5. SOLUTIONS OF SCHRÖDINGER'S WAVE EQUATION IN 1-D

We are interested in solutions of $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\phi + V(x)\phi = E\phi$ subject to $\phi(x\to\pm\infty)\to 0$

Let's first consider an approximate solution that displays the general features all solutions will have. We make a transformation $\phi(x) = e^{i/\hbar\,\sigma(x)}$ so that the wave eqn becomes

$$-i\hbar\sigma''(x) + (\sigma'(x))^2 + 2m(V(x)-E) = 0$$

We will <u>approximately</u> solve this by treating $\hbar$ as a small parameter & expanding in it

$$\sigma(x) = \sigma_0(x) + \hbar\,\sigma_1(x)$$

$$\Rightarrow\quad -i\hbar\sigma_0''(x) + (\sigma_0'(x))^2 + 2\hbar\,\sigma_0'(x)\sigma_1'(x) + 2m(V(x)-E) = 0 \quad \text{to } \mathcal{O}(\hbar)$$

$$\mathcal{O}(1):\ (\sigma_0'(x))^2 = 2m(E-V(x)) \qquad\Rightarrow\qquad \sigma_0'(x) = \pm\sqrt{2m(E-V(x))} \equiv \pm k_0(x)$$

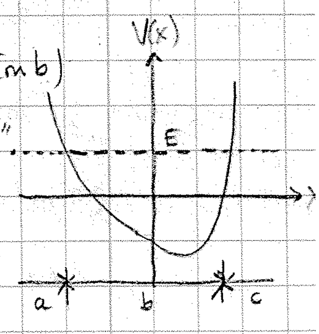
$$\mathcal{O}(\hbar):\ -i\sigma_0''(x) + 2\sigma_0'\sigma_1' = 0$$

$$\sigma_0(x) = \pm\int dx\, k_0(x)$$

$$\&\ \sigma_1' = i\,\sigma_0''/2\sigma_0' = \frac{i}{2}\frac{d}{dx}\ln\sigma_0' = i\frac{d}{dx}\ln\sqrt{\sigma_0'} = i\frac{d}{dx}\ln\sqrt{k_0(x)} \quad\Rightarrow \sigma_1(x) = i\ln\sqrt{k_0(x)}$$

$$\Rightarrow\quad \phi(x) = e^{i/\hbar\,\sigma(x)} \simeq N\exp\left[\frac{i}{\hbar}\left(\pm\int dx\,k_0(x) + i\hbar\ln\sqrt{k_0(x)}\right)\right]$$

$$\underline{\phi(x) \simeq \frac{N}{\sqrt{k_0(x)}}\, e^{\pm i/\hbar\int dx\,k_0(x)}} \qquad k_0 = \sqrt{2m(E-V(x))}$$

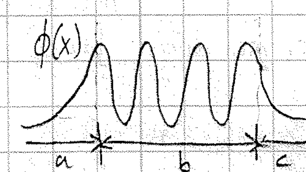


(eg. region b)

Suppose that $E > V(x)$ – such a situation is "classically allowed".
In this case k_0 is real and $\phi(x)$ is an <u>oscillatory function</u>

Now suppose that $E < V(x)$ – such a situation is "classically forbidden"
(eg regions a, c)

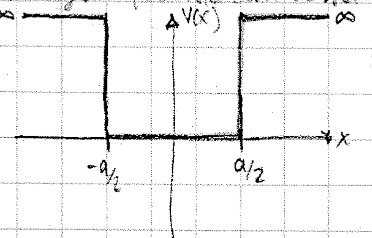
In this case k_0 is imaginary so that $\phi(x)$ rises or falls exponentially. Clearly to have a normalisible solution it must fall exponentially.



(THE INFINITE SQUARE WELL)

Let's consider a system where the Schrödinger equation can be solved exactly.

$$V(x) = \begin{cases} 0 & \text{for } -\frac{a}{2} < x < \frac{a}{2} \\ \infty & \text{elsewhere} \end{cases}$$



In order for any state to have finite energy, the wavefunction must vanish outside $-\frac{a}{2} < x < \frac{a}{2}$. Hence we have boundary conditions $\phi(-\frac{a}{2}) = \phi(\frac{a}{2}) = 0$.

In $-\frac{a}{2} < x < \frac{a}{2}$ we should solve $-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} = E\phi \longrightarrow \frac{d^2\phi}{dx^2} + k^2\phi = 0$ $\left(k^2 = \frac{2mE}{\hbar^2}\right)$

The solutions to this equation are known: $\underline{\phi(x) = A\cos kx + B\sin kx}$

[manual solution by Fourier transform is trivial: $\phi(x) = \int dp\, e^{ipx}\varphi(p) \Rightarrow \phi''(x) = \int dp\,(-p^2)\, e^{ip.x}\varphi(p)$
$\Rightarrow \int dp\, e^{ipx}(k^2 - p^2)\varphi(p) = 0 \Rightarrow \varphi(p) = \delta(p \pm k) \Rightarrow \phi(x) = \alpha e^{ikx} + \beta e^{-ikx} = A\cos kx + B\sin kx$]

To this general solution we should apply the boundary conditions:

$$\left.\begin{aligned} 0 = \phi(\tfrac{a}{2}) &= A\cos\tfrac{ka}{2} + B\sin\tfrac{ka}{2} \\ 0 = \phi(-\tfrac{a}{2}) &= A\cos\tfrac{ka}{2} - B\sin\tfrac{ka}{2} \end{aligned}\right\} \left.\begin{aligned} 0 &= A\cos\tfrac{ka}{2} \\ 0 &= B\sin\tfrac{ka}{2} \end{aligned}\right\} \begin{aligned} &A = 0,\ \sin\tfrac{ka}{2} = 0 \quad (1) \\ \text{or } &B = 0,\ \cos\tfrac{ka}{2} = 0 \quad (2) \end{aligned}$$

in case (1) $\sin\frac{ka}{2} = 0 \Rightarrow \frac{ka}{2} = \bar{n}\pi$ ($\bar{n}$ integer) $\Rightarrow k_n = \frac{2\bar{n}\pi}{a} = \underline{\frac{n\pi}{a}}$ n = even integer

in case (2) $\cos\frac{ka}{2} = 0 \Rightarrow \frac{ka}{2} = \frac{n\pi}{2}$ (n = odd integer) $\Rightarrow k_n = \underline{\frac{n\pi}{a}}$

$$\boxed{\phi_n(x) = N_n \begin{cases} \cos n\pi\frac{x}{a} & n \text{ odd} \\ \sin n\pi\frac{x}{a} & n \text{ even} \end{cases}} \qquad \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \left(\frac{\hbar^2\pi^2}{2ma^2}\right)n^2}$$

since $\int_{-a/2}^{a/2} dx\, \cos^2 n\pi\frac{x}{a} = \int_{-a/2}^{a/2} dx \sin^2 n\pi\frac{x}{a} = \frac{a}{2} \longrightarrow \phi_n(x) = \begin{cases} \sqrt{\frac{2}{a}}\cos n\pi\frac{x}{a} & n \text{ odd} \\ \sqrt{\frac{2}{a}}\sin n\pi\frac{x}{a} & n \text{ even} \end{cases}$

It is straightforward to check that these wavefunctions are orthogonal:

n odd: $\int dx\, \phi_n^*(x)\phi_m(x) = \frac{2}{a}\int_{-a/2}^{a/2} dx\, \cos n\pi\frac{x}{a}\cos m\pi\frac{x}{a} = \frac{2}{\pi}\int_{-\pi/2}^{\pi/2} dy\, \cos ny \cos my = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} dy\left(\cos(n-m)y + \cos(n+m)y\right)$
$= \delta_{n,m}$

n even: $\int dx\, \phi_n^*(x)\phi_m(x) = \frac{2}{a}\int_{-a/2}^{a/2} dx\, \sin n\pi\frac{x}{a}\sin m\pi\frac{x}{a} = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} dy\left(\cos(n-m)y - \cos(n+m)y\right)$
$= \delta_{n,m}$

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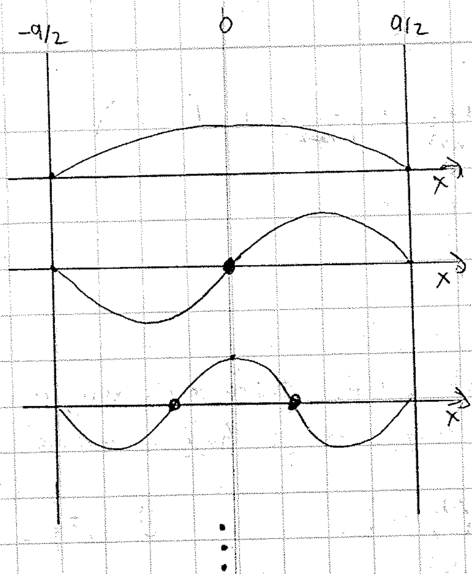
en, odd: $\int dx\, \phi_n^*(x)\phi_m(x) = \frac{2}{a}\int_{-a/2}^{a/2} dx\, \sin n\pi\frac{x}{a}\cos m\pi\frac{x}{a} = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} dy\left(\sin(n-m)y + \sin(n+m)y\right) = 0.$



$n=1$ $\cos\pi\frac{x}{a}$ $\rightarrow E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ "ground state"

$n=2$ $\sin 2\pi\frac{x}{a}$ $\rightarrow E_2 = 4\cdot\frac{\hbar^2\pi^2}{2ma^2}$ "1st excited state"

$n=3$ $\cos 3\pi\frac{x}{a}$ $\rightarrow E_3 = 9\cdot\frac{\hbar^2\pi^2}{2ma^2}$ "2nd excited state"

$\vdots$

The general solution of the time-dependent wave equation can be written

$$\psi(x,t) = \sqrt{\frac{2}{a}}\sum_{k=1}^{\infty}\left(A_k e^{-i/\hbar E_{2k-1}t}\cos(2k-1)\pi\frac{x}{a} + B_k e^{-i/\hbar E_{2k}t}\sin 2k\pi\frac{x}{a}\right)$$

where A_k, B_k are the amplitudes to find each energy eigenstate at $t=0$.

