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The Infinite Tilted-Well: An Example of Elementary Quantum Mechanics with Applications toward Current Research*

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The quantum-mechanical problem of a particle under the simultaneous influence of a linear potential and one-dimensional infinite square-well is considered. A graphical technique is described whereby approximate solutions are obtained for the general case, and some analytical methods are discussed by which exact solutions may be obtained for various special cases. The results should provide insight into a problem of current theoretical and experimental interest: the behavior of electrons in solids under the influence of an applied electric field.

INTRODUCTION

Because of its easy solution and simple interpretation, the problem of a single particle in an infinitely deep square-well[1] (ISW), is usually one of the first examples given to students learning elementary quantum mechanics. Among the various problems that can be used to follow up this introductory example, one of the most popular is the finite square-well problem[2] (FSW) in which one considers a modified square-well having a finite, rather than an infinite, depth.

The purpose of this paper is to point out that although the two square-well examples discussed above are familiar to most teachers of quantum mechanics, there is another example, relatively unknown, which not only fits into the same general category of easy-to-solve potential-well problems, but demonstrates some new and useful features as well. This relatively unexploited problem is defined by the potential energy function

$$v(x) = eE'x, \qquad \text{if } |x| \leq L/2,$$
$$= \infty, \qquad \text{if } |x| > L/2. \qquad (1)$$

The potential-well defined in Eq. (1) will be called an "infinite tilted-well" (ITW), since V(x) may be regarded as a superposition of an infinite square-well potential and the "tilted" potential, $eE'x$. Such a potential would arise, for example, if an ISW containing an electron of charge $-e$ were placed in a uniform, static electric field E'.

Although a number of the features of the FSW and the ITW are analogous, the ITW problem has some features which have no analog in the FSW. For example, one can obtain algebraic approximations to the solution of the ITW problem for the two limiting cases of intense field and weak field. For the weak field case, one obtains closed-form expressions, valid to second and higher orders of perturbation, which reduce to the well-known ISW results when E' is reduced to zero.

There are also some practical aspects of the ITW problem in addition to the pedagogical aspects mentioned above. In particular, this problem should help to develop useful insight concerning the effect of crystal boundaries on the behavior of an electron moving in a crystal under the influence of an electric field. This is important since the behavior of these Bloch electrons in the presence of applied fields is currently a subject of considerable theoretical and experimental interest.[3,4]

In view of certain similarities between the two problems, it is difficult to see why this potentially useful ITW problem has remained in a state of near obscurity while the FSW has not.

In Sec. I, by means of a linear transformation, the problem is first expressed in terms of a new coordinate, z, since the graphical technique is most easily understood in terms of z space. The graphical technique itself is described in Sec. II,

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[1] A. Messiah, *Quantum Mechanics, Vol. I* (Wiley-Interscience, Inc., New York, 1961), p. 86.

[2] Reference 1, p. 88.

[3] J. Zak, Phys. Rev. **168**, 686 (1968).

[4] G. H. Wannier, Phys. Rev. **125**, 1910 (1962).

