A new approach to one-dimensional scattering

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remarkable accomplishment that remains untarnished by this curious error.

ACKNOWLEDGMENT

The author would like to thank Noel Swerdlow for his invaluable help in this research.

[1] *Philosophiæ Naturalis Principia Mathematica*, hereafter abbreviated *Principia*, was first published in 1687. I have used the English translation of 1729 of the third and final edition by Andrew Motte, revised by Florian Cajori (Ref. 3). For prior editions of the *Principia*, I have used a marvelous compilation by Koyré and Cohen (Ref. 11), which does a meticulous job of reporting the three editions of the *Principia*, and the various interleaved, annotated copies.

[2] Though we are mainly concerned with the final edition of 1726 which was translated into English, it should be noted that the format of Newton's argument evolved following the first edition, where the "Rules of Philosophy" and "Phenomena" had not been separate (see Ref. 11).

[3] Sir Isaac Newton, *Sir Isaac Newton's Mathematical Principles of Natural Philosophy and his System of the World*, translated by Andrew Motte in 1729, edited by Florian Cajori (University of California Press, Berkeley, 1934), Book III, Prop. VII, p. 414.

[4] Colin Maclaurin, *An Account of Sir Isaac Newton's Philosophical Discoveries* (The Royal Society, London, 1748; reprinted by Johnson Reprint Corporation, New York and London, 1968), p. 288.

[5] Reference 3, Book III, Prop. VIII, Cor. I, p. 416.

[6] There is an interesting discussion about the lack of consensus on the value of the solar parallax in Chaps. 12 and 13 of A. Van Helden, *Measuring the Universe* (The University of Chicago Press, Chicago, 1985).

[7] Reference 6, pp. 143, 144.

[8] Reference 6, p. 147.

[9] Reference 6, p. 152.

[10] Reference 3, Book III, Prop. VIII, Cor. II, p. 416.

[11] Sir Isaac Newton, *Isaac Newton's Philosophiæ Naturalis Principia Mathematica*, edited by Alexandre Koyré, I. Bernard Cohen, and Anne Whitman (Harvard U. P., Cambridge, 1972), Vol. 2, p. 581 (note to line 15).

[12] Reference 11, Vol. 2, p. 567 (note to line 9).

[13] According to Ref. 6, pp. 154–155, the figure of 10.5″ represents an average of the upper and lower limits of 12″ and 9″ for the solar parallax, as calculated by Bradley and Pound.

A new approach to one-dimensional scattering

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An alternative approach to the one-dimensional scattering problem is presented in which the potential is replaced by a sequence of flat barriers or wells. The resulting problem is solved exactly and the transmission coefficient obtained via multiplication of a string of 2×2 matrices.

I. INTRODUCTION

The phenomenon of tunneling never fails to bring home the magical nature of the microscopic world to new students of quantum mechanics. The one-dimensional potential barrier of height V and width w, treated in nearly all introductory texts, suffices to dispel the classical illusion that particles cannot pass through a barrier whose height V exceeds their energy E. A simple solution of Schrödinger's equation shows that the wave function is zero neither inside the barrier nor on the transmission side and hence that the probability for tunneling is always finite.

For barriers more complicated than the simple flat one, which itself is exactly solvable, one usually resorts to approximation schemes as outlined for example by French and Taylor[1] or somewhat more rigorously utilizing the WKB method as in Bohm.[2] It is our purpose here to show that even for this more general case of nonconstant potential, one need not go beyond the simplest exactly solvable flat barrier, since an arbitrary one can always be made up, to any level of approximation, from a string of individually constant barriers. We show that the composite effect is obtained by multiplying a string of 2×2 real matrices, a calculation that is easily envisaged and readily performed on even the most humble PC. Furthermore, the method is immediately applicable to calculating transmission/reflection coefficients for any potential that is nonzero over a finite range and not just potential barriers, and as such should represent an instructive and rapid way of exploring the subtleties of one-dimensional quantum scattering.

Although the general approach of approximating potentials by segments of constant height is not new, the systematic development of such a procedure enabling it to cope with a large number of segments n, has to our knowledge not been developed. Thus, for example, both Wichman[3] and Gasiorowicz[4] use a string of flat barriers to arrive at the standard approximation for the tunneling probability through a nonconstant barrier, but they do not at the same time develop the full potential inherent in the procedure. Merzbacher,[5] on the other hand, introduces a 2×2 matrix approach similar to our own, but then, due to an overemphasis of the single barrier transmission problem, fails to write down the equivalent of our real matrix K, where one such matrix is defined for each segment and is parametrized by the height and width of that segment *only*. It is this matrix which points the way to the ease and elegance of a calculation with arbitrary n.

