1. The infinite square well

First we will revise the infinite square well which you did at level 2. Instead of the well extending from 0 to a, in all of the following sections we will use a well that extends from $-a$ to a, that is, twice as wide and centred at 0. Of course the solutions are the same: they're just shifted and scaled (see Robinett, chapter 5).

The potential is

$$V(x) = \begin{cases} 0, & \text{for } -a \le x \le a, \\ \infty, & \text{for } |x| > a, \end{cases}$$

Outside the well where the potential is infinite there is no probability for the particle to be found and so $\psi(x) = 0$ for $|x| > a$. Inside the well the potential is zero so the time independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$$

which we write

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -k^2\psi$$

and

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

There are no normalisable solutions for $E < 0$ and so k is real and the general solution is

$$\psi(x) = A\sin kx + B\cos kx$$

The boundary conditions are

$$\psi(-a) = \psi(a) = 0$$

so

$$A\sin ka + B\cos ka = 0$$
$$-A\sin ka + B\cos ka = 0$$

Adding or subtracting these we get either

$$A\sin ka = 0 \qquad \text{or} \qquad B\cos ka = 0$$

Because the potential has inversion symmetry, $V(-x) = V(x)$, it is natural that the solutions fall into two classes: *even parity* solutions having $\psi(-x) = \psi(x)$, and *odd parity* solutions having $\psi(-x) = -\psi(x)$. And the two possible boundary conditions give rise to one of these sets each. Specifically since we cannot have both A and B equal to zero (since then $\psi = 0$ everywhere and this cannot be normalised) the two sets correspond respectively to either $A = 0$ or $B = 0$.

The boundary condition $A = 0$ leads to the even parity solutions. In this case we have $\cos ka = 0$ which is true if

$$k = k_m^{\mathrm{e}} = \left(m - \frac{1}{2}\right)\frac{\pi}{a} = \frac{(2m-1)\pi}{2a}, \qquad m = 1, 2, 3, \cdots$$

and the eigenfunctions of the even solutions are

$$\psi_m(x) = B\cos k_m^{\mathrm{e}} x$$

The other case, $B = 0$ leads to the odd parity solutions with boundary condition $A \sin ka = 0$ implying

$$k = k_m^{\rm O} = \frac{m\pi}{a} = \frac{2m\pi}{2a}, \qquad m = 1, 2, 3, \cdots$$

with eigenfunctions

$$\psi_m(x) = A \sin k_m^{\rm O} x$$

We note that the eigenfunctions can be written as

$$\psi_n(x) = \begin{cases} C \cos k_n x, & n = 2m - 1 \;\; i.e., \; n \text{ odd} \\ C \sin k_n x & n = 2m \qquad i.e., \; n \text{ even} \end{cases}$$

and

$$k_n = \frac{n\pi}{2a}, \qquad n = 1, 2, 3, \cdots$$

The boundary condition fixes the allowed wavelength $\lambda_n = 2\pi/k_n$. k_n is called a *quantum number* and generally speaking quantum numbers arise as labels which dictate the allowed solutions under the given boundary conditions. The allowed energies are the *eigenvalues* associated with the values of k_n. Since we will have $k_n = \sqrt{2mE_n}/\hbar$ it follows that

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$

To find the constant C, we normalise the wavefunction.

$$\int_{-a}^{a} |C|^2 \cos^2 kx \, \mathrm{d}x = \int_{-a}^{a} |C|^2 \sin^2 kx \, \mathrm{d}x = a\,|C|^2 = 1$$

and so we can take $C = 1/\sqrt{a}$.

Please note that these $\psi_n(x)$ are *eigenvectors.* A stationary state of the infinite square well is

$$\Psi_n(x, t) = \psi_n \, e^{iE_n t/\hbar}$$

Now comes an important point. The eigenvectors

$$\psi_n(x) = |n\rangle$$

provide a *basis* in which to express *any* wavefunction that satisfies the boundary conditions laid down by the potential (in this case the infinite square well) just like the basis vectors $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$ are a basis for any cartesian vector. Mathematically we can write the *state* of any particle in the infinite square well as a linear combination

$$\begin{aligned} \psi(x) &= \sum_{n=1}^{\infty} c_n \, \psi_n(x) \\ &= \sum_{n=1}^{\infty} c_n \, |n\rangle \end{aligned}$$

(In the second line I have used the vector notation to describe the eigenvector.) Unlike cartesian space, this space is *infinite dimensional.* It's exactly the same as Fourier analysis which says that any function in some interval, which is zero at the ends, can be expanded in sines and cosines having the same boundary conditions. Using Fourier analysis we find the important result that the coefficients c_n in the expansion above can be found using an integral,

$$\begin{aligned} c_n &= \int_{-a}^{a} \psi_n^*(x)\, \psi(x) \mathrm{d}x \\ &= \langle n \,|\psi\rangle \end{aligned}$$

And, again, I have indicated the alternative vector notation that emphasises this as a *scalar product* between the state and one of the eigenstates. Another property of the basis functions is that they are *orthonormal*,

$$\begin{aligned} \int_{-a}^{a} \psi_m^*(x)\, \psi_n(x)\, \mathrm{d}x &= \delta_{mn} \\ \langle m\,|n\rangle &= \delta_{mn} \end{aligned}$$

where δ_{mn} is the "Kronecker delta," it's zero if $m \neq n$ and one if $m = n$. The fact that the scalar product between two eigenstates is zero unless they are identical is completely analogous to the orthogonality between the cartesian unit vectors, $\hat{\mathbf{i}}$, $\hat{\mathbf{j}}$ and $\hat{\mathbf{k}}$. For example

$$\hat{\mathbf{j}} \cdot \hat{\mathbf{k}} = 0$$

but

$$\hat{\mathbf{i}} \cdot \hat{\mathbf{i}} = 1$$

This will become a lot clearer when I do an example in class.

