Appendix 17: Delta Function

A17.1. General

A delta function (also called Dirac delta function) is a mathematical function, which is defined as:

$$\delta(x) = \infty \text{, for } x = 0$$

$$\delta(x) = 0 \text{, for } x \neq 0 \tag{A17.1.1}$$

$$\text{and } \int_{-\infty}^{\infty} \delta(x) dx = 1$$

i.e. a function which is only non-zero at $x = 0$ with a total area equal to one.

The delta function is symmetric:

$$\delta(-x) = \delta(x) \tag{A17.1.2}$$

and when multiplied with a function $F(x)$ and integrated, yields this function's value at $x = 0$:

$$\int_{-\infty}^{\infty} F(x)\delta(x) dx = F(0) \tag{A17.1.3}$$

Similarly, a shifted delta function will result in the function's value at that point:

$$\int_{-\infty}^{\infty} F(x)\delta(x-\xi) dx = F(\xi) \tag{A17.1.4}$$

A17.2. Solving Schrödinger's equation with a delta function potential

The one-dimensional Schrödinger's equation with a delta function potential with area, M, and located at $x = x_0$ is as follows:

$$-\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2} + M\delta(x - x_0)\Psi(x) = E\Psi(x) \tag{A17.2.1}$$

The general solutions are the same as for $V(x) = 0$ on either side of $x = x_0$:

$$\Psi(x) = A\sin kx + B\cos kx \text{ for } x < x_0$$

$$\Psi(x) = C\sin kx + D\cos kx \text{ for } x > x_0 \tag{A17.2.2}$$

$$\text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

and the constants A, B, C and D must be determined from the boundary conditions.

The boundary condition at the delta function is obtained by integrating Schrödinger's equation just around the delta function, yielding:

$$\int_{x_0-\varepsilon}^{x_0+\varepsilon} (-)\frac{\hbar^2}{2m}\frac{d^2\Psi}{dx^2}dx + \int_{x_0-\varepsilon}^{x_0+\varepsilon} M\delta(x-x_0)\Psi(x)dx = \int_{x_0-\varepsilon}^{x_0+\varepsilon} E\Psi(x)dx \tag{A17.2.3}$$

Which reduces in the limit where $\varepsilon \to 0$ to:

$$\left.\frac{d\Psi}{dx}\right|_{x_0+\varepsilon} - \left.\frac{d\Psi}{dx}\right|_{x_0-\varepsilon} = \frac{2m}{\hbar^2}M\Psi(x_0) \tag{A17.2.4}$$

The boundary conditions at $x = x_0$ are: 1) the continuity of the wave function at x_0 and 2) a discontinuity of the derivative of the wave function at x_0 with the difference in slope given by A17.2.4.[1]

The resulting equations are:

$$\Psi(x_0) = A\sin kx_0 + B\cos kx_0 = C\sin kx_0 + D\cos kx_0$$

and

$$kA\cos kx_0 - kB\sin kx_0 = kC\cos kx_0 - kD\sin kx_0 + \frac{2m}{\hbar^2}M\Psi(x_0) \tag{A17.2.5}$$

$$\text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

[1] This boundary condition can easily be generalized for any potential that includes one or more delta functions.

A17.3. Example: tunneling through a delta function

As an example we consider an incoming wave with amplitude 1 incident on the delta function with area, *M*, and located at $x = 0$. The incident, reflected and transmitted waves are then described by:

$$\Psi_i(x) = \exp ikx = \cos kx + i \sin kx$$

$$\Psi_r(x) = r \exp(-ikx) = r \cos kx - ir \sin kx \tag{A17.3.1}$$

$$\Psi_t(x) = t \exp(ikx) = t \cos kx + it \sin kx$$

Where *r* is the amplitude of the reflected wave and *t* is the amplitude of the transmitted wave. The sum of the incident and reflected wave is the wave function for $x < 0$ and the transmitted wave function is the wave function for $x > 0$, so that:

$$A = i(1 - r),\ B = 1 + r,\ C = it \text{ and } D = t \tag{A17.3.2}$$

The boundary conditions at x = 0 then become:

$$\Psi(x_0) = 1 + r = t \ \text{ and } \ ik(1-r) = ikt + \frac{2m}{\hbar^2} Mt \tag{A17.3.3}$$

So that

$$ik(2-t) = ikt + \frac{2m}{\hbar^2} Mt \ \text{ or } \ t = \frac{ik\hbar^2}{mM + ik\hbar^2}$$
$$\text{and } \ r = t - 1 = \frac{-mM}{mM + ik\hbar^2} \tag{A17.3.4}$$

Note that both *r* and *t* are complex numbers, which accounts for a phase shift relative to the incident wave.

The corresponding transmission and reflection are:

$$T = tt^* = \frac{k^2\hbar^4}{m^2M^2 + k^2\hbar^4} = \frac{2E\hbar^2}{mM^2 + 2E\hbar^2}$$
$$\text{and } \ R = rr^* = \frac{mM^2}{mM^2 + 2E\hbar^2} \tag{A17.3.5}$$

Confirming that $T + R = 1$.