Effects of Finite Boundaries on a One-Dimensional Harmonic Oscillator

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In the study of the effects of finite boundaries on the magnetic properties of a solid, one encounters the problem of finding the energy eigenvalues of a one-dimensional linear harmonic oscillator located in a potential enclosure. The WKB method is employed to solve this problem for an oscillator whose center is fixed at some arbitrary position inside a potential box. Both numerical and analytical approximations of the WKB method are employed to find the energy eigenvalues over a wide range of the parameters of the problem. Numerical methods are also used on the exact series solutions of a bound oscillator to find the exact eigenvalues for the first few quantum states. A comparison of the two methods show that, in general, the WKB eigenvalues are accurate to much better than 1% except when the classical turning points are near the wall. Here the difference is of the order of 10% for the worst possible cases. The eigenvalues of a bound oscillator are shown to reduce to unbound-oscillator energy eigenvalues if the classical turning points are inside the potential enclosure and not near the walls. At the other extreme the eigenvalues are shown to become plane wave box eigenvalues when the separation of the classical turning points is large compared to the size of the enclosure. Also included is the relationship of the WKB solution to the Bohr-Sommerfeld quantization rule for the bound oscillator.

I. INTRODUCTION

THE problem of calculating the magnetic properties of a metallic solid can be reduced (by the usual assumptions of the one-electron approximation of a solid[1]) to studying the magnetic properties of an electron gas. If one wants to take into account the effects of finite boundaries on the magnetic properties, then the problem of interest will be to find the energy eigenvalues of a single electron in a magnetic field which is also in a potential box. This problem can be reduced (among other things) to that of solving a one-dimensional harmonic oscillator in a box with a shifted origin. Because such a bound oscillator is in itself significant for other applications, in addition to its relation to the surface effects of a solid, the purpose of this paper is to find the energy eigenvalues of a bound harmonic oscillator by means of both the WKB approximation and an exact method.

The exact method consists of a numerical extraction of the eigenvalues from the exact series solutions of the bound-oscillator differential equation. Because of practical difficulties, this method is restricted to the first few quantum states and to boxes whose sizes are small.[2]

We will be more interested in using the WKB method to find the eigenvalues because:

(a) In the problem of a solid, the majority of the quantum states will be in the semiclassical region. For example, a typical Fermi energy of 1 eV will correspond to a quantum number of around 10 000 for the unbound oscillator associated with a 1-kG field.

(b) The WKB method gives the exact results for the eigenvalues of an unbound oscillator, and we do not expect the introduction of finite boundaries to radically change the accuracy of this method. Our results will show that this is indeed the case.

(c) The WKB method turns out to be a more convenient procedure for finding the eigenvalues than procedures using the exact eigenfunctions. Also the WKB method gives us some analytical results, whereas the exact procedures usually only produce numerical results.

The studies of a bound oscillator so far (using the exact solutions which take the form of confluent hypergeometric functions in these cases) give the energy eigenvalues only for certain asymptotic or limiting ranges of the parameters of the problem.[3–6] In addition, they fix the position of the center of the oscillator at the middle of the box. Both of these limitations are intolerable if one is interested in knowing the energy-level structure of a metallic solid in order to calculate its magnetic properties. Here one must know the energy eigenvalues over large ranges of the size of the box, position of the center of the oscillator, and the quantum number n of the oscillator. As we shall see, the WKB method will allow us to find the energy eigenvalues over these ranges.

The Hamiltonian of a harmonic oscillator in a box (located in the interval $[a,b]$) with its center shifted by x_0 is given by

$$H=(1/2m)p^2+\tfrac{1}{2}m\omega^2(x+x_0)^2+V(x)\,,$$

where

$$V(x)=0 \quad a<x<b$$
$$=\infty \quad x\leq a \text{ or } x\geq b.$$

The effect of requiring that the box act like an infinitely

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[1] See any text on solid-state physics. For an especially good review article see Max Dresden, Rev. Mod. Phys. 33, 265 (1961).

[2] For the precise meaning of a small box and more on the use of the exact solutions see Sec. V and Refs. 3–6.

[3] F. C. Auluck and D. D. Kothari, Proc. Cambridge Phil. Soc. 41, 175 (1945).

[4] J. S. Baijal and K. K. Singh, Progr. Theoret. Phys. (Kyoto) 14, 214 (1955).

[5] P. Dean, Proc. Cambridge Phil. Soc. 62, 277 (1966).

[6] T. E. Hull and R. S. Julius, Can. J. Phys. 34, 914 (1956).

deep potential well is equivalent to imposing the boundary conditions that the wave functions vanish at the edges of the box. Changing to the dimensionless variable $\tau\equiv(m\omega/\hbar)^{1/2}x$, the problem of finding the eigenvalues of this Hamiltonian is reduced to solving the Sturm Liouville-type differential equation

$$\psi''(\tau)+[\lambda-(\tau+\tau_0)^2]\psi(\tau)=0, \tag{1a}$$

with the boundary conditions

$$\psi(\tau_a)=\psi(\tau_b)=0, \tag{1b}$$

and where

$$\tau_0\equiv(m\omega/\hbar)^{1/2}x_0, \quad \lambda\equiv 2E/\hbar\omega,$$
$$\tau_a\equiv(m\omega/\hbar)^{1/2}a, \quad \tau_b\equiv(m\omega/\hbar)^{1/2}b,$$
$$l\equiv\tau_b-\tau_a=(m\omega/\hbar)^{1/2}(b-a).$$

For this set of variables Eq. (1) represents the differential equation of a harmonic oscillator placed in a box of length l with the center of the oscillator shifted by τ_0. Here λ not only represents the energy eigenvalues of (1) but $\sqrt{\lambda}$ is the classical turning point of an unbound oscillator. A change of coordinates to $\xi\equiv\tau+\tau_0$ reduces (1) to

$$\psi''(\xi)+(\lambda-\xi^2)\psi(\xi)=0, \tag{2a}$$

with

$$\psi(\xi_a)=\psi(\xi_b)=0, \tag{2b}$$

and where

$$\xi_a\equiv\tau_a+\tau_0, \quad \xi_b=\tau_b+\tau_0.$$

In this set of coordinates the harmonic potential is fixed about the origin but now the location of the walls depends on τ_0 (see Fig. 1). The difference between these two representations of the Hamiltonian is the difference between letting the center of the oscillator be shifted by τ_0 and letting the center of the box be shifted by τ_0.

