_g t)^2}{1+t^2\alpha^2\,(\Delta k)^4}\right] \tag{1.51}$$

The probability $|\psi|^2$ has the dependence on space and time given by

$$|\psi(x,t)|^2 = \exp\left[-\frac{(\Delta k)^2\,(x-x_0-v_g t)^2}{1+\alpha^2 t^2\,(\Delta k)^4}\right] \tag{1.52}$$

This is a Gaussian distribution centered around $x = x_0 + v_g t$ and the mean width in real space is given by

$$\begin{aligned}\delta x &= \frac{1}{\Delta k}\sqrt{1+\alpha^2 t^2\,(\Delta k)^4} \\ &= \delta x(t=0)\sqrt{1+\frac{\alpha^2 t^2}{[\delta x(t=0)]^4}}\end{aligned} \tag{1.53}$$

For short times such that

$$\alpha^2 t^2\,(\Delta k)^4 \ll 1 \tag{1.54}$$

the width does not change appreciably from its starting value, but as time passes, if $\alpha \neq 0$, the wavepacket will start spreading.

分類：
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Wave Properties of Particles

1924 de Broglie : particles should have wave properties under certain circumstances

Louis V. de Broglie, who first suggested that electrons might have wave properties. [*Courtesy of Culver Pictures.*]

de Broglie : To a particle of energy E and momentum p there is matter wave with frequency ν and wavelength λ given by

$$\nu = \frac{E}{h} \quad , \quad \lambda = \frac{h}{p}$$

The phase velocity

$$u = \nu\lambda = \frac{E}{h}\frac{h}{p} = \frac{mc^2}{mv} = \frac{c^2}{v} > c$$

v = velocity of the particle $< c$

$\Rightarrow$ would appear that the particle could not keep up with its own matter wave

The matter wave for a particle $\rightarrow$ wave packet

Group velocity

$$v_g = \frac{d\omega}{dk}$$

$$\omega = 2\pi\nu = 2\pi\frac{E}{h} \qquad d\omega = 2\pi\frac{1}{h}dE$$

$$k = \frac{2\pi}{\lambda} = 2\pi\frac{p}{h} \qquad dk = 2\pi\frac{1}{h}dp$$

$$v_g = \frac{dE}{dp}$$

$$E^2 = p^2c^2 + m_0^2c^4 \leftarrow \text{relativistic}$$

$$E\,dE = c^2 p\,dp$$

$$\frac{dE}{dp} = c^2 \frac{p}{E} = c^2 \frac{mv}{mc^2} = v$$

For non-relativistic free particle $E = \frac{p^2}{2m}$

$$dE = \frac{p\,dp}{m}$$

$$\Rightarrow \quad v_g = \frac{dE}{dp} = \frac{p}{m} = v$$

Other consideration of de Broglie

$(E/c,\ \vec{p})$ is the energy-momentum 4-vector

A plane wave is represented by $e^{i(\vec{k}\cdot\vec{r} - \omega t)}$

$\vec{k}\cdot\vec{r} - \omega t$ is the scalar product of the 4-vectors

$(\omega/c,\ \vec{k})$ and $(ct,\ \vec{r})$

There might be some analogy between $(\frac{E}{c},\ \vec{p})$ and $(\frac{\omega}{c},\ \vec{k})$

The matter wave associated with the electron in the hydrogen atom will lead to the Bohr quantization condition.

$\underset{\text{stationary state}}{\text{condition for}} \longleftrightarrow \underset{\text{standing wave of the matter wave}}{\text{condition for}}$

$$2\pi a = n\lambda$$

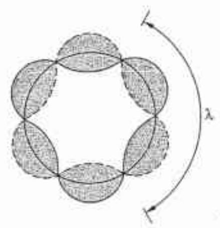
With $\lambda = \frac{h}{p}$

$$2\pi a = n\frac{h}{p}$$

$$\Rightarrow \quad 2\pi p a = nh$$

$$\Rightarrow \quad L = nh/2\pi = n\hbar$$

Bohr's quantization condition

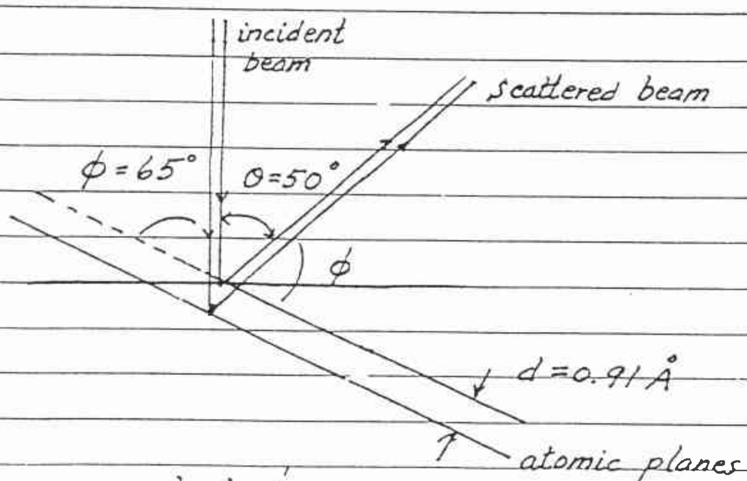


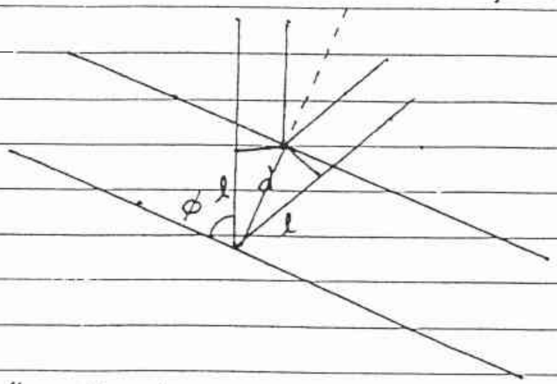
Standing waves around the circumference of a circle. In this case the circle is 3λ in circumference. If the vibrator were, for example, a steel ring that had been suitably tapped with a hammer, the shape of the ring would oscillate between the extreme positions represented by the solid and broken lines.

Experimental confirmation of de Broglie's postulate

1927 Davisson and Germer — Nobel prize 1937
G. P. Thomson

Electron diffraction





$\cos(90^\circ - \phi) = \frac{l}{d}$

$l = d\sin\phi$

Path differences $= 2l$
$= 2d\sin\phi$

Bragg condition
$2d\sin\phi = n\lambda$

$n = 1 \Rightarrow$ "first order" diffraction maximum is usually most intense

Maximum of electron distribution occur at an angle of $\theta = 50^\circ$ with the original beam when a beam of 54 eV (kinetic energy) electrons was directed at the nickel target

$n\lambda = 2d\sin\phi \qquad n=1,\ d = 0.91\,\text{Å},\ \phi = 65^\circ$
$\Rightarrow \lambda = 1.65\,\text{Å}$

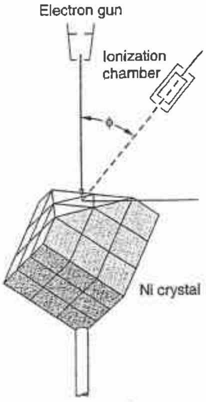
de Broglie wavelength for 54 eV electron

$p = \sqrt{2mT}$

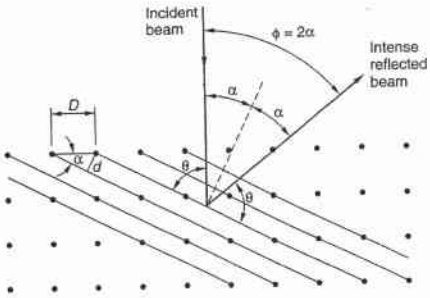
$\lambda = \frac{h}{p}$

$\Rightarrow \lambda = 1.66\,\text{Å}$

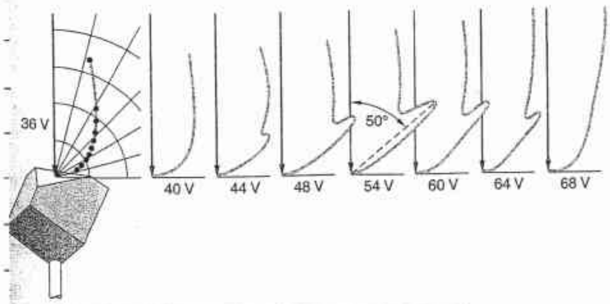
Neutron diffraction has also been observed and is widely used tool for studying the crystal structure



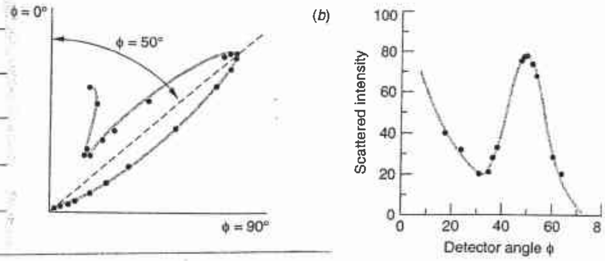
The Davisson-Germer experiment. Low-energy electrons scattered at angle ϕ from a nickel crystal are detected in an ionization chamber. The kinetic energy of the electrons could be varied by changing the accelerating voltage on the electron gun.

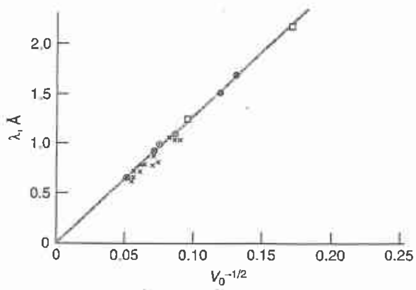


Scattering of electrons by a crystal. Electron waves are strongly scattered if the Bragg condition $n\lambda = 2d \sin\theta$ is met. This is equivalent to the condition $n\lambda = D \sin\phi$.



A series of polar graphs of Davisson and Germer's data at electron accelerating potentials from 36 V to 68 V. Note the development of the peak at $\phi = 50°$ to a maximum when $V_0 = 54$ V.





Test of the de Broglie formula $\lambda = h/p$. The wavelength is computed from a plot of the diffraction data plotted against $V_0^{-1/2}$, where V_0 is the accelerating voltage. The straight line is $1.226V_0^{-1/2}$ nm as predicted from $\lambda = h(2mE)^{-1/2}$. These are the data referred to in the quotation from Davisson's Nobel lecture. (× From observations with diffraction apparatus; ⊗ same, particularly reliable; □ same, grazing beams. ⊙ From observations with reflection apparatus.) [*From* Nobel Prize Lectures: Physics *(Amsterdam and New York: Elsevier, © Nobel Foundation, 1964).*]

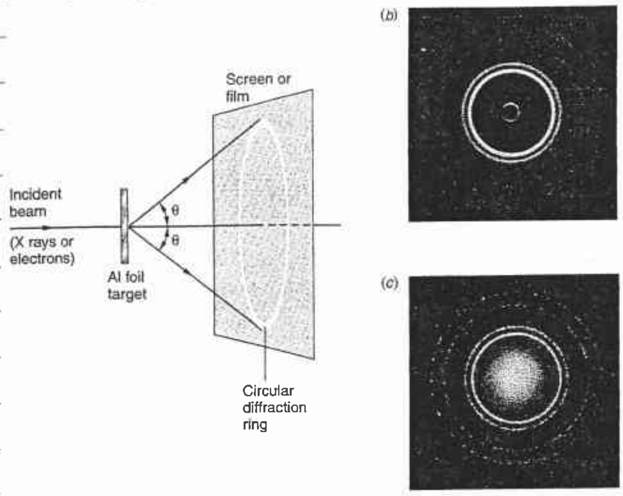


Fig. 5-8 (*a*) Schematic arrangement used for producing a diffraction pattern from a polycrystalline aluminum target. (*b*) Diffraction pattern produced by x rays of wavelength 0.071 nm and an aluminum foil target. (*c*) Diffraction pattern produced by 600-eV electrons (de Broglie wavelength of about 0.05 nm) and an aluminum foil target. The pattern has been enlarged by 1.6 times to facilitate comparison with (*b*). [*Courtesy of Film Studio, Education Development Center.*]

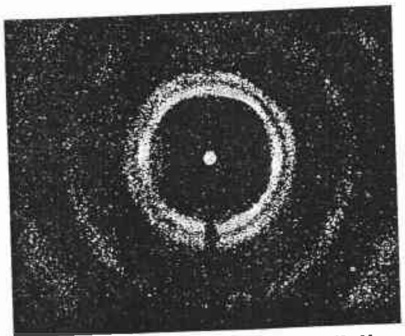


Fig. 5-10 Diffraction pattern produced by 0.0568-eV neutrons (de Broglie wavelength of 0.120 nm) and a target of polycrystalline copper. Note the similarity in the patterns produced by x rays, electrons, and neutrons. [*Courtesy of C. G. Shull.*]

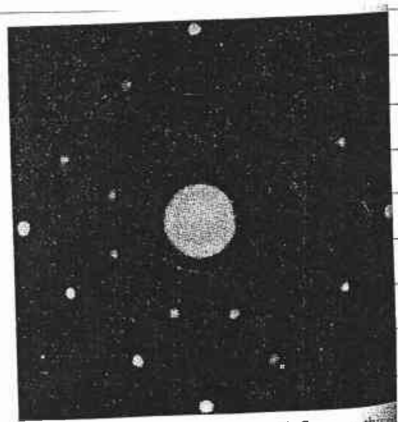


Fig. 5-11 Neutron Laue pattern of NaCl. Compare this with the x-ray Laue pattern in Figure 3-14. [*Courtesy of E. O. Wollan and C. G. Shull.*]

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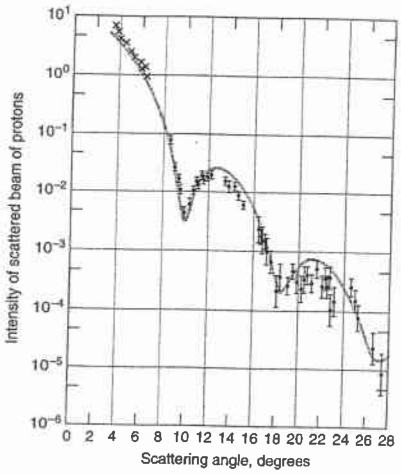

Nuclei provide scatterers whose dimensions are of the order of 10^{-15} m. Here the diffraction of 1-GeV protons from oxygen nuclei results in a pattern similar to that of a single slit.

Particle - Wave duality

Einstein's light quanta

$E = h\nu$; $E = pc$ $\lambda\nu = c$

special relativity

$$\Rightarrow \quad p = \frac{h\nu}{c}$$

$\vec{p}$ is in the direction of $\vec{k}$

$$k = \frac{2\pi}{\lambda}$$

$$p = \frac{h\frac{c}{\lambda}}{c} = h\,\frac{2\pi}{\lambda}\,\frac{1}{2\pi} = \hbar k$$

$$\Rightarrow \quad \vec{p} = \hbar\vec{k} \qquad \hbar = \frac{h}{2\pi}$$

Photoelectric effect
Compton scattering

wave $\vec{k}$, ω
(λ, ν)

$$\Rightarrow \quad E, \ \vec{p}$$

de Broglie

electron (particle) $(\vec{p}, E)$

$(\vec{k}, \omega)$

$$\lambda = \frac{h}{p}, \quad \nu = \frac{E}{h}$$

λ: de Broglie wavelength

Davisson - Germer 1927

G. P. Thomson

Particle - Wave duality.

Complementarity principle

Uncertainty principle.

Correspondence principle

Probability interpretation
Feynman's thought experiment

The Wave - Particle Duality

In classical physics energy is transferred either by waves or by particles.

Experiments compelled one to use both particle and wave model for the same entity

Radiation

Diffraction → wave

Photoelectric effect, Compton effect → particle

Electron

e/m, ionization trial in matter → particle

diffraction → wave

However, in any given measurement only one model applies

Principle of complementiarity (Bohr)

Wave and particle models are complementiarity

If a measurement proves the wave character of radiation or matter, then it is impossible to prove the particle character in the same experiment, and conversely

Furthermore, our understanding of radiation, or of matter, is incomplete unless we take into account measurements which reveal the wave aspects and also those that reveal the particle aspects.

Radiation and matter are not simply waves nor simply particles.

↓

More complicated model is needed to describe their behavior

In wave mechanics, an electron is described by a wave function

$\psi(\vec{x},t)$

Together with principle of superposition

↓

account for the wave properties

$|\psi(\vec{x},t)|^2 d\vec{x}$: probability of finding the electron in the interval $\vec{x}$ and $\vec{x}+d\vec{x}$ at time t

account for the particle aspect.

The Wave-Particle Duality

Principle of complementarity.

↓

inco porate into the
formulation of
quantum mechanics.

Feynman's suggestion of double slit experiment

↓

1989 A Tonomura's experiment

↓

First principle of
Quantum Mechanics

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"Quantum mechanics" is the description of the behavior of matter and light on an atomic scale.

