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, $-L/2 < x < L/2$. L should be much lager than any characteristic length scale in the problem we're considering. We shall apply <u>periodic</u> 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 $p_n = \frac{2\pi\hbar}{L} \cdot n$.

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

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

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

$$= \frac{\hbar}{2\pi\hbar}\int_{-\infty}^{\infty} dk\, e^{ik(x'-x)} = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x'-x)}$$

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

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

The average position can be found using the representation of the position operator in momentum space:
$$\langle p'|\hat{x}|p\rangle = \delta(p'-p)\, i\hbar \frac{\partial}{\partial p}$$
$$\langle x(t)\rangle = i\hbar \int_{-\infty}^{\infty} dp \left[\varphi(p)e^{-i/\hbar E(p)t}\right]^* \frac{\partial}{\partial p}\left[\varphi(p)e^{-i/\hbar E(p)t}\right]$$
$$\& \quad \langle x^2(t)\rangle = -\hbar^2 \int_{-\infty}^{\infty} dp \left[\varphi(p)e^{-i/\hbar E(p)t}\right]^* \frac{\partial^2}{\partial p^2}\left[\varphi(p)e^{-i/\hbar E(p)t}\right].$$

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

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

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

so the uncertainty in momentum remains constant.

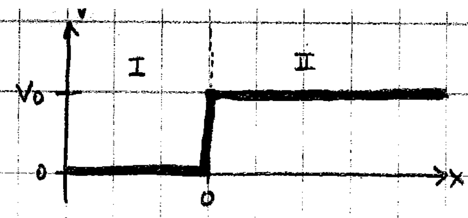
I leave it as an exercise to show that for this particular wavepacket
$$\langle x(t)\rangle = x_0 + \frac{p_0}{m}t \qquad \& \qquad \langle x^2(t)\rangle = \frac{\hbar^2}{2\sigma^2} + \frac{\sigma^2 t^2}{2m^2} + \left(x + \frac{p_0}{m}t\right)^2$$

so that
$$\langle(\Delta x)^2\rangle = \frac{\hbar^2}{2\sigma^2}\left(1 + \frac{t^2}{\left(\frac{\hbar^2 m^2}{\sigma^4}\right)}\right).$$

Hence the wavepacket becomes more diffuse, or "spreads" as time increases, having the absolute minimum 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 $x>0$.

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

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

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

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

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 solutions 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

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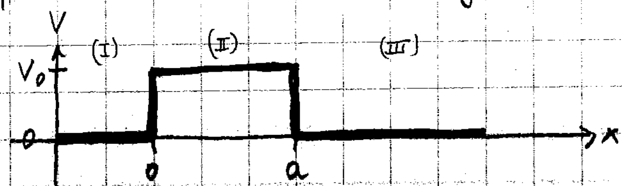
Notice that even in case 1 there was some probability to find the particle past the barrier ($x > 0$). This remains true even if the wavepacket has negligable amplitude to have $E(p) > V_0$. Suppose the barrier has only finite length, then the particle can 'tunnel' through a classically forbidden region

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 $x=a$:

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

these simultaneous equations can be solved yielding

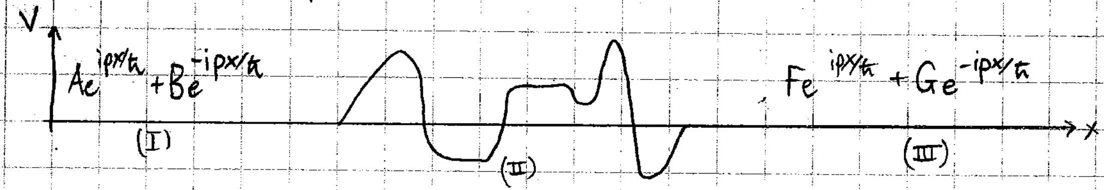
$$B = -A\frac{q+p}{q-p}\frac{1 - e^{-2iqa/\hbar}}{1 - \left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}} \qquad C = -A\frac{2p(p+q)}{(q-p)^2}\frac{e^{-2iqa/\hbar}}{1 - \left(\frac{q+p}{q-p}\right)^2 e^{-2iqa/\hbar}}$$