The objective of this paper has now been reduced to solving Eqs. (1) or (2) for the energy eigenvalues λ. It is comforting to note that the Sturm-Liouville theory guarantees the existence of a countable set of monotonically increasing eigenvalues λ for these equations. Moreover, Sturm-Liouville theory guarantees that the associated solution can be chosen in such a way that the eigenvalues form a complete set of orthonormal states.

II. WKB APPROXIMATIONS

The point $\lambda-\xi^2=0$ is not only the classical turning point of the oscillator, but it is also a point of inflection of the wave functions $\psi(\xi)$, where they change from oscillatory behavior in the region $\xi^2<\lambda$ to exponential behavior in the region $\xi^2>\lambda$.[7] Setting $U(\xi)=\lambda-\xi^2$, we find that the WKB solutions exhibit this behavior by approximating the exact solution by wave functions of the form

$$[-U(\xi)]^{-1/4}\exp\left\{\pm\int[-U(\xi)]^{1/2}d\xi\right\}$$

for $U(\xi)<0$ and

$$[U(\xi)]^{-1/4}\exp\left\{\pm i\int[U(\xi)]^{1/2}d\xi\right\}$$

for $U(\xi)>0$. It is convenient to let

$$F(\xi)\equiv\int(\sqrt{U})d\xi=\tfrac{1}{2}[\xi(\lambda-\xi^2)^{1/2}+\lambda\sin(\xi/\sqrt{\lambda})],$$

$$K(\xi)\equiv\int(\sqrt{-U})d\xi=\tfrac{1}{2}\{\xi(\xi^2-\lambda)^{1/2}-\lambda\ln[\xi/\sqrt{\lambda}+(\xi^2/\lambda-1)^{1/2}]\},$$

and note that

$$F(\pm\sqrt{\lambda})=\pm\tfrac{1}{4}\pi\lambda, \quad K(\sqrt{\lambda})=0.$$

In order to apply the WKB method we must match the above approximate solutions across the turning points by use of the connection relations. Since we also impose finite boundaries, we must consider the relationships of the turning points to the boundaries so that we can properly apply the boundary conditions. For a given energy eigenvalue λ we have the following possibilities:

(a) *Both turning points are inside the box.*

$$\lambda<\min\{\xi_a^2,\xi_b^2\}.$$

If both turning points are inside the box, then the center of the oscillator must lie inside the box and we must consider the three regions I, II, and III in Fig. 1 for values of λ less than ξ_a^2 and ξ_b^2. In these regions the general WKB solutions can be written as

$$\psi_{\mathrm{I}}(\xi)=(-U)^{-1/4}\left[A_1\exp\left(-\int_{\xi}^{-\sqrt{\lambda}}(-U)^{1/2}d\xi\right)+A_2\exp\left(+\int_{\xi}^{-\sqrt{\lambda}}(-U)^{1/2}d\xi\right)\right],$$

$$\psi_{\mathrm{II}}{}^{-}(\xi)=U^{-1/4}\left[B_1\exp\left(i\int_{-\sqrt{\lambda}}^{\xi}U^{1/2}d\xi\right)+B_2\exp\left(-i\int_{-\sqrt{\lambda}}^{\xi}U^{1/2}d\xi\right)\right],$$

$$\psi_{\mathrm{II}}{}^{+}(\xi)=U^{-1/4}\left[B_1'\exp\left(i\int_{\sqrt{\lambda}}^{\xi}U^{1/2}d\xi\right)+B_2'\exp\left(-i\int_{\sqrt{\lambda}}^{\xi}U^{1/2}d\xi\right)\right],$$

$$\psi_{\mathrm{III}}(\xi)=(-U)^{-1/4}\left[C_1\exp\left(\int_{\sqrt{\lambda}}^{\xi}(-U)^{1/2}d\xi\right)+C_2\exp\left(-\int_{\sqrt{\lambda}}^{\xi}(-U)^{1/2}d\xi\right)\right].$$

[7] We follow closely the method used by C. Lanczos, *Linear Differential Operations* (D. Van Nostrand Co., Inc., London, 1961).

Here ψ_{II}^{+} and ψ_{II}^{-} represent the same wave functions. They are written in this manner so that it is easier to use the connection relation across the points $U(\xi)=0$. Since

$$\int_{-\sqrt{\lambda}}^{+\sqrt{\lambda}} U^{1/2}d\xi=\int_{-\sqrt{\lambda}}^{\xi} U^{1/2}d\xi+\int_{\xi}^{+\sqrt{\lambda}} U^{1/2}d\xi,$$

ψ_{II}^{+} and ψ_{II}^{-} will be identical if

$$B_1=B_1'\exp\left(-i\int_{-\sqrt{\lambda}}^{+\sqrt{\lambda}} U^{1/2}d\xi\right)=B_1'e^{-i\pi\lambda/2},$$

$$B_2=B_2'\exp\left(+i\int_{-\sqrt{\lambda}}^{+\sqrt{\lambda}} U^{1/2}d\xi\right)=B_2'e^{+i\pi\lambda/2}.$$

Applying the boundary condition $\psi_I(\xi_a)=0$, we find

$$A_2=-A_1e^{-2K(-\xi_a)}.$$

At the other end, $\psi_{III}(\xi_b)=0$ gives

$$C_1=-C_2e^{-2K(\xi_b)}.$$

The connection relations for a transition from the exponential region I to the periodic region II is given by

$$B_1=e^{-i\pi/4}(A_1+\tfrac{1}{2}iA_2),$$
$$B_2=e^{+i\pi/4}(A_1-\tfrac{1}{2}iA_2).$$

