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Numerical self-consistent-field method to solve the Kohn-Sham equations in confined many-electron atoms

Jorge Garza, Rubicelia Vargas, and Alberto Vela
Departamento de Química, División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa,
Apartado Postal 55-534, México Distrito Federal 09340, Mexico

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A method to solve the Kohn-Sham equations numerically in confined many electron atoms is presented. The method combines a very efficient matrix approach to locate approximate orbital eigenvalues with a shooting method to integrate the radial equations, and an extrapolation to further refine the spin-orbital energies. The confinement is imposed on the atom by requiring that the electron density vanishes for distances greater than or equal to a confinement radius R_c. The algorithm is tested with the confined hydrogen atom. The role of local and nonlocal exchange-only functionals in confined many-electron atoms is analyzed and compared with Hartree-Fock results. [S1063-651X(98)14808-0]

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I. INTRODUCTION

Density functional theory (DFT) has become a very important tool to study the electronic structure of atoms, molecules and extended systems [1–4]. From the practical point of view, the Kohn-Sham method [5] is the most successful variant inside DFT, since it has been largely impelled by the resources of current technology and the design of new exchange-correlation functionals. The strategy to solve the differential equations that arise in this theory depends on the boundary conditions imposed on the system. For example, in atoms and molecules, the electronic density is built such that it vanishes at large distances. On the other hand, in the study of solids it is important to use the translation symmetry that the system exhibits in order to impose periodic conditions on the electronic density.

Up to now, few efforts have been made in trying to implement another type of boundary condition for the solution of the Kohn-Sham equations. In particular, under Dirichlet's boundary conditions the electronic density cancels at an arbitrary distance and not exclusively in the infinite, so confining an atom or a molecule. These boundary conditions can be used to simulate the effect of high pressure in the electronic structure of atoms or molecules, and, thus, to analyze the equation of state under extreme conditions.

Imposing these boundary conditions on atoms is not new. A great amount of work related to the hydrogen atom [6–20] under these conditions exists, and fewer authors have studied the helium atom [16,17,21,22]. To the authors' knowledge, there are only two papers dealing with the variational solution of the electronic structure of many-electron atoms under confinement. One of these is related with the Hartree-Fock (HF) solution [23], and the other one with the Kohn-Sham [24] solution of confined many-electron atoms.

In order to carry out the study at the HF level, Ludeña [23] used Slater-type orbitals within the formalism of Roothan and Bagus [25]. He imposed the confinement by multiplying the basis functions by a cutoff function such that the wave function cancels at a given distance. This methodology was applied for atoms of the first row in the Periodic Table, and centers its attention on the behavior of the total and orbital energies of these atoms as a function of the confining radius. Using the same methodology, electron correlation was included by performing configuration interaction (CI) calculations [22]. Unfortunately, due to the intrinsic computational difficulties of the CI method, Ludeña and Gregory only reported results for two electrons atoms.

On the other hand, Boeyens [24] solved the Hartree-Fock-Slater equations, modifying the Herman-Skillman code [26] in order to incorporate a cutoff function like Ludeña, but with a different functional form. This allowed Boeyens to obtain the electronic structure of confined atoms over the whole Periodic Table.

The main objective of this work is to present a methodology that allows one to solve the spin-polarized Kohn-Sham equations for atoms, imposing Dirchlet's boundary conditions. To properly compare the results of the proposed approach with the results reported by Ludeña and Boeyens, only exchange functionals are considered in the present work.

This work is organized as follows. In Sec. II, a brief description of Kohn-Sham theory, and the numerical approach to solve these equations subjected to Dirichlet's boundary conditions, are presented. To show the reliability of the algorithm proposed, in Sec. III results for the hydrogen atom in a spherical box are presented, and they are compared with previous works. Confinement effects on several atomic properties of many-electron atoms using an exchange-only formalism are presented and discussed in Sec. IV. Conclusions are contained in Sec. V.

