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David Branson

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Continuity conditions on Schrödinger wave functions at discontinuities of the potential

David Branson

Mathematics Department, University of Essex, Colchester CO4 3SQ, England

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Several standard arguments which attempt to show that the wave function and its derivative must be continuous across jump discontinuities of the potential are reviewed and their defects discussed. Three arguments which it is hoped are more satisfactory are then presented.

I. INTRODUCTION

Most introductions to quantum mechanics include a discussion of the square-well potential, since it illustrates important physical ideas while at the same time avoiding the distraction of complicated mathematics. The boundary conditions imposed on the Schrödinger wave function at the edges of the well are: (a) the wave function vanishes, if the potential jump is infinite, (b) the wave function and its first derivative are continuous, if the potential jump is finite.

Condition (a) may be justified by treating the infinite potential jump as the limit of a finite jump. If one investigates the limiting process one sees that conditions (b) reduce to (a) in the limit. This is well treated in many textbooks,¹ but has the pedagogical disadvantage that one usually wishes to treat the infinite well first because of its mathematical simplicity. However, it is the justification for conditions (b) that is the subject of this paper.

In Sec. II we describe why most textbook explanations of conditions (b) are, in our view, unsatisfactory, and in the remaining sections we present arguments which are, we hope, more acceptable. The treatment described in Sec. III uses a momentum-space argument; Sec. IV is probably inappropriate for most students taking a first quantum-mechanics course because it involves distribution theory. By contrast, the argument of Sec. V is very simple: it treats the discontinuous potential as the limit of a continuous potential.

II. UNSATISFACTORY ARGUMENTS

We restrict ourselves to the one-dimensional case, so that we are dealing with the Schrödinger equation

$$(-\hbar^2/2m)\phi''(x) + V(x)\phi(x) = E\phi(x), \quad (1)$$

where $V(x)$ has a finite jump discontinuity at (say) $x = 0$ (and possibly discontinuities at other points also). When students first encounter the strange world of quantum mechanics, (b) must be one of the least puzzling and most readily acceptable statements that they meet. But the more thoughtful student may be a little worried. If the first and second derivatives of ϕ were to exist everywhere it would be necessary that ϕ and its first derivative should be everywhere continuous. It follows that the second term on the left-hand side of (1) would have a simple jump discontinuity at $x = 0$ which would have to be balanced by a similar discontinuity in ϕ'' . However, this is impossible, for a derivative which exists at every point of an interval cannot have a jump discontinuity at some point of that interval.³ We conclude that ϕ'' does not exist at $x = 0$, and hence Eq.

(1) is undefined there. The connection between the two regions $x < 0$ and $x > 0$ is thus lost, and there no longer seems to be any compelling reason for insisting on the continuity of ϕ and ϕ' at $x = 0$. If the potential exhibits violent behaviour at $x = 0$, why should not the wave function and its derivative?

The standard textbooks are not very convincing on this question. Many merely state conditions (b) without justification. In Ref. 1 we read:

The time-independent wave equation is a second-order linear differential equation in $\mathbf{r}$. Thus so long as $V(\mathbf{r})$ is finite, whether or not it is continuous, a knowledge of the wave function and its gradient along a surface makes it possible to integrate the equation to obtain the wave function at any point. It is reasonable, therefore, to require that the wave function and its gradient be continuous, finite and single valued at every point in space, in order that a definite physical situation can be represented uniquely by a wave function. These requirements also have the consequence that the position probability density $P(\mathbf{r})$ and the probability current density $\mathbf{S}(\mathbf{r})$ are finite and continuous everywhere.

This argument certainly is "reasonable" but not completely compelling since the wave equation ceases to be defined at $x = 0$. We could also obtain a unique wave function by imposing some other (less "reasonable") criteria for matching the solution in $x < 0$ with that in $x > 0$. In addition, as we shall see below, conditions (b) are not necessary to ensure the continuity of the position probability density and the probability current density.

