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A study of barrier penetration in quantum mechanics

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The Schrödinger equation is solved for the truncated Gaussian potential barrier using a power series solution and a general expression is obtained for the transmission coefficient. For this potential barrier, computer calculations show only a trace of the oscillatory behavior that characterizes the penetration of a rectangular barrier. The oscillations diminish rapidly as the discontinuity in the potential function approaches zero. The results indicate that it is the unrealistic discontinuities in potential models that cause such oscillatory behavior.

I. INTRODUCTION

It is comonplace in an introduction to quantum mechanics to include a discussion of tunneling using the rectangular potential barrier as a model. A graph of the transmission coefficient versus the energy, such as the graph shown in Fig. 1,[1] reveals the interesting feature that the coefficient varies in an oscillatory fashion for energies greater than the barrier height. The question was raised in a recent class as to whether this oscillatory behavior is peculiar to the rectangular shape or characteristic of other potential barriers as well. The pursuit of the answer to this question led to a study of barrier penetration in the case of a truncated Gaussian potential. This potential was chosen because it allows a convenient comparison of results for barriers with different amounts of abrupt change. The problem turns out to be quite instructive and requires some computer programming.

The initial task will simply be to solve the Schrödinger equation for the assumed potential function. It will be found that even and odd power series solutions are readily obtained and these are used in a derivation of the transmission coefficient T. A calculation of T is carried out for a number of energies. The results for two different barrier widths, presented graphically, are readily compared and provide the basis for the final discussion and conclusions.

II. THE GAUSSIAN POTENTIAL BARRIER

The specific one-dimensional potential function considered is expressed as

$$V(x)=\begin{cases}V_0e^{-\beta^2x^2}, & |x|<b,\\ 0 & |x|>b,\end{cases} \tag{1}$$

where V_0 denotes the barrier height and β and b are parameters that determine the shape and range. The general form of this function is shown in Fig. 2. The development proceeds then with a statement of the Schrödinger equation for the region $|x|<b$:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}+V_0e^{-\beta^2x^2}\psi=E\psi\,. \tag{2}$$

By introducing the dimensionless variable $\xi=\alpha x$, where $\alpha=(2mV_0/\hbar^2)^{1/2}$, and denoting $\gamma=E/V_0$, one finds that Eq. (2) reduces to

$$\frac{d^2\psi}{d\xi^2}-e^{-\beta^2\xi^2/\alpha^2}\psi+\gamma\psi=0,\quad |\xi|\leqslant\alpha b\,. \tag{3}$$

A Maclaurin series expansion of $e^{-\beta^2\xi^2/\alpha^2}$ together with the series substitution

$$\psi=\sum_{n=0}^{\infty}a_n\,\xi^n \tag{4}$$

leads to the recursion formulas

$$a_2=(1-\gamma)a_0/2\,,$$
$$a_3=(1-\gamma)a_1/2\,,$$
$$a_n=\frac{1}{n(n-1)}\left[(1-\gamma)a_{n-2}+\sum_{l=1}^{l'}\frac{(-1)^l}{l!}\left(\frac{\beta}{\alpha}\right)^{2l}a_{n-2l-2}\right],\quad n\geqslant 4\,, \tag{5}$$

where $l'=(n-2)/2$ if n is even, and $l'=(n-3)/2$ if n is odd. The choices ($a_0=1$, $a_1=0$) and ($a_0=0$, $a_1=1$) then yield separate, well-defined even and odd series solutions, denoted as u rather than ψ:

$$u_e=\sum_{n\ \mathrm{even}}a_n\,\xi^n=1+\frac{(1-\gamma)\xi^2}{2\cdot 1}+\frac{[(1-\gamma)^2/2-(\beta/\alpha)^2]}{4\cdot 3}\xi^4+\cdots, \tag{6a}$$

$$u_o=\sum_{n\ \mathrm{odd}}a_n\,\xi^n=\xi+\frac{(1-\gamma)\xi^3}{3\cdot 2}+\frac{[(1-\gamma)^2/6-(\beta/\alpha)^2]}{5\cdot 4}\xi^5+\cdots. \tag{6b}$$

Now one finds that the multiterm recursion relation (5) thwarts any attempt to display these series in such a way that a pattern of successive terms is seen by inspection. However, for the purpose of numerical calculation, such a display is quite unnecessary. In an evaluation of these sums by means of a simple computer program, successive terms are determined easily by means of Eq. (5), and that is all that is needed.

