alcohol, but only electron and hard gamma-rays when a counter filled with helium and alcohol was used. A one-percent counting efficiency was assumed for these x-rays determined with the argon-alcohol-filled counter. This figure could probably be in error by a factor of ten. An analogous situation existed for Os^{185}. In this case, the 0.75-Mev gamma-ray was assumed to be detectable with a one percent counting efficiency.

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On Nuclear Quadrupole Moments

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The correction to nuclear quadrupole moments on account of the quadrupole moment induced in the electron shells has been obtained by solving the Schroedinger equation for the perturbed core wave functions for Li, Al, and Cl. The correction factor by which the average $\langle 1/r^3\rangle$ over the valence electron function in the equation for the quadrupole coupling should be multiplied to take account of the induced effect is 1.11, 0.83, and 0.68, respectively. The previously described Thomas-Fermi calculation of this effect has been carried out for 13 additional elements.

I. INTRODUCTION

The correction to nuclear quadrupole moments on account of the quadrupole moment induced in the electron shells has been previously estimated by means of the Thomas-Fermi model.[1] In the first part of this paper we present a calculation of this effect by solving the Schroedinger equation for the cases of Li, Al, and Cl. It was found that the inclusion of exchange, which is not contained in the Thomas-Fermi model, may change the quadrupole correction considerably. In general, the exchange terms have sign opposite to the direct terms. For Al and Cl they are larger than the direct terms, so that the sign of the effect is reversed, the complete quadrupole correction being such as to increase the interaction energy for a given value of the nuclear quadrupole moment. Moreover, it was found that the statistical model represents only a part of the perturbation of the electron core by the nuclear moment Q, namely, those excitation modes in which there is only angular displacement of the charge, the charge contained in any spherical shell remaining constant. This part always gives rise to a shielding of Q. The other part of the perturbation consists of radial displacements of the charge which may shield or reinforce the effect of the nucleus, depending on the shell structure and the valence electron wave function.

In the second part of the paper, we discuss the effect of including the induced moment in the perturbation which rearranges the electron cloud. We also list the results of calculations of the Thomas-Fermi value of the correction for 13 additional elements, which make it possible to interpolate the Thomas-Fermi correction for all elements.

II. WAVE FUNCTION CALCULATIONS

The perturbed wave function of the core electrons was obtained by solving numerically the Schroedinger equation for the atomic potential as perturbed by the nuclear Q. The procedure will be shown first by considering the perturbation of the $1s$ state for Al. Let H_0 and H_1 be the unperturbed and the perturbed part of the hamiltonian, respectively; u_0 and u_1 will denote the unperturbed and the perturbed part of the wave function times r. We have

$$H_0=-(\hbar^2\nabla^2/2m)+V_0, \qquad (1)$$

where V_0 is the central potential of the atom which was taken as the Thomas-Fermi potential. The perturbation H_1 is given by

$$H_1=-Q(3\cos^2\theta-1)/2r^3, \qquad (2)$$

where r is the length of the radius vector from the nucleus and θ is the angle included by this vector and the axis of the nuclear quadrupole moment Q; lengths are in units of the Bohr radius a_H, and H_1 is in ry units. If E_0 denotes the unperturbed $1s$ energy, the Schroedinger equation becomes

$$(H_0+H_1)(u_0+u_1)=E_0(u_0+u_1), \qquad (3)$$

since the first-order perturbation of the energy is zero for s states. Upon subtracting $H_0u_0=E_0u_0$, and to the first order in Q, we obtain

$$(H_0-E_0)u_1=-H_1u_0. \qquad (4)$$

In the following the zero-order functions u_0 will be written

$$u_0=u_0'(r)\Theta(\theta,\phi), \qquad (5)$$

where u_0' is the radial and Θ is the angular part of the

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* Research carried out under contract with the AEC.

[1] R. Sternheimer, Phys. Rev. **80**, 102 (1950).

wave function; the normalization is

$$\int_0^\infty u_0'^2 dr = 1, \tag{5a}$$

$$\int_0^\pi |\Theta(\theta,\phi)|^2 \sin\theta d\theta = 1. \tag{5b}$$

For s states, $\Theta = 1/\sqrt{2}$. The unperturbed functions for Al were obtained by integration in the Thomas-Fermi potential.

In view of Eq. (2), u_1 has angular dependence $(3\cos^2\theta - 1)$. If we write

$$u_1 = Qu_1'(3\cos^2\theta - 1)/2\sqrt{2}, \tag{6}$$

where u_1' is a function of r only, Eq. (4) becomes

$$-(d^2u_1'/dr^2) + (6u_1'/r^2) + V_0u_1' - E_0u_1' = u_0'/r^3, \tag{7}$$

where V_0 and E_0 are in ry units. For small r we may expand the potential V_0:

$$V_0 = -(2Z/r) + A_0 + A_1r + \cdots, \tag{8}$$

where Z is the atomic number and A_0, A_1, $\cdots$ are constants. Similarly, u_0' can be written

$$u_0' = c_1r + c_2r^2 + \cdots, \tag{9}$$

where the c_i are constants. Thus, the right-hand side of Eq. (7) behaves as c_1/r^2. The term with the lowest power of r on the left is $6u_1'/r^2$. Hence, the expansion of u_1' starts with a constant term $c_1/6$. The complete expansion is of the form:

$$u_1' = a_0 + a_1r + a_2r^2 + a_3r^3 + a_4r^4 + \cdots + b_3r^3 \log r + b_4r^4 \log r + \cdots) \tag{10}$$

where the a_i and b_i are constants. If we use only two terms in the expansions (8) and (9), we find

$$A_0 = -82, \quad c_1 = 8.88, \quad c_2 = -97.7.$$

With $E_0 = -98$ ry, we obtain the following equations determining the a_i and b_i:

$$\begin{aligned} 6a_0 &= 8.88, \\ 6a_1 - 26a_0 &= -97.7, \\ 4a_2 - 26a_1 + 180a_0 &= 0, \\ -5b_3 - 26a_2 + 180a_1 &= 0, \\ -7b_4 - 6a_4 - 26a_3 + 180a_2 &= 0, \\ -6b_4 - 26b_3 &= 0. \end{aligned} \tag{11}$$

