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GENERAL AND APPLIED PHYSICS

Some Problems with the Dirac Delta Function: Divergent Series in Physics

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Abstract
The completeness relation for the eigenfunctions of a self-adjoint operator generally involves a divergent series or integral. In this paper, we show, using the eigenfunctions of the infinite square well as an example, that these divergent objects can be interpreted as distributions. This should be obvious since the right-hand side of these completeness relations is the Dirac delta function but the direct calculation of the right-hand side can be very laborious, but instructive.

Keywords Divergent series · Dirac delta function

1 Introduction

It is well known that the eigenfunctions of a self-adjoint operator form a complete set; see, for instance, [1] or [2]. However, it is not so well known that the closure relation [3] (see Eq. (4)) does not converge [4–7]. This fact is not emphasized in quantum mechanics books.

This fact is so well known in mathematics that it is somewhat surprising to see a recent article by Bender et al. [8] draw attention to this mathematical fact. They show that there is a problem with the closure relation (its left side diverges) and they present a solution to this problem, that is to use a summation method to fix this. To be fair with Bender et al. [8], although the "problem" with the completeness relation (4) was suggested by Dirac in the first edition of his book on quantum mechanics [9], this "problem" they raise is not well explained in quantum mechanics books. The objective of this note is to present an alternative solution to the "problem" discussed by Bender et al. [8] that we think is more natural, and well known to mathematicians.

In Sect. 2, we discuss the problem by considering the infinite square well problem, that is a particle moving in the interval $[0, \pi]$ of the real axis. As is well known, this system has a purely discrete spectrum. In Sect. 3, we discuss an alternative solution to the divergence problem. As mentioned, such a solution is not new and it consists in considering these infinite series as distributions. An early paper on this subject is Braga and Schönberg [7]. Finally in Sect. 4, we discuss some other problems when dealing with divergent series or integrals in Physics.

In this paper, we shall use remarks to point out that some concepts and manipulations used in Physics are not rigorous from the mathematical point of view. These remarks can be ignored by a reader that is used to the physical literature in the subject.

2 The System to be Considered

To follow Bender et al. [8], we consider a particle moving freely in the interval $[0, \pi]$ of the real axis whose Hamiltonian action is

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$$H = -\frac{1}{2}\frac{d^2}{dx^2}\,. \tag{1}$$

As is well known, the normalized eigenfunctions of Hamiltonian, that vanish at $x = 0$ and $x = \pi$, are

$$\varphi_n(x) = \sqrt{\frac{2}{\pi}}\sin(nx) \tag{2}$$

and the corresponding eigenvalues are

$$E_n = \frac{1}{2}n^2\,. \tag{3}$$

It is well known the eigenfunctions of a such a system satisfy the following completeness (closure) relation

$$\sum_{n=1}^{\infty}\varphi_n^*(x)\varphi_n(y) = \frac{2}{\pi}\sum_{n=1}^{\infty}\sin(nx)\sin(ny) = \delta(x-y)\,. \tag{4}$$

The problem raised by Bender et al. [8], that as mentioned before should be well known, is that the series on the left side with the functions given by Eq. (2) diverges. Although not mentioned by Bender et al. [8], the right-hand side $\delta(x-y)$ is not a function but a distribution, the so-called Dirac delta function.

Bender et al. [8] showed that the divergent series can be summed. We think that it is preferable to show that the mathematical object

$$\sum_{n=1}^{\infty}\varphi_n^*(x)\varphi_n(y) = \frac{2}{\pi}\sum_{n=1}^{\infty}\sin(nx)\sin(ny) \tag{5}$$

can be interpreted in the sense of distributions and is in fact the Dirac delta function distribution, as written in Eq. (4). We show this is the next section.

3 Infinite Series Interpreted as Distributions

3.1 A Brief Recapitulation of the Approaches to Distributions: Schwartz [10] and Temple [11, 12] Frameworks

The concept of distribution [10–12] is presented in almost all books on mathematical physics. For completeness, we recapitulate here a few concepts that will be used in the sequel.

3.1.1 The Schwartz Definition

A distribution is a linear operator (a functional) that when acting on a good function (called a test function in the mathematical literature) produces a number. A simple example of a functional is a function $F(x)$ that acts on a good function $f(x)$ as follows

$$\int_{-\infty}^{\infty} dx\, F(x)f(x) = \text{Number}\,. \tag{6}$$

We say that $F(x)$ generates the functional of Eq. (6).

