Quantum tunnelling with two, or more, potential barriers.

Domenico Oricchio

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Abstract

I write the quantum tunnelling using the Laplace transform to obtain the solutions for multiple barriers.

The Laplace transform contain the initial condition of the Schrödinger equation, so that it is possible to connect the solutions in the boundaries of the potentials.

The Laplace transform of the Schrödinger equation for the generic potential barrier is:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + U(x)\Psi(x) = E\Psi(x)$$
$$\mathcal{L}\left\{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + U(x)\Psi(x)\right\} = \mathcal{L}\left\{E\Psi(x)\right\}$$
$$-\frac{\hbar^2}{2m}\left[s^2\mathcal{L}\{\Psi(x)\} - s\Psi(0) - \frac{d\Psi(0)}{dx}\right] = (E-U)\mathcal{L}\left\{\Psi(x)\right\}$$

so that in the free space ($U_2 = U_0 = 0$), and in the barriers $U_3 \neq 0$ and $U_1 \neq 0$

$$\left[s^2 + \frac{2m(E-U)}{\hbar^2}\right]\mathcal{L}\{\Psi(x)\} = \left[s^2 + K^2\right]\mathcal{L}\{\Psi(x)\} = s\Psi(0) + \frac{d\Psi(0)}{dx}$$
$$\mathcal{L}\{\Psi(x)\} = \frac{s\Psi(0) + \frac{d\Psi(0)}{dx}}{s^2 + K^2}$$

the solution of the Laplace transform is:

$$\Psi(x) = \cos(Kx)\Psi(0) + \frac{\sin(Kx)}{K}\Psi'(0)$$

that I write for each boundary:

$$\Psi(x) = \cos(K(x-x_i))\Psi(0) + \frac{\sin(K(x-x_i))}{K}\Psi'(0)$$
$$\Psi'(x) = -\sin(K(x-x_i))\Psi(0) + \cos(K(x-x_i))\Psi'(0)$$

this can be write like a transformation matrix for $x_i \le x \le x_{i+1}$, for a single potential barrier:

$$\begin{pmatrix} \Psi(x) \\ \Psi'(x) \end{pmatrix} = \begin{pmatrix} \cos(k(x-x_1)) & \dfrac{\sin(k(x-x_2)}{k} \\ -k\sin(k(x-x_2)) & \cos(k(x-x_2)) \end{pmatrix} \begin{pmatrix} \cos(K_1\Delta_1) & \dfrac{\sin(K_1\Delta_1)}{K_1} \\ -K_1\sin(K_1\Delta_1) & \cos(K_1\Delta_1) \end{pmatrix} \begin{pmatrix} \Psi(x_0) \\ \Psi'(x_0) \end{pmatrix}$$

the inverse of the transformation matrix is simple:

$$\begin{pmatrix} \Psi(x_0) \\ \Psi'(x_0) \end{pmatrix} = \begin{pmatrix} \cos(K_1\Delta_1) & -\dfrac{\sin(K_1\Delta_1)}{K_1} \\ K_1\sin(K_1\Delta_1) & \cos(K_1\Delta_1) \end{pmatrix} \begin{pmatrix} \Psi(x_1) \\ \Psi'(x_1) \end{pmatrix}$$

so that I can obtain the transformation matrix for a final wavefunction that it is only a progressive wavefunction $e^{ik(x-x_1)}$, that it is the transmitted wavefunction from the initial wavefunction; the final state in x_1 is the $\Psi(x_1) = 1$ and $\Psi'(x_1) = ik$, so that the initial state with this final condition is

$$\begin{pmatrix} \Psi(x_0) \\ \Psi'(x_0) \end{pmatrix} = \begin{pmatrix} \cos(K_1\Delta_1) & -\dfrac{\sin(K_1\Delta_1)}{K_1} \\ K_1\sin(K_1\Delta_1) & \cos(K_1\Delta_1) \end{pmatrix} \begin{pmatrix} 1 \\ ik \end{pmatrix} = \begin{pmatrix} \cos(K_1\Delta_1) - i\dfrac{k}{K_1}\sin(K_1\Delta_1) \\ ik\cos(K_1\Delta_1) + K_1\sin(K_1\Delta_1) \end{pmatrix}$$