II. THEORETICAL AND NUMERICAL APPROACH

Within spin-polarized DFT [1], Kohn-Sham(KS) equations are obtained by minimizing the functional (in atomic units)

$$E_{\mathrm{KS}}[\rho^{\alpha},\rho^{\beta}]=T_s[\{\phi_i^{\sigma}\}]+J[\rho^{\alpha}(\mathbf{r})+\rho^{\beta}(\mathbf{r})]+E_{\mathrm{xc}}[\rho^{\alpha},\rho^{\beta}]+\int d\mathbf{r}[\rho^{\alpha}(\mathbf{r})+\rho^{\beta}(\mathbf{r})]v(\mathbf{r}), \tag{1}$$

subject to the orthonormality constraint for the set $\{\phi_i^{\sigma}\}$ of KS spin orbitals. In Eq. (1), the first term

$$T_s[\{\phi_i^\sigma\}] = \sum_{\sigma=\alpha,\beta} \sum_i^{occ} \int d\mathbf{r}\, \phi_i^{\sigma *}(\mathbf{r}) \left(-\tfrac{1}{2}\nabla^2\right) \phi_i^\sigma(\mathbf{r}) \quad (2)$$

corresponds to the kinetic energy of noninteracting electrons with the same electron density $\rho(\mathbf{r})$ of the fully interacting system, $J[\rho^\alpha+\rho^\beta]$ is the classical electron-electron Coulombic interaction, $E_{\mathrm{xc}}[\rho^\alpha,\rho^\beta]$ is the exchange-correlation energy functional, and the last term corresponds to the contribution due to the external potential $v(\mathbf{r})$. For atomic systems, $v(\mathbf{r})$ is given by $-Z/r$, where Z is the nuclear charge. In KS theory [1,5], the total electron density $\rho(\mathbf{r})$ is written as

$$\rho(\mathbf{r}) = \sum_{\sigma=\alpha,\beta} \rho^\sigma(\mathbf{r}), \quad (3)$$

where the σ-spin density $\rho^\sigma(\mathbf{r})$ is given by

$$\rho^\sigma(\mathbf{r}) = \sum_i^{occ} |\phi_i^\sigma(\mathbf{r})|^2, \quad \sigma=\alpha,\beta, \quad (4)$$

with the sum running over all occupied σ-spin orbitals.

After minimizing Eq. (2.1) with the constraints, one obtains KS equations

$$\{-\tfrac{1}{2}\nabla^2 + v_{\mathrm{H}}(\mathbf{r}) + v_{\mathrm{xc}}^\sigma[\rho^\alpha,\rho^\beta] + v(\mathbf{r})\}\phi_i^\sigma(\mathbf{r}) = \epsilon_i^\sigma \phi_i^\sigma(\mathbf{r}), \quad (5)$$

where $v_{\mathrm{xc}}^\sigma[\rho^\alpha,\rho^\beta]$ is the functional derivative of the exchange-correlation energy functional with respect to the σ-spin density, and

$$v_{\mathrm{H}}(\mathbf{r}) = \int d\mathbf{r}' \frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \quad (6)$$

For spherically symmetric external potentials, such as those in atomic species, KS spin orbitals can be expressed in terms of spherical harmonics $Y_{lm}(\hat{\mathbf{r}})$ as

$$\phi_{nlm}^\sigma(\mathbf{r}) = R_{nl}^\sigma(r) Y_{lm}(\hat{\mathbf{r}}), \quad (7)$$

where $R_{nl}^\sigma(r)$ are the radial parts that are solutions of the KS radial equations

$$-\frac{1}{2}\frac{d^2R_{nl}^\sigma}{dr^2} - \frac{1}{r}\frac{dR_{nl}^\sigma}{dr} + v_{\mathrm{eff}}^\sigma(r) R_{nl}^\sigma = \epsilon_{nl}^\sigma R_{nl}^\sigma. \quad (8)$$

In this later expression, $v_{\mathrm{eff}}^\sigma(r)$ corresponds to the spherical average of the effective potential,

$$v_{\mathrm{eff}}^\sigma(r) = \frac{l(l+1)}{2r^2} + v_H(r) + v_{\mathrm{xc}}^\sigma(r) - \frac{Z}{r}. \quad (9)$$

By transforming Eq. (8) in the usual manner, i.e., defining $y_{nl}^\sigma(r) = rR_{nl}^\sigma(r)$, KS radial equations take the form

$$-\frac{d^2 y_{nl}^\sigma}{dr^2} + 2[\epsilon_{nl}^\sigma - v_{\mathrm{eff}}^\sigma(r)] y_{nl}^\sigma = 0. \quad (10)$$

It should be noted that, due to the spherical average, KS spin orbitals are labeled by the quantum numbers *n* and *l*, and thus, they are degenerate in *m*, i.e., the multiplet structure is not considered in this work.