In Sec. II we outline the general method of segments and supplement this in Sec. III with some relevant comments on the computer implementation of the procedure. In Sec. IV we give the results of a sample tunneling calculation that is currently of some topical interest.

II. CALCULATION METHOD

We consider a beam of particles of mass m and energy E incident upon a potential barrier from the left as shown in Fig. 1. The continuous potential $V(x)$ is segmented into n discrete flat barriers each of width w and height V_j taken as the linearly interpolated mean value[6]

$$V_j \equiv \tfrac{1}{2}\{V[L+(j-1)w] + V(L+jw)\}, \quad j=1,2,\dots,n.$$

The V_j as drawn in Fig. 1 all satisfy $V_j > E$. However, there is no necessity for this as in a general tunneling situation one can have also $V_j \leqslant E$ in some segments. Defining

$$k \equiv \sqrt{2mE/\hbar^2}, \tag{1}$$

$$\alpha_j \equiv \sqrt{2m(V_j - E)/\hbar^2}, \quad j=1,2,\dots,n, \tag{2}$$

Schrödinger's time-independent equation within the jth barrier is

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V_j - E\right)\psi_j(x) = 0 \tag{3}$$

and has the solution

$$\psi_j(x) = A_j e^{\alpha_j x} + B_j e^{-\alpha_j x}, \tag{4}$$

with A_j, B_j as yet undetermined constants. To the left (input) and right (output) of the overall barrier where $V(x)=0$, the solution is just

$$\psi_{\text{in}} = A_{\text{in}} e^{ikx} + B_{\text{in}} e^{-ikx},$$

$$\psi_{\text{out}} = A_{\text{out}} e^{ikx} + B_{\text{out}} e^{-ikx}.$$

Clearly, we need to set the coefficient $B_{\text{out}} = 0$ (unless we assume further nonzero potential segments to the right).

The requirement that the wave function and its derivative be continuous at $x = L, L+w, L+2w, \dots, L+nw$, establishes a relation between the A,B coefficients. Thus continuity of ψ and ψ' at $x=L$ leads to

$$A_{\text{in}} e^{ikL} + B_{\text{in}} e^{-ikL} = A_1 e^{\alpha_1 L} + B_1 e^{-\alpha_1 L},$$

$$ikA_{\text{in}} e^{ikL} - ikB_{\text{in}} e^{-ikL} = \alpha_1 A_1 e^{\alpha_1 L} - \alpha_1 B_1 e^{-\alpha_1 L}.$$

We rewrite this in a convenient matrix form

$$M[L,ik]\begin{pmatrix} A_{\text{in}} \\ B_{\text{in}} \end{pmatrix} = M[L,\alpha_1]\begin{pmatrix} A_1 \\ B_1 \end{pmatrix}, \tag{5}$$

with the 2×2 matrix $M[x,\alpha]$ defined as

$$M[x,\alpha] \equiv \begin{pmatrix} e^{\alpha x} & e^{-\alpha x} \\ \alpha e^{\alpha x} & -\alpha e^{-\alpha x} \end{pmatrix}. \tag{6}$$

The continuity condition at the next point $x = L+w$ is now immediately available as

$$M[L+w,\alpha_1]\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M[L+w,\alpha_2]\begin{pmatrix} A_2 \\ B_2 \end{pmatrix} \tag{7}$$

and so on for all other boundaries, up to the final one at $x = L+nw$ where

$$M[L+nw,\alpha_n]\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M[L+nw,ik]\begin{pmatrix} A_{\text{out}} \\ B_{\text{out}} \end{pmatrix}. \tag{8}$$

From the series of matrix equations (5), (7), and (8) we get immediately

$$\begin{pmatrix} A_{\text{in}} \\ B_{\text{in}} \end{pmatrix} = M^{-1}[L,ik]M[L,\alpha_1]M^{-1}[L+w,\alpha_1] \times M[L+w,\alpha_2]M^{-1}[L+2w,\alpha_2]\cdots \times M[L+\overline{n-1}w,\alpha_n]M^{-1}[L+nw,\alpha_n]$$

