The Dirac Delta Function

The Dirac delta, \( \delta(x-x_0) \), is a strange mathematical object designed to describe something that is quite ordinary in physics: the density of a point object. If we lived in one dimension \((x)\) and placed a point electron at position \(x_0\), then it has a total charge \(e\) but its size is zero, so its charge density \(\lambda(x) = \text{charge-per-unit-length}\) is

- zero at every position \(x \neq x_0\),
- infinity at position \(x = x_0\), because there \(\lambda = (\text{charge-of-electron}) / (\text{length-of-point-electron}) = e / 0 = \infty\),
- yet the integral \(\int \lambda(x) \, dx\) over all space = the total charge on electron = \(e = \text{NOT infinite}\).

The delta function \(\delta(x)\) is an infinitely tall, infinitely narrow spike with a finite integral.

**Definition #1** = 3 defining properties :

1. \(\delta(x) = 0\) when \(x \neq 0\)
2. \(\delta(x) = \infty\) when \(x = 0\)
3. \(\int_{-\infty}^{\infty} \delta(x) \, dx = 1\)

**Definition #2** = 1 defining property :

\(\int_{-\infty}^{\infty} \delta(x) f(x) \, dx = f(0)\)

These definitions are equivalent: if you assume definition, it is clear that definition 2 is true, and vice versa. Definition #1 better describes the origin of the \(\delta\) function as a way to describe the density of a point object; Definition #2 shows a way in which the \(\delta\) function is often used \(\rightarrow\) to pick out a particular value of a function \(f\).

**Problem 1 : Representations of \(\delta(x)\)**

The Dirac \(\delta\) is a rare instance of a mathematical object that was invented by physicists and then rigorously described by mathematicians. In math, it is not a function at all, but a “generalized function” or “distribution” (wiki those things if you want), and it is most commonly represented as the limit of a series of functions. There are numerous such representations. Let’s absorb some of the most common ones.

(a) Here is the most intuitive representation an infinite spike with an integral of 1 :

\[
\delta(x) = \lim_{n \to \infty} \delta_n(x) \quad \text{where} \quad \delta_n(x) = \begin{cases} 
  n & \text{for } |x| < 1/2n \\
  0 & \text{for } |x| > 1/2n 
\end{cases}
\]

Sketch \(\delta_n(x)\) for \(n = 1, 2, 3\). You will immediately see how this limit-of-a-series definition works.

FYI: Similar but more useful than the box representation above is the Gaussian representation:

\[
\delta(x) = \lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{x^2}{2\sigma^2}}
\]

That Gaussian is normalized so that it always integrates to 1 (as a probability distribution must!), so you just run the width \(\sigma\) to 0 and there you go, delta function.

(c) Take the Fourier transform of the Dirac \(\delta\), using its defining properties (definition #2!) to perform the integral, and you will quickly prove this very useful representation:

\[
\delta(x-x_0) = \int_{-\infty}^{\infty} e^{ik(x-x_0)} \frac{dk}{2\pi}
\]

(d) I often wondered why requirement #2 from the 1st definition was necessary: surely, if the \(\delta\) function is zero everywhere but at \(x = 0\) and it integrates to 1, it much be infinite at \(x = 0\) = the only place where it isn’t zero.
To create an integral of 1 from a function that is zero everywhere but at one point, surely the function must be infinite at that one point. One day I tried this series:

\[
\delta_n(x) = \begin{cases} 
  \frac{1}{n} \left( 1 - \frac{|x|}{n} \right) & \text{for } |x| < n \\
  0 & \text{for } |x| > n
\end{cases}
\]

Sketch that for a couple of \( n \) values to see that \( \lim_{n \to \infty} \delta_n(x) \) does not satisfy Definition #1.1 and #1.3 but not #1.2 … and that, as a result, it does not satisfy the all-important Definition #2.

**Problem 2 : \( \delta \)-Function Barrier**

Remember the infinite potential well, \( V(x) = -\infty \) for \( x \) in some finite range? Great for trapping particles! Well if you flip it upside down, it becomes an infinite potential barrier, which is great for bouncing particles back the way they came. If you make such an infinite barrier infinitely narrow, you get a **delta-function barrier** which is a fairly interesting construction.

First, we must quickly derive a relation that we introduced before, namely the infinite-potential caveat on the second of our wavefunction boundary conditions:

| a. Wavefunctions are always continuous \( \implies \lim_{\varepsilon \to 0} [\psi(x - \varepsilon) - \psi(x + \varepsilon)] = 0 \) |
| b. Wavefunctions have continuous derivatives \( \implies \lim_{\varepsilon \to 0} [\psi'(x - \varepsilon) - \psi'(x + \varepsilon)] = 0 \) except at points where \( V = \pm \infty \); there, the discontinuity in the derivative is \( \lim_{\varepsilon \to 0} \psi'(x + \varepsilon) - \psi'(x - \varepsilon) = \frac{2m}{\hbar^2} \lim_{\varepsilon \to 0} \int_{x-\varepsilon}^{x+\varepsilon} V(x) \psi(x) dx \) |
| c. Wavefunctions are zero in any region where \( V = \infty \) |

The proof of “b” is straightforward: you integrate the SE in a tiny neighborhood around a generic point \( x \), i.e. integrate \( \int_{x-\varepsilon}^{x+\varepsilon} \) … then you take the limit \( \varepsilon \to 0 \) … et voilà! You immediately see if and when a wavefunction’s derivative \( \psi' \) can be discontinuous.

