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The bound states of a segmented potential

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teach introductory relativity. But what is this $\Sigma E_i/c^2$ term in calculating the invariant mass of a system? And how many sophomore and junior students will understand a four-vector approach in the limited time available? Such students often use two-vectors well, but still have trouble with three-vectors. Won't beginning their modern physics instruction with four-vectors make things unnecessarily difficult and obscure the subtle concepts of relativity by moving even further from their experience?

Relativistic mass paints a picture of nature that is beautiful in its simplicity. We should continue to use relativistic mass along with consistent interpretations of Newton's second law and $E = mc^2$ in introductory courses. Insisting on its removal as a useful tool from all textbooks, as Okun does,[10] is a form of unnecessary censorship.

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[7] For example, Clifford Will, "The renaissance of general relativity," in *The New Physics*, edited by Paul Davies (Cambridge U.P., Cambridge, 1989), p. 12.

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[10] Reference 4, p. 117.

The bound states of a segmented potential

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The method of potential segmentation previously developed for scattering situations, is extended to the computation of one-dimensional bound states. The energy eigenvalues are determined by the zeros of a specific transcendental function while the corresponding eigenfunctions are supplied with the aid of a series of 2×2 matrix equations.

In a recent communication to this Journal[1] we outlined the procedure of potential segmentation as it applies to the problem of one-dimensional quantum scattering, emphasizing the ease and elegance of this method for the computation of transmission probabilities. Here we wish to show that the same procedure is readily extended to the calculation of energy eigenvalues and eigenfunctions associated with one-dimensional bound-state problems involving potentials of arbitrary shape. Such a typical binding potential, shown in Fig. 1, is taken to be generally nonconstant in the range $L<x<R(\equiv L+a)$ and to be of fixed value V_L, V_R (nonequal in general) in the left and right bounding regions respectively. On breaking up the nonconstant part of the potential into n segments having "average" heights V_j as outlined in Ref. 1 and of equal widths $w = a/n$ (see Fig. 1) and taking over all definitions and symbols appearing in Ref. 1, we arrive immediately at the series of 2×2 matrix continuity conditions

$$
\begin{aligned}
&M[L,\alpha_L]\begin{pmatrix}A_L\\B_L\end{pmatrix} = M[L,\alpha_1]\begin{pmatrix}A_1\\B_1\end{pmatrix},\\
&M[L+w,\alpha_1]\begin{pmatrix}A_1\\B_1\end{pmatrix} = M[L+w,\alpha_2]\begin{pmatrix}A_2\\B_2\end{pmatrix}\\
&\qquad\qquad\vdots\\
&M[L+(n-1)w,\alpha_{n-1}]\begin{pmatrix}A_{n-1}\\B_{n-1}\end{pmatrix}\\
&\quad = M[L+(n-1)w,\alpha_n]\begin{pmatrix}A_n\\B_n\end{pmatrix},\\
&M[L+nw,\alpha_n]\begin{pmatrix}A_n\\B_n\end{pmatrix} = M[R,\alpha_R]\begin{pmatrix}A_R\\B_R\end{pmatrix}. \qquad (1)
\end{aligned}
$$

Here, the only difference from the corresponding scattering equations (5), (7), and (8) of Ref. 1 is that in the left and right regions of the potential we have replaced the pa-

