The 1-dimensional confined harmonic oscillator revisited

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We study the size effect on the energy levels of the 1–dimensional harmonic oscillator confined within a box of with impenetrable walls and large L. We use the particle in a box basis set to diagonalize the Hamiltonian of the confined harmonic oscillator. In this way we obtain the energy eigenvalues and eigenfunctions as a functions of L. We compare our numerical results with those reported in literature finding good agreement with the exact ones.

Keywords: Confined harmonic oscillator; energy eigenvalues; linear variational method.

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1. Introduction

The idea of the spatial confinement of quantum systems has gained growing interest in recent years due to its potential ability to model a great number of applications in different areas of Physics and Chemistry, as it is shown in several reviews and books [1-8].

A spatially confined quantum system is defined as that in which its state functions satisfy certain boundary conditions for a finite value of the spatial coordinates [1]. The one–dimensional (1–D) harmonic oscillator limited by impenetrable walls is called 1–D confined harmonic oscillator (CHO).

The 1-D confined harmonic oscillator has been used as a model to study some more complicated systems, as for example: the proton–deuteron transformation to generate energy in dense stars [9-10]; in the theory of white dwarfs [11]; in the escape velocity of a star from a galaxy or a globular cumulus [12]; in the calculation of the specific heat of a crystal subjected to high external pressures [14]; in magnetic properties of metals [15]; in the study of color centers. More recently, the dynamics of a CHO subjected to a static electric field and a strong laser field has been studied [39], it has called attention because it could be used to understand some aspects of the dynamics of ions caught in a Paul trap and in the study of the time of the revival of a particle in a CHO. Also few studies have been made on the transition probabilities and Einstein coefficients of the 1-D confined harmonic oscillator [20,34,35] as a function of the box size, showing that new allowed transitions appear as a result of the confinement, this fact may be of technological interest.

Perhaps the first ones who studied the problem of the 1–D confined harmonic oscillator were Kothari and Auluck [9-11]. In the decade of the 40's. They found that the eigen-functions of the system could be written in terms of Kummer's functions. To obtain the values of the energy they needed to find the zeroes of the confluent hypergeometric function. They decided to carry out expansions and approaches to the hypergeometric function to obtain an analytical expression for the energy as a function of box size. They found the correct qualitative behavior; the energy of the levels of the CHO increases fast as the size of the box diminishes. Few years ago Baijal and Singh [20] decided to get the zeroes of the hypergeometric function in a numerical way but their results were not accurate. Vawter [26,27] improved the numerical results found by Baijal and Singh [20]. At the beginning of 1980, Aguilera-Navarro *et al*. [30] used the linear variational method to find, in a numerical way, the eigen–energies and eigen–functions of the CHO problem. They diagonalized the Hamiltonian matrix in the basis set of the free particle in a box of impenetrable walls. They obtained numerical values more accurate than those reported previously. However, the accuracy of their results is lower than the number of decimals that they reported.

The purpose of this work is to show the way in which the results of Aguilera–Navarro *et al*. [30] can be improved.

The content of this work is as follows: In Sec. 2 we present the exact solution of the CHO problem. In Sec. 3 we use the linear variational method to obtain the energy eigenvalues. Finally, in section 4 we discuss our results and we give our conclusions.

2. The exact solution

The Schrödinger equation for the *free 1-D harmonic oscillator* (in natural units, $m = \omega = \hbar = 1$) is given by

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2\right)\psi(x) = E\psi(x), \tag{1}$$

where the unit of the distance is $\sqrt{\hbar/m\omega}$ and the energy is in units of $\hbar\omega$.

In order to find the solutions of Eq. (1) we make the following substitution

$$\psi(x) = f(x)e^{-\frac{1}{2}x^2}, \tag{2}$$

where $f(x)$ satisfies the following equation

$$\frac{d^2f(x)}{dx^2} - 2x\frac{df(x)}{dx} + (\mu - 1)f(x) = 0, \tag{3}$$

where $\mu = 2E$.

