Quadrupole moment of atoms in the $nP_{1/2}$ state

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It is shown for the first time that atoms with the principal term $^2P_{1/2}$ have a quadrupole moment approximately five orders of magnitude larger than that of the nuclei of these atoms.

It has been established elsewhere[1] that the quadrupole moment of any particle, structured or structureless, with a spin 1/2 is strictly zero. In the present letter we consider the quadrupole moment of the atoms of the third column of the periodic system, whose electronic shell has $j = 1/2$. The quadrupole moment of these atoms is nonetheless nonvanishing and large: $Q \sim 10^{-20}$ cm^2.

The Breit potential for the interaction of electrons with a nucleus has terms similar to the tensor nuclear forces which account for the nonzero quadrupole moment of the deuteron. These terms also account for the quadrupole moment in a ground-state hydrogen atom, as was initially pointed out in Ref. 2. The numerical value of this quadrupole moment is $Q_{1s}^{(H)} = 7.55 \times 10^{-25}$ cm^2 (Ref. 3).

Amusia and Yakhontov[4] have recently predicted the existence of a much larger quadrupole moment in the $2p_{1/2}$ excited state of hydrogen and mesic hydrogen, in which it occurs as a result of the admixture of the $2p_{3/2}$ level to the $2p_{1/2}$ level through the hyperfine interaction. Since the energies of the $2p_{1/2}$ and $2p_{3/2}$ states are nearly the same, the quadrupole moment increases by approximately a factor of $\alpha^{-2} \sim 2 \times 10^{+4}$ in comparison with $Q_{1s}^{(H)}$, whereas the calculated value is $Q_{2p}^{(H)} = 4 \times 10^{-19}$ cm^2. A mixing of the $np_{1/2}$ and $np_{3/2}$ states also accounts for a large quadrupole moment of the atoms considered by us.

This value of the quadrupole moment is determined by the average value of the z component of the quadrupole-moment tensor of the "electron + nucleus" system in the initial $2p_{1/2}$ state. We easily see that $Q = 0$ if the hyperfine interaction W in the system under consideration is ignored.

Let us now consider the W-induced admixture of only the $np_{3/2}$ level to the $np_{1/2}$ level because of its close proximity to the initial level in terms of energy: $E_{p_{3/2}} - E_{p_{1/2}} = \Delta E_{fs} \sim Z^2\alpha^2 m_e e^4/\hbar^2 \ll e^2/a_B$ (Ref. 5), where Z is the nuclear charge, α is the fine-structure constant, and a_B is the Bohr radius of the hydrogen atom. The nonvanishing quadrupole moment in the $p_{1/2}$ state, which arises when W is taken into account in first order perturbation theory, is given by

$$\langle Q \rangle = 2\eta \langle np_{1/2} IFM \,|\, \hat{Q} \,|\, np_{3/2} IFM \rangle . \tag{1}$$

Here $\hat{Q}$ is the quadrupole-moment operator, and η is the factor for the mixing of the $np_{3/2}$ and $np_{1/2}$ levels which is given by

$$\eta = \langle np_{1/2} IFM \,|\, \hat{W} \,|\, np_{3/2} IFM \rangle (E_{p_{1/2}} - E_{p_{3/2}})^{-1} . \tag{2}$$

The small (proportional to α^2) difference in the radial functions of the $np_{1/2}$ and $np_{3/2}$ states may be disregarded (i.e., they may be assumed to be nonrelativistic) in the calculation of the quadrupole moment. In this approximation, the mixing factor η, as follows from (2), is determined within a numerical factor by

$$\eta \sim \frac{E_{F=1}(np_{1/2}) - E_{F=0}(np_{3/2})}{E_{p_{1/2}} - E_{p_{3/2}}} \sim \frac{\mu}{IZ} \frac{m_e}{m_p} , \tag{3}$$

where μ is the magnetic moment of the nucleus in nuclear-magneton units, and I is its spin.

We have used (1) and (2) to calculate the quadrupole moments of the atoms under consideration. We carried out both semiempirical calculations, i.e., with allowance for the fine + hyperfine splitting of the $np_{1/2}$ level, and analytical calculations. The analytical calculations yielded

$$Q = \frac{8}{15}\frac{Zm_e^2 - \mathcal{M}_я^2}{(m_e + \mathcal{M}_я)^2}\frac{\mu}{Z}\frac{m_e}{m_p}\langle r^2\rangle \begin{cases} 1 \quad , & F = I + 1/2 \\ -\dfrac{I-1}{I}\dfrac{2I-1}{2I+1} \, , & F = I - 1/2 \, , \end{cases} \tag{4}$$

where $\mathcal{M}_n$ is the nuclear mass. We used the nonrelativistic Hartree-Fock approximation to calculate $\langle r^2\rangle$. The calculated quadrupole moments of the hyperfine-structure sublevels with $F = I + 1/2$ of the ^{27}Al and ^{203}Tl, for example, are as follows: $Q = -3.2\times 10^{-20}\,\text{cm}^2$ and $Q = -3.0\times 10^{-21}\,\text{cm}^2$—calculated from (4) and $Q = -4.4\times 10^{-20}\,\text{cm}^2$ and $Q = -6.8\times 10^{-21}\,\text{cm}^2$—calculated semiempirically.

Analysis shows that $Q_{np1/2}$ is on the order of $10^{-21}\,\text{cm}^2$ for each hyperfine-structure sublevel of the atoms under study. This quadrupole moment is nearly a factor of 10^4 larger than the quadrupole moments of the nuclei of these atoms as well as $Q_{1s}^{(H)}$. We should emphasize that for states with $F = I + 1/2$ and $F = I - 1/2 Q_{np1/2}$, as follows from (4), has different signs, decreasing smoothly with increasing Z. As we move from the ground state to the excited $n'p_{1/2}$ states, the quadrupole moment increases rapidly—as n' (Ref. 4) because of the increase of $\langle r^2\rangle \sim n'$.[4]

A large quadrupole moment of the atoms with the principal term $^2P_{1/2}$ should have a large quadrupole moment when these atoms interact with matter, because, according to (4), the average quadrupole moment of the sample (i.e., one that takes into account the statistical weight $2F+1$ of each hyperfine-structure sublevel) is nonvanishing. Because the quadrupole moment is large, it can be observed experimentally and it can also be measured.

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