Chapter 2 - Time Independent Schrodinger Equation

In general, solving partial differential equations is incredibly complicated. Some equations we still don't know if they have physical solutions. The Sch. Eq. has several nice features.

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

If $\Psi_1(x,t)$ and $\Psi_2(x,t)$ are solutions then
$\Psi(x,t) = C_1 \Psi_1(x,t) + C_2 \Psi_2(x,t)$ <u>also</u> a solution

Put into Sch. Eq.

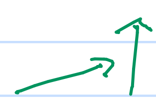
$$i\hbar \frac{\partial \Psi}{\partial t} = C_1 i\hbar \frac{\partial \Psi_1}{\partial t} + C_2 i\hbar \frac{\partial \Psi_2}{\partial t} = C_1\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_1}{\partial x^2} + V\Psi_1\right) + C_2\left(-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi_2}{\partial x^2} + V\Psi_2\right)$$

$$\checkmark = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

When adding different solutions, the concept of linear independence is important.

Examples from vectors

N-vectors are linearly independent if you <u>can't</u> find C_j so $C_1\vec{a}_1 + C_2\vec{a}_2 + C_3\vec{a}_3 + \dots C_N\vec{a}_N = 0$

Are these 2 linearly independent? 

Can you find 3 vectors that lie in a plane and are linearly independent?

N-functions of x are linearly independent if you <u>can't</u> find C_j so

$C_1 f_1(x) + C_2 f_2(x) + \dots C_N f_n(x) = 0$ for every x

Interesting point: Because x is continuous there is an ∞ number of independent functions for any range of x.

Example: For $0 \leq x \leq L$ $\quad f_n(x) = \sin\left(\frac{n\pi x}{L}\right)$ are all independent $n = 1, 2, 3, \ldots \infty$

Important consequence: When possible, find a set of linearly independent solutions of Sch. Eq. and add them up to get <u>any</u> solution.

$$\Psi(x,t) = C_1 \Psi_1(x,t) + C_2 \Psi_2(x,t) + C_3 \Psi_3(x,t) + \ldots$$

A general case where it is possible to find all $\Psi_j(x,t)$ is when $V(x,t) = V(x)$ Time independent potential

One possible set of solutions have the simple form

$\Psi_j(x,t) = \psi_j(x)\, \varphi_j(t)$ Note lower case $\psi_j(x)$ on right hand side

<u>Separation of variables</u>

To find the equations for ψ_j and φ_j substitute

$$\psi_j(x)\, i\hbar \frac{d\varphi_j(t)}{dt} = \varphi_j(t)\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_j(x)}{dx^2} + V(x)\psi_j(x)\right]$$

notice partial derivs $\longrightarrow$ regular derivs

Divide from left by $\psi_j\, \varphi_j$

$$\Rightarrow \quad i\hbar \frac{1}{\varphi_j(t)}\frac{d\varphi_j(t)}{dt} = \frac{1}{\psi_j(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2\psi_j(x)}{dx^2} + V(x)\psi_j(x)\right]$$

The right hand side is only a function of x while the left hand side is only a function of t. The only way they can be equal is if they both equal the same constant.

By dimensional analysis, the constant has the same units of $\hbar$/time $= J\cdot s/s = \underline{\underline{J}}$. The constant has units of energy.

$$\underbrace{i\hbar \frac{d\varphi_j(t)}{dt} = E_j \varphi_j(t) \quad \text{and} \quad -\frac{\hbar^2}{2m}\frac{d^2\psi_j(x)}{dx^2} + V(x)\psi_j(x) = E_j\psi_j(x)}_{\text{same}}$$

$$\varphi_j(t) = \cancel{C}^{\,1} e^{-iE_jt/\hbar} = e^{-iE_jt/\hbar} \qquad \text{By convention } C=1$$

The time independent Sch Eq. depends on V(X) so needs to be solved for each V(x).

I'm now going to start using a notational convenience. A hat means an operator

Examples: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$ and $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$

These states with separable solutions have some very important properties.

(1) Expectation value of <u>all</u> time indep. operators is time independent.

$$\langle \hat{Q}(\hat{x},\hat{p})\rangle = \int \psi_j^*(x)\, e^{iE_jt/\hbar}\, \hat{Q}(\hat{x},\hat{p})\, e^{-iE_jt/\hbar}\, \psi_j(x)\,dx$$

$$= \int \psi_j^*(x)\, \hat{Q}(\hat{x},\hat{p})\, \psi_j(x)\, dx$$

$\boxed{\text{Stationary states}}$

(2) They have a definite energy.

$$\langle \hat{H} \rangle = \int_{-\infty}^{\infty} \psi_j^*(x) \left(\hat{H} \psi_j(x) \right) dx = E_j \int_{-\infty}^{\infty} \psi_j^*(x)\, \psi_j(x)\, dx = E_j$$

$$\langle \hat{H}^2 \rangle = \int_{-\infty}^{\infty} \psi_j^*(x) \left[\hat{H} \left(\hat{H} \psi_j(x) \right) \right] dx = E_j \int_{-\infty}^{\infty} \psi_j^*(x) \left(\hat{H} \psi_j(x) \right) dx$$

$$= E_j^2$$

$$\sigma_E^2 = \langle \hat{H}^2 \rangle - \langle \hat{H} \rangle^2 = E_j^2 - E_j^2 = 0$$

When the variance is 0, then the probability is 1 for E_j and 0 for all others.

$\hat{H}$ is called the Hamiltonian in analogy to the classical quantity

$$H = \frac{p^2}{2m} + V(x)$$

(3) Superposition - Any $\Psi(x,t)$ can be constructed like

$$\Psi(x,t) = C_1 \Psi_1(x,t) + C_2 \Psi_2(x,t) + \ldots$$

$$= \sum_{j=1}^{\infty} C_j \Psi_j(x,t) \qquad C_j \text{ are all constant}$$

$$= \sum_{j=1}^{\infty} C_j e^{-iE_j t/\hbar} \psi_j(x)$$

(4) The E_j are all real.

If $\mathrm{Im}(E_j) > 0$ then $e^{-iE_j t/\hbar} \to \infty$ as $t \to \infty$

" " < 0 " " " " $-\infty$

(5) The $\int_{-\infty}^{\infty} \psi_j^*(x)\psi_{j'}(x)\,dx \begin{array}{l} = 1 \quad \text{if } j = j' \\ = 0 \quad \text{if } j \neq j' \end{array} \Bigg] = \delta_{jj'}$
Kronecker delta

For $j \neq j'$ $\quad \int_{-\infty}^{\infty} \psi_j^*(x)\left(\hat{H}\psi_{j'}(x)\right)dx = E_{j'} \int_{-\infty}^{\infty} \psi_j^*(x)\psi_{j'}(x)\,dx$

and $\quad \int_{-\infty}^{\infty} \left(\hat{H}\psi_j(x)\right)^* \psi_{j'}(x)\,dx = E_j \int_{-\infty}^{\infty} \psi_j^*(x)\psi_{j'}(x)\,dx$

