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Singular potentials in one dimension

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In quantum mechanics of one dimension it is shown for potentials which become infinite at a point but are continuous elsewhere, that the singularity acts as an impenetrable barrier if the potential is not integrable up to the singularity, but if the potential is integrable the behavior is not essentially different from that of a potential which does not become infinite.

I. INTRODUCTION

The one-dimensional Schrödinger equation will be considered for potentials $V(x)$ which are continuous everywhere except that $|V(x)| \to \infty$ as $x \to +0$. It makes no difference to the discussion whether the infinite value be attractive or repulsive. We will divide such potentials into suitable classes and then consider which solutions of the Schrödinger equation are physically acceptable. This will lead to the conclusion that if the potential is integrable then, for each energy, there are two solutions which are acceptable as far as their behavior at $x = 0$ is concerned and the physics is no different from that of a nonsingular potential. If the potential is not integrable (but not so singular as to lie outside the scope of our investigation), then only one solution is acceptable on either side of the singularity, which acts as an impenetrable barrier. It is intuitively reasonable that a repulsive singular potential might act as an impenetrable barrier; perhaps it is more surprising that an attractive potential is equally potent in this regard.

In considering discontinuities or infinities of the potential in quantum mechanics, it can be argued that such behavior is to be regarded only as a convenient model of the true situation in which the singularities would inevitably be smoothed out. In any case it is important to know whether the singular potential does predict the same physical consequences as result when a negligibly small amount of smoothing is present. Obviously a smoothed potential is never impenetrable, but for the case of a smoothed nonintegrable potential it is shown that the transmission of particle flux tends to zero as the smoothed potential approaches the singular form.

The one-dimensional hydrogen atom (for which $V = -C|x|^{-1}$) is an example of a singular potential which has been discussed in earlier contributions[1-3] to this Journal. In Appendix B these contributions are reexamined.

II. CLASSIFICATION OF POTENTIALS

The Schrödinger equation is $\psi'' - V(x)\psi + E\psi = 0$ (units have been chosen such that $\hbar = 2m = 1$). We assume that $|V(x)| \to \infty$ as $x \to +0$, and if there is any asymmetry about $x = 0$, it will be assumed that the behavior as $x \to -0$ is not more singular than it is for $x \to +0$. It will be convenient to divide these singular potentials into three classes. The notation $\int_0 f(x)\,dx$ will be used to denote

$$\lim_{\epsilon \to 0} \int_\epsilon^a f(x)\,dx$$

for any choice of a with $a > \epsilon > 0$.

Class MS (mildly singular) with $\int_0 V\,dx < \infty$. Potentials in this class are singular (in the sense that they become infinitely large at $x = 0$) but not as singular as the one-dimensional hydrogen atom (H1) with $V = C|x|^{-1}$.

Class S with $\int_0 x|V(x)|\,dx < \infty$ but with $\int_x V(y)\,dy \to \infty$ as $x \to 0$. This class includes H1.

Class XS with $\int_0 x|V(x)|\,dx$ divergent. New problems arise in this class and it will not be considered here. Some potentials in this class have been considered by Case.[4] Note that many authors use the term *singular potential* to apply only to this class.

III. ACCEPTABLE SOLUTIONS WITH SINGULAR POTENTIALS

It is a basic premise of quantum mechanics that physical quantities must be represented by Hermitian operators. In our context then p^2 and V (and therefore $H = p^2 + V$) must be Hermitian. In particular, $\langle V \rangle$ must exist (allowing for the nonnormalizability of the wave function in the case of positive energy states). Thus $\int_0 |\psi|^2 V\,dx$ must exist. In Appendix A it is shown that, if $V(x)$ is in class MS or S, there will be a regular solution F and an irregular solution G such that, for small x, $F \sim x$ and $G \sim 1$. Hence $\int_0 F^2 V\,dx$ exists, whereas $\int_0 G^2 V\,dx$ exists if V is in class MS but diverges for class S. Thus for class S only the regular solution F is acceptable, while for class MS both solutions F and G can be admitted.

When there is only one allowable solution at the singular point, there can be no particle flux. The function F is real and the flux $\mathbf{j} = i[(\nabla F)^* F - F^*(\nabla F)]$ is then zero. Complex linear combinations of two independent real solutions are required to give a flux. Therefore there can be a particle flux for class MS but there can be none for class S. Now the question of how to match left to right becomes clear. For class MS the situation is just as for a nonsingular potential: the wave functions and their derivatives are well behaved and match in magnitude and derivative as usual. In case S the singularity isolates left from right, and there is no reason to try to match the wave functions.

If the potential is integrable up to $x = 0$ from the left but not from the right, then only the regular solutions are to be used. We have already established for such a potential that admissable wave functions must vanish as $x \to +0$; to make the momentum operator Hermitian we then require that wave functions vanish as $x \to -0$. In physical terms the potential on the right acts as an impenetrable barrier and for all forms of impenetrable barrier the wave function must vanish.

