

The confined two-dimensional hydrogen atom in the linear variational approach

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In this work we analyze the problem of a two-dimensional hydrogen atom confined in a circular region of impenetrable walls. We study the size effect on the energy eigenvalues as a function of the radius of the circle ρ_0 . We used the linear variational method with the basis set of a free particle in a circle. We compare our results with those obtained by perturbation theory and the Rayleigh-Ritz variational method reported previously.

Keywords: Hydrogen atom; quantum confinement; two dimensional systems.

En este trabajo analizamos el problema de un átomo de hidrógeno bidimensional confinado al interior de una región circular de paredes impenetrables. Estudiamos los efectos de tamaño sobre los valores propios de la energía como función del radio del círculo. Usamos el método variacional lineal con la base de la partícula libre en un círculo. Comparamos nuestros resultados con los obtenidos mediante la teoría de perturbaciones y el método Rayleigh-Ritz que habían sido reportados previamente.

Descriptores: Átomo de hidrógeno; confinamiento cuántico; sistemas bidimensionales.

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1. Introduction

Many pages of some journals have been devoted to discussing the problem of free one-dimensional (1D) and two-dimensional (2D) hydrogen atoms [1-18]. For the particular case of 2D hydrogen atom, some authors have used the coulombian potential in two dimensions as the interaction potential between the electron and the nucleus [8-13,16-17], whereas others have used a logarithmic potential [14-15]. These kinds of systems are of much interest in the field of quantum confined systems at the mesoscopic level, in Condensed Matter and Solid State Physics and also in Atomic and Molecular Physics. One of its first applications was developed by Khon and Luttinger [18] 50 years ago, when they studied the 2D hydrogen atom as a limit case of an anisotropic crystal impurity. Recently, the interest in this system has been renewed due mainly to applications, as for example, the study of H-like atoms subject to high magnetic fields [19], very intense and high frequency laser fields [20], quantum wells and superlattice systems [21], thermal compression of 2D atomic hydrogen gas [22], interaction of atomic hydrogen with *Ag* surface phase [23], proton-hydrogen collisions in 2D Cartesian space [24], among others.

In this paper we discuss the problem of a 2D hydrogen atom confined in a circular region of impenetrable walls [25-26], *i.e.* a hydrogen twice confined. First, we consider that both the nucleus and the electron are restricted to move in the same bidimensional plane, and second, the electron motion is confined to the interior of a circular region that is centered around the nucleus. We take the interaction between charges as the coulombian potential. Some authors argue [15,17] that this potential is not physical because it does not obey the Gauss Law in two-dimensions and, instead of this, we must use a logarithmic potential. Certainly, the

coulombian potential does not satisfy the Gauss law in two-dimensions, but for our purpose it is not relevant, because we are going to be dealing with a tridimensional system whose dynamics are restricted to bidimensional planar regions.

The Hamiltonian of the 2D confined hydrogen atom is [25]

$$H' = \frac{p'^2}{2m_0} - \frac{Ze^2}{\rho'} + V(\rho'). \quad (1)$$

where the potential $V(\rho')$ is given by

$$V(\rho') = \begin{cases} 0, & 0 \leq \rho' < \rho'_0, \\ +\infty, & \rho' \geq \rho'_0, \end{cases} \quad (2)$$

where ρ' is the distance from the nucleus to the electron, m_0 is the electron mass and Ze is the nuclear charge. The prime ' indicates variables with dimensions.

The first approximate solution to this problem was given by Aquino and Castaño [25] using first order perturbation theory (PT) to compute the energy for ground state and the two first excited states. The expressions obtained with this approximation are:

$$\begin{aligned} E_{10}(\rho) &= \frac{2.8916}{\rho_0^2} - \frac{3.5135}{\rho_0}, \\ E_{20}(\rho) &= \frac{15.2356}{\rho_0^2} - \frac{4.3576}{\rho_0}, \\ E_{21}(\rho) &= \frac{7.3010}{\rho_0^2} - \frac{2.0540}{\rho_0}, \end{aligned} \quad (3)$$

where the variables without ' are dimensionless variables given by $\rho' = a_B \rho$, in which a_B is the Bohr radius, and the energy is given in hartrees.