This gives

$$\begin{aligned} &a_0 = 1.48, \quad a_1 = -9.86, \quad a_2 = -131, \\ &b_3 = 325, \quad b_4 = -1408, \quad a_4 = -4.33a_3 - 2287, \end{aligned} \tag{12}$$

a_3 is arbitrary. To obtain the solution for large r, Eq. (7) was integrated inward from infinity, making use of the asymptotic behavior, $u_1' \sim A \exp(-|E_0|^{\frac{1}{2}}r)$, where A is a constant. The inward integration was carried out for several A. The values of A and a_3 were then determined from the two equations expressing the continuity of u_1' and du_1'/dr at the radius r_1 (of order $0.03a_H$) where the two solutions were joined. We note that the perturbation of the wave function, u_1'/r goes as a_0/r and thus diverges at $r=0$ (although it is square integrable over the volume element). Moreover, Q/r^3 is no longer small compared with V_0 for very small r. Our procedure is nevertheless valid, as is seen from the following argument. We may assume that the quadrupole moment is distributed over the nucleus. If the moment is due to a surface density over a sphere of radius r_0, the potential is given by $-(Qr^2/2r_0^5)(3\cos^2\theta - 1)$ for $r<r_0$ and thus decreases with decreasing r. For Al, with $r_0 = 4.5\times10^{-13}$ cm (nuclear radius) and[2] $Q = 0.156\times10^{-24}$ cm^2, we obtain

$$(Q/2Zr_0^2) = 0.03$$

for the maximum of the perturbation relative to the coulomb potential. Similarly small values are obtained for Li and Cl. Inside $r=r_0$, Eq. (19) can be fitted to a solution for the potential ($\sim r^2$) given previously; this solution u_1' goes as r^3 near $r=0$ and is consequently regular. As would be expected, the matching of the solutions at the nuclear radius has a negligible effect on the constants a_i and b_i of Eq. (10), so that the calculations can be carried out with Eq. (10) as stated above.

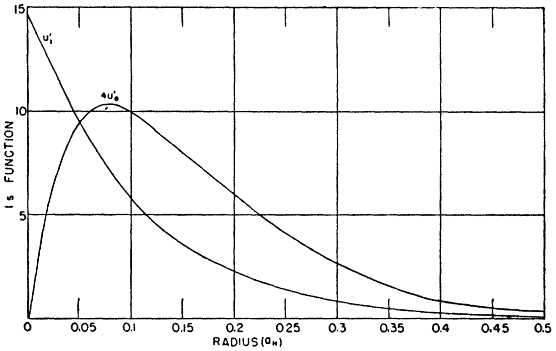

FIG. 1. 1s function u_0' and excited d function u_1' for Al.

Figure 1 shows u_0' together with the perturbation u_1'. The perturbation of the density of the 1s electrons, denoted by $\Delta\rho_{1s}$, is given by

$$\Delta\rho_{1s} = (4u_0u_1)/r^2 = Qu_0'u_1'(3\cos^2\theta - 1)/r^2. \tag{13}$$

Hence, the induced moment ΔQ_{1s} due to the 1s electrons is

$$\Delta Q_{1s} = Q\int_0^\infty u_0'u_1'r^2dr \int_0^\pi (3\cos^2\theta - 1)^2 \sin\theta d\theta = (8/5)Q\int_0^\infty u_0'u_1'r^2dr. \tag{14}$$

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[2] J. E. Mack, Revs. Modern Phys. 22, 64 (1950).

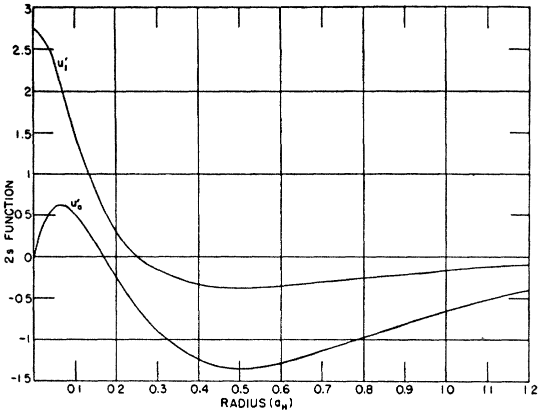

FIG. 2. 2s function u_0' and excited d function u_1' for Al.

The perturbation of the 2s and 3s functions is obtained in the same way as for 1s. By following the inward integration it turns out that u_1' has nodes at approximately the same r as u_0' and has the same sign as u_0' (see Fig. 2). Consequently, $u_0'u_1'$ is generally positive, and the electrons concentrate in the region where $(3\cos^2\theta-1)>0$. This leads to a shielding of the nuclear moment and corresponds to the effect found in the Thomas-Fermi model.

To obtain the moment induced in the 2p shell, we first consider the p state with magnetic quantum number $m=0$. The unperturbed wave function u_0 may be written [see Eq. (5)]

$$u_0=u_0'(\sqrt{3}/\sqrt{2})\cos\theta. \tag{15}$$

The first-order perturbation of the energy E_1 is given by

$$E_1=-\tfrac{1}{2}Q\int_0^\pi\int_0^\infty[u_0^2(3\cos^2\theta-1)/r^3]\sin\theta d\theta$$
$$=-(2/5)Q\langle 1/r^3\rangle_{2p}. \tag{16}$$

The perturbation u_1 obeys the equation:

$$(H_0-E_0)u_1=-(H_1-E_1)u_0, \tag{17}$$

where E_0 is the unperturbed 2p energy. From Eqs. (2) and (16), we obtain

$$-H_1u_0=\frac{\sqrt{3}}{\sqrt{2}}\frac{Qu_0'}{r^3}\left[\left(\frac{3}{2}\cos^3\theta-\frac{9}{10}\cos\theta\right)+\frac{2}{5}\cos\theta\right]. \tag{18}$$

The factor in brackets is written as the sum of an f function and a p function. Equation (17) now gives

$$(H_0-E_0)u_1=Q\frac{\sqrt{3}}{\sqrt{2}}\left(\frac{3}{2}\cos^3\theta-\frac{9}{10}\cos\theta\right)\frac{u_0'}{r^3}$$
$$+Q\frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2}{5}\cos\theta\right)u_0'\left(\frac{1}{r^3}-\left\langle\frac{1}{r^3}\right\rangle_{2p}\right). \tag{19}$$

Accordingly, u_1 is given by

$$u_1=Q\frac{\sqrt{3}}{\sqrt{2}}\left(\frac{3}{2}\cos^3\theta-\frac{9}{10}\cos\theta\right)u_{1,f}'$$
$$+Q\frac{\sqrt{3}}{\sqrt{2}}\left(\frac{2}{5}\cos\theta\right)u_{1,p}', \tag{20}$$

where the radial functions $u_{1,f}'$ and $u_{1,p}'$ are obtained from

$$-\frac{d^2u_{1,f}'}{dr^2}+\frac{12u_{1,f}'}{r^2}+V_0u_{1,f}'-E_0u_{1,f}'=\frac{u_0'}{r^3}, \tag{21}$$

$$-\frac{d^2u_{1,p}'}{dr^2}+\frac{2u_{1,p}'}{r^2}+V_0u_{1,p}'-E_0u_{1,p}'$$
$$=u_0'\left(\frac{1}{r^3}-\left\langle\frac{1}{r^3}\right\rangle_{2p}\right). \tag{22}$$

The calculation of $u_{1,f}'$ is similar to the calculation of u_1' for s states. Near $r=0$, we have the expansion:

$$u_{1,f}'=a_1r+a_2r^2+a_3r^3+a_4r^4+\cdots b_4r^4\log r+\cdots, \tag{23}$$

where the a_i and b_i are determined by equations similar to Eq. (11). For large r, $u_{1,f}'$ goes as $A\exp(-|E_0|^{\frac{1}{2}}r)$, where A is a constant. Its value is determined by matching the external solution with the series (23), in which a_4 is arbitrary. Figure 3 shows $u_{1,f}'$ together with u_0'. Since $u_0'u_{1,f}'$ is positive and $[\frac{3}{2}\cos^4\theta-(9/10)\cos^2\theta]>0$ close to the polar axis, the excitation to f states leads to a shielding effect, similar to the excitation of s states discussed above.