We know that if we <u>start in a stationary state</u>, that the time-evolution is trivial,

e.g.
$$\psi(x,t=0) = \sqrt{\frac{2}{a}}\cos\pi x/a \quad\Rightarrow\quad A_1=1,\ A_{k\neq1}=0,\ B_k=0$$

$$\Rightarrow \psi(x,t) = e^{-i/\hbar E_1 t}\sqrt{\frac{2}{a}}\cos\pi\frac{x}{a}.$$

We also know that the time evolution of the expectation value of an observable is also trivial,

e.g. $$\langle\hat{x}\rangle = \int dx\,\psi^*(x,t)\,x\,\psi(x,t) = \left|e^{-i/\hbar E_1 t}\right|^2\frac{2}{a}\int_{-a/2}^{a/2}dx\ x\cdot\cos^2\pi\frac{x}{a} = 0\quad\forall t$$

or $$\langle\hat{x}^2\rangle = \int dx\,\psi^*(x,t)\,x^2\,\psi(x,t) = \left|e^{-i/\hbar E_1 t}\right|^2\frac{2}{a}\int_{-a/2}^{a/2}dx\ x^2\cos^2\pi\frac{x}{a}$$

$$= \frac{\pi^2-6}{12\pi^2}a^2$$ <u>independant of time!</u>

Now suppose we start in a superposition of two stationary states,

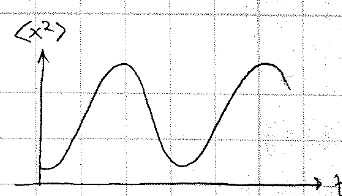
e.g. $$\psi(x,t=0) = \sqrt{\frac{1}{3}}\left(\sqrt{\frac{2}{a}}\cos\pi\frac{x}{a}\right) + \sqrt{\frac{2}{3}}\left(\sqrt{\frac{2}{a}}\cos 3\pi\frac{x}{a}\right)$$

then $$\psi(x,t) = \sqrt{\frac{1}{3}}e^{-i/\hbar E_1 t}\left(\sqrt{\frac{2}{a}}\cos\pi\frac{x}{a}\right) + \sqrt{\frac{2}{3}}e^{-i/\hbar E_3 t}\left(\sqrt{\frac{2}{a}}\cos 3\pi\frac{x}{a}\right)$$ * ANIMATION *

now $$\langle\hat{x}\rangle = \int dx\,\psi^*(x,t)\,x\,\psi(x,t) = \frac{1}{3}\int dx\ x\cdot\frac{2}{a}\cos^2\pi\frac{x}{a} + \frac{2}{3}\int dx\ x\cdot\frac{2}{a}\cos^2 3\pi\frac{x}{a}$$
$$+ \frac{\sqrt{2}}{3}\cdot 2\cos\left(\frac{E_3-E_1}{\hbar}t\right)\int dx\ x\cdot\frac{2}{a}\cos\pi\frac{x}{a}\cos 3\pi\frac{x}{a} \quad = 0$$

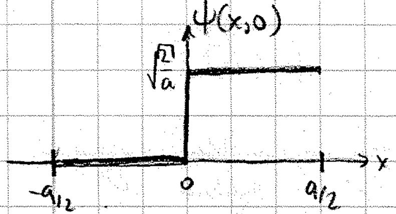
$$\langle\hat{x}^2\rangle = \frac{1}{3}\int dx\ x^2\frac{2}{a}\cos^2\pi\frac{x}{a} + \frac{2}{3}\int dx\ x^2\frac{2}{a}\cos^2 3\pi\frac{x}{a} + \frac{\sqrt{2}}{3}\,2\cos\left(\frac{E_3-E_1}{\hbar}t\right)\int dx\ x^2\frac{2}{a}\cos\pi\frac{x}{a}\cos 3\pi\frac{x}{a}$$

$$\langle \hat{x}^2 \rangle = \frac{1}{3}\cdot\frac{\pi^2-6}{12\pi^2}a^2 + \frac{2}{3}\cdot\frac{3\pi^2-2}{36\pi^2}a^2 + \frac{2\sqrt{2}}{3}\cos\left(\frac{4\hbar\pi^2}{ma^2}t\right)\cdot\left(-\frac{3}{8\pi^2}a^2\right)$$



for non-stationary states, expectation values vary with time.

We can consider a more complicated initial wavefunction to demonstrate the full mathematics of orthogonal functions. Suppose that initially there is an equal amplitude to find the system between 0 & $a/2$, and zero amplitude to find it between $-a/2$ & 0.



$$\psi(x,0) = \sqrt{\frac{2}{a}}\,\theta(x)\,\theta(a/2 - x) \qquad \theta(x) = \begin{cases} 0 & x<0 \\ 1 & x>0 \end{cases}$$

We'd like to express this function as a linear superposition of energy eigenstates

$$\psi(x,0) = \sqrt{\frac{2}{a}}\,\theta(x)\,\theta(a/2-x) = \sqrt{\frac{2}{a}}\sum_{k=1}^{\infty} A_k \cos(2k-1)\pi\frac{x}{a} + B_k \sin 2k\pi\frac{x}{a}$$

We use the orthonormality of the energy eigenfunctions to project out the A_k, B_k (in this case, this corresponds to the Fourier series expansion)

$$A_k = \sqrt{\frac{2}{a}}\int_{-a/2}^{a/2} dx \cos(2k-1)\pi\frac{x}{a}\,\psi(x,0) \qquad \& \qquad B_k = \sqrt{\frac{2}{a}}\int_{-a/2}^{a/2} dx \sin 2k\pi\frac{x}{a}\,\psi(x,0)$$

$$= \frac{2}{a}\int_0^{a/2} dx \cos(2k-1)\pi\frac{x}{a} \qquad\qquad = \frac{2}{a}\int_0^{a/2} dx \sin 2k\pi\frac{x}{a}$$

$$= \frac{2}{a}\cdot\frac{a}{(2k-1)\pi}\left[\sin(2k-1)\pi\frac{x}{a}\right]_0^{a/2} \qquad\qquad = \frac{2}{a}\left(-\frac{a}{2k\pi}\right)\left[\cos 2k\pi\frac{x}{a}\right]_0^{a/2}$$

$$A_k = \frac{2}{(2k-1)\pi}\sin\frac{(2k-1)\pi}{2} = \frac{2}{(2k-1)\pi}(-1)^{k+1} \qquad\qquad B_k = -\frac{1}{k\pi}\left(\cos k\pi - 1\right) = \frac{1}{k\pi}\left(1-(-1)^k\right)$$

ANIMATION

Even a simple-looking initial wavefunction in a dynamically simple system can have complicated quantum time evolution. Expansion in terms of energy eigenstates gives us a mathematical description of this evolution. We could, for example, compute the expectation value of the position operator in this state:

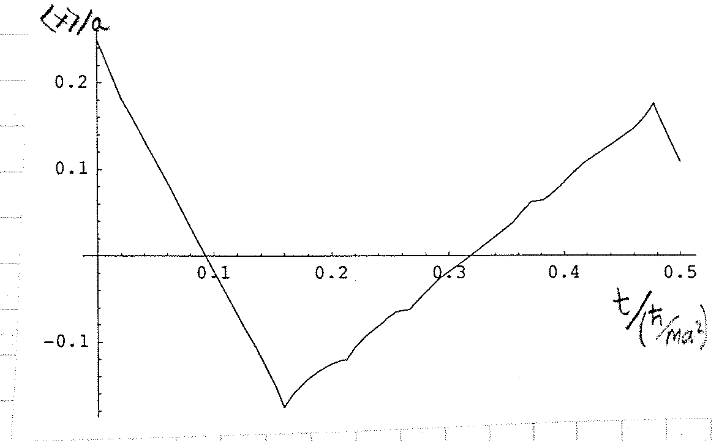
$$\langle \hat{x} \rangle(t) = \int dx\, \psi^*(x,t)\cdot x\cdot\psi(x,t)$$

$$= \frac{2}{a}\int_{-a/2}^{a/2} dx\, x \sum_{k=1}^{\infty}\left(A_k e^{-i/\hbar E_{2k-1}t}\cos(2k-1)\pi\frac{x}{a} + B_k e^{-i/\hbar E_{2k}t}\sin 2k\pi\frac{x}{a}\right)$$

$$\times\sum_{k'=1}^{\infty}\left(A_{k'} e^{-i/\hbar E_{2k'-1}t}\cos(2k'-1)\pi\frac{x}{a} + B_{k'} e^{-i/\hbar E_{2k'}t}\sin 2k'\pi\frac{x}{a}\right)$$

(hard work left as an exercise)

$$= \frac{64a}{\pi^4} \sum_{k=1}^{\infty} \sum_{k'=1}^{\infty} \frac{1-(-1)^{k'}}{\left[(2k-1)^2-4k'^2\right]^2} \cos\left[\frac{\hbar\pi^2}{2ma^2}\left((2k-1)^2-4k'^2\right)t\right]$$



Notice that our eigenfunctions are of definite symmetry about $x=0$. The odd numbered solutions are even under reflection and the even numbered are odd. That this is so is a consequence of the <u>symmetry</u> of the Hamiltonian, namely that it is even under the parity operator.