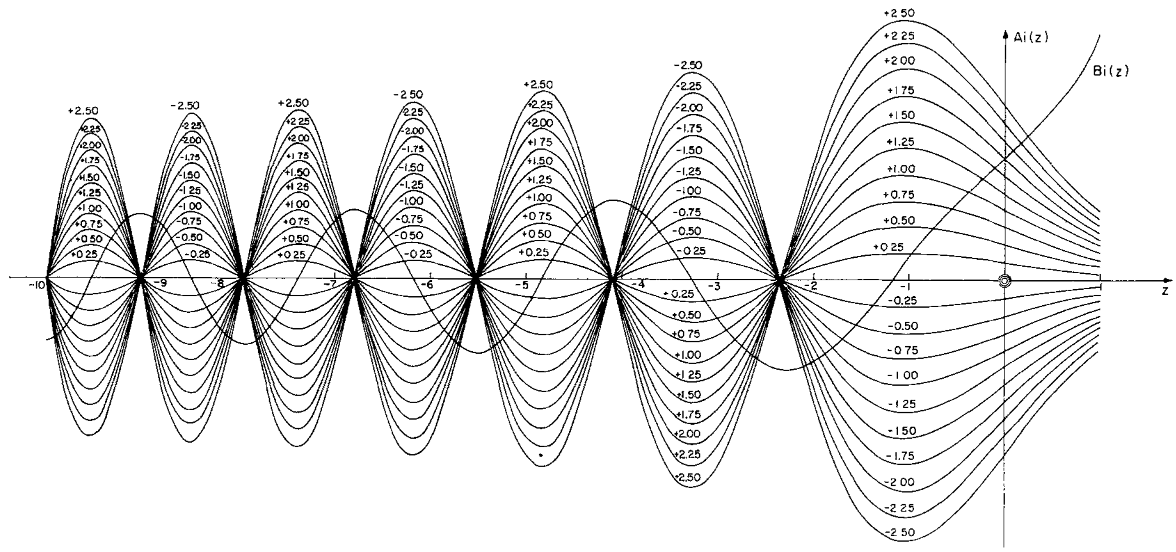

FIG. 1. The Airy Functions. The curves $Ai(z)$ and $Bi(z)$, as well as a family of curves proportional to $Ai(z)$, are shown. (Each member of the family is labeled with its appropriate scale factor.)

while the general features of the results are discussed in Sec. III.

I. TRANSFORMATION TO z SPACE

For the potential-well defined in Eq. (1), the time-independent Schrödinger equation becomes

$$[-(\hbar^2/2m)(d^2/dx^2)+eE'x]\psi=U'\psi. \qquad (2)$$

This can be simplified by introducing the variables, E and U, according to definitions

$$E=2meE'/\hbar^2,$$
$$U=2mU'/\hbar^2, \qquad (3)$$

and by introducing the dimensionless coordinate[5]

$$z=z_U(x,E)=E^{1/3}x-UE^{-2/3}. \qquad (4)$$

In terms of these definitions, Eq. (2) becomes

$$d^2\psi/dz^2-z\psi=0. \qquad (5)$$

This equation has solutions of the form

$$\psi_U(x,E)=\alpha Ai(z)+\beta Bi(z), \qquad (6)$$

where α and β are normalization factors, and where $Ai(z)$ and $Bi(z)$ are the Airy functions[6] (see Fig. 1). These functions are related to the Bessel functions by the relations[7]

$$Ai(-z)=\tfrac{1}{3}z^{1/2}[J_{1/3}(\lambda)+J_{-1/3}(\lambda)], \qquad (7)$$

$$Bi(-z)=\tfrac{2}{3}z^{1/2}[J_{-1/3}(\lambda)-J_{1/3}(\lambda)], \qquad (8)$$

$$\lambda=\tfrac{2}{3}z^{3/2}. \qquad (9)$$

Although one could in principle determine unique values for both α and β in Eq. (6) by requiring normalized wavefunctions, it will not be convenient for the present discussion. Therefore we relax this restriction and (except for the special case where $\beta=0$) work with the unnormalized function

$$\phi=\psi/-\beta=CAi(z)-Bi(z), \qquad (10)$$

where $C=-\alpha/\beta$.

The allowed energy levels, $U_n(E,L)$, and the amplitudes $C_n=-\alpha_n/\beta_n$ are determined by requiring that the wavefunction vanish at $x=+L/2$, and at $x=-L/2$. When applied to Eq. (10), these boundary conditions yield the relationships

$$CAi(\zeta+W/2)=Bi(\zeta+W/2), \qquad (11)$$

$$CAi(\zeta-W/2)=Bi(\zeta-W/2), \qquad (12)$$

where we have defined

$$\zeta=z_E(0,E)=-UE^{-2/3}, \qquad (13)$$

[5] We will assume that $E>0$. To obtain correct results for the case $E<0$, merely replace x by $-x$ in the following equations.

[6] H. A. Antosiewicz, *Handbook of Mathematical Functions*, M. Abramowitz and I. A. Stegun, Eds. (U. S. Dept. of Commerce, National Bureau of Standards, Washington, D. C., 1964); Appl. Math. Ser. **55**, p. 446.

