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When the Classical and Quantum Mechanical Considerations Hint to a Single Point; A Microscopic Particle in a One Dimensional Box with Two Infinite Walls and a Linear Potential Inside It

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ABSTRACT

In this paper we have solved analytically the Schrödinger equation for a microscopic particle in a one-dimensional box with two infinite walls, which the potential function inside it, has a linear form. Based on the solutions of this special quantum mechanical system, we have shown that as the quantum number approaches infinity the expectation values of microscopic particle position and square of the linear momentum are equal to the classical time average of particle position and its square of the linear momentum, respectively.

Keywords: One-dimensional Schrödinger equation; Bessel generalized differential equation; Bessel functions of fractional order; Integrals of Bessel functions; Second Lommel integral.

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 example discussed in a beginning course in quantum mechanics [1]. The slightly more complicated situation is where the potential inside the well has a linear form.

Now, imagine that a single microscopic particle of mass "m" bounces back and forth between the walls of a one dimensional box, as in the following figure. Moreover we shall assume that the walls of the box are infinitely hard, so the microscopic particle does not lose energy each time it strikes a wall, and that its velocity is sufficiently small so that we can ignore relativistic effects.

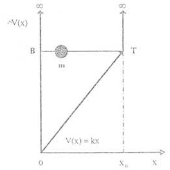

Figure (1): The graphical representation of a single microscopic particle which moving in one dimension, x, and subject to the potential energy function of Eq. (1).

At $x = 0$, and x_0, and at all points beyond these limits the particle encounters an infinitely repulsive barrier, in the other words, because of the microscopic particle cannot have an infinite amount of energy, it can never tunnel into a region of infinite potential energy. So the following mathematical potential form describes the above figure and its physical behavior.

$$V(x) = \begin{cases} \infty & \text{if} \quad x < 0 \\ kx & \text{if} \quad 0 \le x \le x_0 \\ \infty & \text{if} \quad x_0 > x \end{cases} \quad (1)$$

In this system as we discussed in the next section, and for $\langle x \rangle$ and $\langle p^2 \rangle$, the classical mechanics and quantum physics, as the quantum number approaches infinity, yield the identical results. It is an instructive example of corresponding principle from the pedagogical point of view.

DISCUSSION

Average values of position and square of linear momentum according to the classical mechanics.

From the classical mechanics, for one dimensional motion, the conservative force is the negative of the derivative of the potential energy function [2].

$$F(x) = -\frac{dV(x)}{dx} \qquad (2)$$

So classically, for the microscopic particle which it moves under the Eq. (1), we can write

$$F(x) = \begin{cases} \infty & \text{if} \quad x < 0 \\ -k & \text{if} \quad 0 \le x \le x_0 \\ \infty & \text{if} \quad x_0 < x \end{cases} \qquad (3)$$

It is seen from the above equation, the microscopic particle moves with constant acceleration in the interval of $[0, x_0]$.

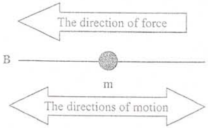

Figure 2. Classically, along the path of TB, the microscopic particle has the maximum mechanical energy. The microscopic particle under the constant force which its direction has been shown has an oscillatory motion. In this motion the microscopic particle has the maximum velocity at the point of B.

Alternatively, from the kinematical point of view, the equation of its motion is equal to

$$x(t) = -\frac{k}{2m}t^2 + v_i t + x_i \qquad (4a)$$

where v_i, and x_i are the initial velocity and position of microscopic particle. Now, according to Figures (1) and (2), if the microscopic particle initially at rest at $x = x_0$, then we can write

$$x(t) = -\frac{k}{2m}t^2 + x_0 \qquad (4b)$$

On the basis of the Eq. (4b), it is obvious that

$$t_{max} = \sqrt{\frac{2mx_0}{k}} \qquad (4c)$$

So

$$\overline{x} = \frac{\int_0^{t_{max}} x(t)dt}{t_{max}} = \frac{2}{3}x_0 \qquad (5)$$

On the other hand, for this classical system we have

$$\overline{v^2} = \frac{\int_0^{t_{max}} (-\frac{k}{m}t)^2 dt}{t_{max}} = \frac{2kx_0}{3m} \qquad (6)$$

And finally, it is obvious that

$$\overline{p^2} = \frac{2mkx_0}{3} \qquad (7)$$

So classically, if the microscopic particle moves along TB path (as be specified in figure), its average of position and average of square of linear momentum can be determined according to the Eqs. (5) and (7), respectively.

Average values of position and square of linear momentum according to the quantum mechanics.