Subtract top line from bottom line

$$\frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\left[\psi_j^*(x)\frac{d^2\psi_{j'}}{dx^2} - \frac{d^2\psi_j^*}{dx^2}\psi_{j'}\right]dx = (E_j - E_{j'})\int_{-\infty}^{\infty}\psi_j^*(x)\psi_{j'}(x)\,dx$$

$$= \frac{\hbar^2}{2m}\int_{-\infty}^{\infty}\frac{d}{dx}\left[\psi_j^*\frac{d\psi_{j'}}{dx} - \frac{d\psi_j^*}{dx}\psi_{j'}\right]dx$$

$$= \frac{\hbar^2}{2m}\left[\psi_j^*(x)\frac{d\psi_{j'}(x)}{dx} - \frac{d\psi_j^*(x)}{\partial x}\psi_{j'}(x)\right]\Bigg|_{-\infty}^{\infty} = 0$$

This means $(E_j - E_{j'})\int \psi_j^*(x)\psi_{j'}(x)\,dx = 0$

Either $E_j = E_{j'}$ or $\int \psi_j^*(x)\psi_{j'}(x)\,dx = 0$

For 1D $E_j \neq E_{j'}$ if $j \neq j'$

(6) <u>All</u> of the $\psi_j(x)$ are linearly independent

Show $c_1\psi_1(x) + c_2\psi_2(x) + \dots \equiv F(x) \neq 0$ for every x

$\int_{-\infty}^{\infty} F^*(x)F(x) \neq 0$ if $F(x) \neq 0$

$$= \int_{-\infty}^{\infty}\left(c_1^*\psi_1^*(x) + c_2^*\psi_2^*(x) + \dots\right)\left(c_1\psi_1(x) + c_2\psi_2(x) + \dots\right)dx$$

$= |c_1|^2 + |c_2|^2 + \dots \geq 0$ unless every $c_j = 0$

what happened to terms like $c_1^* c_2$?

(7) The normalization of $\Psi(x,t)$ becomes

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = |C_1|^2 + |C_2|^2 + \ldots = 1$$

$|C_j|^2$ = probability you will measure energy equal E_j

For a time independent $\hat{H}$, you can have motion by superposing two states with different E_j.

To simplify choose $\psi_j(x)$ and C_j real (and j')

Two states: $\Psi(x,t) = C_j e^{-iE_jt/\hbar}\psi_j(x) + C_{j'}e^{-iE_{j'}t/\hbar}\psi_{j'}(x)$

$$\langle\hat{Q}\rangle(t) = C_j^2 \int_{-\infty}^{\infty}\psi_j(x)\,\hat{Q}\,\psi_j(x)\,dx + C_{j'}^2\int_{-\infty}^{\infty}\psi_{j'}(x)\,\hat{Q}\,\psi_{j'}(x)\,dx$$
$$+ C_jC_{j'}\Big[e^{-i(E_j-E_{j'})t/\hbar}\int_{-\infty}^{\infty}\psi_{j'}(x)\,\hat{Q}\,\psi_j(x)\,dx +$$
$$e^{i(E_j-E_{j'})t/\hbar}\int_{-\infty}^{\infty}\psi_j(x)\,\hat{Q}\,\psi_{j'}(x)\,dx\Big]$$

Really important $e^{i\theta} = \cos\theta + i\sin\theta$

Very important
$$e^{i(\theta+2\pi)} = e^{i\theta}e^{i2\pi}$$
$$= e^{i\theta}\left[\cos(2\pi) + i\sin(2\pi)\right]$$
$$= e^{i\theta}$$

For the 2 state Ψ, every expectation value repeats when $(E_j - E_{j'})t/\hbar = \pm 2\pi, \pm 4\pi, \ldots$

Period $T = \dfrac{2\pi\hbar}{|E_j - E_{j'}|} = \dfrac{h}{|E_j - E_{j'}|} \Rightarrow \dfrac{h}{T} = hf = |E_j - E_{j'}|$

Why does this look so familiar???

Intuition about quantum mechanics: Use the previous expression to build up expectations. For states J and $J+1$, the quantum and classical frequencies should be approx. same.

$$E_{J+1} - E_J \cong \left.\frac{dE}{dJ}\right|_{J+1/2} \simeq h\, f_{cl}(E_{J+1/2})$$

Examples

Harmonic oscillator $\quad f_{cl} = f = \text{const}$

$$\frac{dE}{dJ} = hf \quad \Rightarrow \quad \boxed{E_J = hfJ}$$

Particle bouncing in box $\quad T = \frac{2L}{v} \quad \Rightarrow \quad f = \frac{\sqrt{\frac{2E}{m}}}{2L}$

$$\frac{dE}{dJ} = \frac{h\sqrt{\frac{2}{m}}}{2L} E^{1/2} \qquad \frac{dE}{E^{1/2}} = \sqrt{\frac{h^2}{2mL^2}}\, dJ$$

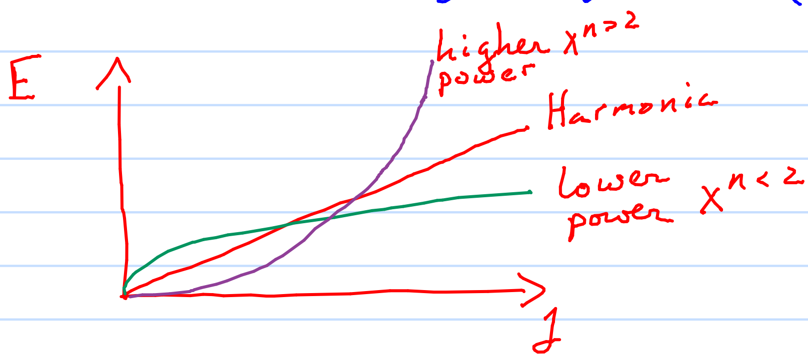
$$2E^{1/2} = \left(\frac{h^2 J^2}{2mL^2}\right)^{1/2} \quad \Rightarrow \quad \boxed{E_J = \frac{h^2 J^2}{8mL^2}}$$

Particle bouncing on ground $\quad t = \frac{2v}{g} \quad \Rightarrow \quad f = \frac{g}{2\sqrt{\frac{2E}{m}}}$

$$\frac{dE}{dJ} = \left(\frac{h^2 g^2 m}{8}\right)^{1/2} \Big/ \sqrt{E} \qquad E^{1/2}\, dE = \left(\frac{h^2 g^2 m}{8}\right)^{1/2} dJ$$

$$\frac{2}{3} E^{3/2} = \left(\frac{h^2 g^2 m}{8}\right)^{1/2} J \quad \Rightarrow \quad E = \left(\frac{3}{2}\right)^{2/3} \left(\frac{h^2 g^2 m}{8}\right)^{1/3} J^{2/3}$$

Generic behavior of E vs J



Infinite square well: $V(x) = 0 \quad 0 \le x \le a$
$= \infty \quad x \le 0 \text{ or } a \le x$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} = E_n\psi_n(x) \Rightarrow \frac{d^2\psi_n(x)}{dx^2} = -k_n^2\psi_n(x) \qquad E_n = \frac{\hbar^2 k_n^2}{2M}$$

$$\psi_n(x) = A\sin(k_n x) + B\cos(k_n x)$$

Must have $\psi_n(0) = 0$ and $\psi_n(a) = 0$ Why?

