

Notes for Quantum Mechanics

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Lecture 21- 1 dimensional barrier problems

OK so now we have looked at a couple different potentials- the square potential and the SHO potential - both in 1 dimension. We will continue to stay in one dimension. In each of these cases, the potentials were infinite at the sides, so the particles were always bound. We know that is not true in real life. Bonds break; Springs break; we might guess that these things lead to decays, and other funny things like tunneling. We will start looking at such cases - and take as a first model, just square shaped potentials - to make things easy.

We will start with the time independent schrodinger eqn - that is we will look at solutions which have a particular defined energy (eigenfunctions of energy). Such solutions also have a defined momentum (up to a sign) and hence are not localized. Here we can think of a couple of examples. The first is a beam of particles. Classically you think of a beam of particles like a stream of bullets from a machine-gun. Well localized things that come one after another. Quantum mechanically though, we think of a wave coming in. That is why we can consider a beam as an unlocalized thing, i.e. Δx is large. A second example is a particle in a finite potential well. You may think its localized, but its not. It can leak out since some of the wavefunction (in the position representation) $\langle x|\alpha\rangle$ has to lie outside the well - since the particle is NOT localized. Hence the phenomenon of decay. We will look at beams hitting finite barriers and potential wells first, then move on to particles stuck in a finite potential.

Beams and currents

Clearly a wavefunction for a beam will need a different normalization procedure. Before we required that $\int_{-\infty}^{\infty} |\psi(x)|^2 dx$ be finite. For beam which extends to ∞ this would be infinite, so what we do is to define $\int_a^b |\psi(x)|^2 dx$ be finite. This should count up the number of particles in the interval (b-a). So $\int_a^b |\psi(x)|^2 dx = N$, i.e. the number of particles between a and b . This means $|\psi(x)|^2 dx = \rho(x)dx = dN$ where $|\psi(x)|^2 = \rho(x)$ has units of particles/unit length, giving $\psi(x)$ units of $\text{length}^{-1/2}$. In 3-D $\rho(x)$ has units of length^{-3} , so $\psi(x)$ has units of $\text{length}^{-3/2}$. As a 1-D example a beam of 10^4 neutrons/cm with momentum $\hbar k$ would have a wave function $\psi(x) = 10^{4/2} e^{i(kx - \omega t)}$ $\text{cm}^{-1/2}$. Note that "particles" does not have a unit.

A beam of particles is a current, so we need to think about the current density \vec{J} which is a vector quantity. Lets think about this in 3-D first and think about electric charge and electric current. We have the continuity eqn $\frac{d\rho}{dt} + \nabla \cdot \vec{J} = 0$. This just says that if you look at some unit volume, the change in the charge inside that unit volume is just the divergence of the current - i.e. the amount of water in the sink is equal to the current of the water coming in the faucet - the water going out the drain. Now in 1-D we can just write this as $\frac{d\rho}{dt} + \frac{dJ_x}{dx} = 0$. Now $\rho(x) = |\psi(x)|^2$, so what is J? We want to figure out what $\frac{d\rho}{dt}$ is. Hopefully it will be a derivative of x and then we can find J. The only eqn we have around to help us is the Schroedinger eqn. We will use the time dependent one we found in lecture $i\hbar \frac{d}{dt} |\alpha, t\rangle = \hat{H} |\alpha, t\rangle$. We will need to put this into the x representation. $i\hbar \frac{d}{dt} \langle x|\alpha, t\rangle = \langle x|\hat{H}|\alpha, t\rangle$

$$\langle x|\hat{H}|\alpha, t\rangle = \langle x|\frac{\hat{p}^2}{2m} + V(x)|\alpha, t\rangle = \frac{1}{2m} \langle x|\hat{p}^2|\alpha, t\rangle + V(x) \langle x|\alpha, t\rangle$$

$$\langle x|\hat{p}^2|\alpha, t\rangle = \langle x|\hat{p}\hat{p}|\alpha, t\rangle = \int dx' \langle x|\hat{p}|x'\rangle \langle x'|\hat{p}|\alpha, t\rangle = -\hbar^2 \int dx' \frac{d}{dx} \delta(x-x') \frac{d}{dx'} \langle x'|\alpha, t\rangle = -\hbar^2 \frac{d}{dx} \frac{d}{dx} \langle x|\alpha, t\rangle = -\hbar^2 \frac{d^2}{dx^2} \langle x|\alpha, t\rangle$$

$$\langle x|\alpha, t\rangle \text{ So } i\hbar \frac{d}{dt} \langle x|\alpha, t\rangle = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \langle x|\alpha, t\rangle + V(x) \langle x|\alpha, t\rangle \quad \text{and setting } \psi(x,t) = \langle x|\alpha, t\rangle$$

