Chapter 5 The Schrodinger Eq.

This chapter motivates the nonrelativistic approximation to the quantum mechanical wave function. (Chap 5 slide 1)

For no forces, the coefficients in the wave equation can't depend on $\vec{r}, t$. For 1D, the wave equation looks like

$$A\,\Psi(x,t) + B\frac{\partial\Psi(x,t)}{\partial t} + C\frac{\partial\Psi}{\partial x}(x,t) + \ldots = 0$$

with

$$\Psi(x,t) = \text{const}\; e^{i(kx-\omega t)}$$

Put into equation

$$A + B(-i\omega) + C\,ik + \ldots$$

Our condition is $\hbar\omega = \frac{\hbar^2 k^2}{2m}$

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2}$$ gives our relation

Memorize this!

Why $\hbar^2\frac{\partial^2\Psi}{\partial t^2} = \left(\frac{\hbar^2}{2m}\right)^2\frac{\partial^4\Psi}{\partial x^4}$ not OK?

What are the units of $\hbar\frac{\partial}{\partial t}$ or $\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$?

If there are conservative forces, the Schrodinger eq. is

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

Time dependent Schrodinger eq.

potential energy

$\Psi(x,t)$ is a complex function. Measurements of any experimental quantity must be real!

We have our wave equation but what does it mean?

The probability for detecting the particle between x and $x+dx$ is

$$\text{Prob} = \Psi(x,t)\,\Psi^*(x,t)\,dx = |\Psi(x,t)|^2\,dx$$ (Chap 5 slide 2-4)

What is the probability to detect between x_0 and x_f?

" " " " " somewhere?

Chap 5 slide 5 $\quad i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}$

$\Psi = e^{i(kx+\omega t)} \qquad -\hbar\omega = \frac{\hbar^2 k^2}{2m} \longrightarrow -E = P^2/2m \qquad$ no

$\Psi = e^{-i(kx+\omega t)} \qquad \hbar\omega = \frac{\hbar^2 k^2}{2m} \longrightarrow E = P^2/2m \qquad$ yes

$\Psi = e^{-i(kx-\omega t)} \qquad -\hbar\omega = \frac{\hbar^2 k^2}{2m} \longrightarrow -E = P^2/2m \qquad$ no

$\Psi = e^{i(Px-Et)/\hbar} \qquad \hbar E/\hbar = \frac{\hbar^2 (P/\hbar)^2}{2m} \longrightarrow E = P^2/2m \qquad$ yes

$\Psi = \sin(kx-\omega t) \qquad -i\hbar\omega \cos(kx-\omega t) \neq \frac{\hbar^2 k^2}{2m}\sin(kx-\omega t) \qquad$ no

$\Psi = \cos(kx)\, e^{-i\omega t} \qquad \hbar\omega = \frac{\hbar^2 k^2}{2m} \longrightarrow E = P^2/2m \qquad$ yes

$\Psi = \cos(kx)\, e^{i\omega t} \qquad -\hbar\omega = \frac{\hbar^2 k^2}{2m} \longrightarrow -E = P^2/2m \qquad$ no

$e^{i(kx-\omega t)} \longrightarrow$ right $\qquad e^{-i(kx+\omega t)} \longrightarrow$ left

$\Psi(x,t)$ is always a continuous function of x

$\frac{\partial \Psi}{\partial x}(x,t)$ is a continuous function of x if $U(x,t) =$ finite

Go through some typical behavior of $\Psi(x,t)$ (Chap 5 slides 6-32)

Because the Sch. eq. is linear in $\Psi(x,t)$, if you have two solutions, $\Psi_1(x,t)$ and $\Psi_2(x,t)$, then any combination

$$\Psi(x,t) = \underbrace{A_1 \Psi_1(x,t) + A_2 \Psi_2(x,t)}_{A_1,\,A_2\ \text{constants}} \quad \text{is a solution}$$