$\psi_n(0) = 0$ means $B = 0$

$\psi_n(a) = 0$ means $\sin(k_n a) = 0 \Rightarrow k_n a = n\pi$
$n = 1, 2, 3, \ldots$

Why $n = 0$ not OK?

$$E_n = \frac{\hbar^2\pi^2 n^2}{2Ma^2} = \frac{h^2 n^2}{8Ma^2}$$

Does this match expectation?

To normalize the $\psi_n(x)$ use $\int_0^a A^2\sin^2(k_n x)\,dx = A^2\frac{a}{2}$

$$\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$$

Important general properties

1) $\psi_n(x)$ alternate even and odd about center of symmetric potential.
2) $E_1 < E_2 < E_3 \ldots$ and number of nodes (zeros) not at the endpoints $= n-1$
3) $\int \psi_{n'}^*(x)\psi_n(x)\,dx = \delta_{nn'}$
4) They are complete $f(x) = \sum_{n=1}^{\infty} C_n\psi_n(x)$
and $C_n = \int \psi_n^*(x) f(x)\,dx$

If $\Psi(x,t) = \sum_n C_n \psi_n(x) e^{-iE_n t/\hbar}$ then

$C_n = \int \psi_n^*(x)\, \Psi(x,0)\, dx$

For time independent $\hat{H}$, the $\langle \hat{H} \rangle$ = constant (Energy conservation)

$$\langle \hat{H} \rangle = \sum_{n n'} C_{n'}^* e^{iE_{n'}t/\hbar} C_n e^{-iE_n t/\hbar} \int \psi_{n'}^*(x)\, \hat{H}\, \psi_n(x)\, dx$$

$$= \sum_n \sum_{n'} C_{n'}^* e^{iE_{n'}t/\hbar} C_n e^{-iE_n t/\hbar} E_n \int \psi_{n'}^*(x)\, \psi_n(x)\, dx$$

$$= \sum_n |C_n|^2 E_n$$

This bolsters the interpretation: $|C_n|^2$ is the probability to measure energy E_n.

Prob 2.4 Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$, σ_x and σ_p for the $\psi_n(x)$.

$$\langle x \rangle = \langle x - \tfrac{a}{2} \rangle + a/2 \overset{\text{symmetry}}{=} 0 + a/2$$

$$\langle x^2 \rangle = \frac{2}{a} \int_0^a x^2 \sin^2(k_n x)\, dx = \frac{2}{a}\left[\frac{a^3}{6} - \frac{a}{4k_n^2}\right] = \frac{a^2}{3} - \frac{a^2}{2(n\pi)^2}$$

$\langle p \rangle = 0$ for eigenstates in 1D

$$\langle p^2 \rangle = 2M \langle \hat{H} \rangle = 2M E_n = \frac{n^2\pi^2\hbar^2}{a^2}$$

$$\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{a^2}{3} - \frac{a^2}{2(n^2\pi^2)} - \frac{a^2}{4} = \frac{a^2}{12} - \frac{a^2}{2n^2\pi^2}$$

$$\sigma_p^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{n^2\pi^2\hbar^2}{a^2}$$

$$\sigma_x \sigma_p = \frac{\hbar}{2}\, n\pi \left(\frac{1}{3} - \frac{2}{n^2\pi^2}\right)^{1/2} = \frac{\hbar}{2} \times (\overset{n=1}{1.136}, \overset{n=2}{3.341}, \ldots$$

Harmonic Potential is often useful approximation near a potential minimum

$$V(x) = \frac{1}{2} k x^2 = \frac{1}{2} m\omega^2 x^2$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi_n(x) = E_n \psi_n(x)$$

First step change variables $x = \left(\frac{\hbar}{m\omega}\right)^{1/2} \xi$

Units of $\left(\frac{\hbar}{m\omega}\right)^{1/2} = \left(\frac{J\,s}{kg/s}\right)^{1/2} = \left(\frac{kg\frac{m^2}{s^2}s^2}{kg}\right)^{1/2} = m$ This means ξ is dimensionless

$$-\frac{\hbar^2}{2m}\frac{1}{\left(\frac{\hbar}{m\omega}\right)}\frac{d^2\psi_n}{d\xi^2} + \frac{1}{2} m\omega^2 \frac{\hbar}{m\omega}\xi^2\psi_n = E_n\psi_n$$

$$-\frac{\hbar\omega}{2}\frac{d^2\psi_n}{d\xi^2} + \frac{\hbar\omega}{2}\xi^2\psi_n = K_n\frac{\hbar\omega}{2}\psi_n \qquad E_n \equiv \frac{\hbar\omega}{2}K_n$$

$$\frac{d^2\psi_n}{d\xi^2} = (\xi^2 - K_n)\psi_n$$

Although this is a simple differential equation, the $\psi_n(\xi)$ is a complicated power series. Strategy, exactly remove the large ξ behavior.

$$\psi_n(\xi) = h_n(\xi)e^{-\xi^2/2}$$

(actually $e^{\xi^2/2}$ also works in the diff. eq. Why not use it?)

$$\frac{d\psi_n}{d\xi} = \left(\frac{dh_n}{d\xi} - \xi h_n\right)e^{-\xi^2/2}$$

$$\frac{d^2\psi_n}{d\xi^2} = \left(\frac{d^2h_n}{d\xi^2} - h_n - \xi\frac{dh_n}{d\xi} - \xi\left(\frac{dh_n}{d\xi} - \xi h_n\right)\right)e^{-\xi^2/2}$$

$$= \left(\frac{d^2h_n}{d\xi^2} - 2\xi\frac{dh_n}{d\xi} + (\xi^2-1)h_n\right)e^{-\xi^2/2}$$

$$\frac{d^2h_n}{d\xi^2} - 2\xi\frac{dh_n}{d\xi} + (K_n-1)h_n = 0$$

An important property is $h_n(\xi) = \pm h_n(-\xi)$. You can see this because you get the same equation when $\xi \to -\xi$.

The convention for harmonic oscillator is $n = 0, 1, 2, 3 \ldots$
start at 0

Power series for $h_n(\xi) = a_0 + a_1 \xi^1 + a_2 \xi^2 + \ldots$

$$\xi \frac{dh_n}{d\xi} = 1 \cdot a_1 \xi^1 + 2 \cdot a_2 \xi^2 + 3 a_3 \xi^3 + \cdots$$

$$\frac{d^2 h_n}{d\xi^2} = 1.2\, a_2 + 2.3\, a_3 \xi + 3.4\, a_4 \xi^2 + \ldots$$

Terms $O(\xi^0)$ $\quad 1.2\, a_2 - 2 \cdot 0 \cdot a_0 + (K_n - 1) a_0 = 0$
" $O(\xi^1)$ $\quad 2.3\, a_3 - 2 \cdot 1 \cdot a_1 + (K_n - 1) a_1 = 0$
" $O(\xi^2)$ $\quad 3.4\, a_4 - 2 \cdot 2 \cdot a_2 + (K_n - 1) a_2 = 0$
$\vdots$
$O(\xi^j)$ $\quad (j+1)(j+2) a_{j+2} - (2 \cdot j + 1 - K_n) a_j = 0$

This is a recursion relation. If you specify K_n and a_0, a_1, then all other terms are determined.