The Dirac delta function is the following distribution

$$\text{Dirac}\quad\text{Delta}\,(x-y)\,\text{acting}\quad\text{on}\, f(x) = f(y)\,. \tag{7}$$

Note that there is no ordinary function that generates this functional. Nevertheless in physics, we usually write (7) as

$$\int_{-\infty}^{\infty} dx\,\delta(y-x)f(x) = f(y) \equiv \delta_y[f]\,. \tag{8}$$

Remark 1 The above equation is wrong from the mathematical point of view. This integral does not exist because the symbol $\delta(y-x)$ is not a function. The delta is a functional that acting on a function $f(x)$, $\delta[f]$ produces a number $\delta[f] = f(0)$. However, most physicists interpret the above formula as

$$\int_{-\infty}^{\infty} dx\,\delta(y-x)f(x) = \lim_{N\to\infty}\int_{-\infty}^{+\infty} dx\,\delta_N(x-y)f(x) = f(y) \tag{9}$$

where $\delta_N(x-y)$ is a delta converging sequence; see, for instance, [13, 14]. This definition of distribution or generalized function as they are also called is due to Temple [11, 12].

Distributions that are "generated" by functions like in Eq. (6) are called **regular** distributions. Distributions that are not generated by functions are called **irregular**. The Dirac delta function is an irregular distribution. See [15] for the use of delta function relations without worrying with mathematical details as physicists usually do.

Some distributions are defined just in a part of the real axis, for example, in a interval $[a, b]$. In this case, the Eq. (8) becomes

$$\int_a^b dx\,\delta(x-y)f(x) = f(y) \text{ if } y \in (a,b)\,. \tag{10}$$

For further information, see [16].

3.1.2 The Temple Definition

The Temple definition is based on the concept of weak convergence. A sequence of differentiable functions $\varphi_n : R \to R$, $n = 1, 2, 3 \ldots$ is said to be weakly convergent if for any **test function** $f(x)$ the limit of numbers

$$\lim_{n\to\infty}\int_{-\infty}^{\infty} dx\, f(x)\varphi_n(x) \tag{11}$$

exists.

A distribution (or generalized function) D is an equivalent class of weakly convergent sequences of functions $[\varphi_n]$ and we write

$$\int dx\, D(x) f(x) = \lim_{n\to\infty} \int_{-\infty}^{\infty} dx\, f(x)\varphi_n(x)\,. \tag{12}$$

Two weakly convergent sequences $[\varphi_n]$ and $[\psi_n]$ are equivalent if their difference converges weakly to zero.

As an example of a weakly convergent sequence, that shall use below, we prove that

$$\lim_{\alpha\to\infty} \frac{\sin(\alpha x)}{\pi x} = \delta(x)\,. \tag{13}$$

This result is classical: see Lichthill [17] or Perelemov and Zel'dovich [18] for a graphical interpretation or Braga [19], whose rigorous demonstration we reproduce below.

Let $f(x)$ be a test function whose support, that is, the interval where $f(x)$ is different from zero, is contained in the interval $[-A, A]$. Then, we can write

$$\int_{-A}^{A} dx\, \frac{\sin(\alpha x)}{x} f(x) = \int_{-A}^{A} dx\, \sin(\alpha x) x \left[\frac{f(x) - f(0)}{x}\right] + f(0) \int_{-A}^{A} dx\, \frac{\sin(\alpha x)}{x}\,. \tag{14}$$

Now we define $\psi(x) = (f(x) - f(0))/x$, which is infinitely differentiable and its value and the value of its derivatives at zero can be calculated by L'Hospital rule. Then, integrating by parts the first integral we have

$$\int_{-A}^{A} dx\, \sin(\alpha x)\psi(x) = - \frac{\cos(\alpha x)}{\alpha}\psi(x)\Big|_{-A}^{A} + \frac{1}{\alpha}\int_{-A}^{A} dx\, \cos(\alpha x)\frac{d\psi(x)}{dx}\,, \tag{15}$$

which goes to zero as $\alpha \to \infty$. The remaining integral in Eq. (14) is well known, see reference [22], and when $\alpha \to \infty$ it goes to π. Therefore, we have

$$\lim_{\alpha\to\infty} \int_{-\infty}^{\infty} dx\, \frac{\sin(\alpha x)}{x} f(x) = \pi f(0)\,, \tag{16}$$

which demonstrates Eq. (13).

3.2 Distribution Interpretation of Eq. (4)

Our task now is to show that the object on left-hand side of Eq. (4) is in fact the Dirac delta function. To accomplish this, we shall prove that this object can be associated to a sequence that converges to the Dirac delta function. Another proof is to show that it satisfies the property (10) and we take this as a definition of the Dirac delta function.

