

DELTA-FUNCTION WELL - BOUND STATE

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Reference: Griffiths, David J. (2005), *Introduction to Quantum Mechanics*, 2nd Edition; Pearson Education - Sec 2.5.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.3.

If the potential function in the Schrödinger equation goes to infinity at infinite distance (as is the case in the infinite square well and the harmonic oscillator), then the only allowed energies of a particle in such a system are discrete, quantized energy states. A particle moving in such a potential can exist only in a bound state, where the probability of finding the particle tends to zero beyond some finite distance. In the infinite square well, the particle is bounded by the infinitely high walls, and the probability of finding it outside these walls is rigorously zero. In the harmonic oscillator, where the potential tends to infinity gradually, the particle can exist at greater distances if its energy is higher (just as in classical physics, a mass with higher energy will have a larger range of oscillation on a spring), but for any given energy state, the probability of finding the particle in any region where the potential is greater than the energy drops rapidly to zero.

Such potentials offer insurmountable barriers to the particle, so the notions of scattering from, or transmission through a region do not arise (in a scattering experiment, the particle is assumed to travel in from infinity in one direction and scatter back to infinity in the opposite direction; with an infinite potential, this is not possible). The only way we can talk about scattering or transmission of particles is to deal with cases where the particle has the possibility of travelling arbitrarily far. In such cases, infinitely high barriers cannot appear.

Unfortunately, the mathematics for such cases tends to get a bit more complicated than in those cases with infinite barriers (and as we've seen in the case of the harmonic oscillator, the mathematics is adequately hard even there!). One case that is often analyzed as an introduction to scattering and transmission is that of the *delta-function well*. The Dirac delta-function $\delta(x)$ is a mathematical curiosity in that it is zero everywhere except at $x = 0$, is infinite at that one point, and has an integral equal to 1 provided that the interval of integration includes the point $x = 0$ (the integral is zero otherwise).

Clearly the delta-function doesn't describe any real physical situation, since no known potential function is a delta-function. However, the function does have its uses as an approximation in many areas of physics, notably electrodynamics (where in fact the representation of an electron as a point charge just might actually be realistic - electrons have what appears to be zero size, or something very close to it). The delta-function does allow one of the simpler analyses of scattering and transmission, however, so it's useful to have a look at it before tackling more realistic cases.

The potential we'll consider is

$$V(x) = -\alpha\delta(x) \quad (1)$$

where α is a positive constant, so this represents a potential well of infinite depth at the origin, but with infinitesimally small width. Note that, from the properties of the delta-function, this is the same as writing

$$V(x) = -\delta(x/\alpha) \quad (2)$$

Since $\delta(x)$ is infinite at $x = 0$, no matter what the value of α , α does not measure the depth of the well; rather it might be thought of more as measuring the 'strength' of the potential in some sense. As we'll see, α *does* turn up in the energy levels and in the probabilities of scattering and transmission, so it's not an irrelevant parameter.

Since $\delta(x) = 0$ everywhere except $x = 0$, the Schrödinger equation at these points reduces to

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi \quad (3)$$

We'll consider bound states here and leave the scattering states to another post. For bound states, the energy E has to be negative, since it has to be less than the potential on either side of the (infinitesimally narrow) well, which has its top at $V(x) = 0$. So we can rewrite this as

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi \quad (4)$$

where

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \quad (5)$$

Since E is negative, κ is real and can be assumed positive.

Now we have to be careful here. The general solution of 4 is quite simple:

$$\psi(x) = Ae^{-\kappa x} + Be^{\kappa x} \quad (6)$$

as can be checked by direct substitution. The constants A and B , one might think, can be determined by some boundary conditions or by normalization. But we have in fact two distinct regions in which we have to find the solution: $x < 0$ and $x > 0$ (we'll get to what happens at $x = 0$ in a moment). Clearly if we want the solution to be normalizable, we can't use the same solution in both regions, since for $x < 0$, the $Ae^{-\kappa x}$ term tends to infinity for large negative x , and for $x > 0$, the *other* term $Be^{\kappa x}$ tends to infinity for large positive x . So we need a separate solution in each area. If we take 6 as the solution for $x < 0$, then we can propose another function with different constants as the solution for $x > 0$:

$$\psi_-(x) = Ae^{-\kappa x} + Be^{\kappa x} \quad (7)$$

$$\psi_+(x) = Ce^{-\kappa x} + De^{\kappa x} \quad (8)$$

We can dispose of two of the constants immediately by requiring the wave functions tend to zero at infinity. This gives us $A = 0$ and $D = 0$, so we have

$$\psi_-(x) = Be^{\kappa x} \quad (9)$$

$$\psi_+(x) = Ce^{-\kappa x} \quad (10)$$

Somehow we have to join up these functions across $x = 0$. We can refer to Born's conditions on the wave function and note that if the wave function is continuous at $x = 0$, then we must have $B = C$, so we're now down to

$$\psi_-(x) = Be^{\kappa x} \quad (11)$$

$$\psi_+(x) = Be^{-\kappa x} \quad (12)$$

However, since the potential is infinite at $x = 0$, we can't require that the derivative of the wave function be continuous.

