Exact Solution of the Energy Shift in each Quantum Mechanical Energy Levels in a One Dimensional Symmetrical Linear Harmonic Oscillator

Hendry Izaac Elim∗)1)

1) Department of Physics, Pattimura University, Ambon, Indonesia

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Abstract

An exact solution of the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator has been investigated. The solution we have used here is firstly derived by manipulating Schrödinger differential equation to be confluent hypergeometric differential equation. The final exact numerical results of the energy shifts are then found by calculating the final analytical solution of the confluent hypergeometric equation with the use of a software (Mathcad Plus 6.0) or a program programmed by using Turbo Pascal 7.0. We find that the results of the energy shift in our exact solution method are almost the same as that in Barton et. al. approximation method. Thus, the approximation constants appeared in Barton et. al. method can also be calculated by using the results of the exact method.

1. Introduction

In 1990, Barton et. al. had already published an approximation method to calculate the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator. They found a formula of the energy shifts either for the ground state or for the excited states calculated in a finite interval $L$. The explanation about the use of their approximation formula is for bound states in one dimensional symmetrical linear harmonic oscillator with a potential $V(x)$ which is proportional to $x^2$. However promising their method, the exact energy shifts in each energy levels have not been solved until now yet. In this paper we use another method to solve the problem. Instead of using the Barton et. al. approximation method, we apply a new method by changing Schrödinger differential equation to a confluent hypergeometric differential equation. After finding the confluent hypergeometric differential equation, we solve exactly the equation and then use a certain program or software to calculate the final exact energy shifts.

This paper is organized as follows. In section 2, we will perform the exact solution method of the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator and will also compare our results with the results in ref.[1]. Section 3 is devoted for discussions and conclusions.

2. Exact solution method of the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator

A particle with mass $m$ moving in a one dimensional space from $-\infty$ to $\infty$ with the influence of a potential $V(x)$ obeys the following Schrödinger differential equation\cite{1}

\[
\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_0(x) = E_0\psi_0(x), \quad -\infty < x < \infty.
\]  

(2.1)

On the other hand, if the motion of the particle is restricted by a finite interval $-\frac{L}{2} < x < \frac{L}{2}$ in the same potential,

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*email: hendry202@cyberlib.itb.ac.id
the wave function $\psi(x)$ and the energy $E$ can be obtained by solving the following time independent Schrödinger differential equation
\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) = E\psi(x), \quad -\frac{L}{2} < x < \frac{L}{2}.
\]

(2.2)

Even though the energy shift $\Delta E \equiv E - E_0$ is small for the large $L$, this case is not included in a classical perturbation theory.

Based on this simple physical phenomena, Barton et. al. derived generally an approximation method for calculating the energy changes or the energy shifts in each quantum mechanical energy levels including the systems in linear harmonic oscillator and hydrogen atom. They got the following formulas
\[
\Delta E = \frac{\hbar^2}{m} \left[ \int_0^{L/2} \frac{dx_1}{\psi_0^2(x_1)} \right]^{-1}, \text{ for ground state},
\]

(2.3a)

and
\[
\Delta E \simeq \frac{\hbar^2}{m} \left[ \int_a^{L/2} \frac{dx_1}{\psi_0^2(x_1)} \right]^{-1}, \quad (0 < a < \frac{L}{2}, \text{ and } x_1 \sim \frac{L}{2}),
\]

(2.3b)

for excited states. However, for the calculation of the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator with a potential $V(x) = m\omega^2 x^2/2$, they found
\[
\frac{\Delta E^{(0)}}{E_0} = \frac{2}{\pi^{1/2}} \frac{L}{T} \exp \left( -\frac{L^2}{4T^2} \right) \left( 1 + O \left( \frac{T^2}{L^2} \right) \right), \quad \text{for ground state}
\]

(2.4a)

where $\psi_0(x) = (\frac{1}{\sqrt{\pi L}}) \exp \left( -\frac{x^2}{4L} \right)$, $l = (\frac{\hbar}{m\omega})^{1/2}$, and the initial energy is $E_0 = \frac{1}{2} \hbar\omega$. And for the excited states, they got
\[
\frac{\Delta E^{(n)}}{E_0^{(n)}} = \frac{2}{(2n + 1)^{1/2}!2^{2n}} \frac{L}{T}^{2n+1} \exp \left( -\frac{L^2}{4T^2} \right) \left( 1 + O \left( \frac{T^2}{L^2} \right) \right),
\]

(2.4b)

where $\psi_0^{(n)}(x) = (\pi^{1/2}2^n!)^{-1/2} H_n \left( \frac{x}{\sqrt{L}} \right) \exp \left( -\frac{x^2}{4L} \right)$ and $E_0^{(n)} = \left( \frac{1}{2} + n \right) \hbar\omega$, $n = 1, 2, 3, \ldots$. For the large $x$, $H_n \left( \frac{x}{\sqrt{L}} \right) \sim 2^n \left( \frac{x}{\sqrt{L}} \right)^n$.

