

The isotropic bounded oscillators

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1997 J. Phys. A: Math. Gen. 30 2403

(<http://iopscience.iop.org/0305-4470/30/7/020>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.112

The article was downloaded on 02/06/2010 at 06:15

Please note that [terms and conditions apply](#).

The isotropic bounded oscillators

N Aquino

Depto. de Física, Universidad Autónoma Metropolitana, Av. Michoacán y Purísima, Apartado Postal 55-534, 09340 México, DF, México

Received 9 July 1996, in final form 6 December 1996

Abstract. We study the three-dimensional isotropic harmonic oscillator confined within spherical impenetrable walls. The potential in the box is of the harmonic oscillator type but outside the box the potential is infinite. The energy eigenvalues and some position expectation values are computed with great accuracy for different box sizes; our results are more accurate than previous calculations. By using the bounded harmonic oscillator wavefunctions as a basis set we obtain with the variational method the energy eigenvalues of a confined hydrogen atom.

1. Introduction

It is well known that very simple quantum systems such as the hydrogen atom and the three-dimensional isotropic harmonic oscillator have analytical solutions. However, when these quantum systems are confined in spherical boxes with impenetrable walls, the solutions of the Schrödinger equation are not trivial and the energy eigenvalues have not been determined analytically.

The study of bounded quantum systems is interesting due to the existence of many problems in different fields of physics that can be considered as bounded quantum systems, and is interesting as a method to compute the energy eigenvalues of free quantum systems when the analytical solution is unknown.

Some models of bounded quantum systems have been developed to study atoms and molecules under high pressures [1–13], near-surface donor states [14], impurity binding energies in quantum wells [15, 16], the confinement of electron holes in microcrystals [17–21], nuclear deformations [22], superconductivity [23] and others [12].

In particular the study of the bounded harmonic oscillators is interesting because they were used in the study of the fundamental mass-radius relation in the white dwarf theory [24], the specific heat of solids [25] and the magnetic properties of a system of electrons within a cylinder [26].

On the other hand, the bounded quantum systems are used to obtain the energy eigenvalues and eigenfunctions of free quantum systems as, for example, the one-dimensional anharmonic oscillator [27–29], the Morse oscillator [30], the Mitra potential [31] and the NH_3 inversion spectra [32, 33].

Until now investigation has been mainly devoted to the study the one- and two-dimensional bounded harmonic oscillators [24–26, 34–37]. A study of a three-dimensional isotropic bounded harmonic oscillators was done independently by Marin and Cruz [38] and by Fernández and Castro [39]. Marin and Cruz [38] used the direct variational method, choosing as a trial function the product of the wavefunction of a free harmonic oscillator times a function, χ , such that $\chi(r_0) = 0$, where r_0 is the box radius. The method

developed by Fernández and Castro [39] is a combination of the hypervirial theorems and the perturbation theory; the results obtained by this method were more accurate than those obtained by Marin and Cruz [38]. However, when the radius of the box increases, the energy eigenvalues produced by this method become less accurate. In this work we compute the energy eigenvalues and some position expectation values with great accuracy for the radii of several boxes.

The present paper is organized as follows. Section 2 introduces the general method for one-dimensional potentials and in section 3 we develop the particular calculations for the three-dimensional isotropic harmonic oscillators. In section 4 we compute $\langle r^{-2} \rangle$, $\langle r^2 \rangle$ and $\langle r^4 \rangle$. Section 5 is devoted to compute the energy eigenvalues for the 1s and some excited states for the confined hydrogen atom diagonalizing its Hamiltonian in the bounded oscillator wavefunctions. Finally, in section 5 the conclusions of this work are given.

2. The method

The method was first introduced by Campoy and Palma [27, 28] to solve free quantum systems, while Aquino [9] showed that the same method can be used for the study of bounded hydrogen atoms.

We begin with the time-independent Schrödinger equation for an arbitrary one-dimensional potential $V(x)$, which in atomic units can be written as

$$\psi'' = 2[V(x) - \epsilon]\psi \quad (1)$$

where ϵ represents the energy eigenvalue. One of the main features of the method is the assumption that ψ must be a function of both position and energy, i.e.

$$\psi = \psi(x, \epsilon). \quad (2)$$

The derivative of equation (1) with respect to the energy is

$$\partial\psi''/\partial\epsilon = 2[V(x) - \epsilon](\partial\psi/\partial\epsilon) - 2\psi. \quad (3)$$

To confine the system we introduce an impenetrable barrier at point x_0 , and therefore the function ψ must vanish at this point for the exact energy only, i.e.

$$\psi(x_0, \epsilon_{\text{exact}}) \equiv 0. \quad (4)$$

The problem of finding the energy eigenvalues of equation (3) is then reduced to finding the zeros of the function ψ at x_0 . One procedure is as follows. Given an initial approximation ϵ_i , equations (1) and (3) are solved numerically for ψ and $\partial\psi/\partial\epsilon$, respectively, to obtain $\psi(x_0, \epsilon_i)$ and $\partial\psi(x_0, \epsilon_i)/\partial\epsilon$. A correction for the energy is then computed through the Newton–Raphson method [40–42],

$$\epsilon_{i+1} = \epsilon_i - \psi(x_0, \epsilon_i)/[\partial\psi(x_0, \epsilon_i)/\partial\epsilon]. \quad (5)$$

With this new value of the energy we iterate equations (1) and (3) until we obtain the eigenvalue ϵ_f with the desired accuracy.

