

On approximating the free harmonic oscillator by a particle in a box *

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Abstract

The main purpose of this paper is to demonstrate and illustrate, once again, the potency of the variational technique as an approximation procedure for the quantization of quantum mechanical systems. By choosing particle-in-a-box wavefunctions as trial wavefunctions, with the size of the box as the variation parameter, approximate eigenenergies and the corresponding eigenfunctions are obtained for the one dimensional free harmonic oscillator.

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1 Introduction

This paper was inspired by the 1965 work of Padnos, as reported in reference [1]. Using the variation ansatz with normalized wavefunctions of a particle in a box as trial wavefunctions, he obtained approximate values for the ground state energy and the first excited state energy of the one dimensional quantum harmonic oscillator. Padnos' work was preceded by and is an improvement upon the work of Rich [2], who approximated the oscillator by a particle in a one dimensional box whose size was the classical range of the oscillator.

One of the reasons Padnos was discouraged from extending the calculations to higher energy levels was the belief that the calculation becomes more tedious as one must introduce extra terms to orthogonalize the new function to the ones already found (for example, the second excited state must be chosen to be orthogonal to both the ground state and the first excited state). The authors of this present paper have no need to introduce any extra terms since the eigenstates of the particle in a box can all be chosen to be mutually orthogonal, as simple trigonometric functions (see section 2.1).

Another notable paper which employed the variational method for harmonic oscillator quantization is reference [3], where different sets of basis functions, built from non-orthogonal monomials, were used as trial wavefunctions.

A particle of mass m , free to move *only* in a ‘box’ of size $2L$, so that the potential, $V(x)$, is

$$V(x) = \begin{cases} 0, & |x| \leq L \\ \infty, & |x| > L \end{cases},$$

is described by the Hamiltonian

$$H_F = T(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}, \quad |x| \leq L.$$

The eigenfunctions of H_F are non-degenerate and are given by

$$\phi_r(x) = \begin{cases} \sqrt{\frac{1}{L}} \cos \left[\frac{(r+1)\pi x}{2L} \right], & r = 0, 2, 4, \dots \\ \sqrt{\frac{1}{L}} \sin \left[\frac{(r+1)\pi x}{2L} \right], & r = 1, 3, 5, \dots, \end{cases}$$

with corresponding eigenvalues

$$\varepsilon_r = (r + 1)^2 \varepsilon, \tag{1}$$

where $\varepsilon = \varepsilon_0 = \hbar^2 \pi^2 / 8mL^2$. The eigenfunctions $\phi_r(x)$ can be written more compactly as

$$\phi_r(x) = \sqrt{\frac{1}{L}} \cos \left[\frac{\pi}{2} \sin^2 \left(\frac{r\pi}{2} \right) - \frac{(r+1)\pi x}{2L} \right], \quad r = 0, 1, 2, 3, \dots \tag{2}$$

If the particle is not free in the box but is instead under the influence of a potential, $V(x)$, where

$$V(x) = \begin{cases} \frac{1}{2} m \omega^2 x^2, & |x| \leq L \\ \infty, & |x| > L \end{cases},$$

then the system becomes a ‘confined’ quantum harmonic oscillator (CHO), and is now described by the Hamiltonian

$$H_{CHO} := -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2, \quad |x| \leq L,$$

where ω is the classical frequency of the oscillator. Although the confined quantum harmonic oscillator has been studied for a long time (see references [4, 5, 6, 7, 8, 9] and the references therein), it does not seem to enjoy the same popularity as its $L \rightarrow \infty$ limit, the ‘free’ quantum harmonic oscillator (FHO), with

$$H_{FHO} := -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} m \omega^2 x^2, \quad -\infty < x < \infty.$$

It is our aim in this paper to apply the variation procedure to quantize H_{FHO} through H_{CHO} . Since H_F and H_{CHO} live in the same Hilbert space we will use the complete set of functions $\phi_r(x)$ (eigenstates of H_F) as trial wavefunctions in the variation ansatz. The size of the box, L , then enters, naturally, as the variation parameter.

2 The free harmonic oscillator as the variational limit of the confined harmonic oscillator

2.1 The choice of trial wavefunctions

The functions $\phi_r(x)$ as given in (2), being non-degenerate eigenstates of a Hermitian operator, H_F , are a complete set of vectors spanning an infinite dimensional Hilbert space. In particular $\phi_r(x)$ being mutually orthogonal in the interval $|x| \leq L$ and satisfying the boundary conditions $\phi_r(\pm L) = 0$ are a suitable choice of trial wavefunctions for the confined harmonic oscillator Hamiltonian, H_{CHO} , whose eigenfunctions are also required to satisfy the same boundary conditions. The box size, L , then serves as the variation parameter which will be optimized to get the approximate eigenfunctions and eigenvalues of the free harmonic oscillator. Henceforth, any quantity derived for the free harmonic oscillator by optimization will be indicated with an asterik on its symbol.

