PHYSICAL REVIEW A VOLUME 22, NUMBER 5 NOVEMBER 1980

Modified Sternheimer equation for polarizability

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(Received 9 June 1980)

The Sternheimer equation for atomic polarizability is modified to account for the self-consistent field. The equations are quite simple for closed-shell ions. Numerical results are presented.

In a weak external field, a closed-shell ion develops a moment proportional to the field. The coefficient of proportionality is called the polarizability. The best known is the dipole polarizability, which gives the dipole moment. However, the idea is easily generalized to higher moments, and often it is useful to know others such as quadrupole, octupole, etc. The Mth moment is in response to the Mth field, and this field has the general form

$$\delta V_M(\vec{r}) = r^M P_M(\cos\theta)\epsilon_M , \qquad (1)$$

where P_M is the Legendre function and ϵ_M is the infinitesimal field. In response to this field, the atom or ion will develop a moment p_M given by

$$p_M = \alpha_M \epsilon_M . \qquad (2)$$

The polarizability α_M can be dipole ($M=1$), quadrupole ($M=2$), octupole ($M=3$), etc. These polarizabilities are useful in a wide variety of atomic and solid-state applications.

In 1954 Sternheimer[1] suggested a method of evaluating the polarizability which has become widely used. In fact, it is employed in nearly all calculations.[2-8] Even Hartree-Fock calculations are recast in terms of the Sternheimer equation.[4] Recently I used the density-functional method to evaluate the Sternheimer equation for many closed-shell ions and atoms.[7,8]

The Sternheimer equation relies on a one-particle picture of the atom. Recently Stott and Zaremba[9] (SZ) showed that a consideration of electron-electron interactions requires the polarizability to be evaluated in a many-particle framework. When the atom polarizes, in response to the external field, the polarizations on different orbitals interact via electron-electron interactions, which affect the polarizability in a substantial fashion. One has to calculate the polarizability self-consistently, by taking into account the mutual interaction of different polarizations. Stott and Zaremba showed that calculating self-consistently reduced the dipole polarizability by typically 40%. Zangwill and Soven[10] (ZS) have used the identical method to calculate the polarizability and also the optical absorption, and both are quite accurate. The method of self-consistent field (SCF), when applied to atomic polarizability, greatly improves the accuracy and must be regarded as a great step forward.

Here we would like to do three things: (1) Show that the method of SCF can be recast as a modified Sternheimer equation; (2) show for a closed-shell ion that the modified Sternheimer equation has very simple angular-momentum characteristics. (These two features make the SCF very easy to solve numerically, and one can very quickly obtain accurate self-consistency); and (3) present a table of values for the first four moments ($M=1, 2, 3, 4$) of most closed-shell ions. One of the features of the present method is that the calculation is equally easy for any value of M. Our numerical results show that the dipole polarizability is indeed reduced by 40% when the fields are made self-consistent, in agreement with SZ and ZS. However, the higher moments are only altered by ±2% by the SCF so the effect is usually negligible except for $M=1$.

I. MODIFIED STERNHEIMER EQUATION

The derivation is cast in the language of the density-functional method.[11,12] Most recent work has used this formalism to evaluate the polarizability.[7-10] Here the electron potential in the ground state of the closed-shell ion has terms from the interaction with the nucleus, the other electrons, and the exchange-correlation potential which is taken to be a local function of the electron density $n(\vec{r})$:

$$V(r) = -2\frac{Z}{r} + 2\int d^3r \frac{n(r')}{|\vec{r}-\vec{r}'|} - V_{xc}(n(\vec{r})) . \qquad (3)$$

Each electron orbital in the ion is given by the Schrödinger-type equation

$$\begin{aligned} &[-\nabla^2 + V(\vec{r})]\psi_i(\vec{r}) = E_i\psi_i , \\ &n(\vec{r}) = \sum_i |\psi_i|^2 , \end{aligned} \qquad (4)$$

and the density $n(\vec{r})$ is found by adding up the densities of the occupied orbitals. These equations are a self-consistent set which have been solved to describe successfully many atomic properties.[11-14]