There are 2 independent solutions ($a_0 = 1, a_1 = 0$ and $a_0 = 0, a_1 = 1$) for any $K_n = 2 E_n / \hbar\omega$. Where are the quantized energies?

If the recursion doesn't stop, the solutions diverge as $\xi \to \pm\infty$.

The only allowed solution is $K_n = 2n + 1$. The highest term in the power series is $j = n$.

$$E_n = \frac{\hbar\omega}{2} K_n = \hbar\omega \left(n + \tfrac{1}{2}\right)$$

$$a_{j+2} = \frac{2j + 1 - K_n}{(j+1)(j+2)} a_j = -\frac{2(n-j)}{(j+1)(j+2)} a_j$$

The $h_n(\xi)$ are proportional to Hermite polynomials.

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}\, x\right) e^{-\frac{m\omega}{2\hbar}x^2}$$

$$H_0(\xi) = 1 \qquad H_1(\xi) = 2\xi \qquad H_2(\xi) = 4\xi^2 - 2 \quad \ldots$$

When using this kind of function there are useful properties

Recursion examples $\quad H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi)$

$$\frac{dH_n}{d\xi} = 2n\, H_{n-1}(\xi)$$

Rodrigues Formula $\quad H_n(\xi) = (-1)^n e^{\xi^2} \dfrac{d^n e^{-\xi^2}}{d\xi^n}$

Generating Function $\quad e^{-z^2 + 2z\xi} = \displaystyle\sum_{n=0}^{\infty} \frac{z^n}{n!} H_n(\xi)$

To see why these might be useful, I will use Rodrigues formula to show orthonormality.

Assume $n' \leq n$

$$\int_{-\infty}^{\infty} \psi_{n'}(x)\psi_n(x)\,dx = \frac{1}{\sqrt{2^n n!}} \frac{1}{\sqrt{2^{n'} n'!}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} H_{n'}\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right) e^{-\frac{m\omega}{\hbar}x^2} \sqrt{\frac{m\omega}{\hbar}}\,dx$$

$$= \left(\frac{1}{\sqrt{2^n n!}} \frac{1}{\sqrt{2^{n'} n'!}} \frac{1}{\sqrt{\pi}}\right) \int_{-\infty}^{\infty} H_{n'}(\xi)\, H_n(\xi)\, e^{-\xi^2}\, d\xi$$

$$= (\qquad\qquad) \int_{-\infty}^{\infty} H_{n'}(\xi)\, (-1)^n \frac{d^n e^{-\xi^2}}{d\xi^n}\, d\xi$$

Integrate by parts n times

$$= (\qquad\qquad) \int_{-\infty}^{\infty} \frac{d^n H_{n'}(\xi)}{d\xi^n}\, e^{-\xi^2}\, d\xi$$

If $n' < n \quad \dfrac{d^n H_{n'}}{d\xi^n} = 0 \qquad$ If $n' = n \quad \dfrac{d^n H_n}{d\xi} = 2^n \dfrac{d^n \xi^n}{d\xi^n} = n!\, 2^n$

$$\int_{-\infty}^{\infty} \psi_{n'}(x)\psi_n(x)\,dx = \frac{\delta_{n'n}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\xi^2}\, d\xi = \delta_{n'n}$$

Can also use operator method to get Ψ_n and E_n

Book calls this the algebraic method. Use "raising" and "lowering" operators.

$$\hat{a}_\pm = (2\hbar m\omega)^{-1/2}\,(m\omega\hat{x} \mp i\hat{p})$$

Useful to look at the classical analog

$$X_{cl}(t) = A\cos(\omega t + \delta) \qquad A = \text{amplitude} \quad \delta = \text{phase}$$
$$P_{cl}(t) = -m\omega A\sin(\omega t + \delta)$$

$$a_\pm^{cl} = (2\hbar m\omega)^{-1/2}\, m\omega A\,[\cos(\omega t+\delta) \mp i(-\sin(\omega t+\delta))]$$
$$= \frac{Ae^{\pm i\delta}}{\sqrt{2\hbar/m\omega}}\, e^{\pm i\omega t} \qquad (\text{Notice } \hbar\omega\, a_-^{cl} a_+^{cl} = \tfrac{1}{2}m\omega^2 A^2 = E \text{ cool})$$

Magnitude constant, rotation ($\pm$) in complex plane.

Back to quantum

$$\hbar\omega\,\hat{a}_-\hat{a}_+ = \frac{1}{2m}(i\hat{p} + m\omega\hat{x})(-i\hat{p} + m\omega\hat{x}) = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2 - \frac{i\omega}{2}(\hat{x}\hat{p} - \hat{p}\hat{x})$$
$$= \hat{H} - \frac{i\omega}{2}[\hat{x},\hat{p}]$$

$[\hat{x},\hat{p}]$ is the <u>commutator</u> of $\hat{x}$ + $\hat{p}$

The trick to figuring out is have it act on a function

$$[\hat{x},\hat{p}]f(x) = x\frac{\hbar}{i}\frac{\partial f}{\partial x} - \frac{\hbar}{i}\frac{\partial(xf(x))}{\partial x} = x\frac{\hbar}{i}\frac{\partial f}{\partial x} - \frac{\hbar}{i}f - x\frac{\hbar}{i}\frac{\partial f}{\partial x} = i\hbar f$$

Substitute into above

$$\hbar\omega\,\hat{a}_-\hat{a}_+ = \hat{H} + \frac{\hbar\omega}{2} \quad \Longrightarrow \quad \hat{H} = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \tfrac{1}{2}\right)$$
$$= \hbar\omega\left(\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right)$$

How can these be the same?

The two expressions for $\hat{H}$ can be the same if

$$\hat{a}_- \hat{a}_+ - \hat{a}_+ \hat{a}_- = 1$$

The only way to get this result is to plug in expression

$$\frac{1}{2\hbar m\omega}\left((ip + m\omega x)(-ip + m\omega x) - (-ip + m\omega x)(ip + m\omega x) \right)$$

$$= \frac{1}{2\hbar m\omega}\left((p^2 + m^2\omega^2 x^2 + im\omega(px - xp)) - (p^2 + m^2\omega^2 x^2 + im\omega(xp - px)) \right)$$

$$= \frac{1}{2\hbar m\omega}\left(im\omega \frac{\hbar}{i} - im\omega(i\hbar) \right) = 1 \checkmark$$

Now use the $\hat{a}_+$ and $\hat{a}_-$ to find all eigenstates and energies. If ψ_n is an eigenstate of $\hat{H}$ it is also an eigenstate of $\hat{a}_+\hat{a}_-$.