3. Energy eigenvalues of the isotropic bounded oscillators

The Hamiltonian for the three-dimensional isotropic bounded harmonic oscillator (IBHO), in atomic units, is given by

$$H = -\frac{1}{2}\nabla^2 + r^2/2 + V'(r) \quad (6)$$

where

$$V'(r) = \begin{cases} +\infty & r > r_0 \\ 0, & r \leq r_0 \end{cases} \quad (7)$$

r_0 is the radius of the box in units of $(\hbar/m\omega)^{1/2}$. Since the problem is separable we solve the radial equation only.

The method described in section 2, was originally developed for polynomial potentials. However, we can use it for the IBHOs if we write the corresponding Schrödinger equation as follows:

$$r^2\psi'' = -2r\psi' + l(l+1)\psi + r^4\psi - 2\epsilon r^2\psi \quad (8)$$

where l is the angular momentum of the particle.

The wavefunction, ψ , is now developed through a Taylor series expansion around the point $r = a$.

$$\psi(r) = \sum_k T_k(a, r) \quad (9a)$$

where

$$T_k(a, r) = (\psi^{(k)}(a)/k!)(r - a)^k \quad (9b)$$

which can be evaluated in a very simple way. The p th derivative of equation (8) relative to r , becomes:

$$[r^2\psi^{(2)}]^{(p)} = -2[r\psi^{(1)}]^{(p)} + l(l+1)\psi^{(p)} - [r^4\psi]^{(p)} - 2\epsilon[r^2\psi]^{(p)} \quad (10)$$

where the superscript quantities in parentheses represent derivative orders. Now using the well known formula for the derivative of a product, together with equations (9a, b), and evaluating in $a = 0$, we finally obtain

$$T_{p+2} = r^2[r^2T_{p-2} - 2\epsilon T_p]/[(p+2)(p+3) - l(l+1)] \quad \text{with } p \geq 0. \quad (11)$$

Hence the wavefunction can be calculated directly using (9a). From (9a) the following expression is also obtained:

$$\partial\psi/\partial\epsilon = \sum_m \partial T_m/\partial\epsilon = \sum_p \dot{T}_p \quad (12)$$

where \dot{T}_p denotes the derivative of T_p relative to the energy, obtained from equation (11), i.e.

$$\dot{T}_{p+2} = r^2[r^2\dot{T}_{p-2} - 2\epsilon\dot{T}_p - 2T_p]/[(p+2)(p+3) - l(l+1)] \quad \text{with } p \geq 0 \quad (13)$$

where T_p and \dot{T}_p are zero for $p < 0$.

We choose $a = 0$ because, we know the value of wavefunctions at this point. To compute $\psi(r_0)$ and $\partial\psi(r_0)/\partial\epsilon$ simply we evaluate equations (9a) and (12) together with equations (11) and (13) in $r = r_0$. From the relations (11) and (13), we can build any eigenstate, using the initial conditions: for $l = 0$ (the s-states), we let $\psi_n(0) = 1$ (or $T_0 = 1$), and the value of the first derivative $\psi'_n(0) = 0$ (or $T_1 = 0$), then we obtain $T_2 = -\epsilon r_0^2/3$ from (11); for $l = 1$ (the p-states), we let $\psi_n(0) = 0$ and $\psi'_n(0) = 1$; and for $l = 2$ (the d-states), we let $\psi_n(0) = 0$, $\psi'_n(0) = 0$, $\psi''_n(0) = 1$.

Once the energy eigenvalue, ϵ_n , has been obtained, we can compute the expansion coefficients for the wavefunction by substituting the values of ϵ_n into equation (11) and evaluating T_p at $r = 1$. Thus, we have the following relation:

$$\psi_n(r) = \sum_m T_m(r = 1, \epsilon_n)r^m. \quad (14)$$

Table 1. Energy eigenvalues $\epsilon(r_0)$ for the three-dimensional bounded harmonic oscillator as a function of the radius of the box (r_0). The energies are in units of $\hbar\omega$ and the radii is in units of $(\hbar/m\omega)^{1/2}$.

r_0	ϵ^a	ϵ^b	ϵ^c	Present
Ground state $n = 0, l = 0$				
0.5		19.774 534		19.774 534 1792
1.0	5.1313	5.075 5820	5.0755	5.075 582 0152
$(\frac{3}{2})^{1/2}$		3.500 0000		3.500 000 0000
1.5	2.5265	2.504 9761	2.5050	2.504 976 1785
2.0	1.7739	1.764 8087	1.7648	1.764 816 4387
2.5	1.5567	1.551 66	1.5514	1.551 421 6545
3.0	1.5105		1.5061	1.506 081 5272
4.0	1.5033		1.5000	1.500 014 6030
5.0	1.5025		1.5000	1.500 000 0036
First excited state $n = 0, l = 1$				
1.0	10.3188		10.2822	10.282 256 9390
1.5	4.9169		4.9036	4.903 590 4194
2.0	3.2514		3.2469	3.246 947 0987
2.5	2.6901		2.6881	2.688 143 9638
3.0	2.5337		2.5313	2.531 292 4666
4.0	2.5015		2.5001	2.500 143 7781
5.0	2.5012		2.5000	2.500 000 0584

^a Using the method described in [38]

^b Using the method described in [39]

^c These values were computed in [38] using the method developed by Ley-Koo and Rubinstein [3]

A major advantage of this method is that the computation of the energy eigenvalues is very accurate and fast. Table 1 shows the energy eigenvalues ϵ_n for the ground state and the first excited state with nine figures of precision for each value of the (impenetrable) wall distance r_0 .