The argument in some other textbooks⁴ may be summarized as follows. "A finite probability density requires the wave function to be finite everywhere. Equation (1) then implies that ϕ'' is finite, so that ϕ' and, *a fortiori*, ϕ are continuous." However, there is no basic principle which demands that the probability density be finite (one requires only that its integral be finite); in Appendix A we show that the finiteness of ϕ does in fact follow from other considerations, but nevertheless ϕ'' does not exist at $x = 0$, so that we are certainly not justified in stating that it is finite at that point.

Other textbooks⁵ argue unconvincingly, as in the previous paragraph, that ϕ'' is finite everywhere and then claim that the equation

$$\phi'(x) = \phi'(a) + \int_a^x \phi''(t) dt \quad (a < 0) \quad (2)$$

implies that $\phi'(x)$ is continuous. The right-hand side of (2) is certainly continuous [the fact that $\phi''(0)$ does not exist

is no problem in this respect] but it is equal to the left-hand side if, and only if, $\phi'(x)$ is continuous. Thus one certainly cannot use (2) to prove the continuity of ϕ' . If ϕ' is not continuous at $x = 0$, Eq. (2) remains true when $x < 0$, but when $x > 0$ it should be replaced by

$$\phi'(x) = \phi'(a) + \phi'(+)-\phi'(-) + \int_a^x \phi''(t)dt,$$

where, for example,

$$\phi'(+)=\lim_{x\rightarrow 0+}\phi'(x).$$

(The existence of the one-sided limits is demonstrated in Appendix A.)

It might be thought that conditions (b) follow from the requirements (i) the expectation value of the momentum operator $(-i\hbar d/dx)$ must be real, i.e., $-i\hbar \int_{-\infty}^{\infty} \phi^* \phi' dx$ is real for all ϕ ; (ii) the expectation value of the momentum-squared operator $(-\hbar^2 d^2/dx^2)$ must be real, i.e., $-\hbar^2 \int_{-\infty}^{\infty} \phi^* \phi'' dx$ is real for all ϕ . In investigating these conditions we accept the *a priori* possibility of discontinuities at $x = 0$ (hereinafter we suppose that V is discontinuous only at this point) and divide the integrals in (i) and (ii) into integrals over $(-\infty, 0]$ and $[0, \infty)$. If we then integrate (i) by parts once and (ii) by parts twice, and note that ϕ and ϕ' vanish at infinity (see Appendix A), we find that (i) implies

$$\phi^*(+)\phi(+) = \phi^*(-)\phi(-), \quad (3)$$

that is, the probability density is continuous, whereas (ii) implies

$$\begin{aligned} \phi^*(+)\phi'(+)-\phi^{*'}(+)\phi(+) \\ = \phi^*(-)\phi'(-)-\phi^{*'}(-)\phi(-), \end{aligned} \quad (4)$$

that is, the probability current density is continuous.

A little manipulation shows that (3) and (4) are equivalent to

$$\phi(+) = \exp(i\alpha)\phi(-), \quad (5)$$

$$\phi'(+)=\exp(i\alpha)[\phi'(-)+\beta\phi(-)], \quad (6)$$

where α and β are real constants, independent of ϕ . Thus conditions (5) and (6), while being more general than conditions (b) nevertheless satisfy conditions (i) and (ii) above, and also guarantee the continuity of the probability density and current density.

At a more technical level, we might suppose that the requirement that the Hamiltonian be self-adjoint would force us to adopt (b). However, this is not the case. Let us consider the subset $\mathcal{S}$ of L^2 consisting of functions which are twice differentiable everywhere except at $x = 0$, whose second derivatives belong to L^2 , and which satisfy (5) and (6). Then $\mathcal{S}$ is dense in L^2 , and the operator T defined by $T\phi = -(\hbar^2/2m)\phi''$ for all $\phi \in \mathcal{S}$ is symmetric, i.e.,

$$\int_{-\infty}^{\infty} \phi_1^*(T\phi_2)dx = \int_{-\infty}^{\infty} (T\phi_1)^*\phi_2 dx$$

for all $\phi_1, \phi_2 \in \mathcal{S}$. If α equals 0 or π (and possibly for all other values) T is also a real operator in the sense of Ref. 6. The potential-energy operator V , restricted to the domain $\mathcal{S}$, is clearly symmetric also, and is real when T is real. Thus we can conclude that for some, and possibly all, values of α , and for all β , $T + V$ is a real symmetric operator and hence, by theorem 9.14 of Ref 6, it can be extended in at

least one way to a self-adjoint Hamiltonian. Thus (5) and (6) allow self-adjointness, and there is no necessity to adopt the more restrictive conditions (b).

