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A new teaching approach to quantum mechanical tunneling

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Abstract

The transfer matrix method has been used to investigate quantum mechanical tunneling in introductory quantum mechanics. The method is applied first to calculate the transmission coefficient for tunneling through a rectangular barrier and is then extended to the problem of potential barriers of arbitrary shape, in particular, to radioactive decay. This approach uses matrix methods that are accessible to a broader range of undergraduates than other numerical techniques, the connection between the rectangular barrier problem and potential barriers of arbitrary shape is transparent, and it can be readily executed by undergraduates. The classroom experience with this approach is discussed. © 1999 Elsevier Science B.V. All rights reserved.

1. Introduction

Tunneling through a one-dimensional potential energy barrier is a topic routinely investigated in introductory quantum mechanics and provides one of the most striking departures of quantum physics from classical physics. A particle that is bound by some attractive nuclear force (for example, a ^{4}He nucleus moving inside a larger atomic nucleus) is able to escape from the parent system even though it lacks the energy to overcome the attractive force. Classical physics predicts that such behavior is impossible. The ^{4}He nucleus or α particle would have to acquire enough additional energy from some source to reach 'escape velocity' before it could leave the parent nucleus. However, the 'fuzziness' of Nature at the subatomic scale implies that precise knowledge of the α particle's trajectory within the nucleus is unobtainable. This uncertainty means the particle has a small, but non-zero probability of being outside the nucleus where the Coulomb repulsion will push it away from the residual nucleus. We say it has 'tunneled' through a potential energy barrier created by the attractive nuclear force. The treatment of this phenomenon in many introductory texts has become rather standard [1–6]. In this paper a method is presented for investigating quantum mechanical tunneling that is readily accessible to undergraduates, permits the solution of a broad range of problems, and takes advantage of increasingly common computational tools. It is part of a program at the University of Richmond to incorporate these tools using a 'hands-on' laboratory environment.

The phenomenon is usually approached by first considering the problem for a highly idealized potential energy curve, the rectangular barrier shown in Fig. 1. The problem is dealt with by solving a set of simultaneous equations generated by applying the appropriate boundary conditions to the solution of the one-dimensional Schrödinger equation shown here [1–6].

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x). \tag{1}$$

The constants E and m are the energy and mass of a particle moving in a potential $V(x)$ and $\hbar$ is Planck's constant divided by 2π. Potential barriers of arbitrary shape are then treated using the Wentzel, Kramers,

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Brillouin (WKB) approximation [1–6]. This pattern of development has several drawbacks. The rectangular barrier problem has limited applicability (few potential barriers are described adequately by it) while the WKB approximation requires either precious class time to rigorously justify the method or resorting to a less substantial, 'cookbook' approach. In addition, the two methods of solution are inconsistent with one another. Applying the WKB approximation to the rectangular barrier does not recover the original result obtained by solving the set of simultaneous equations [7]. Finally, from an undergraduate's perspective, the solutions to the two problems use different techniques (solving a set of simultaneous equations versus performing an integral) whose underlying connections are often unseen or misunderstood.

The use of transfer matrices to solve the rectangular barrier problem is a well established technique used to solve the rectangular barrier problem [8,9]. The method can be extended quickly and naturally to potential barriers of arbitrary shape while retaining a transparent connection to the original rectangular barrier problem. It also has the pedagogically useful features of introducing powerful matrix methods in a new context and takes advantage of current teaching technologies.

In Section 2 an overview of the solution of the rectangular barrier problem with the transfer matrix formalism will be developed and extended to potential barriers of arbitrary shape. More detailed discussions of the technique have been done by others [8–10]. In Section 3 some results from the application of the technique to a specific example will be displayed, the response of students to this approach discussed, and a comparison made with other computational methods.