These formulas produce good results [25] only for small radii less than 2 au, whereas for radii greater than 2.0 au it

is necessary to use a different approach. An alternative treatment was applied through the Rayleigh-Ritz method. Aquino and Castaño [25] used the following trial functions for the ground state, and the first two excited states:

$$\begin{aligned} R_{10}(\rho) &= e^{-\alpha_1 \rho}(\rho_0 - \rho), \\ R_{20}(\rho) &= e^{-\alpha_2 \rho}[\rho_1(\alpha_2) - \rho](\rho_0 - \rho), \\ R_{21}(\rho) &= \rho e^{-\alpha_3 \rho}(\rho_0 - \rho), \end{aligned} \tag{4}$$

where, α_1 , α_2 and α_3 are variational parameters and $\rho_1(\alpha_2)$ is the node of the radial function R_{20} that is determined by the orthogonality condition $\langle R_{10} | R_{20} \rangle = 0$.

It is well known that the linear variational method is more accurate than PT and Rayleigh-Ritz methods, when the basis set used to diagonalize the Hamiltonian is large. In this work we are going to use the linear variational method with the free particle in a circle basis set to find the energy eigenvalues and eigenfunctions of the 2D confined hydrogen atom.

The rest of this work is organized as follows: In Sec. 2, we apply the linear variational method to the 2D confined hydrogen atom problem. In Sec. 3, we compare the results obtained in this work with those obtained by perturbation theory and the Rayleigh-Ritz method. Finally, in Sec. 4, we give our conclusions.

2. The method

The Schrödinger equation to solve is

$$H' \Psi' = E' \Psi', \tag{5}$$

where H' is the Hamiltonian of Eq. (1), and the wavefunction Ψ' is subjected to the following boundary condition

$$\Psi'(\rho' = \rho'_0, \phi) = 0. \tag{6}$$

It is convenient to introduce a change of variable

$$\rho' = a_B \rho, \tag{7}$$

where ρ is a dimensionless variable and $a_B = \hbar^2/m_0 e^2$ is the Bohr radius. Substituting (7) in (1) we found that

$$H' = \epsilon_0 H, \tag{8}$$

where the new Hamiltonian H is given as

$$H = \frac{p^2}{2} - \frac{Z}{\rho} + V(\rho). \tag{9}$$

This is the Hamiltonian (1) written in natural or atomic units, where $\hbar = m = e = 1$, and from Eq. (5)

$$E' = \epsilon_0 E, \tag{10}$$

where E are the eigenvalues of H and

$$\epsilon_0 = \frac{m_0 e^4}{\hbar^2} = 1 \text{ hartree},$$

is the energy unit.

Before applying the linear variational method, it is convenient to write the Hamiltonian (9) as follows

$$H = H_0 - \frac{Z}{\rho}. \tag{11}$$

In this equation H_0 represents the Hamiltonian of a free particle inside a circle with an impenetrable wall whose energy eigenvalues (in atomic units) and eigenfunctions are well known [19-20].

$$E_{nk}^{(0)} = \frac{(x_{n|k|})^2}{2\rho_0^2}, \quad n=1, 2, \dots, \quad k=0, \pm 1, \pm 2, \dots \tag{12}$$

where n is the quantum radial number, whereas k is the angular quantum number. We must note that for $k \neq 0$ the system is two fold degenerate with eigenfunctions given by

$$\psi_{nk}(\rho, \phi) = \frac{C_{nk}}{\sqrt{2\pi}} J_k(x_{nk} \rho/\rho_0) e^{(ik\phi)}, \tag{13}$$

where J_k is the Bessel function of first kind of order k , x_{nk} is the n th zero of J_k , and the normalization constant is given by

$$C_{nk}^2 = \frac{2}{\rho_0^2 J_{|k|+1}^2(x_{nk})}. \tag{14}$$

The basis set $\{\psi_{nk}\}$ is a complete orthonormal set,

$$\langle \psi_{nk} | \psi_{n'k'} \rangle = \delta_{n'n} \delta_{k'k}, \tag{15}$$

where $\delta_{j'j}$ is the Kronecker delta.

