Bounds for the atomic electronic density: The near nuclear region

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Some upper bound estimates for the atomic electron density are derived using Block's inequality. A rough bound for the density is obtained in terms of the number of electrons, the nuclear charge, and the electronic energy. The bounds derived in this work are tested for some members of the helium isoelectronic series using electronic densities derived from 20 term Hylleraas type wave functions. A comparison is also made with some previously derived upper bound estimates for the electronic density. The bounds presented do not diverge in the near nuclear region like r^{-n}, a feature which characterizes presently available bounds.

INTRODUCTION

A number of rigorously derived bounds for the atomic electronic density have been published recently.[1-11] Much of this activity has involved investigation of rigorous bounds for the long-range behavior of the electronic density. In a key paper by the Hoffmann-Ostenhof's,[4] fairly satisfactory upper bound estimates for the electronic density $\rho(\mathbf{r})$ were obtained provided the region close to the nucleus is avoided.

The bounds derived by the Hoffmann-Ostenhof's exhibit one of the following relations:

$$\rho(r) \propto 1/r \quad \text{as } r \to 0, \tag{1a}$$

$$\rho(r) \propto 1/r^2 \quad \text{as } r \to 0, \tag{1b}$$

and consequently, the upper bound estimates for $\rho(r)$ in the region near the nucleus are rather unsatisfactory.

The literature on rigorous relationships describing the behavior of $\rho(r)$ near the nucleus is very limited. The work of Rédei[12] and Bazley and Fankhauser[13] is of interest.

Hoffmann-Ostenhof, Hoffmann-Ostenhof, and Thirring[1] derived a bound *specifically* for the electronic density at the nucleus:

$$\rho(0) \leq \frac{ZN}{2\pi} \langle \Psi \mid r^{-2} \mid \Psi \rangle, \tag{2}$$

where Z is the nuclear charge, N is the number of electrons, and

$$\rho(\mathbf{r}_1) = N \int \mid \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) \mid^2 d\mathbf{r}_2 \cdots d\mathbf{r}_N. \tag{3}$$

Tal and Levy[2] have suggested a generalization of Eq. (2).

In the present work, bounds for the atomic electronic density which yield finite values at the nucleus are derived. This avoids the difficulty, expressed by Eqs. (1), which other bound formulas suffer.

THEORY

The approach taken in this study employs one of a class of inequalities which are referred to as Block's inequalities.[14,15] In a previous paper,[6] the author examined some applications of one of the principal Block inequalities to the problem of finding bounds for the electronic density. That investigation employed fairly tight bounds for the function $y(r)$, expressed in terms of integrals involving $y(r)^2$ and $[y(r)']^2$ (prime denotes differentiation). The class of Block inequalities that were employed impose the constraints:

$$y(r) \to 0 \quad \text{as } r \to 0, \tag{4a}$$

$$y(r) \to 0 \quad \text{as } r \to \infty. \tag{4b}$$

These constraints are satisfied with the choice

$$y(r)^2 = r^2 \rho(r). \tag{5}$$

The divergent character of previously derived bounds, expressed by Eqs. (1a) and (1b), arises directly from the r^2 factor in Eq. (5). The difficulty cannot be resolved by simply removing this factor, since the constraint imposed by Eq. (4a) is no longer satisfied.

The above complication can be avoided by utilizing another of the general Block inequalities. In fact, only a special case of a much more general result is employed. Block's results do not appear to be very widely known. The fundamental bound used in this paper is[14]

$$\mid y(r) \mid^2 \leq \frac{\cosh \alpha(b-r) \cosh \alpha(r-a)}{\alpha \sinh \alpha(b-a)} \times \int_a^b \{[y(r)']^2 + \alpha^2 y(r)^2\}\, dr, \tag{6}$$

where $y(r)$ and its derivative are assumed continuous on $a < r < b$. No other constraints are placed on the function $y(r)$. The quantity α appearing in Eq. (6) is an arbitrary positive parameter. We are specifically interested in Eq. (6) for the case $a \to 0$ $b \to \infty$, the result is

$$\mid y(r) \mid^2 \leq \tfrac{1}{2}(1 + e^{-2\alpha r}) \int_0^\infty \{(1/\alpha)[y(r)']^2 + \alpha y(r)^2\}\, dr. \tag{7}$$

In order for the integrals appearing in Eq. (7) to be convergent, we impose the constraint that $y(r)$ exhibit the asymptotic behavior $y(r) \to 0$ as $r \to \infty$, in such a manner as to lead to convergent integrals, otherwise Eq. (7) is vacuous. However, there is no need to impose the condition expressed by Eq. (4a), and this is a key ingredient in the derivation.

