AAPT PHYSICS EDUCATION | AMERICAN JOURNAL of PHYSICS

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Noble M. Johnson and John N. Churchill

Citation: American Journal of Physics **38**, 487 (1970); doi: 10.1119/1.1976371
View online: http://dx.doi.org/10.1119/1.1976371
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/38/4?ver=pdfcov
Published by the American Association of Physics Teachers

Position Expectation Values for an Electron in an Infinite Tilted Well

NOBLE M. JOHNSON AND JOHN N. CHURCHILL
University of California, Davis, California 95616
(Received 18 August 1969; revision received 10 November 1969)

A numerical technique is used to determine the manner in which the expectation values of position for an electron in an infinite tilted well depend on the potential gradient and quantum state of the system. The results are compared to the classical case and to the exact analytic expression for the special case in which the total energy of the electron is equal to the maximum value of the linear potential.

I. INTRODUCTION

An attempt to understand and explain a physical phenomenon often begins with the consideration of a highly idealized, simplified model amenable to analytic techniques. Though such models do not provide a complete description or explanation of a phenomenon, they are quite effective in illustrating fundamental concepts. Hence, in an introductory course in quantum mechanics or solid-state physics, the problem of a single particle in an infinitely deep square-well potential (ISW) is used to illustrate the concept of discrete energy levels. Likewise, the Kronig–Penney (KP) model of a periodic potential is highly instructive in presenting the concept of energy bands for electrons in solids. This paper concerns a simple physical model which, although less familiar than the ISW or KP models, nevertheless demonstrates some interesting features which the more familiar models do not.

This model, which is defined by the potential energy function

$$V'(x) = e\mathcal{E}'x, \qquad 0 \leq x \leq L$$
$$= \infty, \qquad \text{elsewhere,} \qquad (1)$$

is called the "infinite tilted well" (ITW) because $V'(x)$ may be regarded as a superposition of an ISW potential and a "tilted" potential $e\mathcal{E}'x$. Since the infinite square well is often used as an idealized model of an electron in a "one-dimensional metal," one should be able to use the ITW as an idealized model of an electron of charge $-e$ in a similar environment but with the addition of a uniform electric field $\mathcal{E}'$.

Specifically, this article presents numerical results for the expectation value of position $\langle x \rangle$ of an electron in an ITW and compares these results with the time average of position for the corresponding classical problem. Since calculations of $\langle x \rangle$ have previously been limited to the special case in which the total energy of the particle is equal to the maximum value of the linear potential,[1,2] and since no such limitation is imposed here, the present work represents a generalization of the previous discussions. Thus, the purpose of this paper is not only to further clarify the relationship between the quantum-mechanical and the classical results but to furnish a more encompassing view of the entire ITW problem as well.

In contrast to most of the common examples of quantized systems (e.g., the infinite square well, the harmonic oscillator, and the hydrogen atom), the ITW does not possess inversion symmetry. For this reason, the expectation value of position does not in general fall at the center of the well as it does in the more familiar cases. In fact it will be shown that for the ITW this value depends not only on the well parameters $\mathcal{E}'$ and L but also on the quantum numbers designating the stationary states of the system. This is one of several rather distinctive features which makes the ITW problem a valuable example of elementary quantum mechanics.

Although the techniques presented by Churchill and Arntz[3] are useful for finding energies and wave functions for the ITW potential, they are not the most convenient way to obtain values for $\langle x \rangle$. Hence, a numerical algorithm was developed for calculating these values. For a given set of well parameters, this program computes the energy eigenvalues and wave functions and calculates the expectation value of position for each stationary quantum state. This algorithm is discussed briefly in Sec. II. In Sec. III the results of the analysis are presented and compared to corresponding results

for the classical time average of position. In Sec. IV an exact analytic expression for $\langle x\rangle$ is presented which is valid for the special case in which the total energy of the electron is equal to $V'(L)$. Numerical values calculated from this exact analytic expression confirm the accuracy of the numerical results presented in Sec. III.