2. The finite square well

The potential is

$$V(x) = \begin{cases} -V_0, & \text{for } -a \le x \le a, \\ 0, & \text{for } |x| > a, \end{cases}$$

with $V_0 > 0$. We first consider states with energy $E < 0$. Classically they would be confined within the well. In quantum mechanics a particle is represented by a solution to the time independent Schrödinger equation. The strategy is to find solutions in the three regions, left of the well, in the well and right of the well. To the left, $x < -a$, the potential is zero and we have

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi$$

which we write

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = \kappa^2\psi \tag{1a}$$

with

$$\kappa = \frac{1}{\hbar}\sqrt{-2mE} \tag{1b}$$

The general solution is

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$$

but we must have $A = 0$ or this blows up at large negative x.

Inside the well the time independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} - V_0\psi = E\psi$$

which we write

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -l^2\psi \tag{2a}$$

with

$$l = \frac{1}{\hbar}\sqrt{2m(E + V_0)} \tag{2b}$$

While $E < 0$ it's also true that $E > -V_0$ because there is no normalisable solution in the well for energy less than $-V_0$ (why not?). Please note the signs on κ and l on the right hand sides of (1a) and (2a). Solutions of equations like (1a) with positive coefficent are always exponentially decaying, like $e^{\pm\kappa x}$, while if the coefficient is negative as in (2a) the solution is oscillatory like $e^{\pm ilx}$ which we can also equally correctly write in terms of sines and cosines:

$$\psi(x) = C\sin lx + D\cos lx$$

Note it is conventional to use the symbols k or l for the quantum number in the oscillatory case and to use the symbol κ in the decaying case. In your level 2 notes you used α rather than κ as I shall also do in handwritten notes, since k and κ look very similar.

To the right of the well the potential is again zero and the energy of the state is less than this so the particle is classically forbidden this region. The signature of this is an exponentially decaying wavefunction just as to the left of the well. So for $x > a$ we have

$$\psi(x) = Fe^{-\kappa x}$$

The procedure is one we will use in all problems of this type. First we write down the wavefunction and its first derivative with respect to x in the three regions.

$$\psi(x) = \begin{cases} Be^{\kappa x}, & \text{for } x < -a \\ C\sin lx + D\cos lx, & \text{for } -a \leq x \leq a, \\ Fe^{-\kappa x}, & \text{for } x > a \end{cases}$$

$$\psi'(x) = \begin{cases} \kappa Be^{\kappa x}, & \text{for } x < -a \\ lC\cos lx - lD\sin lx, & \text{for } -a \leq x \leq a, \\ -\kappa Fe^{-\kappa x}, & \text{for } x > a \end{cases}$$

The task at hand is to find those values of the constants B, C, D and F that render the wavefunction continuous and differentiable over the whole range of x. I will show later for the case of states with $E > 0$ how this is done in a general way. We approach this particular problem, $E < 0$, in a way that exploits the *symmetry* of the potential, namely that it is symmetrical about $x = 0$ so that the wavefunction solutions must be either of even parity ($\psi(x) = \psi(-x)$) or of odd parity ($\psi(x) = -\psi(-x)$). We then seek first the even solutions and then the odd solutions. For the even solutions we have

$$\psi(x) = \begin{cases} \psi(-x), & \text{for } x < -a \\ D\cos lx, & \text{for } -a \leq x \leq a, \\ Fe^{-\kappa x}, & \text{for } x > a \end{cases}$$

For ψ to be continuous at $x = a$ we must have

$$Fe^{-\kappa a} = D\cos la$$

and to be differentiable we need

$$-\kappa Fe^{-\kappa a} = -lD\sin la$$

Dividing these two equations one by the other we get

$$\kappa = l\tan la \qquad \text{even solutions} \tag{3}$$

and this is the answer. Looking at (1b) and (2b) you see that the allowed energies, E, are those which result in κ and l obeying (3). For each allowed energy, we get κ and l which we plug into the wavefunctions in the three regions. At the same time we can solve for the constants F and D (one of which is arbitrary and can be chosen to normalise the wavefunction over the range of x).

Now, for the odd solutions we write

$$\psi(x) = \begin{cases} -\psi(-x), & \text{for } x < -a \\ C\sin lx, & \text{for } -a \leq x \leq a, \\ Fe^{-\kappa x}, & \text{for } x > a \end{cases}$$

and matching value and slope at $x = a$ results in

$$\psi(a) = Fe^{-\kappa a} = C\sin la$$
$$\psi'(a) = -\kappa Fe^{\kappa a} = lC\cos la$$

which when we divide one by the other, we arrive at

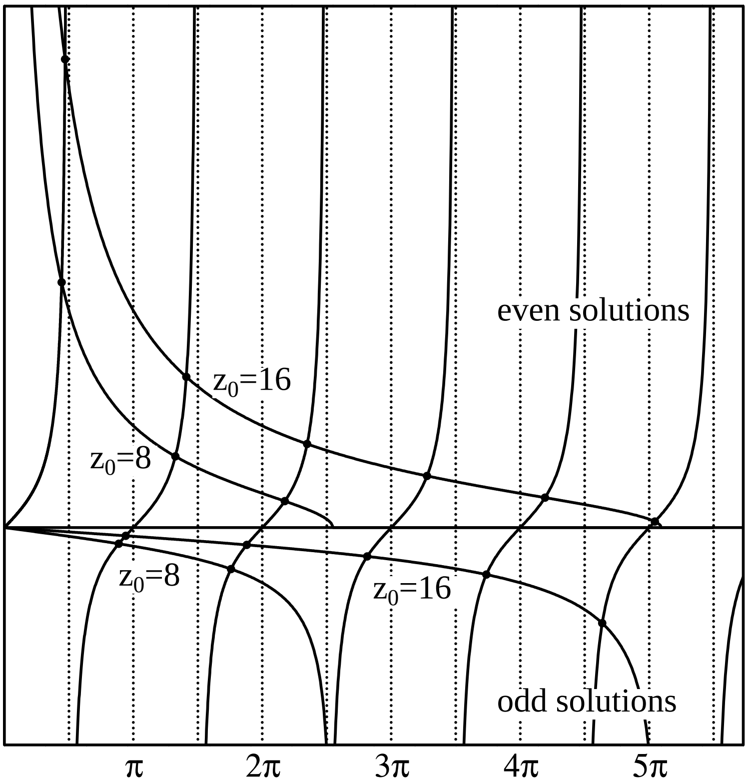
$$-\kappa = \frac{l}{\tan la} \qquad \text{odd solutions} \tag{4}$$

