Upper and lower bounds on the radial electron density in atoms

J. Antolín*
Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain

A. Zarzo
Departamento de Matemática Aplicada, Escuela Técnica Superior de Ingenieros Industriales, Universidad Politécnica de Madrid, 28006 Madrid, Spain

J. C. Angulo
Departamento de Física Moderna, Facultad de Ciencias, Universidad de Granada, 18071 Granada, Spain
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Rigorous upper and lower bounds on the atomic spherically averaged electron density are found for all radial values in terms of the charge density at the nucleus, $\rho(0)$, and the first few radial expectation values. Moment-theory methods and Chebyshev inequalities are used to obtain the bounds. This type of result can be employed to compare diverse information obtained by using different models, numerical approximations or experimental data. In order to study the goodness of the bounds, a computation in a Hartree-Fock framework is done. The accuracy of our simplest upper bound is similar to a previous one found by King [J. Chem. Phys. **78**, 2459 (1983)] using very different methods and information. Other bounds, containing more information, clearly improve the aforementioned result. The same method allows one to obtain bounds on the derivative and primitive functions of the electron density as well as on the atomic charge.

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I. INTRODUCTION

The study of the atomic charge density $\rho(\mathbf{r})$ has a relevant role in obtaining physical properties of those systems in a density-functional-theory framework [1]. However, not much rigorous information has been obtained about the atomic charge density, in spite of the efforts of many authors during the past years. Because of that, rigorous results, such as lower and upper bounds at any point r, would be desirable.

It is interesting to work with the spherically averaged charge density

$$\rho(r)=\frac{1}{4\pi}\int_{\Omega}\rho(\mathbf{r})d\Omega\ , \tag{1}$$

for which some rigorous properties are known [2,3]. Among them, we should mention its non-negativity and its behavior near and far from the nucleus, i.e.,

$$\begin{aligned}&\rho'(0)=-2Z\rho(0)\ ,\\ &\rho(r)\underset{r\to\infty}{\sim}r^{\beta}e^{-\alpha r}\quad(\text{for } r\to\infty)\ .\end{aligned} \tag{2}$$

Equation (2) is the so-called "Kato cusp condition" [2], which relates the values of the density and its derivative at the nucleus.

Moreover, it has been shown numerically that $\rho(r)$ is a monotonically decreasing function of the radial distance [4] [i.e., $\rho'(r)\leq 0$] and that, to a very good degree of approximation, is also convex [5] [i.e., $\rho''(r)\geq 0$] for all ground-state atoms. Other interesting monotonicity properties have also been studied [6,7].

On the other hand, tight upper and lower bounds to the atomic charge density at the nucleus $\rho(0)$ [5,8] as well as rigorous inequalities among radial expectation values [6,9]

$$\langle r^{\alpha}\rangle=\int r^{\alpha}\rho(\mathbf{r})d\mathbf{r}\quad(\alpha>-3) \tag{3}$$

are also known. Throughout the paper, we use the normalization $\langle r^0\rangle=N$, N being the number of electrons of the atom.

Many numerical calculations of the radial expectation values $\langle r^{\alpha}\rangle$ within different models are found in the literature [10], as well as relationships among them and other significant atomic quantities [9,11,12] (e.g., first ionization potential [13], information entropies [14], frequency moments [15]). Moreover, some of these values are experimentally accessible (e.g., by means of electron [16,17] or photon [18,19] scattering by atoms) and/or physically relevant. Let us mention here that the Langevin-Pauli diamagnetic susceptibility χ is expressed [20] in terms of $\langle r^2\rangle$,

$$\chi=-\tfrac{1}{6}\alpha^2\langle r^2\rangle\ ,$$

where α is the fine-structure constant. On the other hand, the quantity $\langle r^{-1}\rangle$ is proportional [20] to the electron-nucleus attraction energy E_{eN},

$$E_{eN}=-Z\langle r^{-1}\rangle\ ,$$

as well as to the nuclear magnetic screening constant [21] or diamagnetic screening factor σ

$$\sigma=\tfrac{1}{3}\alpha^2\langle r^{-1}\rangle\ .$$

Additionally, one should take into account that the recently obtained [22] relationships among radial expectation values of both position and momentum spaces provided another tool for getting information on the quantities $\langle r^\alpha \rangle$ from the knowledge of $\langle p^\beta \rangle$,

$$\langle p^\beta \rangle = \int p^\beta \gamma(\mathbf{p}) d\mathbf{p} \ .$$

Thus we have relevant but limited information on the radial expectation values of the density, either from experimental data, or by using different models or rigorous relationships among quantities of both position and momentum spaces. In this work it is shown that the knowledge (from any source) of the first few radial expectation values of the density imposes strong restrictions on the values of such density at any point.