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

and writing \hat{H} as $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ (i.e. \hat{H} in the position representation) we can write $\hat{H}\psi(x,t) = i\hbar \frac{d}{dt}\psi(x,t)$ so

$$\frac{d}{dt}\psi(x,t) = -\frac{i}{\hbar}\hat{H}\psi(x,t) \quad \text{and its complex conjugate} \quad \frac{d}{dt}\psi^*(x,t) = \frac{i}{\hbar}\hat{H}\psi^*(x,t)$$

Now $\frac{d}{dt}\psi^*\psi = \psi^*\frac{d}{dt}\psi + \psi\frac{d}{dt}\psi^* = -\psi^*\frac{i}{\hbar}\hat{H}\psi(x,t) + \psi\frac{i}{\hbar}\hat{H}\psi^*(x,t)$ now since $V(x)=0$

$$\frac{d}{dt}\psi^*\psi = \frac{i\hbar}{2m} \left(\psi^* \frac{d^2}{dx^2}\psi - \psi \frac{d^2}{dx^2}\psi^* \right) = -\frac{d}{dx} \left[\frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \right] \quad \text{so}$$

$$\frac{d}{dt}\psi^*\psi + \frac{d}{dx} \left[\frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \right] = 0 \quad \text{and comparing this to} \quad \frac{d\rho}{dt} + \frac{dJ_x}{dx} = 0 \quad \text{we see that}$$

$$\text{in 1-D } J_x = \frac{\hbar}{2mi} \left(\psi^* \frac{d\psi}{dx} - \psi \frac{d\psi^*}{dx} \right) \quad \text{in 3-D } \vec{J} = \frac{\hbar}{2mi} (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*)$$

The units are time^{-1} for 1-D and $\text{length}^{-2} \text{time}^{-1}$ for 3-D

Note on the units of J for 1-D and 3-D.

3-D $\frac{d\rho}{dt} + \vec{\nabla} \cdot \vec{J} = 0 \quad \int_{\text{volume}} |\psi(\vec{r})|^2 d^3r = \int_{\text{volume}} \rho(\vec{r}) d^3r = N \rightarrow$ units of $\rho(\vec{r})$ are $1/L^3 \rightarrow$ units of $\frac{d\rho}{dt}$ are $1/(L^3T) \rightarrow$
units of $\vec{\nabla} \cdot \vec{J}$ are $1/(L^3T) \rightarrow$ units of \vec{J} are $1/(L^2T)$ i.e. like charge/cm²/sec

1-D $\frac{d\rho}{dt} + \frac{dJ_x}{dx} = 0 \quad \int_a^b |\psi(x)|^2 dx = \int \rho(x) dx = N \rightarrow$ units of $\rho(x)$ are $1/L \rightarrow$ units of $\frac{d\rho}{dt}$ are $1/(LT) \rightarrow$ units of $\frac{d}{dx} J$ are $1/(LT) \rightarrow$ units of J are $1/T$ i.e. like charge/sec

We want to think about a beam hitting some sort of barrier. Some of it gets reflected and some get transmitted. Lets assume that before and after the barrier its just represented by a plane wave, over some potential that changes only at the barrier, e.g. a step function. There is an incoming wave function, a reflected wave function, and a transmitted wave function.

$V=0$ before the barrier and V after the function

$$\psi_{\text{inc}} = A e^{i(k_1 x - \omega_1 t)} \quad E_{\text{inc}} = \hbar\omega_1 = \frac{\hbar^2 k_1^2}{2m}$$

$$\psi_{\text{refl}} = B e^{i(k_1 x + \omega_1 t)} \quad E_{\text{refl}} = E_{\text{inc}}$$

$$\psi_{\text{trans}} = C e^{i(k_2 x - \omega_1 t)} \quad E_{\text{trans}} = \hbar\omega_2 = \frac{\hbar^2 k_2^2}{2m} + V$$