For transition from II to III the connection relations are

$$B_1'=e^{+i\pi/4}(-\tfrac{1}{2}iC_1+C_2),$$
$$B_2'=e^{-i\pi/4}(\tfrac{1}{2}iC_1+C_2).$$

We now have eight equations involving the eight unknown coefficients in the wave functions. Intrasubstitutions of these above equations give the consistency relation

$$\beta e^{-i\pi\lambda/2}-\beta^{*}e^{i\pi\lambda/2}=0,$$

where

$$\beta\equiv e^{i\pi/2}(1+\tfrac{1}{2}ie^{-2K(-\xi_a)})(1+\tfrac{1}{2}ie^{-2K(\xi_b)}).$$

Since this relation must hold if the WKB method is to give approximate solutions of (1), solving it for λ will give us the energy eigenvalues. Although we cannot solve it exactly, we can take into account its transcendenta lnature. Using trignometric identities, it reduces to

$$\cos(\tfrac{1}{2}\pi\lambda+\theta)=0,$$

where

$$\theta\equiv\tan^{-1}(\mathrm{Re}\beta/\mathrm{Im}\beta).$$

Therefore the consistency relation will hold if $\frac{1}{2}\pi\lambda+\theta=\frac{1}{2}\pi(2n+1)$, so that

$$\lambda=2n+1+(2/\pi)\times\tan^{-1}\left\{\frac{e^{-2K(-\xi_a)}+e^{-2K(\xi_b)}}{2-\frac{1}{2}\exp\{-2[K(-\xi_a)+K(\xi_b)]\}}\right\}. \quad (3a)$$

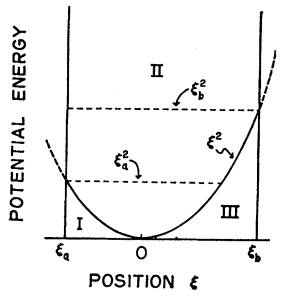

FIG. 1. Potential energy of a dimensionless harmonic oscillator in an infinitely high potential well.

Recalling that $K(\xi)$ is also dependent on λ, we see that Eq. (3a) does not give us the energy eigenvalues. We must solve (3a) for λ to find the eigenvalues as a function of the boundaries ξ_a and ξ_b and the quantum number n.

(b) *The left turning point is outside the box but the right one is inside the box,* $\xi_a^2<\lambda<\xi_b^2$. For this case we need only consider regions II and III of Fig. 1 for values of λ between ξ_a^2 and ξ_b^2. The WKB wave functions can then be written as

$$\psi_{II}^{-}(\xi)=U^{-1/4}\{B_1\exp i[F(\xi)-F(\xi_a)]+B_2\exp -i[F(\xi)-F(\xi_a)]\},$$
$$\psi_{II}^{+}(\xi)=U^{-1/4}\{B_1'\exp i[F(\xi)-F(\sqrt{\lambda})]+B_2'\exp -i[F(\xi)-F(\sqrt{\lambda})]\},$$
$$\psi_{III}(\xi)=(-U)^{-1/4}[C_1\exp K(\xi)+C_2\exp -K(\xi)].$$

Here ψ_{III}^{+} and ψ_{III}^{-} will be identical if

$$B_1=B_1'\exp\{-i[\tfrac{1}{4}\pi\lambda-F(\xi_a)]\},$$
$$B_2=B_2'\exp\{i[\tfrac{1}{4}\pi\lambda-F(\xi_b)]\}.$$

The connection relations for transition from region II to III and the boundary condition relations at ξ_b are identical to those found in case (a). At ξ_a the boundary condition $\psi_{III}^{-}(\xi_a)=0$ implies $B_1+B_2=0$. These relations give the consistency relation $\delta-\delta^{*}=0$, where

$$\delta\equiv(1+\tfrac{1}{2}ie^{-2K(\xi_b)})\exp\{-i[\tfrac{1}{4}\pi(\lambda-1)-F(\xi_a)]\}.$$

In a manner similar to that used in case (a) we can reduce the problem of solving this relation for λ to solving

$$\lambda=4n+3+(4/\pi)F(\xi_a)+(4/\pi)\tan^{-1}(\tfrac{1}{2}e^{-2K(-\xi_b)}) \quad (3b)$$

for λ. This relation is valid regardless of whether or not the center of the oscillator lies inside the box, the only difference being that $\xi_a<0$ when the center is inside and $\xi_a>0$ when the center is outside for case (b).

(c) *The right turning point is outside the box but the left one is inside,* $\xi_b^2<\lambda<\xi_a^2$. This case is nearly identical with (b) and gives a consistence relation of the form

$$\lambda=4n+3-(4/\pi)F(\xi_b)+(4/\pi)\tan^{-1}(\tfrac{1}{2}e^{-2K(-\xi_a)}). \quad (3c)$$

(d) *Both turning points are outside the box,*

$$\lambda>\max\{\xi_a^2,\xi_b^2\}.$$

Here we need only consider region II with the WKB wave function

$$\psi_{II}(\xi)=U^{-1/4}\{B_1\exp i[F(\xi)-F(\xi_a)]+B_2\exp -i[F(\xi)-F(\xi_a)]\}.$$

The boundary condition $\psi_{II}(\xi_a)=0$ again implies $B_1=-B_2$, so that

$$\psi_{II}(\xi)=U^{-1/4}2iB_1\sin[F(\xi)-F(\xi_a)].$$

Applying the other boundary condition, $\psi_{II}(\xi_b)=0$ gives us the consistency relation

$$F(\xi_b)-F(\xi_a)=(n+1)\pi, \qquad (3d)$$

which we must solve to find the energy eigenvalues λ. Note that we have written the consistency relations in all four cases in such a way that the possible values of n are 0, 1, 2, $\cdots$. Also the relations (3) are valid even if the center of the oscillator does not lie inside the box.