This kind of results allows one to study the compatibility of different models, because the restrictions on the density imposed by the knowledge of some moments calculated within a model can be compared with densities provided by other models or calculated by extrapolation of experimental data or numerical approximations.

The aim of this work is to obtain rigorous upper and lower bounds to the spherically averaged density $\rho(r)$ at any point $r \geq 0$, in terms of the above-mentioned quantities $\rho(0)$ and $\langle r^\alpha \rangle$. The results obtained suggest that a greater effort in the knowledge of radial expectation values would be desirable. For illustration, we show the bounds to the atomic charge density $\rho(r)$ by using Hartree-Fock moments, although the validity of the technique is model independent and its usefulness has been pointed out in the preceding paragraph.

Until now, only some upper bounds to $\rho(r)$ based on Block's inequality have been reported [23]. They are expressed in terms of the kinetic energy of the physical system, $T = \langle p^2 \rangle / 2$, and the two radial expectation values of lowest order, namely, $\langle r^{-1} \rangle$ and $\langle r^{-2} \rangle$. The procedure described below has not been previously used in this field to bound the atomic charge density $\rho(r)$. So, we cover the range of intermediate values of r for which rigorous results are very scarce [23]. It is interesting to note that these bounds depend only on a few low-order moments $\langle r^\alpha \rangle$.

This procedure applies the so-called Chebyshev inequalities [24] to some functions related to the charge density $\rho(r)$. These functions are (a) the charge density $\rho(r)$, (b) the cumulative density $\psi(r) = \int_0^r \rho(r) dr$, (c) the number of electrons contained in a sphere of radius r, i.e.,

$$Q(r) = \int_0^r 4\pi r^2 \rho(r) dr \ ,$$

and (d) the first derivative $\rho'(r)$ of the charge density. Related techniques have been applied in other fields, such as, e.g., particle physics [25,26], photoeffect studies in Hilbert space [27], or to bound thermodynamic quantities [28].

In Sec. II a review of results about moment theory, Padé approximants, and orthogonal polynomials is given, in order to show how the bounds are obtained. In Sec. III the results described in the preceding section are applied to the four above-mentioned charge functions. Finally, Sec. IV contains some concluding remarks.

II. CHEBYSHEV BOUNDS FOR THE CUMULATIVE WEIGHT

Many physical quantities of great interest are related to integral transforms of non-negative functions

$$H(z) = \int_0^\infty F(r,z) g(r) dr \ , \quad g(r) \geq 0 \ , \quad r \in [0, \infty) \ . \tag{4}$$

The estimation of these quantities using only a limited number of parameters is an old and controversial problem (see, e.g., Ref. [24]). In its usual form, the known parameters consist of the moments of the weight $g(r)$ or of a differentiable distribution $f(r)$ [24,29],

$$\mu_k = \int_0^\infty r^k g(r) dr = \int_0^\infty r^k df(r) \ , \quad k = 0,1,2, \ldots \ . \tag{5}$$

Moment theory provides approximations or rigorous bounds [30] on the average $H(z)$ of $F(r,z)$ by using the properties of the orthogonal polynomial system associated with the weight $g(r)$. However, sometimes this is not sufficient and information on the actual weight $g(r)$, or on the distribution $f(r)$, is also needed.

The practical and physical situations are such that only a few moments are available, either from experimental measurements or from theoretical calculations, so a unique reconstruction of $f(r)$ is impossible in view of this limited information.

Nevertheless, there are approximation procedures for constructing sequences of functions $g_N(r)$, such that their moments are the known ones

$$\int_0^\infty r^k g_N(r) dr = \mu_k \ , \quad k = 0,1,2, \ldots, N \ , \tag{6}$$

and which eventually converge to the true weight $g(r)$ when N tends to infinity or such that one has the weak convergence for the average

$$H(z) = \lim_{N \to \infty} \int_0^\infty F(r,z) g_N(r) dr \ . \tag{7}$$

Some methods can be used to solve the previous reduced moment problem: orthogonal expansions or reference density methods [31], Bernstein polynomials technique [32], Stieltjes-Chebyshev techniques [33], moment-preserving splines [34], or maximum-entropy techniques [35,36].

