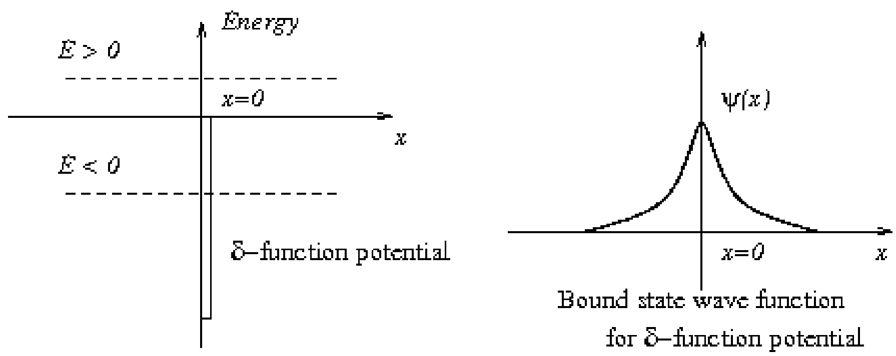
δ-function potential

A delta-function is an infinitely high, infinitesimally narrow spike at the $x = a$ say, where a can also be origin. Let the potential of the form,

$$V(x) \,=\, -\,\alpha\,\delta(x), \tag{70}$$

where, α is some constant of appropriate dimension.



The Schrödinger equation for the delta-function well reads

$$-\,\frac{\hbar^2}{2m}\,\frac{d^2\psi}{dx^2} - \alpha\,\delta(x)\psi \,=\, E\psi. \tag{71}$$

This allows solutions for both the bound states $E < 0$ and scattering states $E > 0$.

Bound state E $<$ 0: In both the regions $x < 0$ and $x > 0$, the potential is $V(x) = 0$ and, with $\kappa^2 = -2mE/\hbar^2$,

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi \,=\, 0 \qquad \left\{ \begin{array}{lcll} \psi(x) & = & A\,e^{-\kappa x} + B\,e^{\kappa x} & x < 0 \\ \psi(x) & = & F\,e^{-\kappa x} + G\,e^{\kappa x} & x > 0 \end{array} \right. \tag{72}$$

However, the term $A\,\exp(-\kappa x)$ blows up as $x \to -\infty$ and $G\,\exp(\kappa x)$ blows up as $x \to \infty$, therefore dropped $A = G = 0$. Hence the solution now is

$$x < 0: \quad \psi \,=\, B\,e^{\kappa x} \qquad x > 0 \;\; \psi \,=\, F\,e^{-\kappa x}.$$

To determine the coefficients and the energy of the bound state (if any), the boundary conditions are used: ψ is always continuous and $d\psi/dx$ is discontinuous because of infinite δ-potential (3). The continuity of wavefunction yields,

$$F \,=\, B \;\;\Rightarrow\;\; \psi(x) \,=\, \left\{ \begin{array}{ll} B\,e^{\kappa x} & x < 0 \\ B\,e^{-\kappa x} & x > 0 \end{array} \right. \tag{73}$$

The discontinuity in $d\psi/dx$ implies,

$$\Delta\left(\frac{d\psi}{dx}\right) \,=\, \left.\frac{\partial\psi}{\partial x}\right|_{+\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{-\epsilon} \,=\, -\,\frac{2m\alpha}{\hbar^2}\,\psi(0)$$

$$x < 0: \left.\frac{\partial\psi}{\partial x}\right|_{-\epsilon} \,=\, B\kappa, \qquad x > 0: \left.\frac{\partial\psi}{\partial x}\right|_{+\epsilon} \,=\, -B\kappa, \qquad \psi(0) \,=\, B$$

$$\Rightarrow\;\; \Delta\left(\frac{d\psi}{dx}\right) \,=\, -\,2B\kappa \,=\, -\,\frac{2m\alpha}{\hbar^2}\,B \;\;\Rightarrow\;\; \kappa \,=\, \frac{m\alpha}{\hbar^2} \tag{74}$$