Next consider the response of the atom when we apply the infinitesimal perturbing field $\delta V_M(\vec{r})$ in Eq. (1). Each wave function $\psi_i(\vec{r})$ will be perturbed by this field. In first order, the change is given by $\bar{\psi}_i$ which is defined by

$$\psi_i \to \psi_i + \bar{\psi}_i \epsilon_M .$$

Of course, this causes the density $n(\vec{r})$ to change, which in first order is given by

$$n(\vec{r}) \to n(\vec{r}) + \delta n(\vec{r})\epsilon_M ,$$
$$\delta n(\vec{r}) = 2\,\mathrm{Re}\left(\sum_i \psi_i(\vec{r})^* \bar{\psi}_i(\vec{r})\right). \tag{5}$$

The potential acting upon the electron also changes. Of course there is the new external perturbation $\delta V_M(\vec{r})$. In addition, the density changes $\delta n(\vec{r})\epsilon_M$ cause a change in $V(\vec{r})$ in (3). The total self-consistent potential is found by combining these effects ($\nu = \cos\theta$),

$$V(\vec{r}) \to V(\vec{r}) + V_{\mathrm{SCF}}(\vec{r})\epsilon_M ,$$
$$V_{\mathrm{SCF}}(\vec{r}) = r^M P_M(\nu) + 2\int d^3r' \frac{\delta n(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|} + \delta n(\vec{r})\left(\frac{\partial V_{xc}}{\partial n(\vec{r})}\right). \tag{6}$$

The final step in the argument is to derive an equation for $\bar{\psi}_i(\vec{r})$. It is obtained from Schrödinger's equation in first-order perturbation theory. Since the energy changes are of order ϵ_M^2 and negligible, we have

$$[-\nabla^2 + V(r) + V_{\mathrm{SCF}}\,\epsilon_M](\psi_i + \bar{\psi}_i\epsilon_M) = E_i(\psi_i + \bar{\psi}_i\epsilon_M) .$$

The component of this equation which is first order in ϵ_M provides the inhomogeneous equation satisfied by $\bar{\psi}_i$,

$$[-\nabla^2 + V(\vec{r}) - E_i]\bar{\psi}_i(\vec{r}) = -V_{\mathrm{SCF}}(\vec{r})\psi_i(\vec{r}) . \tag{7}$$

This equation is defined as the modified Sternheimer equation. The original Sternheimer equation[1] had $r^M P_M(\nu)$ instead of V_{SCF} on the right. The modification uses the self-consistent potential V_{SCF} on the right-hand side of (7). First one does the atomic calculation in order to find the set of atomic wave functions $\psi_i(\vec{r})$, eigenvalues E_i, and potential $V(\vec{r})$. With these in hand, Eqs. (5)–(7) form a self-consistent set of equations to find $\bar{\psi}_i(\vec{r})$ and $\delta n(\vec{r})$. The polarizability is given by

$$\alpha_M = 2a_B^{2M+1}\int d^3r\, r^M P_M(\nu)\delta n(\vec{r}) . \tag{8}$$

Thus the polarizability is rather easily obtained after one has found the self-consistent $\delta n(\vec{r})$.

The above set of equations is exactly equivalent to the set introduced by Stott and Zaremba.[9] They derived them in a different fashion, and solved them using a Green's function method which involved solving an integral equation by diagonalizing big matrices. The present derivation is much simpler. We will also show that for closed shells it is numerically easier to solve directly the modified Sternheimer equation (7).