III. NUMERICAL DETERMINATION OF WKB EIGENVALUES

In order to obtain the energy of eigenvalues of a bound oscillator we must solve directly the consistency relations (3) for λ. Note that these four relations are really only one relation, defined over four disjoint ranges of ξ, which can be solved to give the quantum number n as a function of ξ_a, ξ_b, and λ. We write this in the form $n=N(\lambda,\xi_a,\xi_b)$, where

$$\begin{aligned}N(\lambda,\xi_a,\xi_b)&=\tfrac{1}{2}(\lambda-1)-\pi^{-}(^{1}\tan^{-1}\tfrac{1}{2}e^{-2K(-\xi_a)})\\&\quad-\pi^{-1}\tan^{-1}(\tfrac{1}{2}e^{-2K(\xi_b)})\\&=\tfrac{1}{3}(\lambda-4)-\pi^{-1}F(\xi_a)-\pi^{-1}\tan^{-1}(\tfrac{1}{2}e^{-2K(\xi_b)})\\&=\tfrac{1}{3}(\lambda-4)+\pi^{-1}F(\xi_b)-\pi^{-1}\tan^{-1}(\tfrac{1}{2}e^{-2K(-\xi_a)})\\&=-1+\pi^{-1}F(\xi_b)-\pi^{-1}F(\xi_a).\end{aligned}$$

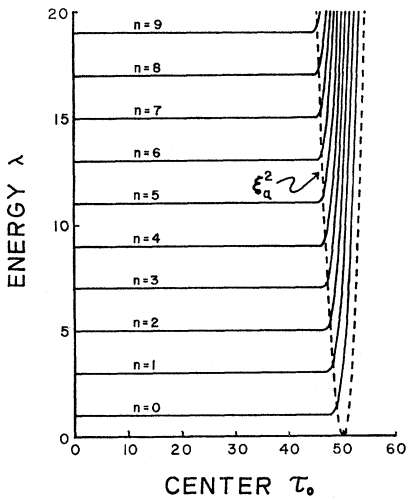

FIG. 2. Energy eigenvalues of a dimensionless harmonic oscillator as the position of the center of the oscillator varies from the center of the box to outside the box. Here $\sqrt{\lambda}\ll l$ and $l=100$.

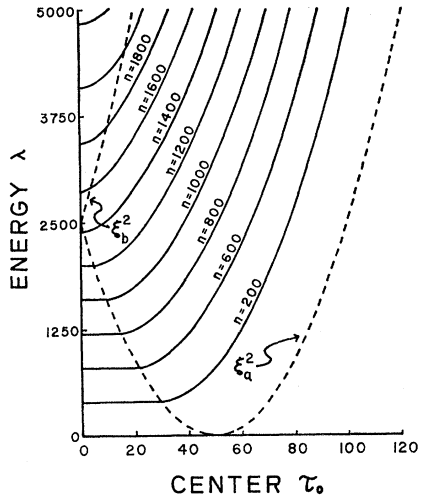

FIG. 3. Energy eigenvalues of a dimensionless harmonic oscillator as the position of the center of the oscillator varies from the center of the box to outside the box. Here $\sqrt{\lambda}\approx l$ and $l=100$.

The ranges are those given in parts (a)–(d), respectively, of Sec. II.

We will use the variables τ_0 and l interchangeably with the variables ξ_a and ξ_b since they are equivalent,

$$\tau_0=\xi_a+\xi_b, \quad l=\xi_b-\xi_a.$$

Placing our original box symmetrically about the origin (letting $b=-a$), it can be shown that the consistency relations are even functions of the dimensionless center τ_0 for this arrangement. This, in turn, implies that the energy eigenvalues λ will also be an even function of τ_0, so that we only need consider positive displacements of the center.

Because of the complex nature of the relations (3) it is not possible to solve them exactly. In certain limiting ranges it is possible to obtain approximate solutions. In all ranges it is possible to solve them using numerical methods and a high-speed digital computer. Fixing n, τ_0, and l, we can find λ by solving for the zeros of $f(\lambda)=n-N(\lambda,\tau_0,l)$. The zeros can be found by an iterative hyperbolic interpolarion.[8] Given an upper and lower bound, and an initial guess $(\lambda_1,\lambda_2,\lambda_3)$, we can fit a unique hyperbola through these three points having the form

$$f(\lambda)=(A\lambda+B)/(C\lambda+D), \quad AD-BC\neq 1.$$

If this hyperbola is taken to approximate $n-N(\lambda,\tau_0,l)$ in the neighborhood of its zeros, then the zeros of the hyperbola approximate the zeros of this function. When the relative difference between successive values of the zeros (i.e., λ) is less than 10^{-4}, we stop the iterations. Since $N(\lambda,\tau_0,l)$ is a monotone function of λ, our procedure will approach the true value of λ even if this value does not lie in the initial bounds given. The lower

[8] A. M. Ostrowski, *Solutions of Equations and Systems of Equations* (Academic Press Inc., New York, 1960).

bound of λ is always $2n+1$ and its upper bound can be found by a procedure like that described by Nordtvedt.[9] The analytical approximations described in Sec. IV give a sufficiently close approximation of λ over its whole range that it can be used as an initial guess, and the upper and lower bound can be placed near it.

Figures 2–4 represent tracings of machine plots of 40 points/in. of the energy eigenvalues found by the above technique as a function of the center τ_0 for various sets of quantum numbers n. The size of the box has been taken to be 100 ξ units in length. The three figures represent the situations when the separation of the classical turning points is much less, comparable with, or greater than the size of the box. The parabolas $\lambda=\xi_a^2$ and $\lambda=\xi_b^2$ represent the boundaries between the regions where the turning points pass through the walls of the box.

IV. ANALYTICAL APPROXIMATIONS OF WKB EIGENVALUES

When the turning points are not near the edges of the box, we can make expansion of terms in the consistency relations in powers of $\xi/\sqrt{\lambda}$ or $(\sqrt{\lambda})/\xi$, depending on whether a turning point is inside or outside the box. If $\xi>\sqrt{\lambda}$, the relations (3) involve terms of the form $\exp[-2K(\xi)]$. Here $K(\xi)$ is positive and monotone if ξ is positive, so that $\exp[-2K(\xi)]$ will be small since K will be fairly large (if ξ is not near $\sqrt{\lambda}$). In the case when both turning points are inside [case (a) of Sec. II] we can obtain the zeroth-order approximation of $\lambda=2n+1$ from (3a) by neglecting the second term on the right in comparison with $2n+1$. These are the energy eigenvalues of an unbound oscillator. We expect this result since the wave functions of a free oscillator fall off like $\exp(-\frac{1}{2}\xi^2)$ after the turning points so that the introduction of finite boundaries should have little effect provided that the walls are not near the turning points. Note that when n is large, we can also neglect the second term on the right in (3a) since its maximum value is always less than unity. This again gives free oscillator states.