Now we make a change of variable, by defining

$$\rho = x^2, \tag{4}$$

then the Eq. (3) is transformed to

$$\rho \frac{d^2 f(\rho)}{d\rho^2} + \left(\frac{1}{2} - \rho\right) \frac{df(\rho)}{d\rho} - \frac{1}{4}(1-\mu) f(\rho) = 0. \tag{5}$$

This equation is identified as the Kummer differential equation. Its general solution, in terms of x, is given by:

$$f(x) = a\, {}_1F_1\left[\frac{1}{4}(1-2E); \frac{1}{2}; x^2\right] + bx\, {}_1F_1\left[\frac{1}{4}(3-2E); \frac{3}{2}; x^2\right], \tag{6}$$

where a and b are constants and ${}_1F_1$ is the hypergeometric function [37,38].

The potential energy of Eq. (1) is a symmetric function of x, therefore the eigenstates of the Schrödinger equation have definite parity; odd or even.

$$\psi^+(x) = Ae^{-x^2/2}\, {}_1F_1\left[\frac{1}{4}(1-2E); \frac{1}{2}; x^2\right],$$
$$\psi^-(x) = Be^{-x^2/2}\, x\, {}_1F_1\left[\frac{1}{4}(3-2E); \frac{3}{2}; x^2\right], \tag{7}$$

where $+$ and $-$ indicate even and odd parity respectively.

In order that the wave functions do not diverge as $x \to \pm\infty$, the hypergeometric function must terminate, this fact requires that there exist some non negative integer n such that

$$E = n + \frac{1}{2}, \quad n = 0,\, 1,\, 2,\, 3, ... \quad . \tag{8}$$

On the other hand, the exact solutions for the *1–D confined harmonic oscillator* are well known [9,10,20,21,25,30], they are obtained as follows. When the harmonic oscillator is symmetrically confined in a box, of length $L = 2a$, of impenetrable walls, the energy quantization results from the boundary conditions on the wave functions

$$\psi^{\pm}(x = -a) = \psi^{\pm}(x = a) = 0. \tag{9}$$

TABLE I. Ground state energy for 1–D confined harmonic oscillator for few states n and different box sizes a. In the first row are the calculations of Aguilera–Navarro *et al*. [30]. In the second row are the calculations of the present work, all calculations were carried out with $N = 35$ functions of the basis set. Finally, in the third row are the exact results obtained with the method described in the Sec. 2 and in the references [16,17].

$n = 1,\ a = 0.5$	$n = 1,\ a = 1.0$	$n = 1,\ a = 5.0$
4.951129323264	1.298459831928	0.4999999999
4.951129323254131	1.298459832032074	0.500000000076717
4.951129323254130411	1.298459832032056693	0.500000000076717131
$n = 2,\ a = 0.5$	$n = 2,\ a = 1.0$	$n = 2,\ a = 5.0$
19.774534178560	5.075582014976	1.5000000035
19.774534179208319	5.075582015226848	1.500000003671584
19.774534179208319898	5.075582015226783066	1.500000003671583931
$n = 3,\ a = 0.5$	$n = 3,\ a = 1.0$	$n = 3,\ a = 5.0$
44.452073828864	11.258825780608	2.500000083
44.452073829740951	11.258825781483075	2.500000084018827
44.452073829740951520	11.258825781482910495	2.500000084018818194
$n = 4,\ a = 0.5$	$n = 4,\ a = 1.0$	$n = 4,\ a = 5.0$
78.996921150976	19.8996964993	3.50000122
78.996921150747461	19.899696501830355	3.500001221456171
78.996921150747460050	19.899696501830088806	3.500001221456053750
$n = 10,\ a = 0.5$	$n = 10,\ a = 1.0$	$n = 10,\ a = 5.0$
493.521634054144	123.53575010	9.53657297
493.521634068787858	123.535750114017713	9.536572972710428
493.521634068787881046	123.535750114015911050	9.536572970482361980
$n = 20,\ a = 0.5$	$n = 20,\ a = 1.0$	$n = 20,\ a = 5.0$
1973.962483650560	493.6466444	24.0826131
1973.962483731369757	493.646644463589652	24.082613154145415
1973.962483731369659659	493.646644463580497219	24.082613059260975237

