

Dirac Delta Function

Paul Dirac introduced some useful formal tools (such as his notation for integrals and operators). One of them is the Dirac delta function $\delta(x)$, an object then unknown to mathematicians, which turned out to be very useful in physics. We may think of it as of a function with the following characteristics¹

- It is nonzero, but very close to $x = 0$, where its value is $+\infty$.
- The surface under its plot equals 1, what is highlighted by a *symbolic* equation:

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

When we look at a straight thin reed protruding from a lake (with the water level = 0), then we have to do with something similar to the Dirac delta function. The only task of the Dirac delta function is its specific behavior, when integrating the product $f(x)\delta(x)$ and the integration *includes the point* $x = 0$; namely:

$$\int_a^b f(x)\delta(x) dx = f(0). \quad (\text{E.1})$$

This result is quite understandable: the integral refers to the surface under the curve $f(x)\delta(x)$, but since $\delta(x)$ is so concentrated at $x = 0$, then it pays to take seriously only those x that are “*extremely close*” to $x = 0$. Over there, $f(x)$ is equal to $f(0)$. The constant $f(0)$ can be extracted from the integral, which itself, therefore, has the form $\int_{-\infty}^{\infty} \delta(x) dx = 1$. This is why we get the right side of the last equation. Of course, $\delta(x - c)$ represents the same narrow peak, but at $x = c$. Therefore, for $a \leq c \leq b$, we have

$$\int_a^b f(x)\delta(x - c) dx = f(c). \quad (\text{E.2})$$

¹ More precisely, this is not a function; it is called a *distribution*. The theory of distributions were developed by mathematicians only after Dirac’s work.

Approximations to $\delta(x)$

The Dirac delta function $\delta(x)$ can be approximated by many functions, that depend on a certain parameter and have the following properties:

- When the parameter tends to approach a limit, then the values of the functions for x distant from 0 become smaller and smaller, while as x gets close to zero, they are getting larger and larger (peaking at close to $x = 0$).
- The integral of the function tends to be equal (or be close to) 1 when the parameter approaches its limit value.

Here are several functions that approximate the Dirac delta function:

- A rectangular function centered at $x = 0$, with the rectangle surface equal to 1 ($a \rightarrow 0$):

$$f_1(x; a) = \begin{cases} \frac{1}{a} & \text{for } -\frac{a}{2} \leq x \leq \frac{a}{2} \\ 0 & \text{for other} \end{cases}.$$

- A Gaussian function² ($a \rightarrow \infty$) normalized to 1:

$$f_2(x; a) = \sqrt{\frac{a}{\pi}} e^{-ax^2}.$$

- Another function is:

$$f_3(x; a) = \frac{1}{\pi} \lim_{a \rightarrow \infty} \frac{\sin ax}{x} \quad \text{when } a \rightarrow \infty.$$

- The last function is (we will use it when considering the interaction of matter with radiation)³:

$$f_4(x; a) = \frac{1}{\pi a} \lim_{a \rightarrow \infty} \frac{\sin^2(ax)}{x^2} \quad \text{when } a \rightarrow \infty.$$

² Let us see how an approximation $f_2 = \sqrt{\frac{a}{\pi}} e^{-ax^2}$ does the job of the Dirac delta function when $a \rightarrow \infty$. Let us take a function $f(x) = (x - 5)^2$ and consider the integral

$$\int_{-\infty}^{\infty} f(x) f_2(x) dx = \sqrt{\frac{a}{\pi}} \int_{-\infty}^{\infty} (x - 5)^2 e^{-ax^2} dx = \sqrt{\frac{a}{\pi}} \left(\frac{1}{4a} \sqrt{\frac{\pi}{a}} + 0 + 25 \sqrt{\frac{\pi}{a}} \right) = \frac{1}{4a} + 25.$$

When $a \rightarrow \infty$, then the value of the integral tends to be $25 = f(0)$, as it must be for the Dirac delta function that is used instead of f_2 .

³ The function under the limit symbol may be treated as $A[\sin(ax)]^2$, with amplitude A decaying as $A = 1/x^2$, when $|x| \rightarrow \infty$. For small values of x , the $\sin(ax)$ changes to ax (as it is seen from its Taylor expansion); hence, for small x , the function changes to a^2 . This means that when $a \rightarrow \infty$, there will be a dominant peak close to $x = 0$, although there will be some smaller side peaks clustering around $x = 0$. The surface of the dominating peak may be approximated by a triangle of the base $2\pi/a$ and the height a^2 , and then we obtain its surface equal to πa . Hence, the “approximate normalization factor” $1/(\pi a)$ in f_4 .