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

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

THE SCATTERING MATRIX

Consider an arbitrary potential localised to a certain region of the x-axis



in general the wavefunction will give relations : $F = S_{11}A + S_{12}G$ *
$B = S_{21}A + S_{22}G$

where S_{ij} are complex numbers. The 'outgoing' waves can be related to the 'incoming' by

$$\begin{bmatrix} F \\ B \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix}\begin{bmatrix} A \\ G \end{bmatrix} = \underline{\underline{S}}\begin{bmatrix} A \\ G \end{bmatrix}$$

Without actually solving a schrödinger eqn we can determine some property of this matrix. Using the conservation of probability flux: $j = \frac{-i\hbar}{2m}\left(\psi^* \frac{\partial}{\partial x}\psi - \psi\frac{\partial}{\partial x}\psi^*\right)$

$$j_I = \frac{-i\hbar}{2m}\Big(\left[A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar}\right]\frac{ip}{\hbar}\left[Ae^{ipx/\hbar} - Be^{-ipx/\hbar}\right]$$
$$- \left[Ae^{ipx/\hbar} + Be^{-ipx/\hbar}\right]\frac{ip}{\hbar}\left[-A^* e^{-ipx/\hbar} + B^* e^{ipx/\hbar}\right]\Big) = \frac{p}{m}\left(|A|^2 - |B|^2\right)$$

$$j_{III} = \frac{p}{m}\left(|F|^2 - |G|^2\right) \quad : \quad j_I = j_{III} \Rightarrow |A|^2 - |B|^2 = |F|^2 - |G|^2$$
$$\Rightarrow |F|^2 + |B|^2 = |A|^2 + |G|^2$$

$$[F^* B^*]\begin{bmatrix} F \\ B \end{bmatrix} = [A^* G^*]\, \underline{\underline{S}}^\dagger \underline{\underline{S}} \begin{bmatrix} A \\ G \end{bmatrix}$$

$|F|^2 + |B|^2 = |A|^2 + |G|^2$ if $\underline{\underline{S}}^\dagger \underline{\underline{S}} = \underline{\underline{1}}$ $\Rightarrow$ $\underline{\underline{S}}$ is a unitary matrix.

Additional constraints follow from time-reversal symmetry and where appropriate, parity symmetry. We'll consider these later when we look at scattering in a formal way.

For now, let's examine the S-matrix for an illustrative simple potential :

$$V(x) = \frac{\hbar^2}{2m}\cdot\frac{\lambda}{a}\,\delta(x-b)$$ [we found the bound state solution to this problem in the homework]

Consider the E>0 solutions. Away from x=b the Schrödinger eqn is $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$
which has solution $\psi(x) = e^{\pm ipx/\hbar}$ with $E = p^2/2m$.

In the immediate vicinity of x=b : $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{\hbar}{2m}\frac{\lambda}{a}\delta(x-b)\psi = E\psi$

integrating from $b-\varepsilon$ to $b+\varepsilon$: $\left.\frac{d\psi}{dx}\right|_{x=b+\varepsilon} - \left.\frac{d\psi}{dx}\right|_{x=b-\varepsilon} = -\frac{2mE}{\hbar^2}\int_{b-\varepsilon}^{b+\varepsilon} dx\,\psi(x) + \frac{\lambda}{\hbar a}\psi(b)$

$$\simeq -\frac{2mE}{\hbar^2}\cdot 2\varepsilon\,\psi(b) + \frac{\lambda}{\hbar a}\psi(b)$$