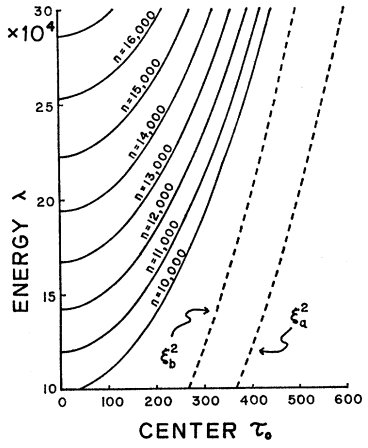

FIG. 4. Energy eigenvalues of a dimensionless harmonic oscillator as the position of the center of the oscillator varies from the center of the box to outside the box. Here $\sqrt{\lambda}\gg l$ and $l=100$.

[9] K. Nordtvedt, Jr., J. Math. Phys. 8, 1406 (1967).

The first-order correction can be found by replacing λ in $K(\xi)$ by $2n+1$,

$$\lambda=2n+1+\frac{2}{\pi}\left[\frac{-\xi_a}{(2n+1)^{1/2}}+\left(\frac{\xi_a^2}{2n+1}-1\right)^{1/2}\right]^{2n+1}\times\exp\{\xi_a[\xi_a^2-(2n+1)]^{1/2}\}+\frac{2}{\pi}\left[\frac{\xi_b}{(2n+1)^{1/2}}+\left(\frac{\xi_b^2}{2n+1}-1\right)^{1/2}\right]^{2n+1}\times\exp\{-\xi_b[\xi_b^2-(2n+1)]^{1/2}\}.$$

Placing the center of the oscillator at the center of the box, $\tau_0=0$, and neglecting $2n+1$ in comparison with the size of the box l, we have

$$\lambda=2n+1+\frac{4}{\pi}\left[\frac{l}{(2n+1)^{1/2}}\right]^{2n+1}e^{-l^2/4}.$$

This approximation agrees with that obtained by Haull and Julius for an asymptotic approximation of the eigenvalues.[10]

When both turning points are outside the box, we note the parabolic dependence of λ on the center τ_0 from the numerical solutions (Fig. 4). We thus expand λ in a Taylor series about $\tau_0=0$.

$$\lambda=\lambda_0+\left.\frac{\partial\lambda}{\partial\tau_0}\right|_0\tau_0+\left.\frac{\partial^2\lambda}{\partial\tau_0^2}\right|_0\tau_0^2+\cdots.$$

From the consistency relation (3d) we can find λ_0 since at $\tau_0=0$ it becomes

$$\alpha(\lambda_0-\alpha^2)^{1/2}+\lambda_0\sin^{-1}(\alpha/\sqrt{\lambda_0})=(n+1)\pi, \qquad (4)$$

where $\alpha\equiv\frac{1}{2}l$. Here λ_0 represents the lowest possible value of λ (consider as a function of τ_0) for a given quantum number n. The partial derivatives can also be obtained from the consistency relation (3d) by direct differentiation with respect to τ_0;

$$\frac{\partial\lambda}{\partial\tau_0}=\frac{(\lambda-\xi_a)^{1/2}-(\lambda-\xi_b)^{1/2}}{\sin^{-1}(\xi_b/\sqrt{\lambda})-\sin^{-1}(\xi_a/\sqrt{\lambda})}.$$

As expected,

$$\partial\lambda/\partial\tau_0|_0=0$$

since λ is known to be an even function of τ_0. Continuing, we find

$$\lambda=\lambda_0+\alpha\tau_0/[(\lambda_0-\alpha^2)\sin^{-1}(\alpha/\sqrt{\lambda_0})].$$

[10] See Ref. 6 and note that their a is equal to our $\frac{1}{2}l$, and that one must use Stirling's approximation to obtain their results.

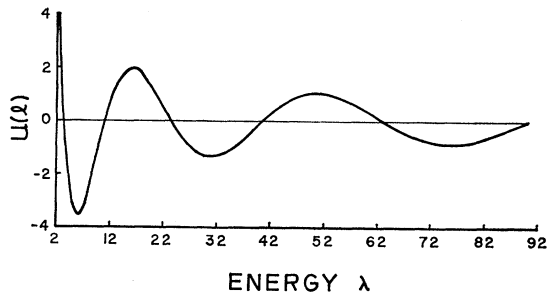

FIG. 5. Plot of $u(l)$ as a function of λ for $c_1=1$.

In the case when λ_0 becomes much larger than α^2 we can make an expansion of (4). To first order this gives

$$\lambda_0=(n+1)^2\pi^2/l^2.$$

Converting back, from dimensionless variables, this last equation takes the form

$$E=(\hbar^2/2m)(n+1)^2\pi^2/L^2, \quad n=1, 0, 2,\cdots$$

of the energy eigenvalues of a particle in a one-dimensional box. This means that if we let $L\rightarrow 0$, then the energy levels go like free-particle box states for the center of the oscillator at zero. This is to be expected since the particle must "bounce" off the walls before it can feel the effects of the oscillator potential. For this same approximation the coefficient of τ_0^2 approaches 1. Thus when the separation of the turning points is large compared to the size of the box, the energy eigenvalues approach

$$\lambda=(n+1)^2\pi^2/l^2+\tau_0^2. \tag{5}$$

From the second-order terms of (4) we find that

$$\lambda_0=\left[\frac{(n+1)\pi}{2l}+\left(\frac{(n+1)^2\pi^2}{4l^2}+\frac{l^2}{24}\right)^{1/2}\right]^2,$$

which can be used to find the second-order correction to λ. It should be added that there are many other approximations that one could make following these same procedures for different ranges of the parameters of the bound-oscillator problem.[11]

For a well of finite depth these same procedures can be used to find the eigenstates.[11] We note that there will be little difference for states with large n. This results from the fact that the depth of well V_0 always appears in terms of the consistency relations which are less than $\frac{1}{2}$.