3.2.1 First Method

Now, we show that in the sense of distributions the object

$$\sum_{n=1}^{\infty} \varphi_n^*(x)\varphi_n(y) = \frac{2}{\pi}\sum_{n=1}^{\infty} \sin(nx)\sin(ny) \tag{17}$$

is the Dirac delta function. This is carried out by the following calculation. First let us note that

$$\sum_{n=-N}^{n=N} e^{in(x-y)} = \frac{e^{-iN(x-y)}(e^{i(2N+1)(x-y)} - 1)}{e^{i(x-y)} - 1} \tag{18}$$

$$= \frac{\sin\left(\left(N + \frac{1}{2}\right)(x-y)\right)}{\sin\left(\frac{1}{2}(x-y)\right)}\,. \tag{19}$$

Taking the limit $N \to \infty$ on both sides of Eq. (19), we have

$$\lim_{N\to\infty} \sum_{n=-N}^{n=N} e^{in(x-y)} = \lim_{N\to\infty}\left[\frac{\sin\left(N + \frac{1}{2}\right)(x-y)}{\sin\left(\frac{1}{2}(x-y)\right)}\right] \tag{20}$$

$$= \lim_{N\to\infty} \frac{\sin(N(x-y))}{\sin\left(\frac{1}{2}(x-y)\right)} = \lim_{N\to\infty} \frac{\left(\frac{1}{2}(x-y)\right)}{\sin\left(\frac{1}{2}(x-y)\right)} \frac{\sin(N(x-y))}{\left(\frac{1}{2}(x-y)\right)} \tag{21}$$

$$= \frac{\left(\frac{1}{2}(x-y)\right)}{\sin\left(\frac{1}{2}(x-y)\right)} \lim_{N\to\infty} \frac{\sin(N(x-y))}{\left(\frac{1}{2}(x-y)\right)} \tag{22}$$

$$= \frac{\left(\frac{1}{2}(x-y)\right)}{\sin\left(\frac{1}{2}(x-y)\right)} 2\pi\delta(x-y) = 2\pi\delta(x-y) \tag{23}$$

since $\lim_{x\to 0} \frac{\sin x}{x} = 1$ and the factor $\frac{\frac{1}{2}(x-y)}{\sin\left(\frac{1}{2}(x-y)\right)}$ is bounded by one and tends to one when $x \to y$.

Then we can write

$$\lim_{N\to\infty} \sum_{n=-N}^{n=N} e^{in(x-y)} = \lim_{N\to\infty} \frac{\sin(N(x-y))}{\frac{1}{2}(x-y)} = 2\pi\delta(x-y)\,, \tag{24}$$

where we have used Eq. (13).

On the other hand, we can write

$$\sin(nx)\sin(ny) = -\frac{1}{2}\left\{\cos\left[n(x+y)\right] - \cos\left[n(x-y)\right]\right\} \quad (25)$$

$$= -\frac{1}{2}Re\left[e^{in(x+y)} - e^{in(x-y)}\right]. \quad (26)$$

Therefore,

$$\sum_{n=-N}^{N} \sin(nx)\sin(ny) = \sum_{n=-N}^{N} (-)\frac{1}{2}Re\left[e^{in(x+y)} - e^{in(x-y)}\right] \quad (27)$$

and we have that object given in Eq. (5) becomes

$$\frac{2}{\pi}\sum_{n=1}^{\infty} \sin(nx)\sin(ny) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty} \sin(nx)\sin(ny) \quad (28)$$

$$= \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} Re\left[e^{in(x-y)}\right] + \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} (-)Re\left[e^{in(x+y)}\right] \quad (29)$$

$$= A + B. \quad (30)$$

To calculate the first term, A, in Eq. (30) we note that it becomes

$$A = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} Re\left[e^{in(x-y)}\right] = \frac{1}{2\pi}Re \lim_{N\to\infty}\sum_{n=-N}^{N} e^{in(x-y)}. \quad (31)$$

Or using Eqs. (19) and (24)

$$A = \frac{1}{2\pi}Re \lim_{N\to\infty}\sum_{n=-N}^{N} e^{in(x-y)} \quad (32)$$

$$= \frac{1}{2\pi}\lim_{N\to\infty}\frac{\sin\left(\left(N+\frac{1}{2}\right)(x-y)\right)}{\frac{1}{2}(x-y)} = \delta(x-y). \quad (33)$$