II. ANGULAR-MOMENTUM THEOREM

For a closed-shell ion or atom, only the radial equation needs to be solved in (7). The wave functions $\psi_i(\vec{r})$ are products of radial functions and angular functions, and $\bar{\psi}_i(\vec{r})$ can be expanded in a similar series

$$\psi_i(\vec{r}) = \frac{U_i(r)}{r} Y_l^m(\theta, \phi) ,$$
$$\bar{\psi}_i(\vec{r}) = \frac{1}{r}\sum_{l'} \bar{U}_{i,l'} Y_{l'}^m(\theta, \phi) . \tag{9}$$

The properties of angular functions can be used to turn (7) into just a radial equation for each $\bar{U}_{i,l}$. The important question is the number of terms needed in the angular-momentum expansion in (9). The answer depends upon the angular dependence of $V_{\mathrm{SCF}}(\vec{r})$ which in turn depends upon the angular dependence of $\delta n(\vec{r})$. Each of these functions can also be expanded in spherical harmonics. For the general case, one can show that the expansions

$$\delta n(\vec{r}) = \sum_L \delta n_L(r) P_L(\nu) ,$$
$$V_{\mathrm{SCF}}(\vec{r}) = \sum_L V_L(r) P_L(\nu) , \tag{10}$$

must have an infinite number of terms: Since parity is conserved, the sum is either over all odd or all even values of L. For a closed-shell ion, our theorem is that the sums in (10) contain only the single term $L = M$, and all other terms vanish.

Theorem

For a closed-shell ion the angular dependence of $\delta n(\vec{r})$ is exactly given by ($\nu = \cos\theta$),

$$\delta n(\vec{r}) = \delta n_M(r) P_M(\nu) . \tag{11}$$

We shall prove this theorem below. One consequence of it is that both $V_{\mathrm{SCF}}(\vec{r})$ and α_M also have a simple form

$$\alpha_M = \frac{8\pi}{2M+1} a_0^{2M+1} \int_0^\infty dr\, r^{2+M} \delta n_M(r) , \tag{12}$$
$$V_{\mathrm{SCF}}(\vec{r}) = V_{\mathrm{SCF},M}(r) P_M(\nu) ,$$

$$V_{\mathrm{SCF},M}(r)=r^M+\frac{8\pi}{2M+1}\int dr'(r')^2\delta n_M(r')\frac{r_<^M}{r_>^{M+1}}$$
$$+\delta n_M\left(\frac{\partial V_{xc}}{\partial n}\right). \qquad (13)$$

We shall prove the theorem by explicitly deriving the form of $\delta n_M(r)$, and showing terms in (10) with $L\neq M$ are zero. For an atom of closed shells, the density change $\delta n(\vec{r})$ is composed of a sum of the contributions from each shell, thus we can sum over the radial and orbital quantum numbers of the occupied shells

$$\delta n(\vec{r})=\sum_{n,l}\delta n^{(n,l)}(\vec{r}),$$
$$\delta n^{(n,l)}(\vec{r})=\delta n_M^{(nl)}(r)P_M(\nu). \qquad (14)$$

The theorem will be proved separately for each angular-momentum state.

s states. The theorem is trivial to prove for s states, and this case is only included for completeness. The original wave function ψ_i and changed part $\bar{\psi}_i$ can be written as

$$\psi_i=\frac{1}{r\sqrt{4\pi}}U_{no}(r),$$
$$\bar{\psi}_i=\frac{1}{r\sqrt{4\pi}}\bar{U}_{no,M}(r)P_M(\nu).$$

The change in density $\delta n(\vec{r})$ is given by (5), and we add an additional factor of two for spin degeneracy:

$$\delta n^{(no)}(\vec{r})=\frac{1}{\pi r^2}U_{no}(r)\bar{U}_{no,M}P_M(\nu),$$
$$\delta n_M^{(no)}(r)=\frac{1}{\pi r^2}U_{no}(r)\bar{U}_{no,M}(r). \qquad (15)$$

the modified Sternheimer equation has the form

$$\left(-\frac{\partial^2}{\partial r^2}+\frac{M(M+1)}{r^2}+V(r)-E_{no}\right)\bar{U}_{no,M}$$
$$=-U_{no}(r)\delta V_{\mathrm{SCF},M}(r). \qquad (16)$$