In the quantum physics, the Schrödinger equation for a single microscopic particle between 0 and x_0, which has been surrounded by Eq. (1), has the following mathematical form

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + kx\psi(x) = E\psi(x) \qquad (8)$$

The fact that $V(x)$ is infinite for $x < 0$ and for $x > x_0$, and that the total energy must be finite, says that $\psi(x)$ must be vanish in these two regions.

If we assume that the total energy of microscopic particle is equal to kx_0, and introduce the following notations

$$\zeta = \frac{2mk}{\hbar^2} \qquad (10)$$

$$\delta = x_0 - x \qquad (11)$$

then Eq. (8) becomes

$$\frac{d^2\psi(x_0-\delta)}{d\delta^2} + \zeta\delta\psi(x_0-\delta) = 0 \qquad (12a)$$

It is concluded that the above equation transforms to the following equation by changing the direction of motion from $0 \to x_0$ to $x_0 \to 0$. So we can write

$$\frac{d^2\psi(\delta)}{d\delta^2} + \zeta\delta\psi(\delta) = 0 \qquad (12b)$$

On the other hand, if d, p, q are nonzero and $(1-a)^2 \geq 4c$, then the following equation represents the general form of the Bessel equation [3].

$$\delta^2\frac{d^2\psi(\delta)}{d\delta^2} + \delta\left(a + 2b\delta^p\right)\frac{d\psi(\delta)}{d\delta} + \left[c + d\delta^{2q} + b(a+p-1)\delta^p + b^2\delta^{2q}\right]\psi(\delta) = 0 \qquad (13)$$

The general solution of this equation can be written as

$$\psi(\delta)=\delta^{\alpha}e^{-\beta\delta^{p}}\left[A_1J_v(\lambda\delta^{q})+A_2Y_v(\lambda\delta^{q})\right] \quad (14)$$

where

$$\alpha=\frac{1-a}{2},\ \beta=\frac{b}{p},\ \lambda=\frac{\sqrt{d}}{q},\ \text{and } v=\frac{1}{2q}\sqrt{(1-a)^2-4c}$$

And A_1 and A_2 are constants. Moreover, for the Eq. (14) there are two following important conditions;

1) If $d<0$, then J_v and Y_v replace with I_v and K_v, respectively.

2) If $v\notin\{1,2,3,\ldots\}$, then we transform $Y_v \to J_{-v}$, and $K_v \to I_{-v}$.

Now, we return to the Eq. (12b) and by comparing this equation with the Eq. (13), the following relations can be concluded

$$a+2b\delta^{p}=0$$

$$c+d\delta^{2q}+b(a+p-1)\delta^{p}+b^2\delta^{2q}=\zeta\delta^{3}$$

And finally we have

$$a=b=c=0,\ d=\zeta,\ p\in\Re-\{0\},\ \text{and } q=\frac{3}{2}.$$

Since the conditions of the Eq. (13) are satisfied, the constants within the Eq. (14) become $\alpha=\frac{1}{2},\beta=0,\lambda=\frac{2\sqrt{\zeta}}{3}$, and $v=\frac{1}{3}$.

So the general solution of Eq. (12b) is equal to

$$\psi(\delta)=\delta^{\frac{1}{2}}\left[A_1J_{\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}\right)+A_2J_{-\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}\right)\right] \quad (15)$$

where [4],

$$J_{\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}\right)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(\frac{4}{3}+k)}\times\left(\frac{\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}}{2}\right)^{\frac{1}{3}+2k} \quad (16a)$$

$$J_{-\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}\right)=\sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(\frac{2}{3}+k)}\times\left(\frac{\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}}{2}\right)^{-\frac{1}{3}+2k} \quad (16b)$$

Therefore, the Eq. (15) can be written in the following form

$$\psi(\delta)=A_1\left\{\frac{3\sqrt{\delta}\,3^{\frac{1}{6}}(\sqrt{\zeta}\delta^{\frac{3}{2}})^{\frac{1}{3}}\Gamma(\frac{2}{3})}{2\pi}-\frac{\sqrt{\delta}\,3^{\frac{1}{6}}(\sqrt{\zeta}\delta^{\frac{3}{2}})^{\frac{7}{3}}\Gamma(\frac{2}{3})}{8\pi}+\ldots\right\}+A_2\left\{\frac{3^{\frac{1}{3}}}{(\sqrt{\zeta})^{\frac{1}{3}}\Gamma(\frac{2}{3})}-\frac{\sqrt{\delta}\,3^{\frac{1}{3}}(\sqrt{\zeta}\delta^{\frac{3}{2}})^{\frac{5}{3}}}{6\Gamma(\frac{2}{3})}+\ldots\right\} \quad (17)$$

This solution is subject to the boundary conditions that $\psi(\delta)=0$ for $x=0$ and for $x=x_0$. Since $\frac{3^{\frac{1}{3}}}{(\sqrt{\zeta})^{\frac{1}{3}}\Gamma(\frac{2}{3})}\neq 0$, the second term of Eq. (17) is an improper term from the physical point of view.