2. The transfer matrix method

To investigate quantum mechanical tunneling one must extract the transmission coefficient from the solution to the one-dimensional, time-independent Schrödinger equation. The transmission coefficient is the ratio of the flux of particles that penetrate a potential barrier to the flux of particles incident on the barrier. It is related to the probability that tunneling will occur. Consider a rectangular potential barrier of

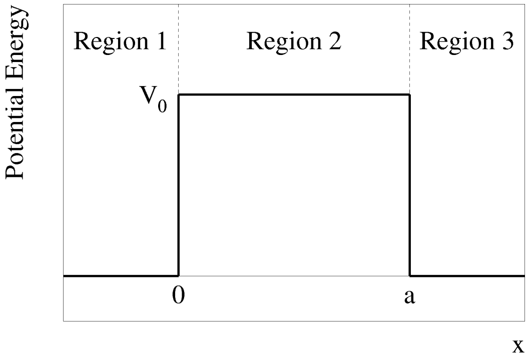

Fig. 1. Potential energy curve for the rectangular potential barrier.

height V_0 as shown in Fig. 1. The general solution of the Schrödinger equation in each region is

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad (x < 0), \tag{2}$$

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \quad (0 \leqslant x \leqslant a), \tag{3}$$

$$\psi_3(x) = Fe^{ik_1x} + Ge^{-ik_1x} \quad (a < x), \tag{4}$$

where $k_1 = \sqrt{2mE/\hbar^2}$ and $k_2 = \sqrt{2m(E - V_0)/\hbar^2}$. This solution can be rewritten as a vector dot product so, for example, in Region 2 of Fig. 1

$$\psi_2(x) = \left(e^{ik_2x} e^{-ik_2x}\right)\begin{pmatrix} C \\ D \end{pmatrix} = \left(e^{ik_2x} e^{-ik_2x}\right)\phi_2, \tag{5}$$

where the ϕ_i are the coefficient vectors representing the wave function in each region. To generate relationships among the coefficients in Eqs. (2)–(4) one requires the wave function and its first derivative to be continuous at the boundaries of each region in Fig. 1. At $x = 0$ this leads to two expressions.

$$A + B = C + D, \tag{6}$$

$$ik_1A - ik_1B = ik_2C - ik_2D. \tag{7}$$

In matrix notation Eqs. (6)–(7) can be expressed in the following way.

$$\begin{pmatrix} 1 & 1 \\ ik_1 & -ik_1 \end{pmatrix}\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ ik_2 & -ik_2 \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}, \tag{8}$$

$$\mathbf{m}\begin{pmatrix} A \\ B \end{pmatrix} = \mathbf{n}\begin{pmatrix} C \\ D \end{pmatrix}. \tag{9}$$

Using the definition of the matrix inverse yields the following result

$$\begin{pmatrix} A \\ B \end{pmatrix} = \mathbf{m}^{-1}\mathbf{n}\begin{pmatrix} C \\ D \end{pmatrix} \tag{10}$$

which can be expressed as

$$\phi_1 = \begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1+\frac{k_2}{k_1} & 1-\frac{k_2}{k_1} \\ 1-\frac{k_2}{k_1} & 1+\frac{k_2}{k_1} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = \mathbf{d}_{12}\phi_2. \tag{11}$$

The matrix, $\mathbf{d}_{12}$, is known as the discontinuity matrix and ‘connects’ the coefficient vectors ϕ_1 and ϕ_2 in Regions 1 and 2.

The wave function and its derivative must also be continuous at $x = a$. At this point, consider a new coordinate system such that the transition from Region 2 to Region 3 takes place at $x' = 0$. By analogy with Eq. (11) one can show that,

$$\phi_2' = \mathbf{d}_{21}\phi_3', \tag{12}$$

where the ϕ_i' are the coefficient vectors in the new coordinate system in the equivalent regions of the potential energy curve and $\mathbf{d}_{21}$ has the same form as $\mathbf{d}_{12}$ in Eq. (3) except for the interchange of the indices. To exploit this result, one must relate the coefficient vectors in the primed coordinate system to the ones in the original coordinates. The original coordinate system is transformed such that $x' = x - a$. The new wave function in Region 2 must satisfy

$$\psi_2(x) = \psi_2'(x-a) \tag{13}$$

which can be written in matrix form and rearranged to yield the following result (recall Eq. (5)).

$$\psi_2(x) = \left(e^{ik_2(x-a)} e^{-ik_2(x-a)}\right)\begin{pmatrix} C' \\ D' \end{pmatrix} = \left(e^{ik_2x} e^{-ik_2x}\right)\begin{pmatrix} C'e^{-ik_2a} \\ D'e^{ik_2a} \end{pmatrix}. \tag{14}$$