Equations (3) and (4) do not have analytical solutions but we can find the answers graphically or by computation. To do this we define some dimensionless parameters,

$$z = la, \qquad \text{and} \qquad z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$$

and (3) and (4) become, in terms of z and z_0

$$\tan z = \begin{cases} \left[(z_0/z)^2 - 1\right]^{1/2}, & \text{even solutions} \\ \left[(z_0/z)^2 - 1\right]^{-1/2}, & \text{odd solutions} \end{cases}$$



To find even and odd solutions we just have to plot $\tan z$ against the right hand sides. The figure shows this plot for two cases, $z_0 = 8$ and $z_0 = 16$. Note that z_0 is proportional to the width and the square root of the depth of the well; it therefore is a measure of the "strength" of the potential well. From (2b) we have

$$E_n + V_0 = \frac{\hbar^2 l^2}{2m} = z^2 \frac{\hbar^2}{2ma^2}$$

In the case of a very deep well, we see from the figure that the intersections occur near the infinities of $\tan z$, namely

$$z_n \to n\pi/2 \qquad \text{as} \qquad z_0 \to \infty$$

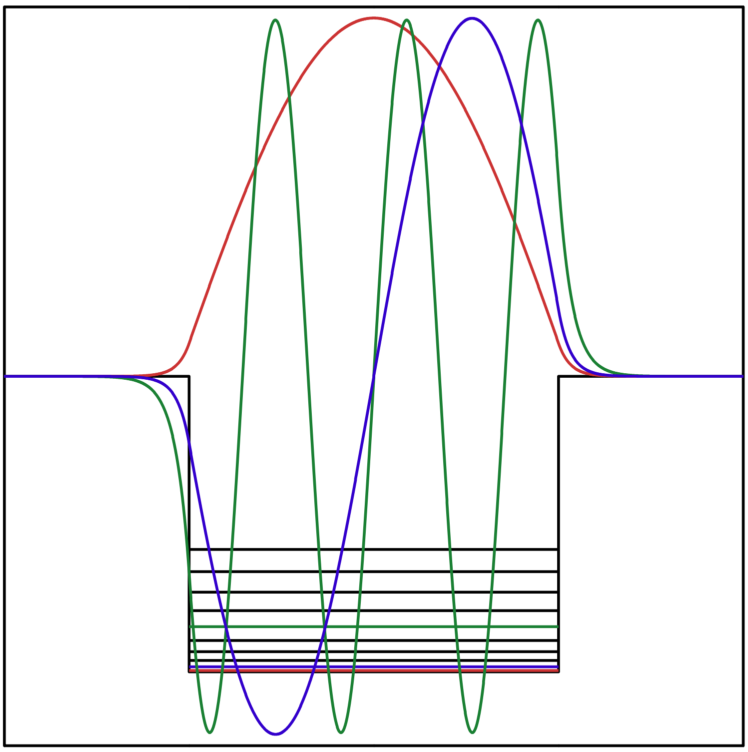
and so in the limit of an infinitely deep well we get that the eigenenergies measured from the bottom of the well, $-V_0$ are

$$\frac{n^2\pi^2\hbar^2}{2m(2a)^2}$$

which are of course the energies of a particle trapped in an infinite square well of width $2a$.

In the other limit, as $z_0 \to 0$, we see from the figure that there are fewer and fewer states "bound by the potential" and for $z_0 < \pi/2$ there are no odd states and just one even state. It is significant that this survives *however weak is the potential*: even the weakest and narrowest square well will bind at least one state.

The next figure shows this lowest energy bound state and also the second and sixth states, which are odd and even respectively, for $z_0 = 16$. These have the shapes of the states of the infinite square well, but unlike classical particles, the quantum mechanics admits a non zero probability that a measurement will find the particle outside the walls even though its energy is less than zero. I also show the eigenvalues of the first 10 bound states. You note that the probability density of a measurement finding the particle *outside* the well increases with the quantum number n. You might think this is inconsistent with Bohr's correspondence principle which asserts that the classical limit corresponds to larger quantum numbers; but in this case the increased probability is due to the energy getting closer to zero after which the states and are free from the well altogether. These states, having $E < 0$, are discussed next.



So those were the particles whose energies were below zero so that they are trapped in or near the well. Now we come to particles whose energies are greater than zero so they can exist as propagating stationary states anywhere in the range of x $(-\infty < x < \infty)$.

I will do this using the general method of "transfer matrices." First we write down the wavefunctions and derivatives in the three regions as before.

