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Unusual situations that arise with the Dirac delta function and its derivative

(Situações não usuais originadas da função delta de Dirac e da sua derivada)

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There is a situation such that, when a function $f(x)$ is combined with the Dirac delta function $\delta(x)$, the usual formula $\int_{-\infty}^{\infty} f(x)\delta(x)dx = f(0)$ does not hold. A similar situation may also be encountered with the derivative of the delta function $\delta'(x)$, regarding the validity of $\int_{-\infty}^{\infty} f(x)\delta'(x)dx = -f'(0)$. We present an overview of such unusual situations and elucidate their underlying mechanisms. We discuss implications of the situations regarding the transmission-reflection problem of one-dimensional quantum mechanics.
Keywords: Dirac delta function, singular functions, quantum mechanics.

Existe uma situação tal que quando uma função $f(x)$ é combinada com a função delta de Dirac, $\delta(x)$, a formula usual $\int_{-\infty}^{\infty} f(x)\delta(x)dx = f(0)$ deixa de ser válida. Uma situação similar pode ocorrer com a derivada da função delta, $\delta'(x)$, com relação à formula $\int_{-\infty}^{\infty} f(x)\delta'(x)dx = -f'(0)$. Nós apresentamos um apanhado destas situaçãoes não usuais e elucidamos os mecanismos por detrás delas. Nós discutimos as implicações destas situaçãoes em relação ao problema de tranmissão-reflexão em mecânica quântica uni-dimensional.
Palavras-chave: função delta de Dirac, funções singulares, mecânica quântica.

1. Introduction

The Dirac delta function $\delta(x)$ is a standard subject that appears in textbooks of quantum mechanics. It is such that

$$\delta(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ \infty & \text{if } x = 0 \end{cases}, \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(x)dx = 1. \qquad (1)$$

It can be interpreted as an infinitely high and infinitesimally narrow spike at the origin [1]. As Dirac himself cautioned, however, $\delta(x)$ is not a function of x according to the usual mathematical definition of a function, which requires a function to have a definite value for each point in its domain.

If $f(x)$ is an "ordinary" function, which we characterize in due course, we obtain

$$\int f(x)\delta(x)dx = f(0), \qquad (2)$$

where the range of the integration contains the origin. If $f(x)$ is discontinuous at $x = 0$, we interpret Eq. (2) as

$$\int f(x)\delta(x)dx = \frac{1}{2}[f(0+) + f(0-)], \qquad (3)$$

where $f(0+)$ and $f(0-)$ are respectively the limits of $f(x)$ when x approaches 0 from the positive and negative sides. Equation (3) implies that, although $\delta(x)$ itself is not well-defined for $x = 0$, when it occurs as a factor in an integrand, the integral has a well-defined value.

There is another commonly used formula, i.e.,

$$\begin{aligned} \int f(x)\delta'(x)dx &= -\int f'(x)\delta(x)dx \\ &= -\frac{1}{2}[f'(0+) + f'(0-)], \end{aligned} \qquad (4)$$

where $\delta'(x) = d\delta(x)/dx$ and $f'(x) = df(x)/dx$. In this case it is understood that $f(0+) = f(0-)$ but $f'(x)$ may be discontinuous at $x = 0$. The range of the integration again contains the origin. In Eq. (4) integration by parts has been done with the understanding that $f(x)\delta(x)$ vanishes at the limits of the integration.

Although Eqs. (3) and (4) look natural they do not necessarily hold for a certain type of functions. Such situations have been known in the literature that we quote

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as we proceed. This problem, however, does not seem to have been mentioned in any textbooks of quantum mechanics. Although the situations are rather unusual we believe that we should at least be aware of such possibilities. In this paper we attempt to present a comprehensive overview of the situations and elucidate their underlying mechanisms. Note that we define $\delta(x)$ by Eq. (1). If one defines $\delta(x)$ by Eq. (3) one may be led to self-contradiction unless one chooses an ordinary function for $f(x)$. We examine Eq. (3) in Sec. 2 and Eq. (4) in Sec. 3. We discuss implications of the unusual situations regarding the transmission-reflection problem of one-dimensional quantum mechanics. A summary is given in Sec. 4.