The eigen–energies are found as the successive roots of the following equations:

$$ {}_1F_1\left[\frac{1}{4}\left(1-2E\right);\frac{1}{2};a^2\right]=0, \quad \text{for even states}$$

$$ {}_1F_1\left[\frac{1}{4}\left(3-2E\right);\frac{3}{2};a^2\right]=0, \quad \text{for odd states} \qquad (10)$$

To determine the energy eigenvalues from these equations, it is necessary to solve numerically for one of the boundary conditions (9) according to the symmetry of the problem. The allowed energies can be determined with high accuracy by using some computer algebra system, Montgomery *et al.* [16-17] used Maple but we can use Mathematica or a Fortran compiler with subroutines of extended precision. The numerical results obtained by solving the Eq. (10) with Mathematica 9 are reported in Table I.

3. Linear variational approach

The Schrödinger equation independent of time is given by

$$H\Psi = E\Psi. \qquad (11)$$

We use the linear variational method to solve the eigenvalue Schrödinger equation. The wavefunction Ψ is expanded as

$$\Psi = \sum_{i=1}^{N} c_i\phi_i. \qquad (12)$$

where $\{c_i\}$ are constants to determine and $\{\phi_i\}$ is an orthonormal basis set.

The solution of eigen–value problem (Eq. 11) is equivalent to find the solutions of

$$(\mathbf{H}-E\mathbf{I})\vec{c}=0, \qquad (13)$$

where $\vec{c}=(c_1,c_2,c_3,...,c_N)$ is the vector of coefficients and **I** is the identity matrix, and

$$H_{ij}=\langle\phi_i|H|\phi_j\rangle\,, \qquad (14)$$

are the elements of the Hamiltonian matrix.

It is convenient to write the CHO Hamiltonian in the following way:

$$H=H^0+H'. \qquad (15)$$

Where $H^{'}=(1/2)x^2$ and H^0 is the Hamiltonian of a free particle in a box:

$$H^0=\frac{p^2}{2}+V_c\,, \qquad (16)$$

in which the potential is given by

$$V_c=\begin{cases} 0, |x|<a \\ \infty, |x|>a\,. \end{cases} \qquad (17)$$

The energy eigenvalues E_n^0 and eigenfunctions ϕ_n of H^0 are well known:

$$E_n^0=\frac{n^2\pi^2}{8a^2}, \qquad (18)$$

and

$$\phi_n(x)=\begin{cases} \sqrt{1/a}\,\cos(n\pi x/2a), & n=1,3,5,... \\ \sqrt{1/a}\,\sin(n\pi x/2a), & n=2,4,6,...\,. \end{cases} \qquad (19)$$

The Hamiltonian matrix elements are:

$$H_{ij}=H_{ij}^0+H_{ij}^{'}, \qquad (20)$$

in which

$$H_{ij}^0=E_i^0\delta_{ij}, \qquad (21)$$

where δ_{ij} is the Kronecker delta.

The Hamiltonian H (Eq. 15) is symmetric, therefore its eigen–functions have definite parity, *even* or *odd*. For even (odd) states, the expansion in (Eq. 12) includes only even (odd) states as given by Eq. (19).

The matrix elements $H_{ij}^{'}$ are analytical.