Because the wave function dose not vanish at $x=0$ or $x=x_0$. Hence we conclude that $A_2=0$.

So we can write

$$\psi(\delta)=A_1\delta^{\frac{1}{2}}J_{\frac{1}{3}}(\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}}) \quad (18)$$

On the other hand for $x=0$, we should have

$$\psi(x_0)=A_1x_0^{\frac{1}{2}}J_{\frac{1}{3}}(\frac{2\sqrt{\zeta}}{3}x_0^{\frac{3}{2}})=0 \quad (19)$$

In the other words, $J_{\frac{1}{3}}(\frac{2\sqrt{\zeta}}{3}x_0^{\frac{3}{2}})=0$, or $\frac{2\sqrt{\zeta}}{3}x_0^{\frac{3}{2}}$ is the nth root of the $J_{\frac{1}{3}}(x)$ [5].

Now by introducing

$$\omega=\frac{2\sqrt{\zeta}}{3}\delta^{\frac{3}{2}} \quad (20)$$

and using the normalization condition, we can write

$$\int_0^{\frac{2\sqrt{\zeta}}{3}x_0^{\frac{3}{2}}}\omega^{\frac{1}{3}}(J_{\frac{1}{3}}(\omega))^2d\omega=A_1^{-2}\zeta^{\frac{1}{2}}\left(\frac{2\zeta^{\frac{1}{2}}}{3}\right)^{\frac{1}{3}}$$

In order to determine the constant of normalization A_1, with respect to the above equation and the Eq. (19), we should apply the following important relation [6],

$$\int x^{-2t-1}(J_{t+1}(x))^2 dx = \frac{-x^{-2t}}{(4t+2)}[(J_t(x))^2 + (J_{t+1}(x))^2] \tag{22}$$

$$\text{Here } t = -\frac{2}{3}, \text{ and } \lim_{x\to 0}(x^{\frac{4}{3}}(J_{-\frac{2}{3}}(x))^2) = 2^{\frac{4}{3}}(\Gamma(\frac{1}{3}))^{-2}.$$

Now, after some algebraic calculations we have

$$A_1 = \left(\left(x_0 J_{-\frac{2}{3}}\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right) \right)^2 - \frac{2^{\frac{4}{3}} x_0^{2}}{\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right)^{\frac{4}{3}} (\Gamma(\frac{1}{3}))^2} \right)^{-\frac{1}{2}} \tag{23}$$

On the other hand, the average value of position of the microscopic particle in this system is equal to

$$\langle x_0 - x \rangle = A_1^2 \left(\frac{3}{2b}\right) \int_0^{\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}} \omega (J_{\frac{1}{3}}(\omega))^2 d\omega \tag{24}$$

In order to calculate the value of $\langle x \rangle$ according to above equation we can use the following equation (a form of the second Lommel integral) [6],

$$\int_0^s x(J_v(x))^2 dx = \frac{s^2}{2}\left[\left(1 - \frac{v^2}{s}\right)(J_v(s))^2 + (J'_v(s))^2\right] \tag{25}$$

Here $s = \frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}$, and so

$$\langle x \rangle = x_0 \left(1 - \frac{\left(J'_{\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right)\right)^2}{3\left(\left(J'_{-\frac{2}{3}}\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right)\right)^2 - R\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right) \right)} \right) \tag{26}$$

where

$$R\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right) = \frac{2^{\frac{4}{3}}}{\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right)^{\frac{4}{3}} \left(\Gamma\left(\frac{1}{3}\right)\right)^2} \tag{27}$$

In order to visualize and better understanding of the mathematical relation of $\langle x \rangle$, we can use the following maple program. Figure (3), and the below table have been produced with the aid of this program.

```
> restart:
> m:=9.109390*10^(-31);
> k:=2;
> h:=6.626076*10^(-34);
> zeta:=(2*m*k)/(h/(2*Pi))^2;
>
X:=(2*((zeta)^(1/2))/3)*x0^(3/2
);
>
R:=evalf((2^(4/3))/((X^(4/3))*(
GAMMA(1/3))^2));
> F:=diff(BesselJ(1/3,x),x);
> x:=X:L:=evalf(F);
>
Averagevalueofposition:=evalf(x
0*(1-(L^2)/(3*((L^2)-R))));
>
plot(Averagevalueofposition,x0=
0.1*10^(-10)..0.2*10^(-
10),y=0..4*10^(-
11),color=black,thickness=1);
>
plot(Averagevalueofposition,x0=
20*10^(-10)..30*10^(-
10),y=10^(-10)..20*10^(-
10),color=black,thickness=1);
>
plot(Averagevalueofposition,x0=
50*10^(-10)..100*10^(-
10),y=0..80*10^(-
10),color=black,thickness=1);
>
plot(Averagevalueofposition,x0=
1000*10^(-10)..10000*10^(-
10),y=0..7000*10^(-
10),color=black,thickness=1);
```