We'll take a brief aside to consider the effect of symmetry operations on states and operators. The parity operator (in 1D) reflects about the origin, so it's effect on an eigenstate of position would be

$$\hat{P}|x\rangle = \eta_p|-x\rangle.$$

Applying the parity operation twice should return us to the original position

$$\hat{P}^2|x\rangle = \hat{P}\eta_p|-x\rangle = \eta_p^2|x\rangle$$

so the arbitrary multiplication constant must be ± 1. We'll assume here the $+1$ option.

$$\hat{P}|x\rangle = |-x\rangle, \qquad \& \quad \hat{P}^2 = 1$$

Now recall the eigen-equation for the position operator $\quad \hat{x}|x\rangle = x|x\rangle$
then

$$\hat{P}\hat{x}|x\rangle = \hat{P}\hat{x}\cdot 1\cdot|x\rangle = \hat{P}\hat{x}\hat{P}\hat{P}|x\rangle = \hat{P}\hat{x}\hat{P}|-x\rangle = x\hat{P}|x\rangle = x|-x\rangle$$

note that the operator transforms as $\hat{P}\hat{x}\hat{P}$ & the only way the eigen equation can still be satisfied is if $\hat{P}\hat{x}\hat{P} = -\hat{x}$ then $-\hat{x}|-x\rangle = x|-x\rangle$

$$\Rightarrow \hat{x}|-x\rangle = -x|-x\rangle \checkmark$$

The effect of parity on momentum can easily be found:

$$\hat{P}|p\rangle = \int dx\, \hat{P}|x\rangle\langle x|p\rangle = \int dx\, |-x\rangle\langle x|p\rangle \qquad \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar} = \langle -x|-p\rangle$$

$$= \int dx\, |-x\rangle\langle -x|-p\rangle = \int d(-x)\, |-x\rangle\langle -x|-p\rangle \qquad \Rightarrow \underline{\hat{P}|p\rangle = |-p\rangle}$$

& hence the effect on the operator is

$$\underline{\hat{P}\hat{p}\hat{P} = -\hat{p}}$$

In terms of position eigenstates the wavefunction is $\psi_n(x) = \langle x|n\rangle$. The space inverted State is $\hat{P}|n\rangle$ with wavefunction $\psi_{\hat{P}n}(x) = \langle x|\hat{P}|n\rangle = \langle -x|n\rangle = \psi_n(-x)$ (since $\langle x|\hat{P} = \langle -x|$)

Suppose the state $|n\rangle$ is an eigenstate of parity $\hat{P}|n\rangle = (\pm 1)|n\rangle$ then

$$\psi_n(x) = \pm\psi_n(-x) \begin{cases} \text{even parity} \\ \text{odd parity} \end{cases}$$

Consider the effect of the parity operation on the Hamiltonian: $\hat{P}\hat{H}\hat{P}$

$$\hat{H} = \hat{p}^2/2m + V(\hat{x}) \quad \Rightarrow \quad \hat{P}\hat{H}\hat{P} = (-\hat{p})^2/2m + \hat{P}V(\hat{x})\hat{P} = \hat{p}^2/2m + V(-\hat{x})$$

if $V(\hat{x})$ is an even function of $\hat{x}$ then $V(-\hat{x}) = V(\hat{x})$ & $\hat{P}\hat{H}\hat{P} = \hat{H}$

or $\underline{[\hat{P},\hat{H}] = 0}$

Then the parity and the energy are <u>compatible observables</u>, which explains why the energy eigenstates can be of definite parity, parity is a "good quantum number" for this system

PROBABILITY CURRENT

Recall that a while ago we suggested that $|\langle x|\alpha\rangle|^2$ is the probability to find the state α in a region of size dx about x. We thus call $\rho(x) = |\psi(x)|^2$, the "probability density". In general the wavefunction is evolving with time so we should write $\rho(x,t) = |\psi(x,t)|^2$. $\psi(x,t)$ satisfies the Schrödinger eqn:

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

the complex conjugate of this is

$$-i\hbar \frac{\partial}{\partial t}\psi^*(x,t) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi^*(x,t) + V(x)\psi^*(x,t)$$ if the potential is a real function

suppose we multiply by ψ^* & by ψ respectively and then subtract:

$$i\hbar\left[\psi^*\frac{\partial}{\partial t}\psi + \psi\frac{\partial}{\partial t}\psi^*\right] = -\frac{\hbar^2}{2m}\left[\psi^*\frac{\partial^2}{\partial x^2}\psi - \psi\frac{\partial^2}{\partial x^2}\psi^*\right]$$

$$\Rightarrow i\hbar\frac{\partial}{\partial t}(\psi^*\psi) = \frac{-\hbar^2}{2m}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*\right]$$

then if we define the "probability current density" by

$$j(x,t) = \frac{-i\hbar}{2m}\left[\psi^*(x,t)\frac{\partial}{\partial x}\psi(x,t) - \psi(x,t)\frac{\partial}{\partial x}\psi^*(x,t)\right]$$

we have $\dfrac{\partial\rho(x,t)}{\partial t} + \dfrac{\partial j(x,t)}{\partial x} = 0$ which is a continuity equation enforcing the conservation of probability

e.g. consider a region $a \le x \le b$, then $\displaystyle\int_a^b dx\,\frac{\partial\rho(x,t)}{\partial t} = \frac{d}{dt}\int_a^b dx\,\rho(x,t) = \frac{d}{dt}P_{ab}(t)$

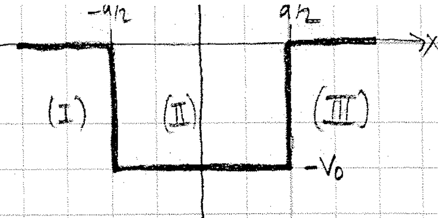
& $\displaystyle\int_a^b dx\,\frac{\partial}{\partial x}j(x,t) = j(b,t) - j(a,t)$ $\quad\Rightarrow \dfrac{d}{dt}P_{ab}(t) = j(a,t) - j(b,t)$

so the change in the probability to be between a and b is the flow of probability in at a, less the flow of probability out at b.

Continuity of the probability current will be used in the next example to set the boundary conditions on the solutions to the Schrödinger eqn.

BOUND STATES OF THE FINITE SQUARE WELL

Consider the potential defined by $V(x) = \begin{cases} 0 & x < -a/2 \quad (\mathrm{I}) \\ -V_0 & -\frac{a}{2} < x < a/2 \quad (\mathrm{II}) \\ 0 & x > a/2 \quad (\mathrm{III}) \end{cases}$



We are interested in "bound" solutions, those with $E<0$.

In regions I & III, the Schrödinger eqn takes the form $\frac{-\hbar^2}{2m}\frac{d^2\phi_E}{dx^2} = -|E|\phi_E$

or $\frac{d^2\phi_E}{dx^2} - \frac{2m|E|}{\hbar^2}\phi_E = 0$ with solutions $\phi_E(x) = Ae^{-Kx} + Be^{+Kx}$ $\left(K = \frac{\sqrt{2m|E|}}{\hbar}\right)$

In region II we have

$$\frac{-\hbar^2}{2m}\frac{d^2\phi_E}{dx^2} - V_0\phi_E = -|E|\phi_E$$ which has solutions $\phi_E = C\cos kx + D\sin kx$ $\quad k = \frac{\sqrt{2m(V_0-|E|)}}{\hbar}$

provided that $|E| < V_0$.

We demand that the wavefunction be normalisable when integrated from $-\infty$ to $+\infty$ $\Rightarrow$

$$\phi_{\mathrm{I}} = Ae^{Kx} \qquad \left(\xrightarrow[x\to-\infty]{} 0\right)$$

$$\phi_{\mathrm{II}} = B\cos kx + C\sin kx$$

$$\phi_{\mathrm{III}} = De^{-Kx} \qquad \left(\xrightarrow[x\to\infty]{} 0\right)$$

We will demand that the probability current $j(x,t)$ is continuous at $x=\pm a/2$ so that no probability is lost in the boundaries.

ie. at $x=-a/2$: $\quad j_{\mathrm{I}}(-a/2) = j_{\mathrm{II}}(-a/2)$

$$\frac{-i\hbar}{2m}\left[\phi_{\mathrm{I}}^*\left(\tfrac{-a}{2}\right)\frac{d\phi_{\mathrm{I}}}{dx}\left(\tfrac{-a}{2}\right) - \phi_{\mathrm{I}}\left(\tfrac{-a}{2}\right)\frac{d\phi_{\mathrm{I}}^*}{dx}\left(\tfrac{-a}{2}\right)\right] = \frac{-i\hbar}{2m}\left[\phi_{\mathrm{II}}^*\left(\tfrac{-a}{2}\right)\frac{d\phi_{\mathrm{II}}(-a/2)}{dx} - \phi_{\mathrm{II}}\left(\tfrac{-a}{2}\right)\frac{d\phi_{\mathrm{II}}^*}{dx}\left(\tfrac{-a}{2}\right)\right]$$

this can be satisfied by making both the wavefunction and its derivative continuous: $\phi_{\mathrm{I}}(-a/2) = \phi_{\mathrm{II}}(-a/2)$ & $\frac{d\phi_{\mathrm{I}}}{dx}\left(\tfrac{-a}{2}\right) = \frac{d\phi_{\mathrm{II}}}{dx}\left(\tfrac{-a}{2}\right)$

The same constraint applies at the other boundary: $\phi_{\mathrm{II}}(+a/2) = \phi_{\mathrm{III}}(a/2)$ & $\frac{d\phi_{\mathrm{II}}}{dx}(a/2) = \frac{d\phi_{\mathrm{III}}(a/2)}{dx}$

Thus: $Ae^{-Ka/2} = B\cos\frac{ka}{2} - C\sin\frac{ka}{2}$ & $KAe^{-Ka/2} = (-kB)(-1)\sin\frac{ka}{2} + kC\cos\frac{ka}{2}$

& $De^{-Ka/2} = B\cos\frac{ka}{2} + C\sin\frac{ka}{2}$ & $-KDe^{-Ka/2} = (-kB)\sin\frac{ka}{2} + kC\cos\frac{ka}{2}$

$$\Rightarrow K = k\,\frac{B\sin ka/2 + C\cos ka/2}{B\cos ka/2 - C\sin ka/2} \quad \& \quad -K = k\,\frac{-B\sin ka/2 + C\cos ka/2}{B\cos ka/2 + C\sin ka/2}$$

$$\Rightarrow \quad B\left(\frac{K}{k}\cos\frac{ka}{2} - \sin\frac{ka}{2}\right) = C\left(\cos\frac{ka}{2} + \frac{K}{k}\sin\frac{ka}{2}\right)$$

$$\& -B\left(\frac{K}{k}\cos\frac{ka}{2} - \sin\frac{ka}{2}\right) = C\left(\cos\frac{ka}{2} + \frac{K}{k}\sin\frac{ka}{2}\right)$$

hence either $B=0$ or $C=0$

odd solution — even solution

$* B=0$: $\quad 0 = \cos\frac{ka}{2} + \frac{K}{k}\sin\frac{ka}{2}$

$$\Rightarrow \underline{K/k = -\cot\frac{ka}{2}} \quad ①$$

$* C=0$: $\quad 0 = \frac{K}{k}\cos\frac{ka}{2} - \sin\frac{ka}{2}$

$$\Rightarrow \underline{K/k = \tan\frac{ka}{2}} \quad ②$$

These equations, which determine the eigen energies, are trancendental, but can be solved numerically. We can visualise the solutions graphically