Now, confinement is introduced by requiring that the total electron density vanishes at the boundaries of the spherical shell that surround the atomic species, that is,

$$\rho(\mathbf{r}) = \begin{cases} \rho(\mathbf{r}) & \text{if } r < R_c \\ 0 & \text{if } r \geqslant R_c, \end{cases} \quad (11)$$

where R_c is the radius of the confining sphere. To guarantee this condition, Eqs. (10) are solved subjected to Dirichlet's boundary conditions

$$y_{nl}^\sigma(0) = y_{nl}^\sigma(R_c) = 0. \quad (12)$$

For free atoms, the conventional procedure to solve Eqs. (10) is by means of shooting methods [27]. These methods require trial eigenvalues to start the inward and outward integrations, and, by an iterative process, they are further refined. In the case of free atoms, Clementi and Roetti's [28] atomic tables or hydrogenic estimates are an excellent source of trial values to start solving KS radial equations. However, in confined atomic systems the one-electron levels change very fast with confinement, differing substantially from the asymptotic values. This latter fact constitutes a drawback in solving the KS radial equations with well known conventional programs such as Herman and Skillman's. An alternative to this problem is to use an efficient method to locate approximate eigenvalues, that afterwards are used in a shooting method to obtain the eigenfunctions and refine the eigenvalues.

In this work, the method proposed by Lindberg [29] to obtain eigenvalues of one-dimensional quantum problems is used. Lindberg's approach is very fast in locating approximate eigenvalues when Dirichlet's boundary conditions are imposed. This algorithm is based on finite differences, and, being a global (matrix) method, does not require trial eigenvalues as input. To apply the eigenvalue finding theorems, two conditions must be satisfied: (i) the differential equations have to be expressed as

$$\frac{d^2 y_i}{dx^2} + [\lambda_i - V(x)] y_i = 0, \quad (13)$$

where $\{y_i\}$ and $\{\lambda_i\}$ are the sets of eigenfunctions and eigenvalues, respectively, and $V(x)$ is a known function of the independent variable x. (ii) Equation (13) has to be discretized in an equally spaced mesh. For atomic systems, the nature of the external potential strongly suggests the use of a dense mesh in the nuclear vicinity and a sparse mesh in the asymptotic region. Trying to comply with the second requirement mentioned above, several transformations have been attempted to write KS radial equations in the form dictated by Eq. (13) and, at the same time, producing a radial mesh that is dense close to the nucleus, but these efforts have been unsuccessful. Even though this drawback is relevant for free or almost free atoms, when the confining radius is small, an equally spaced mesh is appropriate.

TABLE I. Orbital energies of the confined hydrogen atom for two confinements and several values of the grid step (h). All quantities are in atomic units.

		$R_c=2.0$		
h	$1s$	$2s$	$2p$	$3d$
0.020	-0.12498315	3.32721121	1.57595683	3.32741401
0.010	−0.12499579	3.32743467	1.57600330	3.32748537
0.005	−0.12499895	3.32749053	1.57601491	3.32750321
Extrapolated	−0.12500000	3.32750919	1.57601879	3.32750917
Ref. [19]	−0.12500000	3.32750916	1.57601879	–
		$R_c=8.0$		
0.020	−0.49996260	−0.08473741	−0.10445054	0.04605796
0.010	−0.49997197	−0.08473839	−0.10445019	0.04605818
0.005	−0.49997432	−0.08473864	−0.10445010	0.04605823
Extrapolated	−0.49997510	−0.08473872	−0.10445007	0.04605825
Ref. [19]	−0.49997510	−0.08473872	−0.10445007	0.04605825

Using the variable $x=2Zr$, KS radial equations can be written as

$$\frac{d^2y^{\sigma}_{nl}}{dx^2}+[\lambda^{\sigma}_{nl}-v^{\sigma}_{\text{eff}}(x)]y^{\sigma}_{nl}=0, \tag{14}$$

where

$$\lambda^{\sigma}_{nl}=\frac{\epsilon^{\sigma}_{nl}}{2Z^2} \tag{15}$$

and

$$v^{\sigma}_{\text{eff}}(x)=-\frac{1}{x}+\frac{l(l+1)}{x^2}+\frac{1}{2Z^2}[v_{\text{H}}(x)+v^{\sigma}_{\text{xc}}(x)]. \tag{16}$$