The following identification is made for the function $y(r)$:

$$y(r) = \rho(r)^{1/2} \tag{8}$$

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and we assume $\rho(r)$ to be radially symmetric. Substituting Eq. (8) into Eq. (7) leads to the result

$$\rho(r) \leq \tfrac{1}{2}(1+e^{-2\alpha r}) \int_0^\infty \left(\frac{1}{\alpha} \{[\rho(r)^{1/2}]'\}^2 + \alpha \rho(r) \right) dr. \tag{9}$$

The upperbound inequality (9) has one obvious defect, namely the long-range asymptotic behavior of $\rho(r)$ is not correctly described. If bounds for the electronic density for medium to large r are required, inequalities for $\rho(r)$ discussed elsewhere are more appropriate.[4,6] We note in passing that the asymptotic behavior of these other bounds[6] as $r \to \infty$ do not exhibit exponential decay with distance, as we expect on the basis of intuition and a good deal of recent work on the long-range behavior of the electronic density. Because of the above consideration, our further discussion in this work is confined to the near nuclear region. The possibility of deriving a suitable bound for $\rho(r)$ for all r, including the near nuclear region, which has the appropriate long-range exponential decay remains an open question.

Our next objective is to recast Eq. (9) in terms of more readily available quantities. This will also allow the opportunity for comparison with the bound for $\rho(0)$ derived by Hoffmann-Ostenhof *et al.*, Eq. (2).

Equation (9) can be recast in the form

$$\rho(r) \leq \tfrac{1}{2}(1+e^{-2\alpha r})\,[(1/\alpha) I_1 + \alpha I_2], \tag{10}$$

where

$$I_1 = \frac{1}{16\pi} \int \frac{|\nabla \rho(\mathbf{r})|^2 d\mathbf{r}}{r^2 \rho(\mathbf{r})}, \tag{11}$$

$$I_2 = \frac{I}{4\pi} \int \frac{\rho(\mathbf{r})}{r^2} d\mathbf{r}. \tag{12}$$

The integral I_1 may be expressed in the form

$$I_1 < \frac{N}{\pi} \langle \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \,|\, \nabla_1^4 \,|\, \Psi(\mathbf{r}_1, ,,,, \mathbf{r}_N) \rangle. \tag{13}$$

Blau, Rau, and Spruch[16] have derived the following bound:

$$\langle \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \,|\, \nabla_1^4 \,|\, \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \rangle < \frac{4}{N} \{ |E| + [2|E| N\{(N-1)^2 + 4Z^2\}]^{1/2} \}^2, \tag{14}$$

where E is the energy corresponding to the state Ψ. Atomic units are assumed in Eq. (14) and will be employed in the rest of this work.

Combining Eqs. (10)–(14) leads to the upperbound estimate

$$\rho(r) < \frac{1}{8\pi} (1+e^{-2\alpha r}) \left(\alpha N \langle \Psi | r^{-2} | \Psi \rangle + \left(\frac{16}{\alpha} \right) \{ |E| + [2|E| N\{(N-1)^2 + 4Z^2\}]^{1/2} \}^2 \right). \tag{15}$$

Alternatively, $\rho(r)$ may be expressed entirely in terms of E, N, and Z by using the following well known inequality for $\langle \Psi | r^{-2} | \Psi \rangle$ and the virial theorem:

$$\langle \Psi | r_1^{-2} | \Psi \rangle \leq 4 \langle \Psi | -\nabla_1^2 | \Psi \rangle \equiv (8|E|)/N, \tag{16}$$

to yield

$$\rho(r) < \frac{1}{\pi} (1+e^{-2\alpha r}) \left(\alpha |E| + (2/\alpha) \times \{ |E| + [2|E| N\{(N-1)^2 + 4Z^2\}]^{1/2} \}^2 \right). \tag{17}$$