If you dont quite get all this, dont worry, it will become clear in a moment. We then get for the currents

$$J_{\text{inc}} = \frac{\hbar}{2mi} 2ik_1 |A|^2 \quad J_{\text{refl}} = \frac{\hbar}{2mi} 2ik_1 |B|^2 \quad J_{\text{trans}} = \frac{\hbar}{2mi} 2ik_2 |C|^2$$

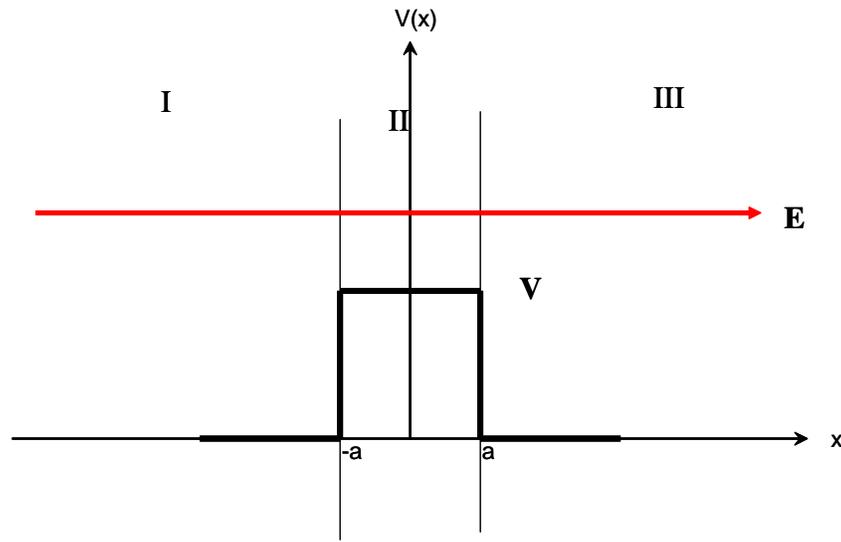
We would like to figure out how much stuff is reflected, and how much is transmitted so we define transmission and reflection coefficients as

$$T = \left| \frac{J_{\text{trans}}}{J_{\text{inc}}} \right| = \left| \frac{C}{A} \right|^2 \frac{k_2}{k_1} \quad \text{and} \quad R = \left| \frac{J_{\text{refl}}}{J_{\text{inc}}} \right| = \left| \frac{B}{A} \right|^2$$

Setting up the problem

We will assume the potential to be square like. That way we can divide the problem up into pieces where the potential is constant (and the Sch eqn is easy to solve) and then just match stuff up at the boundaries. Here is a typical barrier. You can see the height of the barrier which is V , the sides of the barrier are at $\pm a$, the energy of the beam E , and the three

regions where the potential V is just a constant.



$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \varphi(x) = E\varphi(x) \rightarrow -\frac{\partial^2}{\partial x^2} \varphi(x) = \frac{2m}{\hbar^2} (E - V(x)) \varphi(x)$$

Now $V(x)=0$ in regions I and III, and $V(x)=V$ in region II. If we set $k^2 = \frac{2m}{\hbar^2} (E - V(x))$ then the diff eqn is easy to solve in each of the three regions, since k is a constant and in this case positive (in each of the three regions). The solutions are either sines and cosines, or $e^{\pm ikx}$. Either works, but the exponentials are easier since they are eigenfunctions of momentum, and hence you can see which way they are going. The general solution in each of the three regions is a combination of e^{+ikx} and e^{-ikx} . Lets denote $k_1^2 = \frac{2m}{\hbar^2} E$ i.e. the relevant k for regions I and III and $k_2^2 = \frac{2m}{\hbar^2} (E - V)$ for region II. Now we can write down general solutions in all three regions