We now show that the term B, the second term in Eq. (30), is zero in the sense of distributions. In fact, this term is

$$B = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} (-)Re\left[e^{in(x+y)}\right] \quad (34)$$

which can be written

$$B = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} (-)Re\left[e^{in(-x-y)}\right]. \quad (35)$$

Comparing with Eq. (24), we see that if we replace x by $-x$ to get

$$B = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} (-)Re\left[e^{in(-x-y)}\right] \quad (36)$$

$$= -\lim_{N\to\infty}\frac{1}{2\pi}\frac{\sin\left[N(-x-y)\right]}{\frac{1}{2}(x-y)} = -\delta(-x-y). \quad (37)$$

But this is zero because $x \in [0,\pi]$ then $y \in [-\pi, 0]$ and our functions are defined in the interval $[0,\pi]$.

We have therefore shown that

$$\frac{2}{\pi}\sum_{n=1}^{\infty} \sin(nx)\sin(ny) = \frac{1}{\pi}\sum_{n=-\infty}^{\infty} \sin(nx)\sin(ny) = \delta(x-y). \quad (38)$$

3.2.2 Second Method

We now present another demonstration of Eq. (38) that basically consists in showing that property Eq. (10) is satisfied. This property will be taken as a definition of the Delta function. This approach was used in Brownstein [20] and Amaku et al. [21] and is commonly used in the physical literature.

We now define

$$B_N(x,y) = \frac{2}{\pi}\sum_{n=1}^{N} \sin(nx)\sin(ny), \quad (39)$$

to prove that

$$\lim_{N\to\infty}\left(\int_0^{\pi} B_N(x,y)\varphi(y)dy\right) = \varphi(x) \quad (40)$$

The proof of Eq. (40) is as follows:

The first step of the proof is to write Eq. (39) for a finite N in the form

$$B_N(x,y) = \frac{1}{\pi}\sum_{-N}^{N} \sin(nx)\sin(ny), \quad (41)$$

and then to calculate it. Using that

$$\sin(nx)\sin(ny) = -\frac{1}{2}\left[\cos n(x+y) + \cos n(x-y)\right] \quad (42)$$

$$= -\frac{1}{2}Re\left[e^{in(x+y)} - e^{-in(x-y)}\right] \quad (43)$$

we can obtain that

$$B_N(x,y) = \frac{1}{2}\sum_{-N}^{N} Re\left[e^{in(x+y)} - e^{-in(x-y)}\right] \equiv D + E. \quad (44)$$

Calculating the second term in Eq. (44), that is E, we have

$$E = -\frac{1}{2}\sum_{n=-N}^{n=N} Re\, e^{-in(x-y)} \tag{45}$$

$$= \frac{1}{2}\left[\frac{e^{-iN(x-y)}\left(e^{2N+1(x-y)}-1\right)}{e^{i(x-y)}-1}\right] \tag{46}$$

$$= \frac{\sin\left(\left(N+\frac{1}{2}\right)(x-y)\right)}{\sin\left(\frac{1}{2}(x-y)\right)}\,. \tag{47}$$

As explained before, since $\lim_{x\to 0}\frac{\sin x}{x}=1$ we can to simplify the notation by replacing in the denominator of Eq. (47) $\sin\left(\frac{1}{2}(x-y)\right)$ by $\frac{1}{2}(x-y)$. This saves us to carry a factor $\frac{\frac{1}{2}(x-y)}{\sin\frac{1}{2}(x-y)}$, which is bounded by one and when $x\to y$ tends to one, in the rest of the calculation.

We now show that

$$\lim_{N\to\infty}\frac{1}{\pi}\int_0^{\pi} dy\,\frac{\sin\left[\left(N+\frac{1}{2}\right)(x-y)\right]}{\frac{1}{2}(x-y)}\varphi(y) = \varphi(x)\,. \tag{48}$$

In Eq. (48), we now change variables to

$$x-y=x';\;\; y=x'-x \tag{49}$$

note that while $x\in[0,\pi]$, $y\in[0,\pi]$ we have $x'\in[-\pi,\pi]$ so that Eq. (48) becomes

$$\lim_{N\to\infty}\frac{1}{\pi}\int_{-\pi}^{\pi} dx'\,\frac{\sin\left[\left(N+\frac{1}{2}\right)x'\right]}{x'}\,\varphi\left(x-x'\right)dx' = \varphi(x)\,. \tag{50}$$