A slightly superior result to Eq. (17) can be obtained using in place of Eq. (16), a result recently derived by Hoffmann-Ostenhof *et al.*[1] from an inequality of Faris[17]:

$$\langle \Psi | r^{-2} | \Psi \rangle \leq \frac{4|E|}{N} \left[1 + \left(1 - \frac{2|E|}{NZ^2} \right)^{1/2} \right] \tag{18}$$

which leads to

$$\rho(r) < \frac{1}{2\pi} (1+e^{-2\alpha r}) \left(\alpha |E| \left[1 + \left(1 - \frac{2|E|}{NZ^2} \right)^{1/2} \right] + \left(\frac{4}{\alpha} \right) \{ |E| + [2|E| N\{(N-1)^2 + 4Z^2\}]^{1/2} \}^2 \right). \tag{19}$$

BOUNDS FOR $\rho(0)$

If $r \to 0$ in Eq. (10), then the optimum value of α is readily determined to be

$$\alpha = \left(\frac{I_1}{I_2} \right)^{1/2}, \tag{20}$$

which leads to the inequality

$$\rho(0) \leq 2(I_1 I_2)^{1/2}. \tag{21}$$

Employing the approximation for I_1 given by Eqs. (13) and (14) leads to

$$\rho(0) < (Z/\pi)[2|E|N\langle \Psi | r^{-2} | \Psi \rangle]^{1/2} \Gamma, \tag{22}$$

where the factor Γ is

$$\Gamma = (2^{1/2}/Z)[|E|^{1/2} + \{2N[(N-1)^2 + 4Z^2]\}^{1/2}]. \tag{23}$$

Equation (22) has been expressed in the above form to allow comparison with the bound for $\rho(0)$ derived by Hoffmann-Ostenhof *et al.*,[1] Eq. (2). From Eqs. (2) and (16),

$$\rho(0) \leq \frac{NZ}{2\pi} \langle \Psi | r^{-2} | \Psi \rangle \leq \frac{Z}{\pi} [2|E|N \langle \Psi | r^{-2} | \Psi \rangle]^{1/2}. \tag{24}$$

The second of the two inequalities in Eq. (24) is introduced to allow comparison with Eq. (22) above.

Equation (21) may be expressed entirely in terms of E, N, and Z using Eqs. (13), (14), and (18) to yield

$$\rho(0) < \frac{4}{\pi} [|E| + \{2|E|N[(N-1)^2 + 4Z^2]\}^{1/2}] \times \left[|E| \left\{ 1 + \left(1 - \frac{2|E|}{NZ^2} \right)^{1/2} \right\} \right]^{1/2}. \tag{25}$$

NUMERICAL RESULTS FOR $\rho(0)$ INEQUALITIES

For the hydrogen atom, both the integrals I_1 and I_2 [Eqs. (11) and (12)] can be evaluated analytically. Equation (21) is then observed to be satisfied as an equality. Equation (10) holds only as a strict inequality for the hydrogen atom for $r > 0$. See Appendix A for further details on this point.

In order to test the quality of the bound in Eq. (21), several members of the helium isoelectronic series were investigated. The integrals I_1 and I_2 were evaluated by quadrature making use of the electronic densi-

TABLE I. Bounds for $\rho(0)$.

Atom	I_1[a]	I_2[a]	$\rho(0)$[a] exact	$\rho(0)$ Eq. (21)	$\rho(0)$ Eq. (2)
H^-	0.152 125	0.177 474	0.327 011	0.328 624	0.354 949
He	$0.343\,652\times10^{1}$	0.957 783	3.622 83	3 628 46	3.831 13
Li^+	$0.198\,042\times10^{2}$	$0.237\,595\times10^{1}$	$1.370\,97\times10^{1}$	$1.371\,92\times10^{1}$	$1.425\,57\times10^{1}$
B^{3+}	$0.169\,817\times10^{3}$	$0.712\,309\times10^{1}$	$6.954\,21\times10^{1}$	$6.955\,92\times10^{1}$	$7.123\,09\times10^{1}$
O^{6+}	$0.118\,104\times10^{4}$	$0.190\,189\times10^{2}$	$2.997\,19\times10^{2}$	$2.997\,47\times10^{2}$	$3.043\,03\times10^{2}$
Ne^{8+}	$0.294\,111\times10^{4}$	$0.301\,327\times10^{2}$	$5.953\,58\times10^{2}$	$5.953\,94\times10^{2}$	$6.026\,54\times10^{2}$
Mg^{10+}	$0.617\,968\times10^{4}$	$0.437\,930\times10^{2}$	$1.040\,39\times10^{3}$	$1.040\,44\times10^{3}$	$1.051\,03\times10^{3}$

[a]Values determined from the electronic density functions of Benesch (Ref. 18).