In order to obtain bounds for the cumulative weight, i.e., the distribution $f(r)$, we shall use the Stieltjes-Chebyshev procedure related to Padé approximants (PA's) and continued-fraction techniques [33,37,38]. The basic result is that the information contained in the first $N+1$ moments in (6) is sufficient to bound rigorously the cumulative density function $f(r)$ at any point in $[0, \infty)$.

More precisely, the Chebyshev inequalities [24,37,39] provide lower and upper bounds to the values of $f(r)$ through the positive residues of the Padé approximants at points related to the position of the poles.

To obtain these bounds it is convenient to deal with the Stieltjes function

$$H(z) = \int_0^\infty \frac{df(r)}{1 - zr} = \int_0^\infty \frac{g(r)}{1 - zr} dr \ , \quad g(r) \geq 0 \ , \tag{8}$$

which is a particular case of Eq. (4).

The formal [40] series expansion of $H(z)$ is given in

terms of the moments defined in Eq. (5) by

$$H(z)=\sum_{i=0}^{\infty}\mu_i z^i \ . \tag{9}$$

The $[n-1/n]$ Padé approximant to $H(z)$ can be written as

$$[n-1/n](z)=\frac{P_{n-1}(z)}{Q_n(z)}=\sum_{i=1}^{n}\frac{\gamma_i^{(n)}}{1-zr_i^{(n)}} \ , \tag{10}$$

where $P_{n-1}(z)$ and $Q_n(z)$ are polynomials of degree $n-1$ and n, respectively, and can be calculated from the relation

$$H(z)-[n-1/n]=Q(z^{2n}) \ . \tag{11}$$

The parameters $\gamma_i^{(n)}$ and $r_i^{(n)}$ are related to the residues and poles of the PA:

$$[n-1/n]=\sum_{i=1}^{n}\frac{\gamma_i^{*(n)}}{z-r_i^{*(n)}} \ , \quad \gamma_i^{*(n)}<0 \ , \quad r_i^{*(n)}>0 \ , \tag{12}$$

by

$$r_i^{(n)}=\frac{1}{r_i^{*(n)}} \ , \quad \gamma_i^{(n)}=-\gamma_i^{*(n)}r_i^{(n)}>0 \ . \tag{13}$$

The relationship between the moments and the pole positions and residues of the PA is

$$\mu_k=\sum_{i=1}^{n}(r_i^{(n)})^k\gamma_i^{(n)} \ , \quad k=0,1,2,\ldots,2n-1 \ . \tag{14}$$

The sequence $\{q_n\}_{n\geq 0}$ related to the Padé denominators by

$$q_n(z)=z^nQ_n\left[\frac{1}{z}\right] \tag{15}$$

is the orthogonal polynomial family with respect to $g(r)$.

In the same way, we define

$$p_{n-1}(z)=z^{n-1}P_{n-1}\left[\frac{1}{z}\right] \tag{16}$$

so that

$$A_n(z)=\frac{p_{n-1}(z)}{q_n(z)}=\sum_{i=1}^{n}\frac{\gamma_i^{(n)}}{z-r_i^{(n)}} \tag{17}$$

is the n convergent of the continued-fraction approximation to the Stieltjes transform

$$h(z)=\frac{1}{z}H\left[\frac{1}{z}\right]=\int_0^{\infty}\frac{df(r)}{z-r}=\sum_{i=0}^{\infty}\frac{\mu_i}{z^{i+1}} \tag{18}$$

satisfying

$$A_n(z)-h(z)=O\left[\frac{1}{z^{2n}}\right] \ . \tag{19}$$

Many of the bounding properties of the PA are based on the properties of the orthogonal sequence $\{q_n\}_{n\geq 0}$.