For even states they are:

$$H_{ij}^{'}=\begin{cases} \dfrac{L^2\left(-6+(1-2j)^2\pi^2\right)}{24(\pi-2j\pi)^2}, & \text{if} \quad i=j \\ \dfrac{(-1)^{i+j}L^2\left(\frac{1}{(i-j)^2}-\frac{1}{(-1+i+j)^2}\right)}{4\pi^2}, & \text{if} \quad i\neq j,\ i,j=1,2,3,\ldots\,. \end{cases} \qquad (22)$$

Whereas for odd states we have

$$H_{ij}^{'}=\begin{cases} \dfrac{L^2}{48}\left(2-\frac{3}{i^2\pi^2}\right) & \text{if} \quad i=j \\ \dfrac{(-1)^{i+j}L^2\,i\,j}{\left(i^2-j^2\right)^2\pi^2}, & \text{if} \quad i\neq j,\ i,j=1,2,3,\ldots\,. \end{cases} \qquad (23)$$

Where $L=2a$.

4. Results and discussion

The diagonalization of the CHO Hamiltonian was already employed by Aguilera–Navarro, Ley-Koo and Zimerman [30] in 1980, and subsequently used again by Taseli and Safer [36] at the end of the 90's. In Table I we show the calculations obtained in the present work with those obtained by Aguilera–Navarro *et al*. [30] and with the exact ones [16]. Our calculations were made by using Mathematica 9 with real variables with 25 decimal places. For comparison we used the same number of basis set, $N = 35$, as Aguilera–Navarro *et al*. [30].

We compare our results with the exact ones obtained by Montgomery *et al.* [16,17], and we find that the present calculations have the precision shown in Table I.

In Table I we can see that the accuracy in the calculations of reference [30] is lower than the results of the present study. The reason for this difference is due to the fact that in the early 80's the diagonalization subroutines were not as efficient and accurate as they are today, and it could also be due to the fact that the calculations with double precision real variables could only handle 16 decimal places.

As we can see there is an improvement in the accuracy of the energy eigenvalues for boxes with a <5. While for a =5 the accuracy of results of the present report and those of reference [30] is the same. To improve the accuracy of the results of the present work it is necessary to increase the number of functions of the basis set to reach the exact results. In an Appendix we show the Mathematica procedure used to obtain the results presented in this work.

appendix

(* Mathematica procedure to find the energy–eigenvalues *)

```
Clear["Global*"]
delta[n_, m_] := KroneckerDelta[n, m](* Identity matrix*)
(* Even states *)
v[n_, m_] := 1/\[Pi]^2 (-1)^(m + n) a^2 (1/(m - n)^2 - 1/(-1 + m + n)^2)    /;  n !=
m ;(* non-diagonal elements of the harmonic oscillator potential (1/2)x^2 *)
v[n_, m_] := (a^2 (-6 + (1 - 2 n)^2 \[Pi]^2))/(6 (\[Pi] - 2 n \[Pi])^2) /; n == m;(*
Diagonal elements of the harmonic oscillator potential (1/2)x^2*)
d[n_] := ((2 n - 1)^2 \[Pi]^2)/(8 a^2);(* Energy eigenvalues of a particle in a box *)

(* Odd states; replace the three functions defined before by the followin lines *)

v[n_, m_] :=  (4 (-1)^(m + n) a^2 m n)/((m - n)^2 (m + n)^2 \[Pi]^2) /; n != m ;
v[n_, m_] := 1/12 a^2 (2 - 3/(n^2 \[Pi]^2)) /; n == m;
d[n_] := ((2 n)^2 \[Pi]^2)/(8 a^2)*)

Hnm[n_, m_] := SetPrecision[N[ (d[n]) (delta[n, m]) + v[n, m], 25], 25];(* Hamiltonian
matrix *)base = 35;(* Number of functions of the basis set *)
matrizH = Table[Hnm[n, m], {n, 1, base}, {m, 1, base}];
Print[TimeUsed[]]
a = 0.2;(* Box lenght*)
energias = SetPrecision[Eigenvalues[matrizH], 25];(* Energy eigenvalues*)
Sort[SetPrecision[energias, 25]]
```

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