The eigenstates Ψ of Eq. (5) have definite k , so we may expand them in terms of the free particle basis set ψ_{nk} .

$$\Psi = \sum_n a_n |\psi_{kn}\rangle = \sum_n a_n |nk\rangle. \tag{16}$$

For the variational method of the energy, we must minimize the energy

$$\int \Psi^* H \Psi dv$$

subject to the constraint

$$\int \Psi^* \Psi dv = 1,$$

i.e.

$$\delta \left[\int \Psi^* H \Psi dv - \lambda \int \Psi^* \Psi dv \right] = 0, \tag{17}$$

As Ψ is linear in the coefficients a_n , this procedure is equivalent to diagonalising the matrix $|\langle nk | H | n'k \rangle|$ for a fixed

TABLE I. Energy eigenvalues for a few values of the radii ρ_0 of the box and the number N of basis functions.

$\rho = 0.5$				$\rho = 1.0$			
N	$E_{10} (1s)$	$E_{20} (2s)$	$E_{30} (3s)$	N	$E_{10} (1s)$	$E_{20} (2s)$	$E_{30} (3s)$
10	3.919636	52.090189	140.101033	10	-1.328687	10.782790	32.601253
20	3.910523	52.074532	140.077439	20	-1.344187	10.764625	32.575216
30	3.908761	52.071553	140.073078	30	-1.347249	10.761099	32.570303
40	3.908135	52.070498	140.071543	40	-1.348345	10.759841	32.568562
80	3.907524	52.069470	140.070052	80	-1.349420	10.758611	32.566864
100	3.907450	52.069346	140.069872	100	-1.349552	10.758462	32.566658
120	3.907410	52.069278	140.069775	120	-1.349623	10.758381	32.566546
exact[26]	3.907318	52.069124	140.069551	exact[26]	-1.349786	10.758194	32.566289

$\rho = 5$				$\rho = 10$			
N	$E_{10} (1s)$	$E_{20} (2s)$	$E_{30} (3s)$	N	$E_{10} (1s)$	$E_{20} (2s)$	$E_{30} (3s)$
10	-1.755094	-0.130389	0.627801	10	-1.412892	-0.192307	0.003258
20	-1.919101	-0.144237	0.603013	20	-1.750244	-0.210962	-0.011991
30	-1.960842	-0.147357	0.597554	30	-1.866727	-0.216165	-0.015782
40	-1.977082	-0.148532	0.595510	40	-1.918177	-0.218297	-0.017284
80	-1.993950	-0.149731	0.593431	80	-1.976944	-0.220620	-0.018888
100	-1.996090	-0.149881	0.593171	100	-1.984925	-0.220927	-0.019098
120	-1.997267	-0.149964	0.593028	120	-1.989388	-0.221097	-0.019214
exact[26]	-1.999999	-0.150155	0.592697	exact[26]	-2.000000	-0.221500	-0.019488

TABLE II. Energy eigenvalues for few values of the radii ρ_0 of the box and the number N of basis functions.

$\rho = 0.5$				$\rho = 1.0$			
N	$E_{21} (2p)$	$E_{31} (3p)$	$E_{41} (4p)$	N	$E_{21} (2p)$	$E_{31} (3p)$	$E_{41} (4p)$
10	25.213233	93.158157	201.004620	10	5.242815	21.956264	48.743429
20	25.213213	93.158039	201.004254	20	5.242790	21.956128	48.743023
30	25.213211	93.158032	201.004233	30	5.242789	21.956111	48.742999
40	25.213211	93.158030	201.004229	40	5.242788	21.956118	48.742995
50	25.213211	93.158030	201.004229	50	5.242788	21.956118	48.742994
exact[26]	25.213211	93.158030	201.004228	exact[26]	5.242788	21.956118	48.742994

$\rho = 5$				$\rho = 10$			
N	$E_{21} (2p)$	$E_{31} (3p)$	$E_{41} (4p)$	N	$E_{21} (2p)$	$E_{31} (3p)$	$E_{41} (4p)$
10	-0.177109	0.435156	1.456649	10	-0.220363	-0.030396	0.208619
20	-0.177277	0.434764	1.455784	20	-0.221666	-0.031314	0.206902
30	-0.177288	0.434739	1.455730	30	-0.221766	-0.031383	0.206778
40	-0.177291	0.434734	1.455720	40	-0.221784	-0.031395	0.206755
50	-0.177291	0.434733	1.455717	50	-0.221790	-0.031399	0.206749
exact[26]	-0.177291	0.434732	1.455715	exact[26]	-0.221794	-0.031402	0.206744