V. EXACT SOLUTION

It is well known that the harmonic-oscillator differential equation (2) has an exact set of solution which can be expressed in terms of confluent hypergeometric functions.[3–6] For the special case when the center of the oscillator is at the center of the box ($\xi_b=-\xi_a$), Baijal and Singh used numerical methods on these confluent functions to extract the eigenvalues.[12] For the case of a nonsymmetrically placed oscillator their work must be extended in the following way. Instead of using confluent functions as solutions of (2), we look directly for the series solutions of the shifted oscillator differential equation (1). Letting

$$\psi(\tau)=u(\tau)e^{-\frac{1}{2}(\tau+\tau_0)^2},$$

we find that (1) reduces to

$$u''(\tau)-2(\tau+\tau_0)u'(\tau)+(\lambda-1)u(\tau)=0.$$

Assuming the series solution

$$u(\tau)=\sum_{n=0}^{\infty}c_n\tau^n,$$

we obtain the recurrence relation

$$c_n=\frac{2\tau_0}{n}c_{n-1}+\frac{2n-3-\lambda}{n(n-1)}c_{n-2}$$

for $n\geq 2$ and where c_0 and c_1 are arbitrary.

We place our box in the interval $[0,L]$ since $u(0)=0$ implies that $c_0=0$. This eliminates one of the arbitrary constants so that

$$u(\tau)=c_1\{\tau+(2\tau_0)\tau^2/2!+[(2\tau_0)^2+(3-\lambda)]\tau^3/3! +[(2\tau_0)^3+(2\tau_0)(3+5-2\lambda)]\tau^4/4!+\cdots\}.$$

Since c_1 is fixed by normalization, the other boundary condition $u(l)=0$ gives us an equation which fixes the eigenvalues of the shifted oscillator. Figure 5 is a plot of $u(l)$ (for $c_1=1$) as a function of λ for $\tau_0=0$ and $l=2$. We can numerically extract the zeros (i.e., the eigenvalues) of $u(l)$ by the same type of method described in Sec. III (See Tables I and II).

We note that $u(\tau)$ is a slowly convergent function of τ, so that the numerical method above only works satisfactorily for small l (i.e., $l\lesssim 1$). For example, approximately 50 terms are needed for each point plotted of $u(l)$ in Fig. 5. The numerical method also only works satisfactorily for the first few quantum states since the larger λ becomes, the larger the difference between the maximum value of the partial sums and the convergent value of $u(l)$. For example, the partial sums of $u(l)$ in Fig. 5 reach values of the order of 10^9 before they converge back down to values of the order of 1. This means that a large numer of significant figures (in this case 16) must be carried along if the convergent values are to be found correctly.

[11] For more complete details, see R. Vawter, Ph.D. thesis, State University of New York, Stony Brook, 1968 (unpublished).

[12] See Ref. 4 and note that their ξ_0 and n_q are equal to our $2\sqrt{\alpha}$ and $\frac{1}{2}(\lambda-1)$, respectively. Moreover, their states labeled by $q=1,2,3,\cdots$, corresponds to our states $n=1, 3, 5,\cdots$, so that they appear not to have included the even states. Also their eigenstates do not approach $\hbar\omega(n+\frac{1}{2})$ as l becomes large compared to $\sqrt{\lambda}$.

TABLE I. Comparison of exact and WKB eigenvalues of a harmonic oscillator in a box for $l=2$ and $n=0, 1, 2, 3$. Here τ_0 is the distance of the center of the oscillator from the center of the box.

Exact energy	WKB energy	% error	τ_0	Exact energy	WKB energy	% error	τ_0
	$n=0$				$n=2$		
2.596	2.810	8.210	0.00	22.52	22.54	0.103	0.00
2.610	2.827	8.296	0.12	22.53	22.55	0.103	0.12
2.651	2.877	8.547	0.24	22.57	22.60	0.104	0.24
2.718	2.961	8.954	0.36	22.65	22.67	0.104	0.36
2.812	3.079	9.503	0.48	22.75	22.77	0.105	0.48
2.933	3.231	10.176	0.60	22.88	22.91	0.106	0.59
3.080	3.418	10.963	0.72	23.04	23.06	0.107	0.72
3.255	3.212	1.309	0.84	23.23	23.26	0.109	0.84
3.456	3.454	0.068	0.96	23.48	23.48	0.111	0.95
3.685	3.709	0.648	1.08	23.70	23.72	0.113	1.08
3.940	3.979	0.994	1.20	23.97	24.00	0.115	1.20
4.223	4.268	1.088	1.32	24.28	24.31	0.117	1.32
4.532	4.578	1.028	1.44	24.62	24.65	0.120	1.44
4.868	4.911	0.884	1.56	24.98	25.01	0.123	1.56
5.231	5.268	0.706	1.68	25.37	25.41	0.125	1.68
5.621	5.651	0.524	1.80	25.80	25.83	0.128	1.80
6.038	6.059	0.355	1.92	26.25	26.28	0.131	1.92
6.482	6.496	0.206	2.04	26.73	26.77	0.135	2.04
6.954	6.960	0.079	2.16	27.24	27.28	0.138	2.16
7.452	7.451	0.025	2.28	27.78	27.82	0.142	2.28
7.977	7.969	0.110	2.40	28.35	28.39	0.145	2.40
8.530	8.515	0.177	2.52	28.94	28.99	0.148	2.52
9.110	9.089	0.229	2.64	29.57	29.62	0.152	2.64
9.717	9.691	0.268	2.76	30.23	30.27	0.156	2.76
10.35	10.32	0.299	2.88	30.91	30.96	0.160	2.88
11.01	10.98	0.321	3.00	31.63	31.68	0.164	3.00
	$n=1$				$n=3$		
10.15	10.20	0.532	0.00	39.80	39.81	0.032	0.00
10.16	10.22	0.534	0.12	39.81	39.83	0.032	0.12
10.21	10.26	0.539	0.24	39.86	39.87	0.032	0.24
10.28	10.34	0.547	0.36	39.93	39.94	0.033	0.36
10.38	10.44	0.558	0.48	40.03	40.04	0.033	0.48
10.52	10.58	0.572	0.59	40.16	40.17	0.032	0.60
10.68	10.74	0.589	0.72	40.32	40.33	0.033	0.72
10.87	10.93	0.608	0.84	40.51	40.52	0.033	0.84
11.09	11.16	0.630	0.95	40.73	40.74	0.034	0.96
11.34	11.41	0.655	1.08	40.97	40.99	0.034	1.08
11.62	11.70	0.681	1.20	41.25	41.26	0.034	1.20
11.92	12.01	0.709	1.32	41.55	41.57	0.035	1.32
12.26	12.35	0.740	1.44	41.89	41.90	0.035	1.44
12.63	12.72	0.772	1.56	42.25	42.26	0.036	1.56
13.02	13.13	0.806	1.68	42.65	42.66	0.036	1.68
13.45	13.56	0.841	1.80	43.06	43.08	0.037	1.80
13.90	14.02	0.877	1.92	43.51	43.53	0.037	1.92
14.38	14.51	0.914	2.04	43.99	44.01	0.038	2.04
14.90	15.04	0.953	2.16	44.50	44.52	0.038	2.16
15.44	15.59	0.992	2.28	45.04	45.05	0.039	2.28
16.01	16.17	1.032	2.40	45.60	45.62	0.040	2.40
16.61	16.78	1.073	2.52	46.20	46.22	0.040	2.52
17.23	17.43	1.115	2.64	46.82	46.84	0.041	2.64
17.89	18.10	1.158	2.76	47.47	47.49	0.042	2.76
18.58	18.80	1.201	2.88	48.16	48.18	0.042	2.88
19.29	19.53	1.245	3.00	48.86	48.88	0.043	3.00