II. NUMERICAL SOLUTION

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

$$[-(\hbar^2/2m)(d^2/dx^2)+V'(x)]\psi(x)=E'\psi(x). \quad (2)$$

By setting

$$\mathcal{E}=2me\mathcal{E}'/\hbar^2 \quad (3a)$$

and

$$E=2mE'/\hbar^2, \quad (3b)$$

Eq. (2) can be written in the more convenient form

$$[-d^2/dx^2+V(x)]\psi(x)=E\psi(x), \quad (4)$$

where

$$V(x)=[2m/\hbar^2]V'(x).$$

The boundary conditions require that ψ vanish at the edges of the well, i.e.,

$$\psi(0)=0 \quad (5a)$$

and

$$\psi(L)=0. \quad (5b)$$

Any nontrivial solution of Eq. (4) which satisfies Eqs. (5) is an acceptable eigenfunction or wave function and represents an allowed state of an electron in an ITW. The eigenvalue E corresponding to a given wave function is the (rationalized) total energy of an electron in that state.

In order to determine the energy eigenvalues and wave functions numerically, the eigenvalue problem was converted to an initial value problem. This initial value problem is defined by Eq. (4) together with the *initial* conditions

$$\psi(0)=0 \quad (6a)$$

and

$$d\psi/dx\,|_{x=0}=C, \quad (6b)$$

where C is some nonzero constant. The wave functions could be normalized, if desired, by an appropriate choice of C.

The intial value problem defined above is solved by first selecting a trial value for E and then performing a numerical integration of Eq. (4) subject to the initial conditions given by Eqs. (6). The resulting solution is then examined to determine whether or not it satisfies the boundary condition at $x=L$ as given in Eq. (5b). If this boundary condition is *not* satisfied, then by iteration the numerical integration is repeated for a succession of trial values of energy until an acceptable wave function is finally obtained. [Actually Eq. (5b) cannot generally be satisfied *exactly* when $\psi(L)$ has been obtained by a numerical integration. In order to satisfy this boundary condition, it is necessary only to make $|\psi(L)|$ sufficiently small compared to the maximum magnitude of the wave function inside the well.]

Once a wave function is known, the quantum number n can be determined[3] by counting the number of peaks of the function $|\psi(x)|$ in the interval $(0, L)$ and $\langle x\rangle_n$ can be calculated from the formula

$$\langle x\rangle_n=\int_0^L x\,|\psi_n(x)|^2dx \Big/ \int_0^L |\psi_n(x)|^2dx \quad (7)$$

by means of Simpson's rule.[4] The subscript n in $\langle x\rangle_n$ is included to emphasize the dependence of the expectation value of position on the state of the system.

The particular integration technique which was used to produce the results presented in Sec. III was the four-step Adams–Bashforth–Moulton (ABM) predictor–corrector method for evaluating systems of first-order ordinary differential equations. [Equation (4) can be written as a pair of coupled first-order equations.] Since this technique is adequately described elsewhere in the literature,[4,5] no detailed description will be given here. Two points should be made, however, regarding the use of this method.

(a) As is characteristic of any discrete variable technique, the ABM method furnishes an approximate solution to Eq. (4) only on a discrete set of points between $x=0$ and $x=L$.

(b) The ABM method is a multistep method and, as such, requires a special procedure for starting the integration. Thus, given only the initial conditions specified by Eqs. (6) one must begin by estimating the values of the solution at the first three discrete points beyond $x=0$ using a single-step numerical integration technique. After this is done, the more stable ABM method is used

to continue the integration. For the ITW results presented in Sec. III, the fourth-order Runge–Kutta method was used to obtain these starting values.

III. NUMERICAL RESULTS

For a given pair of well parameters, $\mathcal{E}$ and L, the energy eigenvalues E_n, the wave functions ψ_n, and the expectation value of position $\langle x\rangle_n$ for each ψ_n were computed using the techniques described in Sec. II. The expectation values of position for a continuous range of values of $\mathcal{E}$ can be displayed on a single graph by plotting $\langle x\rangle_n$ as a function of the dimensionless energy ratio

$$\xi = E/\mathcal{E}L. \tag{8}$$

This type of plot is especially convenient for displaying the relationship between the classical and the quantum-mechanical results since the classical time average of position $\bar{x}_{cl}$ is a unique function of ξ. Analytic expressions for $\bar{x}_{cl}$ are derived in the Appendix.