p states. For p states and higher angular momentum, the proof is more complicated. The proof proceeds in the fashion of perturbation theory. First we shall assume that there is only the external potential $\delta V_M(\vec{r})$ in (1) which contains only the single angular harmonic $P_M(\nu)$. For the case that ψ_i is ($l=1$, $m=0$), the right-hand side of the Sternheimer equation (7) contains the angular factors νP_M which can be decomposed to P_{M+1} and P_{M-1}. Thus $\bar{\psi}_i$ contains terms with both of these two angular functions. When we evaluate $\delta n(\vec{r})$ in Eq. (5) we have the product of ν from ψ_i and $P_{M\pm1}$ from $\bar{\psi}_i$. These will give the combinations P_{M+2}, P_M, and P_{M-2}. Of course, the new guess at a self-consistent potential now has all three of these angular functions, since the angular dependences of $V_{\mathrm{SCF}}(\vec{r})$ and $\delta n(\vec{r})$ are similar. Thus, when we use this new V_{SCF} in Eq. (7), we will find that the new guess at $\bar{\psi}_i$ has angular functions $P_{M\pm3}$ and $P_{M\pm1}$. The new $\delta n(r)$ has P_M, $P_{M\pm2}$, and $P_{M\pm4}$. Thus each iteration produces more angular harmonics for each function. However, for a closed-shell ion all the terms in $\delta n(\vec{r})$ vanish except P_M. In order to show this, we first need some standard relationships among Legendre functions,

$$\nu P_M(\nu)=\frac{M+1}{2M+1}P_{M+1}+\frac{M}{2M+1}P_{M-1},$$
$$\sin\theta P_M=\frac{1}{2M+1}\left(P_{M+1}^1-P_{M-1}^1\right), \qquad (17)$$
$$\sin\theta P_M^1=\frac{M(M+1)}{2M+1}\left(P_{M-1}-P_{M+1}\right).$$

First we define the auxillary function $\bar{\psi}_i$ associated with the ($l=1$, $m=0$) function ψ_i,

$$\psi_i=\left(\frac{3}{4\pi}\right)^{1/2}\frac{U_{n1}}{r}\nu,$$
$$\bar{\psi}_i=\frac{1}{r}\left(\frac{3}{4\pi}\right)^{1/2}\left(\frac{M+1}{2M+1}\bar{U}_{n1,M+1}P_{M+1}(\nu)\right.$$
$$\left.+\frac{M}{2M+1}\bar{U}_{n1,M-1}P_{M-1}(\nu)\right).$$

Next we do the same for the functions associated with ($l=1$, $m=\pm1$),

$$\psi_i=\left(\frac{3}{8\pi}\right)^{1/2}\frac{U_{n1}}{r}\sin\theta e^{\pm i\phi},$$
$$\bar{\psi}_i=\left(\frac{3}{8}\right)^{1/2}\frac{e^{\pm i\phi}}{r}\left(\frac{1}{2M+1}\right)[\bar{U}_{n1,M+1}P_{M+1}^1(\nu)$$
$$-\bar{U}_{n1,M-1}P_{M-1}^1(\nu)].$$

The coefficients in both of these expansions have been chosen to agree with those in (17). With this choice, the auxiliary functions $\bar{U}_{n1,M\pm1}$ are independent of the magnetic quantum number m. The auxiliary functions obey the radial equation ($M'=M\pm1$),

$$\left(-\frac{\partial^2}{\partial r^2}+\frac{M'(M'+1)}{r^2}+V(r)-E_{n'}\right)\bar{U}_{n1,M'}$$
$$=-U_{n1}(r)V_{\mathrm{SCF},M}(r).$$

The change in density $\delta n(\vec{r})$ is found by adding the product $\psi_i^*\bar{\psi}_i$ for the three states with $m=1,0,-1$. The coefficients of the terms with $P_{M\pm2}$ both vanish, and one is left with

$$\delta n_M^{(n1)}(r)=\frac{3U_{n1}(r)}{\pi r^2}\left(\frac{M+1}{2M+1}\bar{U}_{n1,M+1}(r)\right.$$
$$\left.+\frac{M}{2M+1}\bar{U}_{n1,M-1}(r)\right).$$

Again we have added a factor of two for spin degeneracy. The factor of three essentially accounts for orbital degeneracy.

