

WHY DID DIRAC NEED DELTA FUNCTION

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ABSTRACT

Dirac delta function appears naturally in many physical problems and is frequently used in quantum mechanics. The paradoxical feature of the Dirac delta function is that it is not a function at all. Rather, it is symbol $\delta(x)$ which for certain clearly defined purposes can be treated as if it were a function. The Dirac delta function can be taken as the generalization of the Kronecker delta to the case of the continuous variables. The historical background and some interesting features of the Dirac delta function $\delta(x)$ are discussed in this note.

Key words: delta function, generalized function, distributions

1. Introduction

The delta functions appeared in the early days of 19th century, in works of the Poisson (1815), Fourier (1822) and Cauchy (1823). Subsequently O Heaviside (1883) and G Kirchoff (1891) gave the first mathematical definitions of the delta functions. P A M Dirac (1926) introduced delta function in his classic and fundamental work on the quantum mechanics. Dirac also listed the useful and important properties of the delta function. The uses of the delta function become more and more common thereafter. We call $\delta(x)$ as the Dirac delta function for historical reasons, while it is not a function of x in conventional sense, which requires a function to have a definite value at each point in its domain. Therefore $\delta(x)$ cannot be used in mathematical analysis like an ordinary function. In mathematical literature it is known as generalized function or distribution, rather than function defined in the usual sense. A definitive mathematical theory of distributions was given by L Schwartz (1950) in his *Theorie des Distributions*.

The Dirac delta function is used to get a precise notation for dealing with quantities involving certain type of infinity. More specifically its origin is related to the fact that an eigenfunction belonging to an eigenvalue in the continuum is non-normalizable, *i.e.*, its norm is infinity.

2. Why did Dirac need the delta function?

Now we discuss why did Dirac need the delta function? Let us consider an arbitrary quantum mechanical state $|a\rangle$. We can represent it by an expansion in a complete set of orthonormal basis states $|x_i\rangle$ of a particular representation that is assumed to have n discrete basis states

$$|a\rangle = a_1|x_1\rangle + a_2|x_2\rangle + \dots + a_n|x_n\rangle, \quad (1)$$

where the orthonormality condition is $\langle x_i | x_j \rangle = \delta_{ij}$ (2)

(δ_{ij} is Kronecker delta; $\delta_{ij} = 0$ if $i \neq j$ and $\delta_{ij} = 1$ if $i = j$).

The (probability) amplitude of finding the state $|a\rangle$ in the base state $|x_i\rangle$ is

$$\varphi_i = \langle x_i | a \rangle \quad (3)$$

Due to orthonormality of the $|x_i\rangle$, Eq. (3) gives

$$\varphi_i = a_i \quad (4)$$

i.e., the expansion coefficients (a_i) defining a state $|a\rangle$ in a particular representation are simply amplitudes for finding the arbitrary state in the corresponding basis state.

Eq. (1) can be written as

$$|a\rangle = \sum_i \langle x_i | a \rangle |x_i\rangle \quad (5)$$

We want now to see how these relations must be modified when we are dealing with a continuum of base states. For this, consider the motion of a particle along a line. To describe the state $|\psi\rangle$ of the particle we can use the position representation. In this representation the basis states $|x\rangle$ describe a particle to be found at x and are continuous and non-denumerable. The most general state is

$$|\psi\rangle = a_1|x_1\rangle + a_2|x_2\rangle + \dots, \quad (6)$$

which is in analogy with Eq. (1). Since the states $|x\rangle$ are continuous we must replace sum in Eq. (5) by an integral, *i.e.*,

$$|\psi\rangle = \int f(x)|x\rangle dx, \quad (7)$$

where $f(x)$ is the amplitude of finding the particle at position x . The amplitude of finding the particle at position x' is

$$f(x') = \langle x' | \psi \rangle = \int f(x) \langle x' | x \rangle dx . \quad (8)$$

This relation must hold for any state $|\psi\rangle$ and therefore for any function $f(x)$. This requirement should completely determine the amplitude $f(x')$, which is of course just a function that depends on x and x' .