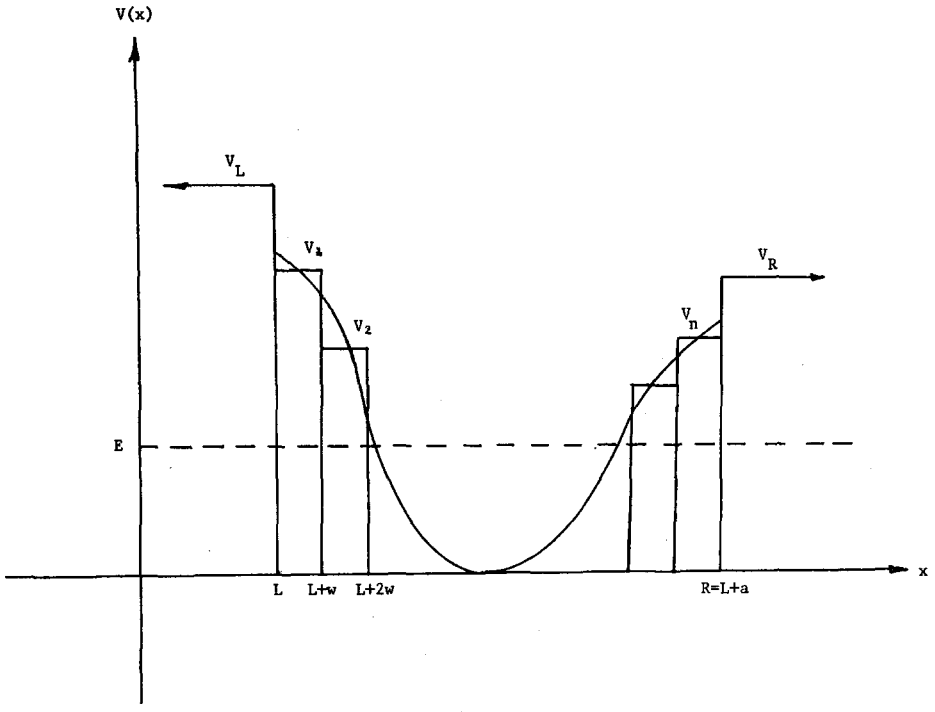

FIG. 1. A general bounding potential and its segmentation.

rameter $ik \equiv \sqrt{2m(-E)}/\hbar$ of scattering according to

$$\begin{aligned} &\text{left:} \quad ik \to \alpha_L \equiv \sqrt{2m(V_L - E)}/\hbar, \\ &\text{right:} \quad ik \to \alpha_R \equiv \sqrt{2m(V_R - E)}/\hbar. \end{aligned} \tag{2}$$

Correspondingly the wave functions in these regions are also replaced as

$$\begin{aligned} &\psi_{\text{in}} \to \psi_L \equiv A_L e^{\alpha_L x} + B_L e^{-\alpha_L x}, \\ &\psi_{\text{out}} \to \psi_R \equiv A_R e^{\alpha_R x} + B_R e^{-\alpha_R x}. \end{aligned} \tag{3}$$

Clearly for bound states (for which α_L, α_R are real) the required vanishing of Ψ_L as $x \to -\infty$ and Ψ_R as $x \to +\infty$, demands that

$$B_L = A_R = 0. \tag{4}$$

Then on eliminating from (1) the intermediate coefficients A_j, B_j for $j = 1,2,\ldots,n$, we obtain the equation

$$\begin{pmatrix} A_L \\ O \end{pmatrix} = M^{-1}[L,\alpha_L]\,\Pi M[R,\alpha_R]\begin{pmatrix} O \\ B_R \end{pmatrix}, \tag{5}$$

where Π is the 2×2 product matrix

$$\Pi = K[\alpha_1,w]K[\alpha_2,w]\cdots K[\alpha_n,w]. \tag{6}$$

Since for a nontrivial solution the coefficient B_R cannot be zero, we conclude from (5) that the (2,2) component of the matrix product $M^{-1}[L,\alpha_L]\,\Pi M[R,\alpha_R]$ must vanish, a condition which on simplification reduces to

$$\Omega(E) \equiv \Pi_{12}\alpha_L\alpha_R - (\Pi_{11}\alpha_L + \Pi_{22}\alpha_R) + \Pi_{21} = 0. \tag{7}$$

This *single*[2] condition determines *all* the bound state energies E as the zeros of the function $\Omega(E)$ for any segmented potential configuration. It is apparent since E enters indirectly into every symbol appearing in Ω via the parameters $\alpha_1,\alpha_2,\ldots,\alpha_n,\alpha_L,\alpha_R$, that Ω itself is in general a complicated transcendental function for all but the simplest cases of $n = 1$ or 2 segments [for which the condition (7) reduces to the standard textbook examples of single and double rectangular wells]. Bounds on the eigenvalues E are, however, readily obtained by the computer monitoring of the function $\Omega(E)$ over a grid of energies extending upward from the lowest potential value to the lower of V_L, V_R, with an eigenvalue located between two such grid values whenever $\Omega(E)$ changes sign over that pair of values. With successive refinement using a finer grid each time, one rapidly improves the bounds and ultimately precision is limited only by round-off errors. In such a calculation the elements of Π are evaluated directly as the product of n real 2×2 K matrices as in (6) with each taking either the "hyperbolic" or "circular" form as discussed in Ref. 1. Only minimal programming skills are required for this straightforward computation.