Why $\int_{\text{all space}} \Psi^*(x,t)\, \Psi(x,t)\, dx = \text{const}$?

$$\left(i\hbar \frac{\partial \Psi}{\partial t}\right)^* = -i\hbar \frac{\partial \Psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi^*}{\partial x^2} + U\Psi$$

$$i\hbar \frac{\partial}{\partial t}\int \Psi^* \Psi\, dx = \int \left[\left(\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} - U\Psi\right)^* \Psi + \Psi^*\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + U\Psi\right)\right] dx$$

$$= \frac{\hbar^2}{2m}\int_{\text{all space}} \frac{\partial^2 \Psi^*}{\partial x^2}\Psi - \Psi^* \frac{\partial^2 \Psi}{\partial x^2}\, dx$$

$$= \frac{\hbar^2}{2m}\int_{\text{all space}} \frac{\partial}{\partial x}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^* \frac{\partial \Psi}{\partial x}\right) dx = \frac{\hbar^2}{2m}\left(\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right)\Big|_{-\infty}^{\infty} = 0 \checkmark$$

Show $\int_{\text{all space}} \Psi_1^*(x,t)\, \Psi_2(x,t)\, dx = \text{const}$

Special case $U(x,t) = U(x)$ Time independent PE

In classical mechanics, this would give energy conservation

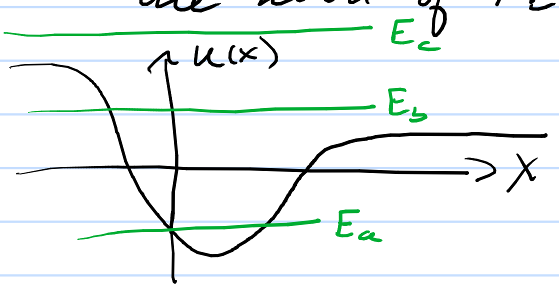
$$\Psi(x,t) = e^{-iEt/\hbar}\, \psi(x)$$

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + U(x)\psi(x)$$ Time independent Schrodinger eq.

For any E, there is always 2 linearly independent solutions.

Example $\psi_a(0) = 1$, $\psi_a'(0) = 0$ and $\psi_b(0) = 0$, $\psi_b'(0) = 1$

How many physical solutions at energy E depends on the kind of PE. Randomly choose E in different region.



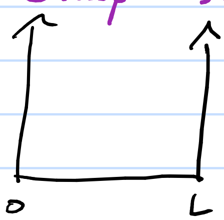
For $E_c \to$ 2 physical linearly independent solutions

For $E_b \to$ 1 physical linearly ....

For $E_a \to$ 0 physical linearly

How can this be? Doesn't this mean the harmonic oscillator has no physical quantum energy states?

Chap 5 slide 33



$$E\psi(x) = -\frac{\hbar^2}{2m}\psi''(x) + U(x)\psi(x)$$

$$\psi(x) = A\sin(kx) + B\cos(kx) \qquad E = \frac{\hbar^2 k^2}{2m}$$

Because $U(0), U(L) \to \infty \Rightarrow \psi(0) = 0$ and $\psi(L) = 0$

$\psi(0) = B = 0$ $\qquad \psi(L) = A\sin(kL) + \cancel{B}^{\,0}\cos(kL) = A\sin(kL)$

For random E $\quad \sin(kL) \neq 0 \Rightarrow A = 0$ which means no solution

What to do?

Find E where $\sin(kL) = 0$!!!

$k_n L = n\pi \qquad n = 1, 2, 3, \ldots$ (why $n=0$ not ok? $n<0$ not ok?)