In table 1 we compare the present calculations with those obtained by Marin and Cruz [38] and by Fernández and Castro [39] with different methods. Fernández and Castro [39] calculated the energy eigenvalues only for the ground state, whereas Marin and Cruz [38] calculated the first excited state also. The results obtained by Fernández and Castro [39] are accurate only for small values of r_0 , whereas they become less precise for values of r_0 higher than 2.0 units in length. The results of Marin and Cruz [38] are less precise than those obtained by Fernández and Castro [39], but the method is very simple and can be employed to compute the energy eigenvalues for higher excited states. In the fourth column of table 1 the calculations are done using the method developed by Ley-Koo and Rubinstein [3]. Although the method of Ley-Koo and Rubinstein can provide the energy eigenvalues with any desired accuracy, the computational task is much more intricate than the method proposed here.

As we mentioned before, with this method we can also compute the excited states. The results of this computation are shown in table 2, where the energy eigenvalues were determined for different values of n and l as functions of the radius of the box r_0 .

It is well known [43–45] that the three-dimensional free isotropic harmonic oscillator (FIHO) is degenerate, its energy is given by $E_N = (N + \frac{3}{2})\hbar\omega$, where $N = 2n + l$. When we confine this system within of an impenetrable box, this degeneracy is broken; for this reason

Table 2. Energy eigenvalues $\epsilon_{nl}(r_0)$ of the three-dimensional bounded harmonic oscillator for different values of n and l as function of the radius r_0 .

r_0	$\epsilon_{00}(r_0)$	$\epsilon_{01}(r_0)$	$\epsilon_{02}(r_0)$
0.5	19.774 534 1792	40.428 276 4970	66.489 756 5349
1.0	5.075 582 0152	10.282 256 9390	16.827 777 1098
1.5	2.504 976 1785	4.903 590 4194	7.871 730 4877
2.0	1.764 816 4387	3.246 947 0987	5.010 040 8656
2.5	1.551 421 6545	2.688 143 9638	3.953 528 9034
3.0	1.506 081 5272	2.531 292 4666	3.598 247 6989
3.5	1.500 399 5211	2.502 910 1642	3.512 580 3181
4.0	1.500 014 6030	2.500 143 7781	3.500 842 0738
4.5	1.500 000 3041	2.500 003 8701	3.500 029 4123
5.0	1.500 000 0036	2.500 000 0584	3.500 000 5567
5.5	1.500 000 0002	2.500 000 0005	3.500 000 0058
6.0	1.500 000 0000	2.500 000 0000	3.500 000 0003
$r_0 = \infty^a$	1.500 000 0000	2.500 000 0000	3.500 000 0000

r_0	$\epsilon_{10}(r_0)$	$\epsilon_{11}(r_0)$	$\epsilon_{20}(r_0)$
0.5	78.996 921 1507	119.402 445 2520	177.693 843 8082
1.0	19.899 696 5018	30.013 487 5924	44.577 171 2285
1.5	9.135 422 0876	13.653 740 8930	20.109 002 9728
2.0	5.584 639 0790	8.159 528 8816	11.764 982 1223
2.5	4.184 261 3183	5.876 767 7360	8.153 436 9588
3.0	3.664 219 6450	4.913 897 6907	6.473 336 6162
3.5	3.523 302 3363	4.580 798 9270	5.758 692 1635
4.0	3.501 691 5385	4.508 330 4308	5.539 421 7970
4.5	3.500 062 3121	4.500 417 4712	5.502 872 2559
5.0	3.500 001 2214	4.500 010 5730	5.500 098 7178
5.5	3.500 000 0132	4.500 000 1425	5.500 001 7124
6.0	3.500 000 0000	4.500 000 0008	5.500 000 0134
$r_0 = \infty^a$	3.500 000 0000	4.500 000 0000	5.500 000 0000

^a These values correspond to the three-dimensional free isotropic harmonic oscillator computed by the analytical formulae of [43–45].

it is convenient to label the energy $E_{nl}(r_0)$. We can confirm this statement by looking at the states $E_{02}(r_0)$ and $E_{10}(r_0)$ in table 2. For small values of r_0 the spectrum is non-degenerate, whereas for large values of r_0 the spectrum is practically degenerate. This behaviour is more evident if we observe figure 1, on its left side it shows the energy levels of the spherical well and on its right side the energy levels of FIHO. The energy levels of BIHO are between the energy spectrum of the well and the FIHO. The continuous lines show how the energy levels of BIHO vary between the energy levels of the well and the FIHO as a function of r_0 . When the size of the spherical box (r_0) diminishes, the energy levels of BIHO leave to be degenerate and their numerical values increase. An unusual fact occurs with levels 1h and 3s when r_0 decreases. For some distance r_0^* , there exists a crossing point of these two levels, and for smaller values than r_0^* , the order of these two levels is inverted. An analogous behaviour is shown for levels 3p and 1i. We must note that the order of the spectrum and the energy splitting between levels are functions of the radius of the impenetrable box (r_0). An estimation of the non-degeneracy is given, for example, by the splitting $\Delta E = E_{10} - E_{02}$. In figure 2, ΔE is plotted as function of r_0 . In this figure we can easily see the above remarks.