$$\xrightarrow{\varepsilon\to 0} \frac{\lambda}{\hbar a}\psi(b) \quad (A)$$

to the left of the potential $\psi_I(x) = Ae^{ipx/\hbar} + Be^{-ipx/\hbar}$

to the right of the potential $\psi_{II}(x) = Fe^{ipx/\hbar} + Ge^{-ipx/\hbar}$

continuity of the wavefunction @ $x=b$: $Ae^{ipb/\hbar} + Be^{-ipb/\hbar} = Fe^{ipb/\hbar} + Ge^{-ipb/\hbar}$

discontinuity of the derivative according to eqn $\textcircled{A}$ $\frac{ip}{\hbar}\left(Fe^{ipb/\hbar} - Ge^{-ipb/\hbar}\right) - \frac{ip}{\hbar}\left(Ae^{ipb/\hbar} - Be^{-ipb/\hbar}\right) = \frac{\lambda}{\hbar a}\left(Ae^{ipb/\hbar} + Be^{-ipb/\hbar}\right)$

$$ip\left(Fe^{ipb/\hbar} - Ge^{-ipb/\hbar}\right) = Ae^{ipb/\hbar}\left(ip + \frac{\lambda}{a}\right) + Be^{-ipb/\hbar}\left(ip + \frac{\lambda}{a}\right)$$

$$ip\left(Fe^{ipb/\hbar} + Ge^{-ipb/\hbar}\right) = Ae^{ipb/\hbar}(ip) + Be^{-ipb/\hbar}(ip)$$

$\oplus$ $2ipFe^{ipb/\hbar} = Ae^{ipb/\hbar}\left(2ip + \frac{\lambda}{a}\right) + Be^{-ipb/\hbar} \cdot \frac{\lambda}{a}$

$\ominus$ $-2ipGe^{-ipb/\hbar} = Ae^{ipb/\hbar}\left(\frac{\lambda}{a}\right) + Be^{-ipb/\hbar}\left(-2ip + \frac{\lambda}{a}\right)$

eliminating B : $\frac{2ip}{\lambda/a} Fe^{ipb/\hbar} = Ae^{ipb/\hbar} \frac{2ip + \lambda/a}{\lambda/a} + Be^{-ipb/\hbar}$

$$\frac{-2ip}{\frac{\lambda}{a} - 2ip} Ge^{-ipb/\hbar} = Ae^{ipb/\hbar} \frac{\lambda/a}{\lambda/a - 2ip} + Be^{-ipb/\hbar}$$

$\ominus$ $$\frac{2ip}{\lambda/a} Fe^{ipb/\hbar} + \frac{2ip}{\lambda/a - 2ip} Ge^{-ipb/\hbar} = Ae^{ipb/\hbar}\left(\frac{2ip + \lambda/a}{\lambda/a} + \frac{\lambda/a}{2ip - \lambda/a}\right)$$

$$F = A \cdot \frac{1}{2ip(2ip - \lambda/a)}(2ip)^2 - G \frac{\lambda/a}{\lambda/a - 2ip} e^{-2ipb/\hbar}$$

$$\underline{F = A \cdot \frac{2ip}{2ip - \lambda/a} + G \frac{\lambda/a}{2ip - \lambda/a} e^{-2ipb/\hbar}}$$

$$\underline{B = Ae^{2ipb/\hbar} \frac{\lambda/a}{2ip - \lambda/a} + G \frac{2ip}{2ip - \lambda/a}}$$

$$\Rightarrow \underline{\underline{S}} = \begin{bmatrix} \frac{2ipa}{2ipa - \lambda} & \frac{\lambda}{2ipa - \lambda} e^{-2ipb/\hbar} \\ \frac{\lambda}{2ipa - \lambda} e^{2ipb/\hbar} & \frac{2ipa}{2ipa - \lambda} \end{bmatrix} = \frac{1}{2ipa - \lambda} \begin{bmatrix} 2ipa & \lambda e^{-2ipb/\hbar} \\ \lambda e^{2ipb/\hbar} & 2ipa \end{bmatrix}$$

it is simple to show that $\underline{\underline{S}}^{+}\underline{\underline{S}} = \underline{\underline{1}}$.