Show $\hat{a}_+\psi_n$ is also eigenstate

If $\hat{a}_+\hat{a}_- \psi_n = N_n \psi_n$ then $\hat{a}_+\hat{a}_-(\hat{a}_+\psi_n) \overset{?}{=} N_{n'}(\hat{a}_+\psi_n)$

$$\hat{a}_+\hat{a}_-(\hat{a}_+\psi_n) = \hat{a}_+(\hat{a}_-\hat{a}_+)\psi_n = \hat{a}_+(1 + \hat{a}_+\hat{a}_-)\psi_n$$

$$= \hat{a}_+\psi_n + \hat{a}_+(\hat{a}_+\hat{a}_-\psi_n) = \hat{a}_+\psi_n + \hat{a}_+ N_n \psi_n = (N_n + 1)\hat{a}_+\psi_n$$

$\hat{a}_+\psi_n$ is an eigenstate with Energy $E_n + \hbar\omega$

1. Find lowest eigenstate ψ_0 and E_0
2. Apply $\hat{a}_+ \rightarrow \hat{a}_+\psi_0 = c_0 \psi_1$
3. Apply again $\hat{a}_+ \rightarrow \hat{a}_+\psi_1 = c_1 \psi_2$

$\vdots$

Can also show $\hat{a}_- \psi_n = d_n \psi_{n-1}$

What happens when $a_- \psi_0 = d_0 \psi_{-1}$???

Find ψ_0 $\quad \hat{a}_- \psi_0 = \frac{1}{\sqrt{2m\hbar\omega}} \left(\hbar \frac{\partial}{\partial x} + m\omega x \right) \psi_0(x) = 0$

Only solution $\quad \psi_0 = B\, e^{-\frac{m\omega}{2\hbar} x^2}$

How to find B? $\quad \int_{-\infty}^{\infty} \psi_0^2(x)\, dx = B^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar} x^2} dx = B^2 \sqrt{\frac{\pi\hbar}{m\omega}}$

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar} x^2}$$

Now we can complete the logic

$\hat{a}_+ \hat{a}_- \psi_0 = \hat{a}_+ 0 = 0 \psi_0$ $\quad$ 0 is the eigenvalue

$\hat{a}_+ \hat{a}_- \psi_1 = (0+1) \psi_1$ $\quad$ 1 " "

$\hat{a}_+ \hat{a}_- \psi_2 = (1+1) \psi_2$ $\quad$ 2 " "

$$\hat{H} \psi_n = \hbar\omega (\hat{a}_+ \hat{a}_- + 1/2) \psi_n = \hbar\omega (n + 1/2) \psi_n \overset{\checkmark}{=} E_n \psi_n$$

Lastly we need to find the normalization

$\hat{a}_- \psi_n = d_n \psi_{n-1}$ $\quad$ and $\quad$ $\hat{a}_+ \psi_n = c_n \psi_{n+1}$

$$c_n = \int_{-\infty}^{\infty} \psi_{n+1} (\hat{a}_+ \psi_n)\, dx = \int_{-\infty}^{\infty} \psi_{n+1} \frac{1}{\sqrt{2\hbar\omega m}} \left(-\hbar \frac{\partial \psi_n}{\partial x} + m\omega x \psi_n \right) dx$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\hbar m\omega}} \left(\hbar \frac{\partial \psi_{n+1}}{\partial x} + m\omega x \psi_{n+1} \right) \psi_n\, dx$$

integrate by parts

$$= \int_{-\infty}^{\infty} (\hat{a}_- \psi_{n+1}) \psi_n\, dx = d_{n+1}$$

Hermitian conjugate

$$\hat{a}_+ \hat{a}_- \psi_n = a_+ d_n \psi_{n-1} = c_{n-1} d_n \psi_n = d_n^2 \psi_n = n \psi_n$$

$d_n = \sqrt{n}$ $\quad$ and $\quad$ $c_n = \sqrt{n+1}$

$$\hat{a}_+ \psi_n = \sqrt{n+1}\, \psi_{n+1} \qquad \text{and} \qquad \hat{a}_- \psi_n = \sqrt{n}\, \psi_{n-1}$$

$$\psi_n = \frac{1}{\sqrt{n!}} \hat{a}_+^n \psi_0 \qquad n! = n\cdot(n-1)\cdot(n-2)\ldots 3\cdot 2\cdot 1$$

The $\hat{a}_+$ and $\hat{a}_-$ are also useful for seeing how $\hat{x}$ and $\hat{p}$ change ψ_n

$$\hat{x} = \left(\frac{\hbar}{2m\omega}\right)^{1/2} (\hat{a}_+ + \hat{a}_-) \qquad \hat{p} = i\left(\frac{\hbar m\omega}{2}\right)^{1/2} (\hat{a}_+ - \hat{a}_-)$$

Some examples worked out.

(1) Suppose $\Psi(x,0) = A\,(2\psi_8 + 3e^{-i\varphi}\psi_9)$. Determine A, $\Psi(x,t)$, $\langle x\rangle(t)$, and $\langle p\rangle(t)$

$$A^2 \int_{-\infty}^{\infty} (2\psi_8 + 3e^{+i\varphi}\psi_9)(2\psi_8 + 3e^{-i\varphi}\psi_9)\,dx = A^2(4 + 9 + \overset{\text{why}}{0})$$

$$A = 1/\sqrt{13}$$

$$\Psi(x,t) = A\,(2\psi_8 e^{-iE_8 t/\hbar} + 3e^{-i\varphi}\psi_9 e^{-iE_9 t/\hbar})$$

$$= A\,(2\psi_8 e^{-i8.5\omega t} + 3e^{-i\varphi}\psi_9 e^{-i9.5\omega t}) \quad \text{pull out average phase}$$

$$= A e^{-i\varphi/2} e^{-i9\omega t} (2\psi_8 e^{i(\omega t+\varphi)/2} + 3\psi_9 e^{-i(\omega t+\varphi)/2})$$

$$\langle x\rangle(t) = \sqrt{\frac{\hbar}{2m\omega}} \langle a_+ + a_-\rangle \qquad \theta(t) = \frac{\omega t+\varphi}{2}$$

$$= \sqrt{\frac{\hbar}{2m\omega}} A^2 \int (2\psi_8 e^{-i\theta} + 3\psi_9 e^{i\theta})(a_+ + a_-)(2\psi_8 e^{i\theta} + 3\psi_9 e^{-i\theta})\,dx$$

$$= \sqrt{\frac{\hbar}{2m\omega}} A^2 \int (2\psi_8 e^{-i\theta} + 3\psi_9 e^{i\theta})\big(2\sqrt{8}\,\psi_7 e^{i\theta} + 3\sqrt{9}\,\psi_8 e^{-i\theta} + 2\sqrt{9}\,\psi_9 e^{i\theta} + 3\sqrt{10}\,\psi_{10} e^{-i\theta}\big)\,dx$$

$$= \sqrt{\frac{\hbar}{2m\omega}} A^2 (6\sqrt{9}\, e^{-2i\theta} + 6\sqrt{9}\, e^{2i\theta})$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \frac{12\sqrt{9}}{13} \cos(\omega t + \varphi)$$

$$\langle p\rangle(t) = i\sqrt{\frac{\hbar m\omega}{2}}\ \langle a_+ - a_-\rangle(t)$$

$$= i\sqrt{\frac{\hbar m\omega}{2}}\ A^2\left(-6\sqrt{9}\,e^{-2i\theta} + 6\sqrt{9}\,e^{2i\theta}\right)$$

$$= -\sqrt{\frac{\hbar m\omega}{2}}\ \frac{12\sqrt{9}}{13}\ \sin(\omega t+\varphi) = m\frac{d\langle x\rangle(t)}{dt} \checkmark$$

The φ is playing the role of shift in phase of oscillation

(2) Sudden approximation. Suppose the wave function is in the ground state of harmonic oscillator ω. Suddenly, the spring constant changes so $\omega \to \alpha\omega$. What is the prob. to still be in ground state?