On the other hand, we know that

$$xJ_{v-1}(x) = xJ'_v(x) + vJ_v(x) \tag{28}$$

Now, based on the above Bessel recurrence relation and for $v = \frac{1}{3}$, and $x = \frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}$, we have

$$J'_{\frac{1}{3}}\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right) = J'_{-\frac{2}{3}}\left(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}}\right) \tag{29}$$

And finally, when $n \to \infty$, according to the figure (3), and the above table the clear result of Eqs. (26) and (29) is

$$\langle x \rangle = \frac{2}{3} x_0 \qquad (30)$$

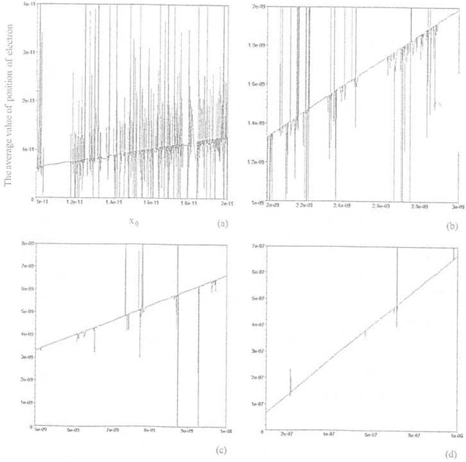

Figure (3): In the each of four above graphs, for $k = 2$, and different ranges of x_0, we plot the average value of position of electron vs. x_0. As we can see, in (a), (b), (c), and (d) the range of x_0 are 0.1-0.2, 20-30, 50-100, and 1000-10000 Angstrom, respectively. The vertical lines show the zeros of $J'_{\frac{1}{3}}(\frac{2\sqrt{\zeta}}{3} x_0^{\frac{3}{2}})$, and if $x_0 \to \infty$, then according to the graph of (d), we have $\langle x \rangle = \frac{2x_0}{3}$.

In order to calculate the average value of the square momentum, we first multiply both sides of Eq. (8) by $\psi(x)dx$, and then integrate over the range of $0 \le x \le x_0$, by assuming that, $E = kx_0$. In the other words

$$-\frac{\hbar^2}{2m}\int_0^{x_0}\psi(x)\frac{d^2\psi(x)}{dx^2}dx + k\int_0^{x_0}x\psi^2(x)dx = kx_0\int_0^{x_0}\psi^2(x)dx \qquad (31)$$

Table1. The value of $\langle x \rangle$ is a function of variations of x_0, and k. As we can see, if $x_0 \to \infty$ then we have $\langle x \rangle = \frac{2}{3}x_0$.

		x_0(Å)						
		0.1	1	10	100	1000	10000	
$k(Jm^{-1})$	2	0.116116	0.654228	6.59729	66.5839	666.357	6665.56	$\langle x \rangle$ (Å)
	4	0.063691	0.653001	6.63623	66.4995	665.150	6665.45	
	6	0.105459	0.659342	5.46106	66.5739	664.094	6664.55	
	8	0.064519	0.645796	6.58281	66.6025	662.968	6665.22	
	10	0.059243	0.660096	6.61651	64.0385	666.377	6666.03	
	12	0.039009	0.658946	6.58624	62.7590	666.478	6665.96	

Since the normalization constant of $\psi(x)$ and the average value of position as $R(\frac{2\sqrt{\zeta}}{3}x_0^{\frac{3}{2}}) \to 0$, have been known, according to the Eq. (31), we can write

$$\langle p^2 \rangle = \frac{2kmx_0}{3} \qquad (32)$$

CONCLUSIONS

Upon the correspondence principle, all the quantum mechanical behaviors that distinguish quantum systems must disappear in some appropriate limits in which we recover the familiar world of classical mechanics [7]. If $\hbar \to 0$, or $m >> m_e$ (m_e is the mass of electron), or as the quantum number approaches infinity, the complete laws of quantum physics must reduce to the classical laws. This principle is inherently unsatisfactory, since it admits of no definite methodology and depends strongly on intuition [8]. Nevertheless, according to the correspondence principle, Eq. (1), figure (2), figure (3), table of data, and from the Eqs. (5), (7), (30), and (32), it is obvious that quantum mechanical calculations and the classical considerations yield the identical results.

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