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A b s t r a c t

The tensor polarizability of the $6p_{\frac{1}{2}}$ and $6p_{\frac{3}{2}}$ states of thallium is calculated.

Measurements of the tensor polarizability (TP) of the $6p_{\frac{1}{2}}$ state in thallium /1/ is a reason of writing the present paper. As it is known, TP of a level with the total electronic momentum $j = \frac{1}{2}$ is different from zero due to hyperfine interaction of the electrons with the nucleus. The tensor polarizability of the $3p_{\frac{1}{2}}$ state in Al has been previously calculated in /2/. In that case, TP is defined by hyperfine mixing of the $3p_{\frac{1}{2}}$ and $3p_{\frac{3}{2}}$ states. Since fine splitting of the $3p$ level in Al is small, the off-diagonal matrix element of the tensor Stark operator between the $3p_{\frac{1}{2}}$ and $3p_{\frac{3}{2}}$ states can be expressed by TP of the $3p_{\frac{3}{2}}$ level, which is known from the experiment. Calculation of TP of the $6p_{\frac{1}{2}}$ level for Tl are essentially different. Fine splitting of the $6p_{\frac{1}{2}}$ and $6p_{\frac{3}{2}}$ levels is comparatively large, therefore it is necessary to take into account the hyperfine mixing of other states. The distinctive feature is the fact that in calculation of the off-diagonal matrix element of the tensor Stark operator between the $6p_{\frac{1}{2}}$ and $6p_{\frac{3}{2}}$ states, the experimental value of TP of the $6p_{\frac{3}{2}}$ level cannot be used, since the radial integrals and energetic denominators for the excitations of the $6p_{\frac{1}{2}}$ and $6p_{\frac{3}{2}}$ electrons for Tl considerably differ. And finally, the Coulomb mixing of the $6s^2 6p$ and $6sns6p$ states plays an important role for Tl.

In the present paper, TP of the $6p_{\frac{3}{2}}$ state, which was measured in /3/ is also calculated (besides TP of the $6p_{\frac{1}{2}}$ state). Our values of TP of the $6p_{\frac{1}{2}}$ and $6p_{\frac{3}{2}}$ states are in good agreement with experimental data /1, 3/.

Our aim in this paper is not only to calculate the tensor polarizability itself, but also to evaluate an accuracy of calculations concerning the parity violation effects in heavy atoms /4-10/. The problem consists in the fact that the results of calculations of these effects, which were performed by various theoretical groups differ up to two times. The opinion has arisen from this, that such a discrepancy is due to the limits of accuracy of calculations for heavy atoms. However, we think that the accuracy of half-empirical calculations /4-6/ is not worse than 10÷20%, that is confirmed by the results of the present paper.

The magnitude of parity violation effects depends on a value of the wave function of the external electron on the nucleus and matrix elements of the electrical dipole moment. It is easy to see that TP of the $p_{\frac{1}{2}}$ state has a similar stricture, since the hyperfine-interaction matrix element is determined by a behavior of the wave function of the electron near by the nucleus, as is the weak-interaction matrix element. Thus, agreement between the calculated and experimental values of TP for the state confirms the correctness of calculations for parity violation effects in Tl, Pb and Bi, which were carried out in /4-6/.

The shift of the levels in an electrical field is expressed by the scalar and tensor polarizabilities as follows:

$$\Delta W = -\frac{1}{2}\alpha_s E^2 - \frac{1}{4}\alpha_t \frac{3M^2 - F(F+1)}{3F^2 - F(F+1)}(3E_z^2 - E^2) \quad (1)$$

where α_s is the scalar polarizability, α_t is the tensor polarizability, F is the total angular momentum of the atom, M is his projection.

