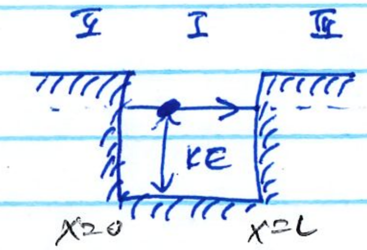
What we learned so far, ...

- Bound states : simple cases (as)
  1. particles in a box (in) the infinite well
  2. particles in a box in the Finite well

Today $\Rightarrow$ 3. The simple Harmonic oscillator

* expectation values, uncertainties, and operator (TBD)
$\longrightarrow$ and maybe go to "Un" bound state

1. Finite P. well

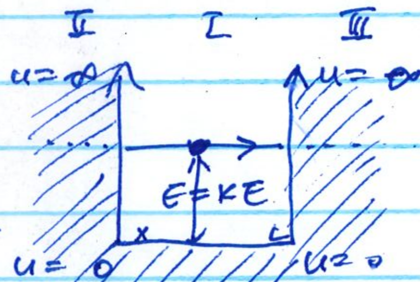


$$\psi(x) = \begin{cases} Ce^{+\alpha x} & (x<0) \\ A\sin kx + B\cos kx & (0<x<L) \\ Ge^{-\alpha x} & (x>L) \end{cases}$$

where $k = \sqrt{\dfrac{2mE}{\hbar^2}}$

$\alpha = \sqrt{\dfrac{2m(U_0 - E)}{\hbar^2}}$

2. infinite P. well



$$\psi_n(x) = \begin{cases} \sqrt{\dfrac{2}{L}}\sin\dfrac{n\pi x}{L} & (0<x<L) \\ 0 & (x<0) \\ & (x>L) \end{cases}$$

$E_n(x) = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$, $kL = n\pi$

$C = B$

$A = \dfrac{\alpha C}{k}$

secant

$\sec x = \dfrac{1}{\cos x}$

$\csc x$

cosecant

- Back to finite potential well (in order to determine A, B, C, G, E)

looked at "continuity" @ $x=0$ and $x=L$.

$\Rightarrow 2\cot kL = \dfrac{k}{\alpha} - \dfrac{\alpha}{k}$ (impossible to solve analytically, but numerical solution is possible)

$\Rightarrow \alpha = \begin{cases} k\tan\frac{1}{2}kL & (2n\pi < kL < 2n\pi + \pi) \\ -k\cot\frac{1}{2}kL & (2n\pi - \pi < kL < 2n\pi) \end{cases}$

$U_0 = \dfrac{\hbar^2 k^2}{2m}\sec^2\dfrac{1}{2}kL$, $2n\pi < kL < 2n\pi + \pi$ $(n = 1, 3, 5 \cdots)$

$\dfrac{\hbar^2 k^2}{2m}\csc^2\dfrac{1}{2}kL$, $2n\pi - \pi < kL < 2n\pi$ $(n = 2, 4, 6 \cdots)$

SHM

$U(x)$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + \frac{1}{2}kx^2\psi(x) = E\psi(x)$$

⇒ one of the few cases that can be solved exactly!!
for the wave f.t & corresponding quantized Es

~~Determine the E & normalized wave f.t in this state,~~

One solution of the Schrödinger eq is of the form $\psi(x) = Ae^{-ax^2}$

☆ Gaussian centered at the origin

$$-\frac{\hbar^2}{2m}\frac{d^2 \cancel{A}e^{-ax^2}}{dx^2} + \frac{1}{2}kx^2 \cancel{A}e^{-ax^2} = E\cancel{A}e^{-ax^2}$$

$$-\frac{\hbar^2}{2m}(-2a+4a^2x^2)\cancel{e^{-ax^2}} + \frac{1}{2}kx^2\cancel{e^{-ax^2}} = E\cancel{e^{-ax^2}}$$

$$\underbrace{\left(\frac{\hbar^2 a}{m}-E\right)}_{0} - \underbrace{\left(\frac{2\hbar^2a^2}{m}-\frac{1}{2}k\right)}_{0}x^2 = 0$$

$$\int_{-\infty}^{+\infty} e^{-a(z-b)^2}dz = \sqrt{\frac{\pi}{a}}$$

$$\frac{2\hbar^2a^2}{m} = \frac{1}{2}k \Rightarrow a = \frac{\sqrt{mk}}{2\hbar}$$

$$E = \frac{\hbar^2 a}{m} = \frac{\hbar^2}{m}\frac{\sqrt{mk}}{2\hbar} = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$$ ☆