The proof is self-consistent, in that if we assume that $\delta n(\vec{r})$ has only the single angular component P_M, then we calculate for it only the same single angular function. We can also think of this proof as proceeding by perturbation theory, in that the applied potential $\delta V_M(\vec{r})$ only has a single angular function P_M, which generates in the self-consistent potential V_{SCF} also only the same angular function.

d states. For d states the algebra is formidable, thus we shall just give the result. The auxiliary function $\bar{\psi}_i$ has three radial components where $M' = M-2$, M, and $M+2$. Each obeys the equation

$$\left(-\frac{\partial^2}{\partial r^2}+\frac{M'(M'+1)}{r^2}+V(r)-E_{n2}\right)\bar{U}_{n2,M'}=-U_{n2}(r)V_{\mathrm{SCF},M}(r)\,.$$

The density is given by

$$\delta n_M^{(n2)}(r)=\frac{5U_{n2}(r)}{\pi r^2}\left(\frac{3M(M-1)}{2(2M-1)(2M+1)}\bar{U}_{n2,M-2}+\frac{M(M+1)}{(2M-1)(2M+3)}\bar{U}_{n2,M}+\frac{3(M+1)(M+2)}{2(2M+1)(2M+3)}\bar{U}_{n2,M+2}\right),$$

where $U_{n2}(r)$ is the radial part of ψ_i.

In summary, there is one auxiliary function $\bar{U}$ for s states, two for p states, three for d states, etc. This number is exactly the same for the old Sternheimer equation. The modification to the self-consistent field does not alter the number of auxiliary functions which must be computed. The only change is that now they must be calculated self-consistently.

The set of equations we have derived is formally equivalent to that given in Refs. 9 and 10. However, the present equations appear numerically simpler and faster, since both Stott and Zaremba, and Zangwill and Soven used a Green's function method which required diagonalizing large matrices. We have previously described[8] the numerical technique for solving the inhomogeneous radial equations for $\bar{U}$. The self-consistent potential $V_{\mathrm{SCF},M}(r)$ was found by iteration, and 0.1% convergence in α_M was obtained after a half-dozen iterations or fewer.

III. RESULTS AND DISCUSSION

Table I shows our calculated values of α_M for $M=1$, 2, 3, 4 for many closed-shell ions.[15] The dipole polarizabilities are compared with the calculations of SZ and ZS. The column labeled "Expt." are the best values deduced from experiments and other theories.[16,17] We followed ZS and used the form of correlation and exchange suggested by Gunnarsson and Lundqvist[12]:

$$V_{xc}=-\frac{1.222}{r_s}-0.0666\ln\left(1+\frac{11.4}{r_s}\right).$$

Thus our calculations are an exact copy of those of ZS, and we should reproduce the four dipole polarizabilities they reported. We do agree with them to within 1%, which is our calculational accuracy, so that we have confirmed their results. Their choice of correlation and exchange was adopted because of the excellent values they obtained for the rare gases. Our results show that this good agreement between theory and experiment is extended to many other closed-shell ions.

The original results of Stott and Zaremba were usually 10% different than ZS and ours. However, they recently found and corrected a numerical error, and their revised values are shown in Table I. They are in excellent agreement with ZS and ours.