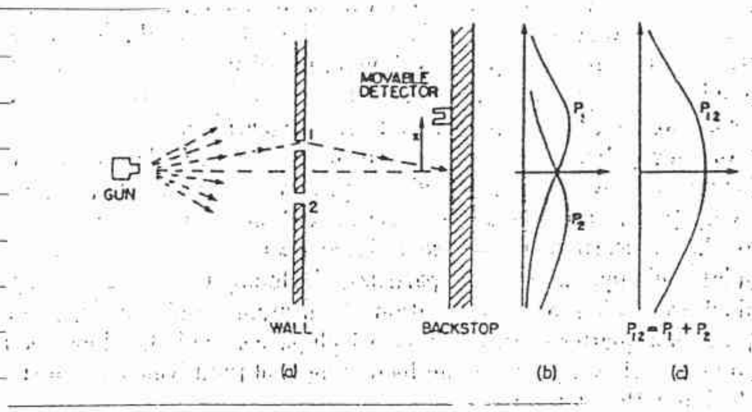
Electrons behave just like light

Have to learn quantum mechanics in a sort of abstract or imaginative fashion and not by connection with our direct experience.

Phenomenon which is impossible to explain in any classical way.

Double Slit Experiment

(1) Bullets



P_1 : slit 1 open, slit 2 clos
P_2 : slit 2 open, slit 1 close

P_{12} : both slit 1 and 2 are open.

Source : a wobby gun that, as it fires, spread the bullets out into the cone, all with the same speed but random directions

Bullets always arrive in "lump"
Lower the rate ⇒ at a given moment either nothing arrive, or one and only one bullet arrive at the backdrop
Size of the lump is independent on the rate of firing the gun
⇒ bullets always arrive in identical lump

Slit 1 open, Slit 2 closed : P_1
Slit 2 open, Slit 1 closed : P_2
Slit 1 and Slit 2 open : P_{12}

$$P_{12} = P_1 + P_2$$

Summary : arrive in identical lump
probability of arrival show no interference.

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"Quantum mechanics" is the description of the behavior of matter and light on an atomic scale.

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Have to learn quantum mechanics in a sort of abstract or imaginative fashion and not by connection with our direct experience.

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Double Slit Experiment

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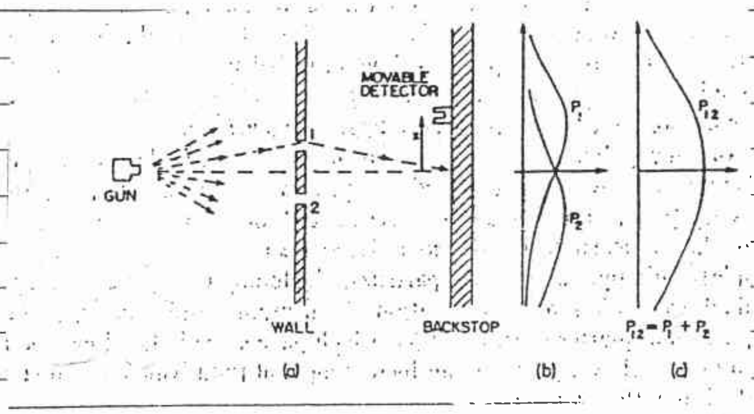

P_1 : slit 1 open, slit 2 clo.
P_2 : slit 2 open, slit 1 clos
P_{12} : both slit 1 and 2 are open.

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Lower the rate ⇒ at a given moment either nothing arrive, or one and only one bullet arrive at the backdrop
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Slit 1 open, Slit 2 closed : P_1
Slit 2 open, Slit 1 closed : P_2
Slit 1 and Slit 2 open : P_{12}

$$P_{12} = P_1 + P_2$$

Summary : arrive in identical lump
probability of arrival show no interference

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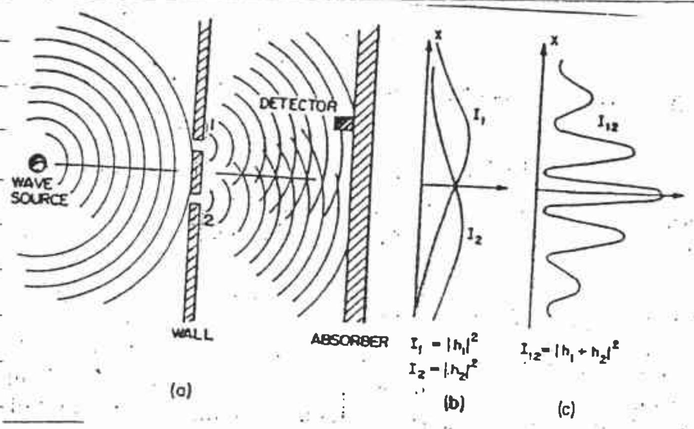
(2) Water Wave

Source : a stone dropped into a large pool of water



Detector measure the "intensity" of the wave motion

↓

proportional to the energy being carried by the wave to the detector

Intensity can have any size

↓

there is no "lumpiness"

Both slits open I_{12}

Slit 1 open, slit 2 closed I_1

Slit 2 open, slit 1 closed I_2

$I_{12} \neq I_1 + I_2 \Rightarrow$ there is "interference" of the two waves

$I_1 = |h_1|^2$

↳ wave amplitude

$I_2 = |h_2|^2$

$I_{12} = |h_1 + h_2|^2$

↓

interference pattern

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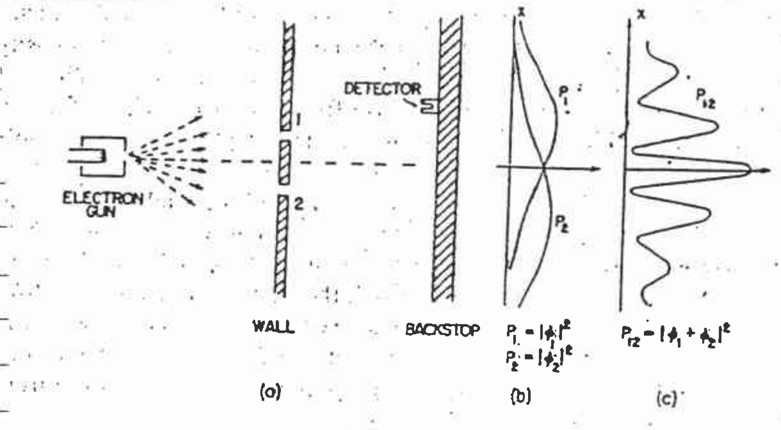
(3) Electrons



Detector: Geiger counter

Sharp "clicks" → all "clicks" are the same
↓
the size of "clicks" is identical

Slit 1 open, slit 2 closed: P_1
Slit 2 open, slit 1 closed: P_2
Slits 1 and 2 open: P_{12}

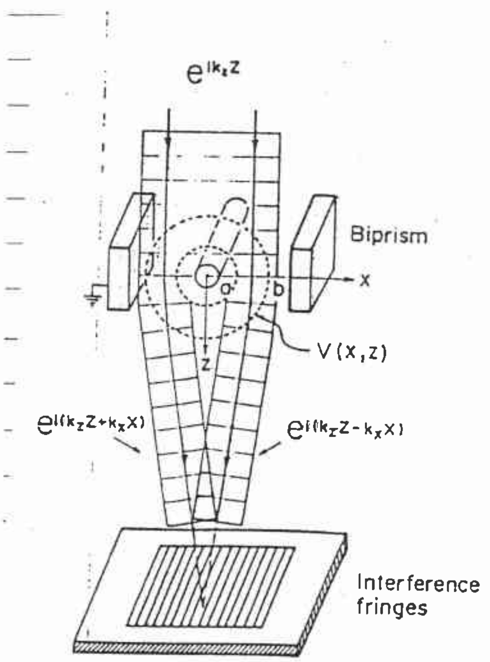
$$P_{12} \neq P_1 + P_2$$

$$P_1 = |\phi_1|^2, \quad P_2 = |\phi_2|^2$$

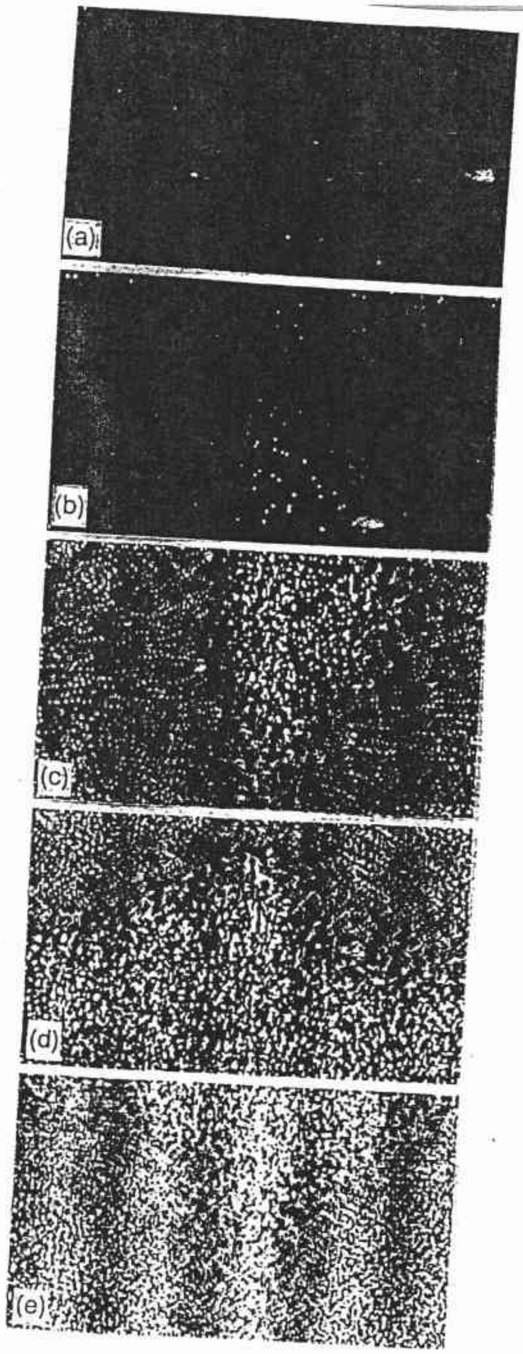
$$P_{12} = |\phi_1 + \phi_2|^2$$

Summary: electrons show wave-like interference in their arrival pattern despite the fact they arrive in lumps like bullets.

Decrease the rate of electron gun until on the average only one electron at a time is in transit between the source and the screen
⇒ interference pattern still appears when a large of electrons are accumulated over a sufficient long time
⇒ interference is the statistical property of a single electron.
↓
each electron acts as a wave, and it does not make sense to ask which slit the electron went throu



Deflection of electron waves by biprism—the case of plane-wave incidence.



The buildup of an electron interference pattern. In photograph (a), the passage of 10 electrons through a double-slit apparatus has been recorded. In (b)–(e) the numbers recorded are 100, 3000, 20 000 and 70 000 respectively. (Reprinted with permission from Tonomura, A., Endo, J., Matsuda, T., and Kawasaki, T. (1989). *American Journal of Physics*, 57, 117–20.)

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First Principle of Quantum Mechanics

(1) The probability of an event in an ideal experiment is given by the square of the absolute value of a complex number ϕ which is called the probability amplitude (wave function)

P = Probability

ϕ = Probability amplitude

$$P = |\phi|^2$$

(2) When an event can occur in several alternative ways, the probability amplitude for the event is the sum of the probability amplitude for each way considered seperately. There is interference

$$\phi = \phi_1 + \phi_2$$

$$P = |\phi_1 + \phi_2|^2$$

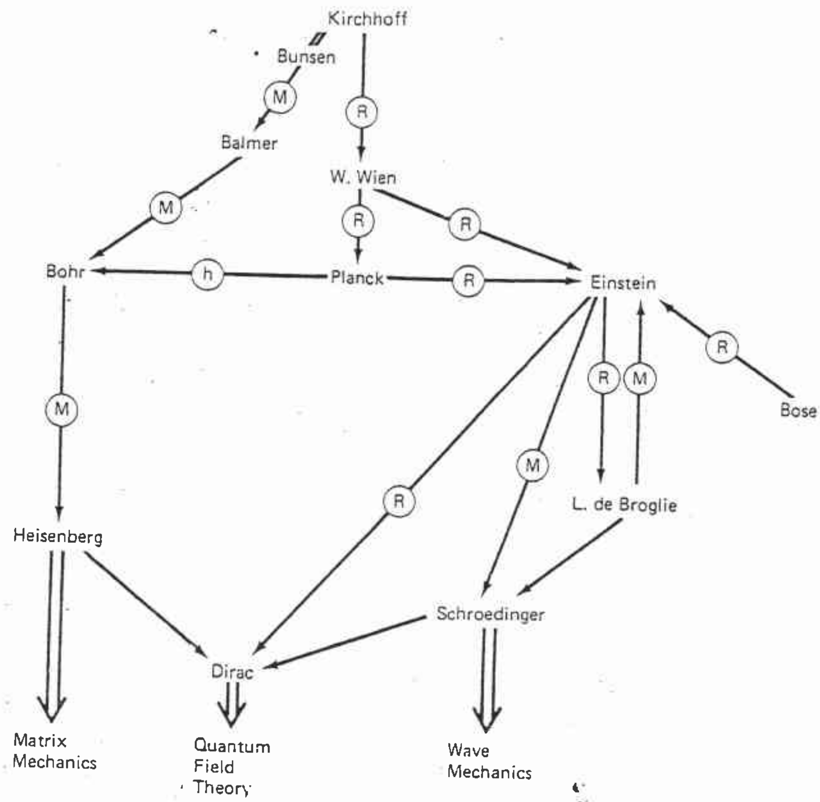
(3) If the experiment is performed which is capable of determining whether one or another alternative is actually taken, the probability of the event is the sum of the probabilities for each alternative. The interference is lost

$$P = P_1 + P_2$$

1895	Wilhelm Conrad Röntgen discovers X-rays: Mysterious radiation that can penetrate cardboard and human flesh $\Longrightarrow$ What is the origin?
1896	Henri Becquerel discovers radioactivity
1890s	It was discovered that specific heat of metals was not explained by classical thermodynamics
1890s	Detailed measurements of thermal radiation from blackbodies could not be understood on the basis of classical thermodynamics
1887	Heinrich Hertz observes photoelectric effect $\Longrightarrow$ could not be understood on the basis of classical electromagnetic theory which treats light as waves
1905	Albert Einstein introduces the concept of a photon to explain the photoelectric effect
1911	Heike Kamerlingh-Onnes discovers superconductivity: Resistance of some materials goes to zero at low temperatures $\Longrightarrow$ completely stumped classical physics
1913	William H. Bragg and Willaim L. Bragg study X-ray diffraction from crystals $\Longrightarrow$ showed that X-rays have wave-like properties
1914	James Franck and Gustav Hertz show evidence for quantized energy levels in atoms: Electrons in atoms do not behave as classical particles
1921	Otto Stern and Walter Gerlach show the need to introduce an intrinsic magnetic moment of electron

Figure 2.1: Some of the key experiments that ushered in the quantum physics age.

4. Einstein



The quantum theory: Lines of influence.

"Atomic Physics"
8th Edition
by
Max Born

Wave-Corpuscles

1. Wave Theory of Light. Interference and Diffraction.

The ideas which we have arrived at in the preceding chapters with regard to the structure of matter all rest on the possibility of demonstrating the existence of fast-moving particles by direct experiment, and indeed of making their tracks immediately visible, as in the Wilson cloud chamber. These experiments put it beyond doubt that matter is composed of corpuscles. We are now to learn of experiments which just as definitely seem to be only reconcilable with the idea that a molecular or electronic beam is a *wave train*. Before we enter upon this, however, we shall briefly recall the main facts of wave motion in general, using the phenomena of optical diffraction as a concrete example.

While in the eighteenth century physicists almost universally adhered to Newton's emission theory (about 1680), according to which light consists of an aggregate of very small corpuscles, which are sent out by the source of light, and the wave theory of Huygens (1690) could claim only a few supporters (among them the great mathematician Euler), the state of matters changed completely when at the beginning of the nineteenth century Young made the discovery that in certain circumstances two beams of light can enfeeble each other, a phenomenon quite incapable of explanation on the corpuscular theory. The results of the further investigations of Young and Fresnel spoke unequivocally in favour of the wave conception of Huygens, for it is impossible to explain interference phenomena except by a wave theory.

We give here a short discussion of Young's *interference experiment* (fig. 1). The source of monochromatic light Q illuminates the double slit in the diaphragm B with parallel light by means of the lens L. On the screen S behind the diaphragm a system of equidistant bright and dark strips (fringes) appears. How this comes about may be explained as follows. From the two openings in the diaphragm spherical waves spread outwards; these are " coherent ", i.e. they are capable of mutual interference. The two wave motions become superimposed, and reinforce each other at those places where a crest of the one wave coincides with a crest of the other; on the contrary, they destroy each other where a crest of the one wave is superimposed on a hollow of the other. Hence we can tell at once at what places on the screen there will

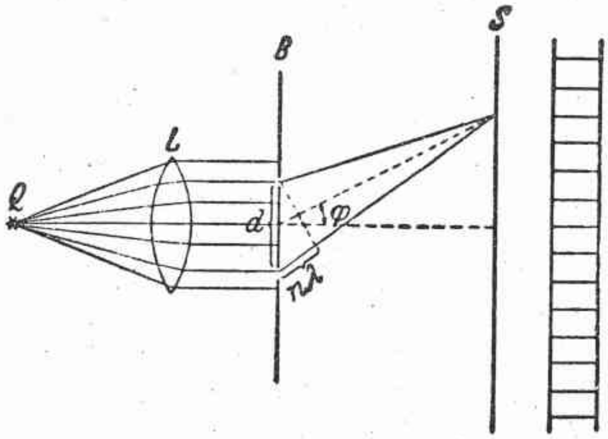


Fig. 1.—Diffraction at two narrow slits close to each other. The diffraction pattern consists of a system of equidistant bright and dark bands (fringes).

be brightness; they are the points whose distances from the two openings in the diaphragm differ exactly by an integral multiple of the wave-length. From fig. 1 we see that the difference of the distances is $d \sin \phi$; there is therefore on the screen

$$\left.\begin{array}{ll} \text{brightness, if } d \sin \phi = n\lambda \\ \text{darkness, if } d \sin \phi = (n + \frac{1}{2})\lambda \end{array}\right\} (n = 0, \pm 1, \pm 2, \ldots),$$

where d is the distance between the two openings, and ϕ is the angle of deflection.