In view of Eq. (11) or, equivalently Eq. (19), the PA is associated with the distribution function $f_n(r)$, given by

$$f_n(r)=\begin{cases}0 & \text{if } 0\leq r<r_1^{(n)}\\ \displaystyle\sum_{i=1}^{p}\gamma_i^{(n)} & \text{if } r_p^{(n)}<r<r_{p+1}^{(n)} \quad (1\leq p<n)\\ \displaystyle\sum_{i=1}^{n}\gamma_i^{(n)}=\mu_0 & \text{if } r_n^{(n)}<r \ ,\end{cases} \tag{20}$$

corresponding to a weight function

$$df_n(r)=\sum_{i=1}^{n}\gamma_i^{(n)}\delta(r-r_i^{(n)})dr \ . \tag{21}$$

Such distributions satisfy the so-called Chebyshev inequalities [24,37,39]

$$\begin{aligned}f_n(r_i^{(n)}-0)&\leq f_{n+1}(r_i^{(n)}-0)\\ &\leq f(r_i^{(n)})\\ &\leq f_{n+1}(r_i^{(n)}+0)\\ &\leq f_n(r_i^{(n)}+0) \ .\end{aligned} \tag{22}$$

The previous inequalities indicate that the Stieltjes values defined by

$$f_n(r_i^{(n)})=\tfrac{1}{2}[f_n(r_i^{(n)}+0)+f_n(r_i^{(n)}-0)] \tag{23}$$

converge monotonically with n at their step points to the correct distribution.

In order to obtain bounds on $f(r)$ at any point in the interval of interest $[0,\infty)$ and not only at the points related to the poles of the approximants, we consider new approximants to the formal series expansion of $H(z)$ or $h(z)$ having a pole in an arbitrary prescribed position on $[0,\infty)$. More precisely, we use the approximants

$$\begin{aligned}\tilde{A}_n(z)&=\frac{\tilde{p}_{n-1}(z)}{\tilde{q}_n(z)}\\ &=\frac{p_{n-1}(z)-[q_n(r)/q_{n-1}(r)]p_{n-2}(z)}{q_n(z)-[q_n(r)/q_{n-1}(r)]q_{n-1}(z)} \ .\end{aligned} \tag{24}$$

Although alternative approximants can be devised [37], the denominators of them are the so-called quasiorthogonal polynomials associated with the distribution function $f(r)$, which have the same properties as the system of orthogonal polynomials except the degree of approximation in quadrature formulas [see Eq. (25)].

The real roots $r_i^{(n)}(r)$ and the positive residues $\gamma_i^{(n)}(r)$ of the new approximants satisfy the moment-problem equations

$$\mu_k=\sum_{i=1}^{n}[r_i^{(n)}(r)]^k\gamma_i^{(n)}(r) \ , \quad k=0,1,2,\ldots,2n-2 \ , \tag{25}$$

where $r=r_i^{(n)}(r)$ for some value of i, since by construction r is one of the roots of $\tilde{q}_n(z)$. As indicated above, $r_i^{(n)}(r)$ and $\gamma_i^{(n)}(r)$ are now functions of r, which can be varied at will over the positive real axis. In terms of these values, the approximants take on the form

$$\tilde{A}_n(z)=\sum_{i=1}^{n}\frac{\gamma_i^{(n)}(r)}{z-r_i^{(n)}(r)} \ , \quad \gamma_i^{(n)}(r)>0 \ , \tag{26}$$

which is similar to Eq. (17)

Rigorous upper and lower bounds on $f(r)$ are obtained from the Stieltjes histogram (20), having now a prescribed spectral point $r=r_j^{(n)}(r)$ with weight $\gamma_j^{(n)}(r)$ and $n-1$ additional points $r_i^{(n)}(r)$ and weights $\gamma_i^{(n)}(r)$, in the form of Chebyshev inequalities

$$\begin{aligned} f_n^C(r-0) &\le f_{n+1}^C(r-0) \\ &\le f(r) \\ &\le f_{n+1}^C(r+0) \\ &\le f_n^C(r+0) \ . \end{aligned} \tag{27}$$

A convergent approximation to $f(r)$ is obtained from the Stieltjes value (20) in the form

$$\begin{aligned} f_n^C(r) &= \tfrac{1}{2}[f_n^C(r-0)+f_n^C(r+0)] \\ &= \sum_{i=1}^{j-1} \gamma_i^{(n)}(r)+\tfrac{1}{2}\gamma_j^{(n)}(r) \ , \end{aligned} \tag{28}$$

which is simply the midpoint of the Chebyshev bounds (27) at $r\equiv r_j^{(n)}(r)$, and can be calculated in terms of the polynomials $\tilde{p}_n(z)$ and $\tilde{q}_n(z)$.