The right-hand columns of Table I show values of α_M for higher values of M. We give the results from both the modified (SCF) and unmodified (r^M) Sternheimer equation. Here the difference is typically ±2%, in contrast to the change in dipole polarizability which is 40%. The higher moments are only slightly affected by making the fields self-consistent. Because the calculated dipole polarizabilities are so accurate when compared with experimental values, it is hoped that the higher moments have a similar accuracy. No reliable experimental values are available for higher polarizabilities.

It is helpful to have a calculational technique which gives the polarizabilities so accurately. Yet we are surprised and troubled by the fact that it works so well. The density-functional scheme we used in these calculations has a feature we regard as unsatisfactory. The Coulomb interaction in Eq. (3) has the full electron density, thus it has the particle interacting with itself. This self-interaction is supposed to be canceled by a like term in V_{xc}. However, when V_{xc} is approximated as a local functional of the density, this cancellation is very incomplete.[18] Bryant showed that much better results were obtained in the density-functional method

TABLE I. Polarizabilities for some closed-shell ions given in angstrom units. In the column labeled "Expt." are the best values deduced from experiments and other theories. The next two columns give the self-consistent results of Stott and Zaremba, and Zangwill and Soven. Our self-consistent results are next, followed by the non–self-consistent results calculated with the unmodified Sternheimer equation. The last six columns give the results for $M=2, 3, 4$ for both self-consistent (SCF) and non–self-consistent (r^M) methods.

		Dipole ($Å^3$)					Quadrupole ($Å^5$)		Octupole ($Å^7$)		2^4 pole ($Å^9$)	
Z	Ion	Expt.[a,b]	Stott[c] and Zaremba	Zangwill[d] and Soven	Present SCF	r	r^2	S_{SCF}	r^3	SCF	r^4	SCF
2	He	0.205	0.24		0.24	0.26	0.134	0.139	0.183	0.188	0.45	0.46
3	Li^+	0.028	0.032		0.032	0.034	0.0057	0.0058	0.0026	0.0026	0.0022	0.0022
4	Be^{2+}				0.0083	0.0087	7.3(−4)	7.3(−4)	1.6(−4)	1.6(−4)	6.6(−5)	6.6(−5)
10	Ne	0.40	0.44	0.43	0.44	0.50	0.40	0.41	0.68	0.70	1.92	1.96
11	Na^+	0.158	0.158		0.157	0.179	0.072	0.073	0.070	0.071	0.090	0.092
12	Mg^{2+}	0.0784			0.075	0.085	0.023	0.024	0.014	0.015	0.011	0.011
18	Ar	1.64	1.75	1.74	1.73	2.57	2.84	2.82	7.25	7.47	26.6	27.5
19	K^+	0.85	0.84		0.83	1.27	0.87	0.84	1.35	1.37	2.65	2.72
20	Ca^{2+}	0.522			0.49	0.75	0.36	0.34	0.40	0.40	0.51	0.52
30	Zn^{2+}				0.42	0.52	0.42	0.41	0.38	0.39	0.61	0.63
31	Ga^{3+}				0.205	0.246	0.13	0.13	0.090	0.092	0.096	0.098
36	Kr	2.48	2.62	2.60	2.58	3.86	5.15	5.11	15.9	16.4	65.	68.
37	Rb^+	1.41	1.40		1.37	2.09	1.84	1.78	3.76	3.78	8.8	9.0
38	Sr^{2+}	0.84			0.87	1.33	0.82	0.80	1.34	1.33	2.13	2.19
47	Ag^+				1.46	2.26	2.90	2.62	4.31	4.47	11.6	12.1
48	Cd^{2+}				0.79	1.18	0.97	0.89	1.07	1.10	1.87	1.93
49	In^{2+}				0.50	0.73	0.44	0.41	0.38	0.38	0.49	0.50
54	Xe	4.04	4.19	4.12	4.15	6.64	11.5	11.0	41.9	42.8	194	203
55	Cs^+	2.42	2.41		2.36	3.74	4.9	4.5	12.1	12.0	34	35
56	Ba^{2+}	1.73			1.56	2.46	2.65	2.36	4.9	4.8	10.0	10.2

[a] Reference 17.
[b] Reference 16.
[c] Reference 9.
[d] Reference 10.

if this self-interaction were removed.[13,14] Others have recently confirmed this improvement.[19,20] Thus it would seem better to calculate the polarizability with the removal of the self-interaction.