value of angular momentum k . Substituting Ψ Eq. (16) into (11), we obtain straightforwardly the following matrix elements:

$$\langle n'k|H|nk\rangle = E_{nk}^{(0)}\delta_{n'n} - Z\langle nk|1/\rho|n'k\rangle. \quad (18)$$

where

$$\begin{aligned} \langle nk|1/\rho|n'k\rangle &= C_{nk}C_{n'k}\rho_0 \int_0^1 J_k(x_{nk}u)J_k(x_{n'k}u)du, \quad (19) \end{aligned}$$

with the integration variable u defined as $u = \rho/\rho_0$.

TABLE III. Energy eigenvalues for few values of the radii ρ_0 of the box and the number N of basis functions.

$\rho = 0.5$				$\rho = 1.0$			
N	$E_{32} (3d)$	$E_{42} (4d)$	$E_{52} (5d)$	N	$E_{32} (3d)$	$E_{42} (4d)$	$E_{52} (5d)$
10	49.291771	137.353919	265.089327	10	11.452383	33.246787	65.030182
20	49.291771	137.353915	265.089307	20	11.452383	33.246783	65.030160
30	49.291771	137.353915	265.089306	30	11.452383	33.246783	65.030160
40	49.291771	137.353915	265.089306	40	11.452383	33.246783	65.030160
exact[18]	49.291771	137.353915	265.089306	exact[18]	11.452383	33.246783	65.030160

$\rho = 5$				$\rho = 10$			
N	$E_{32} (3d)$	$E_{42} (4d)$	$E_{52} (5d)$	N	$E_{32} (3d)$	$E_{42} (4d)$	$E_{52} (5d)$
10	0.168965	0.972907	2.197867	10	-0.057438	0.127074	0.420069
20	0.168964	0.972897	2.197824	20	-0.057444	0.127046	0.419978
30	0.168964	0.972897	2.197824	30	-0.057445	0.127045	0.419976
40	0.168963	0.972897	2.197824	40	-0.057445	0.127045	0.419976
exact[18]	0.168964	0.972897	2.197824	exact[18]	-0.057444	0.127045	0.419976

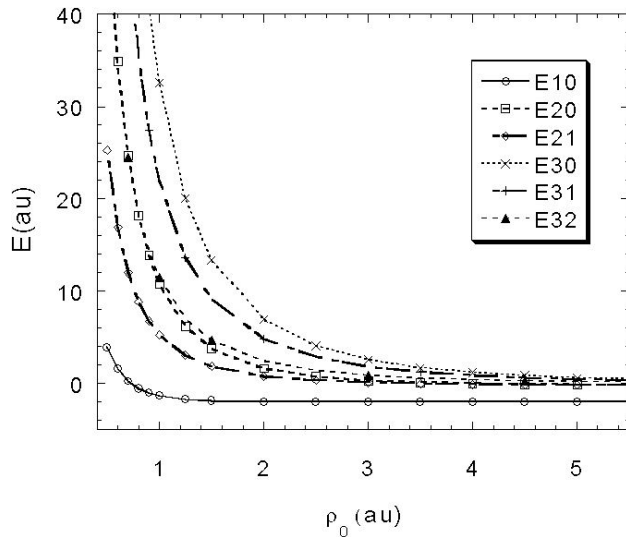


FIGURE 1. Spectrum of the confined 2D hydrogen atom as a function of the Box radius ρ_0 . The energy increases very fast as the box radius diminishes.

Unfortunately, the matrix elements $\langle nk|1/\rho|n'k\rangle$ are not analytical; however they can be easily computed by means a computer program such as Mathematica, Maple, Derive, etc. These kinds of programs have several tools to perform integrations, matrix manipulations and have special built-in functions. We have implemented the above procedure in Mathematica 4.0.

3. Energy eigenvalues and eigenfunctions

In order to calculate the energies of different states, we use the size convergence criteria: for a fixed value of the confinement radius ρ_0 , and for a given value of the angular momentum k , we increase the number of wave functions in the expansion (16), until the computed energies converge to certain definite values with the desired accuracy.