By using the derivative of Eq. (28), it has been shown in Ref. [33] that the Chebyshev weights $g_n^{(C)}(r)$ are real, non-negative, convergent to $g(r)$ in the limit $n\to\infty$, for a continuous weight as in our case. Moreover, the nth-order Chebyshev density is continuous in the real axis, has $2n-4$ continuous derivatives there, and supports $2n-2$ moments.

Solutions of Eqs. (14) and (25) are conveniently obtained from considerations on the continued fraction or Padé representation of the Stieltjes integral (8). Several efficient algorithms can be used in practice: the quotient-difference algorithm [41], the product-difference algorithm [29] related to Lanczos's method, or the S-continued-fraction algorithm [41]. We have checked that these three approaches are satisfactory for the small number of moments used in this work (≤ 15), but instabilities can arise when a large number of moments is used.

III. APPLICATIONS TO ATOMIC SYSTEMS

In this section we apply the bounds given by Eq. (27) to four different weight functions related to the atomic electron density [cases (a)-(d) in Sec. I]. On the other hand, it should be mentioned that all numerical calculations have been performed in the Hartree-Fock framework by using Clementi-Roetti data [42].

(a) $g(r)=-\rho'(r)\ge 0$. This is not yet a theoretically proven inequality, but it has been checked numerically for all ground-state atoms [4]. In this case

$$\mu_k \equiv \int_0^\infty r^k g(r)dr = \begin{cases} \rho(0) \ , & k=0 \\ \dfrac{k\langle r^{k-3}\rangle}{4\pi} \ , & k=1,2,\ldots \ . \end{cases} \tag{29}$$

So, we obtain rigorous upper and lower bounds on the distribution function

$$f(r)=\int_0^r[-\rho'(r)]dr=\rho(0)-\rho(r)$$

and therefore on $\rho(r)$, $r\in[0,\infty)$, in terms of $\rho(0)$ and the first radial expectation values of the one-particle density $\rho(r)$.

Two interesting characteristics of the bounds obtained in this way should be noticed. First, they allow one to obtain rigorous information about the behavior of $\rho(r)$ for some specific and relevant values of r (e.g., the Hoffmann-Ostenhof radius [3] $r_{HO}=Z/I$, I being the ionization potential of the atom), where, until now, there has been no information available in the literature. Second, in a similar way as done in the study of Compton profiles [43], one can give upper and lower bounds on parameters such as r_k $(0<k<1)$, which tell us the radius for which the density takes the value $k\rho(0)$.

In Fig. 1, the upper and lower bounds obtained by using 4, 8, and 12 moments and the density function $\rho(r)$ for the neon ground state have been plotted. As could be expected, it shows that the bounds improve (especially the lower ones) when the number of moments considered increases. Moreover, due to the nested structure of the bounds, their arithmetic mean can be considered as a convergent approximation [33] for $\rho(r)$, which could be used in order to compare the method we have followed here with other approximations, such as the maximum-entropy densities [36] or polynomial expansions [31].

On the other hand, as pointed out in Sec. I, some upper bounds to $\rho(r)$ are known (given by King in Ref. [23]). Among the six different types of King upper bounds, we have chosen for comparison the one which is best [44] for intermediate and large values of r. A numerical Hartree-Fock study has been done for all atoms with $Z\le 54$, showing that King's bound (obtained in terms of the kinetic energy $T=\langle p^2\rangle/2$) and our 4-moment bound [constructed from $\rho(0)$, $\langle r^{-1}\rangle$, and $\langle r^{-2}\rangle$] are of similar accuracy. However, if more information is considered, our bounds clearly improve the King one. As an illustration, Fig. 2 shows the behavior of King's bound with respect to the corresponding 4 and 12 moments and for the neon ground state.

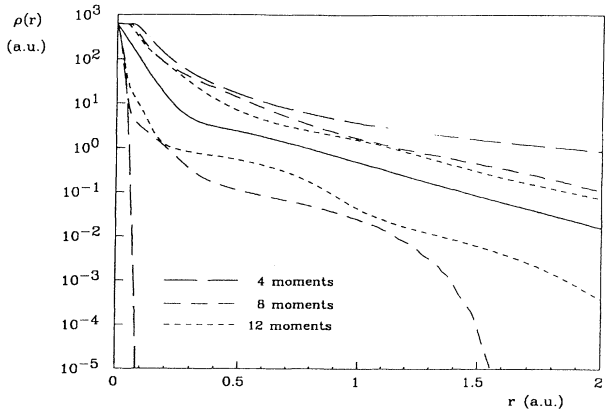

FIG. 1. Spherically averaged charge density $\rho(r)$ (solid line) and upper and lower bounds from 4, 8, and 12 moments for the neon ground state. Atomic units are used.