2. The Dirac delta function

Because $\delta(x) = 0$ for $x \neq 0$, the validity of Eq. (3) [and also of Eq. (4)] only depends on the behavior of $f(x)$ around the origin. By the "ordinary" function we mean $f(x)$ such that it can be expanded around the origin as

$$f(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!}[\theta(x) f^{(n)}(0+) + \theta(-x) f^{(n)}(0-)], \quad (5)$$

where $n = 0, 1, 2, \cdots$, $\theta(x) = 1$ (0) if $x > 0$ ($x < 0$) and $f^{(n)}(0\pm) = \lim_{x\to 0\pm} d^n f(x)/dx^n$. It is understood that $f^{(n)}(0\pm)$ *are all finite*. For such a function, Eq. (3) can be justified in the following manner. Define a rectangular function $\Delta(x)$ by

$$\Delta(x) = \begin{cases} 1/(2\epsilon) & \text{if } -\epsilon < x < \epsilon \\ 0 & \text{otherwise} \end{cases}, \quad (6)$$

where $\epsilon > 0$. Note that $\int_{-\epsilon}^{\epsilon} \Delta(x)dx = 1$. We eventually let $\epsilon \to 0$ so that $\Delta(x)$ becomes $\delta(x)$. The integral $\int \Delta(x) f(x)dx$ with $f(x)$ expanded as Eq. (5) becomes

$$\int \Delta(x) f(x)dx = \frac{1}{2}\sum_{n=0}^{\infty} \frac{\epsilon^n}{(n+1)!}[f^{(n)}(0+) + (-1)^n f^{(n)}(0-)]. (7)$$

In the limit of $\epsilon \to 0$, only the $n = 0$ part remains to contribute to $\int f(x)\Delta(x)dx$ and Eq. (3) follows. Although we assumed the specific form of Eq. (6), the details of the form of $\Delta(x)$ are unimportant. For example we can assume a gaussian form and obtain the same result in the narrow width limit.

If $f(x)$ is a function that is defined by means of a differential equation in which $\delta(x)$ is involved, Eq. (3) may turn out to be inconsistent with the definition of $f(x)$ itself. Such an unusual situation was recognized in relation to the Dirac equation in one dimension [2–4]. More recently Griffiths and Walborn (GW) illustrated such a situation by means of a simple mathematical example [5]. We review GW's example and add further clarification. Consider $f(x)$ that is defined by means of the first order differential equation

$$\frac{df(x)}{dx} = \alpha f(x)\delta(x), \quad (8)$$

where $\alpha \neq 0$ is a constant. (In GW's example, $\alpha = 1$.) From Eq. (8) follows

$$\int_{-\epsilon}^{+\epsilon} \frac{df(x)}{dx}dx = f(\epsilon) - f(-\epsilon) = \alpha \int_{-\epsilon}^{\epsilon} f(x)\delta(x)dx. \quad (9)$$

If Eq. (3) is accepted, Eq. (9) leads to the following boundary condition for $f(x)$ at $x = 0$ in the limit of $\epsilon \to 0$

$$f(0+) - f(0-) = \frac{\alpha}{2}[f(0+) + f(0-)]. \quad (10)$$

It turns out, however, that Eq. (10) is inconsistent with Eq. (8) that defines $f(x)$. In order to see this let us start with

$$\frac{df(x)}{dx} = \alpha f(x)\Delta(x). \quad (11)$$

Before taking the limit of $\epsilon \to 0$, $\Delta(x)$ is finite and $f(x)$ is continuous everywhere. Equation (11) can be solved by

$$f(x) = A \exp\left[\alpha \int_0^x \Delta(y)dy\right] = \begin{cases} Ae^{-\alpha/2} \\ Ae^{\alpha x/(2\epsilon)} \\ Ae^{\alpha/2} \end{cases} \quad \text{if} \quad \begin{cases} x \leq -\epsilon \\ -\epsilon < x < \epsilon \\ \epsilon \leq x \end{cases}, \quad (12)$$

where A is an arbitrary constant. We then obtain $f(\pm\epsilon) = Ae^{\pm\alpha/2}$. (Constant A can be determined if the value of $f(x)$ at a certain point is specified. This, however, is not essential in the present context.) When ϵ is finite, $f(x)$ is continuous everywhere. In the limit of $\epsilon \to 0$, however, $f(x)$ becomes discontinuous at $x = 0$. As x increases through $x = 0$, $f(x)$ jumps from $f(-0) = Ae^{-\alpha/2}$ to $f(0) = A$ and then to $f(0+) = Ae^{\alpha/2}$. We obtain the boundary condition at $x = 0$

$$f(0+) - f(0-) = \tanh(\alpha/2)\,[f(0+) + f(0-)]. \quad (13)$$

Equations (10) and (13) differ through higher order terms with respect to α.