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{for } x < -a \\ C\sin lx + D\cos lx, & \text{for } -a \le x \le a, \\ Fe^{ikx} + Ge^{-ikx}, & \text{for } x > a \end{cases}$$

$$\psi'(x) = \begin{cases} ikAe^{ikx} - ikBe^{-ikx}, & \text{for } x < -a \\ lC\cos lx - lD\sin lx, & \text{for } -a \le x \le a, \\ ikFe^{ikx} - ikGe^{-ikx}, & \text{for } x > a \end{cases}$$

in which

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

and

$$l = \frac{1}{\hbar}\sqrt{2m(E+V_0)}$$

In the well the wavefunction is the same as in the bound state, but outside the well there are now running wave solutions travelling left (e^{-ikx}) and right (e^{ikx}). We need to join the three regions up by matching value and slope at the boundaries of the well as before. So at $x = -a$ we have

$$\begin{aligned} Ae^{-ika} + Be^{ika} &= -C\sin la + D\cos la \\ ikAe^{-ika} - ikBe^{ika} &= lC\cos la + lD\sin la \end{aligned} \tag{5a}$$

and at $x = a$

$$\begin{aligned} C\sin la + D\cos la &= Fe^{ika} + Ge^{-ika} \\ lC\cos la - lD\sin la &= ikFe^{ika} - ikGe^{-ika} \end{aligned} \tag{6a}$$

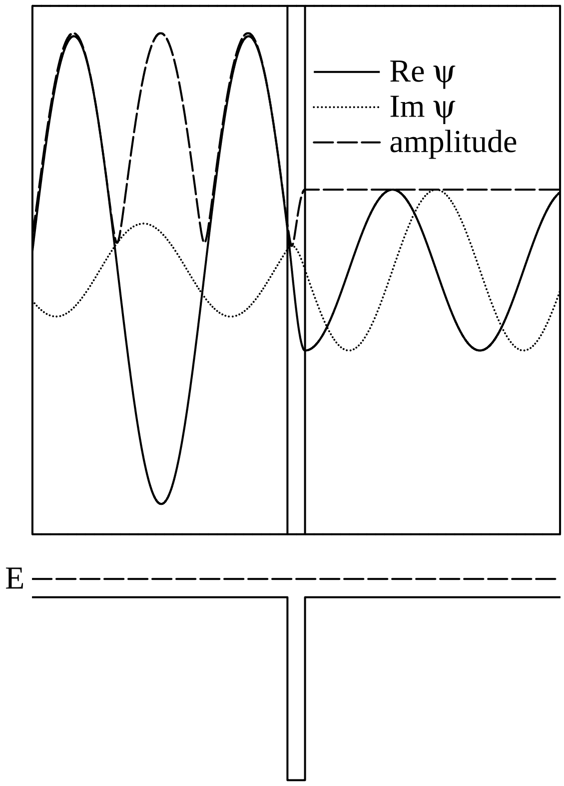
Now the nub. We can solve these as simultaneous equations bit by bit as we did for the bound states by adding and subtracting. But you know that you can usually solve simultaneous equations with matrices. So inspecting these sets of equations for a moment you see they are equivalent to these:

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ ike^{-ika} & -ike^{ika} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -\sin la & \cos la \\ l\cos la & l\sin la \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} \tag{5b}$$

$$\begin{pmatrix} \sin la & \cos la \\ l\cos la & -l\sin la \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix} \begin{pmatrix} F \\ G \end{pmatrix} \tag{6b}$$

Remember the quantum numbers k and l are fixed by the energy E for which we are seeking a solution. What we want are the coefficients A, B, C and D to plug back into the wavefunction. Before doing that let's just look at the physics of this problem. We may well be asking, suppose I launch a wave in from the left at the well. How much probability amplitude is transmitted and how much is reflected? Then I will fix A from the outset by the normalisation of the incoming wave. The amplitude A tells me how much is reflected and the amplitude F how much is transmitted. As long as I don't expect any amplitude coming in from the right (it's my experiment after all) then I may take it that $G = 0$.

The next figure shows such a matched solution for an energy just above zero, $E = 0.1V_0$,



Anticipating ahead, what I really want to know is the *transmission coefficient*

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

In the meanwhile I may want to know what is the wavefunction in the well, so I'll want to know C and D as well.

I will rewrite (5b) and (6b) like this

$$M_1 \begin{pmatrix} A \\ B \end{pmatrix} = M_2 \begin{pmatrix} C \\ D \end{pmatrix} \tag{5c}$$

$$M_3 \begin{pmatrix} C \\ D \end{pmatrix} = M_4 \begin{pmatrix} F \\ G \end{pmatrix} \tag{6c}$$

I can multiply (5c) by the inverse of M_1 and (6c) by the inverse of M_3. Then I substitute (6c) into (5c) and I get

$$\begin{aligned} \begin{pmatrix} A \\ B \end{pmatrix} &= M_1^{-1} M_2 M_3^{-1} M_4 \begin{pmatrix} F \\ G \end{pmatrix} \\ &= P \begin{pmatrix} F \\ G \end{pmatrix} \end{aligned}$$

and P is called the *transfer matrix*. This is a very general way to deduce the relation between waves going in and waves coming out of a one dimensional scattering problem.

There may be more than one well or barrier one after the other and this is the way to tackle such a problem.

For these purposes we just need to solve for A and B in terms of C and D and for C and D in terms of F and G and finally to get all the coefficients so we can plot the wavefunction and extract the transmission coefficient. So firstly I have

$$\begin{pmatrix} A \\ B \end{pmatrix} = M_1^{-1} M_2 \begin{pmatrix} C \\ D \end{pmatrix} \tag{7}$$

It's useful to remember how to invert a 2×2 matrix.

$$\text{if} \qquad T = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \qquad \text{then} \qquad T^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

(Multiply by one over the determinant, swap the diagonals and change the sign of the off diagonals.) We'll get

$$\begin{aligned} M_1^{-1} M_2 &= \frac{i}{2k} \begin{pmatrix} -ike^{ika} & -e^{ika} \\ -ike^{-ika} & e^{-ika} \end{pmatrix} \begin{pmatrix} -\sin la & \cos la \\ l \cos la & l \sin la \end{pmatrix} \\ &= \frac{i}{2k} \begin{pmatrix} e^{ika} (ik \sin la - l \cos la) & -e^{ika} (ik \cos la + l \sin la) \\ e^{-ika} (ik \sin la + l \cos la) & e^{-ika} (-ik \cos la + l \sin la) \end{pmatrix} \end{aligned}$$