A similar diffraction pattern is also obtained when light passes through *one slit*. We can picture it roughly as due to the mutual interference of the elementary Huygens waves spreading out from the individual points of the slit. There are two essential differences, however, as compared with the previous case. In the first place, we easily see that the relation

$$d \sin \phi = n\lambda \qquad (n = \pm 1, \pm 2, \ldots),$$

where d is the slit-width, does not now give the places at which there is brightness, but those where there is darkness. For in the packet of wave trains which spread out from the slit in the direction given by the equation, all "phases" are in this case represented exactly the same number of times; i.e. we find in the packet exactly as many wave trains which reach the screen with a crest, as trains which arrive at it with a hollow; the trains will therefore extinguish each other. We find, further, that the diffraction maxima are not, as before, almost equally bright; but that their intensity falls off very strongly from the middle maximum outwards, in the way indicated in fig. 2 by the wavy line shown at the side. It should also be specially emphasized that *when the slit-width is reduced the diffraction pattern widens out*, as may easily be deduced either from the above equation defining the position of the diffraction minima, or directly from fig. 2.

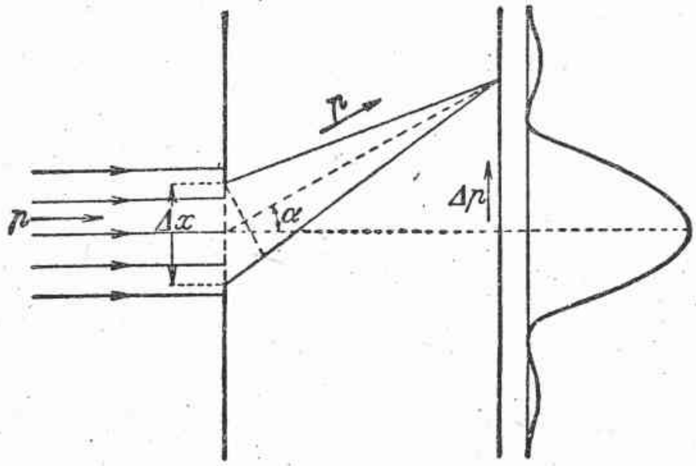


Fig. 2.—Diffraction at a slit. The diffraction pattern shows a strong maximum of intensity for the angle of diffraction $\alpha = 0$, and also a series of equidistant maxima which become progressively weaker as the angle of diffraction increases.

The fact that the form of the diffraction pattern depends essentially on the wave-length of the light makes it possible to carry out spectral investigations by means of interference phenomena (ruled grating, echelon grating, Perot-Fabry plate, Lummer plate). For diffraction patterns to show themselves, it is necessary that the width of the slit employed should be of the order of magnitude of the wave-length of the light. If then we wish to obtain interference phenomena with X-rays, we have to use a grating in which the distance between the rulings is of the order of magnitude of 1 Å. $= 10^{-8}$ cm. Such gratings are put into our hands by nature, as von Laue (1912) has shown, in the shape of crystals, in which the lattice distances are just of this order of magnitude. If a beam of X-rays is passed through a crystal, we do in fact obtain interference phenomena. Following Bragg (1913), we can interpret these as due to interference of the rays reflected at different lattice planes of the crystal (fig. 3). Moreover, Compton (1925) and others succeeded in producing X-ray interference in artificial gratings also, this being found possible at grazing incidence of the rays.

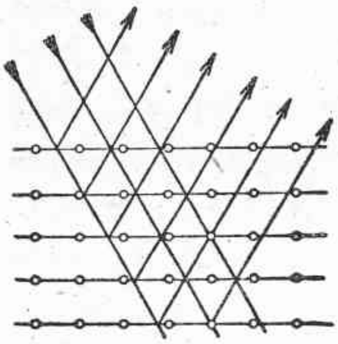


Fig. 3.—Diffraction of X-rays at a crystal. As explained by Bragg, the rays are reflected at the lattice planes of the crystal, and thus made to interfere.

Interference of X-rays supplies a powerful weapon for investigating the structure of crystals. For this purpose we do not even require large pieces of the crystal, but can use it in the form of powder (Debye-Scherrer, 1915; Hull, 1917). The interference figures in the latter case are rings round the direction of the incident beam. Indeed, the powder grains may be of molecular size even. What is more, it is found that the interference phenomena due to the individual atoms of the molecule are by no means completely obliterated by the irregular setting and motion of the molecules in liquids and gases. Circular interference rings are observed, from the intensity distribution of which we can draw conclusions with regard to the distances of the atoms in the molecule (Debye, 1929). However, we shall not enter further into these methods of investigating how matter is built up from atoms.

We add here, in the form of a scale, a summary of the wave-lengths of the types of radiation at present known (fig. 4). The scale is

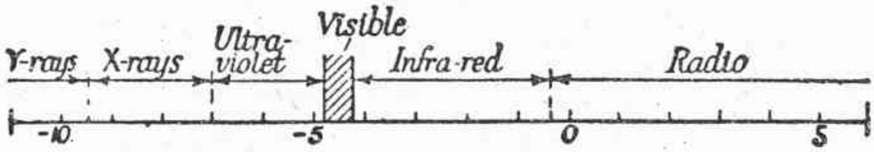


Fig. 4.—Logarithmic scale of wave-lengths; the numbers shown refer to a unit of length $\lambda_0 = 1$ cm., and represent $\log_{10}(\lambda/\lambda_0)$

logarithmic; the numbers shown are therefore indices of powers of 10. As unit $\lambda_0 = 1$ cm. is taken. Next to the wide range of wave-lengths employed in wireless communication comes the region of infra-red waves, which affect our senses as radiant heat. Then comes the relatively narrow stretch of the visible region (7700 to 3900 Å.), followed by the ultra-violet and Schumann regions, which in turn lead into the domain of X-rays (10 to 0·05 Å.). The radioactive γ-radiation reaches to about 0·001 Å. The cosmic radiation contains γ-rays of very short wave-length (10^{-5} Å.) which would lie beyond the scale of our figure.

2. Light Quanta.

Great as has been the success of classical ideas in the interpretation of interference phenomena, their incapacity to account for the processes of absorption and emission of radiation is no less striking. Here classical electrodynamics and classical mechanics absolutely fail.

To give a few examples of this failure, we recall the experimental fact that a hydrogen atom, for example, emits an infinite series of sharp spectral lines (p. 105). Now the hydrogen atom possesses only a single electron, which revolves round the nucleus. By the rules of electrodynamics, an electron accelerated like this sends out radiation continuously, and so loses energy; in its orbit it would therefore necessarily get nearer and nearer the nucleus, into which it would finally plunge. The electron, which initially revolved with a definite frequency, will radiate light of this frequency; in the case when the frequency of revolution changes (continuously) during the radiation process, it will also emit frequencies close to the ground frequency; but how then the spectrum of hydrogen should consist of a discrete series of sharply separated lines, it is quite impossible to understand.

Further, the stability of the atom is inexplicable. We may think by way of comparison of the system of planets circling round the sun, all, when undisturbed, moving in their fixed orbits. Suppose, however, that the whole solar system arrived in the neighbourhood of Sirius, for example; the mere propinquity would suffice to deflect all the planets out of their courses. If then the solar system moved away again to a distance from Sirius, the planets would now revolve round the sun in new orbits with new velocities and periods of revolution. If the electrons in the atom obeyed the same mechanical laws as the planets in the solar system, the necessary consequence of a collision of the atom with another atom would be that the ground frequencies of all the electrons would be completely changed, so that after the collision the atom would radiate light of wave-lengths also entirely different. In direct opposition to this, we have the experimental fact that an atom of a gas, which by the kinetic theory of gases is subjected to something like 100 million collisions per second, nevertheless, after these as before, sends out the same sharp spectral lines.

Finally, classical mechanics and statistics fail with the explanation of the laws of radiation of heat (or energy). We shall not go into this complex question in detail until later (Chap. VII, p. 204), and here merely quote the result to which Planck (1900) was led by the above considerations. To make the laws of radiation intelligible, he found the following hypothesis to be necessary: *emission and absorption of radiant energy by matter does not take place continuously, but in finite "quanta of energy"* $h\nu$ ($h =$ Planck's constant $6{\cdot}62 \times 10^{-27}$ erg sec., $\nu =$ frequency). On the other hand, the connexion with the electromagnetic theory of light is to be maintained to this extent, that the classical laws are to hold for the propagation of the radiation (diffraction, interference).

Einstein (1905), however, went even further than Planck. He not merely postulated quantum properties for the processes of absorption and emission of radiation, but also maintained such properties as inherent in the nature of radiation itself. According to the *hypothesis of light quanta* (*photons*) which he advanced, light consists of quanta (corpuscles) of energy $h\nu$, which fly through space like a hail of shot, with the velocity of light. Daring as at first sight this hypothesis appears to be, there is nevertheless a whole series of experiments which seem scarcely possible to explain on the wave theory, but which can be understood at once if we accept the hypothesis of the light quantum. Some account of these experiments, which were cited by Einstein himself in proof of his hypothesis, will now be given.

The most direct transformation of light into mechanical energy occurs in the photoelectric effect (Hertz (1887), Hallwachs, Elster and Geitel, Ladenburg). If short-wave (ultra-violet) light falls on a metal surface (alkalies) in a high vacuum, it is observed in the first place that the surface becomes positively charged (fig. 5); it is therefore giving off negative electricity, which issues from it in the form of electrons. We can now on the one hand, by capture of the electrons, measure the total current issuing from the metal surface, and on the other hand determine the velocity of the electrons by deflection experiments or by a counter field. Exact experiments have shown that the velocity of the emergent electrons does not depend, as one might at first expect, on the intensity of the light; but that only their number increases as the light becomes stronger, the number being in fact proportional to the intensity of the light. The velocity of the photoelectrons depends only on the frequency ν of the light; for the energy E of the electrons the following relation is found:

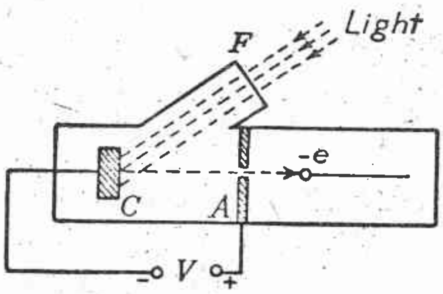


Fig. 5.—Production of photoelectrons (after Lenard). Light entering by the window F strikes the cathode C, and there liberates photoelectrons, which are accelerated (or retarded) in the field between C and A.

$$E = h\nu - A,$$

where A is a constant characteristic of the metal.

From the standpoint of the light quantum hypothesis, both these results can be understood at once. Every light quantum striking the metal and colliding with one of its electrons hands over its whole energy to the electron, and so knocks it out of the metal; before it emerges however, the electron loses a part of this energy equal in amount to the work, A, required to remove it from the metal. The number of electrons expelled is equal to the number of incident light quanta, and this is given by the intensity of the light falling on the metal.

Evidence even more patent for the existence of light quanta is given by the classic experiments of E. Meyer and W. Gerlach (1914) on the photoelectric effect with the small particles of metal dust; by irradiation of these with ultra-violet light photoelectrons are again liberated, so that the metallic particles become positively charged. The advance on the previous case consists in this, that we can now observe the time relations in the process of charging the particles, by causing them to become suspended in an electric field, as in Millikan's droplet method for determining e, the elementary electric charge; a fresh emission of a photoelectron is then shown by the acceleration caused by the increase of charge.

If we start from the hypothesis that the incident light actually represents an electromagnetic alternating field, we can deduce from the size of the particles the time that must elapse before a particle of metal can have taken from this field by absorption the quantity of energy which is required for the release of an electron. These times are of the order of magnitude of some seconds; if the classical theory of light were correct, a photoelectron could in no case be emitted before the expiry of this time after starting the irradiation. But the experiment when carried out proved on the contrary that the emission of photoelectrons set in immediately the irradiation began—a result which is clearly unintelligible except on the basis of the idea that light consists of a hail of light quanta, which can knock out an electron the moment they strike a metal particle.

3. Quantum Theory of the Atom.

Planck's original quantum hypothesis was that to every spectral line there corresponds a harmonic oscillator of definite frequency ν which cannot, as in the classical theory, absorb or emit an arbitrary quantity of energy, but only integral multiples of $h\nu$. Niels Bohr (1913) made the great advance of elucidating the connexion of these "oscillators" with one another and with the structure of the atom. He dropped the idea that the electrons actually behave like oscillators, i.e. that they are quasi-elastically bound. His leading thought was something like this. The atom does not behave like a classical mechanical system, which can absorb energy in portions which are arbitrarily small. From the fact of the existence of sharp emission and absorption lines on the one hand, and from Einstein's light quantum hypothesis on the other, it seems preferable to infer that the atom can exist only in definite *discrete stationary states*, with energies E_0, E_1, $E_2, \ldots$ Thus only those spectral lines can be absorbed for which $h\nu$ has exactly such a value that it can raise the atom from one stationary state to a higher one; the *absorption lines* are therefore defined by the equations $E_1 - E_0 = h\nu_1$, $E_2 - E_0 = h\nu_2, \ldots$, where

E_0 is the energy of the lowest state in which the atom exists in the absence of special excitation.

If the atom is excited by any process, i.e. if it is raised to a state with energy $E_n > E_0$, it can give up this energy again in the form of radiation. It can in fact radiate all those quanta whose energy is equal to the difference of the energies of two stationary states. The emission lines are therefore given by the equation

$$E_n - E_m = h\nu_{nm}.$$

A direct confirmation of this theory can be seen in the following fact. If Bohr's hypothesis is correct, an excited atom has open to it various possible ways of falling back to the ground state by giving up energy as radiation. For example, an atom in the third excited state can either give up its excess of energy relative to the ground state in one elementary process by radiating a line of the frequency ν_{30}; or it can begin with a transition into the first excited state with the energy E_1 and surrender of the energy quantum $h\nu_{31}$, and then in a second radiation process (frequency ν_{10}) fall back into the ground state; and so on (fig. 6). Since the total energy radiated must always be the same, viz. $E_3 - E_0$, the following relation must always exist between the radiated frequencies:

$$\nu_{30} = \nu_{31} + \nu_{10} = \nu_{32} + \nu_{20} = \nu_{32} + \nu_{21} + \nu_{10}.$$

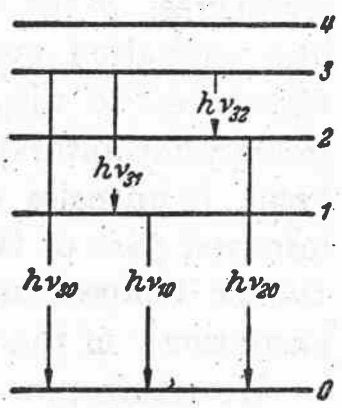


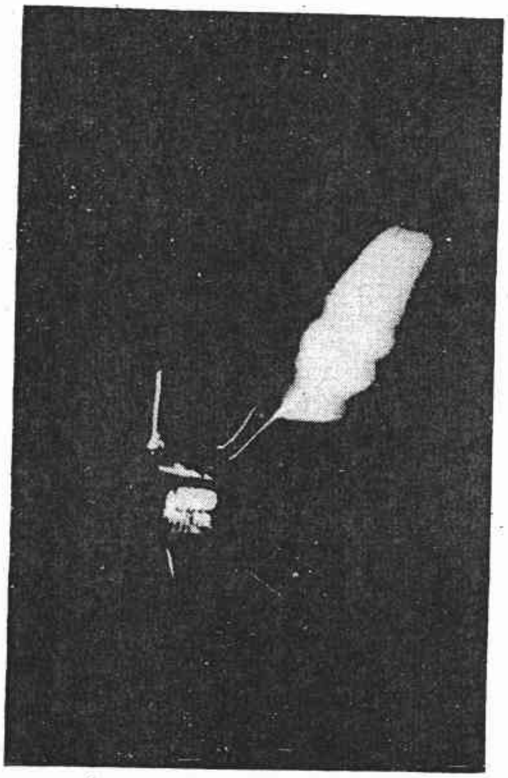
Fig. 6.—Ritz's Combination Principle. An atom in the third excited state can radiate its energy either in the form of a single light quantum of frequency ν_{30}, or as two quanta, the sum of whose frequencies must be exactly ν_{30}.

This *combination principle* must of course hold in all cases, and is a deduction from the theory which can easily be put to the test of experiment. Historically, it is true, the order of these two aspects of the matter was reversed; for Ritz, eight years before Bohr's theory was propounded, deduced this combination principle from collected spectroscopic material which had been obtained by experiment. It is by no means the case, however, that all possible "combination lines" do actually occur with perceptible intensity.