The optimized box size, L^* , is obtained by solving

$$\left. \frac{\partial E_r}{\partial L} \right|_{L=L^*} = 0$$

for L^* , where

$$E_r = \langle \phi_r | H_{CHO} | \phi_r \rangle = \int_{-L}^L \phi_r H_{CHO} \phi_r dx. \quad (3)$$

The optimized approximate energy eigenvalues of the free harmonic oscillator are then given by

$$E_r^* = E_r|_{L=L^*}. \quad (4)$$

Actually, the ε introduced in (1) (ground state energy of the free particle in a box) is more convenient to use as the variation parameter, with its optimum value ε^* being related to the optimum value of the box size L^* by

$$L^{*2} = \frac{\hbar^2 \pi^2}{8m\varepsilon^*}. \quad (5)$$

ε^* is obtained by expressing the E_r of (3) in terms of ε and then solving

$$\left. \frac{\partial E_r}{\partial \varepsilon} \right|_{\varepsilon=\varepsilon^*} = 0 \quad (6)$$

for ε^* . The optimized approximate eigenenergies of the free harmonic oscillator are then obtained from

$$E_r^* = E_r|_{\varepsilon=\varepsilon^*}. \quad (7)$$

2.2 Approximate eigenfunctions and eigenvalues for the free harmonic oscillator

Performing the integration in (3) we have

$$E_r = (r+1)^2 \varepsilon + \frac{1}{\varepsilon} \frac{\varepsilon_\omega^2}{8} \left(\frac{\pi^2}{6} - \frac{1}{(r+1)^2} \right), \quad r = 0, 1, 2, \dots, \quad (8)$$

where $\varepsilon_\omega = \hbar\omega$. Thus

$$E_r = A_r \varepsilon + \frac{B_r}{\varepsilon}, \quad (9)$$

where

$$A_r = (r + 1)^2, \quad B_r = \frac{\varepsilon_\omega^2}{8} \left(\frac{\pi^2}{6} - \frac{1}{(r + 1)^2} \right).$$

From (8) and (6) we have

$$\varepsilon^{*2} = \frac{B_r}{A_r},$$

so that

$$\frac{\varepsilon^*}{\varepsilon_\omega} = \sqrt{\frac{\pi^2(r + 1)^2 - 6}{48(r + 1)^4}} = \gamma(r). \quad (10)$$

From (7) and (9) we have

$$E_r^* = 2\sqrt{A_r B_r},$$

so that the approximate eigenenergies of the free harmonic oscillator, E_r^* , are given by

$$\boxed{E_r^* = \varepsilon_\omega \sqrt{\frac{\pi^2(r + 1)^2 - 6}{12}}, \quad r = 0, 1, 2, 3, \dots} \quad (11)$$

Writing (5) as

$$\frac{1}{L^{*2}} = \frac{8\alpha \varepsilon^*}{\pi^2 \varepsilon_\omega},$$

where $\alpha = m\omega/\hbar$, and using (10) we have

$$\frac{1}{L^*(r)} = \sqrt{\left(\frac{8\alpha}{\pi^2} \gamma(r) \right)}, \quad (12)$$

so that the approximate eigenstates of the free harmonic oscillator are given by

$$\boxed{\phi_r^*(x) = \sqrt{\frac{1}{L^*(r)}} \cos \left[\frac{\pi}{2} \sin^2 \left(\frac{r\pi}{2} \right) - \frac{(r + 1)\pi x}{2L^*(r)} \right], \quad r = 0, 1, 2, 3, \dots} \quad (13)$$

The optimized eigenfunctions $\phi_r^*(x)$ are expected to approximate the eigenstates of the free harmonic oscillator in the interval: $-L^*(r) \leq x \leq L^*(r)$.

