Supplementary Notes for lecture 32 for McGill Phys 357.

1. Matrix Solution to Scattering/Tunneling

Let's try to solve tunneling/scattering exactly. We'll assume there's a plane wave coming in from the left that hits a series of rectangular barriers. We have the tools to solve this problem exactly, and we can approximate any barrier as a series of increasingly narrow rectangles.

Let's start with the simple case of scattering. We'll start with a known energy. This would usually be an input to the problem - you send an electron with 5 eV of kinetic energy towards a barrier of height V_0 and want to see what happens. If we know the energy, then we know the wave vector in all regions, since Schrodinger's equation tells us that $-\hbar^2 q^2/2m \exp(qx) + V_0 \exp(qx) = E \exp(qx)$ for input wave $\exp(qx)$. We can solve this to get $q = \sqrt{2m(V_0 - E)/\hbar^2}$. It may look a little strange to be missing the i's, but we never said that q had to be real. For $E > V_0$, the square root will have a negative input, and we'll get imaginary q, leading to oscillations. As long as we do our math correctly for the case that q is imaginary, we'll get the right answer.

For the case of scattering off a single barrier, we know we'll get a reflected wave and a transmitted wave, so our wave function looks like:

$$\Psi_0 = t_0 \exp(q_0 x) + r_0 \exp(-q_0 x) \tag{1}$$

$$\Psi_1 = t_1 \exp(q_1 x) \tag{2}$$

where Ψ_0 t_0 is the incoming amplitude ("transmitted" from infinity), r_0 is the reflected amplitude in the left region, q_0 is the exponential constant, etc. Since the wave function and its derivative have to be continuous at the boundary, we know that

$$t_0 + r_0 = r_1 \tag{3}$$

$$q_0(t_0 - r_0) = q_1 t_1 \tag{4}$$

It's pretty easy to solve these directly, but instead let's rewrite the equations as a matrix problem. We aren't solving for t_0 - that's the input to the problem, but given t_0 we want to solve for r_0 and t_1. Any term involving those we'll put on the left side of the equals sign as somethign to solve, and anything involving t_0 we'll put on the right. Writing this way, we get:

$$t_1 - r_0 = t_0 \tag{5}$$

$$q_1 t_1 + q_0 r_0 = q_0 t_0 \tag{6}$$

We can write this as a matrix equation:

$$\begin{bmatrix} -1 & 1 \\ q_0 & q_1 \end{bmatrix} \begin{bmatrix} r_0 \\ t_1 \end{bmatrix} = \begin{bmatrix} t_0 \\ q_0 t_0 \end{bmatrix} \tag{7}$$

Now we can just multiply on the left by the inverse of the matrix to get r_0, t_1 in terms of t_0 (and, of course, the $q's$).

2. Finite Barrier

Let's now look at the case of a single finite barrier. In the rightmost region, we still have a single transmitted wave, but inside the barrier, we can have both transmitted/reflected waved or growing/decaying exponentials (depending on if q is real or imaginary), but because the barrier width is finite, both components will be there in general. We'll call the width of the barrier a_1, the transmitted/reflected coefficients t_1, r_1 in the barrier, and the transmitted part of the wave t_2. The matrix will be a lot easier to write down (especially going forward) if we define t_2 to be the amplitude at the right hand edge of the barrier. Under these assumptions, the wave function pieces are

$$\Psi_0 = t_0 \exp(q_0 x) + r_0 \exp(-q_0 x) \tag{8}$$

$$\Psi_1 = t_1 \exp(q_1 x) + r_1 \exp(-q_1 x) \tag{9}$$

$$\Psi_2 = t_2 \exp(q_2 x) \tag{10}$$

Once again, t_0 is an input, and we want to solve for $r_0, t_1, r_1, andt_2$. The continuity/derivative equations at the left edge of the barrier give us

$$t_0 + r_0 = t_1 + r_1 \tag{11}$$

$$q_0(t_0 - r_0) = q_1(t_1 - r_1) \tag{12}$$

At the right edge, we have the similar conditions, except r_2 isn't there. The amplitudes of the transmitted/reflected components also pick up factors of $\exp(\pm q_1 a_1)$ since those components have grown/decayed/oscillated inside the barrier. That gives us the equations:

$$t_1 \exp(q_1 a_1) + r_1 \exp(-q_1 a_1) = t_2 \tag{13}$$

$$q_1(t_1 \exp(q_1 a_1) - r_1 \exp(-q_1 a_1) = q_2 t_2 \tag{14}$$

Since we defined t_2 to be the amplitude at the edge of the barrier, we don't have to worry about where the barrier edge is from t_2's perspective. As before, we can put everything with t_0 on the right to get:

$$-r_0 + t_1 + r_1 = t_0 \tag{15}$$

$$q_0 r_0 + q_1 t_1 - q_1 r_1 = q_0 t_0 \tag{16}$$

$$\exp(q_1 a_1) t_1 + \exp(-q_1 a_1) r_1 - t_2 = 0 \tag{17}$$

$$q_1 \exp(q_1 a_1) t_1 - q_1 \exp(-q_1 a_1) r_1 - q_2 t_2 = 0 \tag{18}$$

Converting to a matrix equation, we get:

$$\begin{bmatrix} -1 & 1 & 1 & 0 \\ q_0 & q_1 & -q_1 & 0 \\ 0 & \exp(q_1 a_1) & \exp(-q_1 a_1) & -1 \\ 0 & q_1 \exp(q_1 a_1) & -q_1 \exp(-q_1 a_1) & -q_2 \end{bmatrix} \begin{bmatrix} r_0 \\ t_1 \\ r_1 \\ t_2 \end{bmatrix} = \begin{bmatrix} t_0 \\ q_0 t_0 \\ 0 \\ 0 \end{bmatrix} \tag{19}$$

Once again, we can pick a value for t_0, and by inverting the matrix and multiplying by the right-hand side vector, we can find all the values for our unknown tranmission/reflection amplitudes.

3. Adding a Second Barrier

We're almost there. If we now add a second barrier immediately adjacent to the first barrier, and have its width by a_2, then the boundary conditions at the junction of the barrier give us

$$t_1 \exp(q_1 a_1) + r_1 \exp(-q_1 a_1) = t_2 + r_2 \tag{20}$$

$$q_1 t_1 \exp(q_1 a_1) - q_1 r_1 \exp(-q_1 a_1) = q_2 t_2 - q_2 r_2 \tag{21}$$

Since the region inside both barriers can have transmitted/reflected components, we need to include them all here. Once again, we have definted t_2, r_2 to be the transmitted/reflected amplitudes at the start of their region. For compactness, we'll define $\gamma_1 \equiv \exp(q_1 a_1)$, and so $\exp(-q_1 a_1) = 1/\gamma_1$. We can write these two equations as

$$\begin{bmatrix} \gamma_1 & 1/\gamma_1 & -1 & -1 \\ q_1\gamma_1 & -q_1/\gamma_1 & -q_2 & q_2 \end{bmatrix} \begin{bmatrix} t_1 \\ r_1 \\ t_2 \\ r_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{22}$$

We can solve the two-barrier problem by inserting Equation **??** into Equation 19, giving:

$$\begin{bmatrix} -1 & 1 & 1 & 0 & 0 & 0 \\ q_0 & q_1 & -q_1 & 0 & 0 & 0 \\ 0 & \gamma_1 & 1/\gamma_1 & -1 & -1 & 0 \\ 0 & q_1\gamma_1 & -q_1/\gamma_1 & -q_2 & q_2 & 0 \\ 0 & 0 & 0 & \gamma_2 & 1/\gamma_2 & -1 \\ 0 & 0 & 0 & q_2\gamma_2 & -q_2/\gamma_2 & -q_3 \end{bmatrix} \begin{bmatrix} r_0 \\ t_1 \\ r_1 \\ t_2 \\ r_2 \\ t_3 \end{bmatrix} = \begin{bmatrix} t_0 \\ q_0 t_0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{23}$$

Once again, we're done. We calculate the q_i and from that we get the γ_i from q_i and a_i. Invert the matrix, multiply by our initial conditions on the right, and get the transmission (which in this case we get from t_3 now).

4. Many Barriers

There's virtualy no difference between the many-barrier case and the two-barrier case. Every time we add in a barrier, we get a set of internal conditions given by Equation **??**, just with $t_1, r_1, q_1, \gamma_1 \to t_i, r_i, q_i, \gamma_i$ and $t_2, r_2, q_2, \gamma_2 \to t_{i+1}, r_{i+1}, q_{i+1}, \gamma_{i+1}$. When we add that barrier, we expand our matrix by 2, and stick a suitable verion of Equation **??** into the matrix. The first two and last two equations stay the same since those are special boundary conditions, and we get the wave function everywhere in space by inverting our new larger matrix.

The code tunneling_exact.py shows how to implement this. It sets up a potential, and calculates the $q's$ and $a's$. It then fills in the first and last two rows, then loops over internal barriers and fills in the rest of the matrix. It also fills in the right hand side, then inverts to calculate the actual amplitudes. The transmitted fraction is then just the last element squared (assuming we've set the initial amplitude to 1). It also calculates the expected tranmission fraction based on $exp(-qa)$ for each barrier where $E < V$ and compares - they do come out quite close in general.

One more fun aspect is perfect tranmission through a rectangular barrier where $V < E$. If you get exactly one wavelength inside the barrier, the reflected parts cancel and you get perfect transmission. The code tranmission.py does this, and shows that indeed we get perfect transmission where the wave function has half-periods inside the barrier. The stars in the plot the script produces are the theoretical estimates of where perfect tranmission should be, which agree with the numerical calculation.