Bounds for the atomic electronic density

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Several upper bound estimates for the atomic electronic density are derived. The bounds are formulated in terms of the kinetic energy and, in some of the cases considered, the expectation values $\langle \Psi \mid r_1^{-1} \mid \Psi \rangle$ or $\langle \Psi \mid r_1^{-2} \mid \Psi \rangle$ are employed. All the inequalities follow from the application of Block's theorem. A numerical test of the bounds has been carried out for some two electron species.

I. INTRODUCTION

There has been considerable activity recently devoted towards the determination of rigorous relationships satisfied by the electronic density. Much of this effort has centered on the determination of bounds for the atomic electronic density,[1-4] investigations of the long-range asymptotic behavior of the electronic density,[5-14] and the derivation of various integral inequalities involving the electronic density.[15-20] The review of Bamzai and Deb[21] provides a survey of some other recent research activity concerning the electronic density.

The purpose of the present study is to expose some new upper bounds for the atomic electronic density. The approach taken involves some ideas due to Block,[22,23] which have not previously been employed in connection with the electronic density. Our objective is to extract the simplest principal bounds from Block's general theorem. In particular, the bound of Hoffmann-Ostenhof and Hoffmann-Ostenhof[2] is obtained as one special case.

Despite the potential utility of accurate bounds for the electronic density, there are very few rigorous results applicable to N electron systems available in the literature. Rédei[24] derived a bound for $|\rho(\mathbf{r}) - \rho_a(\mathbf{r})|$, where $\rho(\mathbf{r})$ is the exact electronic density and $\rho_a(\mathbf{r})$ is the electronic density derived from an approximate trial wave function. Rédei's bound requires information on the ground state and first excited energies and matrix elements of the square of the Hamiltonian operator using the trial wave function. An upper bound for $\rho(0)$ and a generalization have appeared.[3,4] Hoffmann-Ostenhof *et al.*[2] succeeded in deriving an upper bound for $\rho(\mathbf{r})$ in terms of the kinetic energy. The approach taken in this work also leads to upper bound estimates involving the kinetic energy.

II. BLOCK'S THEOREM

Block's work is concerned with the problem of finding upper bounds for the function $|y(x)|$ in terms of integrals involving $y(x)$ and $y(x)'$ (prime denotes differentiation). Block derived the following result:

$$|y(t)|^2 \leq \mathfrak{M}(t) \int_a^b \{f(x)[y(x)']^2 + g(x)\,y(x)^2\}dx \ , \tag{1}$$

where $\mathfrak{M}(t)$, which does not depend on y, is given by

$$\mathfrak{M}(t) = \int_a^b \{f(x)[w(x,t)']^2 + g(x)w(x,t)^2\}dx$$
$$= w(t,t) + f(b)w(b)'\,w(b) - f(a)w(a)'\,w(a) \ . \tag{2}$$

In Eqs. (1) and (2), t satisfies $a<t<b$ and $w(x,t)$ satisfies the following four conditions:

$$\text{(i)}\ (fw')' - gw = 0 \quad \begin{cases} a \leq x < t \\ t < x \leq b \ , \end{cases} \tag{3}$$

(ii) $w(x,t)$ is continuous for $a \leq t \leq b$,

$$\text{(iii)}\ \lim_{\epsilon \to 0} [w(t-\epsilon,t)' - w(t+\epsilon,t)']f(t) = 1 \ , \tag{4}$$

$$\text{(iv)}\ f(a)w(a)'\,y(a) = f(b)w(b)'\,y(b) \ . \tag{5}$$

The successful implementation of Block's inequality [Eq. (1)], depends on the ease with which the function $w(x,t)$ can be determined, which depends on the complexity of the differential equation (3).

III. BLOCK'S INEQUALITY FOR $f(x)>0$

The solution of the above differential equation for the case $f(x)>0$ may be written in terms of the functions $w_i(x)$ $i = 1, 4$, which satisfy the boundary conditions

$$w_1(a) = w_3(b) = w_2(a)' = w_4(b)' = 1 \ , \tag{6}$$

$$w_1(a)' = w_3(b)' = w_2(a) = w_4(b) = 0 \ . \tag{7}$$

The solution is

$$w(x,t) = \begin{cases} A_1(t)w_1(x) + A_2(t)w_2(x) \ , & a \leq x < t \ , \\ A_3(t)w_3(x) + A_4(t)w_4(x) \ , & t < x \leq b \ . \end{cases} \tag{8}$$

Connections between the coefficients $A_i(t)$ can be found using the four constraints listed above. These constraints may be sufficient to determine all the $A_i(t)$ depending on whether or not any additional information about $y(t)$ is employed. Additional constraints on the behavior of $y(t)$ leads to sharper inequalities.