So what can we say about B ? The trick here is to try integrating the Schrödinger equation across the boundary. Putting the delta-function potential into the Schrödinger equation we get

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\delta(x)\psi = E\psi \quad (13)$$

Now if we integrate this equation term by term across the boundary, we get, for some value of ϵ :

$$-\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \frac{d^2\psi}{dx^2} dx - \alpha \int_{-\epsilon}^{\epsilon} \delta(x)\psi dx = E \int_{-\epsilon}^{\epsilon} \psi dx \quad (14)$$

$$-\frac{\hbar^2}{2m} \frac{d\psi}{dx} \Big|_{-\epsilon}^{\epsilon} - \alpha\psi(0) = E \int_{-\epsilon}^{\epsilon} \psi dx \quad (15)$$

If we take the limit as $\epsilon \rightarrow 0$, the integral on the right tends to zero, since it is the integral of a continuous function over an infinitesimally small interval. The first term on the left, however, will *not* be zero, since derivative of the wave function is not continuous when the potential is infinite. However, it does give us a relation which ends up determining the bound state energy. So if we take the limit as $\epsilon \rightarrow 0$, we get

$$-\frac{\hbar^2}{2m} \left[\frac{d\psi}{dx} \Big|_{\epsilon \downarrow 0} - \frac{d\psi}{dx} \Big|_{-\epsilon \uparrow 0} \right] = \alpha B \quad (16)$$

$$\frac{\hbar^2}{m} B\kappa = \alpha B \quad (17)$$

$$\kappa = \frac{m\alpha}{\hbar^2} \quad (18)$$

$$E = -\frac{\hbar^2\kappa^2}{2m} \quad (19)$$

$$= -\frac{m\alpha^2}{2\hbar^2} \quad (20)$$

Just as in the infinite square well, our analysis ends up giving a condition on the energy E rather than on the constant B . B is in fact easily determined by normalizing the wave function:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = |B|^2 \left(\int_{-\infty}^0 e^{2\kappa x} dx + \int_0^{\infty} e^{-2\kappa x} dx \right) \quad (21)$$

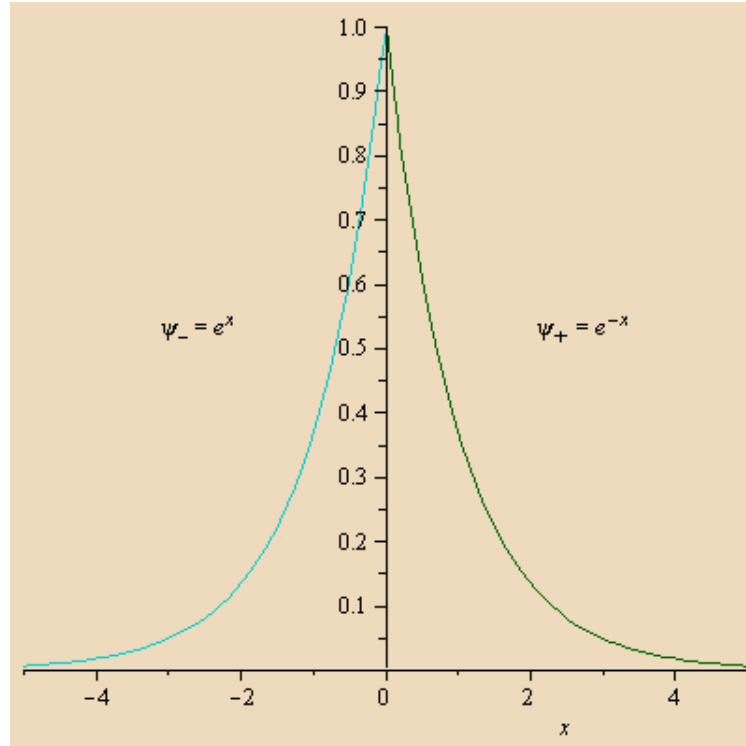
$$= \frac{1}{\kappa} |B|^2 = 1 \quad (22)$$

$$B = \sqrt{\kappa} \quad (23)$$

$$= \frac{\sqrt{m\alpha}}{\hbar} \quad (24)$$

Thus a delta-function well has precisely one bound state, and the energy does depend on the parameter α : the larger α is, the lower (more negative) the energy E is. This is why it makes sense to consider α as the strength of the potential; it regulates how deeply bound the particle in a stationary state is within the well.

The wave function for the bound state looks like this (here we've taken $\kappa = 1$ but it's just the general shape of the curve that's important):



The probability of finding the particle is maximum at $x = 0$ and falls off exponentially on either side. Since the exponent is $\pm\kappa x$ and $\kappa = m\alpha/\hbar^2$, the rate of exponential fall-off depends on the strength of the delta-function. This behaviour is consistent with other bound states. The infinite square well is essentially a well with infinite strength, so the fall off at the boundaries is absolute - there is no exponential decay. With the harmonic oscillator, the wave function oscillates (in space) within the well (although mathematically, the oscillation is due to Legendre polynomials rather than trigonometric functions), but in the regions where the potential is greater than the energy, there is again an exponential decay. In the case of a delta function, since the well itself is infinitesimally narrow, there is no region where the wave nature of the particle is displayed - the exponential fall-off starts immediately either side of the well.

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