IV. SMOOTHING OUT THE SINGULARITY

In this section consideration will be given to the Schrödinger equation when the potential $V(x)$ (which is now taken to be an *even* singular function) is replaced by a nonsingular even potential $U(x)$ for $|x| < b$ while remaining unchanged for $|x| \geq b$. Finding the solutions is straightforward; one matches the solutions for $V(x)$ to those for $U(x)$ in magnitude and derivative at $x = +b$ and at $x = -b$. With the potential $V(x)$ two linearly independent solutions are $F(x)$ and $G(x)$ as described above. Let $u(x)$ and $v(x)$ be two linearly independent solutions with potential $U(x)$. One can take $u(x)$ to be even and $v(x)$ to be odd. If $u(x)$ were neither even nor odd, then even and odd combinations of $u(x)$ and $u(-x)$ could be constructed, while if u and v were both even or both odd, the Wronskian $[u,v] \equiv uv' - u'v$ would vanish at $x = 0$, which is inconsistent with the linear independence of u and v. The Wronskians $[u,v]$ and $[F,G]$ must be independent of x and nonzero. Our choice of F and G gives $[F,G] = -1$; furthermore, we choose $u \sim 1$ and $v \sim x$ so that $[u,v] = 1$.

To find the odd solution $\xi(x)$ with the smoothed potential, a linear combination of F and G is matched to the odd function $v(x)$ at $x = b$. The appropriate linear combination is easily seen to be $\xi = [G,v]_b F - [F,v]_b G$. Similarly, the even solution is $\eta = [G,u]_b F - [F,u]_b G$. For the determination of the form of these solutions as $b \to 0$ (and for the consideration of the transmission coefficient discussed below) we require the behavior for small b of the coefficients of F and G, i.e., the "mixed" Wronskians $[H,w]_b$ in which H stands for F or G and w stands for u or v. These can be determined from the equation

$$\frac{d}{dx}[H,w] = (U - V)Hw,$$

which follows readily from the Schrödinger equations $H'' = (V - K^2)H$ and $w'' = (U - K^2)w$. Unless $[H,w]$ diverges for small x, it follows that

$$[H,w]_b = [H,w]_0 - \int_0^b (V - U)Hw\,dx.$$

For any reasonable smoothing potential $U(x)$ the integral in this relation will be of order $\int_0^b VHw\,dx$ for small b. Thus

$$[F,u]_b \sim -1 + O\left(\int_0^b Vx\,dx\right),$$

$$[G,v]_b \sim 1 + O\left(\int_0^b Vx\,dx\right),$$

$$[F,v]_b \sim O\left(\int_0^b Vx^2\,dx\right),$$

while for $[G,u]$ one must distinguish the class of the potential:

$$[G,u]_b \sim \begin{cases} O\left(\int_0^b V\,dx\right) & \text{for class MS,} \\ O\left(\int^b V\,dx\right) & \text{for class S.} \end{cases}$$

From these results one finds that in the limit as $b \to 0$ the odd solution becomes F while the even solution depends on the class: in class MS the even solution becomes G but in class S the even solution becomes F and the derivative is discontinuous. This agrees with our conclusion above that only the regular solution F is acceptable for class S.

It will now be shown that for class S the transmission from left to right vanishes as $b \to 0$. To have a wave function on the right which is purely outgoing for large x, we must arrange that F and G are in a certain (complex) ratio; the precise ratio is not required—merely that both F and G must be present. When b is small, there is very little of G in either the odd function ξ or the even function η. Therefore a very large amount of ξ and η would be required to give unit flux—a mixture of ξ and η with very large coefficients, the coefficients of F almost cancelling to leave F and G of the same order. Then on the left-hand side the coefficients of F would not cancel, i.e., a very large amplitude wave incident from the left would be almost entirely reflected. Thus the transmission coefficient tends to zero as b does.

This isolation of left from right can be viewed from a different angle. Instead of the odd and even functions formed from F, one could (by taking the sum and difference of these two) form a function which is the same as F on the right but zero on the left and another function which is zero on the right. Any wave function which is zero on the left can be expanded in terms of the eigenfunctions zero on the left and under any nonsingular perturbation will evolve only into states zero on the left.

V. DEGENERACY

So far we have considered only the neighborhood of the singularity. There are also boundary conditions to be satisfied as $x \to \pm\infty$. It is well known[5] that for nonsingular potentials such that $V(x) \to 0$ as $|x| \to \infty$ both of the two solutions for any positive energy are acceptable. Such states are therefore said to be *twofold degenerate* and eigenstates of nonzero flux are possible. There may also be discrete negative-energy solutions (bound states) and these are necessarily *nondegenerate*.

For singular potentials of class MS these conclusions will still hold but for class S we really have two independent systems (left and right) and all states of each half will be nondegenerate. It may happen that some of the bound states on the left have the same energy as those on the right; indeed, if the potential is symmetric, this will be true of every bound state. One could use the term degenerate to apply to such states of the whole system as well as to its positive-energy states.