IV. BLOCK'S INEQUALITY APPLIED TO THE ELECTRONIC DENSITY

The focus of our attention in this paper is the atomic electronic density. By appropriate choice of $y(t)$ we may impose the condition

$$y(a) = y(b) = 0 \ . \tag{9}$$

A more general choice of $y(t)$, which does not impose the constraint $y(a) = 0$, has been investigated in detail, and the results for bounds on the electronic density arising from this case will be discussed elsewhere.

For the case discussed in Sec. IV A, i.e., $f(x)>0$, the conditions (i)–(iv) are not sufficient to determine all the coefficients $A_i(t)$. This leads to flexibility in the

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expression for $\mathfrak{M}(t)$, Eq. (2), and arises directly from the imposed constraint Eq. (9). The $A_i(t)$ may be determined so that $\mathfrak{M}(t)$ is a minimum, with the conditions (i) to (iv) used as constraints. The algebraic details are given in Appendix A. The final expression for $\mathfrak{M}(t)$ is given by Eq. (A5).

In this paper, we choose the function y to be

$$y(r) = r\rho(r)^{1/2} , \tag{10}$$

where $\rho(r)$ is the electronic density, assumed radially symmetric, is given by

$$\rho(\mathbf{r}) = N \int |\Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N)|^2 d\mathbf{r}_2 d\mathbf{r}_3, \ldots, d\mathbf{r}_N . \tag{11}$$

This selection is based on the following criteria. The constraints given in Eq. (9) are satisfied when $a = 0$ and $b = \infty$. Also, this choice allows us to deal with one of the integrals appearing in Block's inequality by employing a lower bound integral inequality for the kinetic energy derived by Hoffmann-Ostenhof *et al.*[1]

A. Case 1: $f(x) = k_1$, $g(x) = k_2$

The simplest possible choice for the functions $f(x)$ and $g(x)$ appearing in Eqs. (1) and (2) is

$$f(x) = k_1 ; \quad g(x) = k_2 , \tag{12}$$

where k_1 and k_2 are positive constants. We will assume that k_1 and k_2 are positive constants throughout this paper. If we set

$$\alpha = (k_2/k_1)^{1/2} , \tag{13}$$

then Eq. (3) reduces to

$$w'' - \alpha^2 w = 0 \tag{14}$$

for which the solutions w_i satisfying Eqs. (6) and (7) are readily determined to be

$$w_1(x) = \cosh \alpha(x - a) , \tag{15}$$

$$w_2(x) = \alpha^{-1} \sinh \alpha(x - a) , \tag{16}$$

$$w_3(x) = \cosh \alpha(x - b) , \tag{17}$$

$$w_4(x) = \alpha^{-1} \sinh \alpha(x - b) . \tag{18}$$

From Eq. (A9) γ_2 (as defined in Appendix A) is found to be zero and a short computation shows that $A_1(x)$ [Eq. (A6)] is also zero, and hence the expression for $\mathfrak{M}(x)$ [Eq. (A5)] simplifies to

$$\mathfrak{M}(x) = A_2(x) w_2(x) \tag{19}$$

which when evaluated leads to the result

$$\mathfrak{M}(x) = \frac{k_1^{-1} \sinh \alpha(x - a) \sinh \alpha(b - x)}{\alpha \sinh \alpha(b - a)} . \tag{20}$$

The Block inequality takes the form

$$|y(r)|^2 \leq \frac{\sinh \alpha(r - a) \sinh \alpha(b - r)}{\alpha \sinh \alpha(b - a)} \times \int_a^b \{[y(x)']^2 + \alpha^2 y(x)^2\} dx , \tag{21}$$

which simplifies in the limit $a \to 0$, $b \to \infty$ to

$$|y(r)|^2 \leq \frac{1}{2\alpha} (1 - e^{-2\alpha r}) \int_0^\infty \{[y(x)']^2 + \alpha^2 y(x)^2\} dx . \tag{22}$$

The inequality Eq. (21) was given by Block and also derived somewhat later by the Hoffmann-Ostenhofs.[25] This specialized Block inequality forms the basis for the bound estimates established by Hoffmann-Ostenhof *et al.*[1,2] The above derivation also makes clear that the bound is governed by one arbitrary parameter and not two as might be inferred from the appearance of Eq. (1).

Substituting Eq. (10) into Eq. (22) and employing the following key inequality established by Hoffmann-Ostenhof *et al.*[1,2]:

$$\int_0^\infty \frac{r^2 |\nabla \rho(r)|^2 dr}{4\rho(r)} \leq \frac{T}{2\pi} \tag{23}$$

leads to the result

$$\rho(r) \leq \frac{1}{8\pi r^2} (1 - e^{-2\alpha r}) \left(\alpha N + \frac{2}{\alpha} T\right) , \tag{24}$$

where T is the kinetic energy. Equation (24) was first proved by Hoffmann-Ostenhof *et al.*[1]

B. Case 2: $f(x) = k_1$, $g(x) = k_2 x^{-1}$

If we define α using Eq. (13) and set

$$\beta = 2\alpha r^{1/2} \tag{25}$$

then $\mathfrak{M}(r)$ is found to be (see Appendix B for details)

$$\mathfrak{M}(r) = \frac{2r}{k_1} I_1(\beta) K_1(\beta) , \tag{26}$$

where $I_n(\beta)$ and $K_n(\beta)$ are the modified Bessel functions of the first and second kind, respectively.