Discretizing Eq. (14) in an equally spaced mesh comprising N elements, each of length $h=x_c/N=2ZR_c/N$, Lindberg's theorems can now be applied to locate the eigenvalues efficiently. Since Lindberg's method is based on Numerov's discretization [30], the error in the eigenvalues is h^4. However, for Coulombic potentials the error is h^2 [31]. Thus a shooting method based on central differences was used to integrate the differential equations and further refine the eigenvalues. Again, the error in this method is h^2 [32]. Originally Lindberg used inverse iteration to find the eigenfunctions, but in several tests it was found that the shooting method was faster than inverse iteration. The shooting method used in the present work relies on the three-term recurrence relation

$$y^{\sigma}_{nl}(j+1)=-y^{\sigma}_{nl}(j-1)+y^{\sigma}_{nl}(j)\{2-h^2F^{\sigma}_{nl}(j)\},$$
$$j=1,2,\ldots,N-1, \tag{17}$$

with

$$y^{\sigma}_{nl}(j)=y^{\sigma}_{nl}(x_j)=y^{\sigma}_{nl}(x=jh) \tag{18}$$

and

$$F^{\sigma}_{nl}(j)=\lambda^{\sigma}_{nl}-v^{\sigma}_{\text{eff}}(j). \tag{19}$$

To use the recurrence relation it is necessary to impose the boundary condition

$$y^{\sigma}_{nl}(0)=y^{\sigma}_{nl}(x=0)=0, \tag{20}$$

and assign a value to $y^{\sigma}_{nl}(1)=y^{\sigma}_{nl}(x=h)$. An alternative to obtain this value is to use a power series expansion to know the behavior near the nuclei, as used by Slater [33] or Froese-Fischer [27]. Another way is to propose that $y^{\sigma}_{nl}(1)=h$, due to the fact that Eq. (14) is a linear differential equation [31]. The eigenfunction is obtained when the eigenvalue λ^{σ}_{nl} is such that $y^{\sigma}_{nl}(N)=0$. Finally, each eigenfunction is normal-

TABLE II. Dependence on the step *(h)* of the expectation values $\langle r^{-1}\rangle$ and $\langle r^2\rangle$ for the lowest lying orbitals of the hydrogen atom in a spherical box of radius $R_c=2$. All quantities are in atomic units.

		$\langle r^{-1}\rangle$			$\langle r^2\rangle$	
h	$1s$	$2s$	$2p$	$1s$	$2s$	$2p$
0.020	1.53515887	1.64630145	0.97234256	0.87482700	1.33207073	1.40566596
0.010	1.53516100	1.64627797	0.97234310	0.87482580	1.33208553	1.40566534
0.005	1.53516153	1.64627210	0.97234324	0.87482549	1.33208923	1.40566519
Extrapolated	1.53516169	1.64627016	0.97234328	0.87482539	1.33209043	1.40566515
Ref. [19]	1.53516171	1.64627014	0.97234328	0.87482539	1.3320904	1.405663

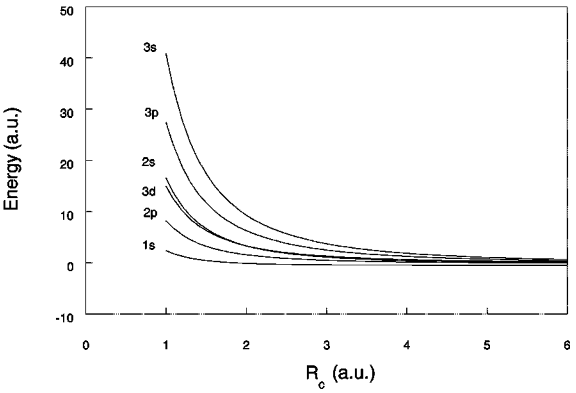

FIG. 1. Orbital energies for the hydrogen atom in a spherical box.

ized using a numerical integration based on the composed Simpson rule [32], requiring an odd number of points in the mesh.

To avoid the problem of having meshes with an unmanageable number of points, a Richardson's extrapolation scheme was implemented [31,32]. In this scheme, solutions are calculated for several steps $(h_1, h_2, \ldots, h_{\mathrm{Ns}})$, and eigenvalues and eigenfunctions are extrapolated to $h=0$. Experience shows that three steps (Ns=3) with $h_1=0.02$ and two successive bisections of this value are enough to achieve nine digit accuracy in the eigenvalues.