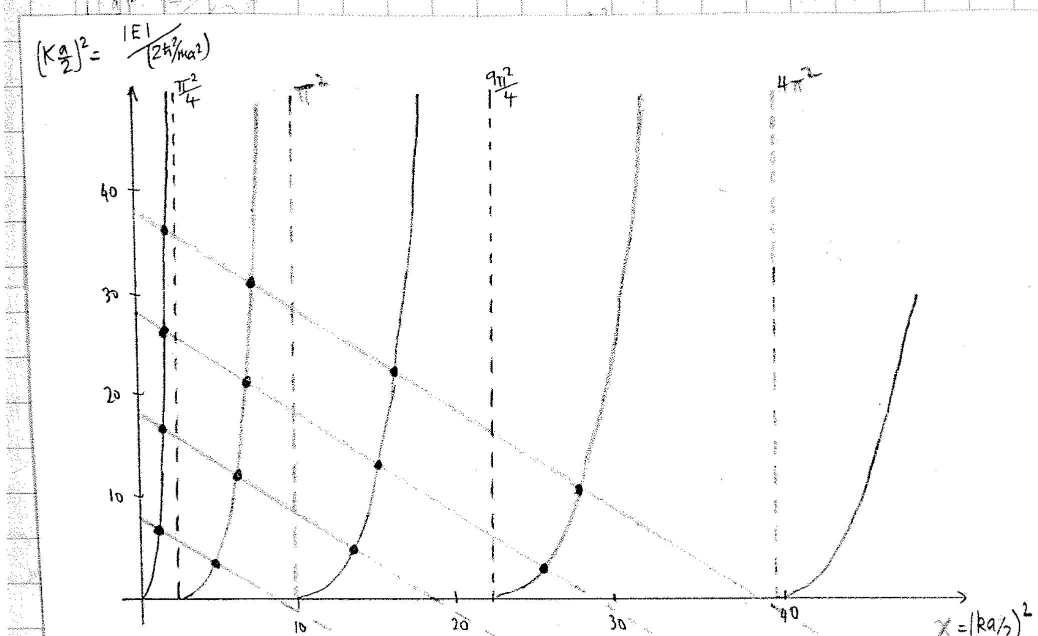
$$k^2 = \frac{2mV_0}{\hbar^2} - \frac{2m|E|}{\hbar^2} \equiv \left(\frac{2}{a}\right)^2\beta^2 - K^2 \quad ; \quad \chi \equiv (ka/2)^2 \quad ; \quad \chi + (Ka/2)^2 = \beta^2$$

$$\boxed{(Ka/2)^2 = \beta^2 - \chi}$$

$$① \rightarrow \frac{Ka/2}{ka/2} = -\cot\frac{ka}{2} \Rightarrow \left(\frac{Ka}{2}\right)^2 = \left(\frac{ka}{2}\right)^2\cot^2\left(\frac{ka}{2}\right) \;\&\; \cot\frac{ka}{2} \le 0$$

$$\boxed{(Ka/2)^2 = \chi\cot^2\sqrt{\chi} \;\&\; \tan\sqrt{\chi} \le 0}$$

$$② \rightarrow \frac{Ka/2}{ka/2} = \tan\frac{ka}{2} \Rightarrow \boxed{\left(\frac{Ka}{2}\right)^2 = \chi\tan^2\sqrt{\chi} \;\&\; \tan\sqrt{\chi} \ge 0}$$



$$\beta^2 = \frac{V_0}{(2\hbar^2/ma^2)}$$

$\Rightarrow$ deeper well gives more bound states

We can solve for the wavefunctions:

* even solution ($C=0$) - $Ae^{-\kappa a/2} = B\cos ka/2$ $\Rightarrow A = B\, e^{\kappa a/2}\cos ka/2$

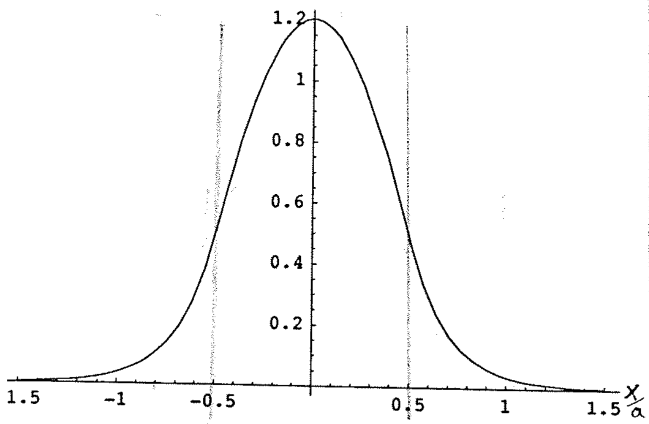
  $De^{-\kappa a/2} = B\cos ka/2$ $\Rightarrow D = B\, e^{\kappa a/2}\cos ka/2$

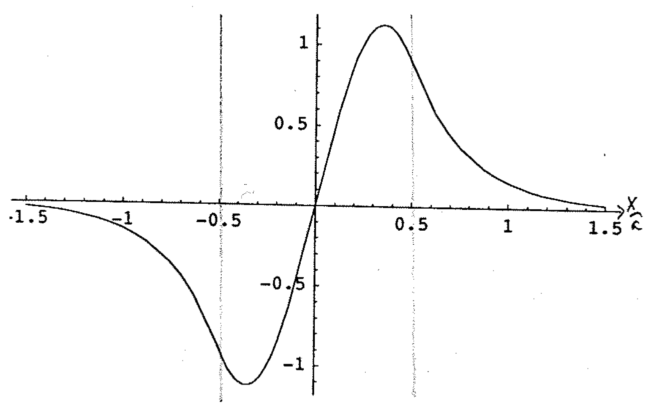
  with B determined by normalisation.

* odd solution ($B=0$) - $A = -Ce^{+\kappa a/2}\sin ka/2$ & $D = Ce^{+\kappa a/2}\sin ka/2$

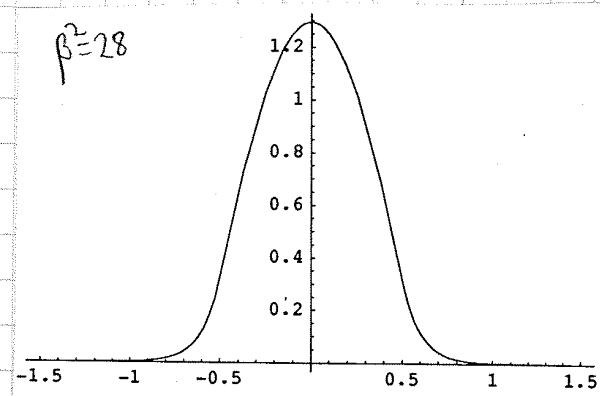
  with C determined by normalisation.

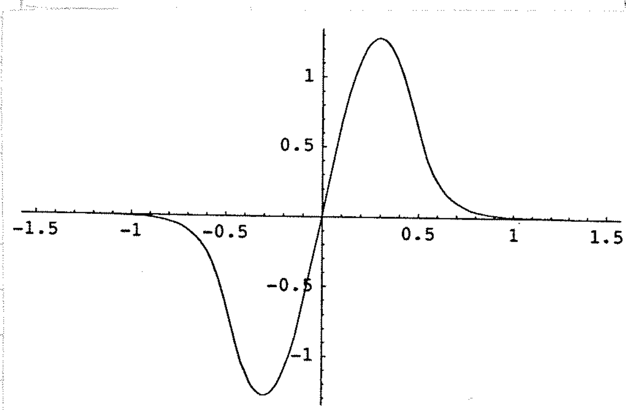
e.g. $\beta^2 = 8$

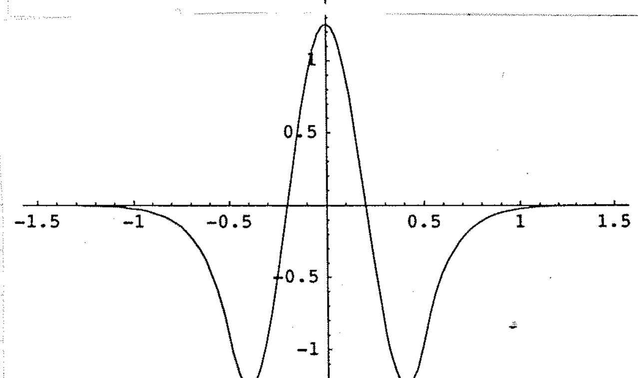


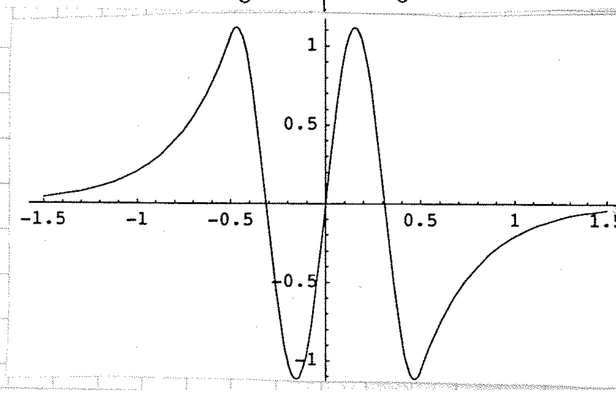


$\beta^2 = 28$









THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

The classical Hamiltonian for this system is $H = \frac{p^2}{2m} + \frac{1}{2}kx^2$. We will rewrite the spring constant in terms of the classical oscillation frequency, $k = m\omega^2$

$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$. The time-independent Schrödinger equation in the position basis is then
$$\frac{-\hbar^2}{2m}\frac{d^2\phi_E(x)}{dx^2} + \frac{1}{2}m\omega^2\phi_E(x) = E\phi_E(x)$$

$$\Rightarrow \frac{d^2\phi}{dx^2} + \left(\frac{2mE}{\hbar^2} - \frac{m^2\omega^2}{\hbar^2}x^2\right)\phi(x) = 0$$

We'll restrict our solutions to those that are square integrable & hence demand the boundary conditions $\phi(x \to \pm\infty) \to 0$.