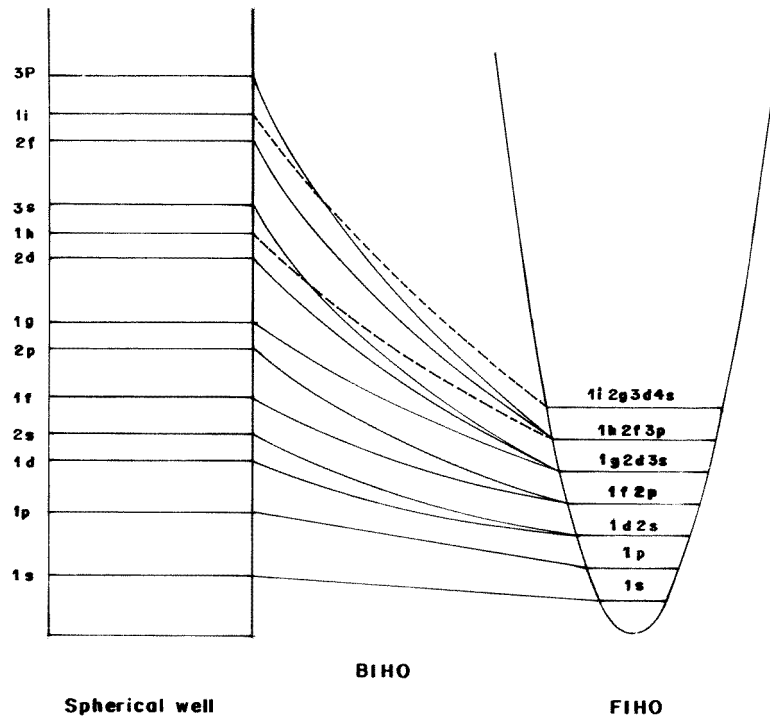


Figure 1. This diagram shows the correspondence of the energy eigenvalues of the BIHO with the spherical well and the FIHO. For small r_0 the energy eigenvalues of the BIHO are very near to the spherical well, for large r_0 the energy eigenvalues are practically the FIHO. It also shows the crossing of some energy levels.

The non-degeneracy of the spectrum for small values of r_0 can be understood as follows. For small values of r_0 we may think of this problem as a particle moving within a spherical box with impenetrable walls (whose spectrum is non-degenerate [43–45]) plus a harmonic oscillator's perturbation r_0^2 , so that the complete problem is non-degenerate. When r_0 is large the problem may be seen as the FIHO perturbed by a box with impenetrable walls, thus the spectrum will be very near to the degenerate one, as expected.

4. The position expectation values

The wavefunction obtained by this procedure is not normalized; this fact is not important for computing the position expectation values because, as Palma remarks [27, 28], these quantities can be computed easily (without the use of the wavefunction) by using the Hellmann–Feynman theorem. We have used this approach in a previous work to compute some position expectation values for the hydrogen atom confined by a box of impenetrable walls [9, 27]. In the present work we use the direct integration of wavefunctions.

The expectation value for r^k is defined by

$$\langle r^k \rangle = \frac{\int_0^{r_0} \psi^2 r^k r^2 dr}{\int_0^{r_0} \psi^2 r^2 dr} \quad \text{with } k = \text{integer.} \quad (15)$$

The integration was done using an extended Simpson's rule [40–42, 46], with this method we obtained a precision of six figures for $\langle r^{-2} \rangle$, $\langle r^2 \rangle$ and $\langle r^4 \rangle$; the results of these calculations

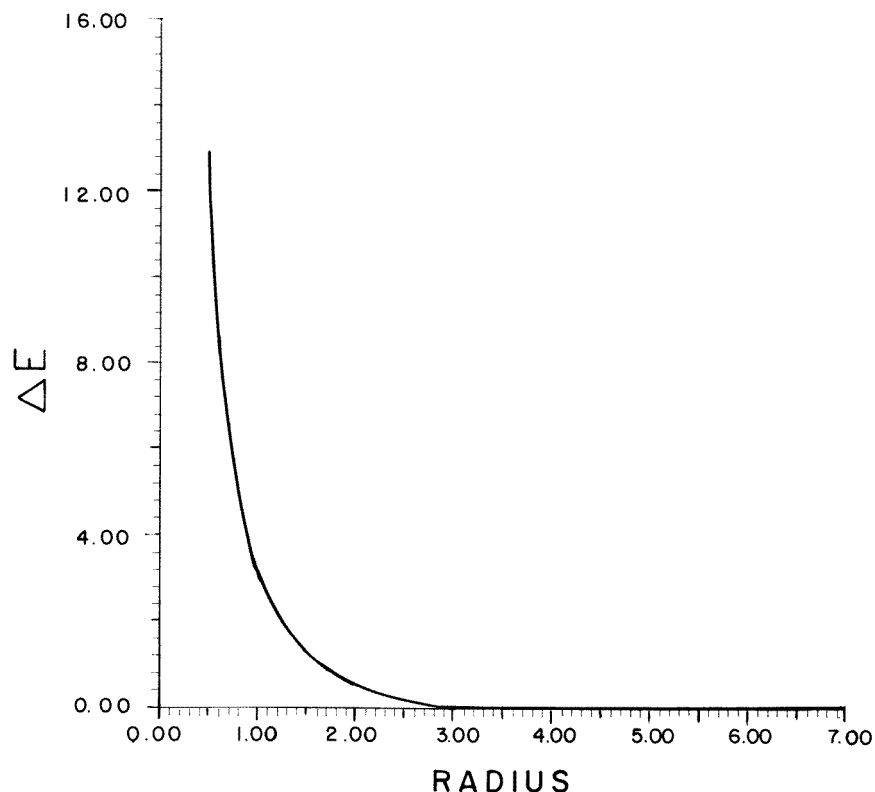


Figure 2. The splitting energy $\Delta E (= E_{10} - E_{02})$ as function r_0 . For small values of r_0 there is not degeneration between these two levels, but when the radius r_0 increases, they approach the degeneration.

are shown in table 3. The behaviour of the expectation values is very similar to that of the energy eigenvalues; they vary monotonically to the values of the FIHO when the radius of the box increases. Interestingly enough, there are no position expectation values reported in previous works [38, 39]. Once we have the energy eigenvalues we can compute the wavefunction ψ (equation (14)) and we can compute $\langle r^k \rangle$ in an analytical way. However, in this work we have computed numerical values of the integrals, because, in the program used to compute the energy eigenvalues, the wavefunctions are obtained at the same time, and they were used immediately to compute the integrals, saving computer time.