III. MOMENTUM-SPACE ARGUMENT

Quantum-mechanical wave-functions $\phi(x)$ must belong to the space L^2 of square-integrable functions. Each such function possesses a Fourier transform defined by

$$\Phi(p) \equiv (\mathcal{F}\phi)(p) = \frac{1}{\sqrt{h}} \int_{-\infty}^{\infty} dx \exp \frac{-ipx}{h} \phi(x). \quad (7)$$

(In this section, in order not to obscure the argument, we assume that all functions vanish sufficiently rapidly at $\pm\infty$ to prevent any convergence problems at these points. If this is not the case, the integral in (7) must be defined via a limit in the L^2 mean, but the conclusions are unaltered.) The function $\Phi(p)$ also belongs to L^2 and the relationship between ϕ and Φ is (1-1) and it preserves the norm. The variable p is identified with momentum and we can regard ϕ and Φ simply as two representations (in configuration space and momentum space, respectively) of the same physical state. Any operator R in configuration space defines an operator $\tilde{R}$ in momentum space by the formula

$$\Phi \rightarrow \tilde{R}\Phi = \mathcal{F}(R\phi), \quad (8)$$

where ϕ and Φ are related by (7).

The operator corresponding to the square of the momentum is defined in configuration space by the usual expression

$$R = -\hbar^2 d^2/dx^2. \quad (9a)$$

(If ϕ belongs to L^2 , then, provided $V(x)$ is well behaved except at the origin, Eq. (1) implies that ϕ'' must also belong to L^2 .) The vital ingredient of this section is the imposition of the following condition: the Schrödinger wave functions must be such that if R is given by (9a), then

$$\tilde{R} = p^2. \quad (9b)$$

Using (7) and (9a), Eq. (8) becomes

$$\tilde{R}\Phi(p) = \frac{-\hbar^2}{\sqrt{h}} \int_{-\infty}^{\infty} dx \exp \frac{-ipx}{h} \frac{d^2\phi}{dx^2}.$$

To accommodate the possibility of discontinuities at $x = 0$, we split the range of integration into $(-\infty, 0]$ and $[0, \infty)$ and integrate by parts twice to obtain

$$\begin{aligned} (\tilde{R}\Phi)(p) = (\hbar^2/\sqrt{h})[\phi'(+)-\phi'(-)] \\ + (ip\hbar/\sqrt{h})[\phi(+)-\phi(-)] + p^2\Phi(p). \end{aligned}$$

In order to satisfy (9b) we must therefore have the continuity conditions $\phi'(+)=\phi'(-)$ and $\phi(+)=\phi(-)$.

IV. DISTRIBUTION THEORY ARGUMENT

In this approach we interpret the ϕ of Eq. (1) not as an ordinary function but as a distribution, and we demand that (1) hold everywhere including the point $x = 0$. In this case there is no problem with the existence of ϕ'' at $x = 0$ because the derivative of a distribution may certainly possess a jump discontinuity.

Since ϕ must belong to L^2 , it must be locally integrable and hence we see from (1) that ϕ'' must also be locally integrable (i.e., it is a "regular distribution"). We now prove

that ϕ' must be a regular distribution which is (absolutely) continuous.

Because ϕ'' is locally integrable we can define a function H by

$$H(x) = \int_a^x \phi''(t) dt,$$

and such a function H is absolutely continuous (and hence locally integrable), and H' exists almost everywhere (ae) and is equal to ϕ'' ae. We now prove that ϕ' and H differ only by a constant. Note that this was the stumbling-block in Sec. II [see discussion following Eq. (2)] where ϕ was regarded as an ordinary function rather than a distribution.

