E. DIRAC DELTA FUNCTION

Paul Dirac introduced some useful formal tools (for example his notation for integrals and operators, p. 19) including an object then unknown to mathematicians, which turned out to be very useful in physics. This is called the Dirac delta function $\delta(x)$. We may think of it as of a function[1]

- which is non-zero only very close to $x = 0$, where its value is $+\infty$;
- the surface under its plot is equal to 1, which is highlighted by a *symbolic* equation

$$\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1.$$

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

$$\int_{a}^{b} f(x)\delta(x)\,\mathrm{d}x = f(0). \tag{E.1}$$

This result is well understandable: the integral means 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 $f(x)$ that are "extremely close" to $x = 0$. Over there $f(x)$ is equal to $f(0)$. The constant $f(0)$ can be taken out of the integral, which itself therefore has the form $\int_{-\infty}^{\infty} \delta(x)\,\mathrm{d}x = 1$. This is why we get the right hand side of the previous equation. Of course, $\delta(x - c)$ represents the same narrow peak, but at $x = c$, therefore, for $a \leqslant c \leqslant b$ we have

$$\boxed{\int_{a}^{b} f(x)\delta(x - c)\,\mathrm{d}x = f(c).} \tag{E.2}$$

1 APPROXIMATIONS TO $\delta(x)$

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

[1] More precisely this is not a function, but what is called a distribution. The theory of distributions was developed by mathematicians only after Dirac.

- when the parameter tends to a limit, the values of the functions for x distant from 0 become smaller and smaller, while for x close to zero they get larger and larger (a peak close to $x = 0$);
- the integral of the function tends to (or is close to) 1 when the parameter approaches its limit value.

Here are several functions that approximate the Dirac delta function:

- a rectangular function centred at $x = 0$ with the surface of the rectangle equal to 1 ($a \to 0$):

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

- a (normalized to 1) Gaussian function[2] ($a \to \infty$):

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

- a function:

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

- the last function is (we will use this when considering the interaction of matter with radiation):[3]

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

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[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 $a \to \infty$. Let us take a function $f(x) = (x-5)^2$ and consider the integral

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

When $a \to \infty$, the value of the integral tends to $25 = f(0)$, as it has to be when the Dirac delta function 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 $|x| \to \infty$. For small values of x, the $\sin(ax)$ changes as ax (as seen from its Taylor expansion), hence for small x the function changes as a^2. This means that when $a \to \infty$, 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 base $2\pi/a$ and height a^2, and we obtain its surface equal to πa, hence the "approximate normalization factor" $1/(\pi a)$ in f_4.

2 PROPERTIES OF $\delta(x)$

Function $\delta(cx)$

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

$$\delta(cx) = \lim_{a\to\infty}\sqrt{\frac{a}{\pi}}\exp\left(-ac^2x^2\right) = \lim_{a\to\infty}\sqrt{\frac{ac^2}{\pi c^2}}\exp\left(-ac^2x^2\right)$$

$$= \frac{1}{|c|}\lim_{ac^2\to\infty}\sqrt{\frac{ac^2}{\pi}}\exp\left(-ac^2x^2\right) = \frac{1}{|c|}\delta(x).$$

Therefore,

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

Dirac δ in 3D

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

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

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

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 3D space) two molecular charge distributions: $\rho_A(\boldsymbol{r})$ and $\rho_B(\boldsymbol{r})$. Each of the distributions consists of an electronic part and an nuclear part.

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

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

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

We put delta functions with the "intensities" equal to the nuclear charges in the nuclear positions . For neutral molecules $\int \rho_{\mathrm{nucl},A}(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r}$ and $\int \rho_{\mathrm{nucl},B}(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r}$ have to give $+N_A$ and $+N_B$, respectively. Indeed, we have

$$\int \rho_{\mathrm{nucl},A}(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r} = \sum_{a\in A} Z_{A,a}\int \delta(\boldsymbol{r}-\boldsymbol{r}_a)\,\mathrm{d}^3\boldsymbol{r} = \sum_{a\in A} Z_{A,a} = N_A,$$
$$\int \rho_{\mathrm{nucl},B}(\boldsymbol{r})\,\mathrm{d}^3\boldsymbol{r} = \sum_{b\in B} Z_{B,b}\int \delta(\boldsymbol{r}-\boldsymbol{r}_b)\,\mathrm{d}^3\boldsymbol{r} = \sum_{b\in B} Z_{B,b} = N_B.$$

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

$$\rho_A(\boldsymbol{r}) = -\rho_{\mathrm{el},A}(\boldsymbol{r}) + \rho_{\mathrm{nucl},A}(\boldsymbol{r}),$$
$$\rho_B(\boldsymbol{r}) = -\rho_{\mathrm{el},B}(\boldsymbol{r}) + \rho_{\mathrm{nucl},B}(\boldsymbol{r}).$$

To demonstrate the difference, let us write the electrostatic interaction of the two charge distributions with and without the Dirac delta functions. The first gives the following expression

$$E_{\mathrm{inter}} = \sum_{a\in A}\sum_{b\in B}\frac{Z_{A,a}Z_{B,b}}{|\boldsymbol{r}_a-\boldsymbol{r}_b|} - \sum_{a\in A}\int \rho_{\mathrm{el},B}(\boldsymbol{r})\frac{Z_{A,a}}{|\boldsymbol{r}-\boldsymbol{r}_a|}\,\mathrm{d}^3\boldsymbol{r}$$
$$-\sum_{b\in B}\int \rho_{\mathrm{el},A}(\boldsymbol{r})\frac{Z_{B,b}}{|\boldsymbol{r}-\boldsymbol{r}_b|}\,\mathrm{d}^3\boldsymbol{r} + \iint \frac{\rho_{\mathrm{el},A}(\boldsymbol{r})\rho_{\mathrm{el},B}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'.$$

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

$$E_{\mathrm{inter}} = \int \frac{\rho_A(\boldsymbol{r})\rho_B(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\,\mathrm{d}^3\boldsymbol{r}\,\mathrm{d}^3\boldsymbol{r}'.$$

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

No matter how the charge distributions looks, whether they are diffuse (the electronic ones) or point-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}.