[7] Reference 6, p. 447.

and

$$W = E^{1/3}L. \quad (14)$$

Notice that ζ is the image of the point $x=0$ under the transformation in Eq. (4), while $\zeta+\frac{1}{2}W$ is the image of the point $x=+L/2$, and $\zeta-W/2$ corresponds to the point $x=-L/2$. In Eqs. (11) and (12), ζ and C are the two unknowns. W has a known value since it is specified by the parameters E' and L given in Eq. (1). As might be expected, we will find that for each given value of W, there is an infinite set of discrete allowed values of the variables ζ and C, denoted by the symbols $\zeta_n(W)$ and $C_n(W)$, respectively. $(n=1, 2, 3, \cdots)$.

The following test can be performed to determine whether or not a proposed value, say ζ, is one of the allowed values, ζ_n. (The graphical method of solution described in Sec. II is merely a systematic way of applying this test.)

First determine which curve of the Ai family of Fig. 1 intersects the single Bi curve at a position $\zeta+\frac{1}{2}W$, located a distance $\frac{1}{2}W$ to the right of the proposed point ζ on the z axis of the figure. The amplitude factor which labels this curve (call it C_R) will automatically satisfy Eq. (11). Next, determine which one of the Ai curves intersects the Bi curve at the related point, $\zeta-\frac{1}{2}W$, located a distance $\frac{1}{2}W$ to the left of the proposed point ζ on the figure. The amplitude of this curve, C_L, will automatically satisfy Eq. (12). If the two amplitudes are *not* equal, then the proposed value, ζ, is *not* an allowed value since it fails to satisfy the boundary conditions. On the other hand, if $C_R=C_L$, then ζ and C_R *are* allowed values, since these values satisfy Eqs. (11) and (12) simultaneously.

II. GRAPHICAL SOLUTION

By sequentially testing every one of the points on the z axis of Fig. 1 in the manner described in Sec. I, one can obtain all of the allowed values $\zeta_n(W)$ and $C_n(W)$. In practice the task of testing points along the z axis can be systematized by the graphical technique described below. The graphical solution utilizes a device which can be constructed by cutting a slot in a 3×5 index card (see Fig. 2). The slot width should be made equal to the numerical value of W by measuring off this amount along the z axis of Fig. 1. In

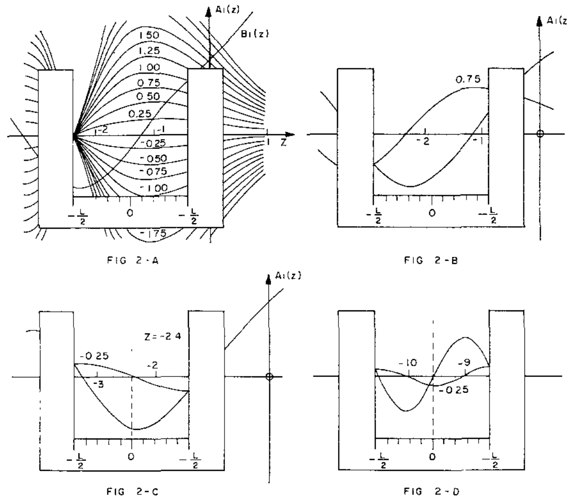

FIG. 2. Examples of indicator card use. (The sketches are drawn to illustrate the case $W=2$.) 2(a) Starting position; 2(b) An unacceptable position; 2(c) An acceptable ground state; 2(d) An acceptable state for $n=2$.

order to test a proposed point, ζ, this card will be laid upon the curves in Fig. 1 so that the center of the slot coincides with the location of the point ζ which is to be tested. Since the slot width is W, the right-hand edge will automatically indicate the location of the point $\zeta+\frac{1}{2}W$, and the left-hand edge will indicate the point $\zeta-\frac{1}{2}W$. Thus, the edges of the slot indicate the two points at which, according to the above test, the amplitude comparisons are to be made.

When the indicator card is positioned over Fig. 1 in this manner, the left edge of the slot will be the image of the point $x=-L/2$ under transformation (4), while the right edge will be the image of the point $x=+L/2$. The center will correspond to the center of the potential-well located at $x=0$. Since Eq. (4) represents a linear mapping of the interval $-L/2<x<+L/2$ onto $\zeta-\frac{1}{2}W<z<\zeta+\frac{1}{2}W$, a linear x scale can be constructed along the bottom of the indicator slot as shown in Fig. 2. Thus, by means of transformation (4), the potential-well defined by Eq. (1) has been mapped onto that part of the z axis of Fig. 1 lying inside the indicator card. The transformed boundary conditions, Eqs. (11) and (12), must be satisfied at the two edges of the slot.