Employing Eqs. (1), (10), (23), and (26) yields the following bound for the electronic density:

$$\rho(r) \leq \frac{I_1(\beta) K_1(\beta)}{2\pi r} [\alpha^2 N \langle \Psi | r_1^{-1} | \Psi \rangle + 2T] . \tag{27}$$

If we employ the following well known inequality[26,27]:

$$\langle \Psi | r_1^{-1} | \Psi \rangle^2 \leq \frac{2}{N} T , \tag{28}$$

then the inequality Eq. (27) may be expressed in terms of T alone:

$$\rho(r) \leq \frac{1}{2\pi r} (2T)^{1/2} I_1(\beta) K_1(\beta) [\alpha^2 N^{1/2} + (2T)^{1/2}] . \tag{29}$$

Alternative inequalities connecting $\langle \Psi | r_1^{-1} | \Psi \rangle$ and T are available if model Hamiltonians are of interest.[28,29] The case $f = k_1$ and $g = k_2/x$ therefore allows the electronic density to be bounded in terms of the kinetic energy and the electron-nuclear energy V_{en} via

$$\rho(r) \leq \frac{I_1(\beta) K_1(\beta)}{2\pi r} \left[2T - \frac{\alpha^2}{Z} V_{en}\right] , \tag{30}$$

where Z is the nuclear charge.

C. Case 3: $f = k_1 x^2$, $g = k_2$

In this case, we do not have $f > 0$ in the interval $[0, \infty)$. In this situation, we do not have to impose the condition $y(a) = y(b) = 0$, Eq. (9), since the constraint given by Eq. (5) is satisfied by imposing $w(b)' = 0$ as $b \to \infty$ and noting that $f(a) \to 0$ as $a \to 0$. For this case, we make the choice

$$y(r) = \rho(r)^{1/2} . \tag{31}$$

Using the expression derived for $\mathfrak{M}(r)$ in Appendix C, and Eqs. (1), (23), and (31), the following bound is obtained:

$$\rho(r) \leq \frac{1}{4\pi r(1+4\alpha^2)^{1/2}} \left[\frac{2T}{\alpha} + \alpha N\langle\Psi|r_1^{-2}|\Psi\rangle\right] . \tag{32}$$

If we employ the well known inequality[26]

$$\langle\Psi|r_1^{-2}|\Psi\rangle \leq \frac{8T}{N} \tag{33}$$

the electronic density bound Eq. (32) may be expressed in terms of the kinetic energy

$$\rho(r) \leq \frac{T}{2\pi r}(1+4\alpha^2)^{1/2} . \tag{34}$$

We note in passing that a slightly refined version of Eq. (33) is available.[3] Since α is an arbitrary positive parameter, the limit $\alpha \to 0$ in Eq. (34) leads to the optimum form of Eq. (34):

$$\rho(r) \leq \frac{T}{2\pi r} . \tag{35}$$

The bound given in Eq. (35) can be shown to be equivalent to the bound formula Eq. (24) in the limit $r \to 0$. We note in passing that the Hoffmann-Ostenhof's[2] also gave a simple bound in terms of T:

$$\rho(r) \leq \frac{1}{4\pi r^2}(2NT)^{1/2} . \tag{36}$$

The dependence of the bound on α in Eq. (32) is sufficiently simple, that an optimum α can be stated. Examination of the derivative of the right-hand side of Eq. (32) with respect to α yields two stationary values. The first, $\alpha = 0$, leads to the bound given in Eq. (35). The second occurs when

$$\alpha^2 = \frac{1}{2}\left(\frac{4T}{N\langle\Psi|r_1^{-2}|\Psi\rangle} - 1\right) . \tag{37}$$

If α^2 is *positive*, and we set

$$\delta = \frac{N\langle\Psi|r_1^{-2}|\Psi\rangle}{4T} , \tag{38}$$

then Eq. (32) becomes

$$\rho(r) \leq \frac{T}{2\pi r}[(2-\delta)\delta]^{1/2} \tag{39}$$

and

$$0 < \delta < 2 . \tag{40}$$

Equation (39) is a superior bound to Eq. (35) if the square root factor in Eq. (39) is less than 1, which is in fact the case for all δ satisfying Eq. (40) except $\delta = 1$.