and the initial solution using the inverse of the transformation matrix is (to simplify I choose $x_0 = 0$):

$$\begin{aligned} \Psi(x) &= \Psi(x_0)\cos(kx) + \Psi'(x_0)\frac{\sin(kx)}{k} = \Psi(x_0)\frac{e^{ikx}+e^{-ikx}}{2} + \Psi'(x_0)\frac{e^{ikx}-e^{-ikx}}{2ik} = \\ &= \frac{1}{2}\left[\Psi(x_0) + \frac{\Psi'(x_0)}{ik}\right]e^{ikx} + \frac{1}{2}\left[\Psi(x_0) - \frac{\Psi'(x_0)}{ik}\right]e^{-ikx} \end{aligned}$$

so that the amplitudes of the e^{ikx} and e^{-ikx} are:

$$\begin{aligned} \Psi_{in}(x) &= \left[\cos(K_1\Delta_1) - i\frac{K_1^2+k^2}{2kK_1}\sin(K_1\Delta_1)\right]e^{ikx} + \left[i\frac{K_1^2-k^2}{2kK_1}\sin(K_1\Delta_1)\right]e^{-ikx} \\ \Psi_{out}(x) &= e^{ikx} \end{aligned}$$

so that I obtain a solution that it is true for each value of E, so that $K_1(E)$ can be a real value, or can be complex value; I can write the wavefunctions:

$$\begin{aligned} \Psi_{in}(x) &= \frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \left[\frac{i\dfrac{K_1^2-k^2}{2kK_1}\sin(K_1\Delta_1)}{\cos(K_1\Delta_1) - i\dfrac{K_1^2+k^2}{2kK_1}\sin(K_1\Delta_1)}\right]\frac{e^{-ikx}}{\sqrt{2\pi\hbar}} = \Psi_\tau\frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \Psi_\rho\frac{e^{-ikx}}{\sqrt{2\pi\hbar}} \\ \Psi_{out}(x) &= \frac{1}{\cos(K_1\Delta_1) - i\dfrac{K_1^2+k^2}{2kK_1}\sin(K_1\Delta_1)}\frac{e^{ikx}}{\sqrt{2\pi\hbar}} \end{aligned}$$

The transmission coefficients is:

$$\tau = \left| \frac{1}{\cos(K_1\Delta_1) - i\dfrac{K_1^2+k^2}{2kK_1}\sin(K_1\Delta_1)} \right|^2 = \frac{1}{\cos^2(K_1\Delta_1) + \left(\dfrac{K_1^2+k^2}{2kK_1}\right)^2 \sin^2(K_1\Delta_1)}$$

the tunnel effect happen when $K_1 = i|K_1|$, so that the energy of the particle is lower of the potential barrier, and the transmission coefficient is:

$$\tau \simeq \Psi_\tau^*\Psi_\tau = \frac{1}{\cosh^2(K_1\Delta_1) + \left(\dfrac{k^2-|K_1|^2}{2k|K_1|}\right)^2 \sinh^2(K_1\Delta_1)}$$

$$\rho \simeq \Psi_\rho^*\Psi_\rho = \frac{\left(\dfrac{K_1^2+k^2}{2kK_1}\right)^2 \sinh^2(K_1\Delta_1)}{\cosh^2(K_1\Delta_1) + \left(\dfrac{k^2-|K_1|^2}{2k|K_1|}\right)^2 \sinh^2(K_1\Delta_1)}$$