Suppose we're interested in the transmission & reflection of probability incident from $x = \pm\infty$; the S-matrix contains the information we need.

e.g. incident wave from $x = -\infty$: $A \neq 0$, $G = 0$; $F \equiv TA$, $B \equiv RA$ $\Rightarrow \begin{bmatrix} T \\ R \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$T = S_{11}$, $R = S_{21}$

$\Rightarrow$ the fraction of flux transmitted $= |T|^2 = |S_{11}|^2$

$$= \frac{4p^2a^2}{4p^2a^2 + \lambda^2} = \left(1 + \left(\frac{\lambda}{2pa}\right)^2\right)^{-1}$$

& the fraction of flux reflected $= |R|^2 = |S_{21}|^2$

$$= \frac{\lambda^2}{4p^2a^2 + \lambda^2} = \left(\frac{\lambda}{2pa}\right)^2 \left(1 + \left(\frac{\lambda}{2pa}\right)^2\right)^{-1}$$

e.g. incident wave from $x = +\infty$: $A = 0$, $G \neq 0$; $F = RG$, $B = TG$ $\Rightarrow \begin{bmatrix} R \\ T \end{bmatrix} = \begin{bmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

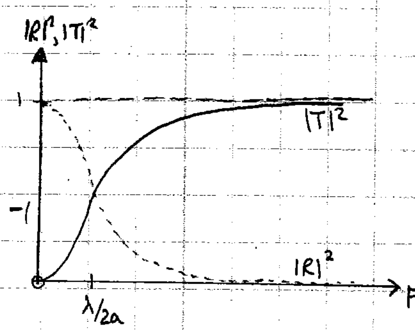
$R = S_{12}$, $T = S_{22}$

$\Rightarrow$ the fraction of flux transmitted $= |T|^2 = |S_{22}|^2$

$$= \left(1 + \left(\frac{\lambda}{2pa}\right)^2\right)^{-1}$$

& the fraction of flux reflected $= |R|^2 = |S_{12}|^2$

$$= \left(\frac{\lambda}{2pa}\right)^2 \left(1 + \left(\frac{\lambda}{2pa}\right)^2\right)^{-1}$$



The S-matrix contains more information than the name "scattering matrix" suggests. In fact it contains all possible information about the solution to the Schrödinger eqn in this case. As an example, we know that for $\lambda < 0$ this potential has a single bound state of energy $-\lambda^2/8ma^2$.

Bound states are embedded as <u>poles</u> of the S-matrix. Notice that we could express $\underline{S}$ as

$$\frac{1}{2ipa - \lambda} \begin{bmatrix} 2ipa & \lambda e^{-2ipb/\hbar} \\ \lambda e^{2ipb/\hbar} & 2ipa \end{bmatrix} = \frac{1}{p - \left(\frac{-i\lambda}{2a}\right)} \begin{bmatrix} p & \frac{-i\lambda}{2a} e^{-2ipb/\hbar} \\ \frac{-i\lambda}{2a} e^{2ipb/\hbar} & p \end{bmatrix}.$$

Clearly there is a pole in each element at $p = -i\lambda/2a$. The energy location of this pole is $E = p^2/2m = -\lambda^2/8ma^2$, ie the bound state energy.

Note that there is still a pole in the case that $\lambda > 0$ where there clearly cannot be a bound state (it is a purely repulsive potential). In this case we talk of a 'virtual bound state' - toward the end of this course we may discuss these in more detail.

7. PERIODIC POTENTIALS IN ONE-DIMENSION

In a metal, ions are arranged in a regular array, giving rise to a potential felt by electrons that is periodic. In this section we'll consider two simple models that exhibit properties which follow from periodicity.

Consider a potential in one-dimension that repeats itself with a period of a: $\quad V(x+a) = V(x)$

Since the kinetic energy term $\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}$ is unchanged by the translation $x \to x+a$, the Hamiltonian is invariant under displacements by a: $H(x+a) = H(x)$.

