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Infinite Square-Well Potential with a Moving Wall

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The problem of a particle in a one-dimensional infinite square-well potential with one wall moving at constant velocity is treated by means of a complete set of functions which are exact solutions of the time-dependent Schrödinger equation. Comparison is made with a first-order perturbation treatment, and numerical results are presented for a particle initially in the ground state.

INTRODUCTION

Because of its simplicity, the problem of a particle in a one-dimensional infinite square-well potential with stationary walls is usually one of the first examples discussed in a beginning course in quantum mechanics. The slightly more complicated situation where one of the walls is allowed to move provides an instructive example of a problem with a time-dependent potential.

If the velocity of the moving wall is low, the problem can be handled by standard first-order time-dependent perturbation theory. In addition, however, if the velocity of the moving wall is constant, there exists a set of exact solutions which form a convenient basis for discussing the behavior for any value of the velocity of the moving wall.

I. PERTURBATION TREATMENT

The potential energy function is zero if $0\leq x\leq L(t)$ and infinite otherwise. The Hamiltonian operator is then

$$\mathcal{H}=-(\hbar^2/2m)(\partial^2/\partial x^2), \qquad 0\leq x\leq L(t). \tag{1}$$

The instantaneous energy eigenfunctions can be used as a basis for expanding the wave function,[1]

$$\psi(x,t)=\sum_n b_n(t)u_n(x,t) \times\exp\left[-(i/\hbar)\int_0^t E_n(\tau)d\tau\right], \tag{2}$$

where

$$u_n(x,t)=(2/L)^{1/2}\sin[n\pi x/L(t)], \tag{3}$$

and

$$E_n(t)=\hbar^2\pi^2n^2/2mL^2. \tag{4}$$

[1] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Co., New York, 1968), 3rd ed., Chap. 8.

Substitution of Eq. (2) into the Schrödinger equation,

$$\mathcal{H}\psi=i\hbar(\partial\psi/\partial t), \tag{5}$$

multiplication by $u_k(x,t)$, and integration over the interval $(0, L)$ yields the equations

$$db_k/dt=-\sum_n b_n\int_0^L u_k(\partial u_n/\partial t)dx \times\exp\left((i/\hbar)\int_0^t (E_k-E_n)d\tau\right). \tag{6}$$

For the special case

$$(dL/dt)=\text{const}, \tag{7}$$

Eq. (6) becomes

$$db_k/d\xi=\sum_{n\neq k} b_n[(-1)^{k+n}/\xi][2nk/(n^2-k^2)] \times\exp[-i(n^2-k^2)\pi^2(1-1/\xi)/4\alpha], \tag{8}$$

where

$$\xi(t)\equiv L(t)/L_0, \qquad L_0\equiv L(0), \tag{9}$$

and

$$\alpha\equiv(m/2\hbar)L_0(dL/dt). \tag{10}$$

Negative values of α correspond to a contracting box and positive values to an expanding box.

So far the treatment is exact. The coupled Eqs. (8) are equivalent to the time-dependent Schrödinger Eq. (5). The first-order approximation consists of replacing the $b_n(t)$ on the right side of Eq. (8) by their values at $t=0$. The indicated integration can then be carried out. Numerical results are presented in Fig. 1 for $|b_2|^2$ as a function of L/L_0 for three different wall velocities for the case

$$b_1(0)=1$$
$$b_n(0)=0, \qquad n\neq 1, \tag{11}$$

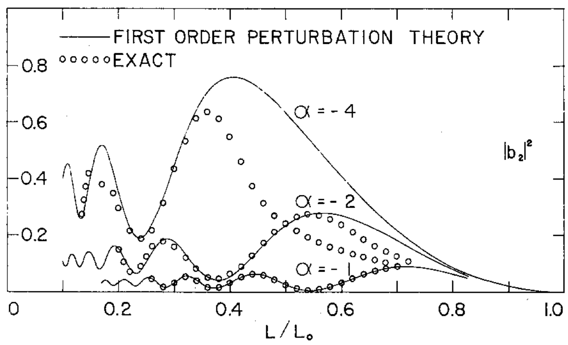

FIG. 1. Comparison of first order perturbation results with an exact calculation for three different compression rates. $|b_2|^2$ is the probability that a particle initially in the energy ground state will be found in the first excited state.

