are the members of the γ-vibrational band via the γ rays of energy 725 and 593 kev, respectively. The transition to the (0,2+) level is also present via the 1600-kev γ ray but its reduced transition probability is about 100 times less than that of the 725-kev γ ray, the 1600-kev γ ray being assumed $E1$. If this 1723-kev level is collective in origin, an assignment of the K value can be made. The experimental ratio of the reduced transition probabilities of 725- and 593-kev γ rays is compared in Table III with theoretical ratios for different K values assumed for the 1723-kev level. As can be seen from Table III, the assignment $K=2$ for this level is clearly favored. Such an assignment explains the relative slowness of the 1600-kev γ transition to (0,2+) level since a transition of $E1$ type is forbidden by the K selection rule. It is interesting to see if any $M2$ mixture, which is allowed by the K selection rule, is present in this γ transition. An identical γ transition of 1189 kev in W^{182} has a 40% $M2$ mixture.[17]

The 2^- levels are found in other deformed even-even nuclei also. Table IV summarizes the presently known 2^- levels occurring in the region of medium-heavy and heavy deformed nuclei. An inspection of this table reveals that such 2^- levels are occurring in regions where there is a shift from a spherical to a deformed nucleus and vice versa. The ratios of the energies of these 2^- levels to the energy of the 2^+ member of the ground-state rotational band (column 3 in Table IV) seem to be grouped into values of about 14, 10, and 20 in the regions of neutron numbers around 90, 110, and 138, respectively; in each region this ratio appears to increase with the increase of deformation.

[17] C. J. Gallagher, Jr. and J. O. Rasmussen, Phys. Rev. **112**, 1730 (1958).

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Antishielding of Nuclear Electric Hexadecapole Moments*

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The antishielding factor η_∞ for a possible nuclear electric hexadecapole moment has been calculated for the Cu^+, Ag^+ and Hg^{++} ions, using the Hartree-Fock wave functions for the $3d$, $4d$, and $5d$ electrons involved. It was found that $\eta_\infty(Cu^+)\cong-1200$, $\eta_\infty(Ag^+)\cong-8050$, and $\eta_\infty(Hg^{++})\cong-63\,000$. The implication of these results is discussed.

IN a previous paper,[1] we have considered the interaction of a possible nuclear electric hexadecapole (16-pole) moment (HDM) with the ion core surrounding the nucleus. It has been shown that for medium and heavy atoms with closed d shells, the interaction energy of the HDM with the fourth-order derivative terms of the potential due to the ionic lattice (for the case of a crystal) will be considerably amplified by antishielding effects of the same type as have been calculated[2] and observed[3] for nuclear quadrupole moments. The antishielding effect arises from the large hexadecapole moment which is induced in the closed d (and possibly f) shells of the ion core. The induced HDM was written as

$$H_{\text{ind}}=-\eta_\infty H, \tag{1}$$

where H is the nuclear HDM, and η_∞ is defined as the hexadecapole antishielding factor, in a completely analogous manner to the antishielding factor[2] γ_∞ for the nuclear quadrupole moment.

In the present paper, we wish to report the results of calculations of η_∞ for the Cu^+ and Ag^+ ions, using the Hartree-Fock wave functions which have been obtained for these ions.[4,5] We have found that $\eta_\infty\cong-1200$ for Cu^+ and $\eta_\infty\cong-8050$ for Ag^+. These values are extremely large, even when compared to typical values of $\gamma_\infty(\sim-100)$, and therefore suggest that it may be possible to detect the nuclear HDM for nuclei with spin $I\geqq2$, by observing the deviation from the relationships between the resonance frequencies which would be expected for a pure quadrupole resonance spectrum.[6]

The predominant contribution to η_∞ for Cu^+ and Ag^+ is due to the $3d\rightarrow d$ and $4d\rightarrow d$ excitations, respectively, produced by the nuclear H. (Although the stable isotopes of Cu and Ag have spin $I=\frac{1}{2}$ and $\frac{3}{2}$, respectively, we assume the presence of a nuclear

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[1] R. M. Sternheimer, Phys. Rev. Letters **6**, 190 (1961). This Letter will be referred to as I.

[2] R. M. Sternheimer, Phys. Rev. **80**, 102 (1950); **84**, 244 (1951); **95**, 736 (1954); **105**, 158 (1957); R. M. Sternheimer and H. M. Foley, *ibid.* **102**, 731 (1956).