Our solution begins by determining how the wavefunction must behave at large $|x|$. Here the potential term $(\sim x^2)$ will dominate over the energy term $(\sim x^0)$

$$\frac{d^2\phi}{dx^2}(x) - \frac{m^2\omega^2}{\hbar^2}x^2\phi(x) = 0 \quad \text{for large } |x|$$

we guess at a trial solution $\phi(x) = e^{-\alpha x^p}$ $\Rightarrow \frac{d\phi}{dx} = -\alpha p x^{p-1} e^{-\alpha x^p}$

$$\& \ \frac{d^2\phi}{dx^2} = e^{-\alpha x^p}\left(-\alpha p(p-1)x^{p-2} + \alpha^2 p^2 x^{2p-2}\right)$$

at large x, $x^{2p-2} >> x^{p-2}$ $\Rightarrow \alpha^2 p^2 x^{2p-2} - \frac{m^2\omega^2}{\hbar^2}x^2 = 0$

$$\Rightarrow \underline{p=2} \ \& \ \underline{\alpha = \frac{m\omega}{2\hbar}}$$

$$\phi(|x| \to \infty) \sim \exp\left(-\frac{m\omega}{2\hbar}x^2\right)$$

Changing to a set of dimensionless variables : $z = \sqrt{\frac{m\omega}{\hbar}}\,x$ & $\varepsilon = \frac{2E}{\hbar\omega}$
we have
$$\frac{d^2\phi}{dz^2} + (\varepsilon - z^2)\phi(z) = 0$$

We'll guess a trial solution which includes the asymptotic behaviour we've determined:
$$\phi(z) = f(z)\exp\left(-z^2/2\right) \Rightarrow \phi' = f'e^{-z^2/2} - zfe^{-z^2/2}$$
$$\& \ \phi'' = \left(f'' - 2zf' - (1-z^2)f\right)e^{-z^2/2}$$

so that we're left with a differential eqn $\underline{f''(z) - 2zf'(z) + (\varepsilon - 1)f(z) = 0}$

$f''(z) - 2zf'(z) + (\varepsilon - 1)f(z) = 0$ which we'll try to solve by a power series

$$f(z) = \sum_{j=0}^{\infty} b_j z^j$$

so that $f'(z) = \sum_{j=1}^{\infty} j b_j z^{j-1}$ & $f''(z) = \sum_{j=2}^{\infty} j(j-1) b_j z^{j-2}$

$$\Rightarrow \sum_{j=2}^{\infty} j(j-1) b_j z^{j-2} - 2\sum_{j=1}^{\infty} j b_j z^j + (\varepsilon - 1)\sum_{j=0}^{\infty} b_j z^j = 0$$

Changing the dummy index in the first sum $k = j-2$ $\quad j = k+2,\ j-1 = k+1$

$$\sum_{k=0}^{\infty} (k+1)(k+2) b_{k+2} z^k - 2\sum_{j=0}^{\infty} j b_j z^j + (\varepsilon - 1)\sum_{j=0}^{\infty} b_j z^j = 0$$

or $$\sum_{j=0}^{\infty} z^j \left[(j+1)(j+2) b_{j+2} + b_j(\varepsilon - 1 - 2j) \right] = 0$$

which is solved for every value of z if $\boxed{b_{j+2} = \frac{2j+1-\varepsilon}{(j+1)(j+2)} b_j}$

This is a recursion relation for the b_j. Since it only connects j to $j+2$, we can treat odd & even j separately.

Notice that for j large $\frac{b_{j+2}}{b_j} \to 2/j$, then the ratio of the $(j+2)$th term in the series to the jth (for large j) is $\frac{b_{j+2} z^{j+2}}{b_j z^j} \to \frac{2}{j} z^2$

Now this is trouble if the series is infinite – consider the series expansion of $e^{z^2(\frac{1}{2}+\Delta)}$ where $\Delta > 0$ $= \sum_{k=0}^{\infty} (z^2)^k \cdot (\frac{1}{2}+\Delta)^k / k!$ $\Rightarrow \frac{a_{k+1}(z^2)^{k+1}}{a_k (z^2)^k} = \frac{\frac{1}{2}+\Delta}{k} z^2$,

so for large j our terms grow faster than this function. Hence the solution will be overall divergent as $z \to \pm\infty$, counter to our demand of normalisable wavefunctions.

If the series is finite, then $f(z)$ is a fixed order polynomial such that $f(z)e^{-z^2/2}$ is convergent. The only way that the series can terminate is if at some point $2j+1-\varepsilon = 0 \Rightarrow \varepsilon = 2j_{max}+1 \equiv 2n+1$ which is a positive integer

Notice that the condition of normalisibility has <u>quantised</u> the allowed energies:

$$E = \frac{\hbar\omega}{2}\varepsilon = \underline{\hbar\omega(n+\tfrac{1}{2})} \qquad n = 0, 1, 2 \ldots$$

Notice that even in the ground state ($n=0$) the energy is not zero, $E_0 = \frac{1}{2}\hbar\omega$ – this energy is often called the zero-point energy and is a consequence of the uncertainty principle. If the zero-point energy had been zero it would have implied that
$\langle 0|p^2|0\rangle = \langle 0|x^2|0\rangle = 0$ which violates the uncertainty principle.

The fixed order polynomials which satisfy the recursion relations are the Hermite polynomials $H_n(z)$ which are the solutions to the differential equation

$$\frac{d^2 H_n(z)}{dz^2} - 2z\frac{dH_n(z)}{dz} + 2n H_n(z) = 0.$$

The first few Hermite polynomials are

$H_0(z) = 1$; $H_1(z) = 2z$; $H_2(z) = 4z^2 - 2$; $H_3(z) = 8z^3 - 12z$; $H_4(z) = 16z^4 - 48z^2 + 12$

They satisfy recurrance relations: $\frac{dH_n(z)}{dz} = 2nH_{n-1}(z)$

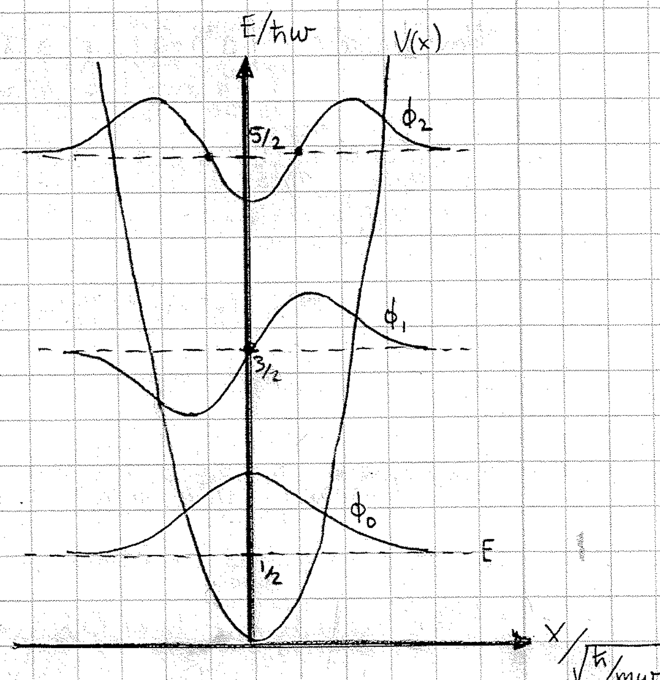
$$H_{n+1}(z) = 2z H_n(z) - 2n H_{n-1}(z)$$

They are orthogonal with a weight e^{-z^2} : $\int_{-\infty}^{\infty} dz\, e^{-z^2} H_m(z) H_n(z) = 2^n n! \sqrt{\pi}\, \delta_{n,m}$

The correctly normalised eigensolutions are thus

$$\boxed{\phi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar}x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)}$$ with $E_n = \hbar\omega(n+\frac{1}{2})$

Notice that the solutions decay rapidly in the classically forbidden region. In general, the solution $\phi_n(x)$ has n nodes in the classically allowed region.



AN OPERATOR-BASED SOLUTION TO THE ONE-DIMENSIONAL HARMONIC OSCILLATOR

It turns out that the harmonic oscillator can also be solved by defining operators which transform states into each other. This technique turns out to be very useful elsewhere in quantum physics so we will devote a little time to it.

The Hamiltonian of interest is $\hat{H} = \hat{p}^2/2m + \frac{1}{2} m\omega^2 \hat{x}^2$.

We can define two non-hermitian operators : $\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}} \left(\hat{x} + i \frac{\hat{p}}{m\omega} \right)$

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

Being non-hermitian they do not correspond to observables, and they cannot be simultaneously diagonalised since they do not commute :

$$[\hat{a}, \hat{a}^{+}] = \frac{m\omega}{2\hbar} \left[\hat{x} + i \frac{\hat{p}}{m\omega}, \hat{x} - i \frac{\hat{p}}{m\omega} \right] = \frac{m\omega}{2\hbar} \left(\cancel{[\hat{x}, \hat{x}]}^{0} + \frac{i}{m\omega} [\hat{p}, \hat{x}] - \frac{i}{m\omega} [\hat{x}, \hat{p}] + \frac{1}{m\omega} \cancel{[\hat{p}, \hat{p}]}^{0} \right)$$

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

Consider $\hat{a}^{+}\hat{a} = \frac{m\omega}{2\hbar} \left(\hat{x} - i \frac{\hat{p}}{m\omega} \right) \left(\hat{x} + i \frac{\hat{p}}{m\omega} \right) = \frac{m\omega}{2\hbar} \left(\hat{x}^2 + \frac{i}{m\omega} [\hat{x}, \hat{p}] + \frac{\hat{p}^2}{m^2\omega^2} \right)$

$$= \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \qquad \& \text{ hence } \qquad \underline{\hat{H} = \hbar\omega \left(\hat{a}^{+}\hat{a} + \tfrac{1}{2} \right)}$$

Then the eigenstates of $\hat{H}$ are the eigenstates of $\hat{a}^{+}\hat{a}$: $\underline{\hat{a}^{+}\hat{a} |n\rangle = n|n\rangle}$

Now consider $[\hat{a}^{+}\hat{a}, \hat{a}] = \hat{a}^{+}\hat{a}\hat{a} - \hat{a}\hat{a}^{+}\hat{a} = \hat{a}^{+}\hat{a}\hat{a} - (1 + \hat{a}^{+}\hat{a})\hat{a} = -\hat{a}$

$\& \ [\hat{a}^{+}\hat{a}, \hat{a}^{+}] = \hat{a}^{+}\hat{a}\hat{a}^{+} - \hat{a}^{+}\hat{a}^{+}\hat{a} = \hat{a}^{+}(1 + \hat{a}^{+}\hat{a}) - \hat{a}^{+}\hat{a}^{+}\hat{a} = \hat{a}^{+}$