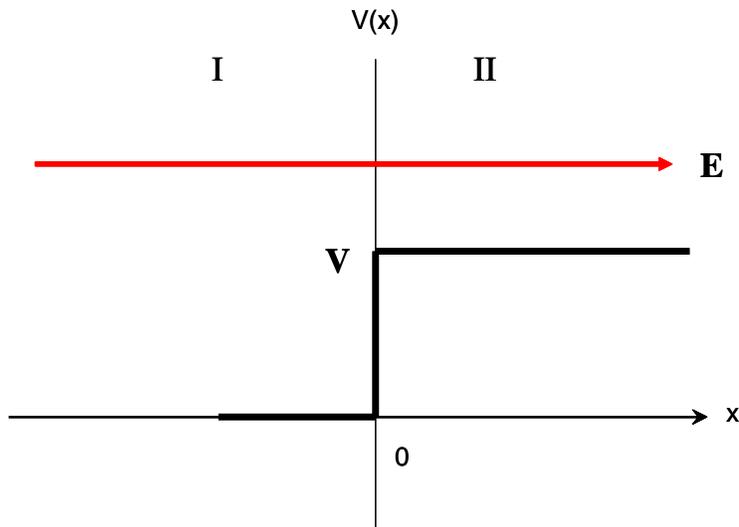
$$\varphi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad \varphi_{II}(x) = Ce^{ik_2 x} + De^{-ik_2 x} \quad \varphi_{III}(x) = Fe^{ik_1 x} + Ge^{-ik_1 x}$$

Solutions like e^{+ikx} have a positive eigenvalue for the momentum so they have positive momentum and are going forward (+x direction). Solutions like e^{-ikx} are going in the -x direction. Now lets clarify our problem. We have a beam coming in from the left. It does something at the boundary at $x=-a$, and something else at the boundary at $+a$. What we expect is that some of the beam is transmitted and some is reflected. You might have a question as to why beam is reflected at $x=+a$, when it is not expected classically - we shall see. In region III however, there is no reflected wave - there is nothing out past $x=a$ to reflect off of. Hence we will set the wave going in the -x direction in region III to zero, i.e. $G=0$. Now we already know what the k 's are. We need to see if we can find out what the coefficients are. We get the transmission coefficient $T = \left| \frac{F}{A} \right|^2 \frac{k_{\text{region III}}}{k_{\text{region I}}}$ and for the reflection coefficient $R = \left| \frac{B}{A} \right|^2$.

There is a normalization condition which sets $A=1$ (i.e. that is the incoming beam). We need to find B and A . The way we do this is to match the wave functions and their first derivatives at the boundaries. Why must these things be matched? If the wave functions did not match then the first derivative would be infinite. Since the momentum is calculated in the x representation as the first derivative - this would give an infinite momentum - an unphysical result. If the first derivatives did not match then the second derivative would be infinite. Looking at the Schrodinger eqn we see that such an infinity in the second derivative would mean the Sch. eqn could not be satisfied at the discontinuity. OK so we will require $\varphi_I(-a) = \varphi_{II}(-a)$, $\varphi_{II}(a) = \varphi_{III}(a)$ and $\frac{d\varphi_I(-a)}{dx} = \frac{d\varphi_{II}(-a)}{dx}$, $\frac{d\varphi_{II}(a)}{dx} = \frac{d\varphi_{III}(a)}{dx}$. Now these will give us 4 eqns which we will have to solve. This is a pain, but I will do it in a second. Lets first take an easier problem to solve algebraically, that is just

a single step.

A single step



Now there are only two regions. $k_1^2 = \frac{2m}{\hbar^2} E$ in region I and $k_2^2 = \frac{2m}{\hbar^2} (E - V)$ for region II.

$\varphi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x}$ $\varphi_{II}(x) = Ce^{ik_2 x}$ and we have set $D=0$ since there is nothing to reflect off of for $x > 0$
 Now $\varphi_I(0) = \varphi_{II}(0)$ and $\frac{d\varphi_I(0)}{dx} = \frac{d\varphi_{II}(0)}{dx}$ are the matching conditions. We will set $A=1$, so we have two eqn's and the two unknowns B and C . So

$$e^{ik_1 x} + Be^{-ik_1 x} = Ce^{ik_2 x} \quad \text{and} \quad k_1 e^{ik_1 x} - Bk_1 e^{-ik_1 x} = Ck_2 e^{ik_2 x} \quad \text{These must be true at } x=0 \text{ so}$$

$$1+B=C \quad \text{and} \quad k_1 - Bk_1 = Ck_2 \rightarrow$$

$$k_1 - Bk_1 = (1+B)k_2 \rightarrow B = \frac{1-k_2/k_1}{1+k_2/k_1} \quad \text{and} \quad C = \frac{2}{1+k_2/k_1} \quad \text{giving us}$$

$$T = |C|^2 \left(\frac{k_2}{k_1}\right)^2 = \frac{4k_2/k_1}{(1+k_2/k_1)^2} \quad \text{and} \quad R = |B|^2 = \left| \frac{1-k_2/k_1}{1+k_2/k_1} \right|^2 \quad \text{where} \quad \frac{k_2}{k_1} = \sqrt{1 - \frac{V}{E}}$$

Lets take some cases. When $V=1/2 E$ then the reflection coefficient is about 3%, so the funny QM effect is small but real.
 Lets vary V .