It is worth mentioning that several aspects of the original Herman-Skillman code were preserved. For instance, the Thomas-Fermi potential is used to start self-consistency, and the mixing scheme and criteria to achieve self-consistency are basically the same as those used by Herman and Skillman. Integration subroutines were replaced by quadratures based in the composed Simpson rule. In this way, three self-consistent calculations are done, storing the eigenfunctions and eigenvalues that are further used in Richardson's extrapolation to obtain the final solution.

III. HYDROGEN ATOM IN A SPHERICAL BOX

The confined hydrogen atom has been extensively studied with different analytical and numerical techniques, and thus is a good testing ground for the approach proposed in Sec. II. To show the sensibility of the method to the grid step, in Table I the $1s$, $2s$, $2p$, and $3d$ orbital eigenvalues corresponding to three step values and two confining radii are reported and compared with an accurate calculation recently reported in the literature. The extrapolated values obtained using the results for these steps is also reported. As it can be seen, the extrapolated values are in almost complete agreement with those reported in Ref. [19]. As expected, coarse meshes $(h=0.02)$ provide results that deviate more from the ''exact'' extrapolated values. These results validate the use of Richardson's extrapolation scheme with steps $h_1=0.02$, $h_2=h_1/2=0.01$, and $h_3=h_1/4=0.005$ to calculate very accurate orbital energies of confined atoms. It is worth to note that for negative eigenvalues the ''exact'' value $(h \rightarrow 0)$ is a lower bound while the situation is reversed when $\epsilon_i > 0$. A similar behavior has been observed in anharmonic potentials [34] and is a consequence of the nonvariational nature of the finite-differences method.

TABLE III. Total energy of the helium atom for several confinements, using two exchange functionals. All quantities are in atomic units.

R_c	LSDA	BECKE	HF[a]
1.0	1.354	1.112	1.061
2.0	−2.384	−2.542	−2.563
3.0	−2.682	−2.826	−2.831
4.0	−2.718	−2.859	−2.859
5.0	−2.723	−2.863	−2.861
6.0	−2.724	−2.863	−2.862

[a] Reference [23].

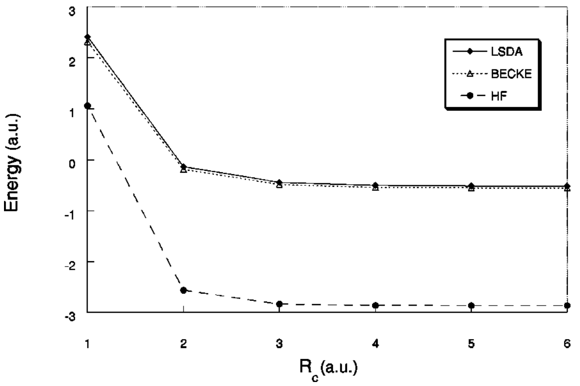

FIG. 2. Exchange-only density functional and Hartree-Fock orbital energies for the ground state of the helium atom in a spherical box.

To test the quality of the wave functions, in Table II the $\langle r^{-1} \rangle$ and $\langle r^2 \rangle$ expectation values of the $1s$, $2s$, and $2p$ orbitals confined in a spherical shell of radius $R_c=2$ are presented. In general, these results are in good agreement with those reported by Aquino [19], but care should be taken in this comparison since these latter values were obtained by numerical differentiation of the eigenvalues, while those presented in this work were calculated by numerical integration.

The behavior of several states as a function of confinement is depicted in Fig. 1. These eigenvalues were calculated using Richardson's three-point extrapolation with $h_1=0.02$, and the bisection procedure mentioned above. A first salient feature is that confinement breaks the existing accidental degeneracy of the free hydrogen atom. Furthermore, states with the same n and different l quantum numbers cross over, while those with the same l never cross. Another known feature of the highly confined hydrogen atom, that is reproduced by the method proposed here, is that the level ordering of the confined atom is noticeably different from that corresponding to the free atom. Again, all these findings are in complete agreement with previous works [7,18].

IV. MANY-ELECTRON ATOMS

In this section, results for He, Ne, and Na neutral atoms under confinement are presented within an exchange-only formalism. The role played by the structure of the exchange functional is analyzed by performing two types of calculations. The local spin density approximation (LSDA) [35] and a semilocal or generalized gradient approximation using

TABLE IV. Total energy of the neon atom for several confinements, using two exchange functionals. All quantities are in atomic units.