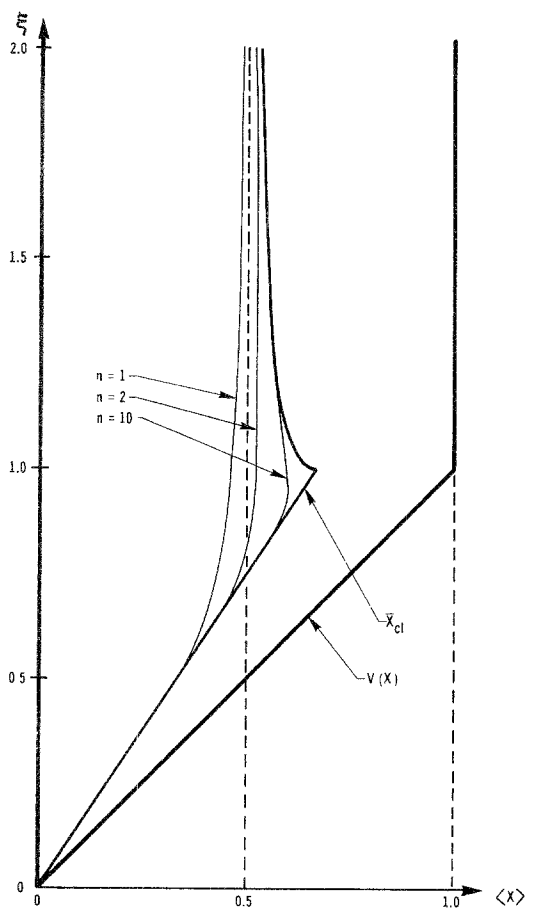

FIG. 1. Position expectation values as functions of ξ for quantum states $n=1$, 2, and 10 of an ITW with $L=1$. The rationalized potential energy function $V(x)$ and the classical time average of position $\bar{x}_{cl}$ are also shown.

Figure 1 displays ξ vs $\langle x\rangle_n$ for the first, second, and tenth stationary quantum states. The rationalized potential energy function $V(x)$ and the classical time average of position are also shown. All numerical calculations were made for a well of unit width, $L=1$. For $\xi \ll 1$, $\langle x\rangle_n$ conforms to $\bar{x}_{cl}$ for all states. As ξ increases in value, the curves begin to diverge from the classical case. As n increases, the point of divergence occurs for larger values of ξ. All the curves, including $\bar{x}_{cl}$, asymptotically approach the center of the well as ξ approaches infinity. From Fig. 1, it is also evident that for the ground state, $n=1$, $\langle x\rangle_1$ approaches the value $\frac{1}{2}$ asymptotically from the left half of the well, whereas all other states approach from the right. Thus, the ground state has a behavior which is unlike that of all other states.

In Fig. 2, a magnified version of Fig. 1 is shown for the first, second, third, fourth, sixth, and tenth stationary states for values of ξ in the vicinity of $\xi=1$. This expanded view illustrates that as n increases, the curves for $\langle x\rangle_n$ conform more and more to $\bar{x}_{cl}$ in accordance with the correspondence principle. In Sec. IV this will be shown to be true analytically for the special case $\xi=1$. Both Figs. 1 and 2 illustrate rather dramatically the manner in which the expectation value of position for an electron in an ITW potential depends upon the quantum numbers as well as the slope of the linear potential.