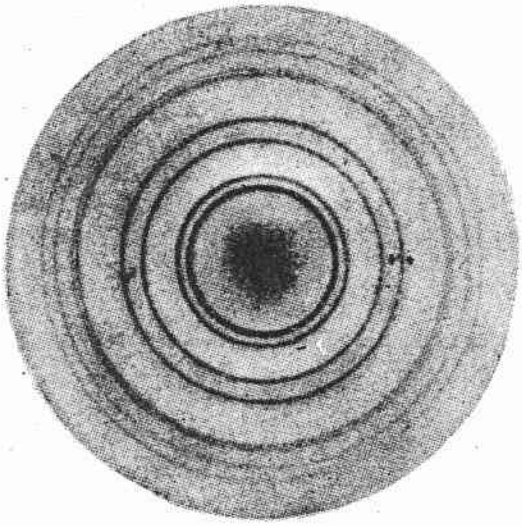
Further direct confirmation of Bohr's theory on the existence of discrete energy levels in the atom was given by the experiments of Franck and Hertz (1914). If the atoms are supplied with energy in any way, e.g. by electronic collision, i.e. by bombarding the atom with electrons, then the atoms can only take up such portions of energy as exactly correspond to an excitation energy of the atoms.

Thus, if we bombard the atoms with electrons whose kinetic energy is less than the first excitation energy of the atoms, no communication of energy from the colliding electron to the atom takes place at all (beyond the trifling amount of energy which is transferred in accordance with the laws of elastic collision, and shows itself only in the kinetic energy of the relative motion of the partners in the collision). With respect to collisions of no great strength the atoms are therefore stable in the ground state. Among such slight collisions are those which a gas atom is subjected to in consequence of the thermal motion of the particles of the gas. This is easily verified, roughly, as follows. The mean kinetic energy of a gas particle, by the results of the first chapter, is given by $\overline{E} = \frac{3}{2}kT$, where $k = R/N_0 = 1{\cdot}37 \times 10^{-16}$ erg/degree; if the whole of this energy were converted at a collision into excitation energy, the energy quantum $h\nu = \frac{3}{2}kT$ would be transferred to the particle struck; where, if we take $T = 300°$ K. (room temperature), ν will be 10^{13} sec^{-1} approximately. On the other hand, frequencies of absorption lines in the visible or even in the infra-red part of the spectrum have values about 10^{14} to 10^{15} sec^{-1}. Higher temperatures will therefore be necessary before "thermal excitation" of the atoms of the gas becomes possible.

We return now to the collision experiments of Franck and Hertz. We see that if the energy E of the electrons is less than the first excitation energy $E_1 - E_0$, the atoms remain in the ground state. If E becomes greater than $E_1 - E_0$, but remains less than $E_2 - E_0$, the atom can be brought by the collision into the first excited state, and consequently when it falls back into the ground state radiates only the line $\nu_1 = \nu_{10}$. If $E + E_0$ lies between E_2 and E_3, the atom which is struck can pass into either the first or the second excited state, and so can radiate the lines ν_{20}, ν_{21}, and ν_{10}; and similarly in other cases (figs. 7*a*, 7*b*, Plate VIII opposite). But we can also measure the energies of the electrons after the collision, by causing them to enter an opposing field of known potential difference, and observing the number of electrons which pass through it. In this way also the energy relation was found to be fulfilled exactly to this extent, that the energy loss of the electron due to the collision with an atom was just equal to an excitation energy $E_n - E_0$ of the atom.



Ch. III, Fig. 11.—Transmutation of lithium on bombardment with protons. Pairs of α-particles are shot out in opposite directions (see p. 71). (From *Proc. Roy. Soc.* A, Vol. 141.)



Ch. IV. Fig. 9.—Diffraction of electrons by thin silver foil. (After H. Mark and R. Wierl.) The velocity of the electrons (accelerating potential 36 kilovolts) corresponds to a de Broglie wave-length of 0·0645 Å. (Exposure $\frac{1}{10}$ sec.) (See p. 93.)

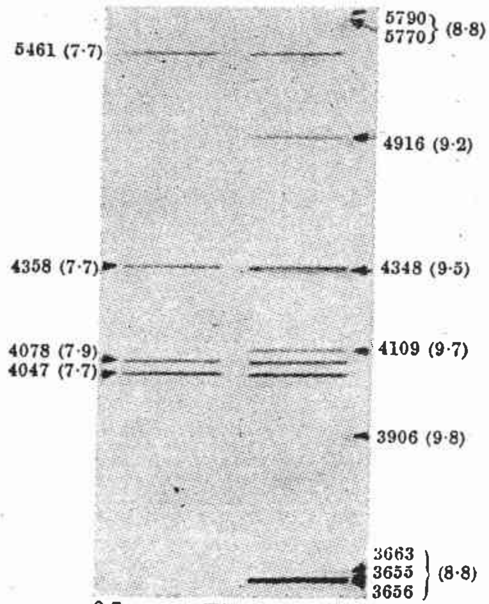


Fig. 7a

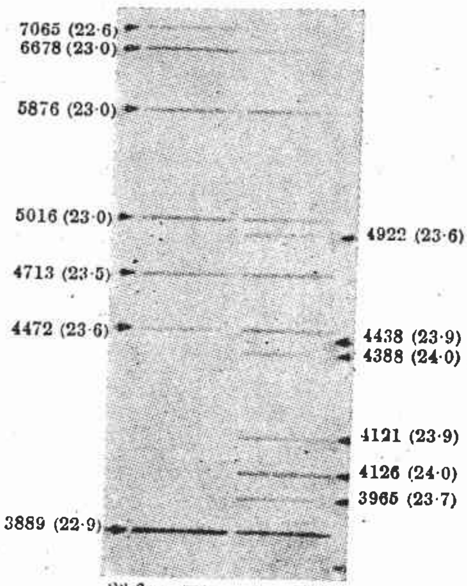


Fig. 7b

Ch. IV, Figs. 7a, 7b.—Excitation of spectral lines by electronic collision (after Hertz). Only those lines appear in the spectrum whose excitation potential (the number in brackets) is smaller than the energy of the electrons (given under the spectra). Fig. 7a refers to mercury, 7b to helium. The wave-lengths are stated in Å (see p. 86).

4. Compton Effect.

The phenomena described up to this point prove only that energy exchange between light and atoms, or between electrons and atoms, takes place by quanta. The *corpuscular nature* of light itself is proved in the most obvious way by the laws of *frequency change in the scattering of X-rays.* We have in an earlier chapter (Chap. III, p. 59) discussed the classical theory of the scattering of X-rays at comparatively weakly bound (nearly free) electrons, and reached the result that the scattered radiation has always the same frequency ν as the primary radiation; for the electron vibrates in the same rhythm as the electric vector of the incident wave and, like every oscillating dipole, generates a secondary wave of equal frequency.

Compton (1922) investigated the scattering of X-rays by a block of paraffin, and found that the radiation scattered at an angle of less than 90° possesses a greater wave-length than the primary radiation, so that the ν' of the scattered wave, contrary to the prediction of the classical theory, is smaller than the ν of the incident radiation. On the principles of the wave theory, this phenomenon is unintelligible.

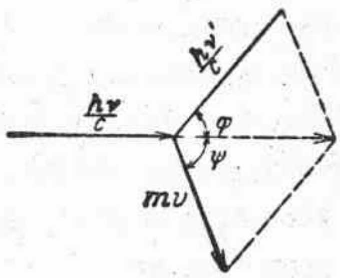


Fig. 8.—Compton Effect. A light quantum on colliding with an electron transfers part of its energy to the latter, and its wave-length becomes greater after the scattering.

The result, however, can be explained at once (Compton and Debye) if, taking the corpuscular point of view, we regard the process as one of elastic collision of two particles, the electron and the light quantum (fig. 8). For if the light quantum $h\nu$ strikes an electron, it will communicate kinetic energy to the electron, and therefore will itself lose energy. The scattered light quantum will therefore have a smaller energy $h\nu'$. The exact calculation of the energy loss proceeds as in the case of the collision of two elastic spheres; the total momentum must be the same after the collision as before, likewise the total energy. The full calculation is given in Appendix X, p. 380; here we merely quote the result. The *Compton formula* for the change of wave-length of the light quantum due to the scattering process runs:

$$\Delta\lambda = 2\lambda_0 \sin^2 \frac{\phi}{2},$$

$$\left(\lambda_0 = \frac{h}{mc} = 0{\cdot}0242 \text{ Å., the Compton wave-length}\right).$$

The increase in the wave-length is accordingly independent of the wave-length itself, and depends only on ϕ, the angle of scattering. The theory is found to be thoroughly in accord with the facts. In the first place, Compton himself confirmed that the change of wave-length is correctly given by the Compton formula. The recoil electrons, which according to the theory are necessarily produced in the scattering process, and take over the energy loss $h\nu - h\nu'$ of the light quanta in the form of kinetic energy, were successfully demonstrated by Compton; and that not only in scattering by solid bodies, but also in the Wilson chamber, where the tracks of the recoil electrons can be seen directly.

But, as has been shown by Compton and Simon, we can take a further step and test experimentally the relation between the angles of scattering ϕ and ψ of the light quantum and the electron. Certainly a light quantum shows no track in the cloud chamber, but all the same we can determine the direction of the scattered quantum, provided it is scattered a second time and again liberates a recoil electron, the direction of the scattered quantum being found as that of the line joining the initial points of the tracks of the two recoil electrons. Although there is a considerable amount of uncertainty in the interpretation of the experiment, owing to the fact that several tracks may be present, and it is not always possible to determine a pair uniquely as corresponding to each other in the foregoing sense (i.e. produced by one and the same quantum), still Compton and Simon were able to establish agreement between theory and experiment with a fair amount of certainty.

Further confirmation of our ideas about the mechanism of the Compton effect was produced by Bothe and Geiger. They caused X-rays to be scattered in hydrogen, and with a Geiger counter recorded when recoil electrons made their appearance; by means of a second counter they determined the instants at which scattered light quanta appeared. They succeeded in this way in establishing that the emission of the recoil electrons took place at the same moment as the scattering of the light quantum.

Investigations by Bothe, Jacobsen and others (1936) first definitely confirmed the simultaneous appearance of the recoiling light quantum and electron.

In the Compton scattering we have therefore a typical example of a process in which radiation behaves like a corpuscle of well-defined energy and momentum; an explanation by the wave theory of the experimental results which we have described seems absolutely impossible. On the other hand, interference phenomena are quite irreconcilable with the corpuscular view of radiation.

5. Wave Nature of Matter. De Broglie's Theory.

The dilemma was still further intensified when in 1925 de Broglie propounded the hypothesis that the same dualism of wave and corpuscle as is present in light may also occur in matter. A material particle will have a matter wave corresponding to it, just as a light quantum has a light wave; and in fact the connexion between the two opposing aspects must again be given by the relation $E = h\nu$. Further, since from the standpoint of the theory of relativity energy and momentum are entities of the same kind (momentum is the spatial part of a relativistic four-vector, whose time component is energy), it is obviously suggested that for consistency we should write $p = h\kappa$; if ν denotes the number of vibrations per unit time, κ must signify the number of waves per unit length, and therefore be equal to the reciprocal of the wave-length λ of the wave motion; hence

$$p = \frac{h}{\lambda}.$$

The extension of the wave idea from optics to mechanics can be carried through consistently. Before we go into this, however, we should like once more to point out the " irrationality " (as Bohr called it) involved in thus connecting the corpuscular and wave conceptions: E and p refer to a point mass of vanishingly small dimensions; ν and κ, on the contrary, to a wave which is infinitely extended in space and time. The imagination can scarcely conceive two ideas which appear less capable of being united than these two, which the quantum theory proposes to bring into such close connexion. The solution of this paradox will occupy us later.

We shall first develop de Broglie's theory further from a formal point of view. A particle of momentum p in the direction of the x-axis and energy E is to be associated, then, with an infinitely extended wave of the form $u(x, t) = Ae^{2\pi i(\nu t - \kappa x)}$ by means of the two relations

$$E = h\nu, \quad p = h\kappa.$$

This wave advances through space with a definite velocity, the *phase* *velocity u.* The value of u we can find at once, by considering the (plane) surfaces of constant phase, viz.

$$\phi \equiv \nu t - \kappa x = \text{const.}, \quad \text{or} \quad x = \frac{\nu}{\kappa} t + \text{const.};$$

it follows that

$$u = \left(\frac{dx}{dt}\right)_{\varphi=\text{const.}} = \frac{\nu}{\kappa} = \nu\lambda.$$

Since ν is in general a function of λ, and conversely, this equation embodies the law of *dispersion of the waves.*

But it must be remarked that the phase velocity is a purely artificial concept, inasmuch as it cannot be determined experimentally. In fact, to measure this velocity it would be necessary to affix a mark to the infinitely extended smooth wave, and to measure the velocity of the mark. But the only way in which we can make a mark on the wave train is by superimposing other wave trains upon it, which mutually reinforce each other at a definite place, and so create a hump in the smooth wave function. We have now to determine the velocity with which this hump moves; it is called the *group-velocity.*

A general method is given in Appendix XI (p. 382); here we confine ourselves to a simple special case, which gives the same result, and brings out the difference between phase-velocity and group-velocity with particular clearness. On the primary wave, which we suppose to have the form of $u(x, t)$ above, we superimpose a wave with the same amplitude and a slightly different frequency ν' and wave-length λ'. In this case, as we know, "beat" phenomena occur, and we make use of one of the beat maxima as the mark in our wave train. What we are interested in, then, is the velocity with which the beat maximum moves.

The superposition of the two wave trains gives us mathematically a vibration of the form

$$u(x, t) = e^{2\pi i(\nu t - \kappa x)} + e^{2\pi i(\nu' t - \kappa' x)}.$$

This expression can be written

$$\begin{aligned} u(x, t) &= e^{2\pi i\left(\frac{\nu+\nu'}{2}t - \frac{\kappa+\kappa'}{2}x\right)}\left\{e^{2\pi i\left(\frac{\nu-\nu'}{2}t - \frac{\kappa-\kappa'}{2}x\right)} + e^{-2\pi i\left(\frac{\nu-\nu'}{2}t - \frac{\kappa-\kappa'}{2}x\right)}\right\} \\ &= 2\cos 2\pi\left(\frac{\nu-\nu'}{2}t - \frac{\kappa-\kappa'}{2}x\right) e^{2\pi i\left(\frac{\nu+\nu'}{2}t - \frac{\kappa+\kappa'}{2}x\right)}. \end{aligned}$$

It therefore represents a vibration of frequency $(\nu + \nu')/2$ and wave-length $2/(\kappa + \kappa')$, the amplitude of which varies slowly (beats) relative to the vibration itself. The phase, as we deduce at once from the formula, moves with the velocity $(\nu + \nu')/(\kappa + \kappa')$. On the other hand, the maximum of the amplitude moves with the velocity $(\nu - \nu')/(\kappa - \kappa')$. In the limit when ν' tends to ν, and therefore κ' to κ, we find from this the value already found for the phase-velocity

$$u = \frac{\nu}{\kappa} = \nu\lambda,$$

while the group-velocity is given by the limiting value

$$U = \lim_{\nu' \to \nu} \frac{\nu - \nu'}{\kappa - \kappa'}.$$

But this is simply, by definition, the derivative (differential coefficient) of the frequency ν with reference to the wave-number κ, if we regard ν as a function of κ (law of dispersion); hence we have

$$U = \frac{d\nu}{d\kappa} = \frac{d\nu}{d(1/\lambda)}.$$

As is shown in Appendix XI (p. 382), this expression for the group-velocity holds perfectly generally.

We now apply these formulæ to the case of a *free particle* with velocity v. Writing β for v/c, and employing the relativistic formulæ for energy and momentum (see p. 372), we have here

$$\nu = \frac{E}{h} = \frac{m_0 c}{h} \frac{c}{\sqrt{(1 - \beta^2)}}, \quad \kappa = \frac{p}{h} = \frac{m_0 c}{h} \frac{\beta}{\sqrt{(1 - \beta^2)}}.$$

The phase-velocity is given by

$$u = \frac{\nu}{\kappa} = \frac{c}{\beta} = \frac{c^2}{v},$$

and is therefore greater than the velocity of light c, if the particle's velocity is less than c. The phases of the matter wave are therefore propagated with a velocity exceeding that of light—another indication that the phase-velocity has no physical significance. For the group-velocity we find

$$U = \frac{d\nu}{d\kappa} = \frac{d\nu}{d\beta} \Big/ \frac{d\kappa}{d\beta};$$

it is exactly equal to the particle's velocity, for

$$\frac{d\nu}{d\beta} = \frac{m_0 c}{h} \frac{c\beta}{(1-\beta^2)^{3/2}},$$

$$\frac{d\tau}{d\beta} = \frac{m_0 c}{h} \frac{1}{(1-\beta^2)^{3/2}},$$

and therefore $U = c\beta = v$.

The relationship thus brought out is very attractive; in particular it tempts us to try to interpret a particle of matter as a wave packet due to the superposition of a number of wave trains. This tentative interpretation, however, comes up against insurmountable difficulties, since a wave packet of this kind is in general very soon dissipated. We need only consider the corresponding case in water waves. If we produce a wave crest at any point of an otherwise smooth surface, it is not long before it spreads out and disappears.

