AMERICAN JOURNAL of PHYSICS

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Citation: American Journal of Physics **36**, 54 (1968); doi: 10.1119/1.1974411
View online: http://dx.doi.org/10.1119/1.1974411
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/36/1?ver=pdfcov
Published by the American Association of Physics Teachers

Agreement Between Classical and Quantum Mechanical Solutions for a Linear Potential Inside a One-Dimensional Infinite Potential Well

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(Received 27 June 1967; revision received 11 August 1967)

For the special case in which the total energy is set equal to the classic maximum potential energy, the Schrödinger equation is solved in closed form and is normalized. It is shown that the expectation value of position is equal to the classical time average of position and that the expectation value of the square of the momentum is equal to the classical time average of the square of the momentum.

I. STATE FUNCTION

FOR a well of width X_o with the left wall at the origin, the potential is specified by

$$V=\infty, \quad X\leqq 0$$
$$V=CX, \quad 0<X<X_o$$
$$V=\infty, \quad X_o\leqq X$$

where C is a constant.

Outside the well, ψ is identically zero. Inside the well,

$$-(\hbar^2/2m)(d^2\psi/dx^2)+CX\psi=E\psi. \quad (1)$$

With

$$2mc\hbar^{-2}=b, \quad (2)$$

and

$$E=CX_o, \quad (3)$$

Eq. (1) becomes

$$d^2\psi/dx^2+b(X_o-X)\psi=0. \quad (4)$$

With

$$\mu=X_o-X, \quad (5)$$

Eq. (4) becomes

$$d^2\psi/d\mu^2+b\mu\psi=0. \quad (6)$$

A general form of the Bessel equation,[1]

$$\mu^2(d^2\psi/d\mu^2)+(1-2\alpha)\mu(d\psi/d\mu)+a^2\beta^2\mu^{2\beta}+\alpha^2-v^2\beta^2)\psi=0, \quad (7)$$

has the solution

$$\psi=\mu^{\alpha}J_v(a\mu^{\beta}), \quad (8)$$

where α, a, β, and v are constants. Comparison of (6) and (7) shows that the solution of (6) is

$$\psi=A_N\mu^{1/2}J_{1/3}[(2/3)b\mu^{3/2}]+B_N\mu^{1/2}J_{-1/3}[(2/3)b^{1/2}\mu^{3/2}], \quad (9)$$

where A_N and B_N are constants.

II. BOUNDARY CONDITIONS

The Bessel series,[1] with the exact form of the coefficients left out for simplicity, is

$$J_v(t)=t^v[1-t^2/(\ \ )+t^4/(\ \ )-\cdots]. \quad (10)$$

Then Eq. (9) may be written as

$$\psi=\{[(2/3)b^{1/2}]^{1/3}A_N\mu+[(2/3)b^{1/2}]^{1/3}B_N\}\left\{1-\frac{[(2/3)b^{1/2}\mu^{3/2}]^2}{(\qquad)}+\cdots\right\}. \quad (11)$$

It is seen from Eq. (11) that B_N must be zero in order that ψ vanish at the right-hand wall. Then

$$\psi_N(X)=A_N[X_o-X]^{1/2}J_{1/3}[(2/3)b^{1/2}(X_o-X)^{3/2}]. \quad (12)$$

It is seen from Eq. (12) that ψ will vanish at the left-hand wall only if

$$(2/3)b^{1/2}X_o^{3/2}=r_N, \quad (13)$$

where r_N is the nth root of the one-third-order Bessel function.

III. NORMALIZATION

With

$$R=2b^{1/2}(X_o-X)^{3/2}/3, \quad (14)$$

[1] A. Bronwell, *Advanced Mathematics in Physics and Engineering* (McGraw–Hill Book Co., New York, 1953).

the normalization condition,

$$1 = A_N{}^2 \int_o^{X_o} (X_o - X)$$

$$\left\{J_{1/3}\left[\frac{2}{3} b^{1/2} (X_o - X)^{3/2}\right]\right\}^2 \ dx,$$

may be written

$$b^{1/2} A_N{}^{-2}\left(\frac{2b^{1/2}}{3}\right)^{1/3} = \int_o^{r_N} R^{1/3} [J_{1/3}(R)]^2 \, dR. \tag{15}$$

From[2]

$$\int s^{-2\mu-1}[J_{\mu+1}(s)]^2 \, ds = \frac{-s^{-2\mu}}{(4\mu+2)} \{[J_\mu(s)]^2 + [J_{\mu+1}(s)]^2\}, \tag{16}$$

and using Eq. (13), the normalization constant is

$$A_N = [J_{-2/3}(r_N)X_o]^{-1}. \tag{17}$$

IV. EXPECTATION VALUE OF POSITION

When the substitution Eq. (14) is made in the integral for $<X>$, the sum of two integrals results, one proportional to the integral in the normalization condition, the other proportional to a form of the second Lommel integral,[1]

$$\int_o^a s[J_N(s)]^2 \, ds = \frac{a^2}{2}\left\{ [J_N'(a)]^2 + \left(1 - \frac{n^2}{a}\right) [J_N(a)]^2 \right\}. \tag{18}$$

Using Eqs. (18), (17), and (13),

$$<X> = X_o\,(1 - [J_{1/3}'(r_N)]^2/\{3[J_{-2/3}(r_N)]^2\}). \tag{19}$$

[2] G. H. Watson, *A Treatise on the Theory of Bessel Functions* (The Macmillan Co., New York, 1962).

The Bessel recurrence relation

$$XJ_v'(X) = XJ_{v-1}(X) - vJ_v(X), \tag{20}$$

with $X = r_N$ and $v = 1/3$, becomes

$$J_{1/3}'(r_N) = J_{-2/3}(r_N), \tag{21}$$

so that

$$<X> = (2/3)X_o. \tag{22}$$

V. EXPECTATION VALUE OF THE SQUARE OF THE MOMENTUM

Since ψ is normalized and $<X>$ is known, $<P^2>$ is obtained from Eq. (1) by setting E equal to CX_o, multiplying both sides by ψdx, and integrating over the length of the well. The result may be written as

$$<P^2>/2m = CX_o/3. \tag{23}$$

VI. CLASSICAL TIME AVERAGES

Classically, for a particle initially at rest at X equals X_o in the potential CX,

$$X = X_o - Ct^2/(2m), \tag{24}$$

and the time required to fall a distance X_o is

$$t_1 = [2mX_o/C]^{1/2}. \tag{25}$$

Then the time average of position is

$$\overline{X} = [t_1]^{-1} \int_o^{t_1} X dt = \frac{2}{3} X_o. \tag{26}$$

In like manner, it is readily shown that

$$m\bar{v}^2/2 = CX_o/3. \tag{27}$$

It is seen from Eqs. (22), (23), (26), and (27) that the quantum calculations and the classical calculations yield identical results. In addition, substitution of typical macroscopic magnitudes into Eq. (13) shows that the allowable well widths are very closely spaced.