Properties of $\delta(x)$

Function $\delta(cx)$

Let us see what $\delta(cx)$ is:

$$\begin{aligned}\delta(cx) &= \lim_{a \rightarrow \infty} \sqrt{\frac{a}{\pi}} \exp(-ac^2x^2) = \lim_{a \rightarrow \infty} \sqrt{\frac{ac^2}{\pi c^2}} \exp(-ac^2x^2) \\ &= \frac{1}{|c|} \lim_{ac^2 \rightarrow \infty} \sqrt{\frac{ac^2}{\pi}} \exp(-ac^2x^2) = \frac{1}{|c|} \delta(x).\end{aligned}$$

Therefore,

$$\delta(cx) = \frac{1}{|c|} \delta(x). \quad (\text{E.3})$$

Dirac δ in 3-D

The 3-D Dirac delta function is defined in the Cartesian coordinate system as

$$\delta(\mathbf{r}) = \delta(x)\delta(y)\delta(z),$$

where $\mathbf{r} = (x, y, z)$. Then, $\delta(\mathbf{r})$ denotes a peak of the infinite height at $\mathbf{r} = \mathbf{0}$, $\delta(\mathbf{r} - \mathbf{A})$ denotes an identical peak at the position shown by the vector \mathbf{A} from the origin. Each of the peaks is normalized to 1; i.e., the integral over the whole 3-D space equals 1. This means that Eq. (E.1) is satisfied, but this time $x \in R^3$.

An Application of the Dirac Delta Function

When may such a concept as the Dirac delta function be useful? Here is an example. Let us imagine that we have (in the 3-D space) two molecular charge distributions: $\rho_A(\mathbf{r})$ and $\rho_B(\mathbf{r})$. Each of the distributions consists of the electronic part and the nuclear part.

How can such charge distributions be represented mathematically? There is no problem with mathematical representation of the electronic parts—they are simply some functions of the position \mathbf{r} in space: $-\rho_{el,A}(\mathbf{r})$ and $-\rho_{el,B}(\mathbf{r})$ for each molecule, respectively. The integrals of the corresponding electronic distributions yield, of course, $-N_A$ and $-N_B$ (in a.u.), or the negative number of the electrons (because the electrons carry a negative charge). How, then, do you write the nuclear charge distribution as a function of \mathbf{r} ? There is no way to do this without the Dirac

delta function. With the function, our task becomes simple:

$$\rho_{nucl,A}(\mathbf{r}) = \sum_{a \in A} Z_{A,a} \delta(\mathbf{r} - \mathbf{r}_a)$$

$$\rho_{nucl,B}(\mathbf{r}) = \sum_{b \in B} Z_{B,b} \delta(\mathbf{r} - \mathbf{r}_b).$$

At the nuclear positions, we put delta functions with “intensities” equal to the nuclear charges. For neutral molecules, $\int \rho_{nucl,A}(\mathbf{r}) d\mathbf{r}$ and $\int \rho_{nucl,B}(\mathbf{r}) d\mathbf{r}$ have to give $+N_A$ and $+N_B$, respectively. Indeed, we have

$$\int \rho_{nucl,A}(\mathbf{r}) d\mathbf{r} = \sum_{a \in A} Z_{A,a} \int \delta(\mathbf{r} - \mathbf{r}_a) d\mathbf{r} = \sum_{a \in A} Z_{A,a} = N_A$$

$$\int \rho_{nucl,B}(\mathbf{r}) d\mathbf{r} = \sum_{b \in B} Z_{B,b} \int \delta(\mathbf{r} - \mathbf{r}_b) d\mathbf{r} = \sum_{b \in B} Z_{B,b} = N_B.$$

Thus, the Dirac delta function enables us to write the total charge distributions and their interactions in an elegant way:

$$\rho_A(\mathbf{r}) = -\rho_{el,A}(\mathbf{r}) + \rho_{nucl,A}(\mathbf{r})$$

$$\rho_B(\mathbf{r}) = -\rho_{el,B}(\mathbf{r}) + \rho_{nucl,B}(\mathbf{r}).$$

To demonstrate the difference, let us write the electrostatic interaction of the two charge distributions both without the Dirac delta functions:

$$E_{inter} = \sum_{a \in A} \sum_{b \in B} \frac{Z_A Z_B}{|\mathbf{r}_a - \mathbf{r}_b|} - \sum_{a \in A} \int \rho_{el,B}(\mathbf{r}) \frac{Z_A}{|\mathbf{r} - \mathbf{r}_a|} d\mathbf{r}$$

$$- \sum_{b \in B} \int \rho_{el,A}(\mathbf{r}) \frac{Z_B}{|\mathbf{r} - \mathbf{r}_b|} d\mathbf{r} + \iint \frac{\rho_{el,A}(\mathbf{r}) \rho_{el,B}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'.$$

The four terms mean, respectively, the following interactions: nuclei of A with nuclei of B, nuclei of A with electrons of B, electrons of A with nuclei of B, electrons of A with electrons of B. With the Dirac delta function, the same expression reads:

$$E_{inter} = \int \frac{\rho_A(\mathbf{r}) \rho_B(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}'.$$

The last expression comes from the definition of the Coulomb interaction and the definition of the integral.⁴

No matter what the charge distributions look like, whether they are diffuse (like the electronic ones) or pointlike (like those of the nuclei), the formula is always the same.

⁴ Of course, the two notations are equivalent because inserting the total charge distributions into the last integral, as well as using the properties of the Dirac delta function, gives the first expression for E_{inter} .