6. Experimental Demonstration of Matter Waves.

In view of the boldness of de Broglie's hypothesis, that matter is to be regarded as a wave process, the question of course at once suggested itself, whether and in what way the hypothesis could be put to the test of experiment. The first answer was given by Einstein (1925), who pointed out that the wave idea gives a simple explanation of the *degeneracy of electrons in metals*, which expresses itself in the abnormal behaviour of metals in regard to their specific heat, and as an experimental fact was known to theoretical physicists before de Broglie. The subject will be discussed in detail in Chapter VII (§ 7, p. 237)

Further, it was known from the investigations of Davisson and Germer (1927) that in the reflection of beams of electrons by metals deviations occurred from the result to be expected on classical principles, more electrons being reflected in certain directions than in others, so that at certain angles a sort of selective reflection took place. The conjecture was first propounded by Elsasser (1925) that we have before us here a diffraction effect of electronic waves in the metallic lattice, similar to that which occurs in X-ray interference in crystals (p. 80). The exact investigations which were then undertaken by Davisson and Germer actually gave interference phenomena in precisely the same form as the known Laue interference with X-rays.

Further experiments by G. P. Thomson, Rupp and others showed that when beams of electrons are made to pass through thin foils (metals, mica), diffraction phenomena are obtained, of the same kind as the Debye-Scherrer rings in X-ray interferences (fig. 9, Plate VIII, p. 86). Moreover, when the conditions of interference and the known lattice distances were used as data, it was found that de Broglie's relation between wave-length and the momentum of the electrons was completely confirmed.

The following rough calculation gives an indication of the kind of wave-lengths we have to deal with in beams of electrons. According to de Broglie, we have $\lambda = h/p$ or, if we confine ourselves to electrons of not too high speed, so that we can leave relativistic corrections out of account, $\lambda = h/mv$. On the other hand, the velocity of the electrons is determined by the potential V applied to the cathode tube: $\frac{1}{2}mv^2 = eV$. Hence $\lambda = h/\sqrt{(2meV)}$, or, on inserting the numerical values ($e = 4{\cdot}80 \times 10^{-10}$ e.s.u., $m = 9{\cdot}1 \times 10^{-28}$ gm., $h = 6{\cdot}62 \times 10^{-27}$ erg. sec.), $\lambda = \sqrt{(150/V)}$ Å., when V is expressed in volts. Thus, to an accelerating potential of 10,000 volts there corresponds a wave-length of 0·122 Å.; the wavelengths of the electronic beams employed in practice therefore lie in approximately the same region as those of hard X-rays.

Although it is astonishing that the discovery of the diffraction of electrons was not made earlier, the fact must nevertheless be considered a piece of great good fortune for the development of atomic theory. What confusion there would have been if, soon after the discovery of cathode rays, experiments had been undertaken simultaneously on their charge and capability of deflection, and on their possibilities in regard to interference! Again, Bohr's theory of the atom, which later was to serve as the foundation of the expansion of atomic theory into wave mechanics, was essentially based on the assumption that the electron is an electrically charged corpuscle.

To-day the technique of electronic diffraction is so far advanced that it is employed in industry instead of the earlier methods with X-rays for the purposes of research on materials. One advantage of using electrons is that decidedly higher intensities are available than there are with X-rays. Thus, for example, an interference photograph which may require an exposure of many hours with X-rays can be produced by means of electrons, with the same working data, in something like one second. Another advantage is that the wave-length of the beams of electrons can be varied at will by changing the tube potential; if the setting of the potentiometer is changed, it can be seen at once on the screen how the whole diffraction image contracts or expands according as the wave-length is made shorter or longer. The third and most important advantage of electronic rays is their deflectability by electric and magnetic fields. There is no known method of constructing lenses for X-rays; but by proper arrangement of condensers and magnetic coils one can focus electronic beams (Busch, 1927), and construct lenses and microscopes. Owing to the short wave-length the resolving power is much higher than for optical instruments; and the theoretical limit is much higher still.

Similarly the wave nature of matter can be demonstrated for the case of slow neutrons and the diffraction patterns resulting from the scattering of neutrons can give considerable information about the crystalline structure of solids. Neutrons have a magnetic moment, so that the scattering is sensitive to the magnetic structure of the scattering material. For thermal neutrons (i.e. neutrons with an energy corresponding to a temperature of 300° K.), the de Broglie wavelength is $\lambda = 1{\cdot}81$ Å.

Very important and impressive was the discovery of Stern and his collaborators (1932) that *molecular rays* (of H_2 and He) also show diffraction phenomena when they are reflected at the surfaces of crystals. It was even possible to separate a beam of molecules of nearly uniform velocity with the help of a device similar to the arrangement for measuring the velocity of light: two toothed wheels rotating on the same axis. De Broglie's equation was confirmed for these particles with an accuracy of about 1 per cent. Here, surely, we are dealing with material particles, which must be regarded as the elementary constituents not only of gases but also of liquids and solids. If we intercept the molecular ray after its diffraction at the crystal lattice, and collect it in a receiving vessel, we find in the vessel a gas which has still the ordinary properties.

These diffraction experiments on whole atoms show that the wave structure is not a property peculiar to beams of electrons, but that there is a general principle in question; classical mechanics is replaced by a new *wave mechanics*. For, in the case of an atom, it is clearly the centroid of all its particles (nucleus and electrons), i.e. an abstract point, which satisfies the same wave laws as the individual free electron. Wave mechanics in its developed form does actually render an account of this.

7. The Contradiction between the Wave Theory and the Corpuscular Theory, and its Removal.

In the preceding sections we have had a series of facts brought before us which seem to indicate unequivocally that not only light, but also electrons and matter, behave in some cases like a wave process, in other cases like pure corpuscles. How are these contradictory aspects to be reconciled?

To begin with, Schrödinger attempted to interpret corpuscles, and particularly electrons, as *wave packets*. Although his formulæ are entirely correct, his interpretation cannot be maintained, since on the one hand, as we have already explained above, the wave packets must in course of time become dissipated, and on the other hand the description of the interaction of two electrons as a collision of two wave packets in ordinary three-dimensional space lands us in grave difficulties.

The interpretation generally accepted at present was put forward by Born. According to this view, the whole course of events is determined by the laws of probability; to a state in space there corresponds a definite probability, which is given by the de Broglie wave associated with the state. A mechanical process is therefore accompanied by a wave process, the guiding wave, described by Schrödinger's equation, the significance of which is that it gives the probability of a definite course of the mechanical process. If, for example, the amplitude of the guiding wave is zero at a certain point in space, this means that the probability of finding the electron at this point is vanishingly small.

The physical justification for this hypothesis is derived from the consideration of scattering processes from the two points of view, the corpuscular and the undulatory. The problem of the scattering of light by small particles of dust or by molecules, from the standpoint of the classical wave theory, was worked out long ago. If the idea of light quanta is to be applied, we see at once that the number of incident light quanta must be put proportional to the intensity of the light at the place concerned, as calculated by the wave theory. This suggests that we should attempt (Born, 1926) to calculate the scattering of electrons by atoms, by means of wave mechanics. We think of an incident beam of electrons as having a de Broglie wave associated with it. When it passes over the atom this wave generates a secondary spherical wave; and analogy with optics suggests that a certain quadratic expression formed from the wave amplitude should be interpreted as the current strength, or as the number of scattered electrons. On carrying out the calculation (Wentzel, Gordon) it has been found that for scattering by a nucleus we get exactly Rutherford's formula (p. 62; Appendix IX, p. 377, and XX, p. 406). Many other scattering processes were afterwards subjected to calculation in this way, and the results found in good agreement with observation (Born, Bethe, Mott, Massey). These are the grounds for the conviction of the correctness of the principle of associating wave amplitude with number of particles (or probability).

In this picture the particles are regarded as independent of one another. If we take their mutual action into account, the pictorial view is to some extent lost again. We have then two possibilities. Either we use waves in spaces of more than three dimensions (with two interacting particles we would have $2 \times 3 = 6$ co-ordinates), or we remain in three-dimensional space, but give up the simple picture of the wave amplitude as an ordinary physical magnitude, and replace it by a purely abstract mathematical concept (the second quantisation of Dirac, Jordan) into which we cannot enter. Neither can we discuss the extensive formalism of the quantum theory which has arisen from this theory of scattering processes, and has been developed so far that every problem with physical meaning can in principle be solved by the theory (Appendix XXV, p. 426). What, then, is a problem with physical meaning? This is for us the really important question, for clearly enough the corpuscular and wave ideas cannot be fitted together in a homogeneous theoretical formalism, without giving up some fundamental principles of the classical theory. The unifying concept is that of probability; this is here much more closely interwoven with physical principles than in the older physics (e.g. the kinetic theory of gases, § 2, p. 3; § 6, p. 9). The elucidation of these relationships we owe to Heisenberg and Bohr (1927). According to them we must ask ourselves what after all it means when we speak of the description of a process in terms of corpuscles or in terms of waves. Hitherto we have always spoken of waves and corpuscles as given facts, without giving any consideration at all to the question whether we are justified in assuming that such things actually exist. The position has some similarity to that which existed at the time the theory of relativity was brought forward. Before Einstein, no one ever hesitated to speak of the *simultaneous* occurrence of two events, or ever stopped to consider whether the assertion of the simultaneity of two events at different places can be established physically, or whether the concept of simultaneity has any meaning at all. In point of fact Einstein proved that this concept must be " relativized ", since two events may be simultaneous in one system of reference, but take place at different times in another. In a similar way, according to Heisenberg, the concepts corpuscle and wave must also be subjected to close scrutiny. With the concept of corpuscle, the idea is necessarily bound up that the thing in question possesses a perfectly definite momentum, and that it is at a definite place at the time considered. But the question arises: can we actually determine exactly both the position and the velocity of the " particle " at a given moment? If we cannot do so—and as a matter of fact we cannot—i.e. if we can never actually determine more than one of the two properties (possession of a definite position and of a definite momentum), and if when one is determined we can make no assertion at all about the other property for the same moment, so far as our experiment goes, then we are not justified in concluding that the "thing" under examination can actually be described as a particle in the usual sense of the term. We are equally unjustified in drawing this conclusion even if we can determine both properties simultaneously, if neither can then be determined exactly, that is to say, if from our experiment we can only infer that this "thing" is somewhere within a certain definite volume and is moving in some way with a velocity which lies within a certain definite interval. We shall show later by means of examples that the simultaneous determination of position and velocity is actually impossible, being inconsistent with quantum laws securely founded on experiment.

The ultimate origin of the difficulty lies in the fact (or philosophical principle) that we are compelled to use the words of common language when we wish to describe a phenomenon, not by logical or mathematical analysis, but by a picture appealing to the imagination. Common language has grown by everyday experience and can never surpass these limits. Classical physics has restricted itself to the use of concepts of this kind; by analysing visible motions it has developed two ways of representing them by elementary processes: moving particles and waves. There is no other way of giving a pictorial description of motions—we have to apply it even in the region of atomic processes, where classical physics breaks down.

Every process can be interpreted either in terms of corpuscles or in terms of waves, but on the other hand it is beyond our power to produce proof that it is actually corpuscles or waves with which we are dealing, for we cannot simultaneously determine all the other properties which are distinctive of a corpuscle or of a wave, as the case may be. We can therefore say that the wave and corpuscular descriptions are only to be regarded as complementary ways of viewing one and the same objective process, a process which only in definite limiting cases admits of complete pictorial interpretation. It is just the limited feasibility of measurements that defines the boundaries between our concepts of a particle and a wave. The corpuscular description means at bottom that we carry out the measurements with the object of getting exact information about momentum and energy relations (e.g. in the Compton effect), while experiments which amount to determinations of place and time we can always picture to ourselves in terms of the wave representation (e.g. passage of electrons through thin foils and observations of the deflected beam).

We shall now give the proof of the assertion that position and momentum (of an electron, for instance) cannot be exactly determined simultaneously. We illustrate this by the example of diffraction through a slit (fig. 10). If we propose to regard the passage of an electron through a slit and the observation of the diffraction pattern as simultaneous measurement of position and momentum from the standpoint of the corpuscle concept, then the breadth of the slit gives the "uncertainty" Δx, in the specification of position perpendicular to the direction of flight. For the fact that a diffraction pattern appears merely allows us to assert that the electron has passed through the slit; at what place in the slit the passage took place remains quite indefinite. Again, from the standpoint of the corpuscular theory, the occurrence of the diffraction pattern on the screen must be understood in the sense that the individual electron suffers deflection at the slit, upwards or downwards. It acquires component momentum perpendicular to its original direction of flight, of amount Δp (the resultant momentum p remaining constant). The mean value of Δp, by fig. 10, is given by $\Delta p \sim p \sin \alpha$, if α is the mean angle of deflection. We know that the experimental results can be explained satisfactorily on the basis of the wave representation, according to which α is connected with the slit-width Δx and the wave-length $\lambda = h/p$ by the equation $\Delta x \sin \alpha \sim \lambda = h/p$. Thus the mean added momentum in the direction parallel to the slit is given by the relation $\Delta p \sim p\, \lambda/\Delta x = h/\Delta x$, or

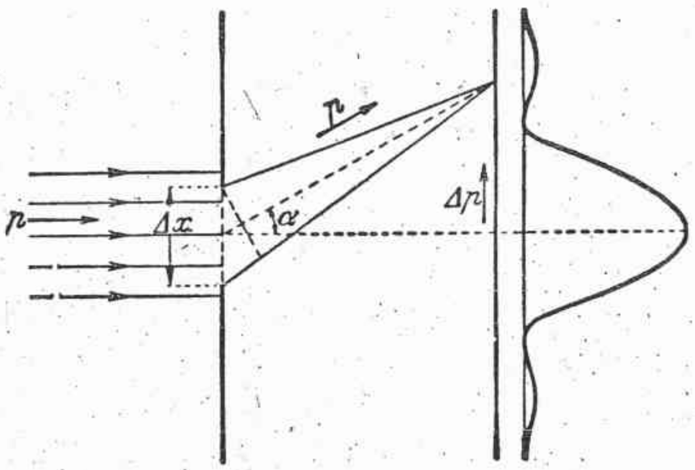


Fig. 10.—Diffraction of electrons at a slit

$$\Delta x \, \Delta p \sim h.$$

This relation, for which a more rigorous derivation will be given in Appendix XII, p. 383, is called *Heisenberg's uncertainty relation*. In our example, therefore, it signifies that, as the result of the definition of the electron's position by means of the slit, which involves the uncertainty (or possible error) Δx, the particle acquires momentum parallel to the slit of the order of magnitude stated (i.e. with the indicated degree of uncertainty). Only subject to this uncertainty is its momentum known from the diffraction pattern. According to the uncertainty relation, therefore, *h represents an absolute limit to the simultaneous measurement of co-ordinate and momentum*, a limit which in the most favourable case we may get down to, but which we can never get beneath. In quantum mechanics, moreover, the uncertainty relation holds generally for any arbitrary pair of "conjugated variables" (p. 385).

A second example of the uncertainty relation is the definition of position by a microscope (fig. 11). Here the order of ideas is as follows. If we wish to determine the position of an electron in the optical way by illuminating it and observing the scattered light, then it is clear, and known as a general rule in optics, that the wave-length of the light employed forms a lower limit to the resolution and accordingly to the exactness of the determination of position. If we wish to define the position as accurately as possible, we will employ light of the shortest possible wave-length (γ-rays). The employment of short-wave radiation implies, however, the occurrence of a Compton scattering process when the electron is irradiated, so that the electron experiences a recoil, which to a certain extent is indeterminate. We may investigate the circumstances mathematically. Let the electron under the miscroscope be irradiated in any direction with

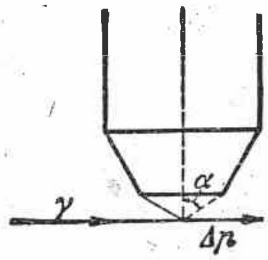


Fig. 11.—Determination of the position of an electron by means of the γ-ray microscope.

light of frequency ν. Then by the rules of optics (resolving power of the microscope) its position can only be determined subject to the possible error

$$\Delta x \sim \frac{\lambda}{\sin \alpha},$$

where α is the angular aperture. Now, according to the corpuscular view, the particle in the radiation process suffers a Compton recoil of the order of magnitude $h\nu/c$, the direction of which is undetermined to the same extent as is the direction in which the light quantum flies off after the process. Since the light quantum is actually observed in the microscope, this indeterminateness of direction is given by the angular aperture α. The component momentum of the electron perpendicular to the axis of the microscope is therefore after the process undetermined to the extent Δp, where approximately

$$\Delta p \sim \frac{h\nu}{c} \sin\alpha.$$

Thus the order of magnitude relation

$$\Delta x \, \Delta p \sim h$$

holds good here also.

Just as every determination of position carries with it an uncertainty in the momentum, and every determination of time an uncertainty in the energy (although we have not yet proved the latter statement), so the converse is also true. The more accurately we determine momentum and energy, the more latitude we introduce into the position of the particle and the time of an event. We give an example of this also, viz. the so-called *resonance fluorescence*. We have seen above (p. 85) that the atoms of a gas which is irradiated with light of frequency ν_{10}, corresponding to the energy difference between the ground state and the first excited state, are raised to the latter state. They then fall back again to the lower state, at the same time emitting the frequency ν_{10}; and if the pressure of the gas is sufficiently low, so that the number of gas-kinetic collisions which occur while the atom remains in the excited state is negligible, then the whole energy which was absorbed will again be emitted. Thus the atom behaves like a classical resonator which is in resonance with the incident light wave, and we speak of resonance fluorescence.