We can write the left-hand side of Eq. (50) as

$$\lim_{N\to\infty}\left\{\frac{1}{\pi}\int_{-\pi}^{\pi} dx'\,\frac{\sin\left[\left(N+\frac{1}{2}\right)\right]x'}{x'}\left[\varphi(x-x')-\varphi(x)\right]\right. \tag{51}$$

$$\left.+\,\varphi(x)\int_{-\pi}^{\pi} dx'\frac{\sin\left[\left(N+\frac{1}{2}\right)\right]x'}{x'}\right\}. \tag{52}$$

At this point, it is convenient to define

$$\Psi(x,x') = \frac{\varphi(x-x')-\varphi(x)}{x'}\,. \tag{53}$$

This function is for each x, continuous and differentiable in x'; the derivative $\frac{\partial}{\partial x'}\Psi(x,x')$ may be computed using l'Hospital rule for $x'=0$. The first integral of Eq. (52) can be integrated by parts writing

$$\sin\left[\left(N+\frac{1}{2}\right)x'\right] = \frac{-1}{\left(N+\frac{1}{2}\right)}\frac{d}{dx'}\cos\left[\left(N+\frac{1}{2}\right)x'\right]. \tag{54}$$

The boundary terms at $+\pi$ and $-\pi$ are zero so we are left with

$$\lim_{N\to\infty}\int_{-\pi}^{\pi} dx'\cos\left[\left(N+\frac{1}{2}\right)x'\right]\frac{\partial}{\partial x'}\Psi(x,x') \tag{55}$$

which is zero.

Now in the term E, the second term of Eq. (52) performs the change of variables

$$x'' = \left(N+\frac{1}{2}\right)x' \tag{56}$$

which gives

$$\varphi(x)\lim_{N\to\infty}\int_{-\pi\left(N+\frac{1}{2}\right)}^{\pi\left(N+\frac{1}{2}\right)} dx''\,\frac{\sin x''}{x''} = \pi\varphi(x)\,. \tag{57}$$

where we have used the result given in reference [22]

$$\int_0^{\infty} dx\,\frac{\sin x}{x} = \frac{\pi}{2} \tag{58}$$

to prove Eq. (50). It remains to demonstrate that term D in Eq. (44) vanishes when $N\to\infty$.

$$\frac{1}{2}\sum_{n=-N}^{n=N} Re\, e^{in(x+y)} = \frac{1}{2}\sum_{n=-N}^{n=N} Re\, e^{in(-x-y)}\,. \tag{59}$$

Comparing the above expression with the left-hand side of Eq. (47), we have that replacing x by $-x$ in Eq. (48) its left-hand side becomes

$$E = \lim_{N\to\infty}\frac{1}{\pi}\int_0^{\pi} dy\,\frac{\sin\left(N+\frac{1}{2}\right)(-x-y)}{\frac{1}{2}(x-y)}\varphi(y)\,. \tag{60}$$

However, note that $x\in[0,\pi]$ and therefore $-x\in[-\pi,0]$ and since $\varphi(x)=0$ in this interval Eq. (60) is zero.

We have therefore proved that Eq. (40), viz.

$$\lim_{N\to\infty}\left(\int_0^{\pi} dy\, B_N(x,y)\varphi(y)\right) = \varphi(x) \tag{61}$$

is true.

Remark 2 The notion of limit in Eq. (61) above may be pictured as $B_N(x,y)$ being $B_N(x-y)$ and approximating for large N the delta function, that is $\lim_{N\to\infty}B_N(x-y)=\delta(x-y)$. Therefore, we could think of Eq. (61) as being

$$\int_0^\pi dy\ \delta(x-y)\varphi(y) = \varphi(x)\,. \tag{62}$$

But the "delta function" is not a function, because it would be $(+\infty)$ at one point and zero elsewhere and since the integral of a function is not altered by changing the function at a discrete set of points the left-hand side of Eq. (62) would be zero.

The definition of the distribution δ_x as a functional, as for example in reference [23], is very simple. It maps a function φ at its value at a given point x. That is we say that it is a functional

$$\delta_x[\varphi] = \varphi(x)\,. \tag{63}$$

Notice that in this language in Eq. (61)

$$\lim_{N\to\infty} B_N[\varphi] \to \delta_x[\varphi] \tag{64}$$

with

$$B_N[\varphi] = \int_0^\pi dy\ B_N(x-y)\varphi(y)\ . \tag{65}$$

B_N is also a "functional," but not defined in the same fashion as δ_x, because for every finite N, $\int_0^\pi dy B_N(x-y)\varphi(y)$ exists. Notice, however, that right-hand side of Eq. (65) becomes more and more concentrated around $x = y$ as N grows. For more of these sequences [17].