Now problem is to find a function $\langle x' | x \rangle$ which when multiplied with $f(x)$ and integrated over x gives the quantity $f(x')$. Suppose we take $x' = 0$ and define the amplitude $\langle 0 | x \rangle$ to be some function of x (say $g(x)$) then Eq. (8) gives

$$f(0) = \int f(x) g(x) dx . \quad (9)$$

What kind of function $g(x)$ could possibly satisfy this? Since the integral must not depend on what values $f(x)$ takes for values of x other than 0, $g(x)$ must clearly be 0, for all values of x except 0. But if $g(x)$ is 0 everywhere, the integral will be 0, too and Eq. (9) will not be satisfied. So we are in a strange situation: *we wish a function to be 0 everywhere except at a point, and still to give a finite result.* It turns out that there is no such mathematical function that will do this. Since we can not find such a function, the easiest way out is just to say the $g(x)$ is defined by the Eq. (9), namely $g(x)$ is that function, which makes Eq. (9) correct, and this relation must hold for any function (numerical, vector or linear operator). ***Dirac first did this and the function carries his name.*** It is written as $\delta(x)$.

3. How $\delta(x-x_0)$ look like?

The Dirac delta function is defined not by giving its values at different points but by giving a rule for integrating its product with a continuous function (Eq. (9)), if the origin is shifted from 0 to some point x_0 then Eq. (9) will be read as

$$f(x_0) = \int \delta(x - x_0) f(x) dx . \quad (10)$$

Obviously, the contribution to the integral in Eq. (10) comes only from $x = x_0$ (i.e., only the first term in the Taylor expansion of the function $f(x)$ around the origin x_0), as for all other values of the function is zero. This relation must hold for any function.

To have an understanding of $\delta(x-x_0)$, let us consider an arbitrary function that is non-zero everywhere except at point x_0 where it vanishes:

$$\begin{aligned} f(x) &= 0 && \text{at } x = x_0 \\ &= \text{non-zero}, && \text{everywhere else } x \neq x_0 \end{aligned} \quad (11)$$

In this case Eq. (10) gives

$$\int \delta(x-x_0)f(x) dx = 0 \quad (12)$$

Since Eq. (12) must hold for any arbitrary form of the $f(x)$ outside of the point x_0 , we conclude that $\delta(x-x_0) = 0$, if $x \neq x_0$. Also from Eq. (10) $\delta(x-x_0) = \infty$, if $x = x_0$. Thus,

$$\begin{aligned} \delta(x-x_0) &= 0 && \text{if } x \neq x_0 \\ &= \infty && \text{if } x = x_0 \end{aligned} \quad (13)$$

If we choose $f(x) = 1$, then defining relation (10) gives

$$\int \delta(x-x_0) dx = 1 \quad (14)$$

i.e., the delta function is normalized to unity.

All of these results show that the $\delta(x-x_0)$ can not thought of as a function in usual sense. However, it can be thought of as a limit of a sequence of regular functions. Schematically the delta function looks like a curve shown in Fig. 1, whose width tends to zero and the peak tends to infinity keeping the area under the curve finite. This curve represents a function of the real variable x , which vanishes everywhere except inside a small domain of length ε about the origin x_0 and which is so large inside this domain that its integral over the domain is unity; then in the limit $\varepsilon \rightarrow 0$, this function becomes $\delta(x-x_0)$. This curve may be visualized as a limit of more

familiar curves, e.g., a rectangular curve of height $1/\varepsilon$ and width ε or isosceles triangles of height $2/\varepsilon$ and base ε . These are plotted in Fig. 2. The area under both the curves is 1 for all values of ε . In the limit $\varepsilon \rightarrow 0$, the height becomes arbitrarily large and width shrinks to zero keeping area still 1. Thus these functions become Dirac delta function in the limit $\varepsilon \rightarrow 0$.