But the energy of excitation of the atoms can also be utilized, not for re-emission of light, but for other actions, by introducing another gas as an indicator. If the latter consists, say, of not too rigidly bound diatomic molecules, the energy transferred in collisions with the excited atoms of the first gas can be utilized for dissociation (Franck, 1922). Again, if the added gas is monatomic, and has a lower excitation level than the first gas, it is itself caused to radiate by the collisions; this is called sensitized fluorescence (Franck). In any case we see that a fraction of the atoms of the first gas is certainly thrown into the excited state by the incident light. We may take the following view of the matter. Excitation by monochromatic light means communication of exact quanta $h\nu_{10}$ to the atom. We therefore know the energy of the excited atoms exactly. Consequently, by Heisenberg's relation $\Delta E \Delta t \sim h$, the time at which the absorption takes place must be absolutely indeterminate. We can satisfy ourselves that this is so, by considering that any experiment to determine the moment in question would necessarily require a mark in the original wave train—an interruption of the train, for example. But that means disturbing the monochromatic character of the light wave, and so contradicts the hypothesis. A rigorous discussion of the circumstances shows that, if the light is kept monochromatic, the moment at which the elementary act happens does actually altogether elude observation.

The uncertainty relation can also be deduced from the following *general idea*. If we propose to build up a wave packet, extending for a finite distance in the x-direction, from separate wave trains, we need for the purpose a definite finite frequency-range in the monochromatic waves, i.e., since $\lambda = h/p$, a finite momentum-range in the particles. But it can be proved generally (Appendix XII) that the length of the wave packet is connected with the requisite range of momenta by the relation

$$\Delta p \Delta x \sim h.$$

The analogous relation

$$\Delta E \Delta t \sim h$$

can be derived in a similar way.

Bohr is in the habit of saying: the wave and corpuscular views are *complementary*. By this he means: if we prove the corpuscular character of an experiment, then it is impossible at the same time to prove its wave character, and conversely. Let us illustrate this further by an example.

Consider, say, *Young's interference experiment* with the two slits (p. 78); then we have on the screen a system of interference fringes. By replacing the screen by a photoelectric cell, we can demonstrate the corpuscular character of the light even in the fringes. It therefore appears as if we had here an experiment in which waves and particles are demonstrated simultaneously. Really, however, it is not so; for, to speak of a particle means nothing unless at least two points of its path can be specified experimentally; and similarly with a wave, unless at least two interference maxima are observed. If then we propose to carry out the "demonstration of a corpuscle", we must settle the question whether its path has gone through the upper or the lower of the two slits to the receiver. We therefore repeat the experiment, not only setting up a photoelectrically sensitive instrument as receiver, but also providing some contrivance which shows whether the light has passed through the upper slit (say a thin photographic film or the like). This contrivance in the slit, however, necessarily throws the light quantum out of its undisturbed path; the probability of getting it in the receiver (the screen) is therefore not the same as it was originally, i.e. the preliminary calculation by wave theory of the interference phenomenon is illusory. Thus, if pure interference is to be observed, we are necessarily precluded from making an observation of any point of the path of the light quantum before it strikes the screen.

We add in conclusion a few general remarks on the philosophical side of the question. In the first place it is clear that the dualism, wave-corpuscle, and the indeterminateness essentially involved therein, compel us to abandon any attempt to set up a *deterministic theory.* The *law of causality*, according to which the course of events in an isolated system is completely determined by the state of the system at time $t = 0$, loses its validity, at any rate in the sense of classical physics. In reply to the question whether a law of causation still holds good in the new theory, two standpoints are possible. Either we may look upon processes from the pictorial side, holding fast to the wave-corpuscle picture—in this case the law of causality certainly ceases to hold; or, as is done in the further development of the theory, we describe the instantaneous state of the system by a (complex) quantity ψ, which satisfies a differential equation, and therefore changes with the time in a way which is completely determined by its form at time $t = 0$, so that its behaviour is rigorously causal. Since, however, physical significance is confined to the quantity $|\psi|^2$ (the square of the amplitude), and to other similarly constructed quadratic expressions (matrix elements), which only partially define ψ, it follows that, even when the physically determinable quantities are completely known at time $t = 0$, the initial value of the ψ-function is necessarily not completely definable. This view of the matter is equivalent to the assertion that events happen indeed in a strictly causal way, but that we do not know the initial state exactly. In this sense the law of causality is therefore empty; physics is in the nature of the case indeterminate, and therefore the affair of statistics.

Phase Velocity and Group Velocity (p. 90.)

In order to give a strict proof of the relationship $U = \partial\nu/\partial\kappa$ given in the text, we in the first instance consider the most general form of a group of waves; it must have the form of a Fourier integral

$$u(x,\ t) = \int a(\kappa)e^{2\pi i(\nu t - \kappa x)}d\kappa,$$

where $\nu = \nu(\kappa)$ is to be regarded as a function of the wave-number κ.

We now assume that the group is very narrow, so that in the integral there occur only those waves of finite amplitude whose wave-numbers differ from the mean wave-number κ_0 by a very small amount. If we put $\kappa = \kappa_0 + \kappa_1$, $\nu(\kappa) = \nu_0 + \nu_1(\kappa_1)$, and $a(\kappa_0 + \kappa_1) = b(\kappa_1)$, the wave-group may be written in the form

$$u(x,\ t) = A(x,\ t)e^{2\pi i(\nu_0 t - \kappa_0 x)},$$

where

$$A(x,\ t) = \int b(\kappa_1)e^{2\pi i(\nu_1 t - \kappa_1 x)}d\kappa_1.$$

Hence the wave-group may be regarded as a single wave of frequency ν_0, wave-number κ_0, and amplitude $A(x,\ t)$ varying from point to point and moment to moment. This assumption is justified, as according to our assumption $A(x,\ t)$ is a function which varies only slowly compared with the exponential function $e^{2\pi i(\nu_0 t - \kappa_0 x)}$; to a first approximation it varies in the rhythm of a mean of the beat frequencies ν_1, which are very small compared with ν_0.

The velocity with which a definite value of the amplitude $A(x,\ t,)$

e.g. its maximum, advances with the wave is called the group velocity. This is accordingly found from the relation

$$\frac{\partial A}{\partial x}\frac{dx}{dt}+\frac{\partial A}{\partial t}=0$$

obtained by differentiating the equation $A(x, t) = \text{const.}$ with respect to the time. If we call the group velocity U to distinguish it from the phase velocity, we have

$$U=\left(\frac{dx}{dt}\right)_{A=\text{const.}}=-\frac{\partial A/\partial t}{\partial A/\partial x}.$$

Now obviously

$$\frac{\partial A}{\partial t}=2\pi i\int b(\kappa_1)\nu_1 e^{2\pi i(\nu_1 t-\kappa_1 x)}d\kappa_1,$$

$$\frac{\partial A}{\partial x}=-2\pi i\int b(\kappa_1)\kappa_1 e^{2\pi i(\nu_1 t-\kappa_1 x)}d\kappa_1.$$

As we have assumed that the group is confined to a very narrow range of wave-length, we can expand $\nu_1(\kappa_1)$ in powers of κ_1:

$$\nu_1(\kappa_1)=\nu(\kappa)-\nu_0=\left(\frac{d\nu}{d\kappa}\right)_0\kappa_1+\ldots.$$

Hence

$$\frac{\partial A}{\partial t}=-\left(\frac{d\nu}{d\kappa}\right)_0\frac{\partial A}{\partial x},$$

and for the group velocity we accordingly have

$$U=\frac{d\nu}{d\kappa},$$

while the phase velocity is given by

$$u=\frac{\nu}{\kappa}.$$

Elementary Derivation of Heisenberg's Uncertainty Relation (p. 98).

We consider a wave packet of finite width. For the sake of simplicity we represent its amplitude at any moment by a Gauss error function (such as actually occurs in the ground state of the harmonic oscillator, Appendices XVI, p. 396, and XXXIX, p. 471):

$$f(x) = Ae^{-x^2/a^2};$$

then Δx the half-width is given by

$$\Delta x = \sqrt{\left(\overline{x^2}\right)} = \sqrt{[\int x^2 f^2(x)dx / \int f^2(x)dx]} = \tfrac{1}{2}a.$$

The Fourier representation of $f(x)$ is

$$f(x) = \int_{-\infty}^{\infty} \phi(\kappa)e^{2\pi i\kappa x}d\kappa,$$

where

$$\phi(\kappa) = \int_{-\infty}^{\infty} f(x)e^{-2\pi i\kappa x}dx$$

is the amplitude of a partial harmonic wave with the wave number κ. Introducing the expression of $f(x)$ in $\phi(\kappa)$ we have

$$\phi(\kappa) = A\int_{-\infty}^{\infty} e^{-(x^2/a^2+2\pi i\kappa x)}dx$$

$$= Ae^{-\pi\kappa a)^2}\int_{-\infty}^{\infty} e^{-(x/a+\pi i\kappa a)^2}dx.$$

This integral is transformed by the substitution $x/a + \pi i\kappa a = y$ into the Gauss integral

$$a\int_{-\infty} e^{-y^2}dy = a\sqrt{\pi}.$$

Therefore

$$\phi(\kappa) = Aa\sqrt{\pi}e^{-(\pi\kappa a)^2} = Aa\sqrt{\pi}e^{-\kappa^2/b^2},$$

where

$$b = \frac{1}{\pi a}.$$

The distribution of the elementary waves composing the wave packet $f(x)$ is again a Gauss function with the half-width $\Delta\kappa = \tfrac{1}{2}b$. Hence we have $\Delta x \,.\, \Delta\kappa = \tfrac{1}{4}ab = \frac{1}{4\pi}$, and introducing the momentum $p = h\kappa$ (p. 89):

$$\Delta x \,.\, \Delta p = \frac{h}{4\pi} = \tfrac{1}{2}\hbar$$

which is the exact expression of Heisenberg's uncertainty law for the special wave packet (see Appendix XL, p. 471). It is evident that with respect to order of magnitude the relation $\Delta x \,.\, \Delta p \sim h$ holds for any form of the wave packet. We shall prove the inequality with an exact numerical coefficient later (see Appendix XXVI, p. 433).

分類:	
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總號:	A-1

Appendix

- Orthogonal Curvilinear Coordinates

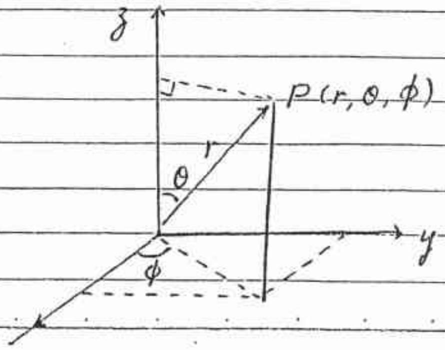
Introduction

Symmetry consideration

↓

Certain coordinates are more convenient than the Cartesian coordinate, e.g for central field problem, it is more convenient to use spherical coordinates

We shall use spherical coordinate as illustration and indicate how these results can be generalized to the case of orthogonal curvilinear coordinate



$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta$$

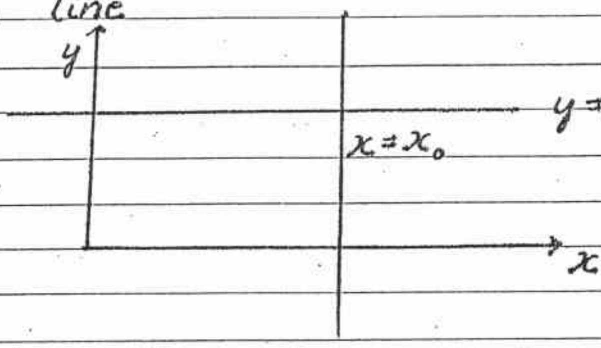
Orthogonal Curvillinear Coordinates

Two dimensional Coordinate

Two dimensional polar coordinate

A point P in two dimension is specified by (x, y) → Cartesian coordinate
or (r, θ) → polar coordinate

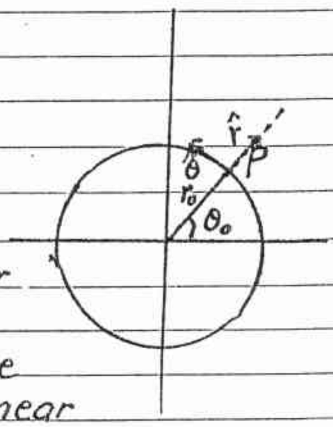
A point $P(x_0, y_0)$ is at the intersection of $x = x_0$ line
$y = y_0$ line



An unit vector along $y = y_0 \rightarrow \hat{i}$
along $x = x_0 \rightarrow \hat{j}$

$\Rightarrow$ form an orthogonal curvillinear coordinate

In polar coordinate $P(r_0, \theta_0)$ is at the intersection of $r = r_0$ (circle), $\theta = \theta_0$ (ray)



We can choose a unit vector $\hat{r}$ along the ray $\theta = \theta_0$
and a unit vector $\hat{\theta}$ along the circle $r = r_0$ as a curvillinear coordinate.
It is obvious that this coordinate is again an orthogonal curvillinear coordinate

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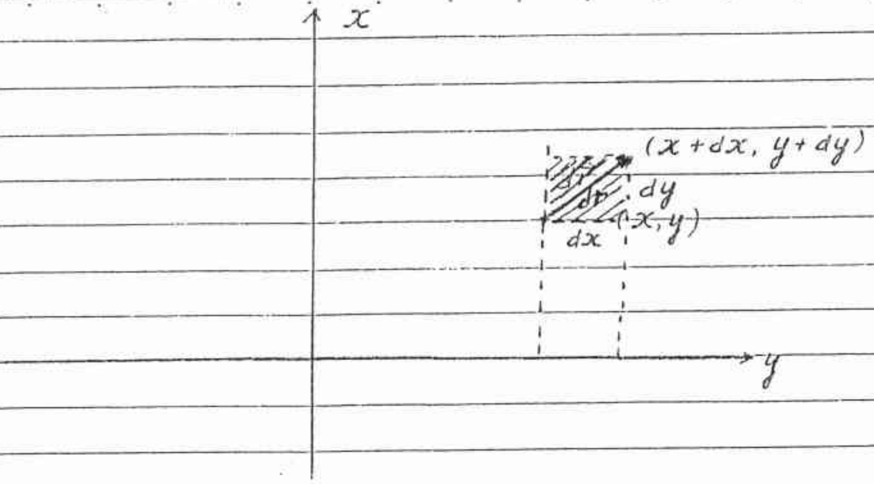
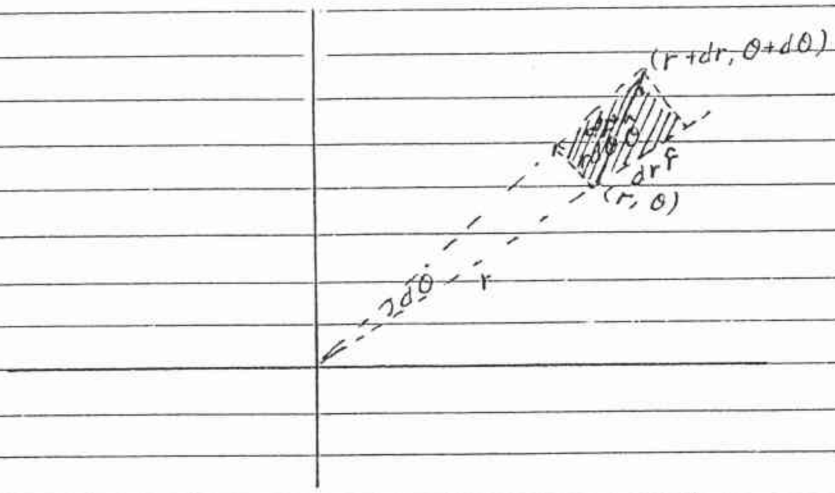
總號： A-3

Two Dimensional Orthogonal Curvilinear Coordinate

Polar Coordinate





$$x = r\cos\theta \qquad\qquad r = \sqrt{x^2+y^2}$$

$$\Longrightarrow$$

$$y = r\sin\theta \qquad\qquad \theta = \tan^{-1}\frac{y}{x}$$

$$d\vec{r} = dx\,\hat{i} + dy\,\hat{j}$$

$$dS = dx\,dy$$

↳ area element

$$d\vec{r} = \alpha\, dr\,\hat{r} + \beta\, d\theta\,\hat{\theta}$$

$\hat{r}$ is a unit vector along $\theta = \text{constant}$

↳ line radiated from the origin

$\hat{\theta}$ is a unit vector along $r = \text{constant}$

↳ circle

Want to find α and β

$\vec{r} = x\hat{i} + y\hat{j}$

$= r\cos\theta\,\hat{i} + r\sin\theta\,\hat{j}$

$d\vec{r}|_\theta = dr\cos\theta\,\hat{i} + dr\sin\theta\,\hat{j}$

$= dr\,[\underbrace{\cos\theta\,\hat{i} + \sin\theta\,\hat{j}}_{\hat{r}}]$

Note $\hat{r}\cdot\hat{r} = 1$

$d\vec{r}|_r = -r\sin\theta\,d\theta\,\hat{i} + r\cos\theta\,d\theta\,\hat{j}$

$= r\,d\theta\,[\underbrace{-\sin\theta\,\hat{i} + \cos\theta\,\hat{j}}_{\hat{\theta}}]$

Note $\hat{r}\cdot\hat{\theta} = 0$
$\hat{\theta}\cdot\hat{\theta} = 1$

$\alpha = 1$, $\beta = r\,d\theta$

$dS = r\,d\theta\,dr$

$\int_0^{2\pi}\int_0^a r\,d\theta\,r = \int_0^{2\pi}\frac{1}{2}a^2\,d\theta = \pi a^2 =$ area of a circle with radius a