Consider the distribution $H - \phi'$ and its distributional derivative $(H - \phi')'$ defined by

$$\langle (H - \phi')', \theta \rangle = - \langle (H - \phi'), \theta' \rangle, \quad (10)$$

for all testing functions θ belonging to the space $\mathcal{D}$ of infinitely smooth functions which vanish outside some finite interval. The right-hand side of (10) is equal to

$$- \langle H, \theta' \rangle + \langle \phi', \theta' \rangle. \quad (11)$$

Using the fact that H is locally integrable the first bracket may be written as

$$- \int_{-\infty}^{\infty} H(x) \theta'(x) dx = \int_{-\infty}^{\infty} H'(x) \theta(x) dx.$$

The integration by parts is justified by the absolute continuity of H ; the terms at infinity vanish because of the properties of θ . Since $H' = \phi''$ ae this expression becomes

$$\int_{-\infty}^{\infty} \phi''(x) \theta(x) dx = \langle \phi'', \theta \rangle = - \langle \phi', \theta' \rangle,$$

where the last step follows from the definition of the derivative of a distribution. It follows that (11) and hence also (10) vanish, i.e., $(H - \phi')$ is a distribution whose derivative is zero. The lemma proved in Appendix B shows therefore that $(H - \phi')$ is a constant distribution. Since H is an absolutely continuous function we conclude that ϕ' is a continuous function.

A similar argument replacing ϕ'' by ϕ' shows that ϕ is also continuous.

V. LIMIT OF A CONTINUOUS POTENTIAL

We consider a continuous potential, illustrated in Fig. 1, which increases linearly between $x = 0$ and $x = a$: $V(x) = V_0 x/a$, $0 \leq x \leq a$; apart from the continuity condition, the potential is unspecified outside the region $0 \leq x \leq a$. We will investigate the limit of solutions as a tends to zero.

For $0 \leq x \leq a$, Eq. (1) may be written

$$\phi'' + (2m/\hbar^2)[E - (V_0 x/a)]\phi = 0. \quad (12)$$

The change of variable

$$y = (2ma^2/V_0^2 \hbar^2)^{1/3} [(V_0 x/a) - E]$$

simplifies (12) to

$$\frac{d^2 W}{dy^2} - yW = 0, \quad (13)$$

where we have written $W(y) = \phi(x(y))$. This is Airy's equation and we may write its solution as⁸

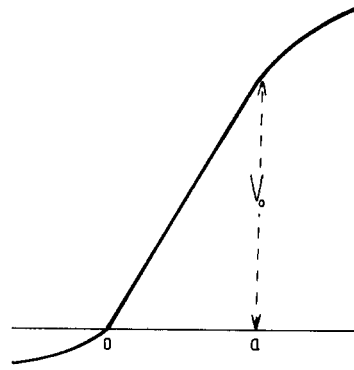


Fig. 1. Potential discussed in Sec. V. We consider the limit as a tends to zero.

$$W(y) = Ff(y) + Gg(y),$$

where

$$f(y) = 1 + y^3/3! + 4y^6/6! + \dots \quad (14)$$

$$g(y) = y + 2y^4/4! + 10y^7/7! + \dots \quad (15)$$

When $x = 0$,

$$y = -(2ma^2/V_0^2 \hbar^2)^{1/3} E = y_0 \quad (16)$$

(say), and when $x = a$,

$$y = (2ma^2/V_0^2 \hbar^2)^{1/3} (V_0 - E) = y_a \quad (17)$$

(say).

We now have a continuous potential, so that Eq. (1) is well-defined everywhere, and we have no hesitation in imposing continuity of ϕ and of $d\phi/dx$ at $x = 0$ and at $x = a$. If we denote by $P(x)$, $Q(x)$ the solutions of Eq. (1) in the regions $x < 0$, $x > a$, respectively, we obtain

$$P(0) = Ff(y_0) + Gg(y_0), \quad (18)$$

$$P'(0) = [Ff'(y_0) + Gg'(y_0)] (2mV_0/a\hbar^2)^{1/3}, \quad (19)$$

$$Q(a) = Ff(y_a) + Gg(y_a), \quad (20)$$

$$Q'(a) = [Ff'(y_a) + Gg'(y_a)] (2mV_0/a\hbar^2)^{1/3}. \quad (21)$$

Since Eq. (13) has no term in dW/dy , the Wronskian $f(y)g'(y) - f'(y)g(y)$ is a constant which we can evaluate at $y = 0$, obtaining the value 1. Using this fact we solve (18) and (19) for F and G :