IV. ANALYTIC SOLUTION FOR $E=\mathcal{E}L$

For the special case in which an energy eigenvalue E_n is equal to the maximum value of the linear potential (i.e., $E_n=\mathcal{E}L$), Dymski[1] found that Eqs. (4) and (5) could be solved in closed form and the solutions normalized. The resulting wave functions are

$$\psi_n(x) = A(L-x)^{1/2} J_{1/3}[\tfrac{2}{3}\mathcal{E}^{1/2}(L-x)^{3/2}], \tag{9}$$

where A is the normalization constant and $J_\nu(\lambda)$ is the Bessel function of the first kind or order ν. At the right-hand edge of the well, x equals L and hence $\psi_n(L)$ is identically zero as required by Eq. (5b). Since ψ_n must also vanish at the left-

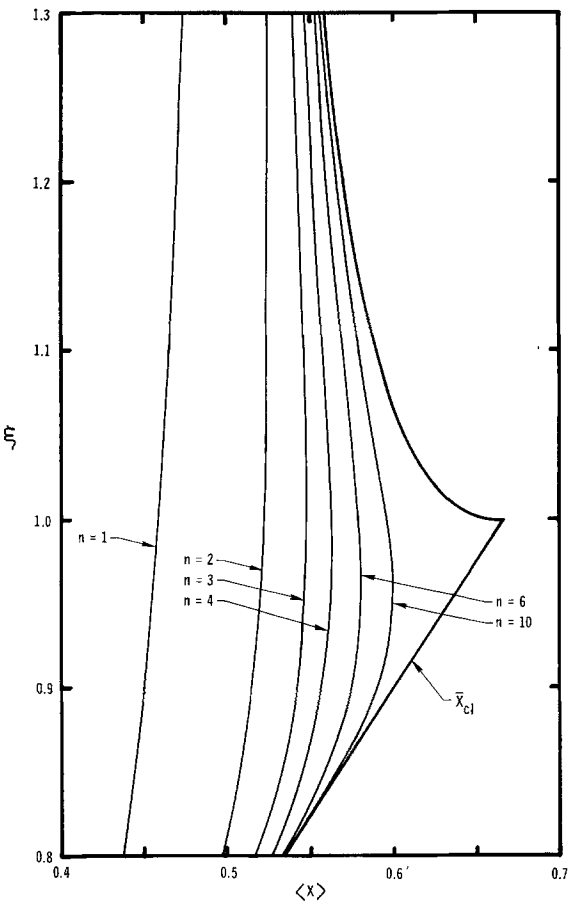

FIG. 2. Position expectation values as function of ξ in the vicinity of $\xi=1$ for quantum states $n=1$, 2, 3, 4, 6, and 10. The classical time average of position $\bar{x}_{cl}$ is also shown. These results are for an ITW with $L=1$.

hand edge of the well it follows that Eq. (9) is an acceptable solution only when

$$\tfrac{2}{3}\mathcal{E}^{1/2}L^{3/2}=r_n, \tag{10}$$

where r_n is the nth root of the one-third-order Bessel function.[6] These roots are assumed to be arranged in the order of ascending values so that the subscript n in r_n continues to denote the quantum number. Thus, for a given well width L only discrete values of $\mathcal{E}$ yield the special case $E_n=\mathcal{E}L$.

Using Eqs. (9) and (10), the normalization constant and the expectation value of position can be calculated. Numerical values for the expectation of position may then be computed from the exact analytic expression and compared to those presented in Sec. III. Following Dymski's method, the normalization constant and the expectation value of position are found to be, respectively,[1,2]

$$A=\{[LJ_{-2/3}(r_n)]^2-3^{4/3}/\mathcal{E}^{2/3}[\Gamma(\tfrac{1}{3})]^2\}^{-1/2} \tag{11}$$

and

$$\langle x\rangle_n\,|_{E_n=\mathcal{E}L}=L-L[J_{-2/3}(r_n)]^2/3\{[J_{-2/3}(r_n)]^2-R\}, \tag{12}$$

where

$$R=3^{4/3}/\mathcal{E}^{2/3}L^2[\Gamma(\tfrac{1}{3})]^2$$

and $\Gamma(\lambda)$ is the gamma function. It follows from Eqs. (10) and (12) that the expectation value of position depends on the quantum number of the state. In addition, it may be seen from Eqs. (10), (12), and (A3) that, as the quantum number n approaches infinity, the expectation value of position reduces to the classical time average of position. That is,

$$\lim_{n\to\infty}\langle x\rangle_n=\tfrac{2}{3}L=\bar{x}_{cl}, \qquad \xi=1.$$

Table I lists values of $\langle x\rangle_n$ and $\mathcal{E}$ for the first eight stationary states as calculated from Eqs. (10) and (12). These values, calculated from the exact analytic expression, confirm the numerically obtained values presented in Sec. III. This agreement is most apparent when the numerical data of Table I are compared with the expanded curves in Fig. 2.

