Chapter 3 Quantum Mechanics

In physics, $e^{i(kr-\omega t)}$ is a $+r$-directionally propagated wave. $\therefore$ A wave function $\Psi \propto e^{i(kr-\omega t)}$, and hence we have $\omega\Psi = i\partial\Psi/\partial t$, $k\Psi = -i\nabla\Psi$, etc. But in EE, $e^{i(\omega t-kr)}$ is a $+r$-directionally propagated wave.

3-1 Schrodinger Equation $i\hbar\,\partial\Psi/\partial t = -\hbar^2\nabla^2\Psi/2m + V\Psi$**, or** $E\Psi = H\Psi$

Total energy=Kinetic energy+Potential energy $\Leftrightarrow E = K + V \Rightarrow hv = 2\pi\hbar\mathbf{v} = p^2/2m + V$

$\Rightarrow \hbar\omega = (h/\lambda)^2/2m + V = (2\pi\hbar/\lambda)^2/2m + V = (\hbar k)^2/2m + V$

Multiply a wave function $\Psi \propto e^{i(kr-\omega t)}$ on both sides of the above equation, and then we have $\hbar\omega\Psi == \hbar^2 k^2\Psi/2m + V\Psi$.

By $\omega\Psi = i\dfrac{\partial\Psi}{\partial t}$, $k\Psi = -i\nabla\Psi \Rightarrow$ **Schrodinger Equation:** $i\hbar\,\partial\Psi/\partial t = -\hbar^2\nabla^2\Psi/2m + V\Psi$

Define $H = -\hbar^2\nabla^2/2m + V$ as a Hamiltonian operator, we have $H\Psi_n = E_n\Psi_n$, where E_n is an eigenvalue of H, and Ψ_n is the corresponding eigenfunction of H.

Table Operators Associated with Various Observable Quantities

Quantity	Operator
Position, x	x
Linear momentum, p	$\dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$
Potential energy, $V(x)$	$V(x)$
Kinetic energy, $KE = \dfrac{p^2}{2m}$	$-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}$
Total energy, E	$i\hbar\dfrac{\partial}{\partial t}$
Total energy (Hamiltonian form), H	$-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V(x)$

Other operators: $p = -i\hbar\nabla$, $x = -i\hbar\nabla_k$, $p_x = -i\hbar\,\partial/\partial x$, $p_y = -i\hbar\,\partial/\partial y$, $p_z = -i\hbar\,\partial/\partial z$, **etc.**

$p\Psi = (h/\lambda)\Psi = (\hbar k)\Psi = -i\hbar\nabla\Psi$,

$\therefore p = -i\hbar\nabla$

Steady-state Schrodinger equation: $\hbar^2\nabla^2\Psi/2m + (E-V)\Psi = 0$

Postulate of quantum mechanics: $|\Psi|^2 = \Psi^*\Psi$ is a probability density function of a particle occurs at r and $\int_{-\infty}^{\infty}|\Psi|^2 dr = 1$.

Expectation (Average) value of f, $\langle f\rangle$: $\langle f\rangle = \int\Psi^* f\Psi dv$

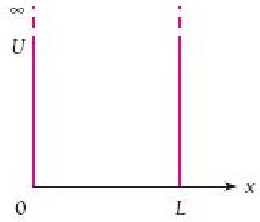
Eg. Show that $\langle px\rangle - \langle xp\rangle = \langle -i\hbar\rangle = -i\hbar$ **.**

(Sol.) $\langle px\rangle - \langle xp\rangle = \int\Psi^* px\Psi dr - \int\Psi^* xp\Psi dr = \int\Psi^*(-ih\partial/\partial x)(x\Psi)dr - \int\Psi^* x(-ih\partial\Psi/\partial x)dr$

$= \int\Psi^*(-i\hbar\,\partial x/\partial x)\Psi dr + \int\Psi^* x(-i\hbar\,\partial\Psi/\partial x)dr - \int\Psi^* x(-i\hbar\,\partial\Psi/\partial x)dr = \int\Psi^*(-i\hbar)\Psi dr$

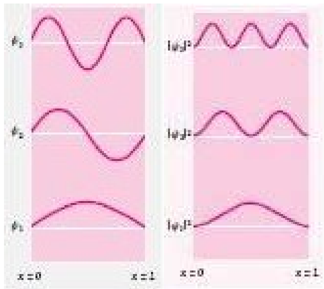
$= \langle -i\hbar\rangle = -i\hbar$

$$\therefore \langle px\rangle - \langle xp\rangle = \langle -i\hbar\rangle = -i\hbar$$



Case 1 Quantum well with infinitely hard walls:

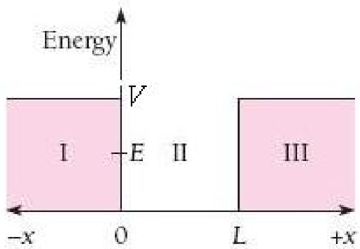
$$V=\begin{cases}0, & 0\le x\le L\\ \infty, & elsewhere\end{cases}$$