R_c	LSDA	BECKE	HF[a]
1.0	−101.512	−102.810	−102.943
1.5	−122.041	−123.206	−123.310
2.0	−126.079	−127.199	−127.231
2.5	−127.076	−128.182	−128.160
3.0	−127.357	−128.458	−128.415
3.5	−127.445	−128.545	−128.495
4.0	−127.474	−128.574	−128.523
4.5	−127.485	−128.584	−128.547

[a] Reference [23].

Becke's exchange functional (BECKE) [36] were tested. All calculations reported were done with the three-point extrapolation scheme described in Sec. III using an initial step value of 0.02. It is worth noting that for very large confinements the total number of mesh points is rather large.

DFT total energies for the ground state of helium under confinement are presented and compared with HF calculations in Table III. The behavior of the total energy of He as a function of confinement is the same for all theoretical levels tested: there is a sharp increase below $R_c=3.0$, and decreases smoothly above this value. As it can be seen, LSDA total energies are the greatest. These results reveal that density inhomogeneities are important, becoming more significant at small confinements. Becke's exchange functional was parametrized to reproduce HF data of noble gases, and the results presented here for helium show that this functional provides essentially the same results as HF, even when the radius of the spherical shell is small.

The behavior of DFT and HF orbital energies for the 1s level of helium is depicted in Fig. 2. LSDA and BECKE behave in a very similar fashion for the whole range of confinements considered, and they differ considerably from HF.

Results for the ground state total energies of neon are presented in Table IV. Similarly to helium, LSDA total energies are considerably greater than HF; discrepancies are larger at small confinements. Semilocal total energies are closer to those obtained with the HF method. Notice that, for both atoms, Becke's total energies are smaller than HF for $R_c \rightarrow \infty$, while for small confinements, these semilocal total energies are larger that those corresponding to HF orbital energies.

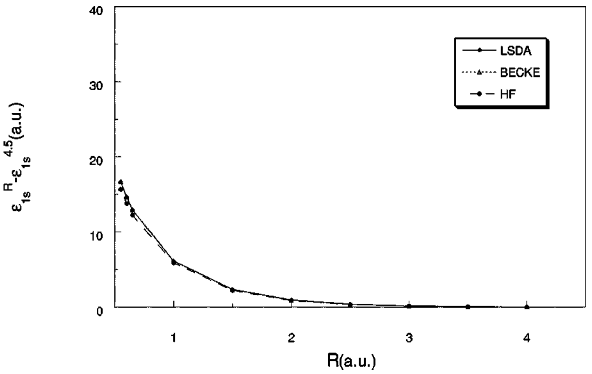

FIG. 3. Differences $\epsilon_i^R - \epsilon_i^{4.5}$ for the 1s orbital energy in the neon atom, using exchange-only density functionals and Hartree-Fock orbital energies.

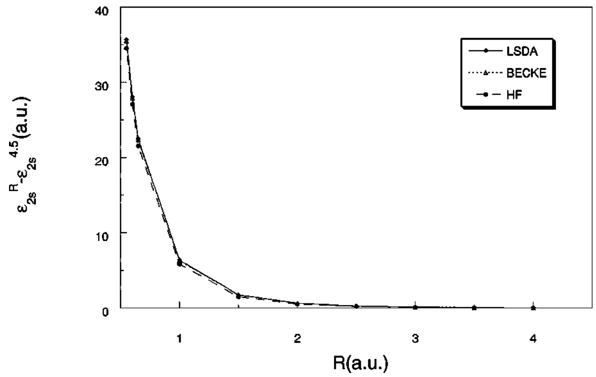

FIG. 4. Differences $\epsilon_i^R - \epsilon_i^{4.5}$ for the 2s orbital energy in the neon atom, using exchange-only density functionals and Hartree-Fock orbital energies.

To see the effect of confinement on the orbital energies, and to compare with Ludeña's results [23], in Figs. 3–5 the differences $\epsilon_i^R - \epsilon_i^{R_0}$, where $R_0=4.5$, are depicted. From these figures it is found that the core level (1s) is less sensitive to confinement than valence levels (2s and 2p). Although DFT and HF orbital eigenvalues have a different physical meaning, their behavior with respect to confinement is similar.