Putting this in (7) you'll find

$$\begin{aligned} A &= \frac{i}{2k} e^{ika} \Big(C \, (ik \sin la - l \cos la) - D \, (ik \cos la + l \sin la) \Big) \\ B &= \frac{i}{2k} e^{-ika} \Big(C \, (ik \sin la + l \cos la) + D \, (-ik \cos la + l \sin la) \Big) \end{aligned}$$

Next we do the same thing with (6c). But we'll now set $G = 0$ as discussed above, and to keep the algebra simpler. (If there *were* amplitude coming in from the right also, then you can retain $G \neq 0$.)

$$\begin{aligned} M_3^{-1} M_4 &= \frac{1}{l} \begin{pmatrix} l \sin la & \cos la \\ l \cos la & -\sin la \end{pmatrix} \begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix} \\ &= \frac{1}{l} \begin{pmatrix} e^{ika} (l \sin la + ik \cos la) & e^{-ika} (l \sin la - ik \cos la) \\ e^{ika} (l \cos la - ik \sin la) & e^{-ika} (l \cos la + ik \sin la) \end{pmatrix} \end{aligned}$$

and (6c) becomes

$$\begin{aligned} C &= F e^{ika} \left(\sin la + i \frac{k}{l} \cos la \right) \\ D &= F e^{ika} \left(\cos la - i \frac{k}{l} \sin la \right) \end{aligned}$$

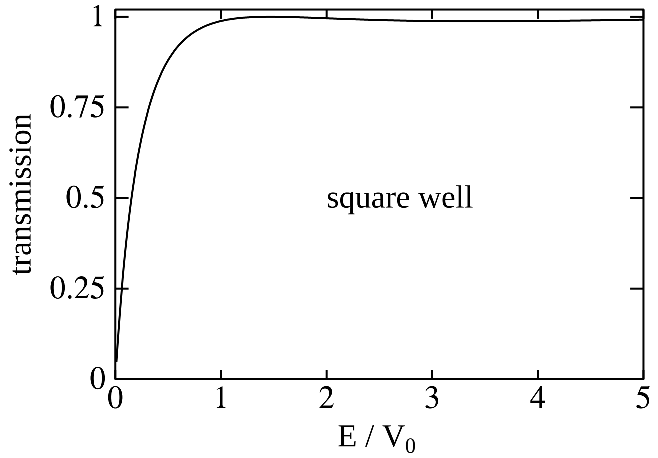
Finally I substitute these into my formulas for A and B to get A and B in terms of F. I find after quite a bit of algebra

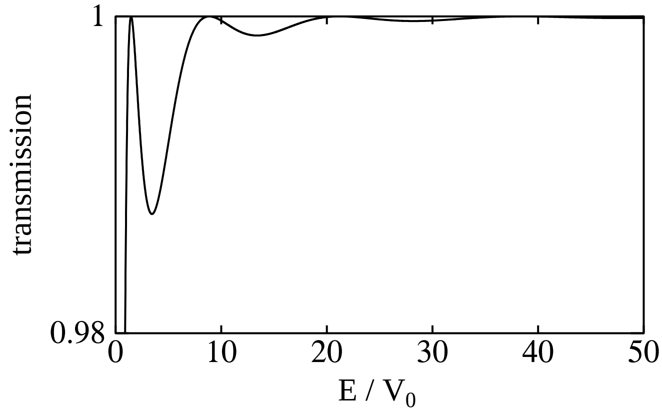
$$\begin{aligned} B &= \frac{iF}{2kl} \left(l^2 - k^2 \right) \sin 2la \\ A &= F e^{2ika} \left(\cos 2la - i \frac{l^2 + k^2}{2kl} \sin 2la \right) \end{aligned}$$

So the transmission coefficient must be given by

$$T^{-1} = \frac{|A|^2}{|F|^2} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right) \tag{8}$$

The next figure shows the transmission coefficient plotted versus the energy (remember this is the energy *above* the top of the well). If the energy is less than zero there are no travelling solutions outside the well, the particle is trapped inside although it can tunnel to the outside as seen in the figure on page 6. Note that the figure below plots the same function twice over, in different ranges of the energy.





You notice that the transmission coefficient periodically becomes one as a function of the energy of the incoming wave. This happens as you see from equation (8) whenever the sine is zero. That is, when

$$\frac{2a}{\hbar}\sqrt{2m(E+V_0)} = n\pi$$

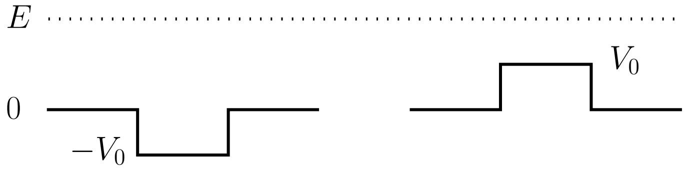
for any integer n. So there is *perfect transmission* (no reflection) whenever

$$E + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} = E_n$$

but these are the energy eigenvalues of the *infinite* square well, measured from the bottom of the well. This is a quite remarkable fact.

3. The square barrier

The square barrier rises above the zero of energy having a constant potential V_0 between $-a < x < a$. If we look for energies greater than V_0 then the problem is the same as for the finite well as you can see from the following figure.