分類:	
編號:	
總號:	A-5

$\hat{r} = \cos\theta\, \hat{i} + \sin\theta\, \hat{j}$

$\hat{\theta} = -\sin\theta\, \hat{i} + \cos\theta\, \hat{j}$

$\vec{r} = r\hat{r}$

$\frac{d\vec{r}}{dt} = r\frac{d\hat{r}}{dt} + \frac{dr}{dt}\hat{r}$

$\frac{d\hat{r}}{dt} = -\sin\theta \frac{d\theta}{dt}\hat{i} + \cos\theta\frac{d\theta}{dt}\hat{j}$

($\hat{i}$, $\hat{j}$ are fixed in space)

$\downarrow$

time independent

$= \dot{\theta}\hat{\theta}$

$\frac{d\hat{\theta}}{dt} = -\cos\theta\,\dot{\theta}\,\hat{i} - \sin\theta\,\dot{\theta}\,\hat{j}$

$= -\dot{\theta}\hat{r}$

$\vec{L} = m\vec{r} \times \frac{d\vec{r}}{dt}$

$= m r\hat{r} \times [r\dot{\theta}\hat{\theta} + \frac{dr}{dt}\hat{r}]$

$= mr^2\dot{\theta}\,\hat{k}$

$\Rightarrow |\vec{L}| = mr^2\dot{\theta}$

$\downarrow$

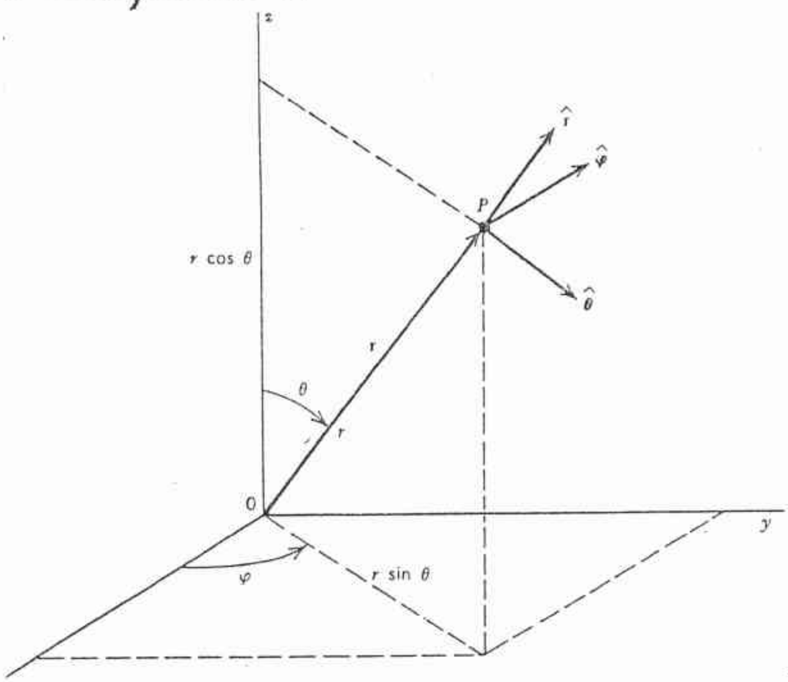
In central force problem

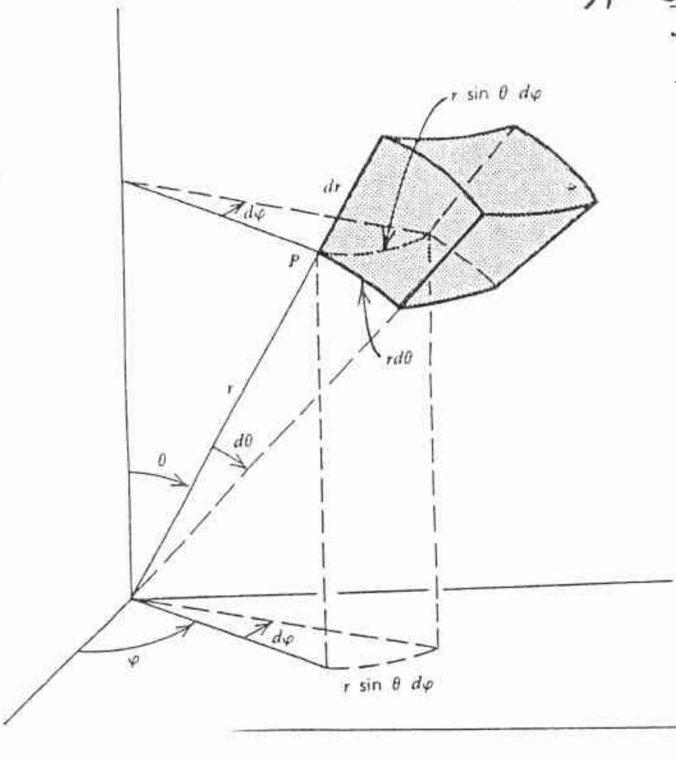
this is a constant of motion.

$\downarrow$

a very useful relation

Spherical Coordinate





Spherical coordinate		General Orthogonal Curvilinear Coordinate
$r = \sqrt{x^2+y^2+z^2}$	$\longleftrightarrow$	$q_1 = q_1(x, y, z)$
$\theta = \cos^{-1}\dfrac{z}{\sqrt{x^2+y^2+z^2}}$	$\longleftrightarrow$	$q_2 = q_2(x, y, z)$
$\phi = \tan^{-1}\dfrac{y}{x}$	$\longleftrightarrow$	$q_3 = q_3(x, y, z)$

Fixed r = constant $\downarrow$ spheres — q_1 = constant $\downarrow$ surfaces

Fixed θ = constant $\downarrow$ cones — q_2 = constant $\downarrow$ surfaces

Fixed ϕ = constant $\downarrow$ planes — q_3 = constant $\downarrow$ surfaces

These three families of surfaces are mutually orthogonal

The intersection of these surfaces, one of each, then defines a point in space P

(r, θ, ϕ) — (q_1, q_2, q_3)

can be seen, from the graph, to be

$$\begin{array}{ccc} dr & r\,d\theta & r\sin\theta\, d\phi \\ \downarrow & \downarrow & \downarrow \\ dl_1 & dl_2 & dl_3 \\ \downarrow & \downarrow & \downarrow \\ h_1 dq_1 & h_2 dq_2 & h_3 dq_3 \end{array}$$

h_1, h_2, h_3 are the most important quantities for orthogonal curvilinear coordinate.

We can find h_1, h_2, h_3 from geometry or from algebra.

We shall now analyze the problem carefully with vector analysis.

Position vector for point P is given by

$$\vec{r} = r\sin\theta\cos\phi\,\hat{i} + r\sin\theta\sin\phi\,\hat{j} + r\cos\theta\,\hat{k}$$

Fixed θ, ϕ, varying $r \rightarrow r + dr$

$$d\vec{r}\,|_{\theta,\phi} = dr\sin\theta\cos\phi\,\hat{i} + dr\sin\theta\sin\phi\,\hat{j} + dr\cos\theta\,\hat{k}$$

is along the intersection line formed by $\theta =$ constant, $\phi =$ constant surfaces.

Define, at point P, $\hat{r}$ to be unit vector perpendicular to $r =$ constant surface, passing through P in the sense of increasing r

$$\Rightarrow \quad d\vec{r}\,|_{\theta,\phi} = \underbrace{|d\vec{r}|_{\theta,\phi}}_{dr}\,\hat{r}$$

$$d\vec{r}\,|_{\theta,\phi} = dr\,\hat{r} \qquad\qquad d\vec{r}\,|_{q_2,q_3} = dl_1\,\hat{q}_1$$

$$\hat{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}$$

Fixed r, ϕ, varying $\theta \to \theta + d\theta$

$$d\vec{r}|_{r,\phi} = r\cos\theta\, d\theta\, \cos\phi\, \hat{i} + r\cos\theta\, d\theta \sin\phi\, \hat{j} + r(-\sin\theta)\, d\theta\, \hat{k}$$

is along the intersection line formed by r = constant, surfaces.

$$d\vec{r}|_{r,\phi} = \underbrace{|d\vec{r}|_{r,\phi}}_{r\,d\theta}\ \hat{\theta} \qquad d\vec{r}|_{q_1,q_3} = dl_2\, \hat{q}_2$$

$$\hat{\theta} = \cos\theta\cos\phi\, \hat{i} + \cos\theta\sin\phi\, \hat{j} - \sin\theta\, \hat{k}$$

Fixed r, θ, varying $\phi \to \phi + d\phi$

$$d\vec{r}|_{r,\theta} = -r\sin\theta\, \sin\phi\, d\phi\, \hat{i} + r\sin\theta\cos\phi\, d\phi\, \hat{j}$$

is along the intersection line formed by r = constant, θ=constan surfaces

$$d\vec{r}|_{r,\theta} = \underbrace{|d\vec{r}|_{r,\theta}}_{r\sin\theta\, d\phi}\ \hat{\phi} \qquad d\vec{r}|_{q_1,q_2} = dl_3\, \hat{q}_3$$

$$\hat{\phi} = -\sin\phi\, \hat{i} + \cos\phi\, \hat{j}$$

It can be shown that $\hat{r}$, $\hat{\theta}$, $\hat{\phi}$ forms an orthogonal coordinate

$$d\vec{r} = dr\, \hat{r} + r\, d\theta\, \hat{\theta} + r\sin\theta\, \hat{\phi} \qquad d\vec{r} = dl_1\, \hat{q}_1 + dl_2\, \hat{q}_2 + dl_3\, \hat{q}_3$$

$$= h_1\, dq_1\, \hat{q}_1 + h_2\, dq_2\, \hat{q}_2 + h_3\, dq_3\, \hat{q}_3$$

$\Rightarrow$ $h_1 = 1$, $h_2 = r$, $h_3 = r\sin\theta$

The volume element enclosed by $r \to r + dr$, $\theta \to \theta + d\theta$, $\phi \to \phi + d\phi$ is $r^2 \sin\theta\, dr\, d\theta\, d\phi$

The volume element enclosed by $q_1 \to q_1 + dq_1$, $q_2 \to q_2 + dq_2$, $q_3 \to q_3 + dq_3$ is $dl_1\, dl_2\, dl_3$
$= h_1 h_2 h_3\, dq_1\, dq_2\, dq_3$

Gradient, Divergence, Curl and Laplacian in Orthogonal Curvilinear Coordinate

Gradient

分類：	
編號：	
總號：	A-9

$$df = \nabla f \cdot d\vec{r}$$

$$\frac{\partial f}{\partial r}\, dr + \frac{\partial f}{\partial \theta}\, d\theta + \frac{\partial f}{\partial \phi}\, d\phi = \nabla f \cdot d\vec{r}$$

Assume $\nabla f = \alpha \hat{r} + \beta \hat{\theta} + \gamma \hat{\phi}$

$d\vec{r}$ is known to be

$$d\vec{r} = dr\, \hat{r} + r\, d\theta\, \hat{\theta} + r\sin\theta\, \hat{\phi}$$

$$\Rightarrow \quad \alpha = \frac{\partial f}{\partial r}, \quad \beta r = \frac{\partial f}{\partial \theta},$$
$$\gamma r \sin\theta = \frac{\partial f}{\partial \phi}$$

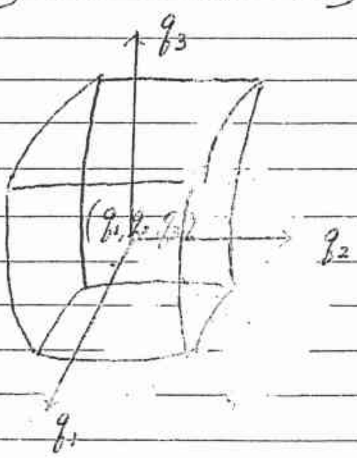
(r, θ, ϕ are independent variable; $\hat{r}, \hat{\theta}, \hat{\phi}$ are orthonormal)

$$\Rightarrow \nabla f = \frac{\partial f}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial f}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f}{\partial \phi}\hat{\phi} \qquad \nabla f = \frac{1}{h_1}\frac{\partial f}{\partial q_1}\hat{q}_1 + \frac{1}{h_2}\frac{\partial f}{\partial q_2}\hat{q}_2 + \frac{1}{h_3}\frac{\partial f}{\partial q_3}\hat{q}_3$$

Note: along z axis, i.e. $\theta = 0$, ∇f is undefined

Divergence

The divergence is the outgoing flux per unit volume



$$\vec{B} = B_1 \hat{q}_1 + B_2 \hat{q}_2 + B_3 \hat{q}_3$$

The central point has coordinates (q_1, q_2, q_3)

The point on the front face

$$\left(q_1 + \frac{dq_1}{2}, q_2, q_3\right)$$

The flux through the front surface

$$\Delta \Phi_f = B_{1f} \, \Delta S_f$$

$\Delta S_f \to dl_2 \, dl_3 = h_{2f} dq_2 \, h_{3f} dq_3$

note h_{1f}, h_{2f} can be function of q's

$$\Delta \Phi_f \cong \left(B_1 + \frac{\partial B_1}{\partial q_1}\frac{dq_1}{2}\right)\left(h_2 + \frac{\partial h_2}{\partial q_1}\frac{dq_1}{2}\right)\left(h_3 + \frac{\partial h_3}{\partial q_1}\frac{dq_1}{2}\right) dq_2 \, dq_3$$

$$\simeq B_1 h_2 h_3 \, dq_2 \, dq_3 + \frac{\partial}{\partial q_1}(B_1 h_2 h_3)\frac{dq_1}{2} \, dq_2 \, dq_3$$

Carry out the calculation for the flux through the back surface

$$\Delta \Phi_B \simeq -B_1 h_2 h_3 \, dq_2 \, dq_3 + \frac{\partial}{\partial q_1}(B_1 h_2 h_3)\frac{dq_1}{2} \, dq_2 \, dq_3$$

$$\Rightarrow \quad \Delta \Phi_{fB} = \frac{\partial}{\partial q_1}(B_1 h_2 h_3) \, dq_1 \, dq_2 \, dq_3$$

Total flux is given by

$$\Delta \Phi = \left[\frac{\partial}{\partial q_1}(B_1 h_2 h_3) + \frac{\partial}{\partial q_2}(B_2 h_3 h_1) + \frac{\partial}{\partial q_3}(B_3 h_1 h_2)\right] dq_1 \, dq_2 \, dq_3$$

$$\to \nabla \cdot \vec{B} \, dV = \nabla \cdot \vec{B} \; h_1 h_2 h_3 \, dq_1 \, dq_2 \, dq_3$$

definition of divergence

$$\Rightarrow \quad \nabla \cdot \vec{B} = \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}(B_1 h_2 h_3) + \frac{\partial}{\partial q_2}(B_2 h_3 h_1) + \frac{\partial}{\partial q_3}(B_3 h_1 h_2)\right]$$

Apply to spherical coordinate, we obtain

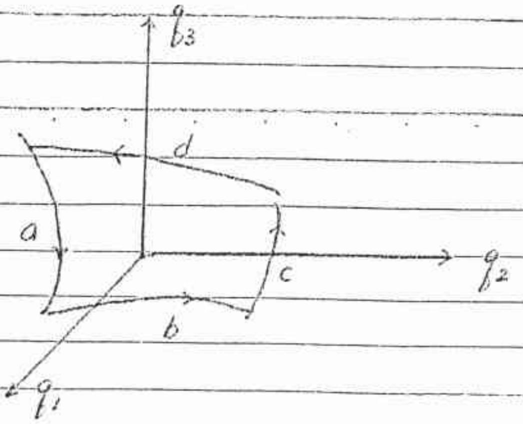
$$\nabla \cdot \vec{B} = \frac{1}{r^2 \sin\theta}\left[\frac{\partial}{\partial r}(B_r r^2 \sin\theta) + \frac{\partial}{\partial \theta}(B_\theta r \sin\theta) + \frac{\partial}{\partial \phi}(B_\phi r)\right]$$

$$= \frac{2}{r} B_r + \frac{\partial B_r}{\partial r} + \frac{B_\theta}{r}\cot\theta + \frac{1}{r}\frac{\partial B_\theta}{\partial \theta} + \frac{1}{r\sin\theta}\frac{\partial B_\phi}{\partial \phi}$$

Curl

$$(\nabla \times B)_1 = \lim_{\Delta S \to 0} \frac{1}{\Delta S} \oint_c \vec{B} \cdot d\vec{l}$$

$c \to$ lie on the surface $\perp$ to $\hat{q}_1$



Contribution from a

$$-B_{3L}\,h_{3L}\,dq_3 \simeq -\left(B_3 - \frac{\partial B_3}{\partial q_2}\frac{dq_2}{2}\right)\left(h_3 - \frac{\partial h_3}{\partial q_2}\frac{dq_2}{2}\right)dq_3$$

$$\simeq -B_3 h_3 dq_3 + \frac{\partial}{\partial q_2}(B_3 h_3)\frac{dq_2}{2}\,dq_3$$

Contribution from c

$$B_{3R}\,h_{3L}\,dq_3 \simeq B_3 h_3\,dq_3 + \frac{\partial}{\partial q_2}(B_3 h_3)\frac{dq_2}{2}\,dq_3$$

Contribution from a and c $\Rightarrow \frac{\partial}{\partial q_2}(B_3 h_3)\,dq_2\,dq_3$

Total contribution from a, b, c, d

$$\Rightarrow \frac{\partial}{\partial q_2}(B_3 h_3)\,dq_2\,dq_3 - \frac{\partial}{\partial q_3}(B_2 h_2)\,dq_2\,dq_3$$

Area $\Delta S = h_2 h_3\,dq_2\,dq_3$

$$\Rightarrow (\nabla\times\vec{B})_1 = \frac{1}{h_2 h_3}\left[\frac{\partial}{\partial q_2}(B_3 h_3) - \frac{\partial}{\partial q_3}(B_2 h_2)\right]$$

Use the same method, we can calculate $(\nabla\times\vec{B})_2$, $(\nabla\times\vec{B})_3$

Put all the results together, we have

$$\nabla\times\vec{B} = \frac{1}{h_1 h_2 h_3}\begin{vmatrix} h_1\hat{q}_1 & h_2\hat{q}_2 & h_3\hat{q}_3 \\ \frac{\partial}{\partial q_1} & \frac{\partial}{\partial q_2} & \frac{\partial}{\partial q_3} \\ h_1 B_1 & h_2 B_2 & h_3 B_3 \end{vmatrix}$$

Apply to spherical coordinate

$$\nabla\times\vec{B} = \frac{1}{r^2\sin\theta}\begin{vmatrix} \hat{r} & r\hat{\theta} & r\sin\theta\,\hat{\phi} \\ \frac{\partial}{\partial r} & \frac{\partial}{\partial\theta} & \frac{\partial}{\partial\phi} \\ B_r & rB_\theta & r\sin\theta\,B_\phi \end{vmatrix}$$

Laplacian

$$\nabla^2 f = \nabla \cdot (\nabla f)$$

$$= \frac{1}{h_1 h_2 h_3}\left[\frac{\partial}{\partial q_1}\left(h_2 h_3 \frac{1}{h_1}\frac{\partial f}{\partial q_1}\right) + \frac{\partial}{\partial q_2}\left(h_3 h_1 \frac{1}{h_2}\frac{\partial f}{\partial q_2}\right) + \frac{\partial}{\partial q_3}\left(h_1 h_2 \frac{1}{h_3}\frac{\partial f}{\partial q_3}\right)\right]$$

Application to spherical coordinate

$$\nabla^2 f = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial f}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial f}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$$

$$= \frac{2}{r}\frac{\partial f}{\partial r} + \frac{\partial^2 f}{\partial r^2} + \frac{\cot\theta}{r^2}\frac{\partial f}{\partial \theta} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 f}{\partial \phi^2}$$

also very useful in studying
central force problem in
quantum mechanics.

