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THE INFLUENCE OF THE ELECTRON CLOUD ON THE NUCLEAR QUADRUPOLE MOMENT

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Using the Sternheimer procedure and the Löwdin–Appel's method for the calculation of atomic functions, the induced quadrupole moment and the energy of interaction between the electron cloud and the quadrupole moment for the Hartree field are calculated.

The present note deals with the influence of the electron cloud on the nuclear quadrupole moment. As is known [1] the change in electron density $\Delta\varrho$ induces a change ΔQ in the nuclear quadrupole moment Q:

$$\Delta Q = \int r^2 \Delta\varrho (3\cos^2\vartheta - 1) d^3r. \tag{1}$$

Starting from the Thomas–Fermi model, Sternheimer [1] estimated the induced moment in the electron shells. According to his result ΔQ is then [1]:

$$\Delta Q = \left[\frac{2 \cdot (1.7707)^{3/2}}{5\pi}\right] Q \int\limits_0^\infty (\chi x)^{1/2} dx. \tag{2}$$

where χ is the screening function in the Thomas–Fermi approximation considered at a point in the electron cloud dependent on the Thomas–Fermi variable $x = \mu r$; $\mu = 0.88534\, Z^{-1/3}$. Q denotes the nuclear quadrupole moment; its numerical values are given in Table I taken from [1].

In this note we assume the screening function of the atomic potential in the analytical form given by Bonham and Strand [2] for a Hartree atom:

$$\chi = Z \sum_{i=1}^{3} \gamma_i \exp(-\lambda_i r) \tag{3}$$

where γ_i and λ_i are parameters for which the numerical values are given in Table II calculated for several atomic number Z by means of the procedure of Bonham and Strand.

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TABLE I

The values of the nuclear quadrupole moment Q taken from [1]

Element	B(10,5)	B(11,5)	Al(27,13)	Ga(69,31)
$Q/10^{-24}$ cm^2	0.06	0.03	0.156	0.232
Element	Ga(71,31)	In(113,49)	In(115,49)	Eu(151,63)
$Q/10^{-24}$ cm^2	0.146	1.114	1.167	1.2
Element	Eu(153,63)	Lu(175,71)	Lu(176,71)	
$Q/10^{-24}$ cm^2	2.5	5.9	7.0	

TABLE II

Numerical values of γ_i and λ_i for several Z values

Z	5	13	31
γ_1	0.0164	0.0478	0.0831
γ_2	0.2452	0.3915	0.4940
γ_3	0.7385	0.5611	0.4233
λ_1	38.7028	25.5703	24.3440
λ_2	5.6204	4.8426	4.8792
λ_3	1.4234	1.4163	1.4452
Z	49	63	71
γ_1	0.1014	0.1108	0.1140
γ_2	0.5316	0.5476	0.5542
γ_3	0.3674	0.3310	0.3125
λ_1	24.7490	25.2363	25.5785
λ_2	5.0858	5.2530	5.3474
λ_3	1.4837	1.5145	1.5319

Next, the Sternheimer's procedure leads to the following expressions for the energy of interaction E_Q with the nuclear quadrupole moment

$$E_Q = -AQ\langle r^{-3}\rangle \tag{4}$$

and for the energy of interaction $E_{\Delta Q}$ with the induced moment:

$$E_{\Delta Q} = \left[\frac{2\cdot(1.7707)^{3/2}}{5\pi}\right] AQ\langle v\rangle. \tag{5}$$

In the formulae (4) and (5) A is a constant:

$$A = 0.64\, Z^{1/3} \tag{6}$$

and we have introduced the usual Sternheimer's symbol for $\langle V\rangle$:

$$\langle v\rangle = \int_0^\infty u_{nl}^2 \left\{ r^{-3} \int_0^r (\chi x)^{1/2} dx + r^2 \int_r^\infty \frac{(\chi x)^{1/2}}{(x\mu)^5}\, dx \right\} dr. \tag{7}$$

We consider only the case of a single valence electron. Then the quantum average values of V and r^{-3} are taken in the single valence electron state. Its radial wave function u_{nl} in our note should be constructed for a Hartree field according to our previous assumptions about the screening function.

The radial wave functions in the Hartree approximation which are complicated in analytical calculations are given in the numerical form (*e.g.*[3]). There exist mathematical methods for a construction of an approximate analytical form of these functions with respect to their numerical values. One of such methods is that given by Löwdin and Appel [4]. It should be applied in our case because the analytical form of the constructed wave functions and of the screening function is the same (expressed by means of exponentional terms). The Löwdin and Appel method assumes the following form for the radial function

$$u_{nl} = r^{l+1}[\pi_i(r_0^{(i)} - r)] \sum_{\nu=1}^{2} A_\nu \exp(-a_\nu r) \tag{8}$$

where $r_0^{(i)}$ denote the zeros of exact radial functions given by the numerical results. The coefficients A_ν, a_ν are chosen by analysing the numerical data. The numerical values of coefficients A_ν, a_ν calculated in this note and $r_0^{(i)}$ taken from [3] are presented in Table III. The functions obtained in this manner for the case discussed in this note agree sufficiently well with their numerical equivalents.

TABLE III

The numerical values of the constants appearing in U_{nl}

Z	A_1	A_2	a_1	a_2	$r_0^{(1)}$	$r_0^{(2)}$	$r_0^{(3)}$
5	0.6754	1.9312	0.6597	1.1656			
13	2.1364	14.4809	1.0426	1.9101	2.03		
31	0.0569	0.3021	0.4618	0.7138	0.828	3.032	
49	0.0434	0.6134	0.5475	0.8185	0.554	1.74	4.668
63	0.0629	0.3894	0.6502	0.9288			
71	0.0159	0.1022	0.4627	0.6759	1.048	3.16	

Our numerical results for the induced quadrupole moment and for the interaction energies calculated for the atom in the Hartree approximation are presented in the Tables. Table IV contains the numerical values of the induced moment ΔQ calculated from Eq. (2). In Table V we have numerical values of $\langle v\rangle$ and $\langle r^{-3}\rangle$ and an additional parameter

$$R = 0.2998\, \langle v\rangle [\langle r^{-3}\rangle]^{-1} \tag{9}$$

usually discussed in the problem presented in [1].

Our numerical values of $\langle r^{-3}\rangle$ and $\langle v\rangle$ obtained for the Hartree field differ from the corresponding values calculated by Sternheimer for the Thomas–Fermi field.

TABLE IV

The numerical values of ΔQ calculated from Eq. (1)

Element	Orbital	$\Delta Q/10^{-24}$ cm^2
B(10,5)	$2p$	0.073
B(11,5)	$2p$	0.036
Al(27,13)	$3p$	0.276
Ga(69,31)	$4p$	0.543
Ga(71,31)	$4p$	0.342
In(113,49)	$5p$	3.042
In(115,49)	$5p$	3.088
Eu(151,63)	$4f$	3.399
Eu(153,63)	$4f$	7.082
Lu(175,71)	$5d$	17.179
Lu(176,71)	$5d$	20.382

TABLE V

The numerical values of $\langle V \rangle$, $\langle r^{-3} \rangle$ and R calculated from Eq. (7) and (9)

Element	R	$\langle V \rangle$	$\langle r^{-3} \rangle$
B	0.1368	0.7849	1.7411
Al	0.0875	1.4609	5.0037
Ga	0.0781	0.5217	2.0013
In	0.0299	2.2215	29.9400
Eu	0.2364	0.7244	0.9186
Lu	0.0327	1.0277	9.3943

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