Before $\Psi = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}$

After $\Psi = \left(\frac{m\alpha\omega}{\pi\hbar}\right)^{1/4} e^{\frac{-m\alpha\omega}{2\hbar}x^2}\, C_0 + \psi_1 C_1 + \psi_2 C_2 + \ldots$

$$C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\alpha^{1/4}\int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}(1+\alpha)x^2}\,dx$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{1/2}\alpha^{1/4}\left(\frac{\pi\hbar}{m\omega}\,\frac{2}{1+\alpha}\right)^{1/2} = \left(\frac{4\alpha}{(1+\alpha)^2}\right)^{1/4}$$

$P_0 = |C_0|^2 = \frac{2\sqrt{\alpha}}{1+\alpha}$ The maximum is when $\alpha = 1 \Rightarrow P_0^{max} = 1$ ✓

What other states get populated? 1?, 2?, ...

(3) When we had Ψ as sum of two states with $\Delta n = 1$, the expectation values oscillated with period $2\pi/\omega$. If $\Delta n = 2$ $\langle x\rangle(t) = 0$? $\langle x^2\rangle(t)$? ... Generalize

$\langle x\rangle(t) = 0$ Why?

$\langle x^2\rangle(t) = (\,)\cos(2\omega t + ?)$ Period $= \frac{2\pi}{2\omega}$ Interpret!

For $\Delta n = 3$ $\langle x^3\rangle(t)$ Period $= \frac{2\pi}{3\omega}$

Now solve for $\psi(x)$ when $V(x) = 0$ everywhere

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\,\psi(x) \qquad \text{define} \quad E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}$$

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

The $e^{\pm ikx}$ are eigenstates of $\hat{p}$

$$\hat{p}\, e^{\pm ikx} = \frac{\hbar}{i}\frac{\partial}{\partial x} e^{\pm ikx} = \pm\hbar k\, e^{\pm ikx}$$

The $e^{\pm ikx}$ represent momentum $\pm\hbar k$

de Broglie? $\quad e^{ik(x+\lambda)} = e^{ikx} = e^{ikx} e^{ik\lambda}$

This happens when $k\lambda = 2\pi \Rightarrow \lambda = \frac{2\pi}{k} = \frac{2\pi\hbar}{\hbar k} = \frac{h}{p}$ ✓

$$\Psi(x,t) = A e^{i(kx - Et/\hbar)} + B e^{i(-kx - Et/\hbar)}$$

For now, we won't worry about how to normalize this wave function. But we need a math detour to understand how to interpret

How to figure out the speed of a wave. There are two interesting definitions: phase velocity and group velocity. For any wave, the formula for ω vs. k is called dispersion relation: $\omega(k)$

Plane wave $\quad e^{i(kx - \omega(k)t)}$

$$\omega_{QM}(k) = \frac{E(k)}{\hbar} = \frac{\hbar k^2}{2m}$$

$$\omega_{light}(k) = ck$$

Add two plane waves $k_\pm = \bar{k} \pm \frac{\delta k}{2}$

If δk is small, $\quad \omega_\pm = \omega(k_\pm) = \omega(\bar{k}) \pm \frac{\delta k}{2}\left.\frac{d\omega}{dk}\right|_{\bar{k}}$

$$= \bar{\omega} \pm \frac{\delta k}{2}\,\omega'(\bar{k})$$

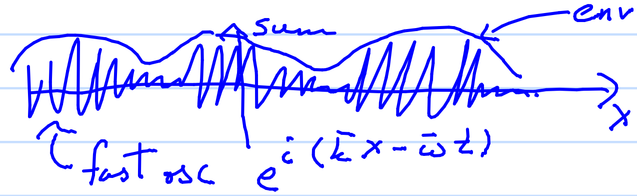
$$\text{Sum} = e^{i(k_+ x - \omega_+ t)} + e^{i(k_- x - \omega_- t)}$$

$$= e^{i(\bar{k}x - \bar{\omega}t)} e^{i\frac{\delta k}{2}(x - \omega' t)} + e^{i(\bar{k}x - \bar{\omega}t)} e^{-i\frac{\delta k}{2}(x - \omega' t)}$$

$$= e^{i(\bar{k}x - \bar{\omega}t)} \, 2\cos\left(\frac{\delta k}{2}(x - \omega' t)\right)$$

envelope $\cos\left(\frac{\delta k}{2}(x - \omega' t)\right)$

At specific time



The fast variation moves in time $\quad \bar{k}x - \bar{\omega}t = \text{const}$

The group moves in time $\quad \frac{\delta k}{2}(x - \omega' t) = \text{const}$

Phase velocity $\quad x = \frac{\bar{\omega}}{\bar{k}} t + \text{const} = V_{phase}\, t + \text{const}$

Group velocity $\quad x = \frac{d\omega}{dk} t + \text{const} = V_{group}\, t + \text{const}$

$$V_{phase}(k) = \frac{\omega(k)}{k} \qquad V_{group}(k) = \frac{d\omega}{dk}$$

Example: light: $\omega = ck \qquad V_{phase} = c \qquad V_{group} = c$

The phase and group velocity are the same. No dispersion

light in matter: $\omega = ck/n(k) \qquad V_{phase} = \frac{c}{n(k)} \qquad V_{group} = \frac{c}{n(k)} - \frac{ck}{n^2}\frac{dn}{dk}$

index of ref

Slow light - large variation in $n(k)$

quantum: $\omega = \frac{\hbar k^2}{2m} \qquad V_{phase} = \frac{\hbar k}{2m} = \frac{p}{2m} \qquad V_{group} = \frac{2\hbar k}{2m} = \frac{p}{m}$

The group velocity corresponds to the motion of the object through space. Does this make sense??

End of math detour.

I'm going to state without proof a math relation that will let us deal with normalization and superposition

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k)\, e^{ikx}\, dk \qquad F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

$F(k)$ is the Fourier transform of $f(x)$
$f(x)$ is the inverse Fourier transform of $F(k)$

Superposition: $\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k)\, e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)}\, dk$

Coefficients: $\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x,0)\, e^{-ikx}\, dx$

What are the analogous eqs. for discrete states?