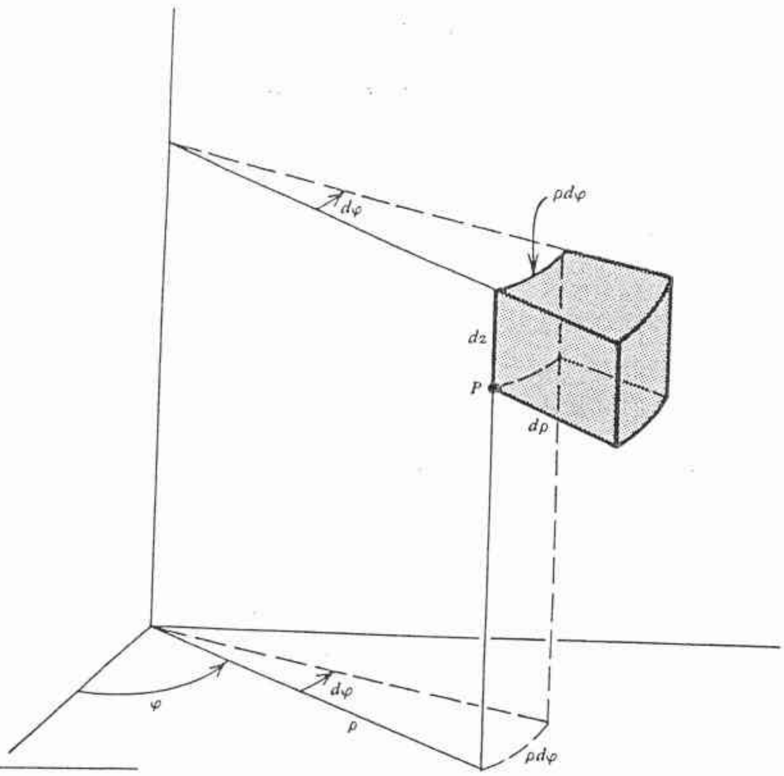
$\nabla^2 \vec{B} \equiv$ Laplacian of a vector field is defined by

$$\nabla^2 \vec{B} = \nabla(\nabla \cdot \vec{B}) - \nabla \times (\nabla \times \vec{B})$$

With the results we have developed, $\nabla^2 \vec{B}$ can be easily calculated.

分類：	
編號：	
總號：	A-13

Cylindrical Coordinate



Volume element in terms of cylindrical coordinates.

Use the same method, we can express ∇t, $\nabla \cdot \vec{V}$, $\nabla \times \vec{V}$ in cylindrical coordinate
(See the textbook)

分類：	
編號：	A-14
總號：	

spherical coördinates

$$\boldsymbol{r} = (x, y, z), \qquad \begin{Bmatrix} x = r\sin\theta\cos\varphi \\ y = r\sin\theta\sin\varphi \\ z = r\cos\theta \end{Bmatrix} \tag{6}$$

$$\therefore \quad \begin{Bmatrix} r^2 = x^2 + y^2 + z^2 \\ \cos\theta = \dfrac{z}{r}, \qquad \tan\varphi = \dfrac{y}{x} \end{Bmatrix} \tag{7}$$

$$\therefore \begin{Bmatrix} \dfrac{\partial r}{\partial x} = \dfrac{x}{r} = \sin\theta\cos\varphi, & \dfrac{\partial r}{\partial y} = \dfrac{y}{r} = \sin\theta\sin\varphi, & \dfrac{\partial r}{\partial z} = \dfrac{z}{r} = \cos\theta \\ \dfrac{\partial\theta}{\partial x} = \dfrac{1}{\sin\theta}\dfrac{xz}{r^3} = \dfrac{\cos\theta\cos\varphi}{r}, & \dfrac{\partial\theta}{\partial y} = \dfrac{1}{\sin\theta}\dfrac{yz}{r^3} = \dfrac{\cos\theta\sin\varphi}{r}, & \dfrac{\partial\theta}{\partial z} = -\dfrac{x^2+y^2}{\sin\theta r^3} = -\dfrac{\sin\theta}{r} \\ \dfrac{\partial\varphi}{\partial x} = -\dfrac{y}{x^2+y^2} = -\dfrac{\sin\varphi}{r\sin\theta}, & \dfrac{\partial\varphi}{\partial y} = \dfrac{x}{x^2+y^2} = \dfrac{\cos\varphi}{r\sin\theta}, & \dfrac{\partial\varphi}{\partial z} = 0 \end{Bmatrix} \tag{8}$$

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x}\frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}$$

$$\begin{aligned}
\frac{\partial^2}{\partial x^2} = {} & \frac{\partial r}{\partial x}\left\{\frac{\partial}{\partial r}\left(\frac{\partial r}{\partial x}\frac{\partial}{\partial r}\right)\right\} + \frac{\partial\theta}{\partial x}\left\{\frac{\partial}{\partial\theta}\left(\frac{\partial r}{\partial x}\frac{\partial}{\partial r}\right)\right\} + \frac{\partial\varphi}{\partial x}\left\{\frac{\partial}{\partial\varphi}\left(\frac{\partial r}{\partial x}\frac{\partial}{\partial r}\right)\right\} \\
& + \frac{\partial r}{\partial x}\left\{\frac{\partial}{\partial r}\left(\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta}\right)\right\} + \frac{\partial\theta}{\partial x}\left\{\frac{\partial}{\partial\theta}\left(\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta}\right)\right\} + \frac{\partial\varphi}{\partial x}\left\{\frac{\partial}{\partial\varphi}\left(\frac{\partial\theta}{\partial x}\frac{\partial}{\partial\theta}\right)\right\} \\
& + \frac{\partial r}{\partial x}\left\{\frac{\partial}{\partial r}\left(\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}\right)\right\} + \frac{\partial\theta}{\partial x}\left\{\frac{\partial}{\partial\theta}\left(\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}\right)\right\} + \frac{\partial\varphi}{\partial x}\left\{\frac{\partial}{\partial\varphi}\left(\frac{\partial\varphi}{\partial x}\frac{\partial}{\partial\varphi}\right)\right\} \\
= {} & \left(\frac{\partial r}{\partial x}\right)^2\frac{\partial^2}{\partial r^2} + \left\{\left(\frac{\partial r}{\partial x}\right)\left[\frac{\partial}{\partial r}\left(\frac{\partial r}{\partial x}\right)\right] + \left(\frac{\partial\theta}{\partial x}\right)\left[\frac{\partial}{\partial\theta}\left(\frac{\partial r}{\partial x}\right)\right] + \left(\frac{\partial\varphi}{\partial x}\right)\left[\frac{\partial}{\partial\varphi}\left(\frac{\partial r}{\partial x}\right)\right]\right\}\frac{\partial}{\partial r} \\
& + \left(\frac{\partial\theta}{\partial x}\right)^2\frac{\partial^2}{\partial\theta^2} + \left\{\left(\frac{\partial r}{\partial x}\right)\left[\frac{\partial}{\partial r}\left(\frac{\partial\theta}{\partial x}\right)\right] + \left(\frac{\partial\theta}{\partial x}\right)\left[\frac{\partial}{\partial\theta}\left(\frac{\partial\theta}{\partial x}\right)\right] + \left(\frac{\partial\varphi}{\partial x}\right)\left[\frac{\partial}{\partial\varphi}\left(\frac{\partial\theta}{\partial x}\right)\right]\right\}\frac{\partial}{\partial\theta} \\
& + \left(\frac{\partial\varphi}{\partial x}\right)^2\frac{\partial^2}{\partial\varphi^2} + \left\{\left(\frac{\partial r}{\partial x}\right)\left[\frac{\partial}{\partial r}\left(\frac{\partial\varphi}{\partial x}\right)\right] + \left(\frac{\partial\theta}{\partial x}\right)\left[\frac{\partial}{\partial\theta}\left(\frac{\partial\varphi}{\partial x}\right)\right] + \left(\frac{\partial\varphi}{\partial x}\right)\left[\frac{\partial}{\partial\varphi}\left(\frac{\partial\varphi}{\partial x}\right)\right]\right\}\frac{\partial}{\partial\varphi} \\
& + 2\left\{\frac{\partial r}{\partial x}\frac{\partial\theta}{\partial x}\frac{\partial^2}{\partial r\partial\theta} + \frac{\partial\theta}{\partial x}\frac{\partial\varphi}{\partial x}\frac{\partial^2}{\partial\theta\partial\varphi} + \frac{\partial\varphi}{\partial x}\frac{\partial r}{\partial x}\frac{\partial^2}{\partial\varphi\partial r}\right\}
\end{aligned} \tag{9}$$

同樣地得$\dfrac{\partial^2}{\partial y^2}$和$\dfrac{\partial^2}{\partial z^2}$，只是把(9)式的 $x \to y, x \to z$

$$\therefore \quad \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

分類：
編號：A-15
總號：

$$= \left[\left(\frac{\partial r}{\partial x}\right)^2 + \left(\frac{\partial r}{\partial y}\right)^2 + \left(\frac{\partial r}{\partial z}\right)^2 \right] \frac{\partial^2}{\partial r^2} + \left[\left(\frac{\partial \theta}{\partial x}\right)^2 + \left(\frac{\partial \theta}{\partial y}\right)^2 + \left(\frac{\partial \theta}{\partial z}\right)^2 \right] \frac{\partial^2}{\partial \theta^2}$$

$$+ \left[\left(\frac{\partial \varphi}{\partial x}\right)^2 + \left(\frac{\partial \varphi}{\partial y}\right)^2 + \left(\frac{\partial \varphi}{\partial z}\right)^2 \right] \frac{\partial^2}{\partial \varphi^2} + 2\left[\frac{\partial r}{\partial x}\frac{\partial \theta}{\partial x} + \frac{\partial r}{\partial y}\frac{\partial \theta}{\partial y} + \frac{\partial r}{\partial z}\frac{\partial \theta}{\partial z} \right] \frac{\partial^2}{\partial r \partial \theta}$$

$$+ 2\left[\frac{\partial \theta}{\partial x}\frac{\partial \varphi}{\partial x} + \frac{\partial \theta}{\partial y}\frac{\partial \varphi}{\partial y} + \frac{\partial \theta}{\partial z}\frac{\partial \varphi}{\partial z} \right] \frac{\partial^2}{\partial \theta \partial \varphi} + 2\left[\frac{\partial \varphi}{\partial x}\frac{\partial r}{\partial x} + \frac{\partial \varphi}{\partial y}\frac{\partial r}{\partial y} + \frac{\partial \varphi}{\partial z}\frac{\partial r}{\partial z} \right] \frac{\partial^2}{\partial \varphi \partial r}$$

$$+ \left\{ \frac{\partial r}{\partial x}\left[\frac{\partial}{\partial r}\frac{\partial r}{\partial x}\right] + \frac{\partial r}{\partial y}\left[\frac{\partial}{\partial r}\frac{\partial r}{\partial y}\right] + \frac{\partial r}{\partial z}\left[\frac{\partial}{\partial r}\frac{\partial r}{\partial z}\right] \right\} \frac{\partial}{\partial r}$$

$$+ \left\{ \frac{\partial \theta}{\partial x}\left[\frac{\partial}{\partial \theta}\frac{\partial r}{\partial x}\right] + \frac{\partial \theta}{\partial y}\left[\frac{\partial}{\partial \theta}\frac{\partial r}{\partial y}\right] + \frac{\partial \theta}{\partial z}\left[\frac{\partial}{\partial \theta}\frac{\partial r}{\partial z}\right] \right\} \frac{\partial}{\partial r}$$

$$+ \left\{ \frac{\partial \varphi}{\partial x}\left[\frac{\partial}{\partial \varphi}\frac{\partial r}{\partial x}\right] + \frac{\partial \varphi}{\partial y}\left[\frac{\partial}{\partial \varphi}\frac{\partial r}{\partial y}\right] + \frac{\partial \varphi}{\partial z}\left[\frac{\partial}{\partial \varphi}\frac{\partial r}{\partial z}\right] \right\} \frac{\partial}{\partial r}$$

$$+ \left\{ \frac{\partial r}{\partial x}\left[\frac{\partial}{\partial r}\frac{\partial \theta}{\partial x}\right] + \frac{\partial r}{\partial y}\left[\frac{\partial}{\partial r}\frac{\partial \theta}{\partial y}\right] + \frac{\partial r}{\partial z}\left[\frac{\partial}{\partial r}\frac{\partial \theta}{\partial z}\right] \right\} \frac{\partial}{\partial \theta}$$

$$+ \left\{ \frac{\partial \theta}{\partial x}\left[\frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial x}\right] + \frac{\partial \theta}{\partial y}\left[\frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial y}\right] + \frac{\partial \theta}{\partial z}\left[\frac{\partial}{\partial \theta}\frac{\partial \theta}{\partial z}\right] \right\} \frac{\partial}{\partial \theta}$$

$$+ \left\{ \frac{\partial \varphi}{\partial x}\left[\frac{\partial}{\partial \varphi}\frac{\partial \theta}{\partial x}\right] + \frac{\partial \varphi}{\partial y}\left[\frac{\partial}{\partial \varphi}\frac{\partial \theta}{\partial y}\right] + \frac{\partial \varphi}{\partial z}\left[\frac{\partial}{\partial \varphi}\frac{\partial \theta}{\partial z}\right] \right\} \frac{\partial}{\partial \theta}$$

$$+ \left\{ \frac{\partial r}{\partial x}\left[\frac{\partial}{\partial r}\frac{\partial \varphi}{\partial x}\right] + \frac{\partial r}{\partial y}\left[\frac{\partial}{\partial r}\frac{\partial \varphi}{\partial y}\right] + \frac{\partial r}{\partial z}\left[\frac{\partial}{\partial r}\frac{\partial \varphi}{\partial z}\right] \right\} \frac{\partial}{\partial \varphi}$$

$$+ \left\{ \frac{\partial \theta}{\partial x}\left[\frac{\partial}{\partial \theta}\frac{\partial \varphi}{\partial x}\right] + \frac{\partial \theta}{\partial y}\left[\frac{\partial}{\partial \theta}\frac{\partial \varphi}{\partial y}\right] + \frac{\partial \theta}{\partial z}\left[\frac{\partial}{\partial \theta}\frac{\partial \varphi}{\partial z}\right] \right\} \frac{\partial}{\partial \varphi}$$

$$+ \left\{ \frac{\partial \varphi}{\partial x}\left[\frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial x}\right] + \frac{\partial \varphi}{\partial y}\left[\frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial y}\right] + \frac{\partial \varphi}{\partial z}\left[\frac{\partial}{\partial \varphi}\frac{\partial \varphi}{\partial z}\right] \right\} \frac{\partial}{\partial \varphi} \qquad (10)$$

把式(8)代入式(10)得：

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{\cos\theta}{r^2 \sin\theta}\frac{\partial}{\partial \theta}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial \varphi^2} \qquad (11)$$