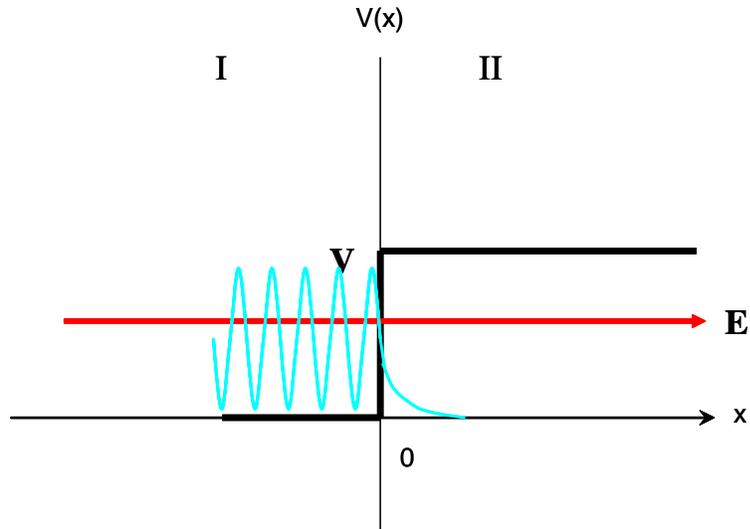
- 1) $V=E$ $\frac{k_2}{k_1}=0$ $T=0$, $R=1$ full reflection
- 2) $0 < V < E$ $0 < \frac{k_2}{k_1} < 1$ T and R non-zero
- 3) $V \sim 0$ $\frac{k_2}{k_1} = 1$ $T=1$ $R=0$ no reflection
- 4) $V < 0$ $\frac{k_2}{k_1} > 1$ T and R non-zero, i.e. there is reflection again!

When V is small compared to E then the reflection coefficient is ~ 0 as we might expect. When $V=E$ then then $T=0$ and the whole beam is reflected. Suppose V is negative, i.e. we are shooting a beam off of a cliff.

Now what happens if $V > E$??? Then $\frac{k_2}{k_1}$ is imaginary. Now we use the incoming beam as the defining beam, which is moving forward so k_1 has to be real. This means that k_2 is imaginary. Since $k_2 = \sqrt{1 - \frac{V}{E}} k_1$ lets write $k_2 = i\kappa_2$ so

$\kappa_2 = \sqrt{\frac{V}{E} - 1} k_1$ which in this case is real. Then we have $\varphi_{II}(x) = C e^{i k_2 x} = C e^{-\kappa_2 x}$

We see that we no longer have a traveling wave, but rather an exponentially dying wave function BUT it actually penetrates into the barrier. As you might guess this sets things up for tunneling.



Back to the tunneling problem

Ok, let's write down the 4 eqn we have from matching the wave functions and the derivatives across the boundaries

$$A e^{-i k_1 a} + B e^{+i k_1 a} = C e^{-i k_2 a} + D e^{+i k_2 a}$$

$$C e^{i k_2 a} + D e^{-i k_2 a} = F e^{i k_1 a}$$

$$-A k_1 e^{-i k_1 a} + B k_1 e^{+i k_1 a} = -C k_2 e^{-i k_2 a} + D k_2 e^{+i k_2 a}$$

$$C k_2 e^{i k_2 a} - D k_2 e^{-i k_2 a} = F k_1 e^{i k_1 a} \quad \text{where we have already set } G=0$$

$$\frac{1}{T} = \left| \frac{A}{F} \right|^2 = 1 + \frac{1}{4} \left(\frac{k_1^2 - k_2^2}{k_1 k_2} \right)^2 \sin^2(2 k_2 a) \quad \text{and plugging in } k_1^2 = \frac{2m}{\hbar^2} E \text{ and } k_2^2 = \frac{2m}{\hbar^2} (E - V) \text{ we get}$$

$$\frac{1}{T} = 1 + \frac{V^2}{4E(E-V)} \sin^2(2 k_2 a) \quad \text{and } R=1-T$$