Hence $(\hat{a}^{+}\hat{a})\, \hat{a}^{+} |n\rangle = \left([\hat{a}^{+}\hat{a}, \hat{a}^{+}] + \hat{a}^{+}\hat{a}^{+}\hat{a} \right) |n\rangle$

$$= \left(\hat{a}^{+} + \hat{a}^{+}\hat{a}^{+}\hat{a} \right) |n\rangle = \hat{a}^{+}(1 + \hat{a}^{+}\hat{a}) |n\rangle$$

$$= \hat{a}^{+}(1 + n) |n\rangle$$

$$\Rightarrow (\hat{a}^{+}\hat{a})(\hat{a}^{+}|n\rangle) = (n+1)(\hat{a}^{+}|n\rangle)$$

$\Rightarrow \hat{a}^{+}|n\rangle$ is an eigenstate of $\hat{a}^{+}\hat{a}$ with eigenvalue $n+1$ $\longrightarrow \hat{a}^{+}|n\rangle = c|n+1\rangle$

Similarly $(\hat{a}^{+}\hat{a})(\hat{a}|n\rangle) = (n-1)(\hat{a}|n\rangle)$ $\Rightarrow \hat{a}|n\rangle$ is an eigenstate of $\hat{a}^{+}\hat{a}$ with eigenvalue $n-1$. $\longrightarrow \hat{a}|n\rangle = c'|n-1\rangle$

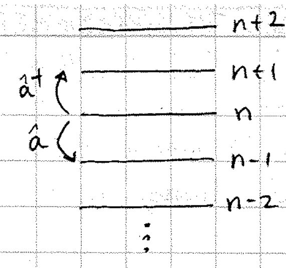
The constants can be determined by normalising the states :

$$|c'|^2 \langle n-1|n-1\rangle = (\langle n|\hat{a}^{+})(\hat{a}|n\rangle) = \langle n|\hat{a}^{+}\hat{a}|n\rangle = n\langle n|n\rangle = n$$

$$\Rightarrow c' = \sqrt{n} \quad \text{real by convention}$$

$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle$ & $\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,|n+1\rangle$

"annihilation op." "lowering ladder op." — "creation op." "raising ladder op."



What can we say about the allowed values of n?

Consider $\langle n|\hat{a}^\dagger\hat{a}|n\rangle = (\langle n|\hat{a}^\dagger)(\hat{a}|n\rangle) \geq 0$ (a mod square)

but $\langle n|\hat{a}^\dagger\hat{a}|n\rangle = \langle n|n|n\rangle = n \Rightarrow n$ must be positive or zero.

If n is not an integer we can repeatedly apply $\hat{a}$ until n lies between 0 & 1. One subsequent application of $\hat{a}$ will take n negative which is not allowed. The only way to prevent this is for the ladder to terminate. If n is limited to the positive integers then for the state $|n=0\rangle$ we'd have

$\hat{a}|0\rangle = \sqrt{0}\,|-1\rangle = 0$, so $-$ve n states cannot be reached.

$\hat{H}|n\rangle = \hbar\omega(\hat{a}^\dagger\hat{a} + \tfrac{1}{2})|n\rangle = \hbar\omega(n+\tfrac{1}{2})|n\rangle \Rightarrow \underline{E_n = \hbar\omega(n+\tfrac{1}{2})}$ $n = 0,1,2\ldots$

excited states can be obtained from the ground state $|0\rangle$ by multiple applications of $a^\dagger$:

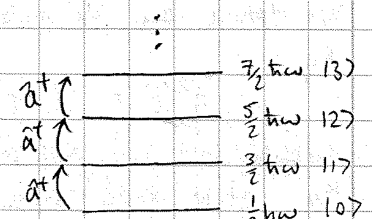
$$|1\rangle = \hat{a}^\dagger|0\rangle$$

$$|2\rangle = \frac{\hat{a}^\dagger}{\sqrt{2}}|1\rangle = \frac{\hat{a}^\dagger\hat{a}^\dagger}{\sqrt{2}}|0\rangle = \frac{(\hat{a}^\dagger)^2}{\sqrt{2}}|0\rangle$$

$$|3\rangle = \frac{\hat{a}^\dagger}{\sqrt{3}}|2\rangle = \frac{(\hat{a}^\dagger)^3}{\sqrt{3}\sqrt{2}}|0\rangle$$

$$\vdots$$

$$\underline{|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}|0\rangle}$$



Matrix elements of a & $a^\dagger$ are simple: $\langle n'|\hat{a}|n\rangle = \sqrt{n}\,\delta_{n',n-1}$

$\langle n'|\hat{a}^\dagger|n\rangle = \sqrt{n+1}\,\delta_{n',n+1}$

From these we can easily obtain matrix elements of $\hat{x}$ & $\hat{p}$ $\left(\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^\dagger)\right.$

$\left.\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}(\hat{a}^\dagger - \hat{a})\right)$

$$\langle n'|\hat{x}|n\rangle = \sqrt{\frac{\hbar}{2m\omega}}\left(\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right)$$

$$\langle n'|\hat{p}|n\rangle = i\sqrt{\frac{\hbar m\omega}{2}}\left(-\sqrt{n}\,\delta_{n',n-1} + \sqrt{n+1}\,\delta_{n',n+1}\right)$$

Obtaining the position-space wavefunctions in this technique is straightforward: for the ground state $a|0\rangle = 0$

$$\left(\hat{x} + i\frac{\hat{p}}{m\omega}\right)|0\rangle = 0 \Rightarrow \langle x|\hat{x} + i\frac{\hat{p}}{m\omega}|0\rangle = 0$$

or $\left[x + \frac{i}{m\omega}\left(-i\hbar\frac{d}{dx}\right)\right]\langle x|0\rangle = 0$ or $\left(\frac{d}{dx} + \frac{m\omega}{\hbar}x\right)\phi_0(x) = 0$

this first-order differential equation can easily be solved $\phi_0(x) = N\exp\left(-\frac{m\omega}{2\hbar}x^2\right)$

ASIDE: THE SCHRÖDINGER & HEISENBERG PICTURES OF TIME EVOLUTION IN QUANTUM MECHANICS

We introduced dynamics in quantum theory by suggesting that states can change over time:

$$|\alpha; t_0; t\rangle = \mathcal{U}(t, t_0)\,|\alpha, t_0\rangle.$$

This approach is called the "Schrödinger picture". In this picture is is only states which change with time, operators remaining constant.

The unitary time evolution does not change state inner products:

$$\langle\beta|\alpha\rangle \to \langle\beta|\mathcal{U}^\dagger\mathcal{U}|\alpha\rangle = \langle\beta|\alpha\rangle$$

but consider the action on a matrix element:

$$\langle\beta|\hat{X}|\alpha\rangle \longrightarrow \langle\beta|\mathcal{U}^\dagger\hat{X}\,\mathcal{U}|\alpha\rangle$$

We could consider this in a different way, treating the states $|\alpha\rangle, |\beta\rangle$ as constant and instead evolving the operator $\hat{X} \to \mathcal{U}^\dagger\hat{X}\,\mathcal{U}$. This second approach is called the "Heisenberg picture". It's useful because it more closely resembles classical mechanics in which observables (like $\vec{x}$) vary with time ($\vec{x}(t)$).

Recall that for time-independent Hamiltonians, $\mathcal{U}(t, t_0=0) \equiv \mathcal{U}(t) = e^{-i/\hbar \hat{H}t}$.
We define the Heisenberg operator A^H in terms of the Schrödinger operator A^S by

$$\hat{A}^H(t) \equiv \mathcal{U}^\dagger(t)\,\hat{A}^S\,\mathcal{U}(t) \qquad \text{where clearly} \quad \hat{A}^H(0) = \hat{A}^S.$$

the state kets co-incide at $t=0$ $\quad |\alpha, t_0=0; t=0\rangle_H = |\alpha, t_0=0\rangle_S$,

but the Schrödinger ket evolves $\quad |\alpha, t_0=0; t\rangle_S = \mathcal{U}(t)\,|\alpha, t_0=0\rangle_S$

while the Heisenberg ket remains frozen $\quad |\alpha, t_0=0; t\rangle_H = |\alpha, t_0=0\rangle_H$.

Expectation values are, as they must be, equal in the two pictures:

$$\begin{aligned}
{}_H\langle\alpha, t_0=0; t|\hat{A}^H|\alpha, t_0=0; t\rangle_H &= {}_H\langle\alpha, t_0=0; t|\,\mathcal{U}^\dagger(t)\hat{A}^S\mathcal{U}(t)\,|\alpha, t_0=0; t\rangle_H \\
&= {}_S\langle\alpha, t_0=0|\,\mathcal{U}^\dagger(t)\hat{A}^S\mathcal{U}(t)\,|\alpha, t_0=0\rangle_S \\
&= {}_S\langle\alpha, t_0=0; t|\hat{A}^S|\alpha, t_0=0; t\rangle_S
\end{aligned}$$

Since in the Heisenberg picture it is operators that evolve in time, there should be an equation describing their dynamics. This is easy to derive, assuming that the operator A^s has no <u>explicit</u> dependence upon time:

$$\frac{d}{dt}\hat{A}^H(t) = \frac{d}{dt}\left(U^\dagger(t)\hat{A}^s U(t)\right) = \frac{\partial U^\dagger}{\partial t}\hat{A}^s U + U^\dagger \hat{A}^s \frac{\partial U}{\partial t}$$

The Schrödinger eq<u>n</u> for the time evolution operator was $i\hbar \frac{\partial}{\partial t}U(t) = \hat{H}U(t)$

$$\text{so } \frac{d}{dt}\hat{A}^H = -\frac{1}{i\hbar}U^\dagger \hat{H}\hat{A}^s U + \frac{1}{i\hbar}U^\dagger\hat{A}^s\hat{H}U$$

$$= -\frac{1}{i\hbar}U^\dagger\hat{H}UU^\dagger\hat{A}^s U + \frac{1}{i\hbar}U^\dagger\hat{A}^s U U^\dagger \hat{H}U \qquad (\text{using } UU^\dagger = 1)$$

$$= -\frac{1}{i\hbar}U^\dagger\hat{H}U\hat{A}^H + \frac{1}{i\hbar}\hat{A}^H U^\dagger\hat{H}U = \frac{1}{i\hbar}\left[\hat{A}^H, U^\dagger\hat{H}U\right]$$

for time-independent Hamiltonians $U(t) = e^{-i/\hbar \hat{H}t} \Rightarrow U^\dagger\hat{H}U = \hat{H}$

$$\& \quad \underline{\frac{d\hat{A}^H}{dt} = \frac{1}{i\hbar}[\hat{A}^H, \hat{H}]} \qquad \text{"Heisenberg equation of motion"}$$