As has been noted, TP of the $6p_{\frac{1}{2}}$ state arises owing to hyperfine mixing, i.e. it takes place in the third order of the perturbation theory:

$$\alpha_{ik} = -2\sum_{n,m}\left[\frac{\langle 0|d_\alpha|n\rangle\langle n|H^{hfs}|m\rangle\langle m|d_\beta|0\rangle}{(E_0-E_n)(E_0-E_m)} + 2\frac{\langle 0|H^{hfs}|n\rangle\langle n|d_\alpha|m\rangle\langle m|d_\beta|0\rangle}{(E_0-E_n)(E_0-E_m)}\right]\times \quad (2)$$

$$\times\left[\frac{1}{2}(\delta_{\alpha i}\delta_{\beta k}+\delta_{\alpha k}\delta_{\beta i}) - \frac{1}{3}\delta_{ik}\delta_{\alpha\beta}\right],$$

$$\alpha_t \equiv \alpha_{zz}$$

where H^{hfs} is the Hamiltonian of hyperfine interaction, d_i is the operator of the electrical dipole moment. The main contribution to TP comes from the following transitions:

$$5d^{10}6s^2 6p_{\frac{1}{2}} \xrightarrow{H^{hfs}} 5d^{10}6s^2 np_{\frac{3}{2}} \xrightarrow{d} i \xrightarrow{d} 5d^{10}6s^2 6p_{\frac{1}{2}}$$

$$n \geq 6,\ i = 5d^{10}6s^2 ms,\ 5d^{10}6s^2 md,$$

$$5d^{10}6s\,6p_{\frac{1}{2}}^2,\ 5d^9 6s^2 6p_{\frac{1}{2}}^2,\ m \geq 7$$

$$6s^2 6p_{\frac{1}{2}} \xrightarrow{H^{hfs}} 6s\,6p_{\frac{1}{2}}\,ns \xrightarrow{d} 6s\,6p_{\frac{1}{2}}^2 \xrightarrow{d} 6s^2 6p_{\frac{1}{2}},\ n \geq 7$$

$$6s^2 6p_{\frac{1}{2}} \xrightarrow{H^{hfs}} 6s\,6p_{\frac{1}{2}}\,ns \xrightarrow{d} 6s^2 ns \xrightarrow{d} 6s^2 6p_{\frac{1}{2}},\ n \geq 7 \quad (3)$$

$$6s^2 6p_{\frac{1}{2}} \xrightarrow{d} 6s^2 ns \xrightarrow{H^{hfs}} 6s^2 ms \xrightarrow{d} 6s^2 6p_{\frac{1}{2}},\ n, m \geq 7$$

$$6s^2 6p_{\frac{1}{2}} \xrightarrow{d} 6s\,6p_{\frac{1}{2}}^2 \xrightarrow{H^{hfs}} 6s\,6p_{\frac{1}{2}}^2 \xrightarrow{d} 6s^2 6p_{\frac{1}{2}}$$

$$6s^2 6p_{\frac{1}{2}} \xrightarrow{d} 6s\,6p_{\frac{1}{2}}\,6p_{\frac{3}{2}} \xrightarrow{H^{hfs}} 6s\,6p_{\frac{1}{2}}^2 \xrightarrow{d} 6s^2 6p_{\frac{1}{2}}$$

It is convenient to write the matrix elements of hyperfine interaction as follows /11/:

$$\langle 6p_{\frac{1}{2}}|H^{hfs}|np_{\frac{3}{2}}\rangle = \frac{1}{9\sqrt{2}}\frac{\Omega}{\nu_6^{\frac{3}{2}}\nu_n^{\frac{3}{2}}} R_{13} K_{13} N_{13} I_z \quad (4)$$

$$\langle ns_{\frac{1}{2}}|H^{hfs}|ms_{\frac{1}{2}}\rangle = \frac{8}{3}\frac{\Omega}{\nu_n^{3/2}\nu_m^{3/2}} R_1 K_{ns,ms}\vec{I}\vec{j} \qquad (5)$$