So, we have proved by using two methods that

$$\frac{2}{\pi}\sum_{n=1}^{\infty} \sin(nx)\sin(ny) = \delta(x-y)\ . \tag{66}$$

4 Another Divergent Series and Other Problems

In their paper, Bender et al. [8] present another problem related to the square well problem. They consider the infinite square well and the completeness relation of its eigenfunctions. The Hamiltonian operator of the system is

$$H = -\frac{1}{2}\frac{d^2}{dx^2} \tag{67}$$

and the completeness relation of its eigenfunctions is, as we have seen,

$$\sum_{n=1}^{\infty} \varphi_n^*(x)\varphi_n(y) = \frac{2}{\pi}\sum_{n=1}^{\infty} \sin(nx)\sin(ny) = \delta(x-y)\,. \tag{68}$$

Bender et al. [8] wanted to calculate the explicit coordinate representation of H, that is,

$$\langle x|H|y\rangle = -\frac{1}{2}\frac{d^2}{dx^2}\delta(x-y)\ . \tag{69}$$

We have

$$\langle x|H|y\rangle = \sum_{n=1}^{\infty} E_n\varphi_n^*(x)\varphi_n(y) = \frac{1}{\pi}\sum_{n=1}^{\infty} n^2\sin(nx)\sin(ny)\,. \tag{70}$$

So it is tempting to write (70) as

$$\langle x|H|y\rangle = -\frac{1}{2}\frac{d^2}{dx^2}\left(\frac{2}{\pi}\sum_{n=1}^{\infty}\sin(nx)\sin(ny)\right) \tag{71}$$

$$= -\frac{1}{2}\frac{d^2}{dx^2}\delta(x-y)\,. \tag{72}$$

But the authors argue that they cannot write Eq. (70) as Eq. (72) because they cannot interchange the sum with the differentiation. This would be allowed only if the sum on the left-hand side of Eq. (72) were absolutely and uniformly convergent. But in fact the left-hand summation of Eq. (70) is divergent, that is, the summation on Eq. (68) is divergent and as we have argued above has to be interpreted in the sense of distribution. We shall elaborate on this on the sequel.

Bender et al. [8] tried to circumvent the problem mentioned above by considering the function

$$K(x,y,t) = \frac{2}{\pi}\sum_{n=1}^{\infty} t^n\sin(nx)\sin(ny) \tag{73}$$

which is absolutely and uniformly convergent for $|t| < 1$. However, the limit $t \to 1^-$ that must be taken to recover Eq. (68) cannot be taken because Eq. (73) does not converge absolutely and uniformly for $t \le 1$. Indeed, as mentioned in the appendix of Bender et al. [8] the convergence as $t \to 1^-$ is in the sense of distributions. However, they do not mention this fact explicitly.

The physical quantities associated to an operator like the one given in Eq. (67) are its expectation values on suitable regular wave functions $f(x)$. Since $f(x)$ vanishes outside the interval $[0,\pi]$ this regularity manifests as the requirement that these wave functions satisfy the conditions

$$f(0) = f(\pi) = 0 \quad \text{and} \quad \frac{df(0)}{dx} = \frac{df(\pi)}{dx} = 0\,. \tag{74}$$

The reader should note that when we write Eq. (4) we have interpreted the wave functions $\varphi_n(x)$ as distributions, in fact regular distributions (see Remark 1). The test functions, $f(x)$, in this case, are infinitely differentiable functions with support in the interval $[0,\pi]$. These functions vanish with their derivatives at the points 0 and π. The operator given by Eq. (67) acts on test functions with the properties given by Eq. (74).

The expectation value of H on such functions is

$$\langle f|H|f\rangle = \int_0^\pi dy f(y)(Hf)(y)\,, \tag{75}$$

$$= \int_0^\pi dy f(y)\left(-\frac{1}{2}\frac{d^2f(y)}{dy^2}\right). \tag{76}$$

If we write

$$(Hf)(x) = \int_0^\pi dy\ \langle x|H|y\rangle f(y) \tag{77}$$

we get, comparing with Eq. (77), that

$$\int_0^\pi dy\ \langle x|H|y\rangle f(y) = -\frac{1}{2}\frac{d^2f(x)}{dx^2}\,. \tag{78}$$