It is crucial that the ordinary function for which Eq. (3) holds is given *independently of the limiting process of* $\lim_{\epsilon\to 0} \Delta(x) = \delta(x)$. In contrast the $f(x)$ defined by Eq. (11) depends on ϵ. Let us examine the integral $\int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx$ with $f(x) = Ae^{\alpha x/(2\epsilon)}$. We expand $f(x)$ as

$$f(x) = \sum_{n=0}^{\infty}(x^n/n!) f^{(n)}(0), \quad f^{(n)}(0) = A(\alpha/2\epsilon)^n. \quad (14)$$

Note that $f^{(n)}(0)$ with $n > 0$ diverges as $\epsilon \to 0$. For the n-th term of the expansion we obtain

$$\frac{1}{n!} f^{(n)}(0) \int_{-\epsilon}^{\epsilon} x^n \Delta(x) dx = \frac{[1-(-1)^{n+1}] A\, \alpha^n}{(n+1)!\, 2^{n+1}}. \quad (15)$$

Unlike in (7) all the terms with even n of the expansion contribute to $\int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx$. This is the cause of the difference between Eqs. (10) and (13). Although we assumed an explicit form of $\Delta(x)$ of Eq. (6), Eq. (13) obtained above is insensitive to the particular form assumed for $\Delta(x)$ [5].

There is another closely related problem. If $f(x)$ is an ordinary function, the following substitution is allowed

$$f(x)\delta(x) \to \delta(x) \int f(y)\delta(y)dy = \delta(x)f(0). \quad (16)$$

When combined with Eq. (16), Eq. (8) becomes

$$\frac{df(x)}{dx} = \alpha\delta(x) \int_{-\epsilon}^{\epsilon} f(y)\delta(y)dy. \quad (17)$$

The $f(x)$ defined by Eq. (17), however, turns out to be different from the one defined by Eq. (8). Substitution (16) is not allowed in this sense. Let us examine this problem by starting with the finite width version of Eq. (17), i.e.,

$$\frac{df(x)}{dx} = \alpha\Delta(x) \int_{-\epsilon}^{\epsilon} f(y)\Delta(y)dy. \quad (18)$$

Its solution, which is continuous everywhere, can be written as

$$f(x) = \left\{ \begin{array}{l} A - \frac{\alpha\lambda}{2} \\ A + \frac{\alpha\lambda x}{2\epsilon} \\ A + \frac{\alpha\lambda}{2} \end{array} \right. \quad \text{if} \quad \left\{ \begin{array}{l} x \le -\epsilon \\ -\epsilon < x < \epsilon \\ \epsilon \le x \end{array} \right. , \quad (19)$$

where A is a constant and

$$\lambda = \int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx. \quad (20)$$

Unlike (14), $f^{(n)}(x) = 0$ if $n > 1$. Equation (19) leads to

$$f(\epsilon) + f(-\epsilon) = 2A, \quad f(\epsilon) - f(-\epsilon) = \alpha\lambda. \quad (21)$$

On the other hand the $f(x)$ of Eq. (19) also yields

$$\int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx = \frac{1}{2\epsilon} \int_{-\epsilon}^{\epsilon} \left(A + \frac{\alpha\lambda x}{2\epsilon} \right) dx = A, \quad (22)$$

which implies $\lambda = A$. In the limit of $\epsilon \to 0$, Eq. (10) follows from Eq. (21). Substitution (16) in Eq. (8) thus changes the boundary condition of $f(x)$ at $x = 0$ from Eq. (13) to Eq. (10).

In the one-dimensional Dirac equation, which is a first order differential equation for a two-component wave function, if there is a potential of the form of $\delta(x)$, Eq. (3) does not hold for the wave function [2–4]. This is essentially for the same reason as the one found in GW's example with Eq. (8). It has also been known that if the potential part of the equation is of the form of $\delta(x)\psi(x)$, where $\psi(x)$ is the Dirac wave function, and if it is replaced by $\delta(x)\int \psi(y)\delta(y)dy$, then Eq. (3) can be used [2, 3, 6]. The interaction in this form can be interpreted as a zero-range "separable potential". The mechanism behind this feature is essentially the same as what we pointed out above regarding Eq. (16).