The induced moment $\Delta Q_{f,0}$ due to the $m=0$ electrons is given by

$$\Delta Q_{f,0}=6Q\int_0^\infty u_0'u_{1,f}'r^2dr\int_0^\pi[\tfrac{3}{2}\cos^4\theta-(9/10)\cos^2\theta]$$
$$\times(3\cos^2\theta-1)\sin\theta d\theta=(216Q/175)\int_0^\infty u_0'u_{1,f}'r^2dr. \tag{24}$$

For the $m=\pm 1$ states, we can write $-H_1u_0$ as follows:

$$-H_1u_0=\frac{\sqrt{3}}{2}\frac{Qu_0'}{r^3}\left[\left(\frac{3}{2}\cos^2\theta\sin\theta-\frac{3}{10}\sin\theta\right)-\frac{1}{5}\sin\theta\right]. \tag{25}$$

The first part of the square bracket gives rise to the f wave excitation. A calculation similar to that which leads to Eq. (24) gives the contribution to the induced moment. We thus obtain the total moment ΔQ_f due to $2p\rightarrow f$:

$$\Delta Q_f=(504Q/175)\int_0^\infty u_0'u_{1,f}'r^2dr. \tag{26}$$

In order to obtain the $2p\rightarrow p$ excitation, we note that the 2p shell is filled; hence, we must require that $u_{1,p}'$

be orthogonal to u_0'. For large r, we write

$$V_0=-C/r, \tag{27}$$

$$u_0'=A'\exp(-|E_0|^{\frac{1}{2}}r), \tag{28}$$

where C and A' are constants. When small terms are neglected, Eq. (22) becomes

$$\frac{d^2u_{1,p}'}{dr^2}-\frac{C}{r}u_{1,p}'-E_0u_{1,p}'=-\left\langle\frac{1}{r^3}\right\rangle_{2p}A'\exp(-|E_0|^{\frac{1}{2}}r). \tag{29}$$

The leading term of $u_{1,p}'$ is of the form $Br\exp(-|E_0|^{\frac{1}{2}}r)$, where the constant B is determined by

$$B=A'\langle 1/r^3\rangle_{2p}/(C-2|E_0|^{\frac{1}{2}}). \tag{30}$$

Thus, the solution of the inhomogeneous equation which goes as $r\exp(-|E_0|^{\frac{1}{2}}r)$ for large r is determined. The general solution is obtained from this by adding a multiple of u_0', since u_0' satisfies the homogeneous equation. Thus if $u_{1,p}'^{(r)}$ denotes the solution obtained by inward integration of $Br\exp(-|E_0|^{\frac{1}{2}}r)$, the excited wave function is given by

$$u_{1,p}'=u_{1,p}'^{(r)}-\alpha u_0', \tag{31}$$

where α is obtained from the orthogonality condition:

$$\alpha=\int_0^\infty u_{1,p}'^{(r)}u_0'dr. \tag{32}$$

In Eq. (30), C was taken as $rV_0(r)$ at the radius where the numerical integration is started. Figure 3 shows $u_{1,p}'$. In view of the orthogonality $u_{1,p}'$ must have a node. At $\theta=0$, the electron density is increased for small $r(u_0'u_{1,p}'>0)$, but for large r there is a decrease of the density. Since large radii are weighted more heavily ($\sim r^2$) for the quadrupole moment, the total induced moment for $2p\rightarrow p$ excitation is negative, so that the potential due to the induced quadrupole at large r has the same sign as the potential due to the nuclear Q ("antishielding effect"). In view of Eq. (19), the contribution of $m=0$ states, denoted by $\Delta Q_{p,0}$, is

$$\Delta Q_{p,0}=(12Q/5)\int_0^\infty u_0'u_{1,p}'r^2dr\int_0^\pi\cos^2\theta\times(3\cos^2\theta-1)\sin\theta d\theta$$
$$=(32/25)Q\int_0^\infty u_0'u_{1,p}'r^2dr. \tag{33}$$

Similarly, we obtain the contribution of $m=\pm1$ states by means of Eq. (25). The total moment due to $2p\rightarrow p$, denoted by ΔQ_p is

$$\Delta Q_p=(48/25)Q\int_0^\infty u_0'u_{1,p}'r^2dr. \tag{34}$$

In calculating the energy splitting we must take into account the penetration of the valence electron inside the core. Thus, if $Qq_0(r)dr$ denotes the induced moment contained between r and $r+dr$, the energy of interaction $E_{\Delta Q}$ with the induced moment for a $3p$ state with $m=0$ is given by

$$E_{\Delta Q}=(2/5)Q\int_0^\infty v'^2\left\{(1/r^3)\int_0^r q_0(r')dr'+r^2\int_r^\infty q_0(r')r'^{-5}dr'\right\}dr. \tag{35}$$

Here v' is the radial part of the $3p$ function, with

$$\int_0^\infty v'^2dr=1. \tag{36}$$

In view of Eqs. (16), (26), and (34), we have

$$q_0=r^2\left[\frac{8}{5}\sum_{n=1}^{3}(u_0'u_1')_{ns}+\frac{504}{175}(u_0'u_{1,f}')_{2p}+\frac{48}{25}(u_0'u_{1,p}')_{2p}\right], \tag{35a}$$

where the subscripts give the quantum numbers for the unperturbed state.

The interaction energy with the nuclear Q is

$$E_Q=-(2/5)Q\int_0^\infty(v'^2/r^3)dr=-(2/5)Q\langle 1/r^3\rangle_{3p}. \tag{37}$$

On account of the penetration, the internal regions of the induced distribution contribute more heavily than the external regions. For Al, the $2p\rightarrow p$ excitation gives a negative moment $-2.19Q$, and the other excited states give a positive moment $1.06Q$, so that the net induced moment is $-1.13Q$ (antishielding). Nevertheless, because of the penetration of $3p$, we find that

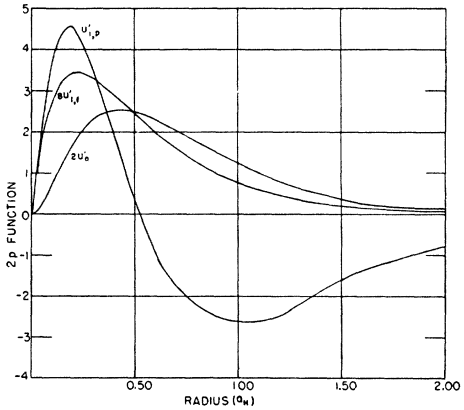

FIG. 3. $2p$ function u_0' and excited p and f functions for Al.