Let's evaluate this in some instructive cases:

1. The free particle in one-dimension: $\hat{H} = \hat{p}^2/2m$. Consider the time-evolution of the momentum operator, $\hat{p}$.

$$\frac{d\hat{p}}{dt} = \frac{1}{i\hbar}[\hat{p}, \hat{H}] = \frac{1}{i\hbar}\left[\hat{p}, \hat{p}^2/2m\right] = 0 \qquad \Rightarrow \underline{\hat{p}(t) = \text{constant} = \hat{p}(0)}$$

Consider now the position operator, $\hat{x}$:

$$\frac{d\hat{x}}{dt} = \frac{1}{i\hbar}[\hat{x}, \hat{H}] = \frac{1}{i\hbar}[\hat{x}, \hat{p}^2/2m] = \frac{1}{2im\hbar}\left([\hat{x},\hat{p}]\hat{p} + \hat{p}[\hat{x},\hat{p}]\right) = \frac{2i\hbar}{2i\hbar m}\hat{p} = \hat{p}/m$$

$$\Rightarrow \frac{d\hat{x}}{dt} = \hat{p}(0)/m \quad \text{which can be solved,} \quad \underline{\hat{x}(t) = \hat{x}(0) + \frac{\hat{p}(0)}{m}t}$$

This looks rather like the classical trajectory of a free particle, but be aware that the position operator at different times does not commute:

$$[\hat{x}(t), \hat{x}(0)] = [\hat{x}(0), \hat{x}(0)] + \frac{t}{m}[\hat{p}(0), \hat{x}(0)] = -i\hbar t/m$$

so that there is an uncertainty relation $\langle(\Delta\hat{x}(t))^2\rangle\langle(\Delta\hat{x}(0))^2\rangle \geq \hbar^2 t^2/4m^2$.

Hence although we might have a well localised particle at one time, it will become less well localised as time goes on. We'll discuss this "spreading of a wavepacket" later.

② a particle in a potential; $\hat{H} = \hat{p}^2/2m + V(\hat{x})$

$$\frac{d\hat{p}}{dt} = \frac{1}{i\hbar}[\hat{p}, \hat{H}] = \frac{1}{i\hbar}[\hat{p}, V(\hat{x})]$$

$$\frac{d\hat{p}}{dt} = -\frac{\partial}{\partial\hat{x}}V(\hat{x})$$

$$\frac{d\hat{x}}{dt} = \frac{1}{i\hbar}[\hat{x}, \hat{H}] = \frac{1}{i\hbar}[\hat{x}, \frac{\hat{p}^2}{2m}]$$

$$= \hat{p}/m$$

$$\Rightarrow \frac{d^2\hat{x}}{dt^2} = \frac{1}{i\hbar}\left[\frac{d\hat{x}}{dt}, \hat{H}\right] = \frac{1}{mi\hbar}\left[\hat{p}, \hat{H}\right]$$

$$= \frac{1}{m}\frac{d\hat{p}}{dt}$$

if $V(\hat{x})$ can be power expanded in $\hat{x}$:
$$V(\hat{x}) = \sum_{n=0}^{\infty} C_n \hat{x}^n,$$

then $[\hat{p}, V(\hat{x})] = \sum_{n=0}^{\infty} C_n [\hat{p}, \hat{x}^n]$.

$[\hat{p}, \hat{x}^2] = [\hat{p}, \hat{x}]\hat{x} + \hat{x}[\hat{p}, \hat{x}] = -2i\hbar\hat{x}$

we can repeatedly apply this to the arbitrary power of $\hat{x}$,

e.g. $[\hat{p}, \hat{x}^3] = [\hat{p}, \hat{x}]\hat{x}^2 + \hat{x}^2[\hat{p}, \hat{x}] = -i\hbar\hat{x}^2 - 2i\hbar\hat{x}^2 = -3i\hbar\hat{x}^2$

$\vdots$

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

$$\Rightarrow m\frac{d^2\hat{x}}{dt^2} = -\frac{dV(\hat{x})}{d\hat{x}}$$ Quantum mechanical analogue of Newton's 2nd law.

considered in an expectation value: $m\frac{d^2\langle x\rangle}{dt^2} = -\left\langle\frac{\partial V}{\partial x}\right\rangle$ "Ehrenfest's theorem"

③ the Harmonic oscillator potential

$$\left.\begin{aligned} \frac{d\hat{p}}{dt} &= -\frac{\partial}{\partial\hat{x}}V(\hat{x}) = -\frac{\partial}{\partial\hat{x}}\left(\tfrac{1}{2}m\omega^2\hat{x}^2\right) = -m\omega^2\hat{x} \\ \frac{d\hat{x}}{dt} &= \hat{p}/m \end{aligned}\right\} \text{coupled differential equations}$$

recall that we defined operators $\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{x} + i\,\hat{p}/m\omega\right)$ & its Hermitian conjugate

then $$\frac{d\hat{a}}{dt} = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{d\hat{x}}{dt} + \frac{i}{m\omega}\frac{d\hat{p}}{dt}\right) = \sqrt{\frac{m\omega}{2\hbar}}\left(\frac{\hat{p}}{m} - i\omega\hat{x}\right) = -i\omega\hat{a}$$

$$\frac{d\hat{a}}{dt} = -i\omega\hat{a} \quad \& \quad \frac{d\hat{a}^\dagger}{dt} = +i\omega\hat{a}^\dagger$$ uncoupled differential equations

$$\underline{\hat{a}(t) = \hat{a}(0)e^{-i\omega t}} \quad \& \quad \underline{\hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{+i\omega t}}$$

N.B. this makes $\hat{a}^\dagger\hat{a}$ & $\hat{H}$ time-independent as we'd expect.

a little rearrangement shows that

$$\hat{x}(t) = \hat{x}(0)\cos\omega t + \frac{\hat{p}(0)}{m\omega}\sin\omega t$$

$$\hat{p}(t) = -m\omega\hat{x}(0)\sin\omega t + \hat{p}(0)\cos\omega t$$

6. SCATTERING IN ONE-DIMENSION

In this section we will attempt to describe quantum mechanically a system where a particle is incident on a potential barrier.

Firstly consider the free-particle solution in position space: $\psi_p(x) = N_p e^{ip.x/\hbar}$ which is an eigenstate of momentum & of energy with eigenvalue $E = p^2/2m$.

This solution is not square-integrable over the range $-\infty < x < \infty$, in fact if we consider the probability current for this state, we have

$$j_p(x) = -\frac{i\hbar}{2m}\left[\psi_p^* \frac{\partial \psi_p}{\partial x} - \psi_p \frac{\partial \psi_p^*}{\partial x}\right] = |N_p|^2 \frac{p}{m}$$

which is independent of x implying that there is a constant creating of probability at $-\infty$ & an annihilation of probability at $+\infty$.

We will propose another approach known as "box normalisation". Here we suppose that the quantum system can be considered to live within a box of large, but finite size, $-L/2 \leq x < L/2$. L should be much lager than any characteristic length scale in the problem we're considering. We shall apply periodic boundary conditions at the walls of the box.

$$\psi(x = -L/2) = \psi(x = L/2)$$

Provided the box is large enough, this non-unique choice should have a negligable impact upon the solution.

For a free-particle solution, the periodic boundary condition enforces the constraint

$$N_p e^{-i/\hbar\, p L/2} = N_p e^{i/\hbar\, p L/2} \Rightarrow e^{i/\hbar\, pL} = 1 \Rightarrow pL = n(2\pi\hbar)$$

n integral.

hence in the box, "free" particles can only have discrete momenta from the set $p_n = \frac{2\pi\hbar}{L}.n$.

These wavefunctions can be normalised on the interval $-L/2 < x < L/2$:

$$1 = |N|^2 \int_{-L/2}^{L/2} dx \left| e^{+i/\hbar \cdot \frac{2\pi\hbar}{L} x} \right|^2 = |N|^2 \int_{-L/2}^{L/2} dx\, 1 = |N|^2 . L$$

$$\Rightarrow \underline{\psi_{p_n}(x) = \frac{1}{\sqrt{L}} e^{i/\hbar\, p_n x}}$$

The completeness relation $1 = \sum_n |n\rangle\langle n|$ in position space is

$$\langle x'|x\rangle = \delta(x'-x) = \sum_n \langle x'|n\rangle\langle n|x\rangle = \sum_n \psi_n(x')\,\psi_n^*(x)$$

in this basis $\sum_n \psi_{p_n}(x')\psi_{p_n}^*(x) = \frac{1}{L}\sum_{n=-\infty}^{\infty} e^{2\pi i\left(\frac{x'-x}{L}\right)n}$ which is a representation of $\delta(x'-x)$.

Then a general free-particle solution to the Schrödinger equation is

$$\psi(x,t) = \frac{1}{\sqrt{L}}\sum_{n=-\infty}^{\infty} c_n\, e^{i/\hbar\, px}\, e^{-i/\hbar\, E_n t}$$

where in order to make the solution normalisable, $\sum_n |c_n|^2 = 1$.

Now suppose we take the limit $L\to\infty$ where we know the spectrum will become continuous. This occurs as the 'distance' between allowed eigenmomenta reduces to zero:

$$\Delta p_n = p_n - p_{n-1} = \frac{2\pi\hbar}{L}n - \frac{2\pi\hbar}{L}(n-1) = \frac{2\pi\hbar}{L} \longrightarrow 0$$

We shall take the limit with $\Delta p_n \cdot \frac{L}{2\pi\hbar} = 1$ kept fixed.

Inserting a judicious 1 into the completeness relation we have

$$\delta(x'-x) = \frac{1}{L}\sum_{n=-\infty}^{\infty}\left(\Delta p_n \frac{L}{2\pi\hbar}\right) e^{i/\hbar\, p_n(x'-x)} = \frac{1}{2\pi\hbar}\sum_n \Delta p_n\, e^{\frac{i p_n}{\hbar}(x'-x)}$$

which in the limit $L\to\infty$ will become an integral $= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, e^{i p/\hbar (x'-x)}$

$$= \frac{\hbar}{2\pi\hbar}\int_{-\infty}^{\infty} dk\, e^{ik(x'-x)} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x'-x)}$$ which is the conventional Fourier representation of $\delta(x'-x)$.