Next let us turn to the $f(x)$ defined by the second order differential equation

$$\frac{d^2 f(x)}{dx^2} = \beta f(x)\delta(x), \quad (23)$$

where β is a constant. In this case we find that $f(x)$ is continuous at $x = 0$ and that Eq. (3) holds. Equation (23) leads to the boundary condition

$$f'(0+) - f'(0-) = \beta f(0). \quad (24)$$

No complication such as those discussed above arises in this case. In order to confirm the validity of Eq. (3), let us start with

$$\frac{d^2 f(x)}{dx^2} = \beta f(x)\Delta(x). \quad (25)$$

Before taking the limit of $\epsilon \to 0$, $f(x)$ and $df(x)/dx$ can be assumed to be continuous everywhere. Solution $f(x)$ for $-\epsilon < x < \epsilon$ can be written as

$$f(x) = Ae^{Kx} + Be^{-Kx}, \quad K = \sqrt{\frac{\beta}{2\epsilon}}, \quad (26)$$

where A and B are constants. From Eq. (26) follows $f(\pm\epsilon) = Ae^{\pm K\epsilon} + Be^{\mp K\epsilon}$. In the limit of $\epsilon \to 0$, we find $K\epsilon \to 0$ and hence $f(x)$ remains continuous, i.e.,

$$f(0+) = f(0-). \quad (27)$$

For x outside the above interval, $d^2 f(x)/dx^2 = 0$ and hence $f(x)$ is a linear function of x. In order to determine the boundary condition for $f(x)$ at $x = 0$ in the limit of $\epsilon \to 0$, however, we do not need $f(x)$ for $|x| > \epsilon$. It is sufficient to know $f(x)$ for $-\epsilon < x < \epsilon$.

Let us examine $\int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx$ with $f(x)$ expanded as Eq. (5). The derivative $f^{(n)}(0) = [A+(-1)^n B]K^n = [A + (-1)^n B](\beta/2\epsilon)^{n/2}$ diverges as $\epsilon \to 0$. When it is combined with $\int_{-\epsilon}^{\epsilon} x^n \Delta(x)dx = [1-(-1)^{n+1}]\epsilon^n/[2(n+1)]$, however, only the $n = 0$ term of the expansion contributes to the integral in the limit of $\epsilon \to 0$. As a consequence, we obtain $\int_{-\epsilon}^{\epsilon} f(x)\Delta(x)dx \to A+B$, which justifies Eq. (3). This is in contrast to the situation found with the $f(x)$ of Eq. (12) for which $f^{(n)}(0) \propto 1/(2\epsilon)^n$. Let us add that substitution (16) in Eq. (23) can be done without affecting the solution.

The Schrödinger equation in one dimension for the stationary state of energy E is,

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \quad (28)$$

where m is the mass of the particle under consideration, $V(x)$ is the potential and $\psi(x)$ is the wave function. Equation (23) can be interpreted as the Schrödinger equation with $E = 0$ and potential $V(x) = (\hbar^2/2m)\beta\delta(x)$. Actually the boundary conditions Eq. (24) and Eq. (27) can be applied to the Schrödinger wave function with any value of E. The effect of the term $E\psi(x)$ on the boundary condition is negligible because $E\int_{-\epsilon}^{\epsilon}\psi(x)dx$ vanishes in the limit of $\epsilon \to 0$. Hence the boundary condition on the wave function at $x = 0$ is independent of energy E.

3. The derivative of the delta function

In this section we turn to the validity of Eq. (4). We consider $\Delta'(x) = d\Delta(x)/dx$, which in its narrow width limit is reduced to $\delta'(x)$. The results that we obtained in Sec. 2 are insensitive to the details of the form assumed for $\Delta(x)$. In contrast to that, what we are going to obtain regarding $\delta'(x)$ in this section depends on what we assume for the form of $\Delta(x)$ and $\Delta'(x)$.

Let us begin with the $\Delta(x)$ of the rectangular form of Eq. (6), which leads to the following dipole form

$$\Delta'(x) = \frac{d\Delta(x)}{dx} = \frac{1}{2\epsilon}[\delta(x+\epsilon) - \delta(x-\epsilon)]. \tag{29}$$

If $f(x)$ is an ordinary function that is continuous at $x = 0$, Eq. (4) can be justified by replacing $\delta'(x)$ with $\Delta'(x)$ of Eq. (29) and letting $\epsilon \to 0$ at the end. Equation (4), however, may not hold if $f(x)$ is a function that is defined by means of a differential equation in which $\delta'(x)$ is involved. GW mentioned this possibility but did not discuss any details; see the last sentence of note 3 of [5].