Previously, we proved that

$$\lim_{N\to\infty}\left(\int_0^\pi dy\ B_N(x,y)f(y)\right) = f(x)\,. \tag{79}$$

Now we have that

$$\int_0^\pi dy\ \left(-\frac{1}{2}\frac{d^2}{dx^2}B_N(x,y)\right)f(y) = \int_0^\pi dy\ \left(-\frac{1}{2}\frac{d^2}{dy^2}B_N(x,y)\right)f(y) = \int_0^\pi dy\ B_N(x,y)\left(-\frac{1}{2}\frac{d^2f(y)}{dy^2}\right), \tag{80}$$

where we used in the first equality that B_N is symmetric under the exchange of x by y and in the second one we just integrated by parts. Taking the limit $N\to\infty$ leads to

$$\lim_{N\to\infty}\int_0^\pi dy\left(-\frac{1}{2}\frac{d^2}{dx^2}B_N(x,y)\right)f(y) = -\frac{1}{2}\frac{d^2f(x)}{dx^2} = \int_0^\pi dy\ \langle x|H|y\rangle f(y)\,, \tag{81}$$

where we used Eq. (79). Therefore, we proved Eq. (72).

Equations (79) and (81) are the precise distributional versions of Eqs. (68) and (72), using the notion of "delta sequences" as explained in the appendix of Bender et al. [8]. That is Eq. (79) is a "delta sequence" definition of the Dirac delta function.

Remark 3 This remark is intended to explain some subtleties involved in Eq. (4). It is only an introduction to the problems overlooked in the physical literature about the infinite square well and will be the subject of a more comprehensive article now in preparation.

The astute reader should note that when we write Eq. (4), we are compelled to interpret the wave functions $\varphi_n(x)$ as distributions, in fact regular distributions; see Remark 1. The test functions, $f(x)$, in this case are infinitely differentiable functions with support in the interval $[0,\pi]$. These functions vanish with their derivatives at the points 0 and π. The usual distributions have test functions with support in R that is in the whole real line.

Is this important? It is because it means that only functions with support in $[0,\pi]$ can be expanded in series of $\varphi_n(x)$. Some excellent textbooks like [24] writes that "any other function, $f(x)$ can be expanded in term of it." This is not entirely correct since it is true only if we periodically extend $f(x)$.

We shall comment below how it is possible to define these distributions that have support in a finite interval of the real line. But first, we show that with this interpretation we can solve one of the questions students ask about the fact that the wave function of the square well have discontinuous derivatives at 0 and π. In fact, the students sometimes ask if the functions

$$\varphi_n(x)\ \sqrt{\frac{2}{\pi}}\sin(\pi x) \tag{82}$$

satisfy the Schödinger equation

$$-\frac{1}{2}\frac{d^2\varphi(x)}{dx^2} = E\varphi(x) \tag{83}$$

with $\varphi(0)=\varphi(\pi)=0$.

They ask this because they learned that if a function is discontinuous, then its derivative have a delta function on the discontinuity. But if $\varphi_n(x)$ is interpreted as a distribution we should differentiate it as a distribution. Distributions are infinitely differentiable. For example, the first derivative D' of say a distribution D acting on a test function f is

$$D'[f] = D[-f']\,. \tag{84}$$

Take, for example, the step function (Heaviside function)

$$\theta(x-x_1)\begin{cases}1 & \text{for } x>x_1\\ 0 & \text{for } x<x_1\end{cases} \tag{85}$$

that we now consider as a distribution with its action defined by Eq. (6). Notice that the space of test functions $(f(x))$ is the set of infinite differentiable function defined in a finite interval of the real numbers containing the point x_1. So, the distribution $\theta(x-x_1)$ is the functional

$$\theta[f] = \int_{-\infty}^{\infty} dx\ \theta(x-x_1)f(x) = \int_{x_1}^{\infty} dx\, f(x)\,. \tag{86}$$

According to Eq. (84), the derivative of $\theta[f]$ is

$$\theta'[f] = -\theta[f'] = -\int_{x_1}^{\infty} dx\, \frac{df}{dx} = -f(\infty) + f(x_1) = f(x_1) \tag{87}$$

where we used that $f(\pm\infty) = 0$. However, this functional is the Dirac delta function defined in Eqs. (7) and (8).