i.e., the particle is initially in the ground state. The explicit expression for the first-order approximation to $b_2(\xi)$ when $\alpha<0$ is

$$\begin{aligned} b_2= & -(4/3)\cos(g)[\mathrm{Ci}(g/\xi)-\mathrm{Ci}(g)] \\ & -(4/3)\sin(g)[\mathrm{Si}(g/\xi)-\mathrm{Si}(g)] \\ & -i(4/3)\cos(g)[\mathrm{Si}(g/\xi)-\mathrm{Si}(g)] \\ & +i(4/3)\sin(g)[\mathrm{Ci}(g/\xi)-\mathrm{Ci}(g)], \end{aligned} \quad (12)$$

where $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$ are the sine and cosine integrals, respectively,

$$\mathrm{Si}(x)=\int_0^x \frac{\sin\tau}{\tau}\,d\tau,$$

$$\mathrm{Ci}(x)=-\int_x^\infty \frac{\cos\tau}{\tau}\,d\tau, \quad (13)$$

and

$$g=-3\pi^2/4\alpha. \quad (14)$$

Also shown in Fig. 1 are the results of an exact calculation described below.

II. EXACT TREATMENT

Substitution of

$$\begin{aligned} \phi_n(x,t)= & (2/L)^{1/2} \\ & \times\exp[i\alpha\xi(x/L)^2-in^2\pi^2(1-1/\xi)/4\alpha] \\ & \times\sin[n\pi x/L(t)] \end{aligned} \quad (15)$$

into the time dependent Schrödinger Eq. (5) will verify that it is a solution if $(dL/dt)=\text{const}$,

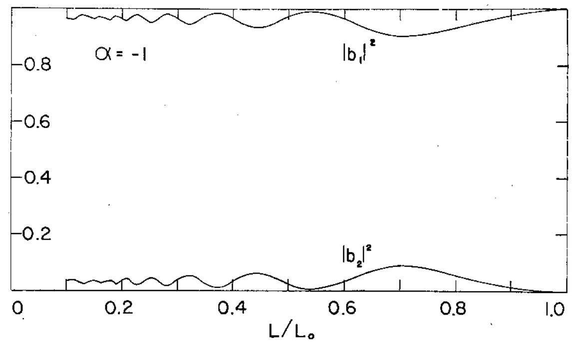

FIG. 2. Probabilities as a function of L/L_0 that the particle will be found in various energy states.

where ξ and α are defined by Eqs. (9) and (10). These functions vanish at $x=0$ and $x=L(t)$ as required, remain normalized as the wall at $x=L(t)$ moves, and form a complete orthogonal set. These functions form a convenient basis because when a wave function is expanded in terms of them,

$$\psi(x,t)=\sum_n a_n\phi_n(x,t), \quad (16)$$

the expansion coefficients a_n remain constant as the wall moves, their values being determined by the wave function at $t=0$ in the usual manner,

$$a_n=\int_0^{L_0}\phi_n^*(x,0)\psi(x,0)\,dx. \quad (17)$$

If the particle happened to be in one of the ϕ-states at $t=0$, it would remain in that state as the wall moved.

Numerical results are presented in Figs. 2–5 for a particle which is initially in the energy

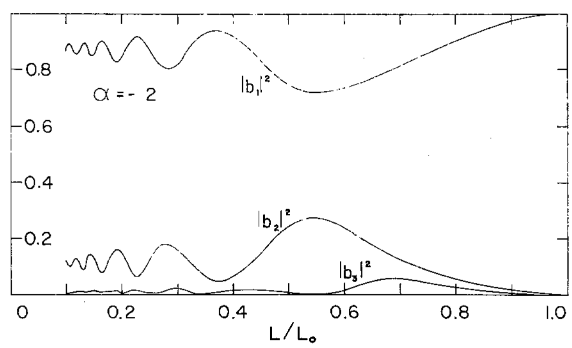

FIG. 3. Probabilities as a function of L/L_0 that the particle will be found in various energy states.