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} = \frac{h^2 n^2}{8mL^2} \qquad n = 1, 2, 3, \ldots$$

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

$$k_n = \frac{2\pi}{\lambda_n} \rightarrow \lambda_n = \frac{2L}{n} \qquad P_n = \frac{hn}{2L}$$

$$\text{Freq. of light} = \frac{E_{n+1} - E_n}{h} = \frac{h}{8mL^2}\left[(n+1)^2 - n^2\right] = \frac{h}{4mL^2}(n + 1/2)$$

$$= \frac{P_{n+1/2}}{m}\frac{1}{2L}$$ (this is the classical frequency at $n + 1/2$)

The $\psi_n(x)$ are the eigenstates of $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) = H$

The E_n are the eigenvalues of H

What are eigenstates and eigenvalues? Idea from linear algebra. Matrix $\underline{\underline{M}}$

$$\underline{\underline{M}}\, \vec{v}_\alpha = \vec{v}_\alpha\, \mu_\alpha$$

eigenvector eigenvalue

Momentum operator $P_{op} = \frac{\hbar}{i}\frac{\partial}{\partial x}$, Hamiltonian $H = \frac{P_{op}^2}{2m} + U(x)$

Find the eigenstates + eigenvalues of P_{op}

eigenstate

$$P_{op}\,\psi_p(x) = p\,\psi_p(x) \qquad \psi_p'(x) = \frac{ip}{\hbar}\psi_p(x)$$

eigenvalue

$$\psi_p = A\, e^{ikx} \quad \text{and} \quad p = \hbar k = \frac{h}{2\pi}\frac{2\pi}{\lambda} = h/\lambda$$

const

Chap 5 Slides 34-38

If the classical motion is bounded, the $\psi_n(x)$ can be "normalized":

$$\int_{\text{all space}} |\psi_n(x)|^2 dx = 1$$

For 1D systems can also show $\int_{\text{all space}} \psi_m^*(x)\,\psi_n(x)\,dx = \begin{cases} 1 & \text{if } m=n \\ 0 & \text{if } m \neq n \end{cases} \rightarrow \delta_{mn}$ Kronecker delta

Go through general features of E_n vs n for 1D (Chap 5 slides 39-43)

Go through general features of $\psi_n(x)$ for 1D (Chap 5 slides 44-48)

Can make structures inside solids (Chap 5 slides 49,50)

Expectation value Given $\Psi(x,t)$, suppose you measure the position with range dx you measure random positions with probability $|\Psi(x,t)|^2 dx$

$$\langle x \rangle (t) = \int_{\text{all space}} x\,|\Psi(x,t)|^2 dx$$

What about momentum? $\langle p \rangle (t) \neq \int_{\text{all space}} \frac{\hbar}{i}\frac{\partial}{\partial x}|\Psi(x,t)|^2 dx$

Need to be able to get phase info

$$\langle p \rangle (t) = \int_{\text{all space}} \Psi^*(x,t)\,\frac{\hbar}{i}\frac{\partial \Psi(x,t)}{\partial x}\,dx = \int_{\text{all space}} -\frac{\hbar}{i}\frac{\partial \Psi^*(x,t)}{\partial x}\,\Psi(x,t)\,dx = \langle p \rangle^*(t)$$

What about energy? $\langle H \rangle (t) = \int_{\text{all space}} \Psi^*(x,t)\,[H\,\Psi(x,t)]\,dx$

Suppose you have a free particle with $\Psi(x,0) = A e^{ik(x-x_0)} e^{-\frac{(x-x_0)^2}{2L^2}}$

Compute $\langle x\rangle(0)$, $\langle p\rangle(0)$, $\langle H\rangle(0)$

First need to find A using

$$\int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx = 1 = A^2 \int_{-\infty}^{\infty} e^{-ik(x-x_0)} e^{-\frac{(x-x_0)^2}{2L^2}} e^{ik(x-x_0)} e^{-\frac{(x-x_0)^2}{2L^2}} dx$$

$$= A^2 \int_{-\infty}^{\infty} e^{-(x-x_0)^2/L^2} dx = A^2 \sqrt{\pi}\, L = 1 \Rightarrow \quad A = \frac{1}{\pi^{1/4}\sqrt{L}}$$