In general, it is necessary to use a larger number of functions to obtain convergence for the states with $l = 0$ than for states with $l \geq 1$, as we can see from Tables I-III. As the radius grows, the size of the basis set increases also. It is necessary to use 120, 50, and 40 functions to assure the convergence of energy eigenvalues for states with $l = 0$, $l = 1$ and $l = 2$, respectively, for $\rho_0 = 10$ au as we can see from Tables I-III.

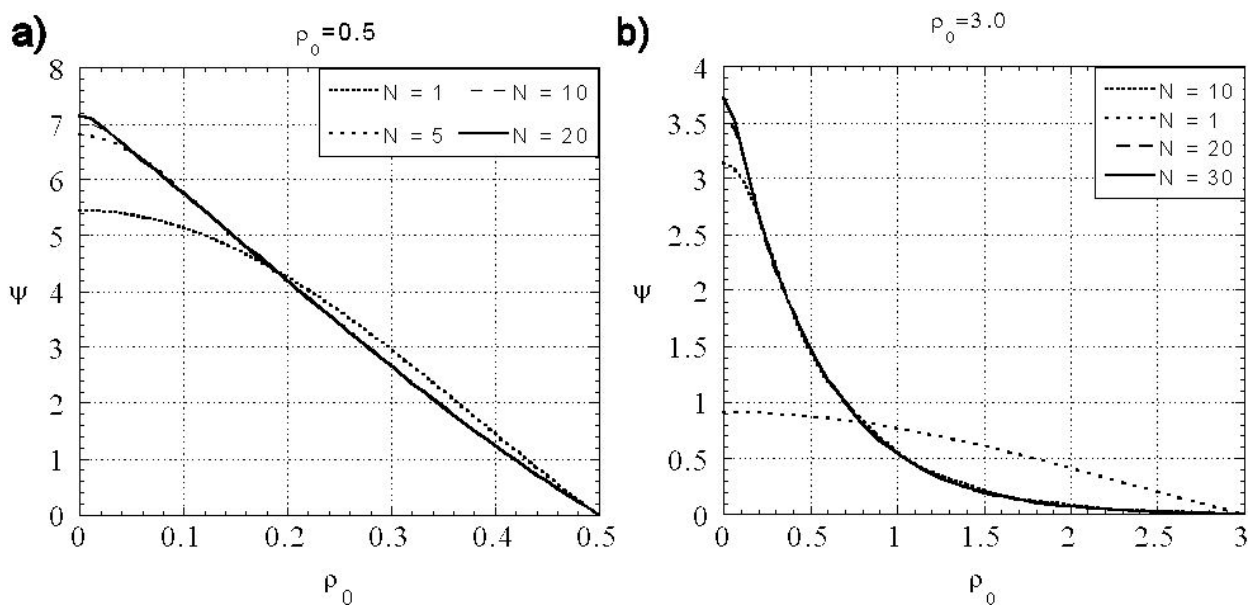
When the box's radius is reduced, the energy of each level increases quickly, as is shown in Fig. 1. An other important fact is that the energy degeneration in the angular momentum is partially broken by the confinement of the system, as it is easy to see from Fig. 1, in which the energy curves for the states $E_{20} (2s)$ and $E_{21} (2p)$ separate as ρ_0 diminishes.

In Table IV, we compare the energy eigenvalues obtained by the Rayleigh-Ritz method with those obtained by the linear variational method for the ground state and the first two excited states. As we can see, the energy values for the ground state obtained by the present method are lower than those obtained by the Rayleigh-Ritz method for boxes with $\rho_0 < 4$, but this situation is reversed for $\rho_0 > 4$, showing that it is necessary to increase the number of functions in the basis set to obtain good convergence in the energy values. For the excited states E_{20} and E_{21} the energy values obtained by the present method are lower than those obtained by the Rayleigh-Ritz method. This is a remarkable fact, because in this problem the energy for the excited states converge before the energy of the ground state.

In Fig. 2a we show the approximate wave function of the ground state for $\rho_0 = 0.5$ au taking $N = 1, 5, 10$, and 20 base functions in its expansion Eq. (16). Upon increasing the number of the basis set functions in the wave function expansion, the obtained energies approach the exact value, and the wave function also approaches the exact one. For $n = 10$ and 20, the graphics of the approximate wave function are

TABLE IV. Energy eigenvalues E_{10} , E_{20} and E_{21} , obtained by present method and those of Ref. 25 as a function of the radii ρ_0 of the box.