D. Case 4: $f = k_1$, $g = k_2 + [k_1 p(p+1)/x^2]$

For this case, where p is a positive constant, we employ the $y(r)$ given in Eq. (10). From Eq. (1), and the expression for $\mathfrak{M}(r)$ (see Appendix D for details) we find the following bound:

$$\rho(r) \leq \frac{I_{p+(1/2)}(\alpha r)K_{p+(1/2)}(\alpha r)}{4\pi r} \times[2T + N\{\alpha^2 + p(p+1)\}\langle\Psi|r_1^{-2}|\Psi\rangle] . \tag{41}$$

If we employ the inequality [Eq. (33)], Eq. (41) can be expressed as

$$\rho(r) \leq \frac{I_{p+(1/2)}(\alpha r)K_{p+(1/2)}(\alpha r)}{4\pi r}[N\alpha^2 + 2T(2p+1)^2] . \tag{42}$$

The Bessel functions have analytic expressions [see Eqs. (D5) and (D6)] when p is an integer.

V. NUMERICAL INVESTIGATION OF BOUNDS

To test the quality of the bounds indicated in Sec. IV, i.e., Eqs. (24), (27), (29), (35), (36), (39), (41), and (42), we have evaluated each bound using the electronic density functions of Benesch[30] which have been derived from the 20 term Hylleraas type wave functions of Hart and Herzberg.[31] Figures 1–6 show the results for the atoms H^-, He, and Mg^{10+}. For the different bounds, the optimum α was determined iteratively for each value of the radial distance. Atomic units are employed in all figures.

Because of the form of the bounds, a simple analytic comparison at finite r is not possible, since the optimum α cannot be determined analytically. However, for the limit $r \to 0$ a comparison can be made. This has already been discussed for case 1 and case 3. For case 2 it may also be shown that the limit $r \to 0$ in Eq. (27) yields Eq. (35). For case 4, the limit $r \to 0$ in Eq. (41) for the case $p = 1$ leads to the result

$$\rho(r) \leq \frac{1}{6\pi r}(T + N\langle\Psi|r_1^{-2}|\Psi\rangle) \tag{43}$$

which is a better result than Eq. (35) if

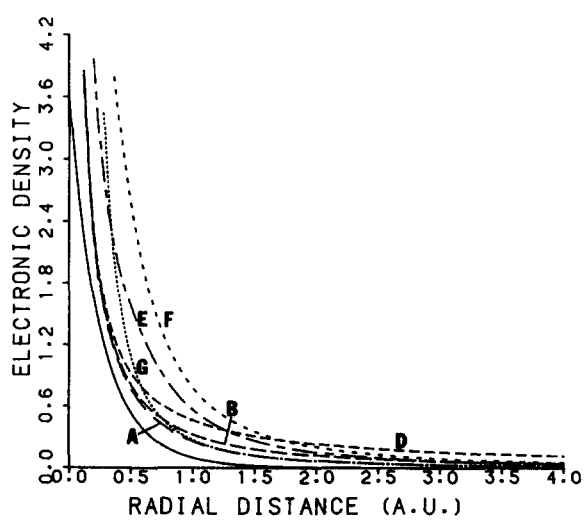

FIG. 1. Bounds for the electronic density for helium. The solid line represents the "exact" electronic density calculated from Benesch's density function. The letter designations are: A is Eq. (24), B is Eq. (27), C is Eq. (29), D is Eq. (35), E is Eq. (41), F is Eq. (42), and G is Eq. (36). Equation (29) is not presented since it coincides very closely with Eq. (27).

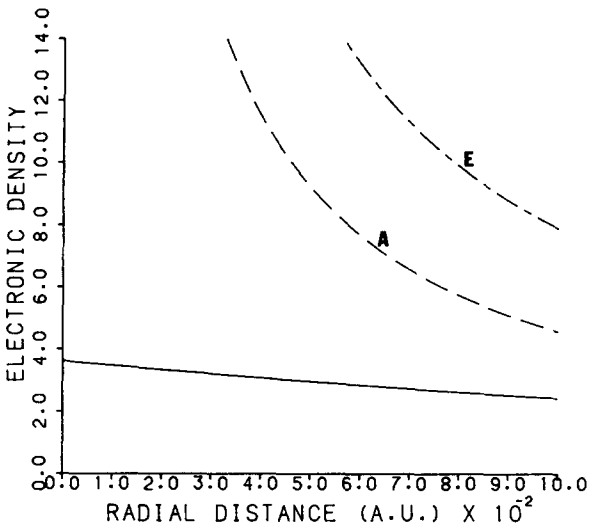

FIG. 2. Bounds for the electronic density for helium in the near nuclear region. The solid line represents the "exact" density. See the caption for Fig. 1 for the correspondence between equation numbers in the text and the letter designations. The bounds given by Eqs. (27), (29), and Eq. (35) are not presented on the graph, since they coincide very closely with the results from Eq. (24). Equations (36) and (42) are off the plot with the given scale.