4. Representations

As noted earlier, the delta function can be thought of a limit of a sequence of regular functions. An infinite number of sequences may be constructed. Here we give some frequently used simple representations of the $\delta(x-x_0)$.

(1) A representation of the $\delta(x)$ is given by

$$\delta(x) = \lim_{L \rightarrow \infty} \left(\frac{\sin Lx}{\pi x} \right) \quad (15)$$

This function for any L looks like a diffraction amplitude with width proportional to $1/L$. For any L the function is regular. As we increase the value of L the function peaks more strongly at $x = 0$, and hence in the limit $L \rightarrow \infty$ it behaves like the delta function. Further, at $x = 0$, $\left(\frac{\sin Lx}{\pi x} \right) \sim \frac{L}{\pi}$ and its value oscillate with a period $\frac{2\pi}{L}$

when x increases.

Also
$$\int_{-\infty}^{\infty} \left(\frac{\sin Lx}{\pi x} \right) dx = 1 \text{ (independent of the value of the } x)$$

and
$$\int_{-\infty}^{\infty} f(x) \left(\frac{\sin Lx}{\pi x} \right) dx = f(0).$$

Thus the
$$\delta(x) = \lim_{L \rightarrow \infty} \left(\frac{\sin Lx}{\pi x} \right)$$
 has all the properties of a $\delta(x)$.

(2) Let us now consider the integral $\int_{-\infty}^{\infty} e^{ikx} dk$: This can be written as

$$\begin{aligned} \lim_{L \rightarrow \infty} \int_{-L}^L e^{ikx} dk &= \lim_{L \rightarrow \infty} \left(\frac{e^{ikx} - e^{-ikx}}{ix} \right) = 2\pi \lim_{L \rightarrow \infty} \left(\frac{\sin Lx}{\pi x} \right) = 2\pi \delta(x) \\ \Rightarrow \delta(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk \end{aligned} \quad (16)$$

The above relation is an alternate representation of $\delta(x)$. Here we immediately note

that $\delta(x)$ is simply the Fourier transform of the constant $\frac{1}{\sqrt{2\pi}}$.

(3) Separating the real and imaginary parts in Eq. (16) we find

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \cos kx dk \quad (17)$$

$$0 = \frac{1}{2\pi} \int_{-\infty}^{\infty} \sin kx dk \quad (18)$$

Eq. (17) is one of the most commonly used explicit expressions for $\delta(x)$.

(4) A useful representation of the $\delta(x)$ is

$$\delta(x) = \lim_{\alpha \rightarrow \infty} \sqrt{\frac{\alpha}{\pi}} e^{-\alpha x^2} \quad (19)$$

This is the normalized Gaussian function of standard deviation $\frac{1}{\sqrt{2\alpha}}$, which tends to

zero as $\alpha \rightarrow \infty$. Its height is proportional to $\sqrt{\alpha}$ and it peaks at $x = 0$.

Some useful representations that are encountered in various applications are

$$(5) \quad \delta(x) = \lim_{\alpha \rightarrow \infty} \frac{1}{\pi} \left(\frac{\alpha}{x^2 + \alpha^2} \right) \quad (20)$$

$$(6) \quad \delta(x) = \frac{d}{dx} \theta(x), \quad (21)$$

where $\theta(x)$ is the step function which is defined as a generalized function through

$$\begin{aligned}\theta(x) &= 0 \quad \text{for } x \leq 0 \\ &= 1 \quad \text{for } x \geq 0\end{aligned}$$