Hence the allowed, and the *only one* available bound state energy is,

$$E = -\frac{\hbar^2\kappa^2}{2m} = -\frac{m\alpha^2}{2\hbar^2} \tag{75}$$

Normalizing the wavefunction ψ:

$$\int_{-\infty}^{+\infty} |\psi|^2 dx = 2|B|^2 \int_0^\infty e^{-2\kappa x} dx = \frac{|B|^2}{\kappa} = 1 \;\Rightarrow\; B = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar} \tag{76}$$

Therefore, the bound state solution of δ-potential is,

$$\psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \;\text{ and }\; E = -\frac{m\alpha^2}{2\hbar^2} \tag{77}$$

Scattering state $\mathbf{E > 0}$: In both the regions $x < 0$ and $x > 0$, the potential is $V(x) = 0$ and, with $k^2 = 2mE/\hbar^2$,

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \qquad \left\{ \begin{array}{lcll} \psi(x) & = & A\, e^{ikx} + B\, e^{-ikx} & x < 0 \\ \psi(x) & = & F\, e^{ikx} & x > 0 \end{array} \right. \tag{78}$$

Imposing the boundary conditions the same way as bound state, from the continuity of ψ at $x = 0$ we have,

$$F = A + B \tag{79}$$

and the discontuity in $d\psi/dx$ at $x = 0$,

$$\begin{aligned} \left.\frac{\partial\psi}{\partial x}\right|_{+\epsilon} - \left.\frac{\partial\psi}{\partial x}\right|_{-\epsilon} &= -\frac{2m\alpha}{\hbar^2}\,\psi(0) \\ ikF - ik(A - B) &= -\frac{2m\alpha}{\hbar^2}\,(A + B) \end{aligned} \tag{80}$$

Solving (79) and (80) for F and B in terms of A, and using $\beta = m\alpha/\hbar^2 k$,

$$F = \frac{1}{1 - i\beta}\,A \qquad \text{and} \qquad B = \frac{i\beta}{1 - i\beta}\,A \tag{81}$$

Therefore, the refelction and transmission coefficients are obtained as,

$$R = \frac{|B|^2}{|A|^2} = \frac{\beta^2}{1 + \beta^2} = \frac{1}{1 + (2E\hbar^2/m\alpha^2)} \tag{82}$$

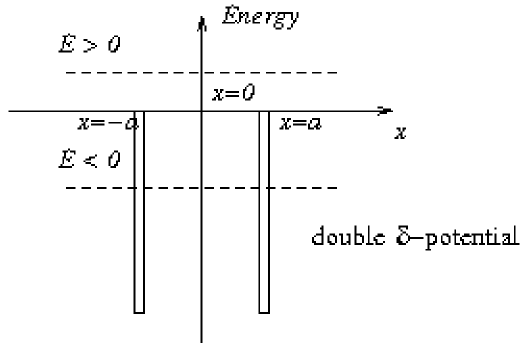
$$T = \frac{|F|^2}{|A|^2} = \frac{1}{1 + \beta^2} = \frac{1}{1 + (m\alpha^2/2E\hbar^2)} \tag{83}$$

The non-zero transmission probability gives us the tunneling phenomenon – higher the energy greater is the probability of tunneling.

Double δ-function potential

Particularly interesting potentials having lot of practical relevances are double or multiple (periodic) square well potentials. These kind of potentials are often found in electronic arrangements in solids or in molecules. First consider an attractive double δ-function potential given by,

$$V(x) = -\alpha\left[\delta(x + a) + \delta(x - a)\right], \quad \text{where } \alpha = \hbar^2/ma. \tag{84}$$



The interest is in $E < 0$ bound states and the Schrödinger equations are solved for wave functions in the regions $I:\ x < -a$, $II:\ -a \le x \le a$ and $III:\ x > a$. In all these regions we have the same Schrödinger equation and the solutions are (discarding those that blow up at $\pm\infty$),

$$\frac{d^2\psi}{dx^2} - \kappa^2\psi \;=\; 0, \qquad \kappa^2 = -\,\frac{2mE}{\hbar^2}$$

$$x < -a \;\;:\;\; \psi(x) \;=\; A\,e^{\kappa x} \tag{85}$$

$$-a \le x \le a \;\;:\;\; \psi(x) \;=\; C\,e^{\kappa x} + D\,e^{-\kappa x} \tag{86}$$

$$x > a \;\;:\;\; \psi(x) \;=\; F\,e^{-\kappa x}. \tag{87}$$

The boundary conditions are applied next to evaluate the unknown constants.