$$\langle x\rangle(0) = A^2 \int_{-\infty}^{\infty} x\, e^{-(x-x_0)^2/L^2} dx = A^2 \int_{-\infty}^{\infty} (x-x_0) e^{-(x-x_0)^2/L^2} dx + x_0 = \underline{x_0}$$

$$p\,\Psi(x,0) = \frac{\hbar}{i} \Psi'(x,0) = A \frac{\hbar}{i} \left[ik - \frac{x-x_0}{L^2} \right] \Psi(x,0)$$

$$\langle p\rangle(0) = A^2 \int_{-\infty}^{\infty} \left(\hbar k + i\hbar \frac{(x-x_0)}{L^2}\right) e^{-(x-x_0)^2/L^2} dx = \underline{\hbar k}$$

$$H\,\Psi(x,0) = -\frac{\hbar^2}{2m} \Psi''(x,0) = -\frac{\hbar^2}{2m}\left(-k^2 - \frac{2ik(x-x_0)}{L^2} + \frac{(x-x_0)^2}{L^4} - \frac{1}{L^2}\right) \Psi(x,0)$$

$$\langle H\rangle(0) = -\frac{\hbar^2}{2m}\left[-k^2 - 0 + \frac{1}{2}\frac{1}{L^2} - \frac{1}{L^2}\right] = \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{4mL^2}$$

Use linearity of Schrodinger eq. The most general solution when $U(x,t) = U(x)$

$$\Psi(x,t) = a_1 \psi_1(x) e^{-iE_1 t/\hbar} + a_2 \psi_2(x) e^{-iE_2 t/\hbar} + a_3 \psi_3(x) e^{-iE_3 t/\hbar} + \dots$$

$a_1, a_2, a_3, \dots$ are constants

Find $\langle H\rangle(t)$

$$H\,\Psi(x,t) = a_1 H \psi_1(x) e^{-iE_1 t/\hbar} + a_2 H \psi_2(x) e^{-iE_2 t/\hbar} + \dots$$
$$= a_1 E_1 \psi_1(x) e^{-iE_1 t/\hbar} + a_2 E_2 \psi_2(x) e^{-iE_2 t/\hbar} + \dots$$

$$\langle H\rangle(t) = \int_{\text{all space}} \left(a_1^* \psi_1^* e^{iE_1 t/\hbar} + a_2^* \psi_2^*(x) e^{iE_2 t/\hbar} + \dots\right)\left(a_1 E_1 \psi_1(x) e^{-iE_1 t/\hbar} + a_2 E_2 \psi_2(x) e^{-iE_2 t/\hbar} + \dots\right) dx$$
$$= |a_1|^2 E_1 + |a_2|^2 E_2 + |a_3|^2 E_3 + \dots$$

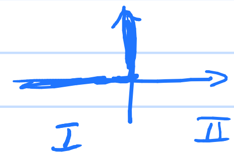
This suggests $|a_n|^2$ is probability to measure E_n

What about when the waves can extend to $+\infty$, $-\infty$, or both? The eigenstates can't be normalized in the way discussed above. Can use Dirac delta function normalization or make an artificial box.

(Chap 5 slides 51, 52)

The idea for pulling out physical info is to use the momentum eigenstates and compare different pieces. Easier to understand by doing some cases

Case 1 $\quad U(x)=0 \quad x<0 \qquad U(x)=\infty \quad x>0$



$x<0 \qquad -\frac{\hbar^2}{2m}\psi_I''(x) = E\,\psi_I(x) \qquad \psi_I(x) = A e^{ikx} + B e^{-ikx} \qquad E = \frac{\hbar^2 k^2}{2m}$