TABLE II. Bounds for $\rho(0)$.

Atom	$\lvert E\rvert$[a]	$\rho(0)$[b] exact	$\rho(0)$[c] Eq. (26)	$\rho(0)$ Eq. (25)
H^-	0.527 644 669 2	0.327 011	0.566 77	4.5366
He	2.903 717 9	3.622 83	5.632 6	4.5407×10^{1}
Li^+	7.279 905 382	$1.370\,97\times10^{1}$	$1.998\,2\times10^{1}$	1.6516×10^{2}
B^{3+}	22.030 959 28	$6.954\,21\times10^{1}$	$9.429\,4\times10^{1}$	8.0646×10^{2}
O^{6+}	59.156 581 537	$2.997\,19\times10^{2}$	$3.841\,6\times10^{2}$	3.3811×10^{3}
Ne^{8+}	93.906 791 9	$5.953\,58\times10^{2}$	$7.454\,0\times10^{2}$	6.6408×10^{3}
Mg^{10+}	136.656 932 8	$1.040\,39\times10^{3}$	$1.279\,7\times10^{3}$	1.1507×10^{4}

[a]From Ref. 19.
[b]Values determined from the electronic density functions of Benesch (Ref. 18).
[c]Bound from Ref. 1.

TABLE III. Bound estimates for various integrals.

Atom	$\langle\Psi\lvert r_1^{-2}\rvert\Psi\rangle$[a]	$\frac{4\lvert E\rvert}{N}\left[1-\frac{2\lvert E\rvert}{NZ^2}\right]^{1/2}$[b]	$\frac{8\lvert E\rvert}{N}$[c]	Estimate for I_1[d]	Γ[e]
H^-	1.1151	1.7806	2.1106	1.8156×10^{1}	7.35
He	6.0179	8.8477	1.1615×10^{1}	3.6604×10^{2}	7.04
Li^+	1.4929×10^{1}	2.0925×10^{1}	2.9120×10^{1}	2.0478×10^{3}	7.01
B^{3+}	4.4756×10^{1}	5.9246×10^{1}	8.8124×10^{1}	1.7243×10^{4}	7.01
O^{6+}	1.1950×10^{2}	1.5086×10^{2}	2.3663×10^{2}	1.1903×10^{5}	7.03
Ne^{8+}	1.8933×10^{2}	2.3417×10^{2}	3.7563×10^{2}	2.9582×10^{5}	7.03
Mg^{10+}	2.7516×10^{2}	3.3503×10^{2}	5.4662×10^{2}	6.2080×10^{5}	7.04

[a]Calculated using density functions of Benesch (Ref. 18).
[b]Upper bound estimate for $\langle\Psi\lvert r_1^{-2}\rvert\Psi\rangle$, see Eq. (18).
[c]Upper bound estimate for $\langle\Psi\lvert r_1^{-2}\rvert\Psi\rangle$, see Eq. (16).
[d]Upper bound estimate for I_1 using Eqs. (13) and (14).
[e]Γ is defined in Eq. (23).

ty functions of Benesch[18] which have been derived from the 20-term Hylleraas type wave functions of Hart and Herzberg.[19] These results are presented in Table I along with $\rho(0)$ evaluated from the inequality Eq. (21) and $\rho(0)$ evaluated from the Hoffmann-Ostenhof *et al.*[1] bound Eq. (2).

For the cases examined in Table I the upperbound to $\rho(0)$ given by Eq. (21) is observed to be in excellent agreement with the "exact" values of $\rho(0)$. The results obtained from the Hoffmann-Ostenhof *et al.* bound are also observed to be in extremely close agreement with the exact $\rho(0)$.