The condition (7) immediately leads to three useful variants wherein one or both of V_L, V_R become infinite. Thus for

(i) $V_L \to \infty, V_R =$ finite: We divide (7) by α_L and set $\alpha_L \to \infty$ to get the eigenvalue condition

$$\Omega_L(E) \equiv \Pi_{12}\alpha_R - \Pi_{11} = 0. \tag{8}$$

(ii) $V_L =$ finite, $V_R \to \infty$: We obtain by a procedure similar to (i)

$$\Omega_R(E) \equiv \Pi_{12}\alpha_L - \Pi_{22} = 0. \tag{9}$$

(iii) $V_L \to \infty, V_R \to \infty$: We divide (7) by $\alpha_L\alpha_R$ and set $\alpha_L \to \infty, \alpha_R \to \infty$ to get

$$\Omega_{LR}(E) \equiv \Pi_{12} = 0. \tag{10}$$

Again, it is easily verified for the simplest case $n = 1$ that these conditions coincide with the corresponding textbook examples of a single rectangular well with one or both bounding walls of infinite height.

Once an eigenvalue E is determined, the corresponding eigenfunction follows simply on evaluating the A,B coefficients of (1). For this purpose it is convenient to rewrite these equations in the form

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = M^{-1}[L+nw,\alpha_n]M[R,\alpha_R]\begin{pmatrix} O \\ B_R \end{pmatrix},$$

$$\begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} = M^{-1}[L+(n-1)w,\alpha_{n-1}] \times K[\alpha_n,w]M[R,\alpha_R]\begin{pmatrix} O \\ B_R \end{pmatrix},$$

$$\vdots$$

$$\begin{pmatrix} A_1 \\ B_1 \end{pmatrix} = M^{-1}[L+w,\alpha_1]K[\alpha_2,w]\cdots \times K[\alpha_n,w]M[R,\alpha_R]\begin{pmatrix} O \\ B_R \end{pmatrix},$$

$$\begin{pmatrix} A_L \\ O \end{pmatrix} = M^{-1}[L,\alpha_L]K[\alpha_1,w]\cdots \times K[\alpha_n,w]M[R,\alpha_R]\begin{pmatrix} O \\ B_R \end{pmatrix}. \quad (11)$$

Then, on selecting the normalization by fixing the value of B_R (e.g., $B_R = 1$), one can evaluate the A,B coefficients directly. It should be noted that all products of K matrices that arise in these equations have already been computed in the preceding eigenvalue calculation stage and they need only be saved there in order to avoid their recomputation in (11). Essentially only real arithmetic is needed throughout this calculation.

For the three subcases (i)–(iii) listed above involving one or two infinite bounding potential walls, the defining equations (1) need to be modified as follows:

(i) The first matrix equation of (1) is to be replaced by

$$B_1/A_1 = -e^{2\alpha_1 L}. \quad (12)$$

(ii) The last matrix equation of (1) is to be replaced by

$$B_n/A_n = -e^{2\alpha_n R}. \quad (13)$$

(iii) The first and last matrix equations of (1) are to be replaced by (12) and (13), respectively.

These conditions are sufficient to ensure that the wavefunction always vanishes at an infinite bounding potential wall.[3] The subsequent solution of the A_j,B_j then proceeds along lines similar to that outlined above.

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Approximating the finite square well with an infinite well: Energies and eigenfunctions

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Polynomial expansions are used to approximate the equations of the eigenvalues of the Schrödinger equation for a finite square potential well. The technique results in discrete, approximate eigenvalues which, it is shown, are identical to the corresponding eigenvalues of a wider, infinite well. The width of this infinite well is easy to calculate; indeed, the increase in width over that of the finite well is simply the original width divided by the well strength. The eigenfunctions of this wider, infinite well, which to first order has the same width for the ground state and all excited states, are also good approximations to the exact eigenfunctions of the finite well. These approximate eigenfunctions and eigenvalues are compared to accurate numeric calculations and to other approximations from the literature.

I. INTRODUCTION

The solution of the time-independent Schrödinger equation for a one-dimensional finite square potential well is an important example of a one-dimensional bound-state problem. The eigenfunction ψ of a particle in a well of width a and depth V_0 obeys the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + V(x)\psi = E\psi, \quad (1)$$

with $\hbar$ Planck's constant divided by 2π, m the mass of the particle, $V(x)$ the potential energy, and E the total energy of the particle. Various authors provide graphical solutions to this problem.[1–6] Eisberg and Resnick[1] give the presentation most often seen in undergraduate quantum-mechanics texts. They solve Eq. (1) for the given potential well subject to the usual continuity conditions and obtain

$$\alpha \tan \alpha = (P^2 - \alpha^2)^{1/2}, \quad (2)$$

for the even-parity solutions, and