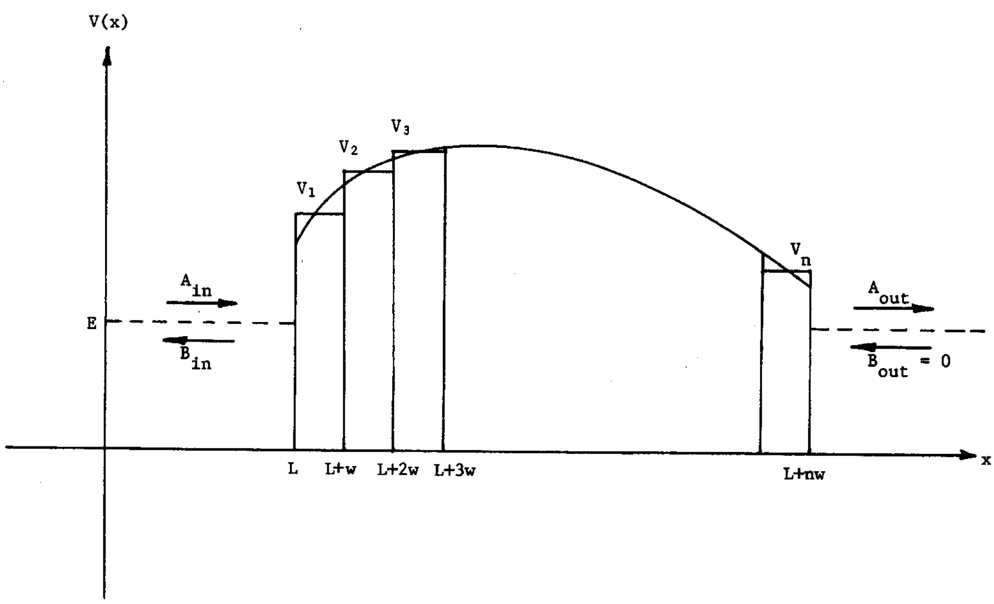

Fig. 1. Approximation of potential by flat barriers.

$$\times M[L+nw,ik]\begin{pmatrix}A_{\text{out}}\\B_{\text{out}}\end{pmatrix}. \quad (9)$$

Defining the matrix

$$K[\alpha,w]\equiv\begin{pmatrix}\cosh\alpha w & -(1/\alpha)\sinh\alpha w\\ -\alpha\sinh\alpha w & \cosh\alpha w\end{pmatrix}, \quad (10)$$

which is *real* for both real and imaginary α, it is readily shown that

$$M[L,\alpha_1]M^{-1}[L+w,\alpha_1]=K[\alpha_1,w],$$
$$M[L+w,\alpha_2]M^{-1}[L+2w,\alpha_2]=K[\alpha_2,w],$$

etc., and hence we obtain the desired scattering relation in the form

$$\begin{pmatrix}A_{\text{in}}\\B_{\text{in}}\end{pmatrix}=M^{-1}[L,ik]K[\alpha_1,w]K[\alpha_2,w]\cdots$$
$$\times K[\alpha_n,w]M[L+nw,ik]\begin{pmatrix}A_{\text{out}}\\B_{\text{out}}\end{pmatrix}. \quad (11)$$

To calculate the transmission probability T, we symbolize the product of K matrices (to be evaluated by computer) arising in (11) as

$$K[\alpha_1,w]K[\alpha_2,w]\cdots K[\alpha_n,w]\equiv\begin{pmatrix}P & Q\\R & S\end{pmatrix}. \quad (12)$$

Then in view of the boundary condition $B_{\text{out}}=0$, we need only evaluate the (1,1) component of the matrix

$$M^{-1}[L,ik]\begin{pmatrix}P & Q\\R & S\end{pmatrix}M[L+nw,ik]$$

in (11) to get

$$A_{\text{in}}=\tfrac{1}{2}e^{iknw}[(P+S)+i(Qk-R/k)]A_{\text{out}}. \quad (13)$$

As expected, this relation is independent of the overall position L of the barrier and leads immediately to the transmission probability

$$T\equiv\left|\frac{A_{\text{out}}}{A_{\text{in}}}\right|^2=\frac{4}{[(P+S)^2+(Qk-R/k)^2]}. \quad (14)$$

The above expression for the transmission probability T is valid not just for the purely tunneling situation wherein $V_j>E$ in all segments j, but also for those potentials in which some or all V_j satisfy $V_j\leqslant E$. The only effect of a segment with $V_j<E$ is to make the corresponding α parameter imaginary, that is $\alpha=i\beta$, in which case the K matrix (10) reduces to the alternative real form

$$K[i\beta,w]=\begin{pmatrix}\cos\beta w & -(1/\beta)\sin\beta w\\ \beta\sin\beta w & \cos\beta w\end{pmatrix}. \quad (15)$$

A whole class of nontunneling scattering situations may thus be profitably tackled in addition to those where the potential peak exceeds the particle energy.