In Table II estimates for $\rho(0)$ using the bound formulas involving E, N, and Z are presented. Equation (25), which employs the inequality estimate for I_1 given by Eqs. (13) and (14) and the inequality Eq. (18) for $\langle\Psi\lvert r^{-2}\rvert\Psi\rangle$ is examined. The Hoffmann-Ostenhof *et al.*[1] bound expressed in terms of E, N, and Z, i.e.,

$$\rho(0)<\frac{2\lvert E\rvert Z}{\pi}\left[1+\left(1-\frac{2E}{NZ^2}\right)^{1/2}\right] \tag{26}$$

is also examined for comparison. It is clear from the results of Table II that both the bound estimates for $\rho(0)$ based on E, N, Z information are considerably weaker than the results presented in Table I. Equation (25) leads to estimates which are approximately a factor of 10 too large. The source of the problem is

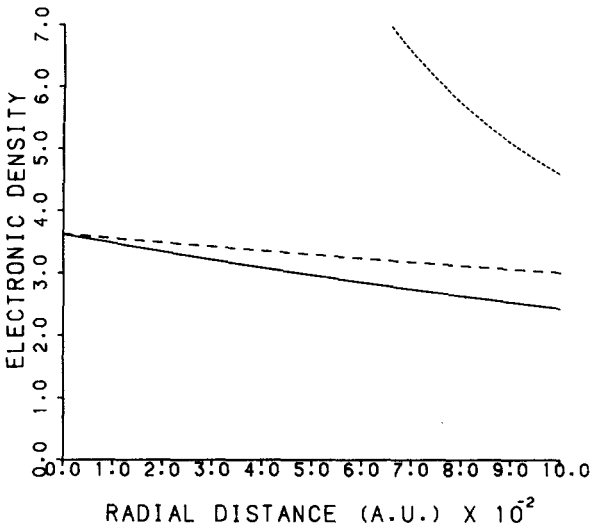

FIG. 1. Bounds for the electronic density for the helium atom. The solid line is the exact density based on Benesch's density function. The short-dashed curve represents Eq. (27) and the medium length dashed curve represents Eq. (10).

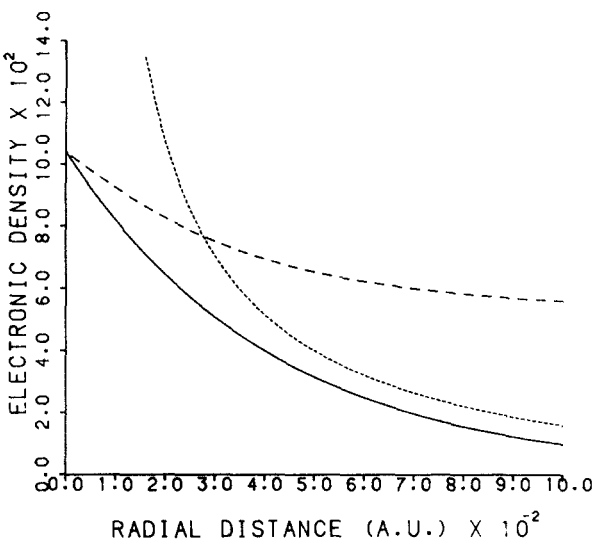

FIG. 3. Bounds for the electronic density for Mg^{10+}. The solid line is the exact density. The short-dashed curve represents Eq. (27) and the medium length dashed curve represents Eq. (10).

the lack of sharpness for the bounds to $\langle\Psi|r^{-2}|\Psi\rangle$, Eq. (18), and in particular, the bound for I_1, Eqs. (13) and (14). In Table III results are presented to indicate the quality of these inequalities. Equation (18) is observed to be a definite improvement over Eq. (16), however the estimate based on Eq. (18) is observed to be approximately 20%–60% too high for the cases examined in Table III. The combined effects of the inequality (13) and the Blau *et al.*[16] estimate in Eq. (14) are observed, on comparing column 5, Table III with I_1 values presented in Table I, to be rather rough estimates for the integrals I_1. The final column in Table III lists values of Γ, Eq. (23) which allows a comparison of the two intermediate inequalities (22) and (24).