Now in the limit $L\to\infty$, the solution will remain normalisable if $\sum_n |c_n|^2 = 1$

i.e. $1 = \sum_{n=-\infty}^{\infty}\left(\Delta p_n \frac{L}{2\pi\hbar}\right)|c_n|^2 \longrightarrow \frac{L}{2\pi\hbar}\int_{-\infty}^{\infty} dp\, |c(p)|^2$ which can only be solved if $c(p) \propto \frac{1}{\sqrt{L}}$

defining $\varphi(p) = \sqrt{\frac{L}{2\pi\hbar}}\, c(p)$ we have $1 = \int_{-\infty}^{\infty} dp\, |\varphi(p)|^2$

& we can form a free-particle solution

$$\boxed{\psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi(p)\, e^{i/\hbar(px - E(p)t)}}$$

which we call a wave packet.

It is straightforward to show that the momentum space wavefunction corresponding to this wavepacket is $\varphi(p)e^{-i/\hbar E(p)t}$.

Thus the average momentum is $$\langle p(t)\rangle = \int_{-\infty}^{\infty} dp \left[\varphi(p)e^{-i/\hbar E(p)t}\right]^* p\left[\varphi(p)e^{-i/\hbar E(p)t}\right]$$
$$= \int_{-\infty}^{\infty} dp\ p\,|\varphi(p)|^2$$

$$\& \ \langle p^2(t)\rangle = \int_{-\infty}^{\infty} dp\ p^2\,|\varphi(p)|^2.$$

The average position can be found using the representation of the position operator in momentum space:
$$\langle p'|\hat{x}|p\rangle = \delta(p'-p)\, i\hbar \frac{\partial}{\partial p}$$

$$\langle x(t)\rangle = i\hbar \int_{-\infty}^{\infty} dp \left[\varphi(p)e^{-i/\hbar E(p)t}\right]^* \frac{\partial}{\partial p}\left[\varphi(p)e^{-i/\hbar E(p)t}\right].$$
$$\& \ \langle x^2(t)\rangle = -\hbar^2 \int_{-\infty}^{\infty} dp \left[\varphi(p)e^{-i/\hbar E(p)t}\right]^* \frac{\partial^2}{\partial p^2}\left[\varphi(p)e^{-i/\hbar E(p)t}\right].$$

Suppose that we form a wavepacket with a gaussian distribution of momenta and a momentum dependent phase:
$$\varphi(p) = \frac{1}{\sqrt{\sigma}\,\pi^{1/4}} \exp\left\{-\frac{(p-p_0)^2}{2\sigma^2} - \frac{i}{\hbar}p x_0\right\}$$

$$\text{then } \langle p(t)\rangle = \frac{1}{\sigma\sqrt{\pi}}\int_{-\infty}^{\infty} dp\, p\, e^{-(p-p_0)^2/\sigma^2} = \frac{1}{\sigma\sqrt{\pi}}\,\sigma \int_{-\infty}^{\infty} dz\,(\sigma z + p_0)e^{-z^2} \qquad \left(z = \frac{p-p_0}{\sigma}\right)$$

$$\left.\begin{array}{l} \underline{\langle p(t)\rangle = p_0} \\ \underline{\langle p^2(t)\rangle = \tfrac{1}{2}\sigma^2 - p_0^2} \end{array}\right\} \langle(\Delta p)^2\rangle = \sigma^2/2$$

so the uncertainty in momentum remains constant.

I leave it as an exercise to show that for this particular wavepacket

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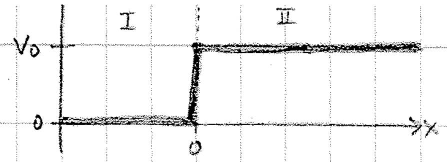
$$+\frac{p_0}{m}t \qquad \& \quad \langle x^2(t)\rangle = \frac{\hbar^2}{2\sigma^2} + \frac{\sigma^2 t^2}{2m^2} + \left(x + \frac{p_0}{m}t\right)^2$$
$$= \frac{\hbar^2}{2\sigma^2}\left(1 + t^2\Big/\left(\frac{\hbar^2 m^2}{\sigma^2}\right)\right).$$

phase velocity / group velocity as homework problem

ecomes more diffuse, or "spreads" as time increases,
imum uncertainty at $t=0$ $\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle = \hbar^2/4$.

ANIMATION

SCATTERING OF A WAVEPACKET FROM A STEP-POTENTIAL



$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & x>0 \end{cases}$$

We'll set up a wavepacket incident from the left such that the center of the packet reaches $x=0$ at $t=0$ when it has minimum uncertainty. We expect some wave to reflect at $x=0$ and be found moving to the left. Additionally there is likely to be some penetration into $x>0$.

$$\psi_I(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi(p)\, e^{i/\hbar(px - p^2/2m\, t)} + \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi_-(p)\, e^{i/\hbar(-px - \frac{p^2}{2m}t)}$$

In region II the allowed sol'ns are plane waves of momentum $q = \pm\sqrt{2m(E-V_0)}$, to match the solutions in region I, where $E = p^2/2m$,

$$q(p) = \pm\sqrt{p^2 - 2mV_0}.$$

$$\& \ \psi_{II}(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi_+(p)\, e^{i/\hbar(q(p)x - \frac{p^2}{2m}t)}$$

At $x=0$, the wavefunctions & their derivatives should match:

$$\psi_I(x=0,t) = \psi_{II}(x=0,t)$$

$$\frac{\partial}{\partial x}\psi_I(x,t)\Big|_{x=0} = \frac{\partial}{\partial x}\psi_{II}(x,t)\Big|_{x=0}$$

$$\Rightarrow \int_{-\infty}^{\infty} dp\, \varphi(p)\, e^{-i/\hbar\, p^2/2m\, t} + \int_{-\infty}^{\infty} dp\, \varphi_-(p)\, e^{-i/\hbar\, p^2/2m\, t} = \int_{-\infty}^{\infty} dp\, \varphi_+(p)\, e^{-i/\hbar\, p^2/2m\, t}$$

$$\rightarrow \underline{\varphi(p) + \varphi_-(p) = \varphi_+(p)}$$

$$\& \int_{-\infty}^{\infty} dp\, \varphi(p)\, \frac{ip}{\hbar}\, e^{-i/\hbar\, p^2/2m\, t} + \int_{-\infty}^{\infty} dp\, \varphi_-(p)\left(\frac{-ip}{\hbar}\right) e^{-i/\hbar\, p^2/2m\, t} = \int_{-\infty}^{\infty} dp\, \varphi_+(p)\, \frac{iq(p)}{\hbar}\, e^{-i/\hbar\, p^2/2m\, t}$$

$$\rightarrow \underline{p(\varphi(p) - \varphi_-(p)) = q(p)\varphi_+(p)}$$

$$\Rightarrow \underline{\varphi_+(p) = \frac{2p}{p+q(p)}\varphi(p)} \quad \& \quad \underline{\varphi_-(p) = \frac{p-q(p)}{p+q(p)}\varphi(p)}$$

Note that we've solved the 'transmission/reflection' problem for all momenta p – we'll see later that this is a handy mathematical shortcut.

The wavepacket solution are then $\psi_I(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi(p)\left[e^{i/\hbar(px - \frac{p^2}{2m}t)} + \frac{p-q(p)}{p+q(p)}\, e^{i/\hbar(-px - \frac{p^2}{2m}t)}\right]$

$$\& \ \psi_{II}(x,t) = \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{\infty} dp\, \varphi(p) \cdot \frac{2p}{p+q(p)}\, e^{i/\hbar(q(p)x - \frac{p^2}{2m}t)}$$

Case 1, $E < V_0 \Rightarrow q(p) = i\sqrt{2m(V_0 - E)} = iQ$ & $\psi_{II}(x,t) \sim e^{-Qx}$ exponentially decaying solution

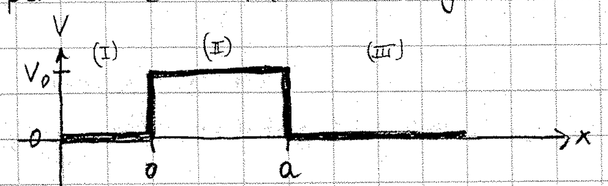
ANIMATION

Case 2, $E > V_0 \Rightarrow q(p) = \sqrt{2m(E-V_0)}$ & $\psi_{II}(x,t)$ is oscillatory

ANIMATION

Notice that even in case 1 there was some probability to find the particle past the barrier $(x>0)$. This remains true even if the wavepacket has negligable amplitude to have $E(p) > V_0$. Suppose the barrier has only finite length, then the particle can 'tunnel' through a classically forbidden region

e.g.



$$V(x) = \begin{cases} 0 & x<0 \\ V_0 & 0<x<a \\ 0 & x>a \end{cases}$$

ANIMATION

We shall now develop the mathematics of these scattering & tunneling processes by considering the individual plane waves that make up a wavepacket.

Consider the potential step above. A time independent plane wave solution can be written (remember that we cannot normalise this soln)

$$\psi_I(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$$
$$\psi_{II}(x) = Ce^{iq(p)x/\hbar} + De^{-iq(p)x/\hbar}$$
$$\psi_{III}(x) = Fe^{ipx/\hbar}$$

where we neglect a term $e^{-ipx/\hbar}$ corresponding to flux coming from $+\infty$.

matching the wavefunctions & first derivatives at $x=0$ and $x=a$:

$$A + B = C + D \qquad Ce^{iqa/\hbar} + De^{-iqa/\hbar} = Fe^{ipa/\hbar}$$
$$p(A-B) = q(C-D) \qquad q(Ce^{iqa/\hbar} - De^{-iqa/\hbar}) = pFe^{ipa/\hbar}$$

these simultaneous equations can be solved yielding

$$B = -A\frac{q+p}{q-p}\frac{1-e^{-2iqa/\hbar}}{1-\left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}} \qquad C = -A\frac{2p(p+q)}{(q-p)^2}\frac{e^{-2iqa/\hbar}}{1-\left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}}$$

$$D = -A\frac{2p}{q-p}\frac{1}{1-\left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}} \qquad F = -A\frac{4pq}{(q-p)^2}\frac{e^{-i(p+q)a/\hbar}}{1+\left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}}$$

insertion of these amplitudes into a wavepacket form gave the animation shown earlier.