where ν_i is the effective principal number of the electron, $\Omega = \frac{\mu}{I} Z\alpha^2 \frac{m_e}{m_p}\frac{m_e e^4}{2\hbar^2}$, μ is the magnetic moment of the nucleus, I is the total angular momentum of the nucleus, $R_1 = \frac{3}{\gamma_1^2(4\gamma_1^2-1)}$ and $R_{13} = -\frac{4\sin[\pi(\gamma_3-\gamma_1)]}{\pi[Z\alpha]^2}$ are the relativistic factors, $\gamma = \sqrt{\varkappa^2-(Z\alpha)^2}$, $\varkappa = (-1)^{j+\frac{1}{2}-l}(j+\frac{1}{2})$, j and l are the total angular and orbital momenta of the electron, K_i is the ratio between the accurate matrix element of hyperfine interaction and the matrix element calculated in the quasiclassical Fermi-Segre approximation /12/; N_{13} is the parameter taking into account the influence of the Coulomb mixing between $6s^2np$ and $6s\kappa s\,mp$ on the matrix element (4). The parameters K_{13} and N_{13} were calculated in /11/ (note that $K_{13}=\sqrt{K_1K_3}$, K_1 and K_3 are the corresponding coefficients for the $p_{\frac{1}{2}}$ and $p_{\frac{3}{2}}$ electrons). The magnitude of hyperfine splitting of the $7s$ level is known from the experiment /13/: $\Delta E_{7s} = 0.417\ \mathrm{cm}^{-1}$. From this, we find that $K_{7s,7s} \approx 0.86$. In /4/ it was shown that $K_{6s,6s} \approx 1$. We determine the remaining K_i as follows: $K_{ms,ns} = K_{7s,7s}$; $K_{6s,ms} = \sqrt{K_{7s,7s}}$, $n,m \geq 7$. The matrix elements of the dipole moment, which are necessary for calculation of TP were found in /14/. The contribution of continuou spectrum is calculated by means of the wave functions obtained by numerical solution of the Dirac equation with the effective potential proposed in /15/.

Using (2)-(5), we find the following value of TP of the state

$$\alpha_t(6p_{\frac{1}{2}}) = -3.7\cdot 10^{-8}\ Hz/(v/cm)^2$$

The experimental value in /1/ is:

$$\alpha_t(6p_{\frac{1}{2}}) = -(3.74\pm 0.09)\cdot 10^{-8}\ Hz/(v/cm)^2$$

Such a good coincidence of calculation with experiment is apparently random, since through strong reduction of contributions to (2), it is doubtful whether the accuracy can be better than 10÷20%.

Calculation of TP for the $6p_{\frac{3}{2}}$ state is essentially simpler compared to that for the $6p_{\frac{1}{2}}$ state, because the former is different from zero and does not take into account the hyperfine interaction. The result of our calculations

$$\alpha_t(6p_{\frac{3}{2}}) = -5.85\cdot 10^{-3}\ Hz/(v/cm)^2$$

agrees well with the experimental value /3/:

$$\alpha(6p_{\frac{3}{2}}) = -(6.04\pm 0.08)\cdot 10^{-3}\ Hz/(v/cm)^2$$

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References

1. H.Gould, Phys.Rev. 14A, 922, 1976.
2. I.R.P.Angel, P.G.H.Sandars and G.K.Woodgate, Proc.R.Soc.Lond. A.338, 95, 1974.
3. F.R.Petersen, H.G.Palmer and I.H. Shirley, Bull.Am.Phys.Soc. 13, 1674, 1968.
4. V.N.Novikov. O.P.Sushkov, I.B.Khriplovich, JeTP, 71, 1665, 1976.
5. O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich. Pis'ma v JeTP 24, 502, 1976.
6. V.V.Flambaum, Yadernaya Fiz. 24, 383, 1976.
7. H.Brimicombe, C.E.Loving and P.G.H.Sandars. J.Phys.B.Atom. Molec.Phys. 9, L 23, 1976.
8. E.M.Henley, L.Wilets. Phys.Rev. A14, 1411, 1976.
9. P.G.H.Sandars, R.M.Sternheimer, Phys.Rev. A11, 473, 1975.
10. E.M.Henley, M.Klapisch, L.Wilets, Phys.Rev.Lett. 39 , 994, 1977.
11. O.P.Sushkov, V.V.Flambaum, I.B.Khriplovich, Optika i spektroskopiya, 44, 3, 1978.
12. E.Fermi and E.Segre, Mem.Acad. d'Italia, 4, 131, 1933.
13. S.Pollack and E.Wong, AmJ.Phys. 39, 1388, 1971.
14. O.P.Sushkov, V.V.Flambaum, J. of Quant.Spectr. and Rad.Transf., to be published.
15. D.V.Neuffer and E.D.Commins. Phys.Rev. 16A, 844, 1977.

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