VI. ERROR OF THE WKB EIGENVALUES

With the numerically determined exact eigenvalues found in Sec. V we can directly compare the WKB eigenvalues with exact eigenvalues.[13] Since the eigenvalues depend on position of the center of the oscillator τ_0, length of the box l, and the quantum number n, we make our comparison for those values of these parameters which give the worst agreement. Before proceeding to determine the regions of worst agreement we note that in this section we will place our original box symmetrically about the origin (letting $b=-a$) as in Sec. III. In this way τ_0 measures the distance the center of the oscillator is displaced from the center of the box.

In general, the WKB method will be at its worst for those energies whose associated turning points are near the walls (the points where $\lambda=\xi_a^2$ or $\lambda=\xi_b^2$). This is expected since the WKB wave functions become singular at these energies and the consistency relations (3) are discontinuous functions at these energies. Moreover, the WKB eigenvalues asymptotically approach the

[13] For an estimate of the relative error of the wave functions see Ref. 11.

TABLE II. Comparison of exact and WKB eigenvalues of a harmonic oscillator in a box for $l=4$ and $n=0$, 1, and 2. Here τ_0 is the distance of the center of the oscillator from the center of the box.

Exact energy	WKB energy	% error	τ_0
	$n=0$		
1.075	1.083	0.716	0.00
1.080	1.089	0.822	0.12
1.095	1.107	1.116	0.24
1.120	1.138	1.523	0.36
1.157	1.178	1.816	0.48
1.206	1.224	1.520	0.60
1.268	1.267	0.056	0.72
1.334	1.514	12.657	0.84
1.436	1.564	8.977	0.96
1.543	1.641	6.398	1.08
1.668	1.743	4.529	1.20
1.811	1.868	3.159	1.32
1.973	2.015	2.150	1.44
2.154	2.184	1.405	1.56
2.356	2.376	0.855	1.68
2.579	2.591	0.450	1.80
2.824	2.829	0.153	1.92
3.091	3.089	0.065	2.04
3.381	3.374	0.223	2.16
3.694	3.682	0.337	2.28
4.030	4.013	0.418	2.40
4.390	4.369	0.473	2.52
4.774	4.750	0.511	2.64
5.183	5.155	0.535	2.76
5.616	5.585	0.548	2.88
6.074	6.041	0.554	3.00
	$n=1$		
3.529	3.357	0.221	0.00
3.543	3.758	6.063	0.12
3.583	3.760	4.942	0.24
3.649	3.791	3.875	0.36
3.742	3.853	2.953	0.48
3.860	3.946	2.216	0.60
4.003	4.069	1.649	0.72
4.171	4.222	1.225	0.84
4.363	4.403	0.908	0.96
4.578	4.609	0.671	1.08
4.818	4.841	0.493	1.20
5.080	5.982	0.358	1.32
5.365	5.379	0.254	1.44
5.674	5.684	0.174	1.56
6.006	6.012	0.111	1.68
6.360	6.364	0.062	1.80
6.738	6.740	0.024	1.92
7.140	7.139	0.007	2.04
7.564	7.562	0.031	2.16
8.013	8.009	0.050	2.28
8.485	8.479	0.065	2.40
8.891	8.974	0.077	2.52
9.501	9.493	0.086	2.64
10.04	10.04	0.094	2.76
10.61	10.60	0.099	2.88
11.21	11.20	0.104	3.00
	$n=2$		
6.799	6.955	2.283	0.00
6.816	6.974	2.324	0.12
6.865	7.033	2.450	0.24
6.946	7.131	2.665	0.36
7.059	7.269	2.978	0.48
7.204	7.449	3.404	0.60
7.380	7.674	3.980	0.72
7.587	7.600	0.167	0.84
7.825	7.870	0.572	0.96
8.092	8.148	0.691	1.08
8.389	8.446	0.673	1.20
8.715	8.766	0.587	1.32
9.068	9.112	0.479	1.44
9.450	9.485	0.373	1.56
9.858	9.886	0.280	1.68
10.29	10.31	0.204	1.80
10.76	10.77	0.144	1.92
11.24	11.25	0.097	2.04
11.75	11.76	0.062	2.16
12.98	12.30	0.034	2.28
12.86	12.86	0.014	2.40
13.45	13.45	0.000	2.52
14.07	14.07	0.012	2.64
14.71	14.71	0.021	2.76
15.38	15.38	0.027	2.88
16.07	16.06	0.032	3.00