$$F = P(0)g'(y_0) - P'(0)g(y_0) (a\hbar^2/2mV_0)^{1/3}$$

$$G = -P(0)f'(y_0) + P'(0)f(y_0) (a\hbar^2/2mV_0)^{1/3}.$$

Substitution of these values into (20) and (21) gives

$$Q(a) = P(0)[f(y_a)g'(y_0) - f'(y_0)g(y_a)] - P'(0)[f(y_a)g(y_0) - f(y_0)g(y_a)] (a\hbar^2/2mV_0)^{1/3}, \quad (22)$$

$$Q'(a) = P(0)[f'(y_a)g'(y_0) - f'(y_0)g'(y_a)] \times (2mV_0/a\hbar^2)^{1/3} - P'(0)[f'(y_a)g(y_0) - f(y_0)g'(y_a)]. \quad (23)$$

We see from (16) and (17) that y_0 and y_a are both proportional to $a^{2/3}$, so (14) and (15) imply that, as a tends to zero, $f(y_0)$, $f(y_a)$, $g'(y_0)$, $g'(y_a)$ all tend to 1, $f'(y_0)$, $f'(y_a)$ tend to zero like $a^{4/3}$, $g(y_0)$, $g(y_a)$ tend to zero like $a^{2/3}$.

Hence our final conclusion from (22) and (23) is that, as a tends to zero, $Q(a) \rightarrow P(0)$, $Q'(a) \rightarrow P'(0)$, that is, in the limit as the potential becomes discontinuous, the wave function and its first derivative remain continuous.

The argument of this section can be generalized to any potential which, in $0 \leq x \leq a$, is of the form $V_0 u(x/a)$ with $u(0) = 0$ and $u(1) = 1$ provided u is analytic in a sufficiently large region centered on the origin. We expand u in a Taylor series about the origin

$$u\left(\frac{x}{a}\right) = \sum_{n=1}^{\infty} \frac{u_n x^n}{a^n} \quad (24)$$

and, by the standard method, obtain a power-series solution to Eq. (1) in the form

$$\phi(x) = \sum_{n=0}^{\infty} c_n(a) x^n,$$

where the coefficients c_n ($n \geq 2$) are given in terms of arbitrary c_0 and c_1 by the recurrence relation

$$(n+2)(n+1)c_{n+2} = \frac{2m}{\hbar^2} \left(V_0 \sum_{i=1}^n \frac{c_{n-i} u_i}{a^i} - E c_n \right). \quad (25)$$

If we first put $c_0 = 1$, $c_1 = 0$, and then put $c_0 = 0$, $c_1 = 1$, we obtain two independent solutions, $\phi_0^a(x)$, $\phi_1^a(x)$, respectively, where the superscripts make explicit the dependence of the solutions on a , arising from the a dependence of the potential.

It is easy to establish that $\phi_0^a(0) = \phi_1^a(0) = 1$, and $\phi_0^a(0) = \phi_1^a(0) = 0$. The Wronskian of the two solutions is again constant and equal to one. A simple induction argument using (25) shows that for ϕ_0^a the coefficients c_n are of order a^{2-n} ($n \geq 2$) as a tends to zero, whereas for ϕ_1^a they are of order a^{3-n} ($n \geq 3$).

We now put $\phi = B_0 \phi_0^a + B_1 \phi_1^a$ $0 \leq x \leq a$, and impose continuity of the wave function and its derivative at $x = 0$ and $x = a$. Eliminating B_0 and B_1 we obtain

$$Q(a) = P(0)\phi_0^a(a) + P'(0)\phi_1^a(a),$$

$$Q'(a) = P(0)\phi_0^a(a) + P'(0)\phi_1^a(a).$$

We now take the limit as a tends to zero. From the remark above we see that $\phi_0^a(a)$ and $\phi_1^a(a)$ are both of the form $1 + \text{an infinite number of terms which are individually of order } a^2$ and $\phi_0^a(a)$ and $\phi_1^a(a)$ consist of an infinite number of terms each of which vanishes with a . Therefore if we are allowed to take the limit term by term we see that $Q(a) \rightarrow P(0)$ and $Q'(a) \rightarrow P'(0)$ as desired. This procedure can be justified⁹ rigorously if the series (24) converges in an interval greater than $|x| \leq 2ea$.