$E_{\Delta Q}/E_Q=-0.0064$, corresponding to a small shielding. The shielding excitations near the nucleus, although their quadrupole moment is smaller, slightly outweigh the $2p\rightarrow p$ excitation at larger radius because the region near the nucleus is more important.

In the preceding calculations we have omitted the exchange terms in the energy. In order to obtain these terms, we first consider the $1s\rightarrow d$ excitation. We assume that the $3p$ electron is in the $m=0$ state. The antisymmetric wave function for $3p$ and the $1s$ electron with spin parallel to $3p$ is

$$\psi=\frac{1}{\sqrt{2}}\begin{vmatrix} \left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}(1) & \left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}(2) \\ \left\{\frac{v'}{r}\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right\}(1) & \left\{\frac{v'}{r}\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right\}(2) \end{vmatrix}, \tag{38}$$

where (1) and (2) indicate that the coordinates are those of the first and second electron, respectively. We are interested in those terms of

$$E_{el}\equiv\int\psi^*(e^2/r_{12})\psi d\tau_1 d\tau_2, \tag{39}$$

which are linear in Q ($d\tau_1$ and $d\tau_2$ are the volume elements for the electrons, r_{12} is their distance of separation). We have

$$\begin{aligned}\psi^*\psi=&\frac{1}{2}\left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}^2(1)\left\{\frac{3}{2}\frac{v'^2}{r^2}\cos^2\theta\right\}(2)\\ &+\frac{1}{2}\left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}^2(2)\left\{\frac{3}{2}\frac{v'^2}{r^2}\cos^2\theta\right\}(1)\\ &-\left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}(1)\left\{\frac{\sqrt{3}}{\sqrt{2}}\frac{v'}{r}\cos\theta\right\}(1)\\ &\left\{\frac{u_0'}{\sqrt{2}r}+\frac{Qu_1'}{r}\left(\frac{3\cos^2\theta-1}{2\sqrt{2}}\right)\right\}(2)\left\{\frac{\sqrt{3}}{\sqrt{2}}\frac{v'}{r}\cos\theta\right\}(2).\end{aligned} \tag{40}$$

The negative term is the exchange effect. In order to evaluate this term we note that we may consider the contribution to Eq. (39) as due to the interaction of the density:

$$\rho_{sp}\equiv-2(u_0'/\sqrt{2})[(\sqrt{3}/\sqrt{2})v'\cos\theta]/r^2, \tag{41}$$

with the potential V_{pd} due to the density:

$$\rho_{pd}\equiv Qu_1'[(3\cos^2\theta-1)/2\sqrt{2}][(\sqrt{3}/\sqrt{2})v'\cos\theta]/r^2. \tag{42}$$

The factor 2 in ρ_{sp} arises from the presence of two such terms in Eq. (40). We write

$$\rho_{pd}=Qu_1'v'(\sqrt{3}/4)\{[(3\cos^3\theta-(9/5)\cos\theta]+(4/5)\cos\theta\}. \tag{43}$$

Only the part of V_{pd} which is due to the $\cos\theta$ term in Eq. (43) interests us, since the other term gives rise to a potential which behaves as an f function, and hence does not interact with ρ_{sp}. The potential V_{pd}' due to $Qu_1'v'(\sqrt{3}/5)\cos\theta$ is

$$V_{pd}'=Q\left(\frac{1}{r^2}\int_0^r u_1'v'r'dr'+r\int_r^\infty u_1'v'r'^{-2}dr'\right)\frac{2e^2}{5\sqrt{3}}\cos\theta. \tag{44}$$

If we denote the function in parentheses by $f_a(r)$ and if V_{pd}' is in ry units, we may write

$$V_{pd}'=(4Q/5\sqrt{3})f_a\cos\theta. \tag{45}$$

The interaction energy E_{sd}' of V_{pd}' with ρ_{sp} is

$$E_{sd}'=\int_0^\infty\int_0^\pi V_{pd}'\rho_{sp}r^2dr\sin\theta d\theta=-(8Q/15)\int_0^\infty u_0'v'f_a dr. \tag{46}$$

By means of Eq. (37), we find

$$E_{sd}'/E_Q=+(4/3)\int_0^\infty u_0'v'f_a dr\Big/\langle 1/r^3\rangle_{3p}. \tag{47}$$

We note that the exchange effect has the opposite sign to the direct (shielding) interaction, provided that the integral in Eq. (47) is positive; this was found to be true for the $s\rightarrow d$ excitations occurring in the present work.

The exchange for the $2p\rightarrow f$ excitation will now be obtained. This will be done first for the $2p$ state with $m=0$. The antisymmetric function for the $3p$ electron ($m=0$) and the $2p$ electron ($m=0$) with spin parallel to $3p$, is

$$\begin{aligned}\psi=&\frac{3}{2\sqrt{2}}\left\{\frac{u_0'}{r}\cos\theta+\frac{Qu_{1,f}'}{r}\left(\frac{3}{2}\cos^3\theta-\frac{9}{10}\cos\theta\right)+\frac{2}{5}\cos\theta\frac{Qu_{1,p}'}{r}\right\}(1)\left\{\frac{v'}{r}\cos\theta\right\}(2)\\ &-\frac{3}{2\sqrt{2}}\left\{\frac{u_0'}{r}\cos\theta+\frac{Qu_{1,f}'}{r}\left(\frac{3}{2}\cos^3\theta-\frac{9}{10}\cos\theta\right)+\frac{2}{5}\cos\theta\frac{Qu_{1,p}'}{r}\right\}(2)\left\{\frac{v'}{r}\cos\theta\right\}(1).\end{aligned} \tag{48}$$

Proceeding in the same way as for the $s \rightarrow d$ wave, we obtain the exchange term $E_{pf,0}'$ for $m=0$ as the interaction of a density:

$$\rho_{pp} \equiv -2\left(\frac{\sqrt{3}}{\sqrt{2}} u_0' \cos\theta\right)\left(\frac{\sqrt{3}}{\sqrt{2}} v' \cos\theta\right)\frac{1}{r^2} \tag{49}$$

with the potential V_{pf} due to the density:

$$\rho_{pf} \equiv Q u_{1,f}' \frac{\sqrt{3}}{\sqrt{2}}\left(\frac{3}{2}\cos^3\theta - \frac{9}{10}\cos\theta\right)\left(\frac{\sqrt{3}}{\sqrt{2}} v' \cos\theta\right)\frac{1}{r^2}. \tag{50}$$