The question of convergence needs to be addressed at this point. The solution given by Eq. (4) is in the form of a Taylor's series expansion about the origin, which is an ordinary point of the differential equation (3). Furthermore, the variable coefficient multiplying ψ in Eq. (3) is regular at $\xi=0$, and the equation has no singular point. It is well known that in such a case, the general solution can be written as a Taylor's series expansion about the origin, which

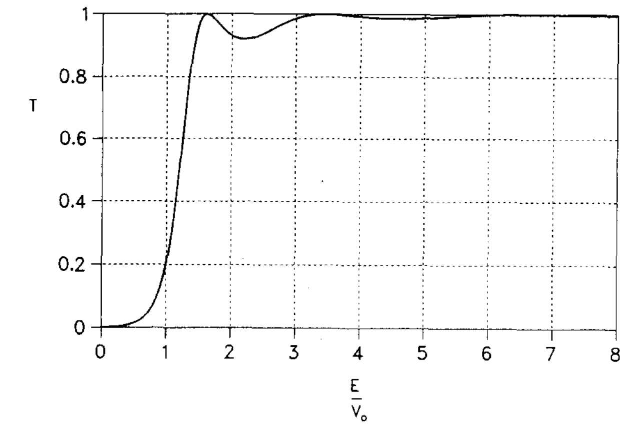

Fig. 1. The transmission coefficient for a rectangular barrier as a function of E/V_0. The barrier height V_0 is equal to $2\hbar^2/mb^2$, where b denotes the barrier half-width.

converges for all ξ.[2] It may be concluded without further ado, the multiterm recursion relation notwithstanding, that the solutions u_e and u_o are convergent for all ξ, and in particular for the range pertinent to this problem, namely, $-\alpha b < \xi < \alpha b$. Indeed, it is knowledge of the foregoing that provides the motivation for a power series solution in the first place.

The barrier height for this study was first assumed to satisfy the relation $(2mV_0 b^2/\hbar^2)^{1/2} = 2$ in order to facilitate a comparison of the final results for the transmission probability with the results of a similar calculation for a rectangular barrier of the same height and width. (Recall Fig. 1.) The width parameter $c = 1.25b$ was then assumed, keeping the same barrier height, i.e., $(2mV_0c^2/\hbar^2)^{1/2} = 2.5$. In both cases the ratio β^2/α^2 characterizing the potential was assumed to have the value 0.4. With these assumptions it was found that the convergence is sufficiently fast that 37 terms represented each of the series u_e and u_o to an accuracy of seven significant figures or more for values of ξ in the interval $-2.5 \leqslant \xi \leqslant 2.5$ and for energies in the range $0 \leqslant E \leqslant 8V_0$. Graphs of these solutions for two arbitrarily chosen energies are shown in Figs. 3 and 4. It may be noted from these figures that for $E < V$ the series u_e and u_o resemble somewhat the functions cosh ξ and sinh ξ, whereas for $E > V$ they are oscillatory in their behavior.

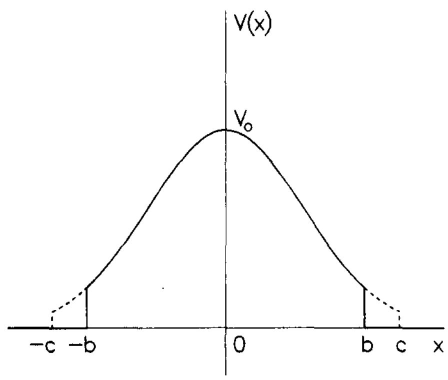

Fig. 2. Truncated Gaussian potential barrier $V_0 e^{-\beta^2 x^2}$ of width $2b$ or $2c$. The constant β^2 is equal to $1.6/b^2$ and the parameter c is equal to $1.25b$. The discontinuous change in the potential at the "edges" of the barrier decreases as the barrier width increases.

