A method for calculating quantum mechanical transmission in 2D potentials

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We describe a method for calculating the quantum mechanical transmission coefficient for waves propagating through a 2D potential geometry, such as the one depicted in Figure 1. In this setup, the particles emerge from the lead on the left. When they encounter the potential stub, some of them are reflected back to the left, and some are transmitted to the right.

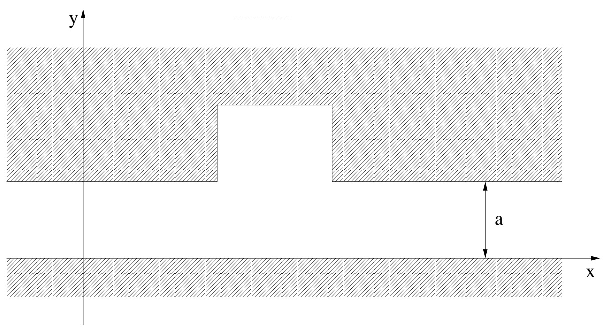

Figure 1: Example of a 2D potential. In the shaded areas $V(x, y) = \infty$, elsewhere $V(x, y) = 0$.

In the asymptotic regions on the potential, the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x, y)\right)\psi(x, y) = E\psi(x, y) \tag{1}$$

is separable to x- and y-components, and the solution can be expressed as a linear combination of wave functions of the form

$$\psi_{n,k}(x, y) = C_{n,k}\phi_n(y)e^{\pm ikx}, \tag{2}$$

where $\phi_n(y) = \sqrt{\frac{2}{a}}\sin(\frac{n\pi y}{a})$ is the transverse infinite-well wave function and $e^{\pm ikx}$ is the freely propagating wave in the $\pm x$-direction.

In order to obtain the transmission coefficient through the structure, we need to calculate the ratio of the amplitudes of the incoming and transmitted waves. Our method is based on the following idea: On the left side, there are waves travelling both to the left and to the right, but on the right side there are only waves propagating to the right. Therefore we can set the wave function on the right side to be

$$\psi^{\rm anal}(x,y) = \phi_{n_f}(y)e^{ikx}. \tag{3}$$

Note that if we begin by writing down the total wave function on left side of the system, the amplitudes of the reflected waves are undetermined and the function can not be used to start the numerical integration.

Now, choose an arbitrary starting point x_1 on the right side, and choose the transmitted mode n_f and wave number k, so that the total energy is $E = \frac{\hbar^2}{2m}(\frac{\pi^2 n_f^2}{a^2} + k^2)$. Then insert these into Eq. (3) and its normal derivative to set the initial values for the integration,

$$\begin{aligned}
\psi^{\rm num}(x_1,y) &= \phi_{n_f}(y)e^{ikx_1} \\
D^{\rm num}(x_1,y) &= -ik\phi_{n_f}(y)e^{ikx_1},
\end{aligned} \tag{4}$$

where $D^{\rm num}(x,y) = -\mathbf{e}_{\rm x}\cdot\nabla\psi(x,y)$. Integrate Eq. (1) with any appropriate numerical method over the region of interest all the way to x_0 on the left side. The general analytic form of the wave function at x_0 is

$$\psi^{\rm anal}(x_0,y) = \sum_{n_i}\phi_{n_i}(y)(A_{n_i,n_f}e^{ik_{n_i}x_0} + B_{n_i,n_f}e^{-ik_{n_i}x_0}), \tag{5}$$

where conservation of energy requires

$$\frac{2m}{\hbar^2}E = \frac{\pi^2 n_i^2}{a^2} + k_{n_i}^2 = \frac{\pi^2 n_f^2}{a^2} + k^2. \tag{6}$$

That is, the summation is over those positive integral values of n_i for which $n_i^2 < n_f^2 + \frac{a^2}{\pi^2}k^2$.

Next we must fit $\psi^{\rm num}$ to $\psi^{\rm anal}$ at x_0 to extract A_{n_i,n_f} and B_{n_i,n_f}. This is accomplished easily due to the orthonormality of the ϕ_n, so that by requiring $\psi^{\rm num} = \psi^{\rm anal}$ we have from (5)

$$\begin{aligned}
A_{n_i,n_f}e^{ik_{n_i}x_0} + B_{n_i,n_f}e^{-ik_{n_i}x_0} &= \int_0^a \phi_{n_i}^*(y)\psi^{\rm num}(x_0,y)dy \\
ik_{n_i}(A_{n_i,n_f}e^{ik_{n_i}x_0} - B_{n_i,n_f}e^{-ik_{n_i}x_0}) &= \int_0^a \phi_{n_i}^*(y)D^{\rm num}(x_0,y)dy.
\end{aligned} \tag{7}$$

To calculate the transmission coefficient we need the quantum mechanical current density, which is defined as

$$\mathbf{J} = \frac{\hbar}{2mi}\left(\psi^*\nabla\psi - \psi\nabla\psi^*\right), \tag{8}$$

and when $\psi_{n,k}$ from (2) is substituted, (8) yields

$$\mathbf{J}_{n,k}(x,y) = \pm|C_{n,k}|^2\frac{2\hbar k}{ma}\sin^2\frac{n\pi y}{a}\;\mathbf{e}_{\rm x}. \tag{9}$$

When this is integrated over $0 \le y \le a$, we have the total current in the x-direction as $J = |C_{n,k}|^2\frac{\hbar k}{m}$. Now, the transmission coefficient from mode n_i to mode n_f at energy E (Eq.(6)) is

$$T_{n_i,n_f}(E) = \frac{|J_{n_f}(E)|}{|J_{n_i}(E)|} = \frac{k}{|A_{n_i,n_f}|^2 k_{n_i}}. \tag{10}$$