ρ_{pf} is the sum of d and g functions; we are interested only in the d function. Let us write

$$\cos^4\theta - (3/5)\cos^2\theta = aP_4 + bP_2, \tag{51}$$

where P_l is the Legendre polynomial of order l; a and b are constants. We obtain

$$b = (5/4)\int_0^{\pi} (\cos^4\theta - \tfrac{3}{5}\cos^2\theta)(3\cos^2\theta - 1)\sin\theta d\theta = 6/35. \tag{52}$$

The d function part of V_{pf} which will be called V_{pf}' is given by

$$V_{pf}' = (9/5)bQP_2 f_b = (54/175)QP_2 f_b. \tag{53}$$

Here $V_{pf,0}'$ is in ry units and f_b is the function:

$$f_b = (1/r^3)\int_0^r u_{1,f}'v'r'^2 dr' + r^2\int_r^{\infty} u_{1,f}'v'r'^{-3}dr'. \tag{54}$$

We thus obtain

$$E_{pf,0}' = \int_0^{\infty}\int_0^{\pi} \rho_{pp} V_{pf}' r^2 dr \sin\theta d\theta = -(216/875)Q\int_0^{\infty} u_0'v'f_b dr, \tag{55}$$

and finally

$$E_{pf,0}'/E_Q = (108/175)\int_0^{\infty} u_0'v'f_b dr \bigg/ \langle 1/r^3\rangle_{3p}. \tag{56}$$

By doing a similar calculation for the exchange of $3p$ with the $2p \rightarrow f$ waves with $m=\pm 1$, one obtains for the ratio of the complete $2p \rightarrow f$ exchange term, denoted by E_{pf}':

$$E_{pf}'/E_Q = (252/175)\int_0^{\infty} u_0'v'f_b dr \bigg/ \langle 1/r^3\rangle_{3p}. \tag{57}$$

In order to obtain the exchange for the $2p \rightarrow p$ excitation, we consider the $2p$ state, $m=0$. The exchange energy may be regarded as resulting from the interaction of the density [see Eq. (48)]:

$$\rho_{pp}' \equiv -\frac{4Q}{5}\left(u_{1,p}'\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right)\left(v'\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right)\frac{1}{r^2}, \tag{58}$$

with the density:

$$\rho_{pp}'' \equiv \left(u_0'\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right)\left(v'\frac{\sqrt{3}}{\sqrt{2}}\cos\theta\right)\frac{1}{r^2}. \tag{59}$$

The potential due to ρ_{pp}' which we denote by V_{pp}' (ry units) is given by

$$V_{pp}' = -(8Q/5)(\tfrac{2}{5}f_c P_2 + gP_0), \tag{60}$$

where the functions f_c and g are as follows:

$$f_c(r) = (1/r^3)\int_0^r u_{1,p}'v'r'^2 dr' + r^2\int_r^{\infty} u_{1,p}'v'r'^{-3}dr', \tag{61}$$

$$g(r) = (1/r)\int_0^r u_{1,p}'v'dr' + \int_r^{\infty} u_{1,p}'v'r'^{-1}dr'. \tag{62}$$

The energy of interaction $E_{pp,0}'$ is

$$E_{pp,0}' = (-32/125)Q\int_0^{\infty} u_0'v'f_c dr - (8/5)Q\int_0^{\infty} u_0'v'g dr. \tag{63}$$

The second term in Eq. (63) is the interaction of the P_0 term of ρ_{pp}' with the P_0 term of ρ_{pp}''. As will be seen subsequently, this term is very important. For the $2p$ states $m=\pm 1$, there is no P_0 term; but the P_2 interaction makes a contribution:

$$E_{pp,1}' = (24/125)Q\int_0^{\infty} u_0'v'f_c dr. \tag{64}$$

We thus obtain for the total $2p \rightarrow p$ energy, denoted by E_{pp}':

$$E_{pp}' = (-8/125)Q\int_0^{\infty} u_0'v'f_c dr - (8/5)Q\int_0^{\infty} u_0'v'g dr. \tag{65}$$

The terms of E_{pp}' will be denoted by $E_{pp}'^{(2)}$ and $E_{pp}'^{(0)}$, respectively. The ratio E_{pp}'/E_Q can be obtained by means of (37).

The preceding calculations were carried out for Al, Cl, and Li. The results are given in Table I, where we have listed the ratios of the induced moment terms to the interaction with the nuclear moment. $E_{\Delta Q}/E_Q$ is due to the direct interaction with the induced moment

TABLE I. Ratio of the induced moment energy to the nuclear quadrupole moment energy.

	Li	Al	Cl
$E_{\Delta Q}/E_Q$	-0.166	-0.0064	-0.094
E'/E_Q	$+0.061$	$+0.033$	$+0.037$
$E'^{(0)}/E_Q$	0	$+0.174$	$+0.472$
R	-0.105	$+0.201$	$+0.415$
R_1(Th-F)	-0.258	-0.121	-0.093

[Eq. (35)]. We have separated the exchange into two parts, E'/E_Q and $E'^{(0)}/E_Q$. The first part includes all terms, except the P_0 interaction and the p shells which is given by $E'^{(0)}/E_Q$. For Al, we have

$$\frac{E'}{E_Q}=\sum_{n=1}^{3}\frac{(E_{sd}')_{ns}}{E_Q}+\frac{(E_{pf}')_{2p}}{E_Q}+\frac{(E_{pp}'^{(2)})_{2p}}{E_Q}, \tag{66}$$

$$E'^{(0)}/E_Q=(E_{pp}'^{(0)})_{2p}/E_Q. \tag{66a}$$

R is the total ratio of the energy splittings, and R_1 is the corresponding Thomas-Fermi result. The numerical calculations were similar in the three cases. For Cl, the $3p$ shell lacks one electron for completion. It can be easily shown that the calculations of the energy ratio can be carried out by considering a $3p$ electron interacting with a complete $3p$ shell. The $3p$ vacancy acts essentially as a $3p$ state with + charge.[3] The Hartree-Fock functions[4] for Cl$^-$ were used for the u_0. The atomic potential V_0 was taken as the Thomas-Fermi potential. For Li there is no quadrupole coupling with the ground ($2s$) state, and the calculations were performed for the valence electron in the $2p$ state. The Li $1s$ function was taken from the work of Fock and Petrashen;[5] to obtain the $2p$ function we used the potential of Seitz.[6]

The disagreement between the present results and the Thomas-Fermi values (see Table I) can be attributed in major part to the fact that the statistical model gives only the direct interaction of the valence electron with the perturbed core but excludes the exchange terms. As is shown by the table, these terms are considerable. In fact, for Cl and Al the P_0 exchange of the valence electron with the p shells determines the sign of the effect.

