Lecture 1: The Schrodinger equation

Read Chap 1 (skip 1.1, 1.3); chap 2.1 – 2.5

1 The time-dependent Schodinger equation

In a (very simplified) history, Einstein and deBroglie came up with these relations, and the interpretation that goes with them:

photoelectric

$\nu\lambda = c$

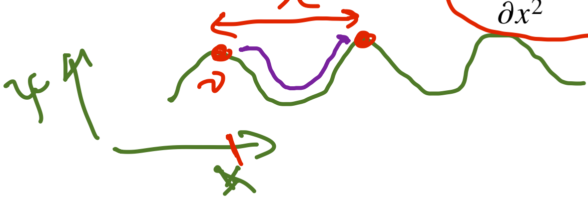
$$\underline{E = h\nu} \ (1\text{-}9) \quad \underline{p = h/\lambda} \ (1\text{-}32)$$

If matter has wave-like properties, Schrodinger investigated treating this via a classical wave equation:

$e^{i\alpha} = \cos(\alpha) + i\sin(\alpha)$

$\psi(x,t)$

$$\frac{\partial^2\Psi}{\partial x^2} = \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} \Rightarrow \underbrace{\Psi = Ce^{i\alpha}} \ (2\text{-}1), (2\text{-}2)$$



$c = \nu\lambda$

$\hbar \equiv \frac{h}{2\pi}$

$$\alpha = 2\pi\left(\frac{x}{\lambda} - \nu t\right) = \frac{xp - Et}{\hbar} \quad (2\text{-}3), (2\text{-}4)$$

differentiat ψ
- wrt t
- wrt x
- wrt x again

$\frac{\partial^2(\psi)}{\partial x^2} \sim -p^2$

$$\underbrace{i\hbar\frac{\partial\Psi}{\partial t} = E\Psi} \quad \underbrace{-i\hbar\frac{\partial\Psi}{\partial x} = p\Psi} \quad (2\text{-}6), (2\text{-}8)$$

K.E. P.E.

$\underset{\sim}{x} \equiv (x, y, z)$

time-dependent Schrodinger equation →

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \quad (2\text{-}11) \rightarrow E\psi$$

$\text{K.E.} = \frac{1}{2}mv^2 = p^2/2m$

$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \equiv \nabla^2$

electrons →
nuclei →

$$\underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + \hat{V}(\underset{\sim}{x})\right]}_{\hat{H}}\psi = i\hbar\,\partial\psi/\partial t$$

$\hat{H}$ in this case, no explicit time dependence

$z = x + iy$
$z^* = x - iy$

$z^* z \equiv |z|^2$ is a ~~po~~ non-negative real number

2 The time-independent Schrodinger equation

First the interpretation that $\Psi^*\Psi$ is a probability density, so that $\Psi^*\Psi dx$ is the probability of finding the particle between x and $x + dx$. (Section 2.2) at time t

Next use the method of separation of variables: Try $\Psi(x,t) = \psi(x)\phi(t)$.

$$\hat{H}\psi\phi = i\hbar\frac{\partial\psi\phi}{\partial t} \Rightarrow \frac{\hat{H}\psi}{\psi} = \frac{i\hbar}{\phi}\frac{\partial\phi}{\partial t} = W \quad \text{(2-25)}$$

constant

Solving first for $\phi(t)$, and then for $\psi(x)$:

$$\phi(t) = e^{-iWt/\hbar}; \quad \hat{H}\psi(x) = \overset{E}{\cancel{W}}\psi(x) \quad \text{(2-28),(2-31)}$$

$\Psi^*\Psi = \psi^*(x)\psi(x)$

$e^{iEt/\hbar} \; e^{-iEt/\hbar}$

$\phi^* \quad \phi$

$e^0 = 1$

time-indenden

The last equation has many solutions, which we index by a *quantum number, i*:

time-independent S.E.

$$\boxed{\hat{H}\psi_i = E_i\psi_i} \quad \boxed{f(x) = \sum_i c_i\psi_i(x) \quad \text{(2-33)}}$$

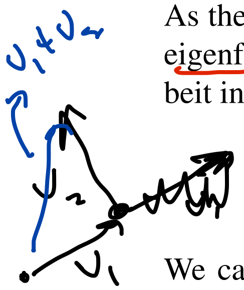
most of semester

$\{\psi_i\}$ forms a complete set

c_i is a (complex) constant

"a superposition of wave functions"

3 The vector interpretation of wavefunctions



As the last equation above implied, we can think about adding together (superimposing) different eigenfunctions of the Hamiltonian. This can be thought of as the analog of addition of vectors, (albeit in a infinite-dimensional vector space!), and drove the development of a very useful notation:

$$\psi_A(x) \Rightarrow |A\rangle \quad \psi_A^* \Rightarrow \langle A| \qquad \langle A|\, A\rangle \Rightarrow \int \psi_A^*(x)\psi_A dx \quad \text{(2-35)}$$

We can often learn a lot in quantum mechanics by considering the properties of these vectors, rather than expanding everything out into wavefunctions. This is the subject of sections 2-4 to 2-8 in your text, which we outline briefly next. Start with *expectation values*:

$$\langle\hat{A}\rangle = \frac{\langle i|\,\hat{A}\,|i\rangle}{\langle i|\,i\rangle} \quad \text{(2-43)}$$