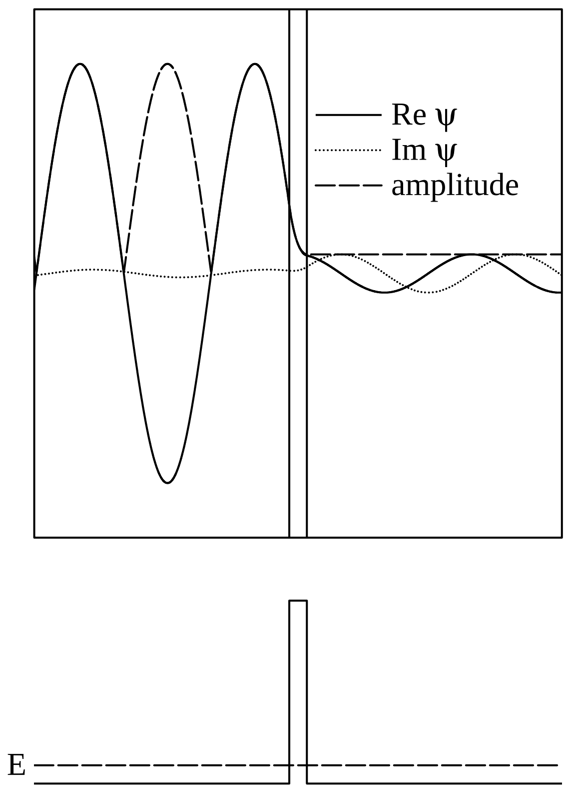
As long as $E > V_0$ then the problem is the same as for the well having $E > 0$, except that the kinetic energy in the barrier is $E - V_0$ rather than $E + V_0$. So the solution is exactly as for the well except that now

$$l = \frac{1}{\hbar}\sqrt{2m(E - V_0)}$$

This means that wavefunctions approaching the barrier are reflected and transmitted with a transmission coefficient given by equation (8) with the sign of V_0 changed,

$$T^{-1} = 1 + \frac{V_0^2}{4E(E - V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E - V_0)}\right) \qquad (9)$$

A classical particle would also fly over the barrier, but what if the energy is less than V_0? This is the most interesting case; classically a particle would bounce off the barrier, but in quantum mechanics there's a finite probability for the particle to "tunnel" through the barrier and appear on the other side.



The figure above shows tunnelling of a particle with energy $E = 0.1V_0$ which you can compare with the figure on page 9. In either case, the amplitude is constant on the right as there is only an outgoing wave and this must have a constant intensity, or energy is not conserved. On the left on the other hand what you see is interference between the incoming and reflected waves, and the combination has a varying amplitude. In the tunnelling case note how the wavefunction is decaying in the barrier and what remains is allowed to "leak out into the vacuum" and propagate.

The transmission coefficient in the tunnelling case, $E < V_0$, as compared to equation (9) is given by

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2\left(\frac{2a}{\hbar}\sqrt{2m(V_0 - E)}\right) \tag{10}$$

I'll now derive this result (you may skip this bit) using the method of transmission matrices. It's almost the same as the case of the potential well. The wavefunction is

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx}, & \text{for } x < -a \\ Ce^{lx} + De^{-lx}, & \text{for } -a \le x \le a, \\ Fe^{ikx} + Ge^{-ikx}, & \text{for } x > a \end{cases}$$

The only difference is that inside the well the wavefunctions are decaying—it's like the case of states bound within a finite well that decay to the outside. These now decay to the inside. The slopes are

$$\psi'(x) = \begin{cases} ikAe^{ikx} - ikBe^{-ikx}, & \text{for } x < -a \\ lCe^{lx} - lDe^{-lx}, & \text{for } -a \le x \le a, \\ ikFe^{ikx} - ikGe^{-ikx}, & \text{for } x > a \end{cases}$$

in which

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

and

$$l = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$$

At $x = -a$

$$Ae^{-ika} + Be^{ika} = Ce^{-la} + De^{la}$$
$$ikAe^{-ika} - ikBe^{ika} = lCe^{-la} - lDe^{la}$$

and at $x = a$

$$Ce^{la} + De^{-la} = Fe^{ika} + Ge^{-ika}$$
$$lCe^{la} - lDe^{-la} = ikFe^{ika} - ikGe^{-ika}$$

$$\begin{pmatrix} e^{-ika} & e^{ika} \\ ike^{-ika} & -ike^{ika} \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} e^{-la} & e^{la} \\ le^{-la} & -le^{la} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}$$
$$\begin{pmatrix} e^{la} & e^{-la} \\ le^{la} & -le^{-la} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} e^{ika} & e^{-ika} \\ ike^{ika} & -ike^{-ika} \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix}$$

By solving these matrix equations in the same way as before you will get these expressions for A and B in terms of C and D,

$$A = \frac{i}{2k}e^{ika}\left(-Ce^{-la}(l + ik) + De^{la}(l - ik)\right)$$
$$B = \frac{i}{2k}e^{-ika}\left(Ce^{-la}(l - ik) - De^{la}(l + ik)\right)$$

and solving for C and D in terms of F (again we set $G = 0$)

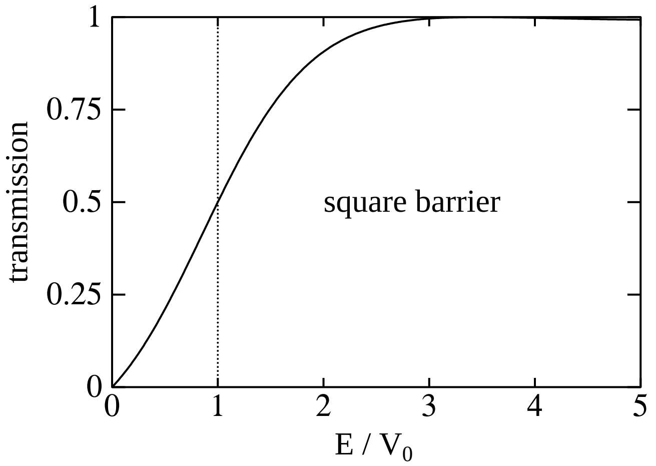
$$C = \frac{F}{2l} e^{ika} \left(e^{-la} (l + ik) \right)$$
$$D = \frac{F}{2l} e^{ika} \left(e^{la} (l - ik) \right)$$