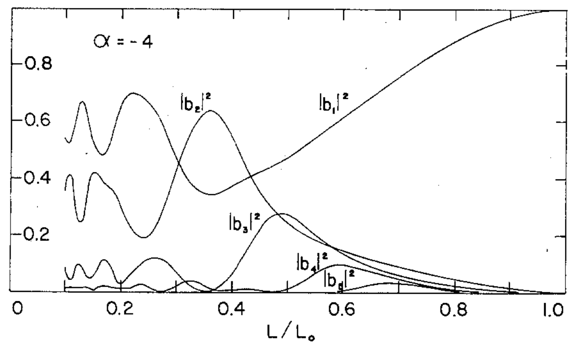

FIG. 4. Probabilities as a function of L/L_0 that the particle will be found in various energy states.

ground state. In this case, Eq. (17) becomes

$$a_n=(2/L_0)\int_0^{L_0}\exp[-i\alpha(x/L_0)^2]\sin(\pi x/L_0)\times\sin(n\pi x/L_0)dx. \quad (18)$$

Unfortunately, the above integral is not elementary, and the best that can be done for numerical evaluation is to reduce it to a combination of terms involving the Fresnel integrals

$$C_1(x)\equiv(2/\pi)^{1/2}\int_0^x \cos\tau^2 d\tau$$

and

$$S_1(x)\equiv(2/\pi)^{1/2}\int_0^x \sin\tau^2 d\tau. \quad (19)$$

In order to find the probabilities that the particle will be found in the various energy eigenstates at a later time, one must re-expand the wave function in terms of the instantaneous energy eigenfunctions $u_k(x,t)$,

$$\psi(x,t)=\sum_n a_n\phi_n(x,t)=\sum_k C_k(t)u_k(x,t), \quad (20)$$

the $u_k(x,t)$ being defined by Eq. (3). The coefficients $C_k(t)$ are related to the previous coefficients $b_k(t)$ by

$$C_k(t)=b_k(t)\exp\left(-(i/\hbar)\int_0^t E_k(\tau)d\tau\right), \quad (21)$$

and

$$|C_k(t)|^2=|b_k(t)|^2. \quad (22)$$

Because of the orthogonality of the $u_k(x,t)$ one finds that

$$C_k(t)=\sum_n a_n\int_0^{L(t)} u_k(x,t)\phi_n(x,t)dx. \quad (23)$$

Again, the integral can be expressed as a combination of Fresnel integrals, and the arithmetic was done on the IBM 360–30 digital computer at the University's Computing Center. Figures 2–4 show the results for the squares of the energy-eigenfunction expansion coefficients versus L/L_0 for three different values of the velocity parameter α. For the values of α shown, it was found that ten terms in the series Eq. (23) were sufficient to give four to five place accuracy for the squares of the coefficients.

The expectation value of the energy of the particle was obtained from

$$\langle E(t)\rangle=\sum_k |C_k(t)|^2E_k(t). \quad (24)$$

Figure 5 shows the ratio of the expectation value of the energy to the energy the particle would have if it remained in the ground state.