In order to determine the allowed values of $\zeta_n(W)$ and $C_n(W)$, the indicator card is used in the following manner. (The sketches in Fig. 2(a)–

2(d) are drawn to illustrate the technique for the particular case where $W=2$.)

Step 1: Lay the indicator card on top of Fig. 1 with the left-hand edge of the slot at the initial position $z=-2.3$, as shown in Fig. 2(a). (It will presently become clear why this particular initial position is used.)

Step 2: Begin sliding the indicator card to the left, a little at a time (i.e., test each prospective point ζ for acceptability), until the position is found for which a *single* member of the family of Ai curves intersects the Bi curve at *both* edges of the slot. This position will represent the ground state of the system. [In Fig. 2(b), the card position illustrates an unacceptable value of ζ, while Fig. 2(c) shows the card position for the ground state of the system for the case $W=2$.]

Step 3: With the card in the ground-state position, record the values ζ_1 from the center of the slot and the value C_1 from the appropriate Ai curve. [From Fig. 2(c) we obtain $\zeta_1=-2.4$ and $C_1=-0.25$ for the case $W=2$.]

Step 4: Use a pair of dividers to obtain a plot of the unnormalized ground-state wavefunction directly from Fig. 1. This is accomplished by measuring the separation between the Bi curve and the appropriate Ai curve at various points along the x scale on the indicator card.[8]

Step 5: Continue moving the indicator card as before toward more negative values of z. Each time an "acceptable" card position is reached, record the appropriate values for ζ_n and C_n and plot the wavefunction from the curves as for the ground state. [Figure 2(d) illustrates the card position corresponding to the case $n=2$. For this case, we read $\zeta_2=-9.6$ and $C_2=-0.25$.]

Once the set of values $\zeta_n(W)$ and $C_n(W)$ has been determined, the energy eigenvalues are obtained from Eq. (13), and an expression for the corresponding wavefunction is obtained from Eq. (10). The results are

$$U_n(E, L) = -\zeta_n E^{2/3} \tag{15}$$

$$\phi = C_n Ai(E^{1/3}X - U_n E^{-2/3}) - Bi(E^{1/3}X - U_n E^{-2/3}). \tag{16}$$

It follows from Eqs. (11), (12), and (14) that the set of allowed values of ζ_n and C_n are determined uniquely by the product $E^{1/3}L$, and not by the individual values of E and L. Because of this, a single set of values ζ_n (i.e., the set determined from a single fixed value of W) is sufficient to determine the energy levels for any combination of E and L for which the product $E^{1/3}L$ is a constant. For example, the result for $W=2$ applies equally well to the case $E=1$, $L=2$ and the case $E=8$, $L=1$. This feature greatly simplifies the construction of plots of $U_n(E, L)$.

By experimenting with the above technique for a sufficient number of different parameters, and by making use of the special cases described in Sec. III which allow analytical solutions, one can quickly obtain a feeling for the general nature of the solutions. A number of these general features are discussed in Sec. III.

III. GENERAL RESULTS

After a few minutes of experimentation with the indicator card, the following interesting facts become apparent.

(1) $\zeta_n - \frac{1}{2}W < -2.3$ for all quantum numbers n and all combinations of E and L. (This is the reason for the initial placement of the indicator card as specified in Sec. II.)

(2) The net effect of the applied field is to squeeze the wavefunction toward the low potential energy end of the well and to change the energy of each quantum state.

(3) The distinguishing feature of the n'th quantum state is that $\phi_n^*\phi_n$ has exactly n peaks in the interval $-\frac{1}{2}L < x < \frac{1}{2}L$. This establishes a one-to-one correspondence with the well-known wavefunctions in the zero-field limit.

(4) If A_n denotes the n'th zero of the function $Ai(z)$, and if the zeros are ordered such that $\cdots < a_{n+1} < a_n < \cdots < a_1 < 0$, then

$$U_n \geq |a_n| E^{2/3} - (EL/2). \tag{17}$$

This inequality, which is valid for all values of E, L, and n, sets a lower bound on the energy levels. The equality holds for the strong-field and/or wide-well case.