We can define a translation operator $T(a)$ such that $T(a)f(x) = f(x+a)$.
Invariance of the Hamiltonian is manifested by $[H, T(a)] = 0$.

The eigenvalue in $T(a)\varphi(x) = \lambda_a \varphi(x)$ can be solved for as follows:

$$f(x) = T(-a)\,T(a)\,f(x) = \lambda_a \lambda_{-a} f(x) \quad \Rightarrow \lambda_a \lambda_{-a} = 1 \quad \Rightarrow \underline{\lambda_a = e^{ka}}$$

Suppose $\varphi(x) = e^{+kx} g(x)$, then $T(a)\varphi(x) = \varphi(x+a) = e^{+ka}\, e^{kx} g(x+a)$

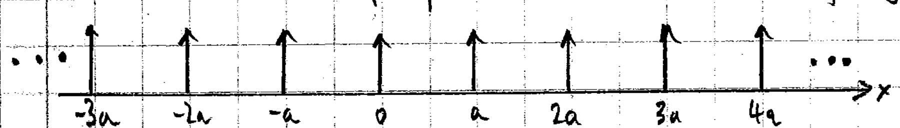
$\Rightarrow$ the eigenfunctions of $T(a)$ are functions $\varphi(x) = e^{kx}\cdot g(x)$ where $g(x)$ is any periodic function of period a: $g(x) = g(x+a)$.

We are interested in square integrable functions which must vanish as $x \to \pm\infty$, implying that k must be pure imaginary, $\quad \varphi(x) = e^{ikx} g(x)$

This is known as 'Bloch's theorem'. The allowed wavefunctions of a periodic system are plane waves modulated by a periodic function.

$$\varphi_p(x) = e^{ipx/\hbar} g_p(x) \quad \& \quad T(a)\varphi_p(x) = e^{ip(x+a)/\hbar} g_p(x+a) = e^{ipa/\hbar}\varphi_p(x) \qquad \left(\lambda_a = e^{ipa/\hbar}\right)$$

We'll consider a simple potential to avoid tricky algebra: $V(x) = \frac{\hbar}{2m}\frac{\lambda}{a}\sum_{n=-\infty}^{\infty}\delta(x-na)$ *



Away from the locations $x = na$, the Schrödinger equation has plane-wave solutions $e^{\pm ipx/\hbar}$ or $\cos\frac{px}{\hbar}$, $\sin\frac{px}{\hbar}$.

*this is a simple version of the "Kronig-Penney" model.

Consider the gap between the $(n-1)^{th}$ potential spike & the n^{th} : $(n-1)a < x < na$

$$\psi(x) = A_n \sin\left[\tfrac{p}{\hbar}(x-na)\right] + B_n \cos\left[\tfrac{p}{\hbar}(x-na)\right]$$

& in the gap between the n^{th} and $(n+1)^{th}$ potential spikes : $na < x < (n+1)a$

$$\psi(x) = A_{n+1} \sin\left[\tfrac{p}{\hbar}(x-(n+1)a)\right] + B_{n+1} \cos\left[\tfrac{p}{\hbar}(x-(n+1)a)\right].$$

At $x = na$, the wavefunctions should match & the derivatives should satisfy

$$\left.\frac{d\psi}{dx}\right|_{a_+} - \left.\frac{d\psi}{dx}\right|_{a_-} = \frac{\lambda}{\hbar a}\psi(a)$$

$$\Rightarrow \quad B_n = -A_{n+1}\sin pa/\hbar + B_{n+1}\cos pa/\hbar$$

$$\& \quad -\frac{p}{\hbar}A_{n+1}\cos pa/\hbar - \frac{p}{\hbar}B_{n+1}\sin\frac{pa}{\hbar} + \frac{p}{\hbar}A_n = \frac{\lambda}{\hbar a}B_n$$

$$\text{or} \quad A_{n+1} = A_n \cos pa/\hbar + \left(\frac{\lambda}{pa}\cos pa/\hbar - \sin pa/\hbar\right)B_n$$

$$\& \quad B_{n+1} = \left(\frac{\lambda}{pa}\sin\frac{pa}{\hbar} + \cos\frac{pa}{\hbar}\right)B_n + A_n \sin\frac{pa}{\hbar}$$

