Low angle/low energy scattering

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What follows is a simple analysis of a model system for scattering of electrons off a potential well. We want to explore what happens in various regimes of weak potential or low scattering angle to the reflection and transmission coefficients.

1 1D potential well

Let's start with the 1D electron scattering problem for a potential well. We have a potential function $U(z)$ which is zero everywhere except for $|z| < a$ where it has the constant negative value $-V$ where $V < 0$: $U(z) = -V\theta(a - |z|)$. We are interested in scattering (unbound) states with energy $E > 0$ and their reflection and transmission through the well. We will work in units where $\hbar^2/m_e = 1$. Then outside the well, the electron state has wave vector $k = \sqrt{E}$ and inside the well has wave vector $k' = \sqrt{E+V}$.

The transmission coefficient $T(E)$ for scattering states is a standard textbook problem and given by

$$\frac{1}{T(E)} = 1 + \frac{\sin^2(2ak')(k'^2 - k^2)^2}{4k^2k'^2} = 1 + \frac{V^2 \sin^2\left(2a\sqrt{E+V}\right)}{4E(E+V)}\,. \tag{1}$$

We can ask for a formal series as $V \to 0$ or more precisely in V/E. Physically, this could mean the energy E is fixed and the potential is being weakened; or both are reduced but $V/E \ll 1$. In this limit, we get

$$\frac{1}{T(E)} = 1 + \left(\frac{V}{E}\right)^2 \cdot \frac{\sin^2\left(2a\sqrt{E}\right)}{4} + O((V/E)^3)\,.$$

Thus the transmission goes to unity as $V/E \to 0$ and the reflection coefficient $R = 1 - T$ is just

$$R(E) = \left(\frac{V}{E}\right)^2 \cdot \frac{\sin^2\left(2a\sqrt{E}\right)}{4} + O((V/E)^3)$$

which is clearly of order V^2 as expected form formal perturbation theory.

A different question is to ask what happens for a given potential well when we reduce E to zero. Here $E/V \ll 1$ or $V/E \gg 1$ which is the opposite limit of above. Going back to the exact formula (1), in this limit we have

$$\frac{1}{T(E)} = 1 + \frac{V}{E} \cdot \frac{\sin^2\left(2a\sqrt{V}\right)}{4} + O((V/E)^0) + O((V/E)^{-1})\,.$$

Basically, $1/T$ becomes divergent like $1/E$ and thus $T \to 0$. Therefore, for low energy scattering off a given potential, the transmission goes to zero and the reflection goes to unity: nothing gets through.

The main physical reason for this is a mismatch of wave vectors. For $E \to 0$, the wave vector outside the well $k = \sqrt{E}$ is getting arbitrarily small (the wavelength is getting very large) but inside the well $k' \to \sqrt{V}$ goes to a finite number. The two waves have very different characters and in the limit can't match up at the boundary. The more detailed logic is this: (a) we must match both value and derivative of wave function at the boundaries $z = \pm a$, (b) in the $U = 0$ regions the wavelength is getting very long so the derivative is getting arbitrarily small, (c) inside the well the wavelength is fixed so the derivative is fixed, and (d) therefore one can't couple the two waves across the boundary and thus everything gets reflected. This perfect reflection is also true for a single potential step up or down instead of a well (i.e., $U = -V\theta(z)$ or $U = -V\theta(-z)$). Conversely, at very high energies we expect perfect coupling and the transmission to be perfect, which is the case.

Before we move to the 3D case, a few remaining observations on the form of the transmission coefficient in equation (1). For comparison, the transmission coefficient for a simple potential step $U(z) = -V\theta(z)$ is given by

$$\frac{1}{T_{step}(E)} = 1 + \frac{(k'-k)^2}{4kk'} = 1 + \frac{\left(\sqrt{E+V} - \sqrt{E}\right)^2}{4\sqrt{E(E+V)}}\,.$$

which has some similarities and differences with the well transmission. Aside form the absence or presence of square roots, the most important difference is that the well problem has the $\sin^2$ term which incorporates the effects of multiple reflection in the well: we multiply wave vector in the well k' by $2a$ (two reflections to get us back to where we started) and take the $\sin^2$ of the phase accumulated. Otherwise the two show very similar behavior: for $E/V \gg 1$ the transmission goes to unity and for $E/V \ll 1$ the transmission goes to zero.