Now, we are going to change the Schrödinger differential equation to become a confluent hypergeometric differential equation. We provide eigen function $H\psi = E\psi$ for a one dimensional symmetrical linear harmonic oscillator with a potential $V(x) = m\omega^2 x^2/2$ into two areas $:l^2$

\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 1/2 \frac{m\omega_+^2 x^2}{2} \right) \psi_+ (x) = E\psi_+ (x), \quad \text{for } x > 0,
\]

(2.5a)

and
\[
\left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + 1/2 \frac{m\omega_-^2 x^2}{2} \right) \psi_- (x) = E\psi_- (x), \quad \text{for } x < 0.
\]

(2.5b)

By substituting parameters $\frac{2mE}{\hbar^2} = \lambda$, and $\frac{m\omega}{\hbar} = \alpha$ or $\alpha = \frac{1}{\beta}$, we find
\[
\frac{d^2\psi_\pm}{dx^2} - \left[ \lambda - \alpha^2 x^2 \right] \psi_\pm = 0, \text{ for } \pm x > 0.
\]

(2.6)
We then introduce parameter $\lambda = \alpha (2n' + 1)$ and a free variable $z = x\sqrt{\alpha}$ to eq.(2.6), we get

$$\frac{d^2\psi_{n'}(z)}{dz^2} - [2n' + 1 - z^2] \psi_{n'}(z) = 0, \text{ for } \pm z > 0,$$

(2.7)

and

$$E_{n'} = \hbar \omega \left( \frac{1}{2} + n' \right).$$

(2.8)

It means that

$$\frac{\omega_-}{\omega_+} = \frac{\omega}{\omega} = \frac{2n' + 1}{2n' + 1} = r = 1,$$

(2.9)

which states that our solution is for a one dimensional symmetrical linear harmonic oscillator.

If $\psi_{n'}(z)$ is the solution of eq.(2.7), then $\psi_{n'}(-z)$ is also the solution. On the other hand, if the Wronskian $W(\psi_{n'}(x\sqrt{\alpha}), \psi_{n'}(-x\sqrt{\alpha}))$ is not the same as zero, then both solutions can be used as a basic solution for implementing boundary conditions whether in $x \to \pm \frac{L}{2}$ or in $x = 0$. To solve eq.(2.7), we firstly substitute the following function

$$\psi_{n'}(z) = \exp \left( -\frac{1}{2} z^2 \right) H_{n'}(z),$$

(2.10)

we then get

$$\left[ \frac{d^2}{dz^2} - 2z \left( \frac{d}{dz} \right) - 2n' \right] H_{n'}(z) = 0,$$

(2.11)

where $H_{n'}(z)$ is a Hermite function. By introducing a new variable $t = z^2$, we find a confluent hypergeometric (CH) differential equation

$$\left[ \frac{t}{dz^2} - \left( \frac{1}{2} - t \right) \left( \frac{d}{dt} \right) - \frac{1}{2} n' \right] H_{n'}(t) = 0,$$

(2.12)

which has a general solution in a linear combination of the following two CH functions

$$A_1 F_1 \left( -\frac{n'}{2}; t = z^2 \right) + B_1 F_1 \left( \frac{1-n'}{2}; \frac{3}{2}; t = z^2 \right).$$

(2.13)

In eq.(2.10), the Hermite function $H_{n'}(z)$ is just a special function of the following equation

$$H_{n'}(z) = \frac{2^n \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( \frac{1}{2} (1-n') \right)} \; \; _1 F_1 \left( -\frac{n'}{2}; \frac{1}{2}; z^2 \right) + \frac{2^n \Gamma \left( -\frac{1}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)} \; \; _1 F_1 \left( \frac{1-n'}{2}; \frac{3}{2}; z^2 \right).$$