III. PROGRAMMING CONSIDERATIONS

Tunneling calculations can often lead to transition probabilities as small as 10^{-100} or smaller, and in order to estimate these correctly one needs to guard against the computer program setting very small numbers to zero (e.g., 10^{-45} is zero in single precision BASIC). To overcome this problem, we have found it convenient when multiplying out the string of K matrices in (12), to extract for each "tunneling" segment $V_j>E$ a factor $e^{\alpha_j w}$ from the matrix $K[\alpha_j,w]$ by writing

$$K[\alpha_j,w]=e^{\alpha_j w}K'[\alpha_j,w], \quad (16)$$

with the K' matrix defined as

$$K'[\alpha,w]\equiv\begin{pmatrix}\frac{1}{2}(1+e^{-2\alpha w}) & -\frac{1}{2\alpha}(1-e^{-2\alpha w})\\ -\frac{\alpha}{2}(1-e^{-2\alpha w}) & \frac{1}{2}(1+e^{-2\alpha w})\end{pmatrix} \quad (17)$$

and then to use K' instead of K for that segment in the product (12). This means that the final transition probability has the modified form

$$T=T'e^{-2G}, \quad (18)$$

where

$$T'\equiv 4/[(P'+S')^2+(Q'k-R'/k)^2], \quad (19)$$

with

$$\begin{pmatrix}P' & Q'\\R' & S'\end{pmatrix}$$

the modified product matrix in (12) and

$$G\equiv w\sum\alpha_j. \quad (20)$$

The sum in (20) is restricted to segments j for which $V_j>E$. The small number problem is now overcome since the computer calculates the exponent $-2G$ separately.

For a pure barrier (i.e., all $V_j>E$) G is in fact just the numerical approximation to the usual Gamow integral

$$G\equiv\int_L^{L+nw}\sqrt{2m[V(x)-E]/\hbar^2}\,dx, \quad (21)$$

with the factor e^{-2G} supplying for most tunneling situations the dominant (small!) part of the transition probability. The term T' in our Eq. (18) is in this case seen to represent a correction factor to the Gamow estimate e^{-2G} for T.

One further practical consideration that needs attention arises from the apparently singular form of the (1,2) component of the K matrix (10) [or the K' matrix (17)] wherein the factor α^{-1} on its own diverges when $\alpha\to 0$ (i.e., if $V_j\cong E$ for some j). However, the overall (1,2) term in (10) and in (17) is nonsingular[7] as may be seen from the respective series expansion near $\alpha=0$, namely,

$$-\frac{\sinh\alpha w}{\alpha}=-w\left(1-\frac{(\alpha w)^2}{3!}+\frac{(\alpha w)^4}{5!}-\cdots\right),$$
$$-\frac{1-e^{2\alpha w}}{2\alpha}=-w\left(1-\frac{(2\alpha w)}{2!}+\frac{(2\alpha w)^2}{3!}-\cdots\right).$$

Thus unlike the WKB approximation, the method of segments proposed here does not break down at or near the classical turning point $\alpha=0$, and demands only that whenever αw in a segment is less than some predetermined small number (say, 0.01) then we evaluate the (1,2) element of K or K' using the appropriate series (with a sufficient number of terms to maintain the desired precision). This action is readily built into a computer program.

IV. A SAMPLE CALCULATION

We consider the example motivated by the recently proposed "cold fusion" scanario[8] in a simplistic version of which one deuteron tunnels head-on into the Coulomb field produced by another. In the center-of-mass system the potential seen by the incident deuteron thus takes the Coulomb form

$$V(x) = e^2/4\pi\epsilon_0 x,$$

with incidence from the right (i.e., x decreasing). We assume the potential to be cut off at $x = 1$ Å (corresponding typically to the lattice spacing of metallic palladium within which the deuterons are closely packed in a "cold fusion" situation) and also at the nuclear fusion distance $x = 4$ F below which the Coulomb repulsion is effectively neutralized by the attractive nuclear forces. We select the energy E as 15.4 eV, thereby giving the incident deuteron about 1 eV of kinetic energy in addition to the potential energy at equilibrium lattice separation of 1 Å.