We are interested in the $f(x)$ defined by

$$\frac{d^2 f(x)}{dx^2} = \gamma f(x)\delta'(x), \tag{30}$$

where γ is a constant. If we accept Eq. (4), Eq. (30) leads to the boundary condition [7]

$$f'(0+) - f'(0-) = -\frac{\gamma}{2}[f'(0+) + f'(0-)]. \tag{31}$$

As we show below, however, Eq. (31) is not valid. Let us start with

$$\frac{d^2 f(x)}{dx^2} = \gamma f(x)\Delta'(x), \tag{32}$$

where $\Delta'(x)$ is the one defined by Eq. (29). Before the limit of $\epsilon \to 0$ is taken, $f(x)$ is continuous everywhere but $f'(x)$ is discontinuous at $x = \pm\epsilon$ because of the $\delta(x \pm \epsilon)$ of Eq. (29). At $x = \pm\epsilon$, $f(x)$ and $f'(x)$ are subject to the boundary conditions (24) and (27) with β replaced by γ. We refer to the three regions, $x < -\epsilon$, $-\epsilon < x < \epsilon$, and $\epsilon < x$ as I, II and III, respectively. In each of the regions, $d^2f(x)/dx^2 = 0$ and hence $f(x)$ is a linear function of x. Let the $f(x)$ in these regions be $f_i(x) = a_i x + b_i$ where $i = 1, 2, 3$ correspond to regions I, II and III, respectively. There are six constants but, if we specify two of them, the others can be determined by using Eqs. (24) and (27) at $x = \pm\epsilon$. If we assume for example that a_2 and b_2 are given, we obtain

$$a_1 = \left(1 + \frac{\gamma}{2}\right)a_2 - \frac{\gamma}{2\epsilon}b_2, \quad b_1 = \frac{\gamma}{2}a_2\epsilon + \left(1 - \frac{\gamma}{2}\right)b_2, \tag{33}$$

$$a_3 = \left(1 - \frac{\gamma}{2}\right)a_2 - \frac{\gamma}{2\epsilon}b_2, \quad b_3 = \frac{\gamma}{2}a_2\epsilon + \left(1 + \frac{\gamma}{2}\right)b_2. \tag{34}$$

In taking the narrow width limit of $\Delta(x)$, let us introduce another parameter η such that $\eta > \epsilon$. We let both of ϵ and η approach zero from the positive side. We integrate both sides of Eq. (32) over the interval $[-\eta, \eta]$. From the left hand side we obtain

$$\int_{-\eta}^{\eta}\frac{d^2 f(x)}{dx^2}dx = f'(\eta) - f'(-\eta) = a_3 - a_1, = -\gamma a_2, \tag{35}$$

where we have used $f(\eta) = f_3(\eta)$ and $f(-\eta) = f_1(-\eta)$ together with Eqs. (33) and (34). The right hand side of Eq. (32) yields

$$\gamma\int_{-\eta}^{\eta} f(x)\Delta'(x)dx = -\frac{\gamma}{2\epsilon}[f(\epsilon) - f(-\epsilon)] = -\gamma a_2, \tag{36}$$

which naturally agrees with Eq. (35). This can also be calculated as

$$\begin{aligned}\gamma&\int_{-\eta}^{\eta} f(x)\Delta'(x)dx \\ &= \gamma[f(x)\Delta(x)]_{-\eta}^{\eta} - \gamma\int_{-\eta}^{\eta}\Delta(x)f'(x)dx \\ &= -\gamma\int_{-\epsilon}^{\epsilon}\Delta(x)f_2'(x)dx = -\gamma a_2,\end{aligned} \tag{37}$$

Note that $\Delta(\pm\eta) = 0$ and $f_2'(x) = a_2$.