Continuity of ψ at $x = -a$:

$$A\,e^{-\kappa a} \;=\; C\,e^{-\kappa a} + D\,e^{\kappa a} \tag{88}$$

Continuity of ψ at $x = a$:

$$F\,e^{-\kappa a} \;=\; C\,e^{\kappa a} + D\,e^{-\kappa a} \tag{89}$$

Discontinuity of $d\psi/dx$ at $x = -a$:

$$\kappa\,\left(C\,e^{-\kappa a} - D\,e^{\kappa a}\right) - \kappa\,A\,e^{-\kappa a} \;=\; -\frac{2m\alpha}{\hbar^2}\,A\,e^{-\kappa a} \;=\; -\frac{2}{a}\,A\,e^{-\kappa a} \tag{90}$$

Discontinuity of $d\psi/dx$ at $x = a$:

$$-\kappa\,F\,e^{-\kappa a} - \kappa\,\left(C\,e^{-\kappa a} - D\,e^{\kappa a}\right) \;=\; -\frac{2m\alpha}{\hbar^2}\,F\,e^{-\kappa a} \;=\; -\frac{2}{a}\,F\,e^{-\kappa a}. \tag{91}$$

The discontinuous boundary equations can be simplified as,

$$\text{For } x = -a:\quad A\,e^{-\kappa a}\left(\kappa - \tfrac{2}{a}\right) \;=\; \kappa\left(C\,e^{-\kappa a} - D\,e^{\kappa a}\right) \tag{92}$$

$$\text{For } x = a:\quad F\,e^{-\kappa a}\left(\tfrac{2}{a} - \kappa\right) \;=\; \kappa\left(C\,e^{-\kappa a} - D\,e^{\kappa a}\right). \tag{93}$$

To determine th allowed energies, we solved the boundary equations (88, 89, 92, 93) for C and D by eliminating A and F,

$$\left.\begin{aligned} C\,e^{-\kappa a} &= D\,e^{\kappa a}(\kappa a - 1) \\ D\,e^{-\kappa a} &= C\,e^{\kappa a}(\kappa a - 1) \end{aligned}\right\}\; C^2 \;=\; D^2 \;\;\Rightarrow\;\; C \;=\; \pm D. \tag{94}$$

This is nothing surprising, because of the symmetry of the potential, we have both even and odd parity solutions

$$\text{Even parity } C = D:\quad \psi \;=\; C\left(e^{\kappa x} + e^{-\kappa x}\right) \;=\; C'\cosh(\kappa x) \tag{95}$$

$$\text{Odd parity } C = -D:\quad \psi \;=\; C\left(e^{\kappa x} - e^{-\kappa x}\right) \;=\; C'\sinh(\kappa x) \tag{96}$$

As for solving for the bound state(s), we solve the transcendental equations,

$$\begin{aligned}
\text{Even} - \;\; C = \;\; D: \quad & e^{-2\kappa a} = \kappa a - 1 \;\; \Rightarrow e^{-2y} = y - 1, \;\; \text{where} \;\; y = \kappa a && (97)\\
\text{Odd} - \;\; C = -D: \quad & e^{-2\kappa a} = 1 - \kappa a \;\; \Rightarrow e^{-2y} = 1 - y, \;\; \text{where} \;\; y = \kappa a && (98)
\end{aligned}$$

The only even bound state solution is $y = \kappa a \approx 1.11$ and therefore,

$$E_{\text{even}} = -\frac{1}{2m}\left(\frac{1.11\hbar}{a}\right)^2. \tag{99}$$

However, we do not have any odd state since the solution corresponding to (98) is $y = \kappa a = 0$ and this leaves bound state wave function non normalizable. But for $\alpha > \hbar^2/ma$, we can get one odd parity bound state also.

If we compare the bound state energy of single delta potential (75) with double delta potential (99), we see double δ-function potential gives lower bound state energy (with $\alpha = \hbar^2/ma$),

$$E_s = -\frac{m\alpha^2}{2\hbar^2} = -\frac{\hbar^2}{2ma^2} \quad \text{and} \quad E_d = -(1.11)^2\frac{\hbar^2}{2ma^2}.$$