(2.14)

Here, we have chosen constants $A$ and $B$ as follows

$$A = \frac{2^n \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( \frac{1}{2} (1-n') \right)};$$

(2.15a)

and

$$B = \frac{2^n \Gamma \left( -\frac{1}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)}.$$

(2.15b)

The boundary conditions in $z$ are
By substituting the boundary condition in eq.(2.19) into eq.(2.18), we find
solution as

\[ H_{n'}(0) = \frac{2^{n'} \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( \frac{1}{2} (1 - n') \right)} \tag{2.16a} \]

and

\[ \frac{dH_{n'}(0)}{dz} = \frac{2^{n'} \Gamma \left( \frac{1}{2} \right) (-\frac{1}{2})}{\Gamma \left( -\frac{1}{2} \right)} = -\frac{2^{n'+1} \sqrt{\pi}}{\Gamma (-\frac{1}{2})} \tag{2.16b} \]

We can also show that

\[ W (\psi_{n'}(x\sqrt{\alpha}), \psi_{n'}(-x\sqrt{\alpha})) = 2^{n'} \sqrt{\pi} \exp (z^2) \tag{2.17} \]

Hence, if \( n' \) is not exactly the same as \( n = 1, 2, 3, \ldots \), then both of the solutions \( H_{n'}(\pm z) \) have a linear independent property. If this is work, then both of the solutions can be chosen as a basic solution of eq.(2.7), we get the general solution as

\[ \psi_{n'}(z) = [AH_{n'}(z) + BH_{n'}(-z)] \exp \left(-\frac{1}{2}z^2\right) \tag{2.18} \]

Here, the boundary condition for the eigen function in \( \pm z = \pm \frac{L}{2}\sqrt{\alpha} \) is

\[ \psi_{n'}(\pm z) = \psi_{n'} \left( \pm \frac{L}{2}\sqrt{\alpha} \right) = 0 \tag{2.19} \]

By substituting the boundary condition in eq.(2.19) into eq.(2.18), we find

\[ \psi_{n'} \left( \pm \frac{L}{2}\sqrt{\alpha} \right) = \left[ AH_{n'} \left( +\frac{L}{2}\sqrt{\alpha} \right) + BH_{n'} \left( -\frac{L}{2}\sqrt{\alpha} \right) \right] \exp \left(-\frac{L^2}{8}\alpha \right) = 0 \tag{2.20} \]

Eq.(2.20) can be divided into two equations with two conditions as follows

(1). For the condition with even parity:

\[ \psi_{n'} \left( \frac{L}{2}\sqrt{\alpha} \right) = \left[ AH_{n'} \left( +\frac{L}{2}\sqrt{\alpha} \right) + BH_{n'} \left( -\frac{L}{2}\sqrt{\alpha} \right) \right] \exp \left(-\frac{L^2}{8}\alpha \right) = 0, \]

or

\[ 2 \left[ \frac{2^{n'} \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( \frac{1}{2} (1 - n') \right)} \right] {}_1F_1 \left( -\frac{n'}{2}; \frac{1}{2}; \frac{L^2}{4}\alpha \right) = 0 \tag{2.21a} \]

(2). For the condition with odd parity:

\[ \psi_{n'} \left( \frac{L}{2}\sqrt{\alpha} \right) = \left[ AH_{n'} \left( +\frac{L}{2}\sqrt{\alpha} \right) - BH_{n'} \left( -\frac{L}{2}\sqrt{\alpha} \right) \right] \exp \left(-\frac{L^2}{8}\alpha \right) = 0, \]

or

\[ 2 \left[ \frac{2^{n'} \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)} \right] \left( \frac{L}{2}\sqrt{\alpha} \right) {}_1F_1 \left( 1 - n'; \frac{3}{2}; \frac{L^2}{4}\alpha \right) = 0 \tag{2.21b} \]