[3] See, for example, M. H. Cohen and F. Reif, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1957), Vol. 5, p. 321; T. P. Das and E. L. Hahn, *Nuclear Quadrupole Resonance Spectroscopy* (Academic Press, Inc., New York, 1958).

[4] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A157**, 490 (1936).

[5] B. H. Worsley, Proc. Roy. Soc. (London) **A247**, 390 (1958).

[6] T. C. Wang, Phys. Rev. **99**, 566 (1955).

HDM for the purpose of the calculations, which will also apply approximately to neighboring elements in the periodic table.) The term $\eta_\infty(nd\to d)$ due to the excitation of the nd electrons into higher d states is given by[1]

$$\eta_\infty(nd\to d) = (80/63)\int_0^\infty u_0'(nd)u'_{1,H}(nd\to d)r^4dr, \quad (2)$$

where $u_0'(nd)$ is r times the radial part of the unperturbed nd function, and $u'_{1,H}(nd\to d)$ is r times the radial part of the perturbation. (The notation of the present paper is the same as in I.) The function $u'_{1,H}(nd\to d)$ is determined by the equation,

$$\left[-\frac{d^2}{dr^2}+\frac{6}{r^2}+V_0-E_0\right]u'_{1,H}(nd\to d) = u_0'(nd)\left[\frac{1}{r^5}-\left\langle\frac{1}{r^5}\right\rangle_{nd}\right], \quad (3)$$

and by the orthogonality condition,

$$\int_0^\infty u_0'(nd)u'_{1,H}(nd\to d)dr=0. \quad (4)$$

In Eq. (3), V_0 and E_0 are the unperturbed potential and energy eigenvalue for the nd state, and $\langle 1/r^5\rangle_{nd}$ is the average of $1/r^5$ for the wave function $u_0'(nd)$.

The perturbed functions $u'_{1,H}(3d\to d)$ for Cu^+ and $u'_{1,H}(4d\to d)$ for Ag^+ were calculated by numerical integration of Eq. (3), using the Hartree-Fock functions $u_0'(3d)$ of Cu^+ and $u_0'(4d)$ of Ag^+, which have been obtained by Hartree and Hartree[4] and by Worsley.[5] The effective values of V_0-E_0 on the left-hand side of (3) were obtained from the function u_0' as follows[2,7]:

$$V_0-E_0+\frac{6}{r^2}=\frac{1}{u_0'}\frac{d^2u_0'}{dr^2}. \quad (5)$$

We note that for Cu^+, $\langle 1/r^5\rangle_{3d}=219.0a_H^{-5}$, and for Ag^+, $\langle 1/r^5\rangle_{4d}=932.3a_H^{-5}$.

The solution $u'_{1,H}$ was obtained by inward numerical integration starting at $r\equiv r_1=6a_H$ (both for Cu^+ and Ag^+), in the same manner as in our previous calculations of the quadrupole antishielding factor[2] $\gamma_\infty(nl\to l)$ and the dipole polarizability[7] α_d. The integration is started with an arbitrary value $u'_{1,H}(r_1)$ at $r_1=6a_H$. The value of $u'_{1,H}$ at $r_1+\delta$ (δ= interval of integration) is then obtained from

$$u'_{1,H}(r_1+\delta)=u'_{1,H}(r_1)\exp\{-[N(r_1)]^{\frac{1}{2}}\delta\}, \quad (6)$$

where N is defined by

$$N(r)\equiv\frac{6}{r^2}+(V_0-E_0)-\frac{I}{u'_{1,H}(r)}, \quad (7)$$

[7] R. M. Sternheimer, Phys. Rev. **96**, 951 (1954); **107**, 1565 (1957); **115**, 1198 (1959).

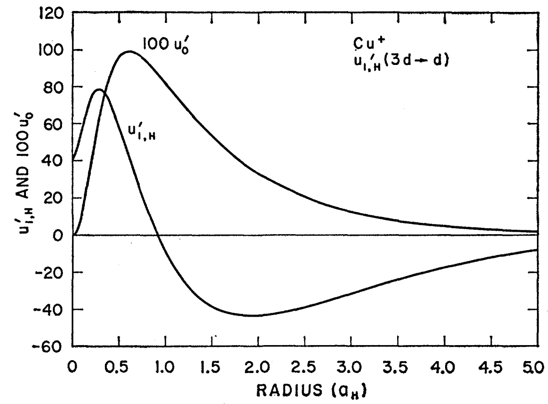

FIG. 1. The $3d$ function $u_0'(3d)$ and the $3d\to d$ perturbation $u'_{1,H}(3d\to d)$ for Cu^+.

and where I is the inhomogeneous term on the right-hand side of Eq. (3). As indicated in Eq. (6), $N(r)$ is to be evaluated at $r=r_1$.