$\int_{k_a}^{k_b} |\phi(k)|^2 dk$ = Probability to measure p between $\hbar k_a$ and $\hbar k_b$

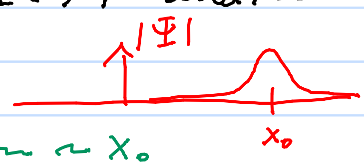
You can show $\int_{-\infty}^{\infty} |f(x)|^2 dx = \int_{-\infty}^{\infty} |F(k)|^2 dk$

This means $\int_{-\infty}^{\infty} |\phi(k)|^2 dk = 1$

Another implication $\langle p^n \rangle = \int_{-\infty}^{\infty} (\hbar k)^n |\phi(k)|^2 dk$

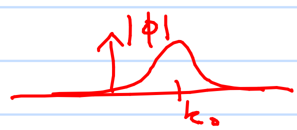
How to quickly interpret $\Psi(x,0)$ and/or $\phi(k)$ without math

$\Psi(x,0) = |\Psi(x,0)|\, e^{ik_0 x}$



momentum $\sim \hbar k_0$ position $\sim x_0$

$\phi(k) = |\phi(k)|\, e^{-ikx_0}$



momentum $\sim \hbar k_0$ position $\sim x_0$

How to interpret $\Psi(x,0) = \psi_{smooth}(x) \cos(k_0 x)$?

How to interpret $\phi(k) = \phi_{smooth}(k) \cos(k x_0)$?

Example $\phi(k) = C\, e^{-\frac{(k-k_0)^2}{2\delta k^2}} e^{-i(k-k_0)x_0}$ Find C and $\Psi(x,0)$

$\int_{-\infty}^{\infty} |\phi(k)|^2 dk = C^2 \int_{-\infty}^{\infty} e^{-(k-k_0)^2/\delta k^2} dk = C^2 \sqrt{\pi}\, \delta k \Rightarrow C = \frac{1}{\pi^{1/4}\sqrt{\delta k}}$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} C \int_{-\infty}^{\infty} e^{-\frac{(k-k_0)^2}{2\delta k^2}} e^{-i(k-k_0)x_0} e^{ikx}\, dk$$

change varible
$y = k - k_0$

$$= \frac{C}{\sqrt{2\pi}} e^{ik_0 x} \int_{-\infty}^{\infty} e^{-y^2/2\delta k^2} e^{iy(x-x_0)}\, dy$$

$$= \frac{C}{\sqrt{2\pi}} e^{ik_0 x} \sqrt{2\pi}\, \delta k\, e^{-(x-x_0)^2 \delta k^2/2}$$

$$= \frac{\sqrt{\delta k}}{\pi^{1/4}} e^{-(x-x_0)^2 \delta k^2/2} e^{ik_0 x}$$

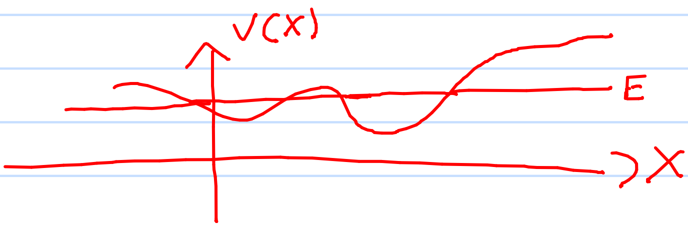
Does it match expectations?

Some generic properties of wave function

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

There are <u>always</u> 2 linearly independent solutions for <u>any</u> E for every $V(x)$. How to reconcile with results from chap 2??

$E > V(\infty)$	and	$E > V(-\infty)$	2 physical solutions (continuum)
$E > V(\infty)$	and	$E < V(-\infty)$	1 " " "
$E < V(\infty)$	and	$E > V(-\infty)$	1 " " "
$E < V(\infty)$	and	$E < V(-\infty)$	0 " " unless find special energy, E_n



When $E > V(x)$ oscillates
When $E < V(x)$ exponential decrease or increase

Another example $V(x) = -\alpha\,\delta(x)$ <u>Delta function</u>

$$\delta(x) = 0 \quad x \neq 0 \qquad \underline{\text{and}} \qquad \int_{-x_0}^{x_0} \delta(x)\, dx = 1$$
$$= \infty \quad x = 0$$

Possible representations $\delta(x) = \lim_{\beta \to 0} \frac{1}{\sqrt{\pi}\,\beta} e^{-x^2/\beta^2}$, $\lim_{x_0 \to 0} \begin{cases} \frac{1}{2x_0} & |x| < x_0 \\ 0 & |x| > x_0 \end{cases}$

The $V(x) = -\alpha\delta(x)$ might have bound state $E<0$
and will have 2 continuum states for every $E>0$.

Bound state?

Except at $x=0$ $\quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad E = -\frac{\hbar^2 k^2}{2m}$

Solution of $\frac{d^2\psi}{dx^2} = k^2\psi \qquad \psi = Ae^{-kx} + Be^{kx}$

$$\left.\begin{aligned}\psi(x) &= Ae^{-kx} && x \geq 0 \\ &= Be^{kx} && x \leq 0\end{aligned}\right] \quad \text{Why?}$$

1) $\psi(x)$ is always continuous
2) $\psi'(x)$ is continuous except when $V(x) = \pm\infty$] continuity conditions

1) means $A = B$ Why?
2) $\psi'(x)$ not continuous at $x=0$

$$\lim_{\varepsilon\to 0}\int_{-\varepsilon}^{\varepsilon} -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\,dx + \int_{-\varepsilon}^{\varepsilon} V(x)\psi(x)\,dx = \int_{-\varepsilon}^{\varepsilon} E\,\psi(x)\,dx$$

$$\lim_{\varepsilon\to 0} -\frac{\hbar^2}{2m}\left(\left.\frac{d\psi}{dx}\right|_{\varepsilon} - \left.\frac{d\psi}{dx}\right|_{-\varepsilon}\right) - \alpha\psi(0) = 0$$

$$= -\frac{\hbar^2}{2m}(-Ak - Ak) - \alpha A = 0 \Rightarrow k = \frac{\alpha m}{\hbar^2}$$

How to find A? Use normalization.

$$1 = \int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2\int_0^{\infty} A^2 e^{-2kx} dx = \frac{2A^2}{2k} e^{-2kx}\Big|_{\infty}^{0} = \frac{A^2}{k}$$

$$A = \sqrt{k}$$

Put it all together $\quad \psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \qquad E = -\frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right) = \frac{-m\alpha^2}{2\hbar^2}$

There are no other bound states.

For $E > 0$ there are two linearly independent solutions for every E.

Not at $x=0$

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad x < 0$$
$$= Fe^{ikx} + Ge^{-ikx} \qquad x > 0$$

Impose the continuity conditions.

$$A + B = F + G$$

$$-\frac{\hbar^2}{2m}\left[ikF - ikG - (ikA - ikB)\right] = \alpha\,(A + B)$$

Two equations and four unknowns $\Rightarrow$ 2 indep. sols.

Find the solution that represents waves coming from the left, some reflect and some keep going.

$G = 0$ $\qquad$ Why?

Define $\beta = m\alpha/(\hbar^2 k)$

$$F = A + B \qquad -iF + iA - iB = 2\beta A + 2\beta B$$

$$-2iB = 2\beta A + 2\beta B \quad \to \quad B = \frac{2\beta A}{-(2i + 2\beta)}$$

$$B = \frac{i\beta}{1 - i\beta} A \quad \text{and} \quad F = \left(1 + \frac{i\beta}{1 - i\beta}\right) A = \frac{1}{1 - i\beta} A$$

Now we have to figure out how to interpret.