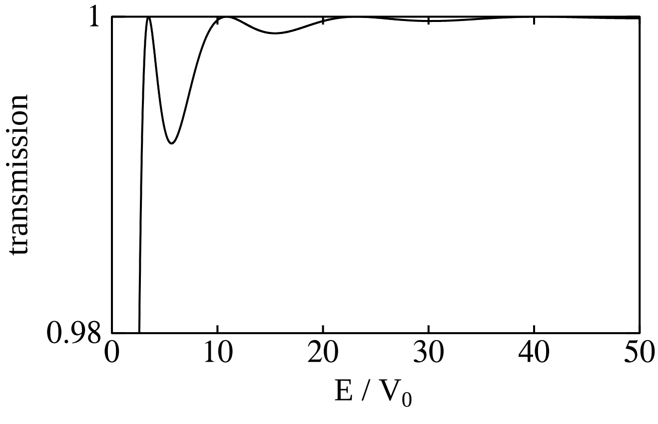
Then

$$\begin{aligned} A &= \frac{iF}{4lk} \left(-e^{2(ik-l)a} (l + ik)^2 + e^{2(ik+l)a} (l - ik)^2 \right) \\ &= \frac{iF}{4lk} e^{2ika} \left(-e^{-2la} \left(l^2 - k^2 + 2ilk \right) + e^{2la} \left(l^2 - k^2 - 2ilk \right) \right) \\ &= \frac{iF}{4lk} e^{2ika} \left(\left(e^{2la} - e^{-2la} \right) \left(l^2 - k^2 \right) - \left(e^{2la} + e^{-2la} \right) 2ilk \right) \\ &= F e^{2ika} \left(\cosh 2la + i \frac{l^2 - k^2}{2lk} \sinh 2la \right) \end{aligned}$$

so finally forming $|A|^2/|F|^2$ we get the inverse of the transmission coefficient

$$T^{-1} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \left(\frac{2a}{\hbar} \sqrt{2m(V_0 - E)} \right) \tag{10}$$





The figure above shows equations (9) and (10) which is the transmission coefficient of the barrier for energies below the barrier (10) left of the dotted line; and above (9) right of the dotted line.

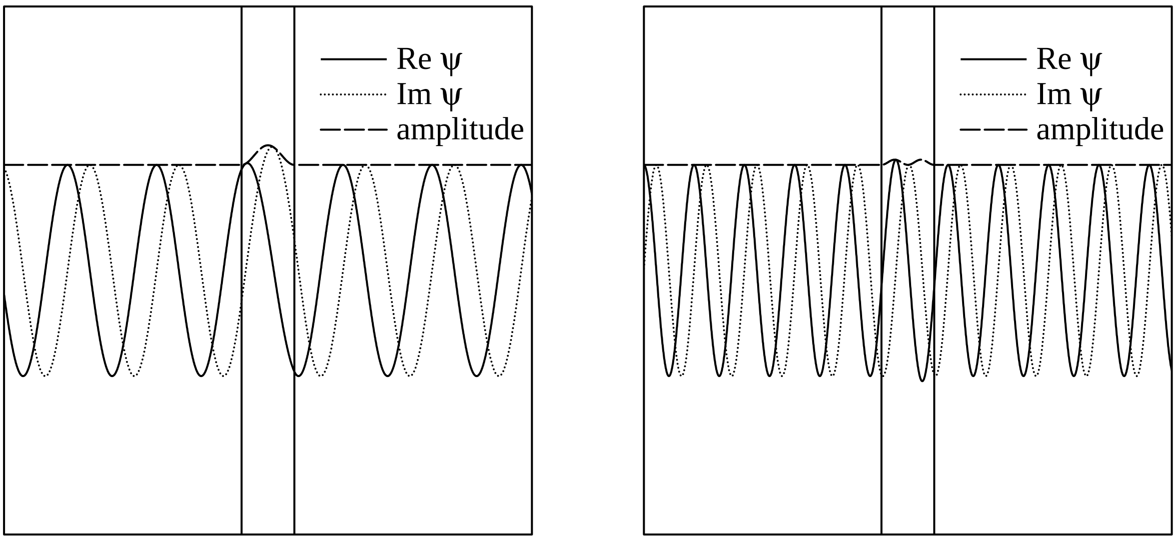
Again we see perfect transmission when the sine in (9) is zero, that is

$$\frac{2a}{\hbar}\sqrt{2m(E-V_0)} = n\pi$$

which is the same as

$$E - V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2} = E_n$$

This happens when the energy measured *from the top of the barrier* is an eigenenergy of an infinite square well whose energy zero is set to the top of the barrier. Maybe this is not too surprising because at those energies the boundary conditions of the infinite well require that exactly one or one-half a wavelength must fit exactly in the well. This allows for the wave reflected from the start of the barrier at $-a$ to interfere maximally with the wave reflected from the end of the well at a when they add up to make the reflected wave in the region $x < -a$. If the interference is destructive then there is no reflected wave and the incoming wave is totally transmitted. This property of reflective coatings is employed in camera lenses to maximise the light entering the camera, and also in non reflective coatings on spectacles. We see as we noted in the Introduction and Revision notes that there is a parallel between interference of the probability amplitude and the interference of waves in optics.



The above figures show this effect, in which the energy E has been set to $V_0 + E_1$, left; and $V_0 + E_2$, right. In each case you can see that the amplitude is completely transmitted from left to right. You can also see that exactly one-half wavelength is contained in the barrier in the left hand plot, and one wavelength in the right hand plot; this is consistent with the boundary conditions on the *infinite* well for quantum numbers $n = 1$ and $n = 2$ as expected.

An example of perfect transmission is the *Ramsauer–Townsend effect* in which low energy electrons impinging on a gas of neon or argon is found to have certain energies for which there is no reflexion.

4. Some manifestations of tunnelling

Here, I will briefly describe some experiments in which tunnelling is revealed.