$x>0 \qquad \psi_{II}(x) = 0$

Continuity $\quad \psi_I(0) = A + B = 0 \rightarrow B = -A$

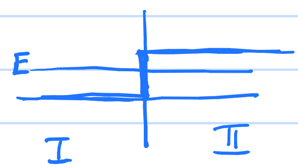
$\psi_I(x) = A\left(e^{ikx} - e^{-ikx}\right) = 2iA\sin(kx)$ ✓

In region I amount traveling to right $\quad \frac{\hbar k}{m}|A|^2$

" " " " " " left $\quad \frac{\hbar k}{m}|B|^2 = \frac{\hbar k}{m}|A|^2$

Gives 100% reflection

Case 2 $\quad U(x)=0 \quad x<0 \qquad U(x) = U_0 > E \quad x>0$



$x<0 \qquad \psi_I(x) = A e^{ikx} + B e^{-ikx}$

$x>0 \qquad \psi_{II}(x) = C e^{\alpha x} + D e^{-\alpha x} \qquad -\frac{\hbar^2\alpha^2}{2m} = -(U_0 - E)$

Must have continuity $\quad \psi_I(0) = \psi_{II}(0) \qquad A + B = C + D$

" " derivative " $\quad \psi_I'(0) = \psi_{II}'(0) \qquad ik(A-B) = \alpha(C-D)$

$\psi(x\to\infty) \rightarrow 0 \qquad C = 0$

$$A + B = D = -\frac{ik}{\alpha}(A-B) \rightarrow B = -A\frac{\left(1+\frac{ik}{\alpha}\right)}{\left(1-\frac{ik}{\alpha}\right)} = -A\frac{\alpha+ik}{\alpha-ik}$$

In Region I amount traveling to right $\quad \frac{\hbar k}{m}|A|^2$

" " " " " left $\quad \frac{\hbar k}{m}|B|^2 = \frac{\hbar k}{m}|A|^2\left(\frac{\alpha+ik}{\alpha-ik}\right)\left(\frac{\alpha-ik}{\alpha+ik}\right)$

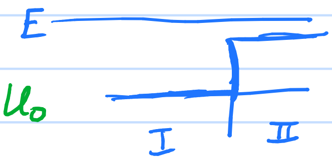
Gives 100% reflection

Note that there is some probability for finding the particle at $x>0$. The distance over which decreases exponentially $L = 1/(2\alpha) = \hbar/\left(2\sqrt{2m(U_0-E)}\right)$ (2 from squaring)

Trends? Larger $m \to$ smaller distance
Smaller $U_0 - E \to$ larger distance

Example electron, $U_0 - E = 1\,eV$ $L = 1.0\times10^{-10}\,m$
proton, " $L = 2.3\times10^{-12}\,m$

Case 3 Same but $E > U_0$



$$\psi_I = A e^{ik_0x} + B e^{-ik_0x} \qquad \hbar^2k_0^2/2m = E$$
$$\psi_{II} = C e^{ik_1x} + D e^{-ik_1x} \qquad \hbar^2k_1^2/2m = E - U_0 \qquad k_1 < k_0$$

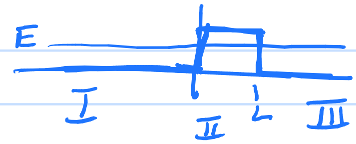
Continuity $\psi_I(0) = \psi_{II}(0)$ $A + B = C + D$
Derivative continuity $\psi_I'(0) = \psi_{II}'(0)$ $ik_0(A-B) = ik_1(C-D)$
No left moving in II $D = 0$ $A + B = C = k_0/k_1\,(A-B)$

$$B = \frac{k_0-k_1}{k_0+k_1}A \qquad C = A+B = \frac{2k_0}{k_0+k_1}A$$

In Region I amount traveling right $\frac{\hbar k_0}{m}|A|^2$
" " " " " left $\frac{\hbar k_0}{m}|B|^2 = \frac{\hbar k_0}{m}\frac{(k_0-k_1)^2}{(k_0+k_1)^2}$
" " II " " right $\frac{\hbar k_1}{m}|C|^2 = \frac{\hbar k_1}{m}\frac{4k_0^2}{(k_0+k_1)^2}$