BOUNDS FOR $\rho(r)$ NEAR THE NUCLEUS

For $r \neq 0$, the optimum value of α appearing in the bound equations has been determined by an iterative approach for each value of r. In Figs. 1–3, the exact density is compared with the bound evaluated from Eq. (10) using the values of I_1 and I_2 (determined by quadrature) listed in Table I for He, H^-, and Mg^{10+}. Also

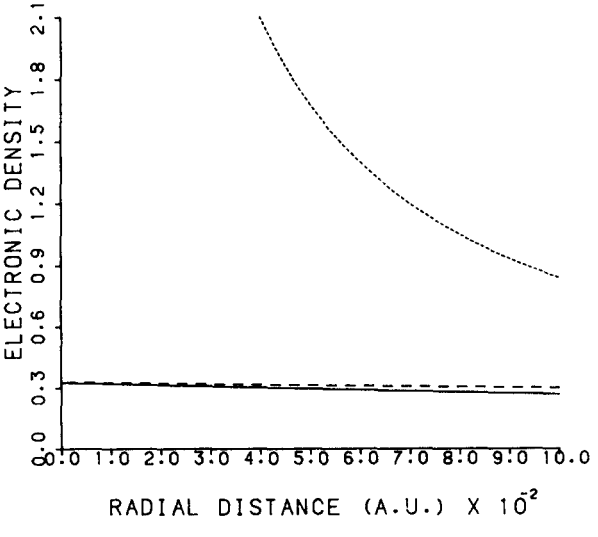

FIG. 2. Bounds for the electronic density for H^-. The solid line is the exact density. The short-dashed curve represents Eq. (27) and the medium length dashed curve represents Eq. (10).

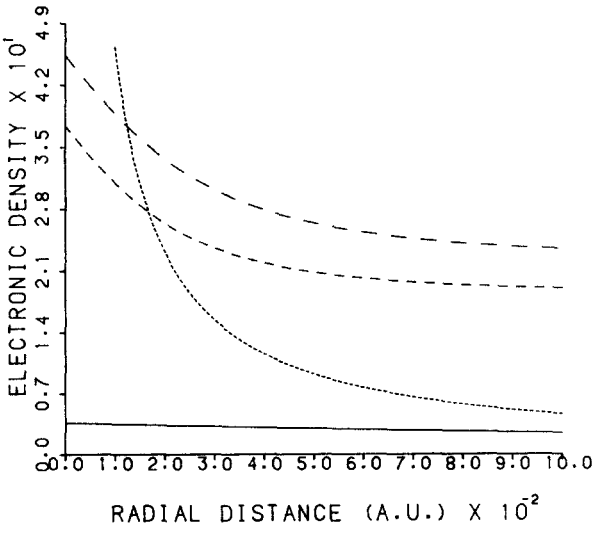

FIG. 4. Bounds for the electronic density for He. The solid line is the exact density. Equation (27) is represented by the short-dashed curve. Equation (15) is represented by the medium length dashed curve and Eq. (19) is represented by the long-dashed curve.

included in these figures are bound estimates derived from the inequality involving the kinetic energy T,

$$\rho(r) \leq \frac{1}{8\pi r^2}\,(1-e^{-2\alpha r})\left(\alpha N + \frac{2T}{\alpha}\right) \tag{27}$$

which has been discussed elsewhere.[4,8] This equation simplifies in the small r limit to

$$\rho(r) \leq T/(2\pi r). \tag{28}$$

The general trend observed from Figs. 1–3 is that Eq. (10) proves a very good upper bound estimate for $\rho(r)$. For Mg^{10+}, where the electronic density is more concentrated in the region close to the nucleus, the bound estimate given by Eq. (27) is satisfactory even for fairly small values of r.

Figures 4, 5, and 6 illustrate the bound estimates based on Eqs. (15) and (19). The bound estimate given in Eq. (27) is also shown for comparison. Equations (15) and (19) are observed to be better bound estimates than Eq. (27) close to the nucleus, however the bound estimates are typically too high by a factor of 10. This can be traced to the lack of sharpness for the combined bounds given in Eqs. (13) and (14).

In this work we have presented some simple upper bound estimates for the atomic electronic density. These bounds provide finite values of $\rho(0)$, and thus avoid the difficulty encountered by other recently derived expressions *which diverge as* $r \to 0$.