$$N\langle\Psi|r_1^{-2}|\Psi\rangle - 2T < 0\ . \tag{44}$$

For the species shown in Figs. 1–6, the condition (44) is not satisfied. Also, α^2 in Eq. (37) is not positive for H^-, He, and Mg^{10+}. From the preceding comments, it is therefore expected that the bounds given for case 1, case 2, and case 3 [Eqs. (24), (27), and (32)] all converge to the same limit as $r \to 0$. This is observed in the figures. The bound given in Eq. (41) for the case $p = 1$, and consequently that given by Eq. (42) (also for $p = 1$) are observed to be less satisfactory.

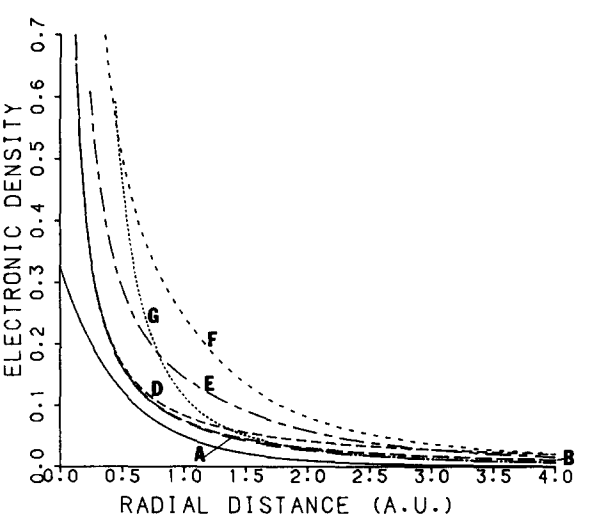

FIG. 3. Bounds for the electronic density for H^-. The solid line represents the exact density. See the caption for Fig. 1 for the correspondence between equation numbers in the text and the letter designations. Equation (29) is not presented since it corresponds very closely with Eq. (27).

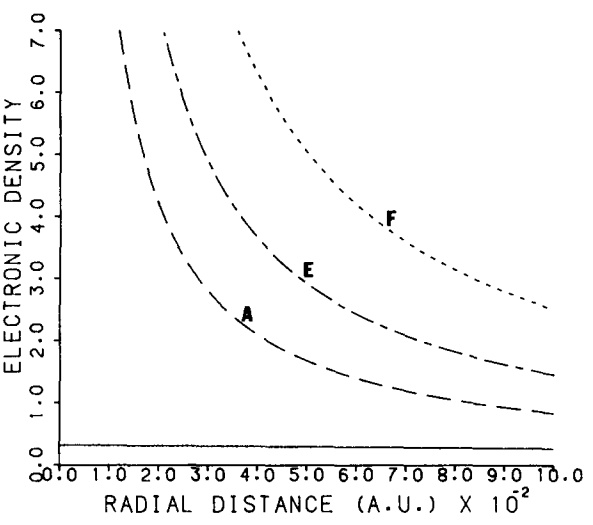

FIG. 4. Bounds for the electronic density for H^- in the near nuclear region. The solid line represents the exact density. See the caption for Fig. 1 for the correspondence between equation numbers in the text and the letter designations. The bounds given by Eqs. (27), (29), and (35) are not presented, since they coincide very closely with the result from Eq. (24). Equation (36) is off the plot with the given scale.

VI. DISCUSSION AND CONCLUSION

The obvious shortcoming of the bounds discussed in Sec. IV is that, in the near nuclear region, each bound diverges as $r \to 0$. This problem is presently under investigation. The problem is directly connected to the condition given by Eq. (9). The bounds considered in this work must therefore be restricted to r values away from the nucleus.

For the numerical studies discussed in Sec. V, Eq.

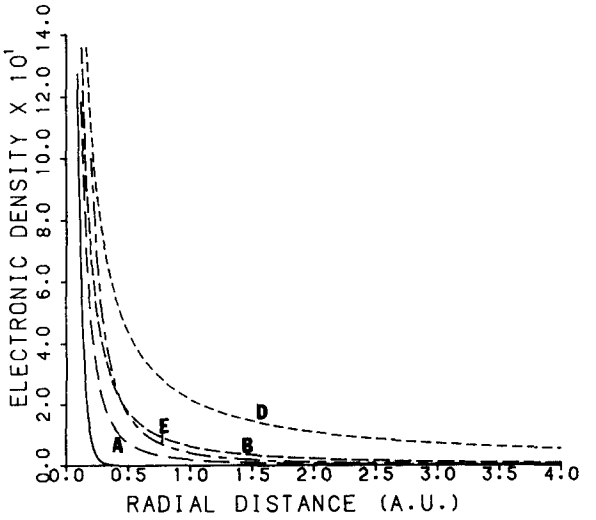

FIG. 5. Bounds for the electronic density for Mg^{10+}. The solid line represents the exact density. See the caption for Fig. 1 for the correspondence between equation numbers in the text and the letter designations. Equation (29) coincides very closely with Eq. (27) and Eq. (36) coincides with Eq. (24). Neither has been plotted.