It is simple to obtain a tunnel effect with two barriers, using the inverse of three transformation matrices:

$$\begin{pmatrix} \Psi(x_0) \\ \Psi'(x_0) \end{pmatrix} = \begin{pmatrix} \cos(K_1\Delta_1) & -\dfrac{\sin(K_1\Delta_1)}{K_1} \\ K_1\sin(K_1\Delta_1) & \cos(K_1\Delta_1) \end{pmatrix} \begin{pmatrix} \cos(k\Delta_2) & -\dfrac{\sin(k\Delta_2)}{k} \\ k\sin(k\Delta_2) & \cos(k\Delta_2) \end{pmatrix} \begin{pmatrix} \cos(K_3\Delta_3) & -\dfrac{\sin(K_3\Delta_3)}{K_3} \\ K_3\sin(K_3\Delta_3) & \cos(K_3\Delta_3) \end{pmatrix} \begin{pmatrix} 1 \\ ik \end{pmatrix}$$

so that:

$$\begin{array}{rccc} \multicolumn{4}{l}{\Psi(x_0) = \sum_{jks} \Lambda_{1j}^{(3)}\Lambda_{jk}^{(2)}\Lambda_{ks}^{(1)}\Psi_s =} \\ \cos(K_1\Delta_1) & \cos(k\Delta_2) & \cos(K_3\Delta_3) & 1+ \\ -\cos(K_1\Delta_1) & \cos(k\Delta_2) & \dfrac{\sin(K_3\Delta_3)}{K_3} & ik+ \\ -\cos(K_1\Delta_1) & \dfrac{\sin(k\Delta_2)}{k} & K_3\sin(K_3\Delta_3) & 1+ \\ -\cos(K_1\Delta_1) & \dfrac{\sin(k\Delta_2)}{k} & \cos(K_3\Delta_3) & ik+ \\ -\dfrac{\sin(K_1\Delta_1)}{K_1} & k\sin(k\Delta_2) & \cos(K_3\Delta_3) & 1+ \\ +\dfrac{\sin(K_1\Delta_1)}{K_1} & k\sin(k\Delta_2) & \dfrac{\sin(K_3\Delta_3)}{K_3} & ik+ \\ -\dfrac{\sin(K_1\Delta_1)}{K_1} & \cos(k\Delta_2) & K_3\sin(K_3\Delta_3) & 1+ \\ -\dfrac{\sin(K_1\Delta_1)}{K_1} & \cos(k\Delta_2) & \cos(K_3\Delta_3) & ik \end{array}$$

$$
\begin{array}{rrrr}
\Psi'(x_0) = \sum_{jks} \Lambda^{(3)}_{2j} \Lambda^{(2)}_{jk} \Lambda^{(1)}_{ks} \Psi_s = & & & \\
K_1 \sin(K_1\Delta_1) & \cos(k\Delta_2) & \cos(K_3\Delta_3) & 1+ \\
-K_1 \sin(K_1\Delta_1) & \cos(k\Delta_2) & \frac{\sin(K_3\Delta_3)}{K_3} & ik+ \\
-K_1 \sin(K_1\Delta_1) & \frac{\sin(k\Delta_2)}{k} & K_3\sin(K_3\Delta_3) & 1+ \\
-K_1 \sin(K_1\Delta_1) & \frac{\sin(k\Delta_2)}{k} & \cos(K_3\Delta_3) & ik+ \\
+\cos(K_1\Delta_1) & k\sin(k\Delta_2) & \cos(K_3\Delta_3) & 1+ \\
-\cos(K_1\Delta_1) & k\sin(k\Delta_2) & \frac{\sin(K_3\Delta_3)}{K_3} & ik+ \\
+\cos(K_1\Delta_1) & \cos(k\Delta_2) & K_3\sin(K_3\Delta_3) & 1+ \\
+\cos(K_1\Delta_1) & \cos(k\Delta_2) & \cos(K_3\Delta_3) & ik
\end{array}
$$