Our earlier calculations[8] of the polarizability were done this way, without self-interaction, although not self-consistent. Removing self-interaction makes $V(r)$ more attractive, makes the eigenvalues larger in magnitude, and makes the ions less polarizable. This explains why the non-SCF polarizabilities reported in Ref. 8 are smaller than those in Table I. When we make the SCF correction to the polarizabilities calculated without the self-interaction, the dipole polarizabilities get about 30% smaller, and become too small when compared with experiment. Thus when we calculate using SCF and eliminate the self-interaction, the dipole results are too small for all cases. The procedure for doing this is complicated, since one must not only eliminate the self-interaction in $n(\vec{r})$ but also in $\delta n(\vec{r})$, which in fact we did only approximately. The step of removing the self-interaction, which generally improves the calculated atomic properties, makes the polarizabilities worse. One exception to this statement is for the first row of the periodic table, where our spin-polarized exchange gave better results for He and Li^+. Another case where the removal of self-interaction improves the result is for the negative halide ions. They cannot be calculated at all with the method of the present paper, since the self-interaction renders the atomic state unstable. The method of Ref. 8 gives nice solutions, although making the dipole polarizabilities self-consistent makes them too small when compared with experiment, in agreement with the other cases.

This research was supported by NSF Grant No. DMR-77-11305.

[1] R. M. Sternheimer, Phys. Rev. **96**, 951 (1954); **107**, 1565 (1957); **115**, 1198 (1959); **183**, 112 (1969); Phys. Rev. A **1**, 321 (1970).

[2] G. Burns, Phys. Rev. **115**, 357 (1959); J. Chem. Phys. **31**, 1253 (1959).

[3] P. W. Langhoff and R. P. Hurst, Phys. Rev. A **139**, 1415 (1965).

[4] P. W. Langhoff, M. Karplus, and R. P. Hurst, J. Chem. Phys. **44**, 505 (1966).

[5] J. Lahiri and A. Mukherji, Phys. Rev. **153**, 386 (1967); **155**, 24 (1967).

[6] C. Litt, Phys. Rev. A **7**, 911 (1973).

[7] G. D. Mahan, Solid State Commun. **33**, 797 (1980).

[8] G. D. Mahan, Solid State Ionics **1**, 29 (1980).

[9] M. J. Stott and E. Zaremba, Phys. Rev. A **21**, 12 (1980); Erratum (in press).

[10] A. Zangwill and P. Soven (unpublished).

[11] B. Y. Tong and L. J. Sham, Phys. Rev. **144**, 1 (1966).

[12] O. Gunnarsson and B. I. Lundqvist, Phys. Rev. B **13**, 4274 (1976).

[13] G. W. Bryant and G. D. Mahan, Phys. Rev. B **17**, 1744 (1978).

[14] G. W. Bryant, Phys. Rev. B **19**, 2801 (1979); **19**, 2864 (1979).

[15] The polarizabilities for Cu^+ are missing from the table because we were unable to find a self-consistent solution to the wave functions with this choice of correlation and exchange. The solution appears unstable. This feature was not encountered for any other case nor for the solutions to Cu^+ with other choices of exchange and correlation.

[16] R. R. Teachout and R. T. Pack, At. Data **3**, 195 (1971).

[17] H. Coker, J. Phys. Chem. **80**, 2078 (1976).

[18] I. Lindgren, Int. J. Quantum Chem. **5**, 411 (1971).

[19] A. Zunger and M. L. Cohen, Phys. Rev. B **18**, 5549 (1978).

[20] J. P. Perdew, Chem. Phys. Lett. **64**, 127 (1979).