Look back at equation (10) for the transmission coefficient of a barrier when the energy is less than the barrier height. If we define some parameters,

$$\alpha = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$$
$$\overline{E} = \frac{4E(V_0 - E)}{V_0^2}$$
$$w = 2a$$

then

$$T^{-1} = 1 + \frac{1}{\overline{E}}\sinh^2 \alpha w$$

We consider the limit that $\alpha w \gg 1$ and the limit of the sinh is

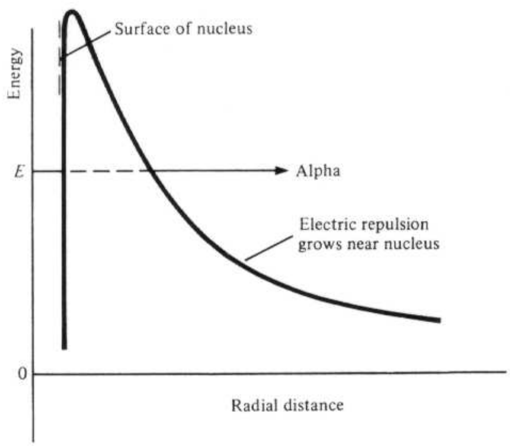
$$\sinh x = \frac{1}{2}(e^x - e^{-x}) \to \frac{1}{2}e^x$$

We then neglect the "one" compared to the $\sinh^2$ and get

$$T = 4\overline{E}\, e^{-2\alpha w}$$

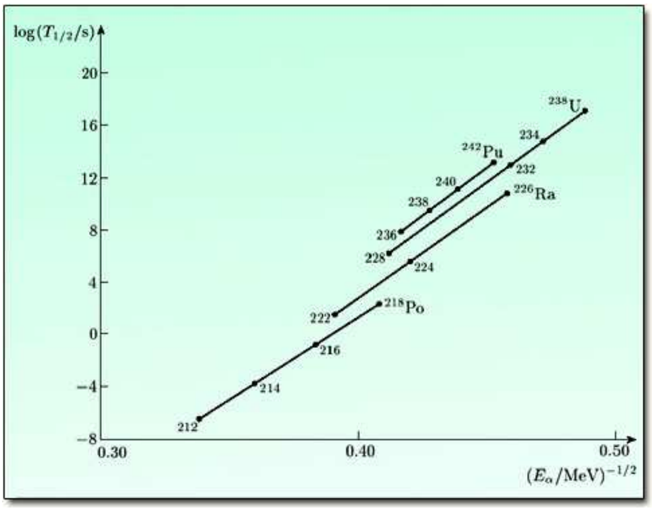
This is the famous "tunnelling law" that says that the fraction of incoming wave that tunnels through a barrier depends exponentially on the thickness, w, of the barrier. So to observe tunnelling you need a large incoming energy or flux and a thin barrier. There is a couple of very important applications of this law.

1. alpha decay. The decay of unstable nuclei by emission of an α-particle (helium nucleus) was understood by Gamow, Condon and Gurney in 1928 as a tunnelling manifestation. The α-particle is bound to the nucleus by the strong nuclear force which attracts positive protons more strongly than the repulsive Coulomb force. However the strong force is very short ranged, acting only over distances of around 10^{-15} m. So a one dimensional representation of the potential looks like this.



Potential barrier around a uranium nucleus presented to an alpha particle. The central well is due to the average nuclear attraction of all the nucleons and the hill is due to the electric repulsion of the protons. Alpha particles with energy E trapped inside the nuclear well may still escape to become alpha rays, by quantum mechanically tunnelling through the barrier.

The combination of the two potential energies (strong and Coulomb) amount to a barrier that the α-particle might tunnel through. The higher the energy of the particle the greater the probability of emission (once it escapes the pull of the strong force it's immediately repelled from the positive nucleus by the Coulomb force). In fact the tunnelling law predicts that the logarithm of the lifetime is proportional to the inverse square root of the α-particle's energy. This is confirmed for a large number of nuclei in the plot below.



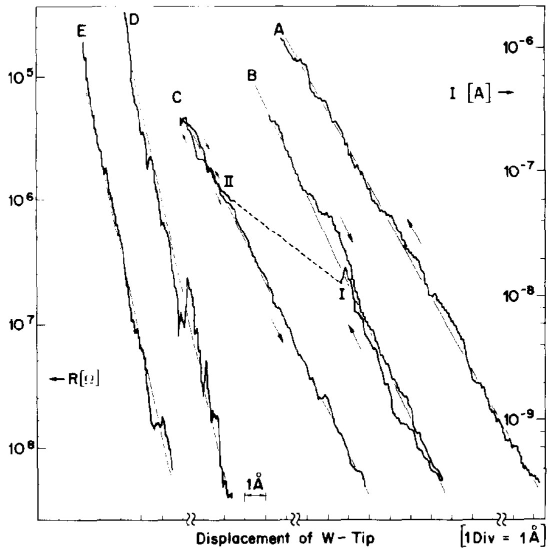


FIG. 2. Tunnel resistance and current vs displacement of Pt plate for different surface conditions as described in the text. The displacement origin is arbitrary for each curve (except for curves B and C with the same origin). The sweep rate was approximately 1 Å/s. Work functions $\phi = 0.6$ eV and 0.7 eV are derived from curves A, B, and C, respectively. The instability which occurred while scanning B and resulted in a jump from point I to II is attributed to the release of thermal stress in the unit. After this, the tunnel unit remained stable within 0.2 Å as shown by curve C. After repeated cleaning and in slightly better vacuum, the steepness of curves D and E resulted in $\phi = 3.2$ eV.

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2. The scanning tunnelling microscope was invented in 1981 by Binnig and Rohrer, who received the Nobel Prize in physics for their invention in 1986. You probably know how it works; here I just want to show a figure from one of their papers showing the logarithmic dependence of the tunnelling current on the gap between the tip and the sample, as predicted by the tunnelling law.