(5) For an infinite set of specific cases, the

[8] Although the wavefunction could also be computed by substituting the values of ζ_1 and C_1 into Eq. (10), this graphical technique is much faster and easier.

given value of W will be equal to the numerical difference between two zeros of either the function $Ai(z)$ or the function $Bi(z)$. For these cases, we can obtain "exact" solutions. (We use the term "exact," in this instance, to indicate solutions which can be read directly from published tables and which do not require either graphical analysis or the solution of a transcendental equation.)

(6) For the low-field/narrow-well limit, the graphical technique makes it evident that one could use the asymptotic expressions[9]

$$Ai(z)\approx K\mid z\mid^{-1/4}\sin(\tfrac{2}{3}\mid z\mid^{3/2}+\tfrac{1}{4}\pi), \quad (18)$$

$$Bi(z)\approx K\mid z\mid^{-1/4}\cos(\tfrac{2}{3}\mid z\mid^{3/2}+\tfrac{1}{4}\pi), \quad (19)$$

where K is a constant. By keeping only second order terms in a Taylor series expansion of the expression $\mid E^{1/3}x-UE^{-2/3}\mid^{3/2}$, one eventually obtains the results

$$U_n\approx(n^2\pi^2/L^2)\{\tfrac{1}{2}+\tfrac{1}{2}[1-(EL^3/\hbar^2\pi^2)]^{1/2}\}^2+\tfrac{1}{2}(EL), \quad (20)$$

$$\phi_n/K(\alpha^2+\beta^2) \approx\sin[U_n^{1/2}(x+\tfrac{1}{2}L)-\tfrac{1}{4}EU_n^{-1/2}(x^2-\tfrac{1}{4}L^2)]. \quad (21)$$

Although Eqs. (20) and (21) actually represent asymptotic expressions, valid for the case of a weak-field and/or a narrow-well, the more restricted case where Eq. (20) is expanded *only* up to second-order in E is also interesting since it allows direct comparison with the well-known results for the ISW. The result is

$$U_n\approx(\pi^2n^2/L^2)+(L^4E^2/4\pi^2n^2). \quad (22)$$

The first term in Eq. (22) is easily recognized as the ISW energy levels and the second term therefore represents the 2nd-order correction to the ISW energy level due to the applied field.

If $W\ll 1$, then Eqs. (20) and (21) apply simultaneously to all quantum states for $n\geq 1$.

IV. REMARKS

As we have seen, the solution to the tilted-well problem combines graphical analysis with both approximate and exact analytical methods. The graphical technique not only provides a quick means of obtaining reasonably accurate energy levels and unnormalized wavefunctions, but points out techniques by which one can sometimes obtain either asymptotic approximations or exact solutions.

Although the discussion has considered only the pedagogical aspects of the tilted-well problem, this problem has some practical aspects as well.[10] These practical aspects are related to the similarities between this simple problem and the more complex but currently important problem of electron behavior in crystalline solids when a uniform electric field is applied. It can easily be shown that for an electron subjected to the simultaneous influence of both a uniform electric field and a periodic potential, the x dependence of the wavefunction must necessarily occur in the form $E^{1/3}x-UE^{-2/3}$. This is the same type of functional dependence which led to the indicator card analysis and also to the weak-field expansion described in the previous section. It is possible to exploit the similarity between this simple ITW problem and the unsolvable crystalline problem in order to acquire some insight into the effect of crystalline boundaries on the behavior of electrons moving in solids under the influence of an electric field. Another practical application is that Eqs. (20) and (21) can be perturbed with a periodic potential to investigate the nature of crystalline surface states in the presence of an applied electric field.

Because of the many instructive features of this problem and because of the relationship between this problem and the currently important analogous problem in crystalline solids, the infinite tilted-well problem ought to be potentially as useful in the classroom as the much better known finite square-well problem.

ACKNOWLEDGMENT

The authors are indebted to Professor R. B. Adler for several illuminating discussions concerning this subject.

[9] H. A. Antosiewicz, Ref. 6, p. 447.

[10] Unpublished report.