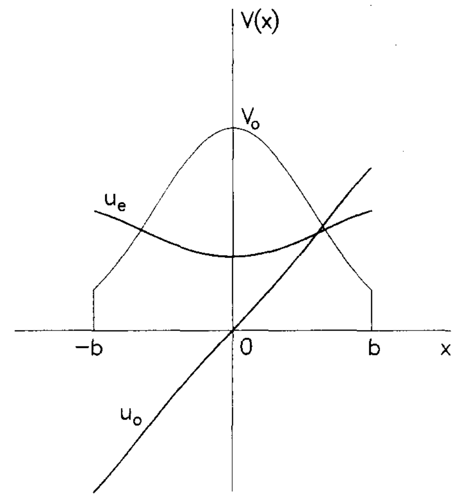

Fig. 3. Even and odd power-series solutions of the Schrödinger equation with a truncated Gaussian potential for the energy $E = 0.5V_0$. The graphs of the solutions are superimposed on the graph of the potential function. The parameters of the potential are the same as those of the potential shown in Fig. 2.

The general solution of the Schrödinger equation then for a particle incident from the left and with energy $E = \hbar^2 k^2/2m$ is of the form

$$\begin{cases} Ae^{ikx} + Be^{-ikx}, & x < -b, \\ Cu_e(\alpha x) + Du_o(\alpha x), & |x| < b, \\ Fe^{ikx}, & x > b, \end{cases} \tag{7}$$

where A, B, C, D, and F denote constants. To proceed with a derivation of the transmision probability, one may impose the boundary conditions that ψ and ψ' be continuous at $x = \pm b$. The matching conditions at $x = b$ give C and D in terms of F, and those at $x = -b$ give C and D in terms of A and B. On eliminating C and D, one finds

$$\frac{F}{A} = -ik\alpha e^{-2ikb} \frac{(u_o' u_e - u_e' u_o)}{(\alpha u_o' - iku_o)(\alpha u_e' - iku_e)},$$

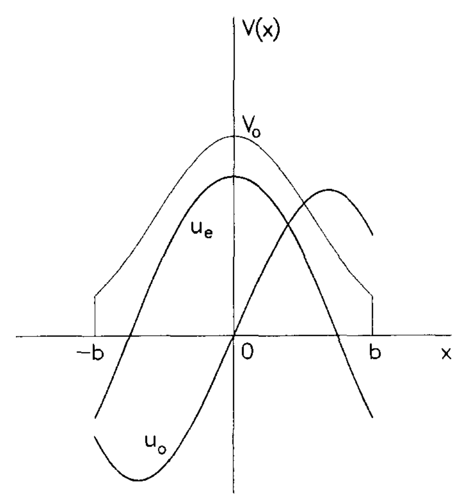

Fig. 4. Even and odd power-series solutions of the Schrödinger equation with a truncated Gaussian potential for the energy $E = 2V_0$. The parameters of the potential are the same as those of the potential shown in Fig. 2.

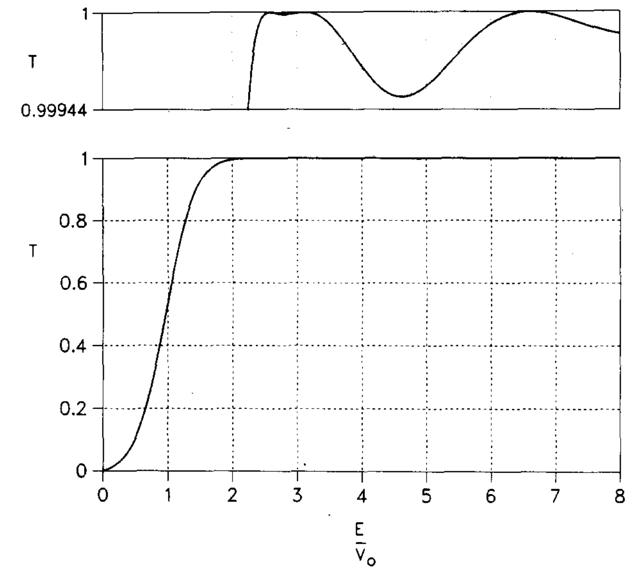

Fig. 5. The transmission coefficient for the truncated Gaussian barrier $V_0e^{-1.6x^2/b^2}$ as a function of E/V_0 for $V_0 = 2\hbar^2/mb^2$. The upper graph shows that the scale for T must be quite large in order that the variations in T be observed for energies considerably greater than the barrier height.