To properly normalize the w.f, calculate the Total Probability

$$1 = \int_{-\infty}^{\infty}|\psi(x)|^2dx = \int_{-\infty}^{\infty}(Ae^{-ax^2})^2dx = A^2\underbrace{\int_{-\infty}^{\infty}e^{-2ax^2}dx}_{\text{Gaussian Integral}} = A^2\sqrt{\frac{\pi}{2a}} = 1$$

$$A = \left(\frac{2a}{\pi}\right)^{1/4} = \left(\frac{2\sqrt{mk}/2\hbar}{\pi}\right)^{1/4} = \left(\frac{mk}{\pi^2\hbar^2}\right)^{1/8}$$

(1) $E = \frac{\hbar}{2}\sqrt{\frac{k}{m}}$ and $\psi(x) = Ae^{-ax^2}$

$$= \left(\frac{mk}{\pi^2\hbar^2}\right)^{1/8} e^{-(\sqrt{mk}/2\hbar)x^2}$$

wave f.t (see Table 5.1)

General solution: $E = (n+\frac{1}{2})\hbar\omega_0$

$(n=0,1,2\ldots)$ $\omega_0 = \sqrt{\frac{k}{m}}$ ... Harmonic oscillator energies

5.8 Expectation Values Uncertainties, & operators.

- QM-cally, we can't know all that we might hope to know, in addition to simple probabilities, another very useful thing is "expectation value"

probability of being found in the interval dx around x

$$= |\psi(x)|^2 dx$$

$$\bar{x} \equiv \int_{\text{all space}} x|\psi(x)|^2 dx, \qquad \overline{x^2} \equiv \int_{\text{all space}} x^2|\psi(x)|^2 dx$$

average or expectation value

$$\Delta x \equiv \sqrt{\int_{\text{all space}} (x-\bar{x})^2 |\psi(x)|^2 dx} = \sqrt{\int_{\text{all space}} (x^2 - 2x\bar{x} + \bar{x}^2) |\psi(x)|^2 dx}$$

uncertainty as standard deviation

$$= \sqrt{\int x^2|\psi(x)|^2 dx - 2\bar{x}\int x|\psi(x)|^2 dx + \bar{x}^2\int |\psi(x)|^2 dx}$$

$$= \sqrt{\overline{x^2} - 2\bar{x}\,\bar{x} + \bar{x}^2} = \sqrt{\overline{x^2} - \bar{x}^2}$$

ex.X) 5-4

An electron is in a state given by the w.f

$$\psi(x) = Ae^{-[(x-b)/2\varepsilon]^2}$$

(a) A ? (b) expectation value of position

(c) uncertainty in position

(a). $$\int_{\text{all space}} |\psi(x)|^2 dx = \int_{-\infty}^{\infty} \left(Ae^{-[(x-b)/2\varepsilon]^2}\right)^2 dx$$

$$= \underbrace{A^2 \int_{-\infty}^{\infty} e^{-(x-b)^2/2\varepsilon^2} dx}_{\text{standard Gaussian integral}} = 1$$

see text's inside cover

$$\downarrow$$

$$\sqrt{2\pi\varepsilon^2}$$

$$\therefore A^2\sqrt{2\pi\varepsilon^2} = 1 \rightarrow A = \frac{1}{\sqrt{\varepsilon}\,(2\pi)^{1/4}}$$

(b) Inserting in $\overline{x} \equiv \int_{\text{all space}} x\,|\psi(x)|^2 dx$

$$= A^2 \int_{-\infty}^{\infty} x\, e^{-(x-b)^2/2\varepsilon^2} dx$$

$$= A^2\, b\sqrt{2\pi\varepsilon^2} = \left(\frac{1}{\sqrt{\varepsilon}\,(2\pi)^{1/4}}\right)^2 b\sqrt{2\pi\varepsilon^2} = b$$