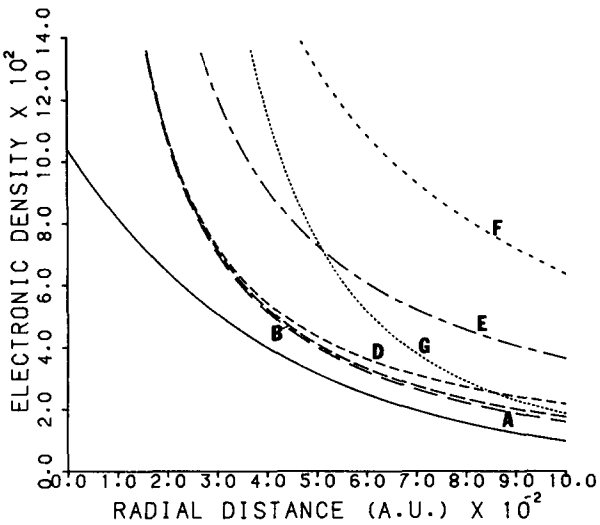

FIG. 6. Bounds for the electronic density for Mg^{10+} in the near nuclear region. The exact density is represented by the solid line. Letter designations are explained in the caption to Fig. 1. Equation (29) has not been plotted because it coincides very closely with Eq. (35).

(24) is the best bound for most values of r. All of the bounds derived herein also apply to the Hartree–Fock electronic density. We have invested these bounds for some larger atomic systems using Hartree–Fock densities.[32] In some cases, the bound given in Eq. (39) is superior to the other bounds at small r. In addition, the bound given in Eq. (27) is the best bound for other values of r near the nucleus. Clearly, there is not a simple answer to the question of which bound for $\rho(r)$ is best.

There is one final point to note. The bounds derived in this study have been based on a rather limited selection of choices for the functions f and g. It may be the case that a more judicious choice for these functions will lead to improved bounds for $\rho(r)$. Studies in this direction would be of interest.

ACKNOWLEDGMENT

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APPENDIX A

In this appendix, the general expression for $\mathfrak{M}(t)$ [Eq. (2)] for the case $f(x)>0$ and $y(a)=y(b)=0$ is derived. Using Eq. (8), $\mathfrak{M}$ is given by

$$\mathfrak{M}(t) = A_1(t)w_1(t) + A_2(t)w_2(t) + f(b)A_3(t)A_4(t) - f(a)A_1(t)A_2(t) \ . \tag{A1}$$

The two constraints (ii) and (iv) yield

$$A_1(t)w_1(t) + A_2(t)w_2(t) - A_3(t)w_3(t) - A_4(t)w_4(t) = 0 \ , \tag{A2}$$

$$A_1(t)w_1(t)' + A_2(t)w_2(t)' - A_3(t)w_3(t)' - A_4(t)w_4(t)' = 1/f(t) \ . \tag{A3}$$

The minimum of $\mathfrak{M}(t)$ with respect to variation of the $A_i(t)$, subject to the constraints Eqs. (A2) and (A3), is found from the function

$$F(t) = \mathfrak{M}(t) + \lambda_1[A_1(t)w_1(t) + A_2(t)w_2(t) - A_3(t)w_3(t) - A_4(t)w_4(t)] + \lambda_2\left[A_1(t)w_1(t)' + A_2(t)w_2(t)' - A_3(t)w_3(t)' - A_4(t)w_4(t)' - \frac{1}{f(t)}\right] \tag{A4}$$

(λ_1 and λ_2 are Lagrange multipliers) by setting $\partial F(t)/\partial A_i(t)=0$, $i=1,4$. Solving the resulting set of four equations together with Eqs. (A2) and (A3) leads to the general result

$$\mathfrak{M}(t) = A_1(t)w_1(t) + A_2(t)w_2(t) - A_1(t)A_2(t)f(a) - \frac{f(b)}{\gamma_3 w_4(t)}(A_1(t)\gamma_1 + A_2(t)\gamma_2)\{A_1(t)[w_1(t) + w_3(t)(\gamma_1/\gamma_3)] + A_2(t)[w_2(t) + w_3(t)(\gamma_2/\gamma_3)]\} \ , \tag{A5}$$

where

$$A_1(t) = [w_4(t)(\gamma_3\gamma_5 - \gamma_2\gamma_6) + \gamma_7(\gamma_2 w_{43}(t) - \gamma_3 w_{24}(t))]/\Gamma \ , \tag{A6}$$

$$A_2(t) = [w_4(t)(\gamma_1\gamma_6 - \gamma_3\gamma_4) + \gamma_7(\gamma_3 w_{14}(t) - \gamma_1 w_{43}(t))]/\Gamma \ . \tag{A7}$$