V. CONCLUSIONS AND DISCUSSION

The expectation value of position for an electron in an ITW potential depends on the quantum numbers denoting the stationary states of the

TABLE I. Values of $\langle x\rangle_n$ and $\mathcal{E}$ obtained analytically[a] for the special case $\xi=1$.

n	$\mathcal{E}$	$\langle x\rangle_n$	n	$\mathcal{E}$	$\langle x\rangle_n$
1	18.96	0.4590	6	777.70	0.5790
2	81.89	0.5222	7	1062.68	0.5846
3	189.22	0.5475	8	1392.08	0.5890
4	340.97	0.5621	⋮	⋮	⋮
5	537.13	0.5719	∞	∞	0.6667[b]

[a] These values were computed from Eqs. (10) and (12) for an ITW of unity width, $L=1$. The numerically-computed values of $\langle x\rangle_n$ shown in Figs. 1 and 2 agree to four significant figures with the corresponding values listed above.

[b] This is also the value of the classical time average of position for $L=1$.

system in addition to the system parameters. This unusual property was illustrated with numerical results and verified with exact analytic results for the special case in which the total energy of an electron is equal to the maximum potential energy inside the well. From the analytic expression for this special case, it was found that the expectation value of position approaches the classical time-average of position as the quantum number approaches infinity. The numerical results also demonstrate this behavior.

The ITW model should find application in introductory courses in quantum mechanics as an example of a bound-state problem in which the potential-energy function does not possess even symmetry. It should also be of use in solid-state physics courses to enable the student to gain insight into the effect of an applied electric field on the wave functions of electrons in solids. In addition, the numerical solution of the one-dimensional, time-independent Schrödinger equation using the algorithm outlined in Sec. II affords an excellent exercise for a physical science-oriented computer programming course.

APPENDIX

Classically, the total energy of a particle of mass m and charge $-e$ placed in an ITW potential is

$$E' = \tfrac{1}{2}mv^2 + e\mathcal{E}'x, \tag{A1}$$

where v is the velocity. The force acting on the particle is

$$m(dv/dt) = -e\mathcal{E}'. \tag{A2}$$

If at a time $t=0$ the particle is at $x=0$ with $v=v_0$, then from Eqs. (A1) and (A2) the displacement of the particle with time is

$$x = (-e\mathcal{E}'/2m)t^2 + v_0 t,$$

where

$$v_0 = (2E'/m)^{1/2}.$$

For $E' \leq e\mathcal{E}'L$, the time required to travel from $x=0$ to $x=E'/e\mathcal{E}'$ is

$$t_1 = mv_0/e\mathcal{E}'$$

and, in terms of the dimensionless energy ratio $\xi = E'/e\mathcal{E}'L$, the time average of position is

$$\bar{x}_{cl} = (t_1)^{-1}\int_0^{t_1} x\,dt = \tfrac{2}{3}\xi L, \qquad \xi \leq 1. \tag{A3}$$

For $E' \geq e\mathcal{E}'L$, the time required to travel from $x=0$ to $x=L$ is

$$t_2 = (m/e\mathcal{E}')[v_0 - (v_0^2 - 2e\mathcal{E}'L/m)^{1/2}],$$

and

$$\bar{x}_{cl} = (t_2)^{-1}\int_0^{t_2} x\,dt = \tfrac{1}{3}L[(\xi+1) - (\xi^2-\xi)^{1/2}], \quad \xi \geq 1. \tag{A4}$$

The results given in Eqs. (A3) and (A4) are shown in Figs. 1 and 2 for the case $L=1$.

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