The integrations were carried out from $r=r_1$ down to a small radius $r_0\sim 0.06a_H$. For small r, one can obtain the power series expansion for $u'_{1,H}$ which is valid near $r=0$. We note that $u'_{1,H}$ is finite at $r=0$, and has the value

$$u'_{1,H}(r=0)=c_3/6, \quad (8)$$

where c_3 is the coefficient of r^3 in the expansion of the $3d$ or $4d$ wave function u_0' near $r=0$. Thus we have

$$u_0'=c_3r^3+c_4r^4+\cdots, \quad \text{for} \quad r\sim 0, \quad (9)$$

where c_3 and c_4 are constant coefficients which can be obtained from the tabulated Hartree-Fock wave functions.[4,5] For Cu^+ $3d$, we have[4] $c_3=244.5$, so that $u'_{1,H}(r=0)=40.75$. Similarly, for the $4d$ function[5] of Ag^+, $c_3=1114$, whence $u'_{1,H}(r=0)=185.7$.

For each case (Cu^+ $3d$ and Ag^+ $4d$), two separate integrations were carried out, with starting values at $r_1=6a_H$ which differ by a factor of ~ 1.5, in order to obtain a check on the calculations. It should be noted that after the numerical integration is completed, the solution $u'_{1,H}$ is made orthogonal to u_0' by adding a suitable multiple of u_0' [see Eq. (4)]. For Ag^+, the resulting two solutions $u'_{1,H}(4d\to d)$ differ by less than 1% in the important region between $r=1a_H$ and $4a_H$, which makes the predominant contribution to the integral of Eq. (2) for $\eta_\infty(4d\to d)$. Correspondingly, the values of $\eta_\infty(4d\to d)$ which are derived from the two solutions, namely -7999 and -8056, differ only by a factor of 1.007. The average of the two results for $\eta_\infty(4d\to d)$ is thus -8028.

For Cu^+, the two solutions $u'_{1,H}(3d\to d)$ differ by less than 3% between $r=2a_H$ and $4a_H$. The resulting values of $\eta_\infty(3d\to d)$ are -1179 and -1214 (average $=-1197$).

We note that these results for both Cu^+ $3d\to d$ and Ag^+ $4d\to d$ are considerably larger (by a factor of 5–8) than the values which would be obtained for hydrogenic

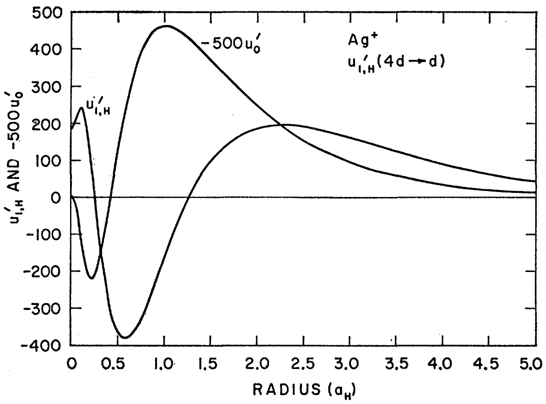

FIG. 2. The $4d$ function $u_0'(4d)$ and the $4d \to d$ perturbation $u'_{1,H}(4d \to d)$ for Ag^+.

wave functions with an effective atomic number $Z_e=1$. As was shown in I, for the hydrogenic case, one finds $\eta_\infty(3d \to d) = -147.2/Z_e$ and $\eta_\infty(4d \to d) = -1680.8/Z_e$. Thus a value of $Z_e=1$, which would be suggested by results for the quadrupole antishielding factor γ_∞, would give $\eta_\infty(3d \to d) \cong -150$ for Cu^+ and $\eta_\infty(4d \to d) \cong -1700$ for Ag^+. The actual values, namely -1197 and -8028 are larger by factors of 8.0 and 4.7, respectively. To put it in another way, the results for $\eta_\infty(nd \to d)$ from the Hartree-Fock wave functions correspond to effective Z values: $Z_e=0.123$ for Cu^+ $3d \to d$, and $Z_e=0.209$ for Ag^+ $4d \to d$. It should, of course, be noted that the Cu^+ $3d$ and Ag^+ $4d$ wave functions differ considerably from hydrogenic wave functions for any value of Z_e, so that one should not expect the hydrogenic formula to apply.