Bloch's theorem insists that $\psi(x+a) = e^{i\bar{p}a/\hbar}\psi(x)$ $\Rightarrow A_{n+1} = e^{i\bar{p}a/\hbar}A_n$ & $B_{n+1} = e^{i\bar{p}a/\hbar}B_n$

$$\text{so that} \quad A_n\left(e^{i\bar{p}a/\hbar} - \cos pa/\hbar\right) = \left(\frac{\lambda}{pa}\cos pa/\hbar - \sin pa/\hbar\right)B_n$$

$$\& \quad B_n\left(e^{i\bar{p}a/\hbar} - \frac{\lambda}{pa}\sin\frac{pa}{\hbar} - \cos\frac{pa}{\hbar}\right) = A_n \sin pa/\hbar$$

$$\Rightarrow \left(e^{i\bar{p}a/\hbar} - \frac{\lambda}{pa}\sin\frac{pa}{\hbar} - \cos\frac{pa}{\hbar}\right)\left(e^{i\bar{p}a/\hbar} - \cos\frac{pa}{\hbar}\right) = \sin\frac{pa}{\hbar}\left(\frac{\lambda}{pa}\cos\frac{pa}{\hbar} - \sin\frac{pa}{\hbar}\right)$$

$$\bar{\varepsilon}^2 - \bar{\varepsilon}(2c + \gamma s) + c(\gamma s + c) = \gamma cs - s^2$$

$$\bar{\varepsilon}^2 - \bar{\varepsilon}(2c + \gamma s) + 1 = 0$$

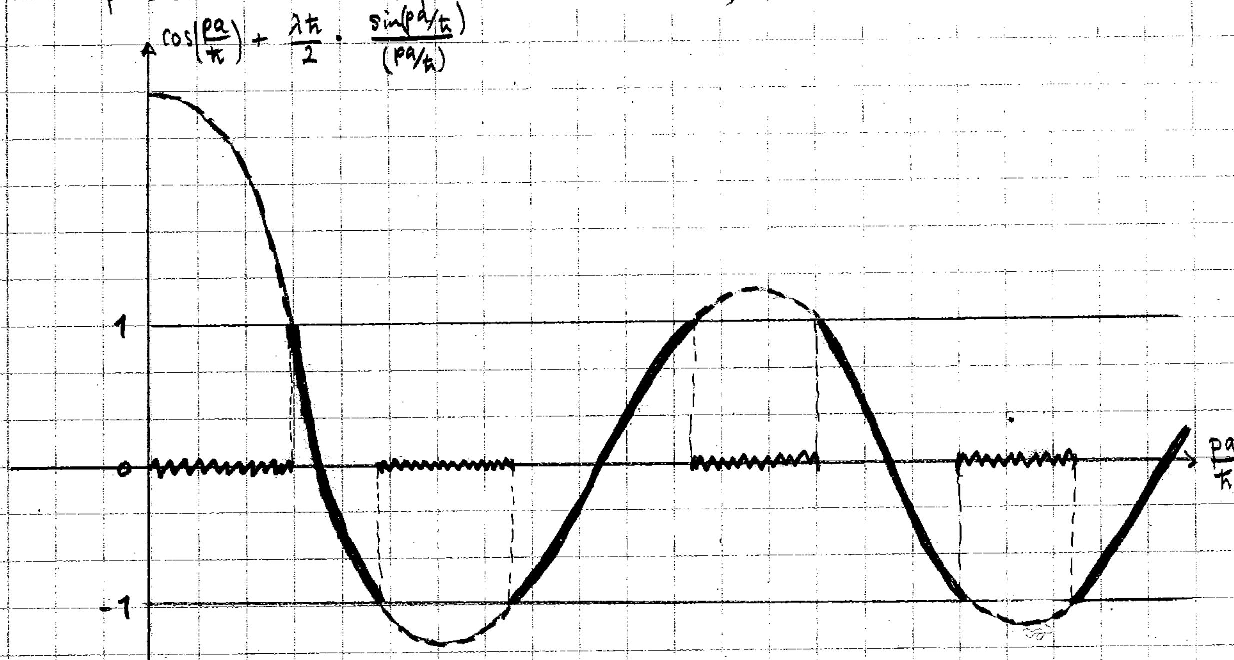
$$\times e^{-i\bar{p}a/\hbar} \quad e^{i\bar{p}a/\hbar} - 2\cos\frac{pa}{\hbar} - \frac{\lambda}{pa}\sin\frac{pa}{\hbar} + e^{-i\bar{p}a/\hbar} = 0$$