Although there is a very good bound available in the literature for the specific point $r=0$[1], there has been little attention devoted to the important region close to the nucleus. Further investigations to determine optimum bounds for the two key expectation values which are important for finding bounds on $\rho(r)$ in the near nuclear region would be welcome.

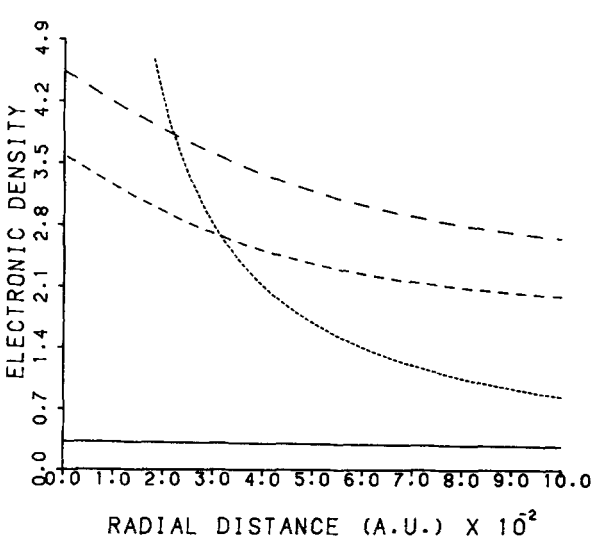

FIG. 5. Bounds for the electronic density for H^-. The solid line is the exact density. Equation (27), (15), and (19) are represented by the short-dashed curve, medium length dashed curve, and long-dashed curve, respectively.

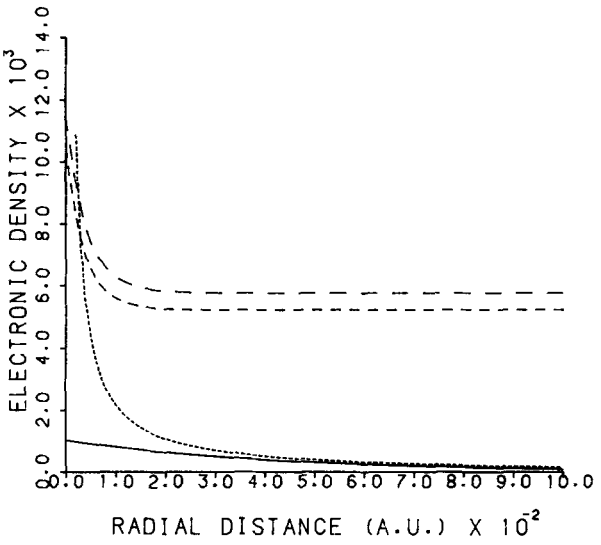

FIG. 6. Bounds for the electronic density for Mg^{10+}. The solid line is the exact density. Equations (27), (15), and (19) are represented by the short-dashed, medium length dashed, and long-dashed curve respectively.

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APPENDIX A

The special case of the Block inequality (7) for the situation $r=0$, with the optimum α employed, is actually a well known inequality.[20] Equation (21) can be shown by inspection to be a strict inequality unless

$$\rho(r) = Ae^{-\beta r}, \tag{A1}$$

where A and β are constants. For the situation represented by Eq. (A1), Eq. (21) is an equality.

The density functions of Benesch that we have employed take the form

$$\rho(r) = \frac{1}{4\pi r^2}\left[\sum_{i=1}^{14} a_i r^i e^{-kr} + \sum_{i=1}^{7} b_i r^i e^{-2kr}\right]. \tag{A2}$$

There are no (simple) connections between the a and b coefficients except $a_1 = -b_1$. If we express $\rho(r)$ in the form

$$\rho(r) = e^{-kr} f(r)\,, \tag{A3}$$

then for small values of r we have that

$$f(r) = \frac{1}{4\pi}\,(ka_1 + a_2 + b_2), \quad r \to 0. \tag{A4}$$

Thus, for the Benesch density functions, Eqs. (A3) and (A4) indicate that the limiting form of the electronic density satisfies Eq. (A1). For this reason, the bound estimate given by Eq. (21) becomes exact in the limit $r \to 0$ for these functions.

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