Here the details of the physics being modelled become important. If some smoothing is present, then there will be a slow leakage from one side to the other. For phenomena occurring over such a short period of time that this leakage is negligible, the two sides are effectively isolated and the notion of degeneracy has no relevance. Over a longer period of time, so that the leakage is important, the model using the singular potential is not strictly accurate and there cannot be exact degeneracy. However, the wave functions and eigenvalues provided by that model may be useful for some purposes. In this case the matter of whether some states are (almost) degenerate may be of significance.

APPENDIX A: SOLUTIONS OF THE SCHRÖDINGER EQUATION NEAR A SINGULARITY

Unfortunately, the theory of the asymptotic behavior of solutions of differential equations is usually presented in a form applicable to large values of the independent variable. However, if one changes to $t = 1/x$ and also to $t\psi(x)$ as dependent function, then a standard theorem[6] becomes applicable. Converting back to the original variables one concludes that, if $\int^0 x|V(x)|\,dx < \infty$, then there are solutions $\psi = F(x)$ and $\psi = G(x)$ such that as $x \to 0$

$$F/x \to 1, \qquad F' \to 1,$$
$$G \to 1, \qquad xG' \to 0.$$

Since one has

$$G'(x) = G'(a) - \int_x^a G''(y)\,dy$$
$$= G'(a) - \int_x^a [V(y) - E]G(y)\,dy,$$

it follows for class S [where $\int_x V(y)\,dy \to \infty$ as $x \to 0$] that $G'(x) \to \infty$ as $x \to 0$, whereas for class MS it follows that $G'(x)$ has a definite limit $G'(0)$ as $x \to 0$. If $G'(0) \neq 0$, then $\bar{G}(x) \equiv G(x) - G'(0)F(x)$ is also a solution of the differential equation with $\bar{G}(0) = 1$ and $\bar{G}'(0) = 0$. Hence, for class MS there is a solution G such that, as $x \to 0$, $G \to 1$ and $G' \to 0$.

A somewhat simpler argument can be made if the potential is assumed to behave as a power of x for small x [thus $V(x) = -Cx^{s-2}$ with $0 < s < 2$]. The Schrödinger equations becomes $\psi'' + (Cx^{s-2} + E)\psi = 0$ and it is clear that for small x the energy term $E\psi$ can be ignored in comparison with the singular potential term. With the independent variable transformed to x^s, the equation $\psi'' + Cx^{s-2}\psi = 0$ becomes amenable to solution in power series. In fact, it becomes a form of Bessel's equation,[7] but the behavior for small x can most simply be obtained by finding the leading terms of the series expansion directly from the equation before transformation. In this way one finds that the regular solution is

$$F \sim x[1 - Cx^s/s(s+1) + \text{higher powers of } x^s],$$

and the irregular solution is (for $s \neq 1$)

$$G \sim 1 - Cx^s/s(s-1) + \text{higher powers of } x^s.$$

As usual these series can be differentiated term by term, and hence $F' \sim 1$ while $G' \sim -Cx^{s-1}/(s-1)$. Thus G' tends to zero with x if $s > 1$ (i.e., for class MS) but diverges if $s < 1$ (i.e., for class S). For $s = 1$ (H1) the solution can be found by standard methods and G' diverges logarithmically.

APPENDIX B: ONE-DIMENSIONAL HYDROGEN ATOM

The potential $V(x) = -C|x|^{-1}$ lies on the boundary of class S, but clearly within it. The integral $\int_0 G^2 V\,dx$ diverges logarithmically, so that G must be rejected. Haines and Roberts[3] admit G as physically acceptable and are led to a continuum of negative-energy eigenstates. This set of states is clearly unacceptable; not only does the expectation value of the potential energy not exist, but eigenstates of different energy are not always orthogonal to each other. For example, any two of their "first continuum wave functions" have no zeros (as shown in their Fig. 1) and are consequently not orthogonal. It follows that the Hamiltonian is not Hermitian with respect to their set of states. The treatment given by Loudon[1] leads to the correct conclusions, apart from a previously noted error.[2]

There is another respect in which Haines and Roberts differ from our conclusions. While admitting the regular function F as an odd solution, they reject it as an even solution on the grounds that it does not then satisfy the Schrödinger equation at $x = 0$. Indeed it does not, since taking the second derivative gives rise to a δ function: if $\psi(x) = F(|x|)$, then $\psi'' = F''(|x|) + 2\delta(x)$. However, this does not matter—since there is an impenetrable barrier at $x = 0$, adding a δ function to it makes no difference. For example the δ function does not affect any matrix elements of the Hamiltonian because all admissible wave functions vanish at $x = 0$.

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[6] W. A. Coppel, *Stability and Asymptotic Behavior of Differential Equations* (Heath, Boston, 1965), Theorem 3, p. 92.
[7] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards, Washington, DC, 1964), Eq. 9.1.51, p. 362.