$$\text{real part} \quad 2\cos\bar{p}a/\hbar - 2\cos pa/\hbar - \frac{\lambda}{pa}\sin\frac{pa}{\hbar} = 0$$

$$\boxed{\cos\frac{\bar{p}a}{\hbar} = \cos\frac{pa}{\hbar} + \frac{\lambda}{2pa}\sin\frac{pa}{\hbar}}$$

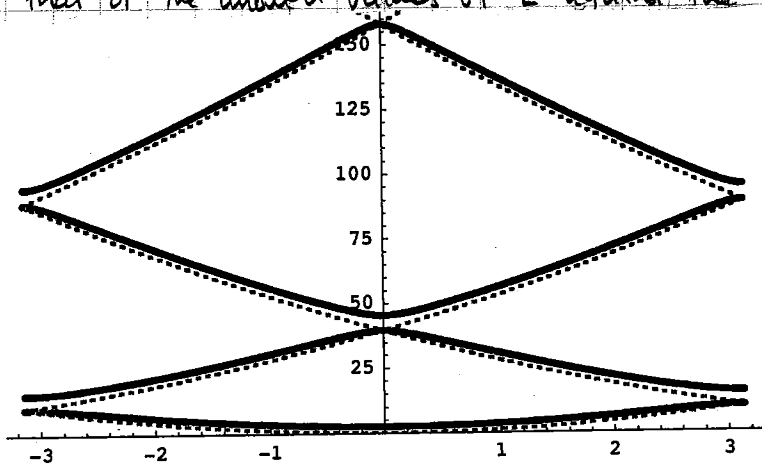
In the limit of no potential $(\lambda \to 0)$ $\bar{p} = p$ is the momentum of a free particle.

Allowed energies, $E = \bar{p}^2/2m$ are the solutions of this equation for all values of $\bar{p}$. Notice though that the LHS is bounded to be between -1 & 1 which limits the possible values of p.



The zig-zag lines represent the forbidden energy bands between the allowed energy bands.

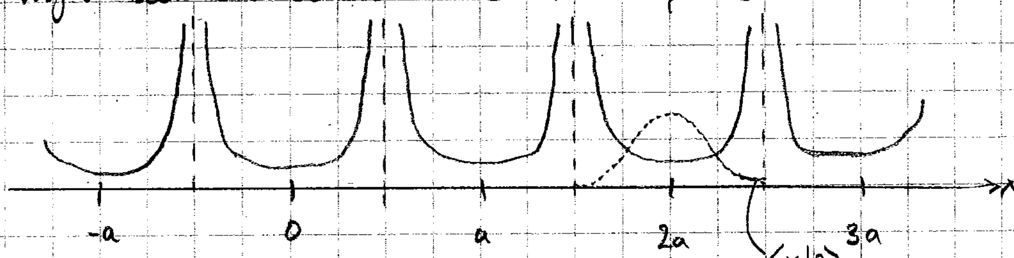
An illustrative plot is that of the allowed values of E against the 'no-potential' momentum