The three-dimensional Dirac delta function can be written by generalizing the one-dimensional function i.e.,

$$\delta^3(\vec{r} - \vec{r}_0) = \delta(x-x_0) \delta(y-y_0) \delta(z-z_0) \quad (22)$$

with $\int \delta^3(\vec{r} - \vec{r}_0) d^3r = \iiint \delta(x-x_0) \delta(y-y_0) \delta(z-z_0) dx dy dz = 1$

and $\int \delta^3(\vec{r} - \vec{r}_0) f(\vec{r}) d^3r = f(\vec{r}_0)$

5. Delta function in physical problems

The Dirac delta function arises naturally in many branches of science and engineering. To appreciate this, let us consider the divergence of function $\vec{A} = \frac{\hat{r}}{r^2}$ (a basic problem of electrodynamics)[1]. As shown in Fig. 3 \vec{A} is spreading radially outward and has a large positive divergence, but we get zero by actual calculation as shown below (in radial coordinates):

$$\vec{\nabla} \cdot \vec{A} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{1}{r^2} \right) = \frac{1}{r^2} \frac{\partial}{\partial r} (1) = 0 \quad (21)$$

The surface integral of \vec{A} over a sphere of radius R centered at origin ($r = 0$) is

$$\oint \vec{A} \cdot \vec{ds} = \int \frac{1}{R^2} (R^2 \sin \theta d\theta d\phi) = \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi = 4\pi \quad (22)$$

On the other hand from divergence theorem, we have

$$\int \vec{\nabla} \cdot \vec{A} dv = \oint \vec{A} \cdot \vec{ds} = 4\pi \quad (23)$$

Thus we are in a paradoxical situation, in which $\vec{\nabla} \cdot \vec{A} = 0$ but its integral is 4π . The source of this inconsistency lies at the origin, where the \vec{A} blows up, although $\vec{\nabla} \cdot \vec{A} = 0$ everywhere except at the origin. From Eq. (23) it is evident that $\int \vec{\nabla} \cdot \vec{A} dv = 4\pi$ for any sphere centered at origin irrespective of its size. Hence $\vec{\nabla} \cdot \vec{A}$ has a strange property that it vanishes everywhere except at the origin, and yet its integral is 4π . We also have the similar problem of a point particle: density (charge density) is zero everywhere except at its location, yet its integral i.e., mass (charge) is finite. No mathematical functions behave like this but we note that these are precisely the defining properties of the Dirac delta function (see Eqs 13 and 14). Hence these contradictions can be avoided by introducing the Dirac delta function; one can write

$$\vec{\nabla} \cdot \frac{\hat{r}}{r^2} = 4\pi \delta^3(\vec{r})$$

6. Properties of the Dirac delta function

We list below some properties of the Dirac delta function without assuming any particular representation. In fact, these properties are equations, which are essentially rules for manipulations for algebraic work involving $\delta(x)$ functions. The meaning of these equations is that the left and right hand sides when used as a multiplying factor under an integrand leads to the same results.

(i) $\delta(x) = \delta(-x)$

(ii) $\delta^*(x) = \delta(x)$

(iii) $x \delta(x) = 0$

$$(iv) \quad \delta(ax) = \frac{1}{a} \delta(x) \quad (a > 0)$$

$$(v) \quad f(x) \delta(x-a) = f(a) \delta(x-a)$$

$$(vi) \quad \int dx \delta(x) f(x) = f(0)$$

$$(vii) \quad \int dx \delta(a-x) \delta(x-b) = \delta(a-b)$$

$$(viii) \quad \delta'(-x) = -\delta'(x) \quad \text{where } \delta'(x) = \frac{d}{dx} \delta(x)$$

$$(ix) \quad \int dx \delta'(x) f(x) = -f'(0)$$

$$(x) \quad \delta(x^2 - a^2) = \frac{\delta(x-a) + \delta(x+a)}{2a} \quad (a > 0)$$

Further suggested reading:

- 1) D J Griffiths, *Introduction to Electrodynamics*, Prentice Hall of India Private Limited, 1997 p. 46.
- 2) R P Feynman, R B Leighton and M Sands, *The Feynman Lectures on Physics* Vol. III *Quantum Mechanics*, Narosa Publishing Housing, New Delhi, 1986 (See chapter 16).
- 3) P A M Dirac, *The Principles of Quantum Mechanics*, Oxford University Press, IV Edition 1985, p 58.
- 4) Ashok Das and A C Melissinos, *Quantum Mechanics A Modern Introduction*, Gordon and Breach Science Publishers, 1986.