2.3 Comparison with the exact results

The free harmonic oscillator is one of the few quantum mechanical systems that can be quantized exactly. Expressions for the eigenenergies and the corresponding wavefunctions are derived in every book on quantum mechanics. For quantum numbers $r = 0, 1, 2, \dots$, the energy eigenvalues are given by

$$E_r = \left(r + \frac{1}{2} \right) \varepsilon_\omega, \quad (14)$$

with corresponding normalized wavefunctions

$$\phi_r(x) = \left(\frac{\alpha}{\pi} \right)^{1/4} \frac{1}{\sqrt{2^r r!}} H_r(x\sqrt{\alpha}) \exp(-\alpha x^2/2), \quad (15)$$

where $H_q(y)$ is the degree q Hermite polynomial in y and, as before, $\alpha = m\omega/\hbar$ and $\varepsilon_\omega = \hbar\omega$. The first few Hermite polynomials are:

$$\begin{aligned} H_0(y) &= 1, & H_1(y) &= 2y, \\ H_2(y) &= 4y^2 - 2, & H_3(y) &= 8y^3 - 12y. \end{aligned}$$

2.3.1 Comparison of energy eigenvalues

We recall expressions (11) and (14) for the approximate and exact eigenenergies of the free one-dimensional linear harmonic oscillator:

$$E_r^* = \varepsilon_\omega \sqrt{\frac{\pi^2(r+1)^2 - 6}{12}}, \quad r = 0, 1, 2, \dots$$

$$E_r = \varepsilon_\omega \left(r + \frac{1}{2} \right).$$

E_r^*/ε_ω and E_r/ε_ω are plotted in Figure 1 as functions of the harmonic oscillator quantum number r . The agreement between E_r^* and E_r is quite remarkable, especially for low quantum numbers.

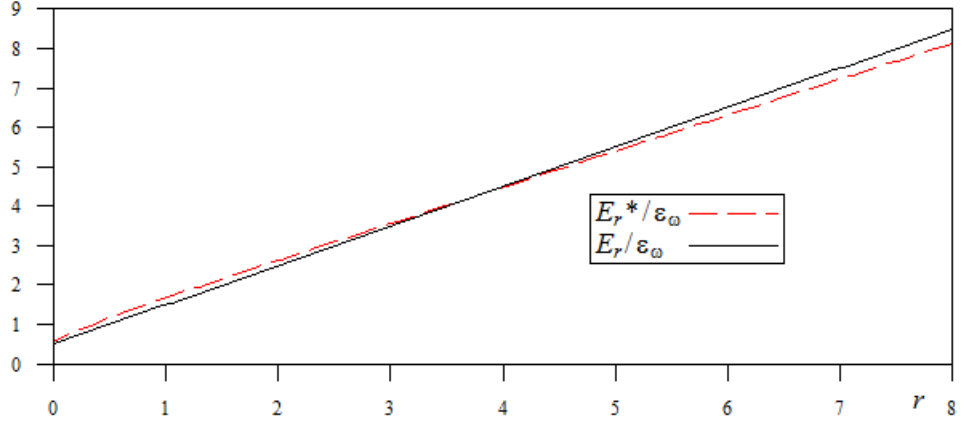


Figure 1: Comparison of the approximate eigenenergies, E_r^* , with the exact eigenenergies, E_r , for the free harmonic oscillator.

2.3.2 Comparison of eigenfunctions

To illustrate the agreement between the variation results and the exact wavefunctions for the free harmonic oscillator, it is instructive to plot the approximate and the exact wavefunctions together, as functions of position. Here we do this for the ground state and the first excited state.

From (13) and (15) we have

$$\phi_0^*(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{2}{\pi}\right)^{1/4} \left(\frac{\pi^2 - 6}{3}\right)^{1/8} \cos \left\{ \left(\frac{\alpha}{2}\right)^{1/2} \left(\frac{\pi^2 - 6}{3}\right)^{1/4} x \right\}$$

and

$$\phi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \exp\left(-\frac{\alpha x^2}{2}\right).$$

The good correlation between $\phi_0^*(x)$ and $\phi_0(x)$ is already obvious from the Taylor series expansion of both functions:

$$\phi_0^*(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{2}{\pi}\right)^{1/4} \left(\frac{\pi^2 - 6}{3}\right)^{1/8} + O(x^2)$$

and

$$\phi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} + O(x^2),$$

with

$$\frac{\phi_0^*(0)}{\phi_0(0)} = \left(\frac{2}{\pi}\right)^{1/4} \left(\frac{\pi^2 - 6}{3}\right)^{1/8} = 0.9221215996$$

The approximate ground state wavefunction $\phi_0^*(x)$ and the exact ground state wavefunction $\phi_0(x)$ of the free harmonic oscillator, with $\alpha = 1$ are shown in Figure 2 as functions of position.