In both eq.(2.21a) and (2.21b), hermite functions \( H_{n'}(\pm \frac{L}{2}\sqrt{\alpha}) \) are

\[ H_{n'} \left( \frac{L}{2}\sqrt{\alpha} \right) = \left[ \frac{2^{n'} \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( \frac{1}{2} (1 - n') \right)} \right] {}_1F_1 \left( -\frac{n'}{2}; \frac{1}{2}; \frac{L^2}{4}\alpha \right) + \left[ \frac{2^{n'} \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)} \right] \left( \frac{L}{2}\sqrt{\alpha} \right) {}_1F_1 \left( 1 - n'; \frac{3}{2}; \frac{L^2}{4}\alpha \right) \tag{2.22a} \]
\[
H_{n'} \left( \frac{L}{2} \sqrt{\alpha} \right) = \left[ \frac{2^{n'} \Gamma \left( \frac{3}{2} \right)}{\Gamma \left( \frac{1}{2} (1 - n') \right)} {}_1F_1 \left( -\frac{n'}{2}, \frac{1}{2}, \frac{L^2}{4} \alpha \right) \right. \\
- \left. \frac{2^n \Gamma \left( \frac{1}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)} \left( L \sqrt{\alpha} \right)^n {}_1F_1 \left( \frac{1 - n'}{2}, \frac{3}{2}, \frac{L^2}{4} \alpha \right) \right], \tag{2.22b}
\]

where
\[
{}_1F_1 \left( \frac{n'}{2}, \frac{1}{2}, \frac{L^2}{4} \alpha \right) = \frac{\Gamma \left( \frac{3}{2} \right)}{\Gamma \left( -\frac{n'}{2} \right)} \sum_{s=1}^{\infty} \frac{\Gamma \left( -\frac{n'}{2} + s \right) \left( \frac{L^2}{4} \alpha \right)^s}{\Gamma \left( \frac{1}{2} + s \right) s!} \\
= 1 - \frac{n'L^2\alpha}{4} + \frac{(n'^2 - 2n') L^4\alpha^2}{96} + \ldots, \tag{2.23a}
\]

and
\[
{}_1F_1 \left( \frac{1 - n'}{2}, \frac{3}{2}, \frac{L^2}{4} \alpha \right) = \frac{\Gamma \left( \frac{3}{2} \right)}{\Gamma \left( \frac{1}{2} - n' \right)} \sum_{s=1}^{\infty} \frac{\Gamma \left( \frac{1 - n'}{2} + s \right) \left( \frac{L^2}{4} \alpha \right)^s}{\Gamma \left( \frac{3}{2} + s \right) s!} \\
= 1 + \frac{(1 - n') L^2\alpha}{12} + \frac{(1 - n')(3 - n') L^4\alpha^2}{480} + \ldots. \tag{2.23b}
\]

From eq.(2.21b), we find a solution for the odd parity,
\[
n' = 1 + 2m'. \tag{2.24a}
\]

On the other hand, the even parity is found by calculating eq.(2.21a), we then get
\[
n' = 2m'. \tag{2.24b}
\]

Here (in eq.(2.24a) and (2.24b)), \( n' \) and \( m' \) are positive real values due to the boundary condition \( z = \pm \frac{L}{2} \sqrt{\alpha} \) where \( \psi_{n'} \left( \pm z \right) = 0 \) vanishes in \( z = \pm \frac{L}{2} \sqrt{\alpha} \). \( n' \) in eq.(2.21a) and (2.21b) can exactly be calculated by using Mathcad Plus 6.0 or a program programmed by using Turbo Pascal 7.0. The results of the calculation are provided in table 1 and 2.

The requirement in eq.(2.24b) produces the bound states quantum mechanical energy with even parity,
\[
E_{n'} = \left( n' + \frac{1}{2} \right) \hbar\omega, \quad n' = 2m'. \tag{2.25a}
\]

and the requirement in eq.(2.24a) produces the bound states quantum mechanical energy with odd parity as follows
\[
E_{n'} = \left( n' + \frac{1}{2} \right) \hbar\omega, \quad n' = 1 + 2m'. \tag{2.25b}
\]

On the other hand, for the calculation of the quantum mechanical energy in the boundary \( z = \pm \infty \), and the boundary condition \( \psi_{n} \left( \pm z \right) \) =finite, we can use an asymptotic formula of \( H_{n} \left( \pm z \right) \) according to ref.[3] as follows
\[
H_{n} \left( \pm z \right) \simeq \left( \pm 2z \right)^n, \text{ for } z \rightarrow \pm \infty \text{ or } |z| \rightarrow \infty \text{ if } |\arg(z)| < \frac{3\pi}{4}, \tag{2.26a}
\]

and
\[
H_{n} \left( \pm z \right) \simeq \left( \sqrt{\pi} \right) \exp \left( z^2 \right) (|z|)^{-n-1}, \text{ for } z \rightarrow \pm \infty. \tag{2.26b}
\]
By substituting the conditions in eq.(2.26a) and (2.26b) into eq.(2.18), we find the bound states quantum mechanical energy with even parity,

\[ E_n = \left( n + \frac{1}{2} \right) \hbar \omega, \quad n = 2m = 0, 2, 4, 6 \ldots \]  