As we mentioned before, we can compute the energy and eigenfunctions through equations (11) and (13), giving initial conditions for the wavefunction and some of its derivatives at the origin $r = 0$, together with the boundary condition at $r = r_0$. The nodes of the wavefunction are also automatically determined by these conditions. We do not need to make any changes to the analytic form of the function equation (11) to compute any state, as is done in other methods [47, 48]. The position of the nodes depends on the size of the impenetrable box; when the size of the box increases, the nodes of IBHO approach the position of the nodes of FIHO, and in the limit $r \rightarrow \infty$ they are identical. In practice we may consider that they are equal when the size of the box r_0 satisfies $r_0 \geq 6$ au. In figure 3 six different states are plotted as functions of r_0 , where we can observe the position shift of nodes. The wavefunctions plotted have not been normalized to unity. The states

Table 3. Position expectation values $\langle r^{-2} \rangle$, $\langle r^2 \rangle$ and $\langle r^4 \rangle$ as a function of the radius of the box (r_0).

r_0	$\langle r^{-2} \rangle$	$\langle r^2 \rangle$	$\langle r^4 \rangle$
$n = 0, l = 0$			
0.5	35.670 362 6921	7.063 332 5319 E - 2	7.124 051 8727 E - 3
1.0	9.024 100 6941	0.280 449 1919	0.112 597 9005
2.0	2.695 851 7746	0.996 925 7335	1.478 304 9734
3.0	2.024 417 3259	1.461 864 1057	3.478 551 3901
4.0	2.000 077 6828	1.499 804 6846	3.747 914 0456
5.0	2.000 000 0216	1.499 999 9191	3.749 998 7701
5.5	2.000 000 0007	1.499 999 9996	3.749 999 9994
$r_0 = \infty^a$	2.000 000 0000	1.500 000 0000	3.750 000 0000
$n = 0, l = 1$			
0.5	15.604 579 0517	9.362 593 5728 E - 2	1.087 150 5434 E - 2
1.0	3.924 711 2835	0.372 964 4642	0.172 728 4387
2.0	1.080 173 3970	1.394 483 9053	2.461 796 8195
3.0	0.694 710 7566	2.337 424 9913	7.377 655 7684
4.0	0.666 856 9583	2.498 236 0443	8.728 662 0820
5.0	0.666 666 7627	2.499 998 7516	8.749 979 2031
5.5	0.666 666 6675	2.499 999 9866	8.749 999 7431
$r_0 = \infty^a$	0.666 666 6667	2.500 000 0000	8.750 000 0000
$n = 1, l = 0$			
0.5	75.009 927 0868	8.017 671 9300 E - 2	1.097 790 5107 E - 2
1.0	18.773 803 8158	0.321 280 0381	0.175 854 6450
2.0	4.774 023 4899	1.313 675 5498	2.837 678 6605
3.0	2.363 160 5071	2.848 497 3047	12.360 529 1432
4.0	2.006 155 6647	3.481 600 7196	18.501 511 1189
5.0	2.000 005 8010	3.499 975 3635	18.749 555 38
6.0	2.000 000 0	3.500 000 000	18.750 000 00
$r_0 = \infty^a$	2.000 000 0	3.500 000 000	18.750 000 00
$n = 2, l = 0$			
0.5	114.459 392 6675	8.193 230 0984 E - 2	1.180 930 2000 E - 2
1.0	28.623 515 5711	0.328 101 1648	0.189 197 6805
2.0	7.186 709 1622	1.335 690 5995	3.087 980 9920
3.0	3.236 711 7630	3.178 497 5904	16.411 451 6391
4.0	2.095 221 1738	5.187 265 1591	40.659 421 4306
5.0	2.000 367 3908	5.498 260 7986	45.713 491 7561
6.0	2.000 000 06	5.499 999 6086	45.749 989 5219
$r_0 = \infty^a$	2.000 000 00	5.500 000 0000	45.750 000 0000

^a These values correspond to the three-dimensional free isotropic harmonic oscillator computed by the analytical formulae of [45].

are labelled with the quantum numbers n and l , thus the state 10 means the function ψ_{10} , etc. The wavefunctions are compressed to the inner of the spherical box, but the symmetry of the wavefunctions and the number of nodes are unaltered.

5. The confined hydrogen atom in terms of BIHO states

For several years the FIHO basis set has been used to solve a great variety of problems of more complexity [49] such as, hydrogen atoms, hydrogen molecules, helium atoms, etc. An

