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Piecewise Function/Continuity Review -Scattering from Step Potential

Piecewise Function/Continuity Review

Continuous piecewise functions are defined as follows:

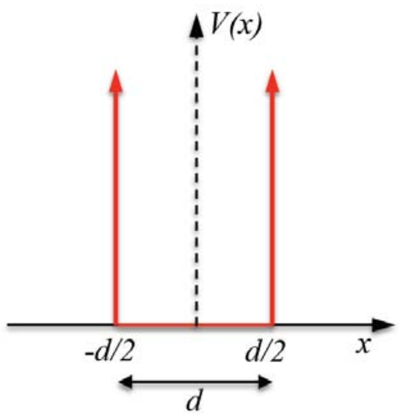
$$f(x) = \begin{cases} f_1(x) & x\epsilon(-\infty, a_1] \\ f_2(x) & x\epsilon[a_1, a_2] \\ \vdots & \vdots \\ f_n(x) & x\epsilon[a_n, \infty) \end{cases}$$

Here we note that the following continuity conditions must be in place for these functions to be piecewise continuous:

$$f_n(a_n) = f_{n+1}\,(a_n)$$
$$\frac{df_n(a_n)}{dx} = \frac{df_{n+1}\,(a_n)}{dx}$$

Wave functions must obey the same boundary conditions. Note however that the potential function *V(x)* does not have to be piecewise continuous, just the wave function. There are many problems of interest where $V(x)$ is a piecewise function and not necessarily continuous such as the particle in a 1D box and barrier and potential well problems.

Example 1: Particle in a box – symmetric about x-axis



Consider the above system with the piecewise potential energy function $V(x)$ for an electron inside the infinite potential well.

$$V(x) = \begin{cases} \infty & x\epsilon\left(-\infty, -\frac{d}{2}\right) \cup \left(\frac{d}{2}, \infty\right) \\ 0 & x\epsilon\left[-\frac{d}{2}, \frac{d}{2}\right] \end{cases}$$

The wave function is 0 outside the middle region since there is 0 probability of finding the electron in the infinite potential regions.

We write Schrödinger's equation for the middle region.

$$\widehat{H}\varphi = E\varphi$$

$$\frac{\hat{p}^2}{2m}\psi = E\psi \rightarrow \left(\frac{\left(-i\hbar\frac{\partial}{\partial x}\right)^2}{2m}\right)\psi = E\psi$$

$$\therefore \frac{-\hbar^2\frac{\partial^2\psi}{\partial x^2}}{2m} = E\psi$$

The general solution of this equation is:

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

with $k^2 = \frac{2mE}{\hbar^2}$

The boundary conditions (BCs) for this problem are:

$$\psi\left(-\frac{d}{2}\right) = 0 \text{ and } \psi\left(\frac{d}{2}\right) = 0$$

The first BC gives:

$$Ae^{\frac{ikd}{2}} + Be^{-\frac{ikd}{2}} = 0$$

The second BC gives:

$$Ae^{-\frac{ikd}{2}} + Be^{\frac{ikd}{2}} = 0$$

Adding these two equations:

$$A\left(e^{\frac{ikd}{2}} + e^{-\frac{ikd}{2}}\right) + B\left(e^{\frac{ikd}{2}} + e^{-\frac{ikd}{2}}\right) = 0$$

or

$$2A\cos\frac{kd}{2} + 2B\cos\frac{kd}{2} = 0$$

$$2(A+B)\cos\frac{kd}{2} = 0$$

Subtracting the second equation from the first equation:

$$A\left(e^{\frac{ikd}{2}} - e^{-\frac{ikd}{2}}\right) - B\left(e^{\frac{ikd}{2}} - e^{-\frac{ikd}{2}}\right) = 0$$

or

$$2iA\sin\frac{kd}{2} - 2iB\sin\frac{kd}{2} = 0$$

$$2i(A-B)\sin\frac{kd}{2} = 0$$

Thus these equations must simultaneously be true:

$$2(A+B)\cos\frac{kd}{2} = 0$$

$$2(A-B)\sin\frac{kd}{2} = 0$$

If $A = B$:

$$\cos\frac{kd}{2} = 0 \ \rightarrow kd = n\pi \text{ with } n \text{ odd}$$

If $A = -B$:

$$\sin\frac{kd}{2} = 0 \ \rightarrow kd = n\pi \text{ with } n \text{ even} > 0$$

Thus the solution to the problem is:

$$\psi_n(x) = \begin{cases} c_{odd}\left(e^{i\frac{n\pi x}{d}} + e^{-i\frac{n\pi x}{d}}\right) \\ c_{even}\left(e^{i\frac{n\pi x}{d}} - e^{-i\frac{n\pi x}{d}}\right) \end{cases} = \begin{matrix} C_{odd}\cos\left(\frac{n\pi x}{d}\right) & n\ odd \\ C_{even}\sin\left(\frac{n\pi x}{d}\right) & n\ even \end{matrix}$$