In the limit of $\eta \to 0$, we obtain $f'(\pm\eta) \to f(0\pm)$, $f(0+) = a_3$ and $f(0-) = a_1$, and then

$$f'(0+) - f'(0-) = a_3 - a_1 = -\gamma a_2, \tag{38}$$

$$\begin{aligned}-\frac{\gamma}{2}[f'(0+) + f'(0-)] &= -\frac{\gamma}{2}(a_3 + a_1) \\ &= -\gamma a_2 + \frac{\gamma^2}{2\epsilon}b_2.\end{aligned} \tag{39}$$

Note that Eq. (39) is different from Eqs. (36) and (37). From Eqs. (38) and (39) we see that Eq. (31) is not valid. It is possible to resurrect Eq. (31) by choosing b_2 such that $b_2/\epsilon = 0$, i.e., either $b_2 = 0$ or b_2 scales with ϵ in such a manner. Such a choice of b_2, however, is artificial. Here the following remark would be in order. One may erroneously think that $[f(\epsilon) - f(0)]/\epsilon \to f'(0+)$ and $[f(0) - f(-\epsilon)]/\epsilon \to f'(0-)$. Both of these are equal to a_2, which is $f_2'(x)$. Note that $f'(0+) = f_3'(x)$ and $f'(0-) = f_1'(x)$.

There is another important aspect of the $f(x)$ that is subject to Eq. (30). In Eqs. (33) and (34) we assumed that $f_2(x)$ is given first and then determined $f_1(x)$ and $f_3(x)$. If instead we start with an assumed $f_1(x)$ and determine $f_2(x)$ and $f_3(x)$, we obtain

$$\begin{aligned} a_2 &= \left(1-\frac{\gamma}{2}\right)a_1 + \frac{\gamma}{2\epsilon}b_1, \\ b_2 &= -\frac{\gamma}{2}a_1\epsilon + \left(1+\frac{\gamma}{2}\right)b_1, \end{aligned} \tag{40}$$

$$\begin{aligned} a_3 &= \left(1-\gamma+\frac{\gamma^2}{2}\right)a_1 - \frac{\gamma^2}{2\epsilon}b_1, \\ b_3 &= -\frac{\gamma^2}{2}a_1\epsilon + \left(1+\gamma+\frac{\gamma^2}{2}\right)b_1. \end{aligned} \tag{41}$$

Let us require that $f_3(x)$ be finite in the limit of $\epsilon \to 0$. This requirement can be satisfied if we choose $b_1 = 0$. Then we find that $b_2 = b_3 = 0$. Alternatively we can assume that b_1 is scaled according to $b_1 = c_1\epsilon$. In this case we again obtain $b_2 = b_3 = 0$. Thus we arrive at the boundary condition,

$$f(0+) = f(0-) = 0. \tag{42}$$

Regarding the relation between $f'(0+)$ and $f'(0-)$, we obtain

$$f'(0+) = \left(1-\gamma+\frac{\gamma^2}{2}\right)f'(0-) - \frac{\gamma^2}{2}c_1, \tag{43}$$

where we assumed $b_1 = c_1\epsilon$. Equation (43) contains c_1 that can be chosen arbitrarily. Hence it is not a legitimate boundary condition.

As we said at the end of the last section, Eq. (30) also can be regarded as the Schrödinger equation with energy $E = 0$ and potential $V(x) = (\hbar^2/2m)\gamma\delta'(x)$. We pointed out that the energy term $E\psi(x)$ has no effect on the boundary condition, that is, Eq. (42) can be applied even when $E \neq 0$. Let us consider the transmission-reflection problem of one-dimensional quantum mechanics with energy $E = k^2/(2m)$ where $k > 0$. Assume that a "plane wave" e^{ikx} is incident from the left. The wave function can be written as

$$\psi(x) = \begin{cases} e^{ikx} + R(k)e^{-ikx} & \text{for } x < 0 \\ T(k)e^{ikx} & \text{for } x > 0 \end{cases}, \tag{44}$$

where $T(k)$ and $R(k)$ are the transmission and reflection coefficients, respectively. The probabilities of transmission and reflection are respectively given by $|T(k)|^2$ and $|R(k)|^2$. Equation (42) requires that

$$\psi(0) = T(k) = 1 + R(k) = 0, \tag{45}$$

so that there is no transmission at any energies. The incident wave is totally reflected at $x = 0$. This means that the two half-spaces of $x > 0$ and $x < 0$ become effectively disjoint. This was pointed out by Šeba a long time ago [8]. In this connection, see Refs. [9, 10] also. The $T(k)$ and $R(k)$ for the potential $V(x) = (\hbar^2/2m)\gamma\Delta'(x)$ with finite ϵ can be worked out explicitly. When $|\epsilon k| \ll 1$ we obtain [10]

$$T(k) = \frac{i\epsilon k}{\gamma^2 + i\epsilon k}, \quad R(k) = \frac{-\gamma^2}{\gamma^2 + i\epsilon k}, \tag{46}$$

which is reduced to Eq. (45) in the limit of $\epsilon \to 0$.