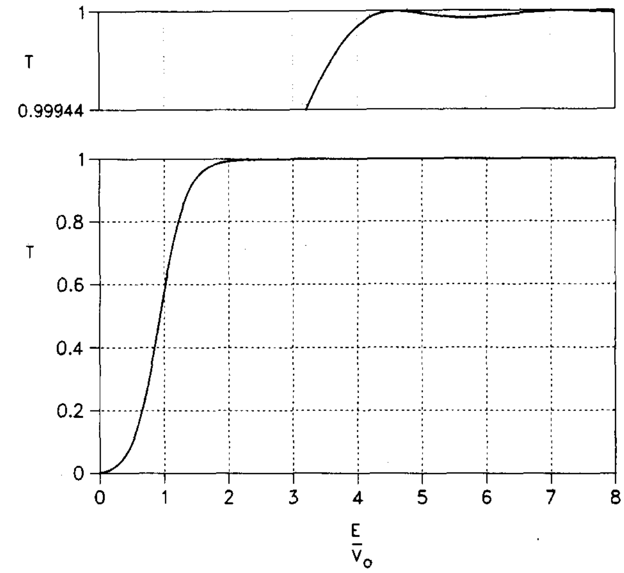

Fig. 6. The transmission coefficient for the truncated Gaussian barrier $V_0e^{-1.6x^2/b^2}$ as a function of E/V_0. The barrier height is equal to $3.125\,\hbar^2/mc^2$, where $2c$ is the barrier width. The upper graph reveals only slight variations in T in spite of the greatly enlarged scale. A comparison with Fig. 5 indicates that the magnitude of the variations decreases rapidly with increasing barrier width.

where u_o' and u_e' denote derivatives of the functions u_o and u_e with respect to ξ, and the suppressed argument for each of these four functions is αb. The expression $u_o'u_e - u_e'u_o$ will be recognized as the Wronskian of u_o and u_e, which is independent of the argument.[3] This constant is easily evaluated using $\xi = 0$, and it is found for this or any other value of ξ (verified by computer program) to have the value of unity. Thus the final expression for the transmission coefficient, written in terms of the ratio $\gamma = E/V_0 = k^2/\alpha^2$, is

$$T = \left|\frac{F}{A}\right|^2 = \frac{\gamma}{(u_o'^2 + \gamma u_o^2)(u_e'^2 + \gamma u_e^2)}. \qquad (8)$$

The matching conditions may be used in a similar way to obtain an expression for the reflection coefficient $R = |B/A|^2$ and to verify the familar relation, $R + T = 1$. This derivation, however, is not necessary to this study and is excluded.

Equation (8) provides a convenient means of computing T for various values of the energy ratio E/V_0. For the barrier widths chosen, one sets $\alpha b = 2$ and $\alpha c = 2.5$, and use is made of Eqs. (6a) and (6b) in the calculation of u_e, u_o, and their derivatives. A graph of the results for the smaller barrier width is shown in Fig. 5, where it is observed that the oscillatory behavior is discernible only on a greatly enlarged scale. Figure 6 gives the results for the greater width; there it is seen that the variations are quite small, even though the scale for T is greatly enlarged. For even greater barrier widths it was found that the oscillations become vanishingly small.

III. DISCUSSION

The rectangular barrier and the first truncated Gaussian barrier considered in this study satisfied the same height–width relation, namely, $mV_0b^2/\hbar^2 = 2$. The Gaussian barrier was then studied using the greater barrier half-width $c = 1.25b$. Listed in this order, these barriers represent a decreasing measure of abrupt change in the potential function at the "edges" of the barrier. On the other hand, a comparison of Figs. 1, 5, and 6 reveals a pronounced decrease in the magnitude of the oscillations in T for $E > V_0$. Relative to the results for the rectangular barrier, the variations are more than two orders of magnitude smaller in the case of the Gaussian barrier with the smaller width, and three orders of magnitude smaller in the case of the Gaussian barrier with the greater width. For even greater barrier widths the variations diminish markedly as significantly less potential is truncated.

It should be mentioned that a similar study was carried out for the parabolic potential barrier

$$V(x) = \begin{cases} V_0(1 - x^2/b^2), & |x| < b, \\ 0 & |x| > b, \end{cases}$$

where $mV_0b^2/\hbar^2 = 2$ was assumed. The results obtained were similar to those reported above for the Gaussian barrier, although the variations in T were not quite as small. The derivation and calculation for this potential are left as a possible exercise for the reader.