The row vector on the right hand side of Eq. (14) is the same as the row vector in Eq. (5) so the coefficient vectors representing $\phi_2(x)$ and $\phi_2'(x)$ are related by

$$\phi_2 = \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} C'e^{-ik_2a} \\ D'e^{ik_2a} \end{pmatrix} = \begin{pmatrix} e^{-ik_2a} & 0 \\ 0 & e^{ik_2a} \end{pmatrix}\begin{pmatrix} C' \\ D' \end{pmatrix} = \mathbf{p}_2\phi_2', \tag{15}$$

where $\mathbf{p}_2$ is the propagation matrix in Region 2. Similarly, one can show that

$$\phi_3' = \begin{pmatrix} e^{ik_1a} & 0 \\ 0 & e^{-ik_1a} \end{pmatrix}\begin{pmatrix} F \\ G \end{pmatrix} = \mathbf{p}_{-1}\phi_3, \tag{16}$$

where $\mathbf{p}_{-1}\phi_3$ shifts the wave function back to the original coordinate system. Combining Eqs. (11), (12), (15), and (16) and setting $G = 0$ since there are no incoming waves in Region 3 one obtains

$$\phi_1 = \begin{pmatrix} A \\ B \end{pmatrix} = \mathbf{d}_{12}\mathbf{p}_2\mathbf{d}_{21}\mathbf{p}_{-1}\phi_3 = \mathbf{t}\phi_3 = \begin{pmatrix} t_{11}F \\ t_{21}F \end{pmatrix}, \tag{17}$$

where $\mathbf{t}$ is the transfer matrix relating the coefficient vectors in Regions 1 and 3. The transmission coefficient is then

$$T = \frac{|Fe^{ik_1x}|^2}{|Ae^{ik_1x}|^2} = \frac{1}{|t_{11}|^2}. \tag{18}$$

This treatment of the rectangular potential barrier problem can be extended to potential barriers of arbitrary shape. Consider the radioactive α-decay of ^{212}Po. The potential barrier is shown as the solid curve in Fig. 2. The central portion of the curve is the Coulomb potential $V(x) = Z_1Z_2e^2/x$, where x is the distance between the nuclear centers and the product of the charges is $Z_1Z_2e^2$. It is divided into a sequence of adjacent barriers (the dot-dashed lines) lying between the nuclear radius, x_0, and the classical turning point, x_{max}, for an α particle of total energy, E. The potential energy is taken to be zero outside these limits in the manner of Condon and Gurney [12]. One can now use the propagation and discontinuity matrices to relate the wave function inside the barrier to the wave function outside ($x > x_{max}$). For the configuration shown in Fig. 2 one chooses the origin at the nuclear radius and the two wave functions are related by

$$\phi_{inside} = \mathbf{d}_{01}\mathbf{p}_1\mathbf{d}_{12}\mathbf{p}_2\mathbf{d}_{23}\mathbf{p}_3\mathbf{d}_{30}\mathbf{p}_{-0}\phi_{outside}, \tag{19}$$

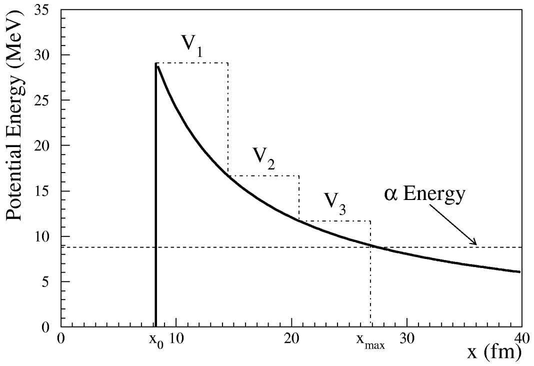

Fig. 2. Potential energy curve for an α particle in the force field of ^{208}Pb, the daughter nucleus of the ^{212}Po decay.