On the basis of Eq. (30) Griffiths [7] proposed Eq. (31) together with

$$f(0+) - f(0-) = \frac{\gamma}{2}[f(0+) + f(0-)], \tag{47}$$

which also relies on Eq. (4). As we have shown explicitly, Eq. (31) is inconsistent with Eq. (30). In a similar manner it can also be shown that Eq. (47) is inconsistent with Eq. (30). It is interesting, however, that Eqs. (31) and (47) together represent a legitimate point interaction that can be related to a self-adjoint extension of the kinetic energy operator [10]. Boundary conditions (31) and (47) can be reinstated if we make the following substitution in Eq. (30) [11, 12],

$$\begin{aligned} f(x)\delta'(x) \quad \to \quad & \delta_p'(x)\int f(y)\delta(y)dy \\ + \quad & \delta(x)\int f(y)\delta_p'(y)dy, \end{aligned} \tag{48}$$

where $\delta_p'(x)$ is defined by

$$f(x)\delta_p'(x) = \tilde{f}(x)\delta'(x), \tag{49}$$

$$\tilde{f}(x) = \begin{cases} f(x) - \frac{1}{2}[f(0+) - f(0-)] & \text{if} \quad x > 0 \\ f(x) + \frac{1}{2}[f(0+) - f(0-)] & \text{if} \quad x < 0 \end{cases}. \tag{50}$$

Boundary conditions (31) and (47), however, should be dissociated from $\delta'(x)$. Note a similarity between substitutions (16) and (48); they respectively resurrect Eqs. (3) and (4). The substitutions, however, change the physics of the models under consideration.

We have interpreted $\delta'(x)$ as the $\epsilon \to 0$ limit of $\Delta'(x)$ of Eq. (29), which is the derivative of the rectangular function $\Delta(x)$ of Eq. (6). A question that arises here is: Does boundary condition (42) depend on the explicit form assumed for $\Delta'(x)$? The answer to this question is somewhat surprisingly affirmative. This is in the following sense. Recently Christiansen et al. [13] re-examined the transmission-reflection problem with a potential of the form of $\delta'(x)$. They assumed the $\delta'(x)$ as the narrow width limit of the following rectangular function [see their Eq. (5)]

$$\Delta_{\mathrm{C}}'(x) = \begin{cases} 0 & \text{if} \quad |x| > 2\epsilon \\ -(x/|x|)(2\epsilon)^{-2} & \text{if} \quad |x| < 2\epsilon \end{cases}. \tag{51}$$

We have replaced their ϵ with 2ϵ so that the ϵ of Eq. (51) corresponds to the ϵ of Eq. (29). The $\Delta_{\mathrm{C}}'(x)$ is the derivative of a triangular function of a unit area. If $f(x)$ is an ordinary function, Eq. (4) with $\delta'(x) = \lim_{\epsilon\to 0}\Delta_{\mathrm{C}}'(x)$ holds.

Christiansen et al. [13] considered the potential

$$V_\sigma(x) = \frac{\hbar^2}{2m}\,\sigma^2\Delta'_{\rm C}(x), \tag{52}$$

where σ is a dimensionless constant. They solved the Schrödinger equation and then took the limit of $\epsilon \to 0$. They showed that, if σ satisfies

$$\tan\sigma = \tanh\sigma, \tag{53}$$

the potential becomes partially transparent with

$$T(k) = \sec\sigma\,{\rm sech}\,\sigma \neq 0. \tag{54}$$

This is in contrast to $T(k) = 0$ of Eq. (45). Equation (53) admits discrete values of σ. They are 3.927, 7.069, 10.210, $\cdots$ in increasing order. Let us add that there are a variety of other forms of $\Delta'(x)$ that lead to non-vanishing but different $T(k)$ [14].

If we assume Eqs. (16) and (47), which are both based on Eq. (4), we obtain

$$T(k) = \frac{4-\sigma^4}{4+\sigma^4}. \tag{55}$$

This follows from Eqs. (38) and (49) of [10] with $c = \sigma^2$. The σ of Eq. (54) is subject to Eq. (53) but there is no such restriction on the σ of Eq. (55). The $T(k)$'s of Eqs. (54) and (55) are clearly different. This means that Eq. (4) with the wave function fails when it is used for $V_\sigma(x)$ with $\epsilon \to 0$.