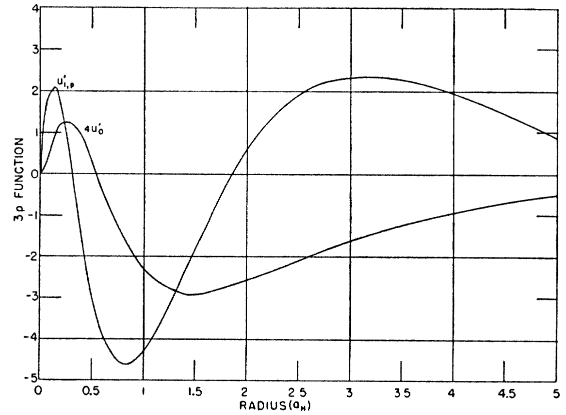

FIG. 4. $3p$ function u_0' and excited p function for Cl.

The change of density predicted by the Thomas-Fermi model [see Eq. (4), reference 1] consists in an angular displacement into the regions with positive $(3\cos^2\theta-1)$ (for $Q>0$); the total charge within any spherical shell $(r, r+dr)$ remains the same. This displacement corresponds to the $ns\rightarrow d$ and $np\rightarrow f$ excitations. The model does not include the $np\rightarrow p$ terms in which charge is displaced radially. In the direct interaction the $np\rightarrow p$ wave may give a net shielding or antishielding effect depending on the valence electron function. For Al, the $2p\rightarrow p$ excitation gives an antishielding effect because the $3p$ electron is external to $2p$ and experiences a considerable antishielding when it is outside the node of $u_{1,p}'$ at $r\sim 0.5a_H$ (see Fig. 3). Hence, the $2p\rightarrow p$ term subtracts from the shielding provided by the $ns\rightarrow d$ and $2p\rightarrow f$ waves; this explains the smallness of $E_{\Delta Q}/E_Q$. For Cl, the $2p\rightarrow p$ excitation leads to an antishielding as for Al (term in $E_{\Delta Q}/E_Q=+0.049$). However, the direct interaction with the $3p\rightarrow p$ excitation leads to shielding. This can be seen from Fig. 4, which shows the unperturbed $3p$ function together with the perturbation $u_{1,p}'$. The maximum of u_0' is at $r\sim 1.5a_H$, while the perturbed density (at $\theta=0$), $(12/5)Qu_0'u_{1,p}'/r^2$ is positive up to the node of $u_{1,p}'$ at $r=1.9a_H$. Hence, the $3p$ electron hole experiences predominantly a shielding, particularly since the most important region is somewhat inside $1.5a_H$, near the maximum of $u_0'^2/r^3$. The $3p\rightarrow p$ term in $E_{\Delta Q}/E$ is -0.079, so that for Cl, the sum of the $np\rightarrow p$ terms gives a net shielding effect.

The Thomas-Fermi R_1 can be directly compared with $E_{\Delta Q}/E_Q$ for Li and with the angular excitation part of $E_{\Delta Q}/E_Q$ for Al and Cl; its values are -0.078 and -0.063, respectively. Thus, R_1 is too large by a factor ~ 1.5. This discrepancy is due at least in part to the fact that the Thomas-Fermi density does not fall off rapidly enough at large r. Figure 5 shows the values of the density of induced moment (in units of Q) for Cl as obtained from the wave functions (angular modes only) and from the Thomas-Fermi model; they are denoted by $\bar{q}_0$ and $\bar{q}_0'$, respectively. The expression for $\bar{q}_0$ is similar to Eq. (35a), but excludes terms involving $(u_0'u_{1,p}')_{np}$. For the statistical model, we obtain

$$\bar{q}_0'=0.2998(\chi x)^{\frac{1}{2}}(x/r), \tag{67}$$

where χ is the Thomas-Fermi function and x is the Thomas-Fermi variable, $x=2.90r/a_H$ for Cl. We see from Fig. 5 that the statistical model gives a reasonably good approximation to $\bar{q}_0$. Of course, the maxima due to shell structure are smoothed over.

In the calculations of the wave functions, it was assumed that the perturbing potential is that of the nuclear quadrupole moment alone. Actually, the induced moment contributes to polarize the core. In order to investigate this effect, the $3p\rightarrow p$ wave for Cl was recalculated, using the potential of the nuclear moment plus the interaction of $3p$ with the induced moment.

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[3] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Macmillan Company, New York, 1935), Ch. VI.

[4] D. R. Hartree, Proc. Roy. Soc. (London) **156**, 56 (1936).

[5] V. Fock and M. Petrashen, Physik. Z. Sowjetunion **8**, 555 (1935).

[6] F. Seitz, Phys. Rev. **47**, 400 (1935).

We obtain the following equation [see Eq. (22)]:

$$-\frac{d^2u_{1,p}'}{dr^2}+\frac{2u_{1,p}'}{r^2}+V_0u_{1,p}'-E_0u_{1,p}'$$

$$=u_0'\left(\frac{1-\beta}{r^3}-\left\langle\frac{1-\beta}{r^3}\right\rangle_{3p}\right)$$

$$+4\beta_e-4u'_{0,(3p)}\cdot\int_0^\infty\beta_eu'_{0,(3p)}dr. \quad (68)$$

Here E_0 is the unperturbed $3p$ energy, $\beta(r)$ is given by

$$\beta(r)=\int_0^r q_0dr'+r^5\int_r^\infty(q_0/r'^5)dr', \quad (69)$$

where Qq_0dr is the induced moment between r and $r+dr$; $\beta_e(r)$ is the function

$$\beta_e(r)=g_{2p}u'_{0,(2p)}+g_{3p}u'_{0,(3p)}, \quad (70)$$

with

$$g_{2p}(r)=(1/r)\int_0^r u'_{1,(2p)}u'_{0,(3p)}dr'$$

$$+\int_r^\infty(u'_{1,(2p)}u'_{0,(3p)}/r')dr', \quad (71)$$

$$g_{3p}(r)=(1/r)\int_0^r u'_{1,(3p)}u'_{0,(3p)}dr'$$

$$+\int_r^\infty(u'_{1,(3p)}u'_{0,(3p)}/r')dr'. \quad (71a)$$

Here, $u'_{0,(2p)}$ and $u'_{0,(3p)}$ are the unperturbed functions for $2p$ and $3p$, respectively [normalized by Eq. (5a)]; $u'_{1,(2p)}$ and $u'_{1,(3p)}$ are the $2p\rightarrow p$ and $3p\rightarrow p$ excitation, respectively. The β-term in Eq. (68) represents the shielding by the induced moment, and β_e gives the P_0 exchange interaction of the $3p$ electron with $2p$ and $3p$ [Eq. (65)]. The other exchange terms are less important, as is shown by Table I (see E'/E_Q), and were omitted for simplicity. We note that

$$\left\langle\frac{1-\beta}{r^3}\right\rangle_{3p}+4\int_0^\infty\beta_eu'_{0,(3p)}dr$$

$$=\left\langle\frac{1}{r^3}\right\rangle_{3p}\left(1+\frac{E_{\Delta Q}+E'^{(0)}}{E_Q}\right)=1.38\left\langle\frac{1}{r^3}\right\rangle_{3p}. \quad (72)$$