Using mean values[6] to define the segment heights V_j, we list in Table I the computed values of T', $2G$, and T for various segment numbers n. The convergence rate in n is seen to be quite satisfactory in view of the steeply rising nature of the Coulomb potential; for slowly varying potentials convergence is much faster. It is noteworthy that T' here contributes about another two negative orders of magnitude to T beside the exceedingly small Gamow estimate $\exp(-2G)$, making the probability of this kind of D–D tunneling highly unlikely. However, the situation can be considerably improved by the addition of screening as shown by the present authors elsewhere.[9]

V. DISCUSSION

In contrast to elementary treatments of potential scattering and the more rigorous WKB method that aims at finding an approximate analytic solution for the wave function, our presentation above supplies an *exact* solution to a problem that *approximates* the desired scattering situation. This approximation improves as the number n of barriers/wells increases, up to a practical limit governed largely by computing time and roundoff errors. Computing time itself is not a serious problem as instanced by our elementary interpreted (slow) BASIC program which evaluates the transition probability for $n = 100$ potential segments in about 5 s, and for a calculation with n of the order of a few hundred and utilizing standard 64-bit double precision arithmetic, the roundoff errors may be virtually neglected.

In essence, our work reduces the analytic problem of scattering to one that requires only straightforward algebraic steps. The residual task of encoding the algebra in a high-level language such as BASIC, FORTRAN, or PASCAL is not expected to cause real problems for today's computer literate students. A useful embellishment to a program is to require it to treat not only prespecified analytic potentials such as the Coulomb or Gaussian but also to handle an arbitrary sequence of flat barriers and wells that one may specify at will. In this way, by varying the particle mass m, the incident energy E, the individual barrier/well heights and their widths (obtained by adding more barriers/wells with the same height and width), much valuable intuitive understanding can be gained about a problem that is otherwise far from mathematically transparent.

We emphasize again that all types of potentials are catered for by the above method. For those potentials that contain one or more tunneling segments, the transition probability is evaluated as a product of two separate factors as in Eq. (18). When there are no tunneling segments, $G = 0$ and T' becomes the only contribution. Though it is customary for the pure tunneling case to take e^{-2G} on its own as a good order-of-magnitude approximation for T, it should be pointed out that the correction factor T' can nevertheless turn out to be quite significant. Taking the single flat barrier as an example, $T' \simeq 16(\alpha/k + k/\alpha)^2$, for low energies ($k$ small) and high barrier (α large); in such cases the factor T' can modify the Gamow part $e^{-2\alpha w}$ by significant negative orders of magnitude. Thus for particles of low energy, tunneling into a steeply rising potential such as a Coulomb barrier discussed above, the correction factor T' turns out to be meaningful.

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Table I. The tunneling probability T and the correction T' to the Gamow factor for D–D penetration at 15.4 eV as described in Sec. IV. The table shows convergence in the number of segments n into which the repulsive Coulomb barrier is divided over the range 1 Å to 4 F.

n	T'	$T = T'e^{-2G}$
100	0.034	1.13×10^{-114}
200	0.027	2.96×10^{-113}
300	0.023	1.03×10^{-112}
400	0.021	1.87×10^{-112}
500	0.020	2.96×10^{-112}
600	0.019	3.79×10^{-112}
700	0.018	4.32×10^{-112}
800	0.017	5.02×10^{-112}
900	0.016	5.18×10^{-112}
1000	0.016	5.81×10^{-112}

[1] A. P. French and Edwin F. Taylor, *An Introduction to Quantum Physics* (Van Norstrand Reinhold, London, 1978), Chap. 9.

[2] David Bohm, *Quantum Theory* (Prentice-Hall, Englewood Cliffs, NJ, 1951), Chap. 12.

[3] E. H. Wichman, *Quantum Physics* (McGraw-Hill, New York, 1971), pp. 287–292.

[4] Stephen Gasiorowicz, *Quantum Physics* (Wiley, New York, 1974), pp. 84–86.

[5] Eugen Merzbacher, *Quantum Mechanics* (Wiley, New York, 1970), Chap. 6.

[6] A more realistic choice would be to take V_j as the mean value

$$V_j \equiv \frac{1}{w}\int_{L+(j-1)w}^{L+jw} V(x)dx,$$

which for analytic potentials may be calculated exactly or suitably approximated.