Table 3. (Continued)

r_0	$\langle r^{-2} \rangle$	$\langle r^2 \rangle$	$\langle r^4 \rangle$
$n = 1, l = 1$			
0.5	28.849 399 1689	8.682 928 6126 E - 2	1.199 162 7564 E - 2
1.0	7.221 200 1399	0.347 621 3689	0.192 061 3526
2.0	1.838 609 7252	1.408 622 1564	3.113 726 3025
3.0	0.880 321 8876	3.200 689 7343	15.257 357 0373
4.0	0.674 417 7243	4.420 593 0777	28.567 342 6176
5.0	0.666 680 5327	4.499 799 2081	29.746 073 9542
6.0	0.666 666 6678	4.499 999 9758	29.749 999 3858
$r_0 = \infty^a$	0.666 666 6667	4.500 000 0000	29.750 000 0000
$n = 0, l = 2$			
0.5	11.471 280 3274	0.109 655 9301	1.398 157 5372 E - 2
1.0	2.878 144 3188	0.437 484 7350	0.222 697 2275
2.0	0.762 891 4153	1.676 456 3054	3.306 502 7796
3.0	0.438 300 9920	3.019 042 3538	11.657 311 5440
4.0	0.400 530 8571	3.490 618 1724	15.623 363 2297
5.0	0.400 000 4600	3.499 988 6907	15.749 795 2218
6.0	0.400 000 0002	3.499 999 9920	15.749 999 8331
$r_0 = \infty^a$	0.400 000 0000	3.500 000 0000	15.750 000 0000

^a These values correspond to the three-dimensional free isotropic harmonic oscillator computed by the analytical formulae of [45].

important question is the following. Is the IBHO basis set as good for complex bounded problems as the FIHO for free problems? We are going to give a partial answer by means of an example.

Some years ago Moshinsky [49] calculated the ground-state energy for the free hydrogen atom using a basis set of free harmonic oscillator states. In this section we are going to show that using this simple idea it is possible to do a similar calculation for the confined hydrogen atom in spherical impenetrable walls using the basis set of BIHO states.

In non-relativistic quantum mechanics we may write the Hamiltonian for the bounded hydrogen atom as follows:

$$H' = \frac{p'^2}{2m} + V(r') \tag{16}$$

where

$$V(r') = \begin{cases} -e^2/r' & \text{if } r < r_0 \\ +\infty & \text{if } r \geq r_0 \end{cases}$$

r_0 is the spherical impenetrable box radius. It is convenient to transform equation (16) adding and subtracting the harmonic oscillator term of frequency w for $r < r_0$:

$$H' = \frac{1}{2m} p'^2 + \frac{1}{2} m w^2 r'^2 - e^2/r' - \frac{1}{2} m w^2 r'^2. \tag{17}$$

Making the change of variable $r' = ar$, where $a = \sqrt{\frac{\hbar}{mw}}$, and the energy equivalence $\hbar w = \frac{me^4}{\hbar^2}$, the Hamiltonian equation (17) is now

$$H' = \hbar w H = \frac{me^4}{\hbar^2} H \tag{18}$$

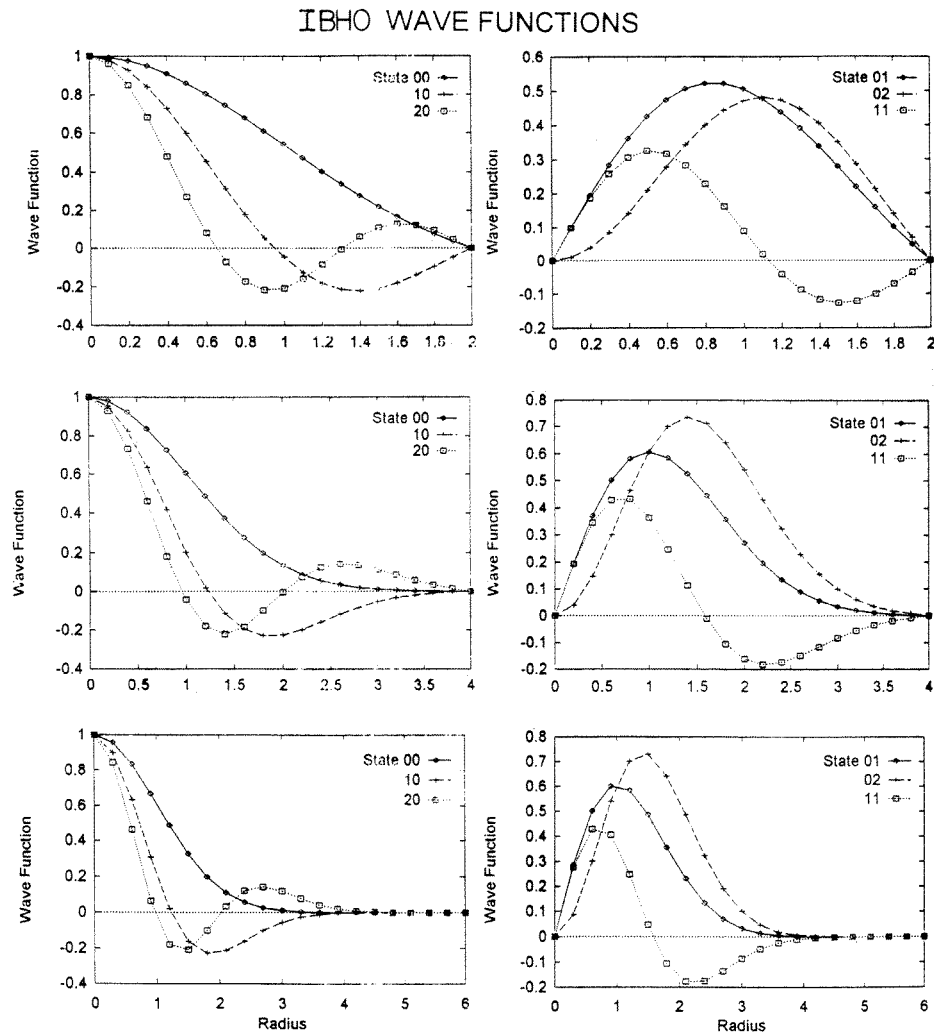


Figure 3. We plot the radial wavefunctions for the ground state and the first five excited states, as function of the box radius r_0 . The wavefunctions plotted have not been normalized to unity. When the radius, r_0 , is small the wavefunctions are compressed, but when r_0 increases they are almost the same that the free wavefunctions. The number of nodes of each wavefunction is the same for every value of r_0 .