I can evaluate the input and output wavefunctions:

$$
\begin{aligned}
&\Psi_{in}(x) = \Big[2\cos(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3) - i\frac{k^2+K_3^2}{kK_3}\cos(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3)+ \\
&-\frac{K_3^2+k^2}{kK_3}\cos(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3) - 2i\cos(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3)+ \\
&-\frac{k^2+K_1^2}{kK_1}\sin(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3) + i\frac{k^4+K_1^2K_3^2}{k^2K_1K_3}\sin(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3)+ \\
&-\frac{K_3^2+K_1^2}{K_1K_3}\sin(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3) - i\frac{k^2+K_1^2}{kK_1}\sin(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3)\Big]\frac{e^{ikx}}{\sqrt{2\pi\hbar}}+ \\
&\Big[-i\frac{k^2-K_3^2}{kK_3}\cos(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3) - \frac{K_3^2-k^2}{kK_3}\cos(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3)+ \\
&-\frac{k^2-K_1^2}{kK_1}\sin(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3) + i\frac{k^4-K_1^2K_3^2}{k^2K_1K_3}\sin(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3)+ \\
&-\frac{K_3^2-K_1^2}{K_1K_3}\sin(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3) - i\frac{k^2-K_1^2}{kK_1}\sin(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3)\Big]\frac{e^{-ikx}}{\sqrt{2\pi\hbar}} = Ae^{ikx}+Be^{-ikx} \\
&\Psi_{out} = \frac{e^{-ikx}}{\sqrt{2\pi\hbar}}
\end{aligned}
$$

I scale the wavefunction to obtain a simple input function:

$$
\begin{aligned}
\Psi_{in}(x) &= \frac{e^{ikx}}{\sqrt{2\pi\hbar}} + \frac{B}{A}\frac{e^{-ikx}}{\sqrt{2\pi\hbar}} \\
\Psi_{out} &= \frac{1}{A}\frac{e^{-ikx}}{\sqrt{2\pi\hbar}}
\end{aligned}
$$

so the transmission an refletion coefficients are:

$$\tau = \frac{|B|^2}{|A|^2}$$
$$\rho = \frac{1}{|A|^2}$$

I write the $|A|^2$ and $|B|^2$ parameters:

$$|A|^2 = \Bigg[2\cos(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3) - \frac{K_3^2+k^2}{kK_3}\cos(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3) + $$
$$+ -\frac{k^2+K_1^2}{kK_1}\sin(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3) - \frac{K_3^2+K_1^2}{K_1K_3}\sin(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3)\Bigg]^2 +$$
$$+ \Bigg[-\frac{k^2+K_3^2}{kK_3}\cos(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3) - 2\cos(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3) +$$
$$+\frac{k^4+K_1^2K_3^2}{k^2K_1K_3}\sin(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3) - \frac{k^2+K_1^2}{kK_1}\sin(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3)\Bigg]^2$$

$$|B|^2 = \Bigg[-\frac{K_3^2-k^2}{kK_3}\cos(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3) - \frac{k^2-K_1^2}{kK_1}\sin(K_1\Delta_1)\sin(k\Delta_2)\cos(K_3\Delta_3) +$$
$$-\frac{K_3^2-K_1^2}{K_1K_3}\sin(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3)\Bigg]^2 + \Bigg[-\frac{k^2-K_3^2}{kK_3}\cos(K_1\Delta_1)\cos(k\Delta_2)\sin(K_3\Delta_3) +$$
$$+\frac{k^4-K_1^2K_3^2}{k^2K_1K_3}\sin(K_1\Delta_1)\sin(k\Delta_2)\sin(K_3\Delta_3) - \frac{k^2-K_1^2}{kK_1}\sin(K_1\Delta_1)\cos(k\Delta_2)\cos(K_3\Delta_3)\Bigg]$$

there are changes in the trigonometric function, when the energy of the free particle is under the potential thresholds: if $U_1 < U_3$ then the energy E can be $E < U_1 < U_3$ so that the parameters K_1, K_3 are complex values, if $U_1 < E < U_3$ then the K_1 is real, and K_3 is complex value, if $U_1 < U_3 < E$ the the K_1, K_3 are reals; the transmission and reflection function have trigonometric function, or hyperbolic functions depending on the E values.

It is possible to write a program to write automatically the transmission and reflection coefficients using the transformation matrices, recursively, using only the barriers potential values and the width of the barriers: the continuity conditions are automatically verified by Laplace transform using the matrix transform.

References

[1] P. Caldirola, R. Cirelli, G. M. Prosperi (1982). Introduzione alla fisica teorica. Utet