In order to evaluate β_e [Eqs. (70), (71)] we used the functions, $u'_{1,(2p)}$ and $u'_{1,(3p)}$ obtained previously from the nuclear perturbation alone. The numerical integration of Eq. (68) proceeds in the same way as for Eq. (22). The solution is made orthogonal to u_0' by adding a constant times u_0' [see Eq. (32)]. The resulting $u_{1,p}'$ follows closely the $u_{1,p}'$ obtained for the nuclear perturbation alone (Fig. 4) but is somewhat larger in magnitude, as is expected, since the exchange term has the same sign as the nuclear perturbation. The increase is about 20 percent. Its relatively small magnitude shows that $u_{1,p}'$ is primarily determined by the nuclear perturbation. With the new $u_{1,p}'$ we recalculated the P_0 exchange term for $3p\rightarrow p$:

$$(E_{pp}'^{(0)})_{3p}/E_Q=4\int_0^\infty g_{3p}u_0'^2dr\bigg/\langle 1/r^3\rangle_{3p}. \quad (65a)$$

Its value is increased by only 10 percent, from 0.37 to 0.41.

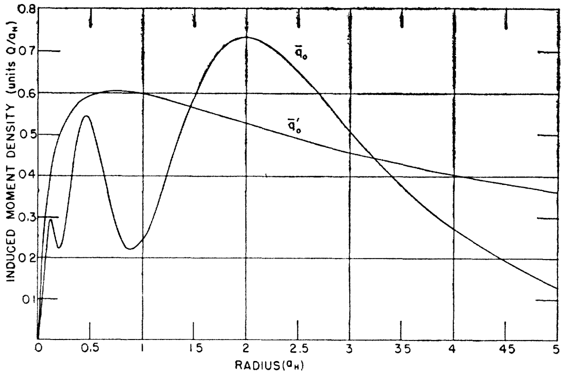

FIG. 5. Induced quadrupole density for Cl from wave functions ($\bar{q}_0$) and from Thomas-Fermi model ($\bar{q}_0'$).

Whereas the radial excitations are increased because of the P_0 exchange, the angular excitations are reduced, since the exchange terms are relatively less important so that the direct interaction (shielding) predominates. The $2s\rightarrow d$ wave for Cl was recalculated [see Eq. (7)], with the perturbing term $u_0'(1-\beta)r^3$ instead of u_0'/r^3. Thus, the shielding of Q by the induced moment was taken into account, but the exchange of $2s$ with the perturbed wave functions was not included. The external minimum of the $2s\rightarrow d$ wave (see Fig. 2) is 0.73 of the minimum obtained for the original wave function. The contribution of $2s$ to $E_{\Delta Q}/E_Q$ is reduced in about the same proportion, from -0.0087 to -0.0066. The actual decrease of u_1' is somewhat smaller because of the neglect of exchange. We estimate that the decrease is of the order of 15 percent for all shells (see Thomas-Fermi calculations subsequently).

Upon correcting the results of Table I for the effect of the induced moment on the excited wave functions, we obtain for the quadrupole correction, $R=-0.10$ for Li, 0.21 for Al, 0.46 for Cl. The experiments[7] from which the present values of Q for Al and Cl have been obtained consist in the measurement of the splittings a and b due to the interaction of the electrons with the magnetic moment μ_I and the quadrupole moment,

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[7] Davis, Feld, Zabel, and Zacharias, Phys. Rev. 76, 1076 (1949). H. Lew, Phys. Rev. 76, 1086 (1949).

respectively. If the interaction were with the valence electron only, a and b would be given by

$$a=(\mu_0\mu_I/hI)[2L(L+1)/J(J+1)]\langle r^{-3}\rangle_{\mathrm{val}}\equiv a'\mu_I\langle r^{-3}\rangle_{\mathrm{val}},$$

$$b=-(e^2Q/h)(2L/2L+3)\langle r^{-3}\rangle_{\mathrm{val}}\equiv b'Q\langle r^{-3}\rangle_{\mathrm{val}},$$

where μ_0 is the Bohr magneton, L and J are the orbital and the total angular momentum of the atom, I is the nuclear spin; the average $\langle r^{-3}\rangle_{\mathrm{val}}$ is taken over the valence electron function. Q is determined from the equation:

$$Q=(ba'/b'a)\mu_I,$$

μ_I being known independently. As we have seen, $\langle r^{-3}\rangle_{\mathrm{val}}$ in the equation for b must be replaced by $\langle r^{-3}\rangle_{\mathrm{val}}(1+R)$. It is not obvious that in the magnetic splitting a, $\langle r^{-3}\rangle_{\mathrm{val}}$ need not be corrected for the distortion of the spherical electron core by the asymmetric potential due to the valence electron. Because of this distortion there may be an interaction of the magnetic moment μ_I with the core, as well as with the valence electron. This effect is being investigated; if it exists, Q will be given by

$$Q=(ba'/b'a)\mu_I(1+R_m)/(1+R),$$

where R_m is a correction to $\langle r^{-3}\rangle_{\mathrm{val}}$, such that

$$a=a'\mu_I\langle r^{-3}\rangle_{\mathrm{val}}(1+R_m)$$

gives the magnetic splitting in terms of $\langle r^{-3}\rangle_{\mathrm{val}}$. Of course, if $R_m=0$, then the corrected moments are just $1/(1+R)$ times the present values.

The uncertainty of the wave functions introduces an important source of error. In order to obtain an estimate of this error, R was recalculated for Cl, assuming that the true $3p$ function is more internal than the Hartree-Fock function[1] and is, in fact, given by

$$u'_{0,(3p)}=u^{\mathrm{HF}}{}_{0,(3p)}+0.1u^{\mathrm{HF}}{}_{0,(2p)}, \tag{73}$$

where $u^{\mathrm{HF}}{}_{0,(np)}$ is the Hartree-Fock function. The inner maximum of $u'_{0,(3p)}$ is 1.5 times larger than for $u^{\mathrm{HF}}{}_{0,(3p)}$, and $\langle 1/r^3\rangle_{3p}$ is increased from $5.7a_H{}^{-3}$ to $11.3a_H{}^{-3}$. With the new $u'_{0,(3p)}$, the perturbation $u_{1,p}'$ was recalculated. The resulting value of the P_0 exchange term $(E_{pp}'^{(0)})_{3p}/E_Q$ [see Eq. (65)] is 0.29, as compared to 0.37 for the original calculation. The decrease is due to the fact that $(E_{pp}'^{(0)})_{3p}$ increases less rapidly than $\langle 1/r^3\rangle_{3p}$ as $u'_{0,(3p)}$ is made more internal. Similarly, $E_{\Delta Q}/E_Q$ is reduced from -0.094 to -0.072. An estimate of the change of the other terms in R gives $R=0.32$, as compared to the value 0.415 in Table I. We conclude that the uncertainty of our values of R is of the order of 30 percent.