where

$$H = H_{bho} - \frac{1}{r} - \frac{1}{2}r^2. \quad (19)$$

The term H_{bho} is the Hamiltonian of the bounded isotropic harmonic oscillator (BIHO) equation (6). The eigenstates ψ of equation (19) have definite l, m thus we may expand them in terms of the BIHO states ψ_{nlm} .

$$\psi = \sum_n |nlm\rangle. \quad (20)$$

To obtain the energy eigenvalues of (19) it is sufficient to diagonalize $\| \langle n'lm|H|nlm\rangle \|$

Table 4. Energy eigenvalues E_{nl} (in atomic units) for confined hydrogen atom as function of the number of quanta N , for $r_0 = 2, 4, 5$ Bohr.

N	E_{00}	E_{10}	E_{20}	E_{30}	E_{40}	E_{50}
$r_0 = 2$						
1	-0.0611					
2	-0.0839	3.4057				
3	-0.1087	3.3776	9.4056			
4	-0.1159	3.3486	9.3708	17.9153		
5	-0.1199	3.3400	9.3398	17.8766	28.9173	
6	-0.1217	3.3349	9.3300	17.8450	28.8763	42.4034
7	-0.1228	3.3325	9.3240	17.8345	28.8448	42.3612
Exact	-0.1250	3.3275	9.3142	17.8161	28.8135	42.2967
$r_0 = 4$						
1	-0.3783					
2	-0.3970	0.8374				
3	-0.4642	0.6220	2.3658			
4	-0.4642	0.4455	2.0791	4.3978		
5	-0.4732	0.4404	1.8981	4.1417	7.0545	
6	-0.4751	0.4277	1.8957	3.9913	6.8500	10.3535
7	-0.4776	0.4270	1.8823	3.9908	6.7159	10.1843
Exact	-0.4833	0.4202	1.8727	3.9665	6.6907	10.0406
$r_0 = 5$						
1	-0.3784					
2	-0.3974	0.8287				
3	-0.4694	0.5778	2.2370			
4	-0.4705	0.2957	1.7409	3.7837		
5	-0.4857	0.2231	1.2669	3.1064	5.4940	
6	-0.4858	0.1579	1.1483	2.5655	4.7643	7.5027
7	-0.4895	0.1523	1.0708	2.4625	4.2573	6.8101
Exact	-0.4964	0.1413	1.0532	2.3823	4.1176	6.2548

for fixed l, m . The matrix elements are

$$\langle n'lm|H|nlm\rangle = E_{bho}\delta_{n'n} - \frac{1}{2}\langle n'lm|r^2|nlm\rangle - \langle n'lm|1/r|nlm\rangle. \quad (21)$$

The term E_{bho} is the energy eigenvalue for the BIHO and some of these values are given in table 2; the calculation of the position expectation values was explained in section 4.

We are interested only in the spherical symmetric states, i.e. 1s, 2s, 3s, etc. For this reason we may fixed $l = m = 0$, thus we need to calculate only the matrix $\| \langle n'00|H|n00\rangle \|$. For up to N quanta we need to diagonalize a $(\frac{1}{2}N + 1)(\frac{1}{2}N + 1)$ matrix, with $n = 0, 1, \dots, \frac{1}{2}N$. The results of our calculation for $r_0 = 2, 4, 5$ bohrs are given in table 4. In this table the ground state and few excited states are reported.

From table 4 we obtained good convergence for the ground state when the number of quanta was 12; the excited states also converge fast for small values of r_0 . However, for $r_0 \geq 5$ the ground state converges first, than the excited states, as in the case of the free hydrogen atom.

6. Conclusions

In a previous work the present method was successfully applied to the problem of a hydrogen atom confined by spherical impenetrable walls [9]. We use the same method to solve the IBHO for different radii of the boxes. We found the energy eigenvalues with a higher precision than previous works, and we also found the correct eigenfunctions, this last assertion is based on the fact that the energy eigenvalues and position expectation values approach the corresponding quantities of the free harmonic oscillator when r_0 increases.

The main advantage of the present method is the possibility of computing the energy eigenvalues, eigenfunctions and the position expectation values with high accuracy for ground and excited states, at a low computational cost.

The calculations resulting from this method could be taken as reference values for future comparisons.

For wavefunctions we can conclude that the total effect of the confinement by impenetrable walls, is a compression of the wave function to the inner of the impenetrable box, but the shape of the confined function is very similar to that of the free function, and the number of nodes of the confined function is the same than the free function. One point we must emphasize, not considered in previous works [38,39], is the following fact: the IBHO, unlike the FIHO, does not have degeneracy in energy, i.e. the impenetrable walls break only the degeneracy in energy, but the symmetry of the problem remains unaltered.

The study of bounded harmonic oscillators is interesting by itself, but it is more important, because it opens the opportunity to solve more complex systems using the IBHO basis set. As an example we solved the confined hydrogen atom.

In the variational calculation of a confined hydrogen atom we can see that the ground state and excited states converge almost at the same time, but when r_0 increases the ground state converges first as in the case of a free hydrogen atom. We conclude, at least for this problem, that the IBHO basis set is as good (for bounded systems) as the FIHO basis set (for free problems).

The method described in this work can be used in other one-dimensional potentials, such as the rotational Morse potential or polynomial potentials with several wells. At present we are working on these problems and future results will be published elsewhere.