[7] For the special case $\alpha_j = 0$, the solution (4) is replaced by $\psi_j(x) = A_j x + B_j$ leading to the matrix

$$M[x,\alpha=0] \equiv \begin{pmatrix} x & 1 \\ 1 & 0 \end{pmatrix}.$$

This is *not* the $\alpha = 0$ limit of the matrix (6) which itself becomes singular in this limit. However, the combination

$$K[\alpha=0,w] \equiv M[x,\alpha=0]M^{-1}[x+w,\alpha=0]$$

$$= \begin{pmatrix} 1 & -w \\ 0 & 1 \end{pmatrix}$$

is the *same* as the $\alpha = 0$ limit of the $K[\alpha,w]$ matrix defined in (10) and so justifies setting $\alpha = 0$ in that definition whenever necessary.

[8] Some samples from the Cold Fusion literature are the paper by J. S. Cohen and J. D. Davis, "The cold fusion family," Nature **338**, 705–707 (1989) and the three related articles of K. Ross and S. Bennington, T. Greenland, and D. Morrison in "Solid state fusion (?)" Phys. World **2**, 15–18 (1989).

[9] A. R. Lee and T. M. Kalotas, "On the feasibility of cold fusion," Nuovo Cimento A **102**, 1177–1180 (1989).

Schrödinger equation in two dimensions for a zero-range potential and a uniform magnetic field: An exactly solvable model

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The spectrum and eigenfunctions of a particle moving in two dimensions under the influence of an external uniform magnetic field and in the presence of a "point interaction" is determined. This is done after an elementary discussion of how to construct a "point interaction" in two dimensions circumventing the well-known difficulties with the Dirac $\boldsymbol{\delta}^2(\mathbf{r})$ interaction.

The delta-function potential is used in the one-dimensional Schrödinger equation to illustrate a number of interesting features. In two and three dimensions, however, the δ-function potential is problematic: The usual limiting procedure for its construction does not work (see discussion below). Recently, however, the theory of point interactions (also called zero-range or contact interactions in the literature) and its application to solid-state physics have been subject of extensive studies.[1–3]

The purpose of this paper is to solve the problem of a charged particle moving in a plane subjected to a magnetic field perpendicular to it and acted upon by an "impurity" represented by a two-dimensional contact interaction. A system like this has been used by Prange[4] in connection to the quantized Hall effect. Prange,[4] however, uses for this contact interaction a delta function that, as we will see, remains "too strong," even in the presence of a magnetic field.

We first review the problem of defining a point interaction in two dimensions without magnetic field. Our treatment is very pedestrian and therefore should serve as an introduction to more powerful methods presented in Ref. 2.

Consider a particle moving in a plane. Let's introduce polar coordinates (ρ,θ) and suppose that the interaction is a square well of depth V_0 and radius δ. Later, we shall let V_0 go to infinity and δ to zero in such a way that the specified energy of the unique bound state remains constant.

We shall consider only S waves, as in the limit $\delta \to 0$ the states with $l \neq 0$ are unaffected by the potential.

The Schrödinger equation for the S waves reads

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{d\rho^2} + \frac{1}{\rho}\frac{d\psi}{d\rho}\right) = E\psi, \quad \text{for} \quad \rho > \delta, \tag{1}$$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi}{d\rho^2} + \frac{1}{\rho}\frac{d\psi}{d\rho}\right) - |V_0|\psi = E\psi, \quad \text{for} \quad \rho < \delta. \tag{2}$$

Suppose there is a bound state of energy $|E_b|$, and as usual call $k = \sqrt{2m|E_b|/\hbar^2}$ and $k_0 = \sqrt{2m/\hbar^2(|V_0| - |E_b|)}$.

The solutions of (1) and (2) are Bessel functions:

$$\psi = K_0(k\rho), \text{ for } \rho > \delta, \tag{3}$$

$$\psi = J_0(k_0\rho), \text{ for } \rho < \delta. \tag{4}$$

Now we have to match the functions and derivatives at $\rho = \delta$. Using[5] the relations

$$J_0'(z) = -J_1(z), \tag{5}$$

$$K_0'(z) = -K_1(z), \tag{6}$$

we get

$$-k_0[J_1(k_0\delta)/J_0(k_0\delta)] = -k[K_1(k\delta)/K_0(k\delta)]. \tag{7}$$

If we now try to let $\delta \to 0$, assuming E_b to remain finite and in such way that $|V_0|\delta^2 \to \Delta$ [so that our potential would approach $-\Delta\,\boldsymbol{\delta}^2(\mathbf{r})$] we find that the left-hand side of Eq. (7) behaves as[5]