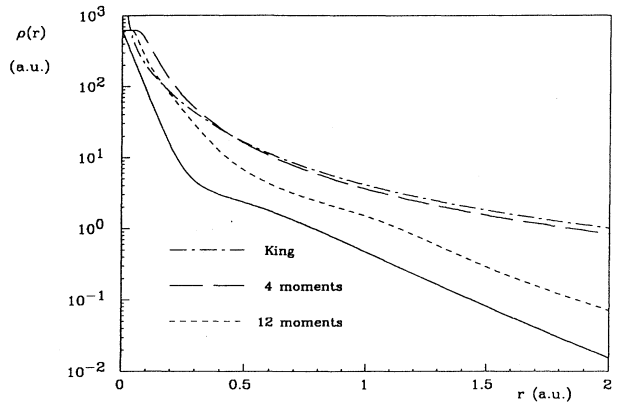

FIG. 2. Comparison between the upper bounds from 4 and 12 moments and the King upper bound (see case A in the last paper of Ref. [23]) for the neon ground state. The solid line represents the spherically averaged charge density. Atomic units are used.

(b) $g(r)=\rho(r)\geq 0$. This is a well-known rigorous property of the electronic density. The moments are now

$$\mu_k=\frac{\langle r^{k-2}\rangle}{4\pi}\ ,\quad k=0,1,2,\ldots\ . \tag{30}$$

The knowledge of the first moments allows us to bound the cumulative density

$$\psi(r)=\int_o^r \rho(r)dr\ ,$$

which shows how the probability density accumulates when r grows. In Fig. 3 the upper and lower bounds from 4, 8, and 12 moments together with the function $\psi(r)$ have been plotted, and also for the neon ground state.

(c) $g(r)=4\pi r^2\rho(r)\geq 0$. This relation allows one to bound the charge [19]

$$Q(r)=\int_0^r 4\pi r^2\rho(r)dr \tag{31}$$

in terms of the moments

$$\mu_k=\int_0^\infty 4\pi r^{k+2}\rho(r)dr=\langle r^k\rangle\ ,\quad k=0,1,2,\ldots\ . \tag{32}$$

This is a relevant quantity because, e.g., it is needed in determining the Thomas-Fermi energy of neutral atoms [19]. However, no information of the type we give here is known in the literature.

Figure 4 includes the behavior of the bounds from 4, 8, and 12 moments and also for the neon ground state. Notice that the above-mentioned nested structure also holds in this case. So, the arithmetic mean of the successive lower and upper bounds can be considered again as approximations for $Q(r)$, which improves when the number of moments considered increases.

(d) $g(r)=\rho''(r)\geq 0$. Convexity is, to a good degree of approximation, a property fulfilled by the electron density of all ground-state atoms [5]. This property allows one to bound $\rho'(r)$ by using this technique together with the cusp condition (2), because

$$\int_0^r \rho''(r)dr=2Z\rho(0)-\rho'(r)\ . \tag{33}$$

In this case the moments are

$$\mu_k=\int_0^\infty r^k\rho''(r)dr=\begin{cases}-\rho'(0)=2Z\rho(0)\ , & k=0\\ \rho(0)\ , & k=1\\ \dfrac{k(k-1)}{4\pi}\langle r^{k-4}\rangle\ , & k=2,3,4,\ldots\ .\end{cases} \tag{34}$$

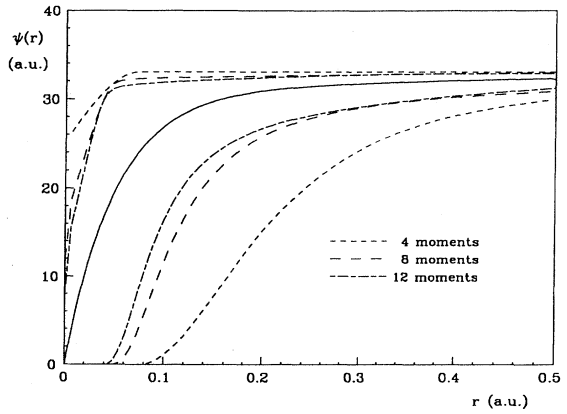

FIG. 3. Cumulative density $\psi(r)$ (solid line) and the corresponding upper and lower bounds obtained by using 4, 8, and 12 moments, for the neon ground state. Atomic units are used.