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I am grateful to Dr. J. L. Bona and to Dr. J. F. Toland for useful conversations.

APPENDIX A

We here prove that both the wave function and its first derivative vanish at infinity, and that, at any points where they are discontinuous, the one-sided limits exist and are finite.

Suppose that the wave function ϕ is discontinuous at $x = b$, but that both ϕ and ϕ' are continuous in the half-open interval $[a, b)$. Then for any x belonging to (a, b) we have

$$2 \int_a^x \phi(t) \phi'(t) dt = \phi^2(x) - \phi^2(a). \quad (A1)$$

The wave function ϕ belongs to L^2 , and, if the momentum operator $(-\hbar d/dx)$ is to be well defined, so does ϕ' and therefore the integral $2 \int_a^b \phi(t) \phi'(t) dt$ exists and is finite and equal to C (say). It follows that the left-hand side of (A1) tends to C as x tends to b from below; therefore, the right-hand side does likewise. The existence of a finite left-hand limit of ϕ at $x = b$ then follows from the continuity of ϕ in $[a, b)$. Similarly all right-hand limits of ϕ exist.

By taking $b = \infty$ a similar argument shows that $\phi(x)$ tends to a finite limit as $x \rightarrow \infty$; since ϕ belongs to L^2 , this limit can only be zero.

We can repeat the argument, replacing ϕ and ϕ' by ϕ' and ϕ'' , respectively, to show that ϕ' tends to zero at infinity and its one-sided limits exist at points of discontinuity.

APPENDIX B

Lemma. If S is a distribution whose derivative is zero then S is a constant.

Let θ_0 be some fixed testing function in $\mathcal{D}$ which satisfies $\int_{-\infty}^{\infty} \theta_0(x) dx = 1$, and let $A = \langle S, \theta_0 \rangle$. Then every θ belonging to $\mathcal{D}$ may be written uniquely as $\theta = k\theta_0 + \xi$, where $k = \int_{-\infty}^{\infty} \theta(x) dx$ and ξ belongs to that subspace of $\mathcal{D}$ whose elements are the derivatives of testing functions in $\mathcal{D}$.¹⁰

Put $\xi = \eta'$ where $\eta \in \mathcal{D}$. Then

$$\langle S, \theta \rangle = k \langle S, \theta_0 \rangle + \langle S, \eta' \rangle$$

$$= A \int_{-\infty}^{\infty} \theta(x) dx - \langle S', \eta \rangle = \langle A, \theta \rangle,$$

since $S' = 0$. Thus S is equal to the constant distribution A .

¹See, for example, L. I. Schiff, *Quantum Mechanics*, 3rd ed. (McGraw-Hill, New York, 1968), p. 32.

²This statement is untrue if we impose the condition $\phi(0) = 0$. However, if we impose also the continuity of $\phi'(x)$ at $x = 0$, then the problem becomes overconstrained, and no solution exists.

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⁵S. Gasiorowicz, *Quantum Physics*, (Wiley, New York, 1974), p. 77; A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1964), Vol. 1, p. 79; D. Park, *Introduction to Quantum Theory* (McGraw-Hill, New York, 1964), p. 77; M. Scharff, *Elementary Quantum Mechanics* (Wiley, New York, 1969), p. 48.

⁶M. H. Stone, *Linear Transformations in Hilbert Space and their Applications to Analysis* (American Mathematical Society, New York, 1932), Chap. IX.

⁷See, for example, B. Epstein, *Linear Functional Analysis: An Introduction to Lebesgue Integration and Infinite Dimensional Problems* (Saunders, Philadelphia, 1970), p. 117.

⁸M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965), p. 446.

⁹I am very grateful to Dr. D. H. Fremlin for providing a proof of this statement.

¹⁰A. H. Zemanian, *Distribution Theory and Transform Analysis* (McGraw-Hill, New York, 1965), p. 68.