Now let's take a look at some cases. In the case we are thinking about where $E > V$, then k_2 is real, and everything makes sense. Suppose, however, that $E < V$. Can it get over the barrier? This is a similar situation to the one we had in the single step. Let's have a look. Again let's set $k_2 = i \kappa_2$, where κ_2 is real. (note- my convention is different than the book) Then

$$\frac{1}{T} = 1 - \frac{V^2}{4E(V-E)} \sin^2(2 i \kappa_2 a).$$

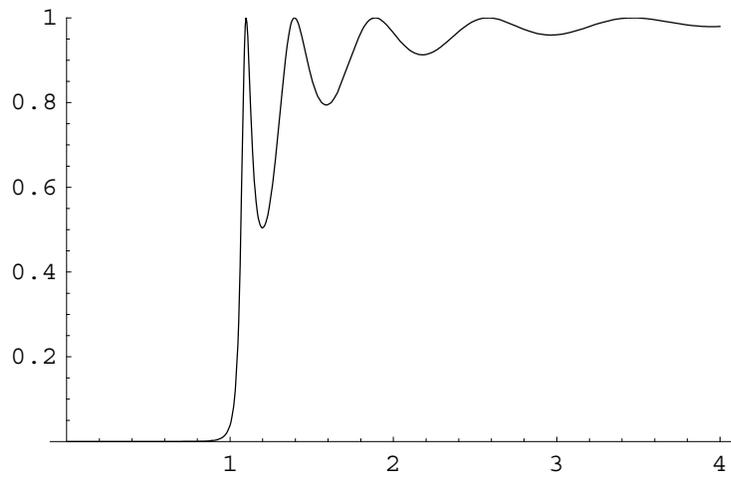
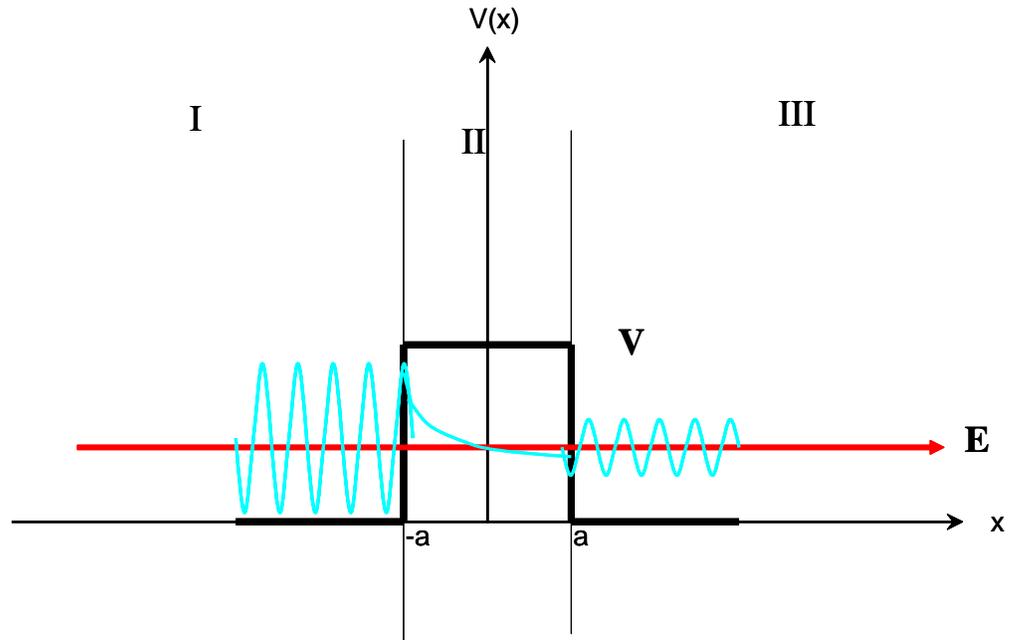
$$\text{What is } \sin(i \kappa) ? \quad \sin \theta = \frac{1}{2i} (e^{i \theta} - e^{-i \theta}) \text{ so } \sin(i \kappa) = \frac{1}{2i} (e^{-\kappa} - e^{\kappa}) = -\frac{1}{2i} (e^{\kappa} - e^{-\kappa}) = -\frac{1}{i} \sinh(\kappa)$$