ρ	E_{10} (1s)		E_{20} (2s)		E_{21} (2p)	
	Eqs. (4)	present	Eqs. (4)	present	Eqs. (4)	present
0.10	260.0222	253.4580		1479.8064	723.4568	713.5168
0.15	106.6756	104.5180		647.9130	316.3071	312.5308
0.20	55.0090	54.1406		358.9271	175.2189	173.2127
0.25	32.0045	31.6218		226.1667	110.4481	109.1977
0.30	20.0015	19.8193	169.1783	154.5892	75.5229	74.6776
0.40	8.7320	8.6741	90.9425	84.1643	41.1536	40.7037
0.50	3.9259	3.9074	56.0313	52.0693	25.4852	25.2132
0.60	1.5308	1.5264	37.3782	34.9073	17.1033	16.9253
0.70	0.2136	0.2133	26.3286	24.7240	12.1270	12.0040
0.80	-0.5613	-0.5615	19.3153	18.2223	8.9476	8.8592
1.0	-1.3460	-1.3496	11.3233	10.7585	5.2922	5.2428
1.2	-1.6824	-1.6895	7.1696	6.8475	3.3711	3.3414
1.4	-1.8383	-1.8475	4.7695	4.5786	2.2514	2.2328
1.6	-1.9144	-1.9240	3.2814	3.1658	1.5497	1.5377
1.8	-1.9529	-1.9618	2.3103	2.2396	1.0856	1.0778
2.0	-1.9732	-1.9805	1.6515	1.6081	0.7659	0.7608
2.2	-1.9841	-1.9901	1.1907	1.1641	0.5382	0.5349
2.4	-1.9902	-1.9947	0.8603	0.8441	0.3719	0.3697
2.6	-1.9938	-1.9970	0.6184	0.6088	0.2476	0.2463
2.8	-1.9959	-1.9980	0.4381	0.4326	0.1531	0.1523
3.0	-1.9972	-1.9985	0.3018	0.2987	0.0802	0.0798
3.4	-1.9986	-1.9986	0.1160	0.1154	-0.0218	-0.0219
3.8	-1.9992	-1.9983	0.0018	0.0022	-0.0867	-0.0867
4.0	-1.9994	-1.9975	-0.0384	-0.0379	-0.1101	-0.1101

FIGURE 2. Ground state wavefunction of confined 2D hydrogen atom for $\rho_0 = 0.5$ au and $\rho_0 = 3.0$ au. See the text for an explanation.

superposed almost entirely. This behavior is maintained for a number greater than 20 base functions, indicating that there is a good convergence of the ground state wavefunction for this radius. In Fig. 2b shows the approximate ground state wave function for $\rho_0 = 3$ au, taking 1, 10, 20, and 30 functions in its expansion Eq. (16). The above comments also apply in this case but, as we can see when ρ_0 grows, it is necessary to take a greater number of basis set functions in the expansion Eq. (16) to guarantee its convergence.

As we mentioned above, the calculations were carried out on an IBM PC with a processor of 900 MHz and using Mathematica 4.0. The greatest amount of time is consumed in the computation of the matrix elements, with the diagonalising of the Hamiltonian matrix and the output of the eigenvalues being very fast. An interesting fact we could mention is that for $l = 0$ states at $\rho_0 = 10$ au, using $N=120$ basis set functions, the computation took about 2 hours.

4. Conclusions

In this work, we showed a systematic way to obtain the energy eigenvalues of the 2D confined hydrogen atom by diagonalising the Hamiltonian matrix in the free particle basis set, which is a complete and orthogonal basis set. The values obtained by this procedure are more accurate than those obtained by the Rayleigh-Ritz method for boxes with radii less than 4 au. The present method is numerically stable for all

values of ρ_0 , but the Rayleigh-Ritz method becomes numerically unstable for the $2s$ state for $\rho_0 < 1$ au, and it is necessary to make an approximation of the wave function before it is possible to compute the energy values. As the box radius ρ_0 grows, it is necessary to use many wave functions of the basis set to assure the convergence of the energy eigenvalues and eigenfunctions of the 2D confined hydrogen atom. For this reason for a larger ρ_0 , it is more efficient to use the Rayleigh-Ritz method. In addition, the trial functions (Eq. 4) tend asymptotically to the exact wavefunctions of the free 2D hydrogen atom.