In the case of the wave functions $\varphi_n(x)$, the corresponding regular distributions are the functional

$$\varphi_n[f] = \int_0^{\pi} dx\, \varphi_n(x) f(x) \tag{88}$$

and the distribution $d\varphi_n/dx$ is

$$\frac{d\varphi_n}{dx}[f] = \int_0^{\pi} dx\, \varphi_n(x) \frac{df(x)}{dx}\,. \tag{89}$$

This functional nor the next derivative has delta functions on the points $x = 0$ or $x = \pi$ because the test functions and all its derivatives vanishes on these points. Is this important? Yes it shows how to use distributions defined with test functions defined in a finite interval of the real axis correctly. In fact, we have more to say about this below.

Distributions that have test functions with support in an interval of the real line are defined, for example in, the paper by Pandey and Pathak [6]. In this paper, they demonstrate the following result: A generalized function (distribution) can be expanded in terms of a complete set of normalized eigenfunctions $\Psi_n(x)$ of a Sturm-Liouville system. Let these eigenfunctions be defined in an interval $I = [a, b]$. Consider a space of test functions $f(x)$ in this interval. Then if $\varphi(x)$ is a generalized function defined in the same interval we define

$$F(n) = \int_a^b dx'\, \Psi_n^{\star}(x') f(x') \tag{90}$$

and we expand $f(x)$ as follows:

$$f(x) = \lim_{N\to\infty} \sum_{N=1}^{N} F(n)\Psi_n(x)\,. \tag{91}$$

Now substituting Eq. (90) into the last expression allows us to write

$$f(x) = \lim_{N\to\infty} \int_a^b dx' \sum_{n=1}^{N} \Psi_n(x)\Psi^{\star}(x') f(x') \tag{92}$$

$$= \int_a^b dx' \left(\lim_{N\to\infty} \sum_{n=1}^{N} \Psi_n(x)\Psi^{\star}(x') \right) f(x')\,. \tag{93}$$

Hence, we have that

$$\lim_{N\to\infty} \sum_{n=1}^{N} \Psi_n(x)\Psi^{\star}(x') = \delta(x - x')\,. \tag{94}$$

If the time independent Schrödinger equation (TISE) has a singular interaction then to interpret the wave function as a distribution is not so simple. For example, if the TISE defined on $(-\infty.\infty)$ has a delta function or a singularity at the origin like in the one-dimensional hydrogen atom we can follow the method of self-adjoint extensions [25] for the case of the delta function and for the case of the Hydrogen atom [26]. A didactic introduction to the self-adjoint extension method can be found in [27] and [28] and references there. On the other hand, the paper [29] explain how to treat the delta function problem as a distribution and [30] treats the hydrogen atom in the same way.

Finally, we would like to comment on a problem that is never mentioned in the quantum mechanics textbooks with the exception of [31]. This problem is that the operator

$$\hat{\mathcal{O}} = -\frac{d^2}{dx^2} \tag{95}$$

operating on functions defined in the interval $[0, \pi]$ with boundary conditions $\varphi(0) = \varphi(\pi) = 0$ is not self-adjoint. To define a self-adjoint operator, we need to restrict the $\hat{\mathcal{O}}$ domain as follows:

$$D(\hat{\mathcal{O}}) = \{\, \varphi(x) \in L^2(I = [0, \pi]) \mid \varphi'(x) \in L^2(I = [0, \pi]) \text{ and } \varphi(0) = \varphi(\pi) = 0 \,\}\,. \tag{96}$$

However, $\varphi'(x)$ is the weak (distributional) derivative of $\varphi(x)$. The operator so defined have the same eigenfunctions and eigenvalues as the usual operator defined in the quantum mechanics textbooks.

The treatment given in [31] is a bit abstract and can be generalized. Therefore, we shall analyze this problem in another paper. The reader could benefit from the more intuitive paper [32] that we also examine in this forthcoming paper. If, however, the reader is anxious to see practical consequence of the non-selfadjointness of the infinite square well potential he/she should see [28].

5 Concluding Remarks

We have shown in this paper that the methods used by Bender et al. [8], in their appendix coincide with the methods of distribution theory explained for example in the book by Schwartz [23] or for sequences of delta functions in the book of Lichthill [17].

The advantages of using distribution theory to explain the problems raised by Bender et al. article [8] are many:

1. One deals with objects that are finite quantities and hence physically motivated. Infinite quantities like the ones in Eqs. (68) and (70) simply do not arise.

2. The methods used are elementary because they require techniques that within the reach of undergraduates physics students.
3. The theory can be used directly. For example, we do not have to use the Euler summation to “reconstruct” a Hamiltonian from its eigenstates and eigenfunctions as proposed by Bender et al. [8].

On the other hand, much more serious infinities arise in applications of mathematics to physics as suggested by Bender et al. [8]. We shall deal with them in a separate paper.

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