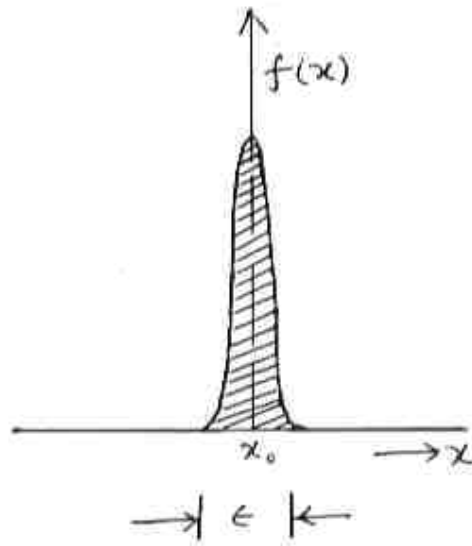


Fig.: 01 Schematic representation of Dirac delta function.

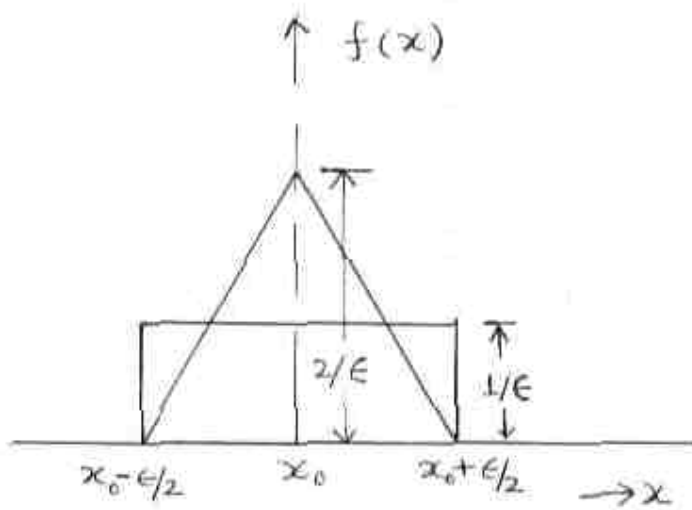


Fig.: 02 Retangular and isosceles traingular curves represnet Dirac delta function in the limit $\epsilon \rightarrow 0$.

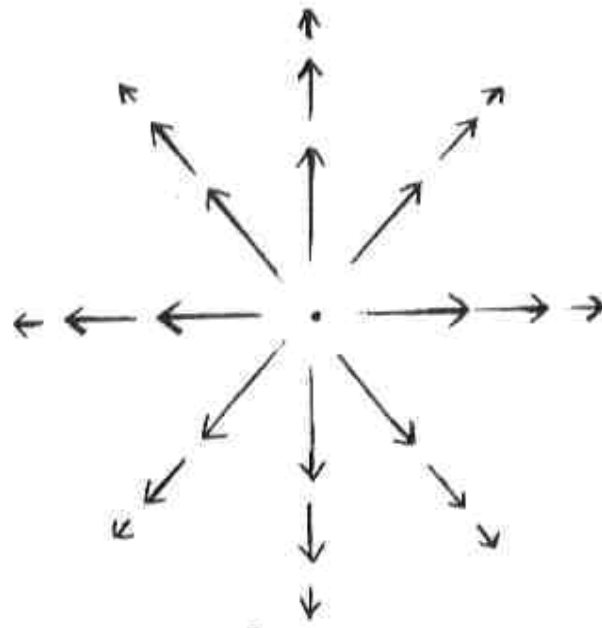


Fig.: 03 The vector function \vec{A} spreading radially outward, having large positive divergence at origin.