Recently, Boeyens presented Hartree-Fock-Slater results for the confined sodium atom. As pointed out in Sec. I, this author modified Herman and Skillman's code, and used a cutoff function to incorporate the confining conditions. Thus, LSDA calculations for the ground state of sodium were carried out to compare with results reported by Boeyens. The ground state orbital energies of the confined sodium atom are depicted in Fig. 6. According to the observation made in the previous paragraph, concerning the effect of confinement on valence and core levels, it is seen that the 3$s(\alpha)$ orbital is far more sensitive to confinement than the 1$s(\alpha)$, 2$s(\alpha)$, and 2$p(\alpha)$ orbitals. This behavior is in contradiction with that presented by Boeyens, where the 3s level is almost insensitive to confinement. Trying to resolve this discrepancy, several tests were done with different steps, but no important changes from those depicted in Fig. 6 were found. Thus, it is

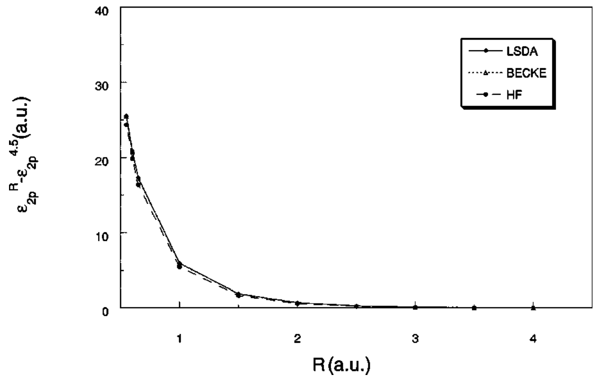

FIG. 5. Differences $\epsilon_i^R - \epsilon_i^{4.5}$ for the 2p orbital energy in the neon atom, using exchange-only density functionals and Hartree-Fock orbital energies.

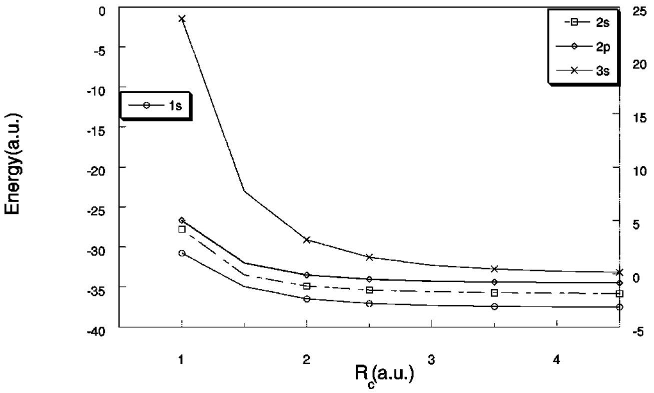

FIG. 6. Alpha spin-orbital energies for the ground state of sodium atom in a spherical box as a function of confinement. The left scale corresponds to $1s(\alpha)$ orbital energy and the right scale to the $2s(\alpha)$, $2p(\alpha)$, and $3s(\alpha)$ orbital energies.

concluded that Boeyens' methodology is in error, or that the cutoff function proposed by this author does not represent correctly the confining conditions.

V. CONCLUSIONS

A method to solve spin-polarized Kohn-Sham equations for atomic systems confined within a spherical box has been presented. Confinement is introduced via imposing Dirichlet's boundary conditions. The method stems from a very efficient matrix method that locates approximate orbital energies to be used as input in a shooting method to find the radial functions and further refine the orbital energies. To have a manageable number of mesh points, a three-point extrapolation scheme is used.

The methodology here presented was tested by applying it to the very well known problem of the hydrogen atom in a spherical box. Results are in full agreement with previous works, showing that the method can be reliably used to study atoms under confinement.

Many-electron atoms under confinement have been studied by solving Kohn-Sham equations in an exchange-only formalism. Two theoretical levels were considered: the local spin density approximation and semilocal (generalized gradient approximation) Becke's functional. Although the total energies obtained with Becke's functional are closer to Hartree-Fock values, the orbital energies differ for every confinement radius. However, the behavior of the orbital energies as a function of confinement is similar for both Hartree-Fock and density functional theory.

Extension of the methodology to include other functionals is straightforward. In particular, the role of electron correlation and self-interaction will be presented elsewhere.

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