(2.27a)

and for the odd parity, we get

\[ E_n = \left( n + \frac{1}{2} \right) \hbar \omega, \quad n = 1 + 2m = 1, 3, 5, \ldots \]  

(2.27b)

Hence, for a one dimensional symmetrical linear harmonic oscillator in the boundary \( z = \pm \infty \), we get its wave function as

\[ \psi_n(x) = [A_n H_n(x \sqrt{\alpha})] \exp \left( -\frac{1}{2} \alpha x^2 \right), \]  

(2.28)

where the constant parameter \( A_n \) can be found by a normalization.

Now, the energy shift in each quantum mechanical energy levels in the one dimensional symmetrical linear harmonic oscillator can exactly be calculated by formulating a simple formula related to eq.(2.25) and eq.(2.27) as follows

\[ \Delta E^{(n)} = E_{n'} - E_n \]

\[ = (n' - n) \hbar \omega, \]  

(2.29)

where \( n = 0, 1, 2, 3, 4, 5 \ldots \) (positive integer) and the values of parameter \( n' \) depend on \( \frac{k}{\sqrt{\alpha}} = 6 \),

\[ n' = 1.55 \times 10^{-15}, (1 + 1.082 \times 10^{-13}), (2 + 3.671 \times 10^{-12}), (3 + 0.805 \times 10^{-10}) \ldots \]

Some results of the energy shift are attached in table 1 and 2.

| \( k = \frac{L}{2} \sqrt{\alpha} \) | Barton et. al. results (1990) (see : eq.(2.4a), \( \Delta E^{(0)} \)) | Our results (\( \Delta E^{(0)} = E_{n'} - E_0 \)) |
|---|---|---|
| 1 | 0.415 (1 + O \( \frac{1}{4} \)) \( \hbar \omega \) | 0.798 \( \hbar \omega \) |
| 3 | 4.177 \times 10^{-4} (1 + \( \frac{1}{10} \)) \( \hbar \omega \) | 3.911 \times 10^{-4} \( \hbar \omega \) |
| 7 | 5.879 \times 10^{-7} (1 + \( \frac{1}{100} \)) \( \hbar \omega \) | 4.908 \times 10^{-7} \( \hbar \omega \) |
| 5 | 7.853 \times 10^{-11} (1 + \( \frac{1}{750} \)) \( \hbar \omega \) | 7.671 \times 10^{-11} \( \hbar \omega \) |
| 6 | 1.570 \times 10^{-15} (1 + \( \frac{1}{2000} \)) \( \hbar \omega \) | 1.550 \times 10^{-15} \( \hbar \omega \) |
| 7 | 4.141 \times 10^{-21} (1 + \( \frac{1}{20} \)) \( \hbar \omega \) | 4.098 \times 10^{-21} \( \hbar \omega \) |
| 10 | 4.197 \times 10^{-43} (1 + \( \frac{1}{2000} \)) \( \hbar \omega \) | 36.769 \times 10^{-43} \( \hbar \omega \) |

Table 1. The energy shift in the ground state of the one dimensional symmetrical linear harmonic oscillator.
3. Discussions and Conclusions

We have presented an exact solution method of the energy shift in each quantum mechanical energy levels in a one dimensional symmetrical linear harmonic oscillator by using the solution of the confluent hypergeometric differential equation. We can conclude that the relationship of the energy shifts is as follows:

\[ \Delta E^{(0)} < \Delta E^{(1)} < \Delta E^{(2)} < \Delta E^{(3)} < \ldots < \Delta E^{(n-1)} < \Delta E^{(n)}. \]

According to the comparison between our results and Barton et. al. results shown in table 1 and 2, we get that their results are almost the same as our results. However, our results are the exact results. On the other hand, our results will be more accurate than their method if in our calculation, we add the series of gamma function in eq.(2.23a) and (2.23b). The longer gamma function series, the more accurate our results. Based on the comparison, we also get the approximation constants (obliquity factors) appeared in Barton et. al. method.

In conclusion, our method is work without a detail calculation of the wave function in each energy levels.

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