Such that:

$$C_{odd} = 2c_{odd} \text{ and } C_{even} = 2ic_{even}$$

The constants *C* and *D* are found by the normalization condition for the total probability of finding the particle:

$$1 = \int_{-\frac{d}{2}}^{\frac{d}{2}} \psi_n^*(x)\psi_n(x)\,dx = \begin{cases} \int_{-\frac{d}{2}}^{\frac{d}{2}} C_{odd}^2\cos^2\left(\frac{n\pi x}{d}\right)dx \rightarrow C_{odd} = \sqrt{\frac{2}{d}} \\ \int_{-\frac{d}{2}}^{\frac{d}{2}} C_{even}^2\sin^2\left(\frac{n\pi x}{d}\right)dx \rightarrow C_{even} = \sqrt{\frac{2}{d}} \end{cases}$$

Therefore:

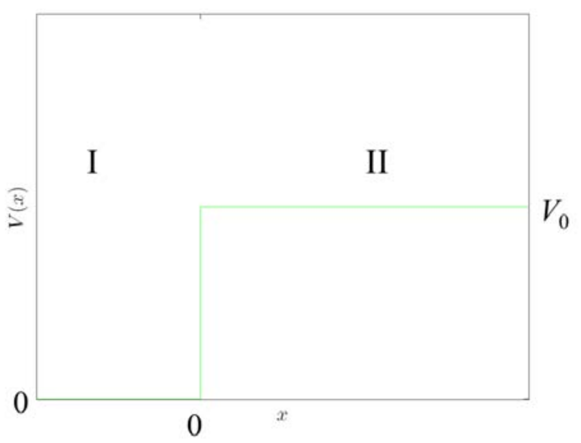
$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{d}}\cos\left(\frac{n\pi x}{d}\right) & n\ odd \\ \sqrt{\frac{2}{d}}\sin\left(\frac{n\pi x}{d}\right) & n\ even \end{cases}$$

The energies of the system are quantized such that:

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2\left(\frac{n\pi}{d}\right)^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{h^2 n^2}{8md^2}$$

Example 2: Scattering off a step potential.
Consider the following piecewise potential energy function $V(x)$ for an electron traveling incident from the left side with total energy $E > V_0$.

$$V(x) = \begin{cases} 0 & x\epsilon(-\infty, 0) \\ V_0 & x\epsilon[0, \infty) \end{cases}$$



Find the general form of the wave functions for this potential energy and the transmission and reflections coefficients for the incident electron, R and T.

First we write Schrödinger's equation in the two regions.

$$\hat{H}\psi = E\psi$$

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

In region I:
$V = 0$

$$\therefore \frac{-\hbar^2 \frac{\partial^2 \psi_{\mathrm{I}}}{\partial x^2}}{2m} = E\psi_{\mathrm{I}}$$

In region II:
$V = V_0$

$$\therefore \frac{-\hbar^2 \frac{\partial^2 \psi_{\mathrm{II}}}{\partial x^2}}{2m} + V_0\psi_{\mathrm{II}} = E\psi_{\mathrm{II}}$$

Since the wave function must be piecewise continuous, we have the following boundary conditions (BCs).

BC are $\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0)$ and $\frac{\partial \psi_{\mathrm{I}}}{\partial x}(0) = \frac{\partial \psi_{\mathrm{II}}}{\partial x}(0)$

Now, to solve these we write the general solutions for the wave function in each region and apply boundary conditions.

Let $k^2 \equiv \frac{2mE}{\hbar^2}$ and $\rho^2 \equiv \frac{2m(E-V_0)}{\hbar^2}$
In region I:

$$k^2\psi_{\mathrm{I}} + \frac{\partial^2\psi_{\mathrm{I}}}{\partial x^2} = 0 \text{ which has solutions of the form } \psi_{\mathrm{I}}(x) = Ae^{ikx} + Be^{-ikx}$$

In region II:

$$\rho^2\psi_{\mathrm{II}} + \frac{\partial^2\psi_{\mathrm{II}}}{\partial x^2} = 0 \text{ which has solutions of the form } \psi_{\mathrm{II}}(x) = Ce^{-i\rho x} + De^{i\rho x}$$

Since the electron is incident from the left, there can never be a rightward propagating wave from the right side.

$$C = 0 \rightarrow \psi_{\mathrm{II}}(x) = De^{i\rho x}$$

The coefficients *R* and *T* are simply related to the coefficients *A*, *B*, and *D* such that *A* corresponds to the incident electron, *B* the reflected electron, and *D* any transmission electron.
The exact correspondence comes from the conservation of the flux of electrons from the left equaling the flux of the electrons on the right.
The probability current/flux is simply the probability amplitudes times the velocity of the electron.

$$v = \frac{p}{m} = \frac{\hbar k}{m}$$
$$F = A^2 v$$

We have 3 probability currents/fluxes, incident, reflected, and transmitted.

$$I + R = T$$
$$A^*A\frac{\hbar k}{m} + B^*B\frac{\hbar k}{m} = D^*D\frac{\hbar\rho}{m}$$

Assuming $I = 1$, we can normalize this current/flux equation by A^*Ak and obtain the following relations for *R* and *T*.
We can thus write $R = \frac{B^*B}{A^*A}$ and $T = \frac{D^*D}{A^*A}\frac{\rho}{k}$.