The magnitude of current density with positive momentum and $x<0$ is $(\hbar k/m)|A|^2$

Negative momentum and $x<0$ $\quad (\frac{\hbar k}{m})|B|^2$

Positive " " $x>0$ $\quad (\hbar k/m)|F|^2$

Negative " " " $\quad 0$

Reflection prob $\equiv R = \frac{\hbar k}{m}|B|^2 / \frac{\hbar k}{m}|A|^2 = \beta^2/(1+\beta^2)$

Transmission " $\equiv T = \hbar k/m\,|F|^2 / \frac{\hbar k}{m}|A|^2 = 1/(1+\beta^2)$

$$R + T \overset{\checkmark}{=} 1 \qquad \beta^2 = \frac{m^2\alpha^2}{\hbar^4 k^2} = \frac{m\alpha^2}{\hbar^2 2E}$$

Is there intuition here? What should happen as $E \to 0$? $E \to \infty$?

$E \to 0 \quad \beta \to \infty \quad R \to 1$ and $T \to 0$

$E \to \infty \quad \beta \to 0 \quad R \to 0$ and $T \to 1$

Another example scattering: $\quad V(x) = 0 \quad x<0$

$\qquad\qquad\qquad\qquad = \infty \quad x>0$

Only one solution for each $E = \frac{\hbar^2 k^2}{2m}$

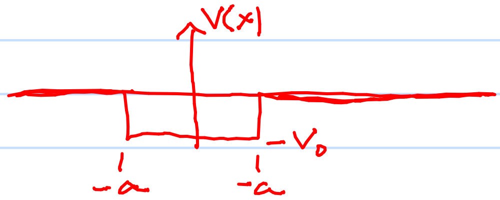
$$\psi(x) = A\sin(kx) \qquad x<0$$
$$= 0 \qquad x>0$$

How much reflected? transmitted? How to see?

$$\psi(x) = \frac{A}{2i}e^{ikx} - \frac{A}{2i}e^{-ikx}$$

$$R = \frac{\hbar k}{m}\left|\frac{A}{2i}\right|^2 / \frac{\hbar k}{m}\left|\frac{-A}{2i}\right|^2 \overset{\checkmark}{=} 1$$

The last standard potential I'll work out is the finite square well



First find the bound states $E_n < 0$ Why?

Because the potential is symmetric $\psi_n(x) = \pm \psi_n(-x)$
They must come in the order $\psi_1(x) = \psi_1(-x)$, $\psi_2(x) = -\psi_2(-x)$
$\psi_3(x) = \psi_3(-x)$, etc
There are a finite number of bound states.

Define $\ell = \frac{\sqrt{2m(E+V_0)}}{\hbar}$ and $k = \frac{\sqrt{-2mE}}{\hbar}$

For $|x| < a$ $\frac{d^2\psi}{dx^2} = -\ell^2 \psi$, $|x| > a$ $\frac{d^2\psi}{dx^2} = k^2 \psi$

Even solutions

$$
\begin{aligned}
\psi(x) &= D\cos(\ell x) & -a \le x \le a \\
&= F e^{-kx} & a \le x \\
&= F e^{kx} & x \le -a
\end{aligned}
$$

Odd solutions

$$
\begin{aligned}
\psi(x) &= C\sin(\ell x) & -a \le x \le a \\
&= F e^{-kx} & a \le x \\
&= -F e^{kx} & x \le -a
\end{aligned}
$$

The total number of bound states can be found from number of ½ wavelengths between $-a$ and a when $E=0$.
N = number of bound states
$(N-1)\pi < 2(\sqrt{2mV_0}/\hbar)a \le N\pi$

Work out the condition for even bound state

Continuity Conditions

$$
\left.
\begin{aligned}
D\cos(\ell a) &= F e^{-ka} \\
-D\ell\sin(\ell a) &= -kF e^{-ka}
\end{aligned}
\right]
$$

take the ratio

$\ell \tan(\ell a) = k$

The scattering case is more difficult because you have to do 2 boundaries (instead of 1).

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \qquad x \le -a \qquad E = \frac{\hbar^2 k^2}{2m}$$
$$= C\sin(lx) + D\cos(lx) \qquad -a \le x \le a$$
$$= Fe^{ikx} \qquad a \le x$$

The reflection probability is $R = \frac{\hbar k}{m}|B|^2 / \frac{\hbar k}{m}|A|^2 = |B|^2/|A|^2$
" transmission " " $T = \ldots = |F|^2/|A|^2$

Do the continuity conditions at $x=-a$
Gives 2 equations in A, B, C, D
Do the continuity conditions at $x=a$
Gives 2 equations in C, D, F

Strategy: use last 2 equations to get C in terms of F and D in terms of F. Substitute into first two equations. Solve for B in terms of A and F in terms of A.

The four continuity equations are

$$\left.\begin{array}{ll} (1) & Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \\ (2) & ik(Ae^{-ika} - Be^{ika}) = l(C\cos(la) + D\sin(la)) \end{array}\right] \quad x=-a$$

$$\left.\begin{array}{ll} (3) & C\sin(la) + D\cos(la) = Fe^{ika} \\ (4) & l(C\cos(la) - D\sin(la)) = ikFe^{ika} \end{array}\right] \quad x=a$$

$$(3)\sin(la) + \frac{\cos(la)}{l}(4) = C = \left[\sin(la) + \frac{ik}{l}\cos(la)\right]e^{ika}F$$
$$(3)\cos(la) - \frac{\sin(la)}{l}(4) = D = \left[\cos(la) - \frac{ik}{l}\sin(la)\right]e^{ika}F$$
etc.

I checked the results in the book

$$B = i\sin(2la)\frac{l^2-k^2}{2lk}F \quad \text{and} \quad F = \frac{Ae^{-2ika}}{\cos(2la) - i\frac{k^2+l^2}{2kl}\sin(2la)}$$

The transmission coefficient $T = \frac{|F|^2}{|A|^2}$

$$T^{-1} = \frac{1}{|e^{-2ika}|^2}\left[\cos^2(2\ell a) + \frac{(k^2+\ell^2)^2}{4k^2\ell^2}\sin^2(2\ell a)\right]$$

$$= 1\left[1 - \sin^2(2\ell a) + \frac{(k^2+\ell^2)^2}{4k^2\ell^2}\sin^2(2\ell a)\right]$$

$$= \left[1 + \frac{(k^2-\ell^2)^2}{4k^2\ell^2}\sin^2(2\ell a)\right]$$

$$= \left[1 + \frac{(E-(E+V_0))^2}{4E(E+V_0)}\sin^2(2\ell a)\right] = 1 + \frac{V_0^2}{4E(E+V_0)}\sin^2\left[\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right]$$

Notice the transmission is 100% when $2\ell a = n\pi$

" " " " 0% when $E \to 0$

The condition for 100% transmission is states in ∞ well with bottom at $-V_0$!!

The peaks in reflection when $2\ell a \simeq \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$