TABLE II. Higher order terms in the induced quadrupole moment.

Element	Z	R_1	R_2	R_3	R'
B	5	0.220	0.075	0.032	0.166
Al	13	0.121	0.045	0.029	0.095
Sc	21	0.452	0.207	0.113	0.320
Ga	31	0.055	0.020	0.013	0.044
In	49	0.038	0.016	0.014	0.031
Eu	63	0.405	0.159	0.069	0.292
Lu	71	0.125	0.051	0.035	0.097
Ac	89	0.116	0.069	0.067	0.092

III. THOMAS-FERMI CALCULATIONS

The Thomas-Fermi calculation[1] of the quadrupole correction can be readily extended to include the effect of the induced moment on the perturbation of the core. We note that the potential due to the density by the nuclear Q is given by[1]

$$V_1(x,\theta)=\beta\left\{(1/x^3)\int_0^x x'^3(\chi x')^{\frac{1}{2}}(1/r'^3)dx' + x^2\int_x^\infty[(\chi x')^{\frac{1}{2}}/x'^2](1/r'^3)dx'\right\} [e^2Q(3\cos^2\theta-1)/4]. \tag{74}$$

Here χ and x are the Thomas-Fermi function and variable, respectively, $x=(Z^{\frac{1}{3}}/0.885a_H)r$, and $\beta=0.2998$. $V_1(x,\theta)$ is due to the density produced by the potential, $-(e^2Q/4r^3)(3\cos^2\theta-1)$. We are now interested in the potential V_2 produced by the perturbed density due to V_1. We obtain

$$V_2(x,\theta)=-\beta\left\{\frac{1}{x^3}\int_0^x x'^3(\chi x')^{\frac{1}{2}}V_1(x',\theta)dx' + x^2\int_x^\infty[(\chi x')^{\frac{1}{2}}]V_1(x',\theta)dx'\right\}. \tag{75}$$

V_2 has the same sign as the nuclear potential and produces a density which tends to shield the nucleus. By iteration, the total induced potential at x is given by

$$V(x,\theta)=-\frac{e^2Q}{4}\frac{Z}{(0.885)^3}(3\cos^2\theta-1)\sum_{i=1}^{\infty}(-\beta)^iI_i(x), \tag{76}$$

where

$$I_i(x)=(1/x^3)\int_0^x(\chi x')^{\frac{1}{2}}x'^3I_{i-1}(x')dx' + x^2\int_x^\infty[(\chi x')^{\frac{1}{2}}/x'^2]I_{i-1}(x')dx'.$$

$$I_0(x)=1/x^3. \tag{77}$$

Finally, the ratio R of the induced to the nuclear splitting may be written

$$R=\sum_{i=1}^{\infty}(-1)^iR_i, \tag{78}$$

where

$$R_i=Z\beta^i\int_0^\infty v'^2I_i(x)dr\Big/(0.885)^3\int_0^\infty(v'^2/r^3)dr. \tag{79}$$

Here v' is r times the radial part of the valence wave function normalized by Eq. (36). Table II lists R_2 and R_3 for the eight cases of reference 1. It is seen that R_2 is substantially smaller than R_1, indicating that the expansion is essentially valid. However, the decrease from R_2 to R_3 is not as great; in fact, for Ac, we have $R_3 \approx R_2$. The reason lies in the failure of the Thomas-Fermi field at large r. Whereas I_1 and I_2 have their maximum at $x=0(I_1(0)=\infty)$, I_3 is peaked at $x=2.0$ and the maximum of I_4 is at $x=5.2$, i.e., in a region where the Thomas-Fermi theory becomes inapplicable because of the low electron density. This difficulty would disappear if χ were replaced by the Thomas-Fermi-Dirac χ (including exchange), which becomes zero at a finite radius.[8] We, therefore, believe that a good approximation to the correction is obtained by taking $R_1-R_2+\frac{2}{3}R_3$. This is given as R' in Table II. We note that R'/R_1 is between 0.7 and 0.8. These results are in fair agreement with the calculation for Cl ($2s\rightarrow d$ excitation). R_1 can be obtained for all elements by interpolation among relatively few values. R_1 depends primarily on the orbital of the valence electron which determines $\langle 1/r^3\rangle$ [see Eq. (79)] and the penetration inside the core. Hence, it varies smoothly and by a relatively small amount as a given external shell is filled. For this reason it is possible to obtain R_1 for an intermediate element if R_1 is known for two cases at the beginning and at the end of the row of the periodic table. Table III presents results for additional elements whose orbitals are the same as in the earlier work[1] and for $4d$, $6p$, and $5f$. The valence wave functions v' were obtained by means of the Thomas-Fermi potential. The last column gives estimates of R' which were made by means of the values of R'/R_1 for the elements of Table II. Tables II and III provide two values of R' for each valence orbital, so that R' can be interpolated for the ground state of all elements. We saw that for Al, Cl, and Li, the Thomas-Fermi R_1 is bigger by a factor ~1.5 than the value calculated from the wave functions for the angular modes. We may conclude that for light atoms $R'/1.5$ gives an estimate of the shielding correction. It is likely that for heavy atoms R' should be reduced by a similar factor. It should be emphasized that R' gives only the angular part of the quadrupole correction.

TABLE III. Effect of the induced quadrupole moment.

Element	Z	Orbital	R_1	$\langle V_1\rangle a_H^3$	$\langle 1/r^3\rangle a_H^3$	R'
F	9	$2p$	0.145	4.29	8.89	0.110
Cl	17	$3p$	0.093	2.56	8.24	0.073
Cu	29	$3d$	0.263	8.23	9.38	0.186
Br	35	$4p$	0.047	3.82	24.1	0.038
Y	39	$4d$	0.242	2.10	2.60	0.180
Ag	47	$4d$	0.155	5.49	10.6	0.115
I	53	$5p$	0.034	2.54	22.1	0.028
La	57	$5d$	0.210	1.12	1.60	0.164
Lu	71	$4f$	0.317	19.0	17.9	0.229
Pt	78	$5d$	0.110	7.26	19.9	0.085
Tl	81	$6p$	0.023	2.20	28.6	0.019
At	85	$6p$	0.022	2.90	38.8	0.019
U	92	$5f$	0.296	6.09	6.17	0.225

I would like to thank Professors I. Rabi and E. Teller, who suggested this problem, for helpful discussions. I am also indebted to Drs. H. Foley and H. Snyder for several valuable discussions.

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[8] The induced moment for the statistical model, Eq. (5a) of reference 1, diverges logarithmically for large x for the same reason. This divergence does not lead to serious error, since v' decreases exponentially in the region where the nuclear Q is strongly shielded.