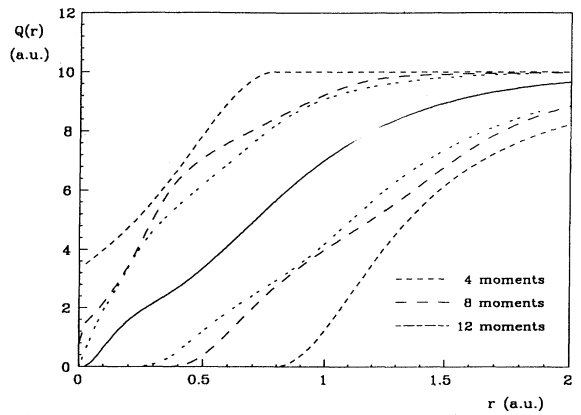

FIG. 4. Neon ground-state charge $Q(r)$ (solid line) and the corresponding upper and lower bounds from 4, 8, and 12 moments. Atomic units are used.

In this way, we have described the information which can be obtained with this method for convex densities. For the sake of completeness we have plotted in Fig. 5 the bounds from 4, 8, and 12 moments together with $-\rho'(r)$.

It is clear that the above results can be extended by means of more restrictive monotonicity properties for functions closely related to $\rho(r)$, e.g., p-order monotonicity [6,7] ($p > 1$), log convexity [45], etc. In particular, if some fermionic density is completely monotonic, it is possible to obtain, by using the same technique, bounds of the Baker-Gammel [46] form $\sum_i A_i \exp(-B_i r)$, where the coefficients A_i and B_i are related again with the residues and poles of the PA associated with the density.

IV. CONCLUDING REMARKS

It has been shown how the knowledge of the first few moments of the derivative of a monotonically decreasing density $\rho(r)$ allows one to obtain rigorous upper and lower bounds on this density for any value of r. These bounds can be systematically improved if the number of known moments increases or if additional information on monotonicity properties of the density is available. Since the bounds are nested, it is also possible to obtain convergent approximations which may be compared with those given by other methods. Moreover, due to the consideration of the approximants given in Eq. (24) having a pole in an arbitrary prescribed position, the method allows one to study how the density decreases for any specific value of the radius.

The test of the bounds in a Hartree-Fock framework suggests that more effort in the model-independent calculations of expectation values would lead to important results. In the same way, the method allows one to study the compatibility of diverse models, numerical approximations, or moment computations (based indirectly on experimental computations).

The method we have used is general and it may be applied to many other problems of the density functional theory. In particular, we should mentioned that it is possible to obtain upper and lower bounds on the Compton profile for several atoms and molecules and, if we consider the moment space, results analogous to those presented in Sec. III can be derived for those physical systems having a monotonically decreasing moment density $\gamma(p)$. This will be done elsewhere.

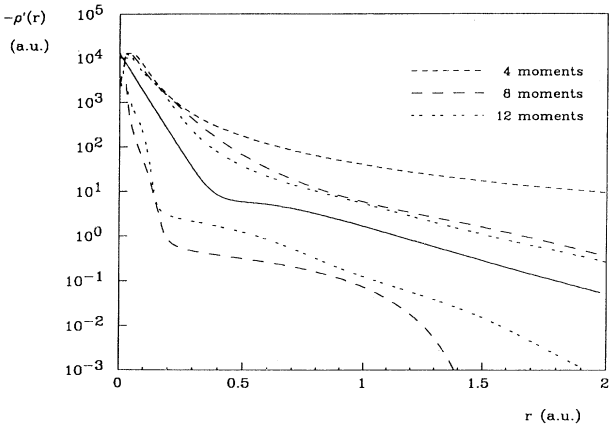

FIG. 5. Derivative of the spherically averaged density $-\rho'(r)$ (solid line) and the corresponding upper and lower bounds from 4, 8, and 12 moments for the neon ground state. Atomic units are used.

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*Permanent address: Dpto. Física Aplicada, E.U.I.T.I.Z., Universidad de Zaragoza, 50009 Zaragoza, Spain.

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