Acknowledgments

I appreciate the comments of I Campos, J L Jiménez, S A Cruz, and one of the referees of this work. This work was partially supported by CONACYT, grant no 400200-5-1399-PE.

References

- [1] Ludeña E V 1977 *J. Chem. Phys.* **66** 468
- [2] Ludeña E V 1978 *J. Chem. Phys.* **69** 1770
- [3] Ley-Koo E and Rubinstein S 1979 *J. Chem. Phys.* **71** 351
- [4] Ley-Koo E and Cruz S A 1981 *J. Chem. Phys.* **74** 4603
- [5] Le Sar R and Herrschbach D R 1981 *J. Chem. Phys.* **85** 2798
- [6] Gorecki J and Byers Brown W 1987 *J. Phys. B: At. Mol. Phys.* **21** 403
- [7] Gorecki J and Byers Brown W 1988 *J. Chem. Phys.* **89** 2138
- [8] Weil J A 1979 *J. Chem. Phys.* **71** 2803
- [9] Aquino N 1995 *Int. J. Quantum. Chem.* **54** 107
- [10] Killinbeck J 1981 *Phys. Lett.* **84A** 95
- [11] Artega G A, Maluendes S A, Fernández F M and Castro E A 1983 *Int. J. Quantum. Chem.* **XXIV** 1969

- [12] Fernández F M and Castro E A 1982 *Kinam* **4** 193
- [13] Fernández F M and Castro E A 1982 *J. Math. Phys.* **23** 1103
- [14] Levine J D 1965 *Phys. Rev. A* **140** 586
- [15] Bastard G 1981 *Phys. Rev. B* **24** 4714
- [16] D'Andrea A and Del Sole R 1985 *Phys. Rev. B* **32** 2337
- [17] Kayanuma Y 1988 *Phys. Rev. B* **38** 9797
- [18] Kayanuma Y and Momiji H 1990 *Phys. Rev. B* **41** 10261
- [19] Lippens P E and Lannoo M 1990 *Phys. Rev. B* **41** 6079
- [20] Einevoll G T 1992 *Phys. Rev. B* **45** 3410
- [21] Porras-Montenegro N and Pérez-Merchancano S T 1992 *Phys. Rev. B* **46** 9780
- [22] Moszkowski S A 1955 *Phys. Rev.* **99** 803
- [23] Osborne M F 1951 *Phys. Rev.* **81** 147
- [24] Auluck F C 1942 *Proc. Natl Inst. Sci., India* **8** 147
- [25] Corson E M and Kaplan I 1947 *Phys. Rev.* **71** 130
- [26] Dingle R B 1952 *Proc. R. Soc. A* **212** 47
- [27] Campoy G and Palma A 1984 *Acta Mex. Ciencia Tecnología* **11** 47
Campoy G 1990 *PhD Thesis* México
- [28] Palma A and Campoy G 1987 *Phys. Lett.* **121A** 221
Campoy G, Palma A and Sandoval L 1989 *Int. J. Quantum Chem.: Quantum Chem. Symp.* **23** 355
- [29] Chaudhuri R N and Mukherjee B 1984 *J. Phys. A: Math. Gen.* **17** 277
Vargas R, Garza J and Vela A 1996 *Phys. Rev. E* **53** 1954
- [30] Ley-Koo E, Mateos-Cortés S and Villa-Torres G 1995 *Int. J. Quantum. Chem.* **56** 175
- [31] Rivas-Silva J F, Campoy G and Palma A 1991 *Int. J. Quantum Chem.* **XL** 405
- [32] Campoy G, Palma A and Sandoval L 1989 *Int. J. Quantum. Chem.: Quantum Chem. Symp.* **23** 355
- [33] Aquino N, Palma A, López J L and Rosales M A 1995 *Pramana J. Phys.* **45** 75
- [34] Kothari D S and Auluck F C 1940 *Science and Culture* **6** 370
- [35] Auluck F C 1941 *Proc. Natl Inst. Sci., India* **7** 133
- [36] Auluck F C 1941 *Proc. Natl. Inst. Sci., India* **7** 383
- [37] Aguilera-Navarro V C, Ley-Koo E and Zimmerman A H 1980 *J. Phys. A: Math. Gen.* **13** 3585
- [38] Marin J L and Cruz S A 1991 *Am. J. Phys.* **59** 931
- [39] Fernández F M and Castro E A 1981 *Phys. Rev. A* **24** 2883
- [40] Press W H, Flannery B P, Teukolsky S A and Vetterling W T 1986 *Numerical Recipes: The Art of Scientific Computing* (New York: Cambridge University Press)
- [41] Dorn W S and McCracken D D 1972 *Numerical Methods with Fortran IV Case Studies* (New York: Wiley)
- [42] Killingbeck J P 1991 *Microcomputer Algorithms, Action from Algebra* (New York: Hilger)
- [43] Davidov A S 1965 *Quantum Mechanics* (Oxford: Pergamon)
- [44] Merzbacher E 1970 *Quantum Mechanics* (New York: Wiley)
- [45] de Lange O L and Raab R E 1991 *Operator Methods in Quantum Mechanics* (Oxford: Clarendon)
- [46] Abramowitz M and Stegun I A 1964 *Handbook of Mathematical Functions* (New York: Dover)
- [47] Marín J L 1992 *PhD Thesis* UNAM, México unpublished
- [48] Fernández F M and Castro E A 1981 *J. Phys. A: Math. Gen.* **14** L485
- [49] Moshinsky M 1969 *The Harmonic Oscillator in Modern Physics: From Atoms to Quarks* (London: Gordon and Breach)