Instead of reviewing it in detail, let us put Christiansen et al.'s analysis in the perspective of the "threshold anomaly" of transmission-reflection problem. With an arbitrarily given potential, the transmission probability usually vanishes at threshold, i.e., $|T(k)|^2 \to 0$ as $k \to 0$. This is because, no matter how small it is, the potential is insurmountably large as compared with the infinitesimal energy of the incident particle. If there is a bound state at threshold (i.e., with zero energy), however, threshold anomaly can occur such that $|T(k)|^2$ remains finite as $k \to 0$ [15]. When the strength parameter σ of the potential is chosen to satisfy Eq. (53), indeed there is a bound state at threshold. There are two types of the anomaly, I and II. We obtain $|T(0)|^2 = 1$ in type I whereas $|T(0)|^2$ can take any value between 0 and 1 in type II. Type II can be found only if the potential is asymmetric as a function of x [16]. The partial transparency that was found in [13] is an illustration of the threshold anomaly of type II. Let us add that threshold anomaly does not occur to a potential of the form of $\Delta'(x)$ of Eq. (29). This can be seen from Eq. (46).

The threshold anomaly refers to $T(k)$ with $k = 0$. The $T(k)$ of Eq. (54) that is due to potential $V_\sigma(x)$, however, is independent of k. In this sense the threshold anomaly holds for all energies. The reason why $T(k)$ becomes independent of k can be seen as follows. Note that $V_\sigma(x) \propto 1/\epsilon^2$ and its spatial range is proportional to ϵ. In the Schrödinger equation with $V_\sigma(x)$, if we introduce dimensionless quantities $y = x/\epsilon$ and $\eta = \epsilon k$, we can eliminate x and k in favor of y and η. The transmission coefficient can be expressed in terms of dimensionless parameters σ and η [13]. In the limit of $\epsilon \to 0$ and $\eta \to 0$, the transmission coefficient is reduced to a function of σ alone, which is independent of k; see Eq. (54). The reason why the $T(k)$ of Eq. (55) is also independent of k can be explained in a similar manner.

4. Summary

Regarding the Dirac delta function $\delta(x)$ and its derivative $\delta'(x)$, Eqs. (3) and (4) appear quite ubiquitously in textbooks of quantum mechanics but we should be aware of some possible danger in using them naively. We presented an overview of unusual situations in which the seemingly natural Eqs. (3) and (4) fail to hold. They can occur when function $f(x)$ is not an arbitrarily given function but is specifically defined by a differential equation in which $\delta(x)$ or $\delta'(x)$ appears.

We illustrated the mechanism behind the failure of Eq. (3) by starting with function $\Delta(x)$ of Eq. (6) that has a finite width 2ϵ and taking its narrow width limit. Equation (3) fails when $f(x)$ is a function that is defined by a *first order* differential equation of the form of Eq. (8). In this case $f^{(n)}(0)$, given by Eq. (14), diverges as $\epsilon \to 0$ for all values of $n > 0$ and this results in the failure of Eq. (3). The commonly used substitution (16) also fails. No such complication arises for $f(x)$ that is subject to a second order differential equation such as the Schrödinger equation. The delta function $\delta(x)$ that we used is the one defined by Eq. (1). Often Eq. (3) is used in defining $\delta(x)$. The $\delta(x)$ so defined, however, is led to self-contradiction as we illustrated by means of the $f(x)$ defined through Eq. (8).

The failure of Eq. (4) is associated with the *second order* differential equation (30) (and also the Schrödinger equation) in which $\delta'(x)$ is involved. For $\Delta'(x)$, the finite width version of $\delta'(x)$, we first considered the traditional dipole form of Eq. (29) and explicitly examined how Eq. (4) fails. We also examined the different version (51) that Christiansen et al. [13] recently considered. Equation (4) again fails in this case. The results obtained in Sec. 2 are insensitive to the details of the form assumed for $\Delta(x)$. In contrast the results obtained in Sec. 3 vary depending on the form of $\Delta'(x)$. We discussed implications that the unusual situations have regarding one-dimensional quantum mechanics. We related the results of [13] to the threshold anomaly of the transmission-reflection problem.

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