exact eigenvalues as the turning points recede from the walls either into the box or outside the box. To obtain an estimate of the region affected around the walls, we recall that the unbound oscillator wave functions decay exponentially (like $e^{-\xi^2/2}$) after the turning points. Thus only those unbound oscillator eigenfunctions whose associated turning points are inside the box and closer than a few ξ units to the walls will have values appreciably different from zero at the walls. Therefore we expect the error to be greater when the turning points are within a few ξ units of the walls. It turns out that the error is the greatest right at the walls due to the discontinuity in the consistency relations (3). In all cases the discontinuity in the energy eigenvalues λ is $\frac{1}{2}-(2/\pi)\times\arctan\frac{1}{2}\approx 0.2$. If λ is large, then this discontinuity will be small, so that this discontinuity error will have its greatest effect when λ has its smallest values. The latter occurs when $n=0$ and $\tau_0=0$ (see Figs. 2–4). For $\tau_0=0$ the discontinuity occurs when $\lambda=(\frac{1}{2}l)^2$, and since the minimum possible value of λ is 1 for $n=0$, then the greatest error will occur when $l\approx 2$. Tables I and II show that this error is never more than $\sim 10\%$.

We emphasize that Tables I and II show the comparison between the exact and WKB eigenvalues in the region of the worst possible agreement. First, we have chosen to look only at the first few quantum states. Second, we have shrunk the size of the box down so that the turning points of the lowest quantum states will always be within a few ξ units of the walls. If l is taken to be less than 1, then the error can be shown to always be less than 1%, independent of τ_0 or n. This happens because the turning points of even the lowest states are always larger than the size of the box. In fact, if $l\lesssim 0.1$, then the analytical equation (5) for λ is always good to at least one part in 10^3. If l is greater than 10, then the error in λ can also be shown to be less than 1% for all τ_0 and n except for the case when $n=0$ and turning points are at the walls. Even this error decreases from a maximum value $\sim 10\%$ as l becomes larger.

VII. RELATION TO BOHR-SOMMERFELD QUANTIZATION RULE

It is well known that the Bohr-Sommerfeld quantization rule $\oint pdq=\hbar(n+\frac{1}{2})$ and the WKB method give

the same result for the eigenstates of unrestricted systems. For a bounded system this quasiquantization rule must be modified by replacing $\frac{1}{2}$ by a factor γ which depends on the boundary conditions. For our infinite-well case the WKB solutions (i.e., the consistency relations) can be written in the form of the modified quasiquantization rule as

$$\int(\lambda-\xi)^{1/2}d\xi=\pi(n+\gamma),$$

where the upper and lower limits of the integral are understood to be taken between the actual classical turning points $\min\{\xi_b,\sqrt{\lambda}\}$ and $\max\{\xi_a,-\sqrt{\lambda}\}$, respectively. Here

$$\begin{aligned}\gamma&=\tfrac{1}{2}+\pi^{-1}\tan^{-1}\tfrac{1}{2}e^{-2K(-\xi_a)}+\pi^{-1}\tan^{-1}\tfrac{1}{2}e^{-2K(\xi_b)}\\&=\tfrac{3}{4}+\pi^{-1}\tan^{-1}\tfrac{1}{2}e^{-2K(\xi_b)}\\&=\tfrac{3}{4}+\pi^{-1}\tan^{-1}\tfrac{1}{2}e^{-2K(-\xi_a)}\\&=1\end{aligned}$$

in the four regions [(a)–(d)] described in Sec. II. Therefore γ depends not only on the size of the enclosure but also on the position of the center of the oscillator τ_0. For a well of finite depth we can likewise write the WKB solutions in the form of a modified Bohr-Sommerfeld quantization rule where γ depends also on the depth of the well.[11]

VIII. SUMMARY

Using the WKB method, we find the introduction of finite boundaries will radically change the structure of the eigenstates of a quantum-mechanical linear oscillator. If the classical path is such that the oscillator will run into the wall, then its eigenstates will be changed from a usual free-oscillator state regardless of whether the boundaries are considered to be those of a well of finite or infinite depth. We have, in general, two limiting cases. If both turning points are inside the enclosure, then the associated eigenstates behave like a free-oscillator state except for the addition of a small term which goes as the exponential negative of the square of size of the enclosure. If the enclosure is small compared to the size of the turning points, so that the oscillator must classically bounce off the walls long before it would reach its normal turning points, then the associated eigenstates behave like free-particle box eigenstages. The intermediate ranges of the eigenstates can be found by numerical methods with the aid of a high-speed computer (Figs. 2–4). We note these facts:

(1) The eigenstates depend on the size of the enclosure, the position of the center of the oscillator, and the height of the walls.

(2) For a symmetrically placed box, the eigenvalues are an even function of the position of the center of the oscillator. If both turning points are inside the well, then the states are independent of τ_0 to a good approximation. When one or more turning points are outside the box, then the eigenstate shows a parabolic dependence on τ_0.

(3) The minimum bound on an eigenstate is always $2n+1$ regardless of position of the center or the depth of the well.

(4) The upper bound for an infinite well is $(n+1)^2\pi^2/l^2+\tau_0^2$.

(5) The consistency relations used to find the eigenstates can be written in the form of a modified Bohr-Sommerfeld quantization rule for a well of finite or infinite depth, where γ is a complicated function of the size of the box, the position center of the oscillator, and the depth of the wall.

(6) A comparison of WKB results with the exact results show that the WKB method gives the eigenvalues for a bound oscillator which are never worse than $\sim 10\%$, and in general are much better than 1%.

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