The gamma factors are defined by

$$\gamma_1 = w_1(t)[w_{34}(t)f(a) + w_{12}(t)f(b)] \ , \tag{A8}$$

$$\gamma_2 = w_2(t)[w_{12}(t)f(b) + w_{43}(t)f(a)] \ , \tag{A9}$$

$$\gamma_3 = 2w_3(t)w_{21}(t)f(b) \ , \tag{A10}$$

$$\gamma_4 = w_2(t)w_{14}(t)f(a) \ , \tag{A11}$$

$$\gamma_5 = -w_2(t)w_{24}(t)f(a) \ , \tag{A12}$$

$$\gamma_6 = -w_2(t)w_{12}(t)f(b) \ , \tag{A13}$$

$$\gamma_7 = f(t)w_2(t)w_4(t)w_{12}(t) \ , \tag{A14}$$

$$\Gamma = f(t)[w_{43}(t)(\gamma_2\gamma_4 - \gamma_1\gamma_5) + w_{24}(t)(\gamma_1\gamma_6 - \gamma_3\gamma_4) + w_{14}(\gamma_3\gamma_5 - \gamma_2\gamma_6)] \ . \tag{A15}$$

w_{ij} denotes the Wronskian $w_i' w_j - w_i w_j'$.

APPENDIX B

For the case $f=k_1$, $g=k_2x^{-1}$, Eq. (3) becomes

$$x^2w'' - \alpha^2 xw = 0 \ , \tag{B1}$$

α is defined in Eq. (13). Equation (B1) is a special case of the generalized Bessel differential equation. The solution is (in terms of arbitrary coefficients c_1 and c_2, which are functions of r)

$$w(x,r) = x^{1/2}[c_1 I_1(2\alpha x^{1/2}) + c_2 K_1(2\alpha x^{1/2})] \ , \quad 0 \le x < r \ , \tag{B2}$$

where I_1 and K_1 are modified Bessel functions of the first and second kind. A similar solution on the interval $r<x<\infty$ exists with c_1 and c_2 replaced by constants c_3 and c_4, respectively.

Because of the asymptotic behavior

$$I_1(z) \sim e^z/z^{(1/2)} \ \text{ as } z \to \infty \ , \tag{B3}$$

we require $c_3=0$.

Employing the conditions (ii) and (iii) in Sec. II and ensuring the term $f(a)w(a)'w(a)$ in Eq. (2) is well behaved as $a \to 0$, is sufficient to determine the coefficients c_1, c_2, c_4. The function $w(x,r)$ is then determined to be

$$w(x,r) = \frac{2(xr)^{1/2}}{k_1} I_1(2\alpha x^{1/2}) K_1(2\alpha r^{1/2}) , \quad 0 \le x < r , \tag{B4}$$

$$w(x,r) = \frac{2(xr)^{1/2}}{k_1} I_1(2\alpha r^{1/2}) K_1(2\alpha x^{1/2}) , \quad r < x < \infty , \tag{B5}$$

Using Eq. (2) and the limit $x \to r$ in either Eq. (B4) or (B5), leads to the expression for $\mathfrak{M}(r)$ given in Eq. (26). The two factors involving f in Eq. (2) vanish in the limits $a \to 0$, $b \to \infty$.

APPENDIX C

The differential equation to be solved for the case $f = k_1 x^2$, $g = k_2$ is

$$x^2 w'' + 2xw' - \alpha^2 w = 0 . \tag{C1}$$

The solutions of Eq. (C1) are elementary and take the form

$$w(x,r) = c_1 x^{m_1} + c_2 x^{m_2} , \quad 0 \le x < r , \tag{C2}$$

$$w(x,r) = c_3 x^{m_1} + c_4 x^{m_2} , \quad r < x < \infty ,$$

where $m_1 = -\frac{1}{2} + (\frac{1}{4} + \alpha^2)^{1/2}$ and $m_2 = -\frac{1}{2} - (\frac{1}{4} + \alpha^2)^{1/2}$. If we examine the conditions $x \to 0$ and $x \to \infty$, then $c_2 = 0$ and $c_3 = 0$. The limit $x \to r$ leads to the result

$$c_4 = c_1 r^{m_1 - m_2} . \tag{C3}$$

To ensure that condition (iv) [Eq. (5)] is satisfied, we require that $w(b)'$ vanish as $b \to \infty$ in such a manner that $f(b)w(b)'w(b)$ is zero. From Eqs. (C2) and (C3),

$$w(x,r)' = \frac{c_1 m_2 r^{m_1 - m_2}}{x^{3/2 + (1/4 + \alpha^2)^{1/2}}} . \tag{C4}$$