The results summarized above, obtained as they were for particular potential functions, do not permit a certain conclusion. They strongly suggest, nevertheless, that the discontinuous change in the potential function and its slope in the case of the rectangular barrier underlie the relatively large variations in T that occur for energies greater than the barrier height. It is also suggested that the remnant of such behavior that occurs in the case of the truncated Gaussian potential stems from the discontinuous change in the function or its slope. One would expect from these results, more generally, that the smaller the abrupt change is in a potential barrier, the smaller will be the variations in T for $E > V_0$. Although the wave nature of the atomic system plays an important role in the existence of these variations, it is the unrealistic discontinuities in the potential models that seem to be responsible.

[1]The graph shown in Fig. 1 was obtained by means of a computer program based on Eqs. (17.5) and (17.7) of L. I. Schiff, *Quantum Mechanics* (McGraw-Hill, New York, 1968), 3rd ed., p. 103. There *a* is used to denote the barrier width. A similar graph appears on p. 104 of the same book.

[2]J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (Benjamin, New York, 1970), 2nd ed., p. 14.

[3]J. L. Powell and B. Crasemann, *Quantum Mechanics* (Addison-Wesley, Reading, MA, 1961), p. 118.

Physics of a ballistic missile defense: The chemical laser boost-phase defense

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The basic physics involved in proposals to use a chemical laser based on satellites for a boost-phase defense are investigated. After a brief consideration of simple physical conditions for the defense, a calculation of an equation for the number of satellites needed for the defense is made along with some typical values of this for possible future conditions for the defense. Basic energy and power requirements for the defense are determined. A summary is made of probable minimum conditions that must be achieved for laser power, targeting accuracy, numbers of satellites, and total sources of power needed.

I. INTRODUCTION

Research and development for a possible space-based ballistic missile defense has been made a national goal with the Strategic Defense Initiative. The feasibility and wisdom of building one has become a major public debate. Much light can be shed on what can and cannot be done and the probable requirements for such a defense through an analysis of the basic physics of the defense.

In this and future articles on the same subject, the goal will be to present such an analysis on specific proposals that have been made for this defense either for the missile boost phase or later stages of the missile. Most of the physics in this analysis will be sufficiently basic that it can be introduced in upper division physics courses at the undergraduate level that would deal with the physics of nuclear weapons or the applications of physics to society.

In Sec. II is a summary of how the chemical laser operates and a discussion of the satellite mode and other basic requirements for a chemical laser defense. Section III is the most important one in the article in which the number of satellites needed for a boost-phase defense is determined through a general equation. In Sec. IV the minimum energy and power requirements for this laser defense are estimated. A summary is made in Sec. V.

II. MECHANISM AND REQUIREMENTS FOR A CHEMICAL LASER DEFENSE

The chemical laser defense would use a hydrogen fluoride (HF) laser or its companion, the deuterium fluoride (DF) laser. The HF laser operates at a wavelength of 2.7 μ, and the DF laser at 3.8 μ. Both wavelengths lie in the infrared.

The pumping energy for the laser is supplied by the chemical reaction:

$$H_2 + F_2 \rightarrow 2HF,$$

where H_2 and F_2 are hydrogen and fluorine in their normal diatomic form. For the high-power continuous-wave lasers needed for missile defense, the F_2 is dissociated into F before reacting with H_2. Part of the energy that is produced by this chemical reaction is absorbed by electrons of the molecule as they are stimulated into a higher-energy vibrational state.

The larger number of hydrogen fluoride molecules with electrons in the upper-energy state, compared to the number with electrons in the lower-energy unexcited state, as a result of the chemical reaction creates a population inversion that is necessary for the lasing to take place. The reaction is kept ongoing by continually pumping new hydrogen and fluorine into the reaction chamber and the laser continually operates as long as this happens.

The infrared beam created by the HF laser would be almost completely absorbed if transmitted through the Earth's atmosphere. Thus the lasers can only be used exoatmospherically. (Very little of the power of a DF laser is absorbed in the atmosphere, however.) The proposed use of these lasers is to base them in satellites in low-Earth orbit a few hundred miles above the Earth's surface. The attempt will be to cover the Soviet ICBM missile fields as well as all possible locations of submarines for launching SLBMs.

Low-Earth orbit satellites have an orbit period of

$$t_{\text{orbit}} = \frac{d_{\text{orbit}}}{v_{\text{orbit}}} = \frac{2\pi R}{(Rg)^{1/2}} = 5078 \text{ s} \sim 1.5 \text{ h}, \quad (1)$$

where R is the radius of the Earth (6400 km) and g is the