III. DISCUSSION

The velocity parameter α can be written as

$$\alpha=\tfrac{1}{4}\pi\tau_0L_0^{-1}(dL/dt), \quad (25)$$

where

$$\tau_0=2L_0/v_0$$

is the period of oscillation of a classical particle with the ground state energy. Examination of Figs. 2–4 shows that if $|\alpha|$ is small, i.e., the fractional change of the well width in one classical

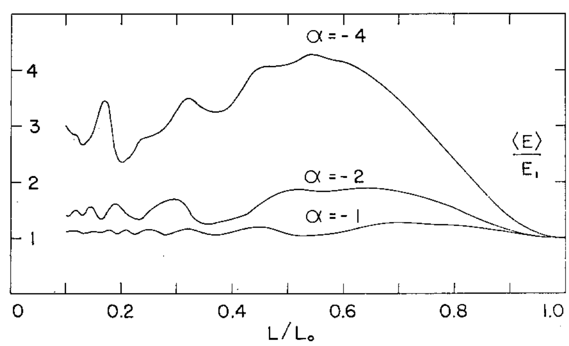

FIG. 5. Ratio of the average energy of the particle to the instantaneous ground state energy as a function of L/L_0 for three different compression rates.

period is small, then the particle will tend to remain in the initial state, a not unexpected result. As the velocity of the moving wall increases, larger amounts of other energy states are mixed in.

Examination of Fig. 1 shows that first order perturbation theory provides a useful approximation to $|b_2|^2$ for $|\alpha|$ as large as 2, a rather surprising result, since $\alpha=-2$ corresponds to a rather rapid compression. For higher values, of course, the deviation between the perturbation result and the exact calculation becomes appreciable.

Figure 5 shows the ratio of the average energy of the particle to the instantaneous ground state energy. One sees that for large compression rates there is a considerable increase in energy over and above the $(1/L^2)$ increase which would be obtained in a quasistatic compression. To this extent, one Schrödinger particle in a box exhibits a behavior similar to that of a real substance when compressed at a finite rate. Such a process is known to be irreversible, the most notable example being that of a shock-wave compression which can lead to a large increase in entropy.

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The Reflection and Transmission of Electromagnetic Waves by a Moving Dielectric Slab. I. Solution in the Moving Frame

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The Darwin scattering method is used to calculate the amplitudes, frequencies and propagation directions of the free space electromagnetic waves reflected and transmitted by a plane-parallel, non-dissipative, isotropic, homogeneous, dielectric slab. The laws of reflection and refraction and the conservation of energy flux follow naturally. Explicit formulas are given for perpendicular polarization but the method is equally applicable to polarization parallel to the plane of incidence. The results of Part I for the reference frame of the moving slab are in a form to be transformed in Part II to the reference frame of a "fixed" observer.

The discussion of the reflection of electromagnetic waves by a moving mirror provides one of the classic applications[1] of the special theory of relativity. Actually, an essentially correct treatment[2] preceded Einstein's 1905 analysis.[3] Quite recently, there have appeared studies of such problems as the reflection and transmission by a moving interface and a moving plasma slab,[4] and the diffraction of electromagnetic waves by moving cylinders[5] and wedges.[6] The method of analysis usually proceeds in two steps. One first obtains a solution when the body under consideration is at rest, and then transforms this solution, through the use of standard relativistic transformations, into a reference frame in which the body is in uniform motion.

In the case of the plane-parallel, nondissipative, homogeneous, isotropic, dielectric slab considered here, the first step is accomplished through the use of the Darwin scattering method, a method which will be shown to lead directly to all the important results associated with the reflection and transmission of electromagnetic waves by the slab. In Part II, these results will be transformed so as to obtain a solution for a fixed observer. The transformed solution will be seen to lead to the usual angle and frequency relations associated with a moving mirror, but it will also be shown that energy conservation can no longer be expressed in the same form as in the static case. In order to obtain a valid expression for energy

[1] A. Sommerfeld, *Optics* (Academic Press, Inc., New York, 1954), p. 72.
[2] W. Pauli, *Theory of Relativity* (Pergamon Press, Inc., New York, 1958), p. 95.
[3] A. Einstein, Ann. Physik **17**, 891 (1905).
[4] C. Yeh, J. Appl. Phys. **36**, 3513 (1965); **37**, 3079 (1966).
[5] S. W. Lee and R. Mittra, Can. J. Phys. **45**, 2999 (1967).
[6] G. N. Tsandoulas, Radio Sci. **3**, 887 (1968).