$$\sin^2(i \kappa) = -\sinh^2(\kappa) \text{ so}$$

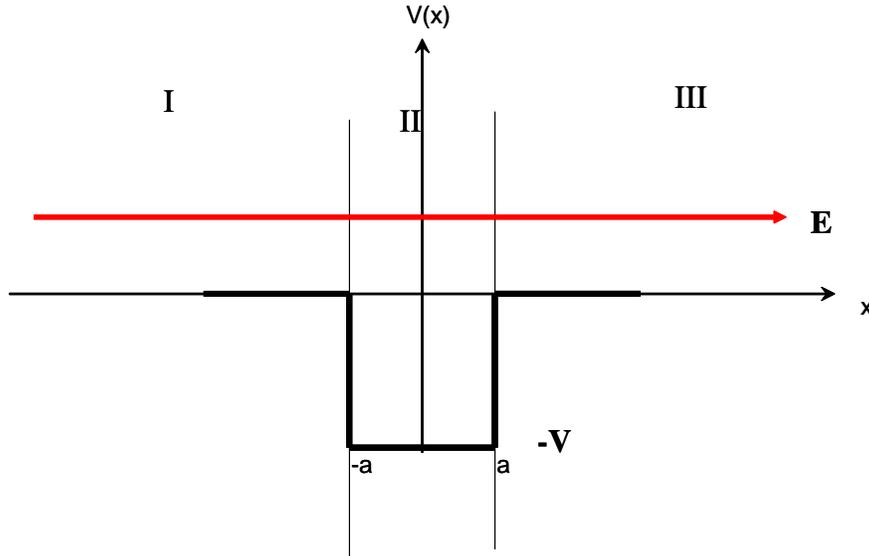
$$\frac{1}{T} = 1 + \frac{V^2}{4E(V-E)} \sinh^2(2 \kappa_2 a) \quad \kappa_2 = \sqrt{\frac{2m}{\hbar^2} (V - E)} \quad \kappa_2 \text{ is real for } E < V$$

Now let's rewrite the three solutions

$$\varphi_I(x) = Ae^{ik_1 x} + Be^{-ik_1 x} \quad \varphi_{II}(x) = Ce^{-\kappa_2 x} + De^{\kappa_2 x} \quad \varphi_{III}(x) = Fe^{ik_1 x}$$



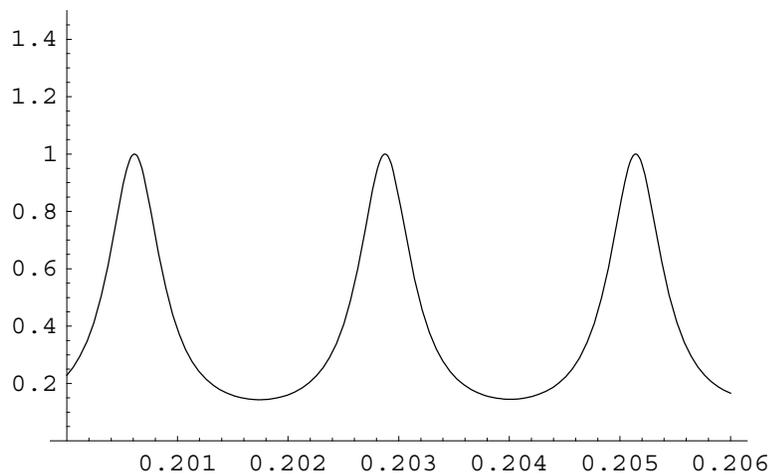
Now let take a look at the following case where the potential energy in region II is negative.