ANIMATION

We see that when $\bar{p}a = n\pi\hbar$, we have the maximal deviation from the no-potential result. This condition on the momentum is that of Bragg reflection, in which the scattering from each potential is in phase and as such standing waves are formed - here they are of the form $\sin n\pi\frac{x}{a}$ and $\cos n\pi\frac{x}{a}$.
From the graph we note that the no-potential degeneracy is broken, with one solution going up in energy, while the other is unperturbed.
The physical origin is simple: the $\sin n\pi\frac{x}{a}$ solution has value 0 at the potential positions & hence does not feel their effect, on the other hand the $\cos n\pi\frac{x}{a}$ solution has the maximal values ± 1 & hence is maximally perturbed by the repulsive ($\lambda > 0$) potentials.

The Kronig-Penney model just presented is solved in such a way that the potential is essentially a perturbation on free-particle solutions. Let's consider the opposite extreme in which each potential has localised states that do not overlap. Suppose for example we had a potential with very high barriers between the $x = na$ points:



$H|n\rangle = E_0|n\rangle$

Then we can form an eigenstate $|n\rangle$ of H that is entirely localised on the n^{th} site (e.g. $|2\rangle$ in the diagram above). While this is an eigenstate of H, it is not an eigenstate of $T(a)$ since $T(a)|n\rangle = |n+1\rangle$ (up to a phase)

A set of simultaneous eigenstates of H & $T(a)$ can be constructed as

$$|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle \quad \text{where} \quad -\pi \le \theta \le \pi$$

$$H|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta} H|n\rangle = E_0|\theta\rangle \qquad \text{(translational invariance)}$$

$$T(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}T(a)|n\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle = e^{-i\theta}|\theta\rangle$$

Now suppose the barrier between the sites is not infinitely high, then there can be some overlap between wavefunctions & an initially localised solution $|n\rangle$ can tunnel into another site. In the "tight-binding" approximation, only tunneling into neighbouring sites is allowed. We parameterise this in the Hamiltonian by

$$\langle n\pm1|H|n\rangle = -\Delta \qquad (\langle n|H|n\rangle = E_0)$$

$$\Rightarrow H|n\rangle = E_0|n\rangle - \Delta|n-1\rangle - \Delta|n+1\rangle$$

but $H|\theta\rangle = H\sum_{n=-\infty}^{\infty} e^{in\theta}|n\rangle = (E_0 - 2\Delta\cos\theta)|\theta\rangle$ so $|\theta\rangle$ is still an eigenstate.

For $\langle x|\theta\rangle$ to satisfy the Bloch condition it must be of the form $e^{i\bar{p}x/\hbar}g(x)$:

$$\langle x|T(a)|\theta\rangle = e^{-i\theta}\langle x|\theta\rangle \text{ by the eigenvalue condition}$$
$$= \langle x-a|\theta\rangle$$

$$\Rightarrow e^{-i\theta}e^{i\bar{p}x/\hbar}g(x) = e^{i\bar{p}(x-a)/\hbar}g(x-a) = e^{i\bar{p}(x-a)/\hbar}g(x)$$

$$\Rightarrow \underline{\theta = \bar{p}a/\hbar}$$

& as θ varies from $-\pi$ to π, $\bar{p}$ varies from $-\frac{\hbar\pi}{a}$ to $\frac{\hbar\pi}{a}$.

Thus we have a continuous set of allowed energies given by

$$E(\bar{p}) = E_0 - 2\Delta \cos \bar{p}a/\hbar$$

, Energies outside the range $E_0 - 2\Delta \to E_0 + 2\Delta$ are not allowed.

In the Kronig-Penney model, we had multiple allowed values of E for each $\bar{p}$, in this case we require there to be more than one possible localised state in the duplicated potential. This is the case for most potentials of sufficient depth.