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COMMENT

Boundary conditions at the derivative of a delta function

David J Griffiths

Department of Physics, Reed College, Portland, OR 97202, USA

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Abstract. We derive the joining conditions on ψ at a point where the potential is the nth derivative of a Dirac delta function.

In a recent letter [1], Bao-Heng Zhao correctly states the joining conditions for the (time-independent) Schrödinger equation, at a potential of the form

$$V(x) = c\delta'(x) \tag{1}$$

to wit†

$$\Delta\psi = \frac{2mc}{\hbar^2}\bar{\psi}(0) \tag{2}$$

$$\Delta\psi' = -\frac{2mc}{\hbar^2}\bar{\psi}'(0). \tag{3}$$

Zhao goes on, however, to impose an incorrect and extraneous constraint‡

$$\Delta\psi = 0 \tag{4}$$

† Zhao sets $\hbar = 1$ and $m = 1/2$, and neglects to mention that the quantities on the right are the *averages* at the discontinuity

$$\bar{f}(0) \equiv \frac{1}{2}[f(0^+) + f(0^-)].$$

‡ Zhao sketches the derivation of (2) and (3), but in support of (4) merely remarks that 'as usual, we require ψ to be continuous at $x = 0$'. The interesting feature of the δ' potential is precisely that ψ is *not* continuous. The reader who may be skeptical about this is encouraged to model $V(x)$ by the 'rectangular' function

$$V_1(x) \equiv \begin{cases} 0 & \text{if } x < -a \\ c/\epsilon^2 & \text{if } -\epsilon \le x < 0 \\ -c/\epsilon^2 & \text{if } 0 < x < \epsilon \\ 0 & \text{if } x > \epsilon \end{cases}$$

or (more simply) by the double delta function

$$V_2(x) \equiv \frac{c}{2\epsilon}[\delta(x+\epsilon) - \delta(x-\epsilon)]$$

in the limit $\epsilon \to 0$.

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which overdetermines the solution. Because this potential has been a source of recurring confusion (Zhao was himself responding to an error by Gesztesy and Holden in [2]), I thought it might be useful to present here a general derivation of the boundary conditions at the nth derivative of a delta function

$$V(x) = c\delta^{(n)}(x). \tag{5}$$

The Schrödinger equation for this potential reads

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + c\delta^{(n)}(x)\,\psi = E\psi. \tag{6}$$

Integrating from $-\epsilon$ to $+\epsilon$

$$-\frac{\hbar^2}{2m}[\psi'(\epsilon) - \psi'(-\epsilon)] + c\int_{-\epsilon}^{\epsilon}\left[\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\delta(x)\right]\psi(x)\,\mathrm{d}x = E\int_{-\epsilon}^{\epsilon}\psi(x)\,\mathrm{d}x. \tag{7}$$

Using integration by parts n times, and noting that all the 'boundary' terms vanish, we find†

$$\int_{-\epsilon}^{\epsilon}\left[\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\delta(x)\right]\psi(x)\,\mathrm{d}x = (-1)^n\int_{-\epsilon}^{\epsilon}\delta(x)\left[\left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^n\psi(x)\right]\mathrm{d}x = (-1)^n\bar{\psi}^{(n)}(0). \tag{8}$$

In the limit $\epsilon \to 0$, the last integral in (7) goes to zero, and we are left with the *first boundary condition*

$$\Delta\psi' = (-1)^n\frac{2mc}{\hbar^2}\bar{\psi}^{(n)}(0). \tag{9}$$

Meanwhile, integrating the Schrödinger equation from $-L$ (with L positive) to x yields

$$-\frac{\hbar^2}{2m}[\psi'(x) - \psi'(-L)] + c\int_{-L}^{x}\left[\left(\frac{\mathrm{d}}{\mathrm{d}x'}\right)^n\delta(x')\right]\psi(x')\,\mathrm{d}x' = E\int_{-L}^{x}\psi(x')\,\mathrm{d}x'. \tag{10}$$

Again we integrate by parts, but this time the 'upper' boundary terms are *not* zero

$$\begin{aligned}\int_{-L}^{x}\left[\left(\frac{\mathrm{d}}{\mathrm{d}x'}\right)^n\delta(x')\right]\psi(x')\,\mathrm{d}x' &= \delta^{(n-1)}(x)\psi(x) - \delta^{(n-2)}(x)\psi'(x)\\ &\quad + \delta^{(n-3)}(x)\psi^{(2)}(x) - \cdots + (-1)^{n-1}\delta(x)\psi^{(n-1)}(x)\\ &\quad + (-1)^n\theta(x)\bar{\psi}^{(n)}(0).\end{aligned} \tag{11}$$

† For functions $f(x)$ that are discontinuous at the origin, the expression

$$\int_{-\epsilon}^{\epsilon}\delta(x)f(x)\,\mathrm{d}x$$

is not, in general, well-defined. However, if we stipulate that the delta function is the limit of a sequence of *even functions*, then

$$\int_{-\epsilon}^{\epsilon}\delta(x)f(x)\,\mathrm{d}x = \bar{f}(0)$$

and it is in this sense that $\delta(x)$ is to be interpreted throughout this paper.

Integrating (10) itself from $-\epsilon$ to $+\epsilon$, and taking the limit $\epsilon \to 0$, we find that

$$-\frac{\hbar^2}{2m}\Delta\psi + c\left\{\int_{-\epsilon}^{\epsilon}\delta^{(n-1)}\psi\,\mathrm{d}x - \int_{-\epsilon}^{\epsilon}\delta^{(n-2)}\psi'\,\mathrm{d}x + \int_{-\epsilon}^{\epsilon}\delta^{(n-3)}\psi^{(2)}\,\mathrm{d}x - \cdots + (-1)^{n-1}\int_{-\epsilon}^{\epsilon}\delta\psi^{(n-1)}\,\mathrm{d}x\right\} = 0. \tag{12}$$

A final set of integrations by parts reduces the term in curly brackets to

$$(-1)^{n-1}n\bar{\psi}^{(n-1)}(0)$$

and we are left with the *second boundary condition*

$$\Delta\psi = (-1)^{n-1}\frac{2mc}{\hbar^2}n\bar{\psi}^{(n-1)}(0). \tag{13}$$

For example, at a simple delta function ($n = 0$), equations (9) and (13) yield the familiar conditions

$$\Delta\psi = 0 \qquad \Delta\psi' = \frac{2mc}{\hbar^2}\psi(0)$$

and for the (first) derivative of a delta function ($n = 1$) we recover equations (2) and (3).

References

[1] Zhao B H 1992 *J. Phys. A: Math. Gen.* **25** L617
[2] Gesztesy F and Holden H 1987 *J. Phys. A: Math. Gen.* **20** 5157