Using Eq. (C4), we see that $f(b)w(b)'w(b) \to 0$ as $b \to 0$. It is also clear that $f(a)w(a)'w(a) \to 0$ as $a \to 0$, so that Eq. (5) is satisfied. The remaining coefficient can be determined from condition (iii) [Eq. (4)], with the result that

$$c_1 = \frac{1}{k_1 (1 + 4\alpha^2)^{(1/2)} r^{1 + m_1}} . \tag{C5}$$

Hence, Eq. (2) becomes

$$w(x,r) = \frac{x^{m_1} r^{-1-m_1}}{k_1 (1 + 4\alpha^2)^{(1/2)}} , \quad 0 \le x < r , \tag{C6}$$

$$w(x,r) = \frac{x^{m_2} r^{-1-m_2}}{k_1 (1 + 4\alpha^2)^{(1/2)}} , \quad r < x < \infty . \tag{C7}$$

The function $\mathfrak{M}(r)$ is thus determined to be

$$\mathfrak{M}(r) = \frac{1}{k_1 r (1 + 4\alpha^2)^{(1/2)}} . \tag{C8}$$

APPENDIX D

The differential equation arising from the choice

$$f = k_1$$

$$g = k_2 + \frac{k_1 p(p+1)}{x^2} \quad \text{(positive } p\text{)} \tag{D1}$$

is

$$x^2 w'' - [p(p+1) + \alpha^2 x^2] w = 0 , \tag{D2}$$

which is a modified Bessel differential equation. The solution of the differential equation is

$$w(x,r) = x^{1/2} [c_1 I_{p+(1/2)}(\alpha x) + c_2 K_{p+(1/2)}(\alpha x)] , \quad 0 \le x < r , \tag{D3}$$

$$w(x,r) = x^{1/2} [c_3 I_{p+(1/2)}(\alpha x) + c_4 K_{p+(1/2)}(\alpha x)] , \quad r < x < \infty . \tag{D4}$$

The solutions hold for general p (integer or noninteger values), however, if p is restricted to integer values, the Bessel functions can be expressed analytically using[33]

$$K_{p+(1/2)}(x) = \left(\frac{\pi}{2x}\right)^{1/2} e^{-x} \sum_{k=0}^{p} \frac{(p+k)!}{k!(p-k)!(2x)^k} , \tag{D5}$$

$$I_{p+(1/2)}(x) = \frac{e^{-x}}{(2\pi x)^{(1/2)}} \sum_{k=0}^{p} \frac{(p+k)!}{k!(p-k)!(2x)^k} [(-1)^k e^{2x} - (-1)^p] . \tag{D6}$$

Since $I_{p+(1/2)}(\alpha x) \sim e^{\alpha x}/[(2\pi\alpha x)^{(1/2)}]$ as $x \to \infty$, we set the coefficient $c_3 = 0$. The limit $x \to 0$ indicates the choice $c_2 = 0$, based on the behavior of $K_{p+(1/2)}(x)$ as $x \to 0$. Equations (D3) and (D4) simplify to

$$w(x,r) = x^{1/2} I_{p+(1/2)}(\alpha x) c_1 , \quad 0 \le x < r , \tag{D7}$$

$$w(x,r) = x^{1/2} K_{p+(1/2)}(\alpha x) c_4 , \quad r < x < \infty . \tag{D8}$$

The coefficients c_1 and c_4 can be determined by examination of the limit $x \to r$ in Eqs. (D7) and (D8) which yields

$$c_1 = \frac{c_4 K_{p+(1/2)}(\alpha r)}{I_{p+(1/2)}(\alpha r)} \tag{D9}$$

and by imposing the condition (iii) Eq. (4). The result for $w(x,r)$ is

$$w(x,r) = \frac{(xr)^{1/2}}{k_1} I_{p+(1/2)}(\alpha x) K_{p+(1/2)}(\alpha r) , \quad 0 \le x < r , \tag{D10}$$

$$w(x,r) = \frac{(xr)^{1/2}}{k_1} I_{p+(1/2)}(\alpha r) K_{p+(1/2)}(\alpha x) , \quad r < x < \infty . \tag{D11}$$

It is straightforward to check that

$$f(b)w(b)'w(b) \to 0 , \quad \text{as } b \to \infty ,$$

$$f(a)w(a)'w(a) \to 0 , \quad \text{as } a \to 0 . \tag{D12}$$

Therefore, from Eq. (2) we find

$$\mathfrak{M}(r) = \frac{r}{k_1} I_{p+(1/2)}(\alpha r) K_{p+(1/2)}(\alpha r) . \tag{D13}$$

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