Rewriting things in terms of $|V|$ to make things easier to think about we get $k_2^2 = \frac{2m}{\hbar^2} (E + |V|)$ we get $\frac{1}{T} = 1 + \frac{V^2}{4E(E+|V|)} \sin^2(2k_2 a)$ and $R=1-T$. Now for both this case and the original case of a positive V when $E > V$ we get perfect transmission for $2k_2 a = n\pi$. In this case $2a\sqrt{\frac{2m}{\hbar^2} (E + |V|)} = n\pi$ and solving for E we get

$$E(\text{perfect transmission}) = \frac{1}{2m} \left(\frac{n\pi\hbar}{2a} \right)^2 - |V|$$

An attractive square wave potential is a reasonable model for the scattering of a beam of electrons by atoms. If you shoot a beam of electrons at a rare gas, at certain energies, the electrons penetrate perfectly - this is the Ramsauer-Townsend effect. Again - a weirdness of QM. Here is a picture of the transmission coefficient vs the energy of the beam in eV. Where $V = -5$ eV and $a = 1000$ angstroms, i.e. a thin layer of gas



For more pictures with labels see qm21cont.pdf

More difficult potentials – e.g. the SHO

There is a standard approximation method called the WKB Approximation (for Wentzel, Kramers, Brillouin) to figure stuff out for more complex potentials. I will not actually derive it here but I will just give you the result.

WKB:

$T = \exp(-2 \int_{x_1}^{x_2} \kappa dx)$ where $\kappa = \sqrt{\frac{2m}{\hbar^2} (V(x) - E)}$ and x_1 and x_2 are the classical turning points, that is the points where $E = V(x)$ (so $V(x_1) = E$ and $V(x_2) = E$)

$$T = \exp\left(-2 \int_{x_1}^{x_2} dx \sqrt{\frac{2m}{\hbar^2} (V(x) - E)}\right)$$

Also the energies allowed in the well will obey the condition

$$\frac{1}{2\pi} \int_{x_1}^{x_2} \sqrt{2m(E - V(x))} dx = \left(n + \frac{1}{2}\right) \frac{\hbar}{2}$$

Let's see these formula at work. First for a couple of non-tunneling problems

How about the infinite potential well with walls at 0 and a ? Here within the well $V=0$

$$\frac{1}{2\pi} \int_0^a \sqrt{2mE} dx = \frac{\sqrt{2mE}}{2\pi} a = \left(n + \frac{1}{2}\right) \frac{\hbar}{2} \quad \text{and we get } 2mE = \frac{4\pi^2}{a^2} \frac{\hbar^2}{4} \left(n + \frac{1}{2}\right)^2 \quad E^{\text{WKB}} = \frac{\hbar^2 \pi^2}{2ma^2} \left(n + \frac{1}{2}\right)^2$$

The right answer is of course $E^{\text{real}} = \frac{\hbar^2 \pi^2}{2ma^2} (n)^2$ which is not bad for n reasonably large. This tells us something - the WKB is a semi-classical approximation and is good for large quantum numbers. Note that in this case the $n=1$ state is off by more than 100% but for $n=10$, it's good to about 10%.

Now the SHO where the edges/walls go to infinity.

$V(x) = \frac{1}{2} m\omega^2 x^2$ and after some work we get $E_n = \left(n + \frac{1}{2}\right) \hbar\omega$ which is exactly the right answer.

Now let's try the only tunneling problem we have done, the square potential barrier. Remember

$$\frac{1}{T} = 1 + \frac{V^2}{4E(V-E)} \sinh^2(2\kappa_2 a). \quad \text{Let's let } E \ll V \text{ so } \kappa_2 = \sqrt{\frac{2m}{\hbar^2} (V - E)} \quad \text{where}$$

we will assume that $2\kappa_2 a$ is large and since $\sinh(z) = \frac{1}{2} (e^z - e^{-z})$ we will assume that the e^{-z} term is negligible

$$T^{\text{real}} \sim 4 \frac{EV}{V^2} \left[\frac{1}{2} \exp\left(2a \sqrt{\frac{2m}{\hbar^2} (V - E)}\right) \right]^{-2} \sim 16 \frac{E}{V} \exp\left(-4a \sqrt{\frac{2m}{\hbar^2} (V - E)}\right) \quad \text{and}$$

$$T^{\text{WKB}} = \exp\left(-2 \int_{x_1}^{x_2} dx \sqrt{\frac{2m}{\hbar^2} (V(x) - E)}\right) = \exp\left(-2 \int_{-a}^a dx \sqrt{\frac{2m}{\hbar^2} (V - E)}\right) = \exp\left(-2 \sqrt{\frac{2m}{\hbar^2} (V - E)} (a + a)\right) = \exp\left(-4a \sqrt{\frac{2m}{\hbar^2} (V - E)}\right) \quad \text{which is off by } 16E/V \text{ (i.e. if } E \sim 1/16V \text{ then it would be exact otherwise it's off)}$$