(a) Here are the advertised steps. Just inspect them and make sure everything is clear:

Integrate SE in tiny neighborhood around \( x \):  

\[-\frac{\hbar^2}{2m} \int_{x-\varepsilon}^{x+\varepsilon} \psi''(x) dx + \int_{x-\varepsilon}^{x+\varepsilon} V(x) \psi(x) dx - E \int_{x-\varepsilon}^{x+\varepsilon} \psi(x) dx = 0 \]

Note:  

- \( \psi \) is continuous and finite \( \implies \lim_{\varepsilon \to 0} \) of right-hand term = \( E \psi(x) \varepsilon \to 0 \)

- integral in left-hand term can be integrated, giving \( \psi'(x) \big|_{x-\varepsilon}^{x+\varepsilon} = \psi'(x + \varepsilon) - \psi'(x - \varepsilon) \)

So:  

\[-\lim_{\varepsilon \to 0} \frac{\hbar^2}{2m} \psi'(x) \big|_{x-\varepsilon}^{x+\varepsilon} + \lim_{\varepsilon \to 0} \int_{x-\varepsilon}^{x+\varepsilon} V(x) \psi(x) dx = 0 \]

\[1 \text{ Q2 (d)} \quad R = \frac{1}{1 + 2\hbar^2 E / (m\alpha^2)}, \quad T = \frac{1}{1 + m\alpha^2 / (2\hbar^2 E)}.\]
Rearranging this gives you the formula “b” in the box. It clearly shows that the wavefunction’s derivative must be continuous \( (\psi'(x)|_{x=0} = 0) \) unless the integrand \( V(x) \) in the second term blows up to infinity. (That is the only way you can integrate \( V(x) \psi(x) \) over the vanishingly small region \( x \pm \epsilon \) and get something finite).

(b) Let’s place a lovely \( \delta \)-function barrier at \( x = 0 \):

\[
V(x) = \alpha \delta(x)
\]

where \( \alpha \) is a positive constant. To the left and right of this barrier — i.e. in the region \( x \neq 0 - V = 0 \), so we have free particles in those regions. Our general solution for a free particle is a superposition of plane waves of definite momentum \( p = \hbar k \) and definite energy \( E = \hbar \omega(k) \). If a particle coming in from the left has definite momentum \( p \) and energy \( E = p^2/2m \) (i.e. is in a plane-wave state = eigenstate of \( \hat{p} \) and \( \hat{E} \)), it will keep that energy \( E \) unchanged as there is nowhere in this system for energy to go except into the kinetic and potential energy of which \( E \) is composed. So: write down an incident plus a reflected wave in the region \( x < 0 \) and a possible transmitted wave in the region \( x > 0 \), all with the same energy and momentum.

(c) Apply the three boundary conditions to your \( x < 0 \) and \( x > 0 \) wavefunctions at the boundary point \( x = 0 \).

(d) Calculate the reflection & transmission coefficients, \( R \) and \( T \), that indicate the probability of the particle being in its reflected or its transmitted state, as compared to its incident state. \( R = \left| A_{\text{reflected}} \right|^2 / \left| A_{\text{incoming}} \right|^2 \) and \( T = \left| A_{\text{transmitted}} \right|^2 / \left| A_{\text{incoming}} \right|^2 \) → go ahead and calculate them.

(e) How do \( R \) and \( T \) behave with the “strength” \( \alpha \) of the barrier? The behaviour you find should make sense! It is a bit odd that the \( \alpha \) in \( V(x) = \alpha \delta(x) \) matters at all, since the height of the \( \delta \) function is already infinite at \( x = 0 \). However, the integral over the delta function is 1, so the integral of \( V(x) \) over the potential barrier is \( \alpha \). The \( \delta \) barrier is the thin limit of a potential wall; if you think back to the box representation from question 1(a), en route to this thin limit, the factor \( \alpha \) does make a difference.

**TUNNELLING**: Thin though it may be, the region inside the \( \delta \) barrier has \( V > E \) so it is classically forbidden. No classical particle could even get into this region, nevermind getting past it to the other side. The transmission coefficient is non-zero and shows that in quantum mechanics, particles can pass through classically-forbidden regions. This phenomenon is called tunnelling.

**Problem 3: \( \delta \)-Function Well**

Now flip the \( \delta \) function upside down to form an infinitely deep and infinitely narrow well:

\[
V(x) = -\alpha \delta(x)
\]

where \( \alpha \) is again a positive constant that sets the “strength” of the well. Consider particles with \( E < 0 \). Last week, such particles were trapped in an infinitely deep well of finite width … can they also be trapped inside an infinitely deep well of zero width?

(a) Write down the most general wavefunction \( \psi_-(x) \) with energy \( E < 0 \) that can exist in the region \( x < 0 \), and the most general wavefunction \( \psi_+(x) \) with the same energy \( E < 0 \) that can exist in the region \( x > 0 \). No need for hand-holding this time: apply the boundary conditions, and see what solutions you get. This time, the wavefunctions \( \psi_-(x) \) and \( \psi_+(x) \) are not plane waves, and they can — must — be normalized. What states and energies are allowed by the \( \delta \)-function well?

\[\text{Q3 (a)} \quad \psi_\pm(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-m\alpha|x|/\hbar^2} \quad \text{and only one energy is allowed:} \quad E = -\frac{m\alpha^2}{2\hbar^2}.\]