(c) According to $\Delta X = \sqrt{\overline{x^2} - \overline{x}^2}$ — ①

need to calculate $\overline{x^2}$

$$\overline{x^2} = \int_{\text{all space}} x^2 |\psi(x)|^2 dx = A^2 \int_{-\infty}^{\infty} x^2 e^{-(x-b)^2/2\varepsilon^2} dx$$

$$= \left(\frac{1}{\sqrt{\varepsilon}\,(2\pi)^{1/4}}\right)^2 (\varepsilon^2 + b^2)\sqrt{2\pi\varepsilon^2} = \varepsilon^2 + b^2$$

now inserting in ①

$$\Delta X = \sqrt{(\varepsilon^2 + b^2) - b^2} = \varepsilon$$

- Now, let us generalize to quantities other than position.
  e.g. position, m/m, E or Angular m/m etc...

- General form for calculating an expected value:

$$\overline{Q} = \int_{\text{all space}} \psi^*(x,t)\, \hat{Q}\, \psi(x,t)\, dx$$

"operator"

For m/m, $\hat{p} = -i\hbar \frac{\partial}{\partial x}$

e.g. $KE = \frac{p^2}{2m} \longrightarrow \hat{KE} = \frac{1}{2m}\hat{p}^2$

$$= \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial x}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)$$

$$= \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial^2 x}$$

Basic operators

m/m	position	E
$\hat{p} = -i\hbar\frac{\partial}{\partial x}$	$\hat{x} = x$	$\hat{E} = i\hbar\frac{\partial}{\partial t}$

- Re-write the Schrödinger eq.

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

$$\Rightarrow \hat{KE}\,\psi(x,t) + \hat{U}(x)\,\psi(x,t) = \hat{E}\,\psi(x,t)$$

- Uncertainty $\Delta Q = \sqrt{\overline{Q^2} - \overline{Q}^2}$ ⟵ see p170

$\Delta x = \sqrt{\overline{x^2} - \overline{x}^2}$

- check out "example 5.5"

5.9 Nonstationary states

$$\Psi(x,t) = \psi(x)\, e^{-i(E/\hbar)t} \longleftarrow \text{5.2 stationary state}$$

A bound ptl will have quantized E,

e.g. $E_1, E_2, E_3, \ldots$

the corresponding solutions of the time-independent Schrödinger eq as $\psi_1, \psi_2, \psi_3 \ldots$

Total w.f in stationary state n is,

$$\Psi_n(x,t) = \psi_n(x)\, e^{-i(E_n/\hbar)t}$$

⇒ now, non-stationary state

: process of jumping from one stationary state to another

$$\Psi(x,t) = \psi_n(x)\, e^{-i(E_n/\hbar)t} + \psi_m(x)\, e^{-i(E_m/\hbar)t}$$

$\Psi^*(x,t)\,\Psi(x,t) \longleftarrow$ its probability density varies w/ time

$$= \left[\psi_n(x) e^{+i(E_n/\hbar)t} + \psi_m(x) e^{+i(E_m/\hbar)t}\right]\left[\psi_n(x) e^{-i(E_n/\hbar)t} + \psi_m(x) e^{-i(E_m/\hbar)t}\right]$$

$$= \psi_n^2(x) + \psi_m^2(x) + 2\,\psi_n(x)\,\psi_m(x)\cos\left(\frac{E_n - E_m}{\hbar}t\right)$$

variation is a periodic f.t of time, of angular frequency,

$$(E_n - E_m)/\hbar = \omega$$

5.11 Well-Defined observables : Eigenvalues

Given an operator $\hat{Q}$,
the function $f(x)$ is an "eigenfunction" of the operator ..

$$\underbrace{\hat{Q}}_{\text{operator}}\ \underbrace{f(x)}_{\text{eigenfunction}} = \underbrace{\lambda}_{\text{eigenvalue}}\ \underbrace{f(x)}_{\text{eigenfunction}}$$

① m/m

$$\hat{p}\, e^{ikx} = -i\hbar \frac{\partial}{\partial x} e^{ikx} = \underbrace{\hbar k}_{\text{eigenvalue of the m/m operator}} e^{ikx}$$

∴ $p = \hbar k$

② E

$$\hat{E}\, e^{-i\omega t} = i\hbar \frac{\partial}{\partial t} e^{-i\omega t} = \underbrace{\hbar\omega}_{\text{eigenvalue of the E op.}} e^{-i\omega t}$$

∴ $E = \hbar\omega$

※ we'll see this later !!