Reflection prob $= \frac{\hbar k_0}{m}|B|^2 \Big/ \frac{\hbar k_0}{m}|A|^2 = \frac{(k_0-k_1)^2}{(k_0+k_1)^2}$
Transmission prob $= \frac{\hbar k_1}{m}|C|^2 \Big/ \frac{\hbar k_0}{m}|A|^2 = 4k_1k_0/(k_0+k_1)^2$
] sum = 1 ✓

Case 4 $U(x) = 0$ $x<0,\ x>L$ $U(x) = U_0 > E$ $0<x<L$



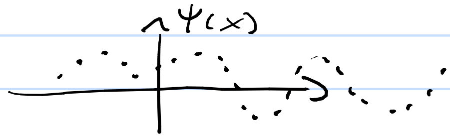
This is more complicated than I want for this class but general idea

Transmission prob $\sim e^{-2\alpha L} = e^{-2\sqrt{2m(U_0-E)}\,L/\hbar}$
Fission, Fusion, μ catalyzed fusion, Scanning Tunneling microscope (Chap 5 slide 53)

In recent times, "quantum computing" has become intense area of research. Why can't quantum computers be simulated by classical computers? Nothing, so far, has hinted at why QM is hard.

Numerical QM.

1) Grid of spatial points



$\psi_j = \psi(x_0 + j\cdot\Delta x)$

$j = 0, 1, \ldots N$

Becomes like linear algebra

$\Psi(x_j, t) = \psi_j(t)$ $\qquad i\hbar \frac{d\psi_j(t)}{dt} = \sum_k H_{j,k}(t)\,\psi_k(t)$

2) Expansion in terms of "basis" functions

$\Psi(x,t) = \sum_j a_j(t)\, \chi_j(x)$

Becomes like linear algebra $\quad i\hbar \frac{da_j(t)}{dt} = \sum_k \tilde{H}_{j,k}(t)\, a_k(t)$

For 1D "all" calculations are "easy" (errors less than ~1%)

What is the 2D Schrodinger eq.?

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

Numerical QM requires $(N_x+1)(N_y+1)$ points $\sim N^2$

3D? $$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right) + U(x,y,z,t)\,\Psi(x,y,z,t$$

Numerical QM requires $(N_x+1)(N_y+1)(N_z+1)$ points $\sim N^3$

What is the Schrodinger eq. for 2 particles in 1D?

$$i\hbar \frac{\partial \Psi(x_1, x_2, t)}{\partial t} = -\frac{\hbar^2}{2m_1}\frac{\partial^2 \Psi(x_1,x_2,t)}{\partial x_1^2} - \frac{\hbar^2}{2m_2}\frac{\partial^2 \Psi(x_1,x_2,t)}{\partial x_2^2} + U(x_1,x_2,t)\,\Psi(x_1,x_2,t)$$

Numerical QM requires $(N_1+1)(N_2+1)$ points $\sim N^2$

2 particles in 3D $\Psi(x_1, y_1, z_1, x_2, y_2, z_2, t)$ $\sim N^6$ points

Numerical QM

1D easy 2D easy(ish) 3D medium 4D hard 5D really hard

6D ~ impossible

Quantum computers 2 points per particle

effort $2^{N_{qbits}}$

$N_{qbit} = 10 \rightarrow \sim 10^3$

" $= 20 \rightarrow \sim 10^6$

" $= 30 \rightarrow \sim 10^9$

" $= 40 \rightarrow \sim 10^{12}$

" $= 50 \rightarrow \sim 10^{15}$

] naive classical calculations run into trouble

Classical 1D $U(x)$ — no chaos

Classical 2D $U(x,y)$ - can have chaos

Quantum corral, Quantum scar (Chap 5, slide 54)

Casimir effect (Chap 5, slide 55)