Now, using the boundary conditions:

$$\psi_{\mathrm{I}}(0) = \psi_{\mathrm{II}}(0) \rightarrow Ae^{ik0} + Be^{-ik0} = De^{i\rho 0} \rightarrow A + B = D$$
$$\frac{\partial\psi_{\mathrm{I}}}{\partial x}(0) = \frac{\partial\psi_{\mathrm{II}}}{\partial x}(0) \rightarrow ik(Ae^{ik0} - Be^{-ik0}) = i\rho De^{i\rho 0} \rightarrow A - B = \frac{i\rho}{ik}D$$

Subtracting the second equation from the 1st times $\frac{ik}{i\rho}$ we can find *R*:

$$\left(1 - \frac{ik}{i\rho}\right)A + \left(1 + \frac{ik}{i\rho}\right)B = 0$$
$$\frac{B}{A} = -\frac{\left(1 - \frac{ik}{i\rho}\right)}{\left(1 + \frac{ik}{i\rho}\right)} = \frac{i\rho - ik}{i\rho + ik} = \frac{\rho - k}{\rho + k}$$

$$R = \frac{B^*B}{A^*A} = \left(\frac{\rho - k}{\rho + k}\right)^2$$

$$R = \left(\frac{\rho - k}{\rho + k}\right)^2$$

$$R = \frac{\frac{2m(E-V_0)}{\hbar^2} - 2\frac{2m\sqrt{E(E-V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}{\frac{2m(E-V_0)}{\hbar^2} + 2\frac{2m\sqrt{E(E-V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}$$

$$\therefore R = \frac{(E-V_0) - \sqrt{E(E-V_0)} + E}{(E-V_0) + \sqrt{E(E-V_0)} + E}$$

Adding the two equations we can find *T*:

$$2A = \left(1 + \frac{i\rho}{ik}\right)D$$

$$\frac{D}{A} = \frac{2}{\left(1 + \frac{i\rho}{ik}\right)} = \frac{2ik}{(ik + i\rho)} = \frac{2k}{k + \rho}$$

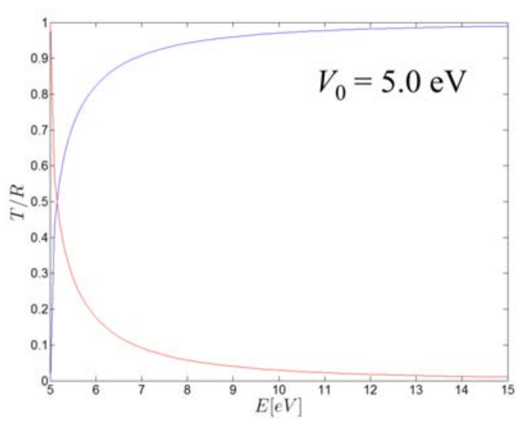
$$T = \frac{D^*D}{A^*A}\frac{\rho}{k} = \left(\frac{2k}{k+\rho}\right)^2\frac{\rho}{k} = \left(\frac{4\rho k}{(k+\rho)^2}\right)$$

$$T = \left(\frac{4\frac{2m\sqrt{E(E-V_0)}}{\hbar^2}}{\frac{2m(E-V_0)}{\hbar^2} + 2\frac{2m\sqrt{E(E-V_0)}}{\hbar^2} + \frac{2mE}{\hbar^2}}\right)$$

$$\therefore T = \frac{4\sqrt{E(E-V_0)}}{(E-V_0) + \sqrt{E(E-V_0)} + E}$$

Note that classically a particle would always reflect, but here there is a finite probability of transmission.

Plotting *R* (red) and *T* (blue) versus *E*.



For the case $E < V_0$, $i\rho$ becomes real, so let $i\rho = \alpha$.

$$\frac{B}{A} = \frac{\alpha - ik}{\alpha + ik}$$

$$R = \frac{B^* B}{A^* A} = \left(\frac{\alpha + ik}{\alpha - ik}\right)\left(\frac{\alpha - ik}{\alpha + ik}\right) = \frac{\alpha^2 + k^2}{\alpha^2 + k^2} = 1$$

For this case, the entire wave is reflected, analogous to the classical case. The wave function in region II is a decaying exponential, which is not classical. This implies even though electrons are reflected if their energy is lower than the barrier potential, they have a finite probability of penetrating the step barrier before being reflected.

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