2 3D potential slab

This is a simple generalization of the 1D case. Here the potential has complete translational symmetry in the xy plane and depends only on z. And along z is it just the potential well.

So $U(x, y, z) = -V\theta(a - |z|)$. The lack of dependence on the xy coordinates mean that an eigenstate of this potential with energy E is of the form

$$\psi_E(x, y, z) = e^{ik_x x + k_y y}\phi_E(z)\,.$$

Both inside and outside the well ϕ_E is a sum of plane waves. Let the wave vector inside be k' and outside be k. Inside, the z component of hte wave vector is k'_z and outside it is k_z. The xy wave vector (k_x, k_y) is obviously the same in all regions. All these quantities are related via

$$E = k^2 = k_x^2 + k_y^2 + k_z^2 \quad , \quad E + V = k'^2 = k_x^2 + k_y^2 + k_z'^2\,.$$

Furthermore, ϕ_E obeys the same differential equation as the 1D potential well only with modified naming of the various wave vectors and energies. Therefore the transmission is

$$\frac{1}{T} = 1 + \frac{\sin^2(2ak'_z)(k_z'^2 - k_z^2)^2}{4k_z^2 k_z'^2}\,.$$

We would prefer to work with more convenient variables such as the total incident energy E of the plane wave as well as the angle θ_i of incidence to the xy plane measured from the plane: $\theta_i = \pi/2$ is normal incidence with $k_x = k_y = 0$ while $\theta_i = 0$ is glancing incidence with $k_z = 0$. We also define the angle of k' with respect to the xy plane to be θ_t (t for transmitted). The precise relations are

$$k_z = k\sin(\theta_i) \quad , \quad k'_z = k'\sin(\theta_t) \quad , \quad k\cos(\theta_i) = \sqrt{k_x^2 + k_y^2} = k'\cos(\theta_t)\,.$$

Using the relations of k^2 and k'^2 to the energies it is easy to show that

$$k_z'^2 - k_z^2 = V\,.$$

Next, we have

$$\begin{aligned} k_z'^2 &= k'^2\sin^2(\theta_t) = (E+V)[1 - \cos^2(\theta_t)] = (E+V)[1 - (k/k')^2\cos^2(\theta_i)] \\ &= (E+V)[1 - (E/(E+V))\cos^2(\theta_i)] = E + V - E\cos^2(\theta_i) \\ &= V + E\sin^2(\theta_i)\,. \end{aligned}$$

Using these two results along with $k_z^2 = k^2\sin^2(\theta_i) = E\sin^2(\theta_i)$ the transmission coefficient becomes

$$\frac{1}{T(E)} = 1 + \frac{V^2\sin^2\left(2a\sqrt{V + E\sin^2(\theta_i)}\right)}{4E\sin^2(\theta_i)\left[V + E\sin^2(\theta_i)\right]}\,.$$

Looking back at the 1D result, this just involves replacing E by $E\sin^2(\theta_i)$ which makes sense: the incident total energy is not relevant but instead what matters is the part of the kinetic energy directed along z and hence the $\sin^2(\theta_i)$.

The main difference between this and the 1D form is that we have two degrees of freedom. For the 1D problem, there was no θ_i degree of freedom we had to reduce E to zero to get zero transmission; mathematically, the 1D case is equivalent to normal incidence at $\theta_i = \pi/2$. For the 3D case, we can still have a finite and even large total energy E but can access various regions of the behavior.

One important consequence of the above result is that even for a weak potential $V/E \ll 1$, there are incident angles small enough so that the perturbative expansion $T = 1 - O(V)^2$ and thus $R = O(V^2)$ breaks down due to $E\sin^2(\theta_i)$ denominator: once θ_i gets very small, the denominator blows up and we get the "non-perturbative" result that $T \to 0$ as $T = O(E/V \sin^{-2}(\theta_i))$ and thus a series expansion in V/E is a complete failure in this limit.

We can even be more specific about what small angles mean. It means that V is much larger than $E\sin^2(\theta_i)$ or $\sin^2(\theta_i) \ll V/E$. Thus even a very weak potential becomes "strong" for small enough incidence angles. Again the transmission going to zero is due to the same physics as in 1D: the interior region has a finite wave vector $k_z' \to \sqrt{V}$ but outside $k_z \to 0$ as $\theta_i \to 0$ so we must get perfect reflection. We can get perfect reflection from a potential that is very weak (but of fixed strength) by going to low enough angles.