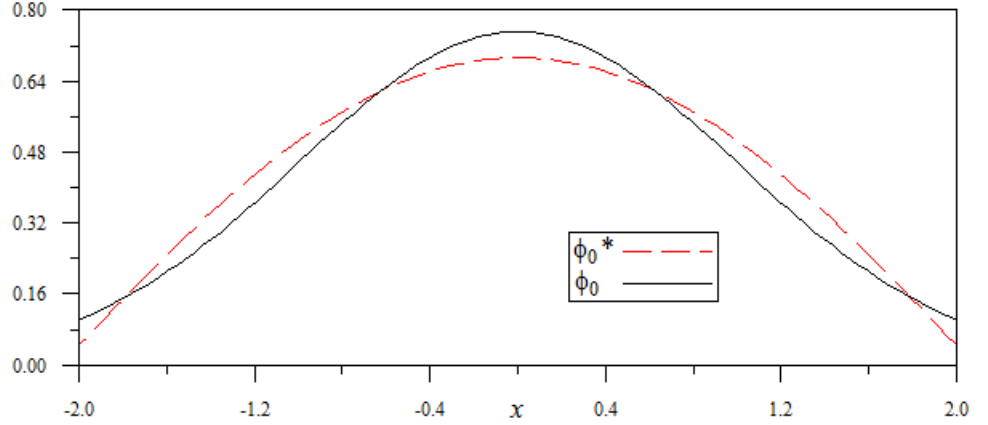


Figure 2: Approximate ground state, $\phi_0^*(x)$, and exact ground state, $\phi_0(x)$ as functions of position, for the free harmonic oscillator, for $\alpha = 1$.

As for the first excited state, we have from (13) and (15) we have

$$\phi_1^*(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{2\pi^2 - 3}{6\pi^2}\right)^{1/8} \sin \left\{ \alpha^{1/2} \left(\frac{2\pi^2 - 3}{6}\right)^{1/4} x \right\}$$

and

$$\phi_1(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} x \sqrt{2\alpha} \exp\left(-\frac{\alpha x^2}{2}\right).$$

The variation of $\phi_1^*(x)$ and $\phi_1(x)$ with respect to position are as shown in Figure 3.

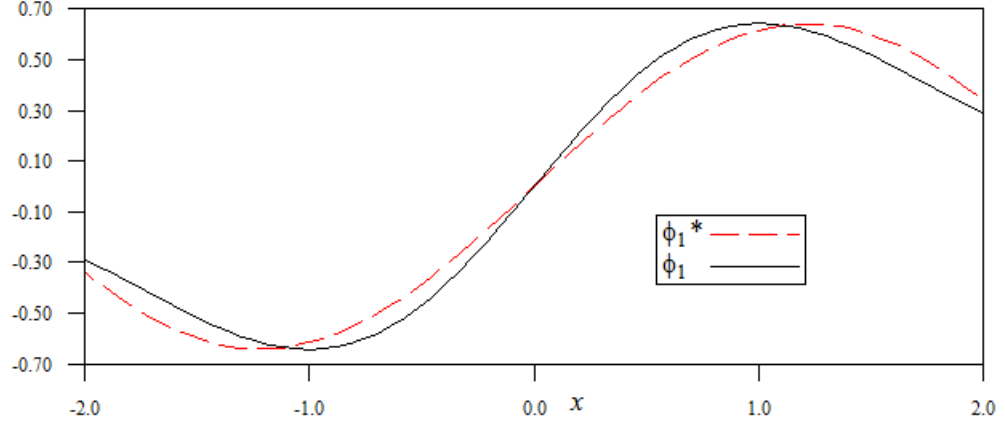


Figure 3: Approximate first excited state, $\phi_1^*(x)$ and exact first excited state, $\phi_1(x)$, as functions of position, for the free harmonic oscillator, for $\alpha = 1$.

3 Summary and conclusion

By using the normalized mutually orthogonal wavefunctions of the free-particle-in-a-box model as trial wavefunctions in variation calculation we have obtained approximate energy eigenvalues and the corresponding eigenstates for the one dimensional free harmonic oscillator of mass m and classical frequency ω . We obtained, for quantum numbers $r = 0, 1, 2, 3, \dots$,

$$E_r^* = \varepsilon_\omega \sqrt{\frac{\pi^2(r+1)^2 - 6}{12}}$$

and

$$\phi_r^*(x) = \sqrt{\frac{1}{L^*(r)}} \cos \left[\frac{\pi}{2} \sin^2 \left(\frac{r\pi}{2} \right) - \frac{(r+1)\pi x}{2L^*(r)} \right],$$

where $\varepsilon_\omega = \omega \hbar$ and

$$\frac{1}{L^*(r)} = \sqrt{\left(\frac{8\alpha}{\pi^2} \gamma(r) \right)}, \quad \gamma(r) = \sqrt{\frac{\pi^2(r+1)^2 - 6}{48(r+1)^4}},$$

with $\alpha = m\omega/\hbar$.

The optimized eigenfunctions $\phi_r^*(x)$ were found to adequately describe the eigenstates of the free harmonic oscillator in the interval: $-L^*(r) \leq x \leq L^*(r)$.

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