However, the interesting behaviour of this system is precisely in the region $\rho_0 \leq 5$ au. We also showed that the states with angular momentum $l \neq 0$ converge faster than those with $l = 0$.

The confinement breaks the degeneracy between states with the same n but different l . This implies that new transitions between states can appear, as for example the transitions $2s \longleftrightarrow 2p$, $3s \longleftrightarrow 3p$, $3p \longleftrightarrow 3d$, etc. at small values of $\rho_0 (\leq 2)$. The computation of these kinds of transitions is now being carried out.

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1. R. Loudon, *Am. J. Phys.* **27** (1959) 649.
 2. L.K. Haines and D.H. Roberts, *Am. J. Phys.* **37** (1969) 1145.
 3. M. Andrews, *Am. J. Phys.* **34** (1966) 1194.
 4. J.F. Gomes and A.H. Zimmerman, *Am. J. Phys.* **48** (1980) 579.
 5. R.E. Moss, *Am. J. Phys.* **55** (1987) 397.
 6. M.M. Nieto, *Phys. Rev. A* **61** (2000) 034901.
 7. A modern point of view of this problem where some unphysical predictions of the original model are reexamined are found in: H.N. Núñez Yepez, C.A. Vargas, and A. Salas-Brito, *Eur. J. Phys.* **8** (1987) 189; H.N. Núñez Yepez and A. Salas-Brito, *Eur. J. Phys.* **8** (1987) 307; Martínez-Romero R., C. A. Vargas, A. Salas-Brito, and H.N. Núñez Yepez, *Rev. Mex. Fis.* **35** (1989) 617; U. Oseguera and M. de Llano, *J. Math. Phys.* **43** (1993) 4575.
 8. G.Q. Hassoun, *Am. J. Phys.* **49** (1981) 143.
 9. T.I. Shibuya and C.E. Wulfman, *Am. J. Phys.* **33** (1965) 570.
 10. B. Zaslow and M.E. Zandler, *Am. J. Phys.* **35** (1967) 1118.
 11. J.W.K. Huang and A. Kozycki, *Am. J. Phys.* **47** (1979) 1005.
 12. B.B. Dasgupta, *Am. J. Phys.* **49** (1981) 189.
 13. I.R. Lapidus, *Am. J. Phys.* **49** (1981) 807.
 14. F.J. Asturias and S.R. Aragón, *Am. J. Phys.* **53** (1985) 893.
 15. K. Eveker *et al.*, *Am. J. Phys.* **58** (1990) 1183.
 16. X.L. Xang, M. Lieber, and F.T. Chan, *Am. J. Phys.* **59** (1991) 231.
 17. X.L. Yang, S.H. Guo, F.T. Chan, K.W. Wong, and W.Y. Ching, *Phys. Rev. A* **43** (1991) 1186.
 18. W. Khon and J.M. Luttinger, *Phys. Rev.* **98** (1955) 915.
 19. A.H. MacDonald and D.S. Ritchi, *Phys. Rev B* **33** (1986) 8336.
 20. J.R.V. De Aldana and L. Roso, *J. Phys. B: Atomic, Molecular and Optical Physics* **33** (2000) 3701.
 21. V.M. Villalba and R. Pino, *J. Phys.: Condens. Matter* **8** (1996) 8067.
 22. S. Vasilyev, J. Järvinen, A.I. Safonov, and S. Jaakkola, *Phys. Rev. A* **69** (2004) 023610.
 23. O. Kubo, J.T. Ryu, M. Katayama, and K. Oura, *Phys. Rev. B* **69** (2004) 045406.
 24. P. Gavras, M.S. Pindzola, D.R. Schultz, and J.C. Wells, *Phys. Rev. A* **52** (1995) 3868.
 25. N. Aquino and E. Castaño, *Rev. Mex. Fis.* **44** (1998) 628.
 26. N. Aquino, Thesis Doctoral, Universidad Autónoma Metropolitana-Iztapalapa, México, D.F. 1997; N. Aquino, G. Campoy, and A. Flores-Riveros, *Int. J. Quantum Chem.* **103** (2005) 267.