$d^2\Psi/dx^2+2mE\Psi/\hbar^2=0$ in $0\leqq x\leqq L \Rightarrow \Psi(x)=A\sin(\frac{\sqrt{2mE}}{\hbar}x)+B\cos(\frac{\sqrt{2mE}}{\hbar}x)$

Boundary conditions: $\Psi(0)=\Psi(L)=0 \Rightarrow B=0$, $E_n=\frac{n^2\pi^2\hbar^2}{2mL^2}$, and $\Psi_n(x)=A\sin(n\pi x/L)$

$\int_{-\infty}^{\infty}|\Psi_n|^2 dv=1 \Rightarrow A=\sqrt{2/L}$, $\therefore \Psi_n(x)=\sqrt{2/L}\sin(n\pi x/L)$



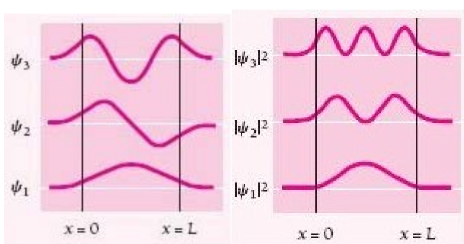
Case 2 Quantum well with finite potential walls V:

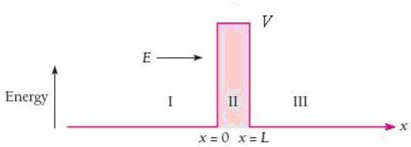
$$V=\begin{cases}0, & 0\le x\le L\\ V, & elsewhere\end{cases}$$

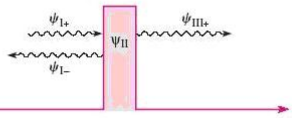
$$\begin{cases}\frac{d^2\Psi_I}{dx^2}+\frac{2m}{\hbar^2}(E-V)\Psi_I=0\\ \frac{d^2\Psi_{II}}{dx^2}+\frac{2m}{\hbar^2}\Psi_{II}=0\\ \frac{d^2\Psi_{III}}{dx^2}+\frac{2m}{\hbar^2}(E-V)\Psi_{III}=0\end{cases}$$

with boundary conditions: $\Psi_I(0)=\Psi_{II}(0)$, $\Psi_{II}(L)=\Psi_{III}(L)$, $\Psi_I'(0)=\Psi_{II}'(0)$, $\Psi_{II}'(L)=\Psi_{III}'(L)$

$$\Rightarrow\begin{cases}\Psi_I(x)=Ce^{\alpha x}\\ \Psi_{II}(x)=A\sin(\frac{\sqrt{2mE}x}{\hbar})+B\cos(\frac{\sqrt{2mE}x}{\hbar})\\ \Psi_{III}(x)=De^{-\alpha x}\end{cases}$$



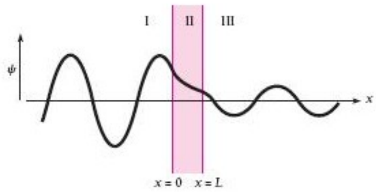




Case 3 Tunnel effect: A barrier of V>E,

$$V=\begin{cases} V(>E), & 0 \le x \le L \\ 0, & elsewhere \end{cases}$$

$$\begin{cases} \dfrac{d^2\Psi_I}{dx^2}+\dfrac{2m}{\hbar^2}E\Psi_I=0 \\ \dfrac{d^2\Psi_{II}}{dx^2}+\dfrac{2m}{\hbar^2}(E-V)\Psi_{II}=0 \\ \dfrac{d^2\Psi_{III}}{dx^2}+\dfrac{2m}{\hbar^2}E\Psi_{III}=0 \end{cases}$$ with boundary conditions: $\Psi_I(0)=\Psi_{II}(0)$, $\Psi_{II}(L)=\Psi_{III}(L)$, $\Psi_I'(0)=\Psi_{II}'(0)$, $\Psi_{II}'(L)=\Psi_{III}'(L)$



$$\Rightarrow \begin{cases} \Psi_I(x)=Ae^{ik_1x}+Be^{-ik_1x} \\ \Psi_{II}(x)=Ce^{-ik_2x}+De^{-ik_2x} \\ \Psi_{III}(x)=Fe^{ik_3x} \end{cases}$$, where $k_1=\dfrac{\sqrt{2mE}}{\hbar}$,

$k_2=\dfrac{\sqrt{2m(V-E)}}{\hbar}$, $k_3=\dfrac{\sqrt{2mE}}{\hbar}=k_1$

$\Rightarrow$ Transmission probability: $T=|\Psi_{III}^+|^2/|\Psi_I^+|^2=|F|^2/|A|^2 \approx [\dfrac{16}{4+(K_2/K_1)^2}]\cdot e^{-2k_2L} \approx e^{-2k_2L}$

Eg. A beam of electrons is incident on a barrier of 5eV high and 0.2*nm* wide. What energy should they have if 50% of them are to get through the barrier?