The perturbed wave functions $u'_{1,H}(3d \to d)$ of Cu^+ and $u'_{1,H}(4d \to d)$ of Ag^+ are shown in Figs. 1 and 2, respectively, together with the corresponding unperturbed radial functions $u_0'(nd)$. We note that the large results for $\eta_\infty(nd \to d)$ are essentially due to two effects: (1) the large values of $u'_{1,H}$ in the region of the outermost maximum of the perturbed wave function; e.g., $u'_{1,H}(4d \to d)$ of Ag^+ reaches a value of 197 at $r=2.3a_H$; (2) the large values of the factor r^4 in the region of the maximum of the integrand $u_0'u'_{1,H}r^4$ of Eq. (2). Thus the maximum of $u_0'u'_{1,H}r^4$ for Ag^+ $4d \to d$ occurs at $r=2.8a_H$, where $u_0'=-0.232$, $u'_{1,H}=176.5$, $r^4=61.47$, whence $u_0'u'_{1,H}r^4=-2517$. The fact that u_0' and $u'_{1,H}$ have opposite sign in the region of large r is responsible for the net antishielding effect of $\eta_\infty(nd \to d)$ (<0), in the same manner as for $\gamma_\infty(nl \to l)$.

For the $3d \to d$ excitation of Ag^+, the perturbed wave function $u'_{1,H}(3d \to d)$ was calculated, and the resulting $\eta_\infty(3d \to d)$ is -18.4. If one uses $\eta_\infty(4d \to d) = -8030$, one thus obtains for the complete η_∞ due to the radial modes, $\eta_{\infty,\mathrm{rad}}(Ag^+) \cong -8048$. Similarly, for Cu^+, we have $\eta_{\infty,\mathrm{rad}}(Cu^+) = -1200$.

As has been discussed in I, the contribution to η_∞ due to the angular modes of excitation of the core ($ns \to g$; $np \to f$, $np \to h$; $nd \to g$, $nd \to i$) can be obtained by means of the Thomas-Fermi model, in the same manner as for the quadrupole shielding factor[2] $\gamma_{\infty,\mathrm{ang}}$. If we interpolate between the results for K^+ ($\eta_{\infty,\mathrm{ang}}=0.58$) and Cs^+ (1.6), as given in I, we obtain $\eta_{\infty,\mathrm{ang}}=0.9$ for Cu^+ and 1.4 for Ag^+. These values are obviously negligible compared to the radial terms $\eta_{\infty,\mathrm{rad}}$ which therefore represent essentially the complete hexadecapole antishielding factor η_∞. Thus we have as our final result: $\eta_\infty(Cu^+) \cong -1200$ and $\eta_\infty(Ag^+) \cong -8050$, with an estimated uncertainty of $\sim 10\%$ due to the procedure of the numerical integration of Eq. (3).

We have also obtained the antishielding factors $\eta_\infty(4d \to d)$, $\eta_\infty(4f \to f)$, and $\eta_\infty(5d \to d)$ for the Hg^{++} ion, using the Hartree $4d$, $4f$, and $5d$ functions for this ion.[8] The results are: $\eta_\infty(4d \to d) = -271$, $\eta_\infty(4f \to f) = -17.6$, and $\eta_\infty(5d \to d) = -62{,}700$. It is expected that the value of $\eta_\infty(3d \to d)$ will be much smaller than $\eta_\infty(4d \to d)$ $[|\eta_\infty(3d \to d)| \lesssim 1]$. Thus the complete antishielding factor η_∞ for Hg^{++} is $\cong -63\,000$. Similarly to the results for Ag^+, where $|\eta_\infty(3d \to d)| \ll |\eta_\infty(4d \to d)|$, it is seen that also for Hg^{++} the outermost d shell makes the predominant contribution to η_∞.

As already pointed out above and in reference 1, these large values of η_∞ may make it possible to detect the presence of a nuclear hexadecapole moment using quadrupole resonance spectra from crystals containing ions with closed d shells. We note that the present results for $\eta_\infty(Cu^+)$ and $\eta_\infty(Ag^+)$ are considerably larger than the estimates made in reference 1 using $Z_e=1$.

[8] D. R. Hartree and W. Hartree, Proc. Roy. Soc. (London) **A149**, 210 (1935).