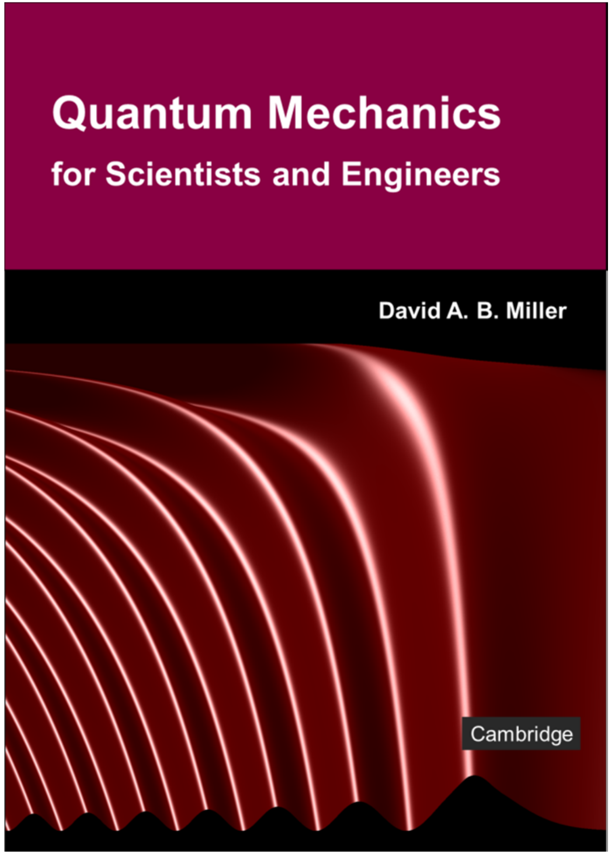
2.2 Schrödinger’s wave equation

Slides: Video 2.2.2 From de Broglie to Schrödinger

Text reference: Quantum Mechanics for Scientists and Engineers

Sections 2.1 – 2.2



Schrödinger's wave equation

From de Broglie to Schrödinger

Quantum mechanics for scientists and engineers

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Electrons as waves

de Broglie's hypothesis is that the electron wavelength λ is given by

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

where p is the electron momentum and

h is Planck's constant

$$h = 6.62606957 \times 10^{-34}\ J\ s$$

Now we want to use this to help construct a wave equation

A Helmholtz wave equation

If we are considering only waves of one wavelength λ for the moment

i.e., monochromatic waves

we can choose a Helmholtz wave equation

$$\frac{d^2\psi}{dz^2} = -k^2\psi \quad \text{with} \quad k = \frac{2\pi}{\lambda}$$

which we know works for simple waves

with solutions like

$\sin(kz)$, $\cos(kz)$, and $\exp(ikz)$

(and $\sin(-kz)$, $\cos(-kz)$, and $\exp(-ikz)$)

A Helmholtz wave equation

In three dimensions, we can write this as

$$\nabla^2 \psi \equiv \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -k^2 \psi$$

which has solutions like

$\sin(\mathbf{k} \cdot \mathbf{r})$, $\cos(\mathbf{k} \cdot \mathbf{r})$, and $\exp(i\mathbf{k} \cdot \mathbf{r})$

(and $\sin(-\mathbf{k} \cdot \mathbf{r})$, $\cos(-\mathbf{k} \cdot \mathbf{r})$, and $\exp(-i\mathbf{k} \cdot \mathbf{r})$)

where $\mathbf{k}$ and $\mathbf{r}$ are vectors

From Helmholtz to Schrödinger

With de Broglie's hypothesis $\lambda = h / p$

and the definition $k = 2\pi / \lambda$

then $k = 2\pi p / h = p / \hbar$

where we have defined $\hbar \equiv h / 2\pi$

so $k^2 = p^2 / \hbar^2$

Hence we can rewrite our Helmholtz equation

$$\nabla^2 \psi = -\frac{p^2}{\hbar^2} \psi$$

or

$$-\hbar^2 \nabla^2 \psi = p^2 \psi$$

From Helmholtz to Schrödinger

If we are thinking of an electron, we can divide both sides by its mass m_o to obtain

$$-\frac{\hbar^2}{2m_o}\nabla^2\psi = \frac{p^2}{2m_o}\psi$$

But we know from classical mechanics that

$$\frac{p^2}{2m_o} \equiv \text{kinetic energy of electron}$$

and in general

Total energy (E)=Kinetic energy + Potential energy ($V(\mathbf{r})$)

From Helmholtz to Schrödinger

So Kinetic energy = $p^2 / 2m_o$

= Total energy (E) - Potential energy ($V(\mathbf{r})$)

Hence our Helmholtz equation $$-\frac{\hbar^2}{2m_o}\nabla^2\psi = \frac{p^2}{2m_o}\psi$$

becomes the Schrödinger equation $$-\frac{\hbar^2}{2m_o}\nabla^2\psi = \left(E - V(\mathbf{r})\right)\psi$$

or equivalently $$\boxed{\left(-\frac{\hbar^2}{2m_o}\nabla^2 + V(\mathbf{r})\right)\psi = E\psi}$$

Schrödinger's time-independent equation

We can postulate a Schrödinger equation for any particle of mass m

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi = E\psi$$

Formally, this is the

time-independent Schrödinger equation

Probability densities

Born's postulate is that

the probability $P(\mathbf{r})$ of finding an electron

near any specific point $\mathbf{r}$ in space

is proportional to the modulus squared $|\psi(\mathbf{r})|^2$

of the wave amplitude $\psi(\mathbf{r})$

$|\psi(\mathbf{r})|^2$ can therefore be viewed as a

"probability density"

with $\psi(\mathbf{r})$ called a "probability amplitude"

or a "quantum mechanical amplitude"