(Sol.) $T=[\dfrac{16}{4+(K_2/K_1)^2}]\cdot e^{-2k_2L} \approx e^{-2k_2L}=0.5$

$\Rightarrow k_2=1.7\times10^9=\dfrac{\sqrt{2m(V-E)}}{\hbar}$, $V=5 \Rightarrow E=4.89\text{eV}$

Case 4 Harmonic oscillator with frequency $\nu=\frac{\sqrt{k/m}}{2\pi}$: $V=kx^2/2$

$d\Psi^2/dx^2+2m(E-kx^2/2)\Psi/\hbar^2=0$. Define $y=\sqrt{\frac{\sqrt{km}}{\hbar}}x=\sqrt{\frac{2\pi m\nu}{\hbar}}x$ and $\alpha=\frac{2E}{\hbar}\sqrt{\frac{m}{k}}=\frac{2E}{h\nu}$

$\Rightarrow d\Psi^2/dy^2+(\alpha-y^2)\Psi=0$. Define $\Psi=f(y)\exp(-y^2/2)\Rightarrow df^2/dy^2-2ydf/dy+(\alpha-1)f=0$

Let $f(y)=\sum_{n=0}^{\infty}A_n y^n \Rightarrow A_{n+2}=\frac{2n+1-\alpha}{(n+2)(n+1)}A_n$. If $\alpha=2n+1\Rightarrow A_{n+2}=A_{n+4}=A_{n+6}=\ldots=0$

$\Rightarrow\Psi=f(y)\exp(-y^2/2)\longrightarrow 0$ as $y\longrightarrow\pm\infty$. ∴ Choose $\alpha=2n+1$.

∵ $\alpha=\frac{2E}{h\nu}=2n+1$, ∴ $E_n=\alpha h\nu/2=(n+1/2)h\nu$

$\int_{-\infty}^{\infty}|\Psi_n|^2 dv=1\Rightarrow\Psi_n=(\frac{2m\nu}{\hbar})^{1/4}(2^n\cdot n!)^{1/2}H_n(y)\exp(-y^2/2)$, where $H_n(y)$ is a Hermite polynomial of order n.

3-2 Uncertainty Principle $\triangle p\cdot\triangle x\geqq\hbar/2$, $\triangle E\cdot\triangle t\geqq\hbar/2$

Consider 1-D case. Define $<\triangle x^2>=\int\Psi^*(x-<x>)^2\Psi dx$, $<\triangle p_x^2>=\int\Psi^*(p_x-<p_x>)^2\Psi dx$, and take $<x>=<p_x>=0$ without any loss of generality.

$p_x=-i\hbar\,\partial/\partial x\Rightarrow<\triangle p_x^2><\triangle x^2>=-\hbar^2\int\Psi^*\frac{\partial^2\Psi}{\partial x^2}dx\cdot\int\Psi^*x^2\Psi dx$

∵ $\int\Psi^*\frac{\partial^2\Psi}{\partial x^2}dx=-\int\Psi^*i\frac{\partial}{\partial x}(i\frac{\partial\Psi}{\partial x})dx=-\Psi^*i\frac{\partial\Psi}{\partial x}\Big|_{-\infty}^{\infty}+\int i\frac{\partial\Psi^*}{\partial x}(i\frac{\partial\Psi}{\partial x})dx=-\int\frac{\partial\Psi^*}{\partial x}(\frac{\partial\Psi}{\partial x})dx$

∴ $<\triangle p_x^2><\triangle x^2>=\hbar^2\int\frac{\partial\Psi^*}{\partial x}(\frac{\partial\Psi}{\partial x})dx\cdot\int\Psi^*x^2\Psi dx$

By Schwarz inequality, $\int ff^*dx\cdot\int gg^*dx\geqq[(\int fg^*dx+\int gf^*dx)/2]^2$

$\Rightarrow<\triangle p_x^2><\triangle x^2>\geqq\frac{\hbar^2}{4}[\int\frac{\partial\Psi}{\partial x}x\Psi^*dx+\int x\Psi\frac{\partial\Psi^*}{\partial x}dx]^2=\frac{\hbar^2}{4}[\int x\frac{\partial\Psi\Psi^*}{\partial x}dx]^2$

$=\frac{\hbar^2}{4}[\Psi\Psi^*x\Big|_{-\infty}^{\infty}-\int\Psi\Psi^*\frac{\partial x}{\partial x}dx]^2=\frac{\hbar^2}{4}$. Define $<\triangle x>=<\triangle x^2>^{1/2}$, $<\triangle p_x>=<\triangle p_x^2>^{1/2}$

$\Rightarrow\triangle p\cdot\triangle x\geqq\hbar/2$

Eg. A typical atomic nucleus is about $5\times10^{-15}m$ in radius. What is the lower limit on the momentum an electron must have if it is to be part of a nucleus?

(Sol.) $\triangle x=5\times10^{-15}m$, $\triangle p\cdot\triangle x\geqq\hbar/2\Rightarrow\triangle p\geqq1.1\times10^{-20}$ Kg · m/sec