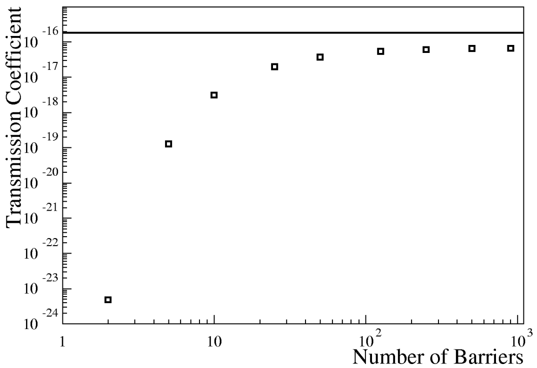

Fig. 3. A test of the convergence of the transmission coefficient calculation. The circles show the dependence of the transmission coefficient calculation for different numbers of adjacent barriers (see Fig. 2).

where $\mathbf{d}_{01}$ is the discontinuity matrix between the region where $V(x) = 0$ and $V(x) = V_1$, $\mathbf{p}_1$ is the propagation matrix where $V(x) = V_1$, and so on. The propagation matrix $\mathbf{p}_{-0}$ returns the wave function to the appropriate coordinate system. The last matrix $\mathbf{p}_{-0}$ is unnecessary for calculating the transmission coefficient since it changes the coordinates, but does not change the ratio of the coefficients. The adequacy of treating the potential energy curve in Fig. 2 as a sequence of adjacent rectangular barriers will improve as the number of barriers increases and should converge to some limiting value. The transmission coefficient will be extracted from the transfer matrix using Eq. (18).

3. Results and discussion

The algorithm described above was programmed using the *Mathematica* software package. As the number of barrier segments increases the calculation of the transmission coefficient should converge to some limiting value close to the result using the WKB approximation. Fig. 3 shows the result for the calculation of the transmission coefficient through the barrier shown in Fig. 2 for different numbers of adjacent rectangular barriers. The calculation converged to a value of 6.1×10^{-17} after dividing the potential barrier into 250 adjacent rectangular barriers. This calculation took about one second on a 400 MHz PC running Linux. The solid line in the figure is the result of a calculation of the transmission coefficient using the WKB approximation. It is within a factor of three of the value the transfer matrix calculation approaches. This level of agreement is about the same as one finds in comparing the calculation of the transmission coefficient through a rectangular barrier using the two methods [7].

In the classroom students were asked to generate the algorithm for solving the rectangular potential barrier problem using *Mathematica*. The method was developed in lecture and then a laboratory was used to introduce the necessary commands. In a later session the extension to barriers of arbitrary shape was made and another laboratory used to introduce any new commands. The results of their transmission coefficient calculations were used to generate the half-lives for a series of radioactive isotopes in the manner of Gurney and Condon and then compared with the measured values found in the literature [11,12].

The pedagogical impact of the method was significant. The simplicity of the algorithm makes it accessible to undergraduates. They were able to program the algorithm with little outside help and as a result spent their time investigating the physics of the problem rather than debugging code. The transition from the rectangular barrier problem to potential barriers of arbitrary shape was transparent. It is analogous to the approach used to introduce the notion of an integral to many of our students so it can be developed with a minimum of class time. The validity of the approach was confirmed by having each student test the convergence of their algorithm as shown in Fig. 3.

The incorporation of computational laboratories (of which this method is part) has been successful. We recently began assessing our graduating seniors' competence using the Educational Testing Service's Field of Study test [13]. During the period 1994–1997 when we started this project and also began testing, the average performance of our seniors was in the 75th percentile in the quantum mechanics portion of the test.

A numerical integration of the Schrödinger equation was explored to solve the tunneling problem. Methods like this one are generally less familiar to undergraduates and hence less accessible to them. One must invest considerable class time to develop the algorithms or else run the risk of treating the solution of differential equations as a mere 'push button' function on a sophisticated calculator like *Mathematica*.

To conclude, the transfer matrix method provides a means for solving some of the typical quantum mechanics problems in a coherent, powerful fashion that can be readily extended to problems inside and outside the usual realm of introductory quantum mechanics courses [8,9,14,15]. The technique is readily accessible to undergraduates and its connection to the simple rectangular barrier problem is transparent. It also acquaints them with powerful matrix methods in a new context and is a vehicle for developing the students' skills with the computational tools that are used outside the classroom.

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