The nature of the strongly forbidden M1 transitions and the g-factor anomalies in heavy atoms

O. P. Sushkov, V. V. Flambaum, and I. B. Khriplovich

Institute of Nuclear Physics, Siberian Division of the USSR Academy of Sciences

(Accepted 3 February 1979)


A new mechanism is proposed for the appearance of strongly forbidden M1-transition amplitudes and corrections to the g factor in a heavy atom with a single outer electron. Expressions are obtained for these quantities in the case of an outer s or p electron. Numerical computations are carried out for cesium and thallium.

1. INTRODUCTION

The question of the causes of the deviation of the g factor of an atom with one outer electron from the g factor of the free electron was actively discussed many years ago at the time of the first measurements of the anomalous magnetic moment of the electron.\(^{11}^{14}\) The strongly forbidden M1 transitions in the heavy atoms have of late attracted attention in connection with the ongoing search for parity nonconservation in these atoms as a result of the weak interaction of the electron with the nucleus.\(^{15}^{16}\)

The g-factor anomalies of the alkali atoms have been measured in a number of experiments.\(^{17}^{19}\) If in the light atoms the corrections to the g factor is almost constant, in the heavy atoms it changes its sign and increases rapidly with Z. Hence we can conclude that the corrections to the g factor in the heavy and light atoms are due to different mechanisms. It is well known that, to explain this anomaly in the light atoms, it is sufficient to take only the relativistic effects into account.\(^{11}^{16}\) As regards the heavy atoms, however, it was proposed long ago that here a large contribution is made by the mixing of the configurations jointly with the spin-orbit interaction.\(^{15}^{16}\) It was natural to assume that the latter effect is important for the strongly forbidden M1 transitions in the heavy atoms.\(^{15}^{16}\) Specifically, in Refs. 5, 6, and 16, the topic of discussion in the corrections arising in fourth-order perturbation theory: second order in the Coulomb mixing of the configurations and second order in the spin-orbit interaction. The corresponding quantitative computations were, however, not carried out. Therefore, the decisive argument in favor of this mechanism was the fact that all the remaining attempts to explain the observed effects, say in cesium, turned out to be untenable. Yet when we carried out the corresponding computation for cesium, we surprisingly found its result to be roughly 100 times smaller than the experimental result. This discrepancy for cesium is also noted in Neuffer and Commins’s paper,\(^{17}^{19}\) with which we became acquainted only after the completion of the present investigation.

In the present paper we propose a new mechanism for the phenomena under discussion. They can arise not in fourth-order, but in third-order, perturbation theory: first-order in the Coulomb mixing of the configurations and second-order in the spin-orbit interaction. We compute the g factors of the 6s\(_{1/2}\) state of cesium and the 5p\(_{1/2}\) and 6p\(_{3/2}\) states of thallium, as well as the amplitudes of the M1 transitions 6s\(_{1/2}\)→7s\(_{1/2}\) in cesium and 5p\(_{3/2}\)→6p\(_{1/2}\) in thallium, taking into account, along with the configuration mixing, the normal relativistic corrections. We do not consider the corrections due to the hyperfine interaction, since their computation is trivial and, besides, they can be experimentally separated out.

2. THE g FACTOR OF CESIUM

To elucidate the cause of the appearance of the g-factor anomaly of cesium, it is convenient to represent the correction due to configuration mixing in the following form:

\[\left|\langle J_{\ell}\rangle - \langle J_{\ell}^{(0)}\rangle\right| = \left|\langle J_{\ell}\rangle - \langle J_{\ell}^{(0)}\rangle\right|\]

In the LS-coupling approximation there is in the cesium atom an outer 6s electron above the filled shells, i.e., the ground state is \(\left|6s_{1/2}\right\rangle\). In order for the matrix element \(\langle L_{\ell}\rangle\) to be different from zero, it is necessary for the admixture into the \(5p_{3/2}\) states of cesium with \(L = 0\) to have a non-zero admixture. Numerical computations are carried out for cesium and thallium, as well as the amplitudes of the M1 transitions 6s\(_{1/2}\)→7s\(_{1/2}\) in cesium and 5p\(_{3/2}\)→6p\(_{1/2}\) in thallium.
Thus far we have carried out the discussion in terms of the LS scheme, treating the spin-orbit interaction as a perturbation. However, the computation looks significantly simpler in the jj scheme with the use of relativistic radial wave functions, where the effect formally arises in first-order perturbation theory. In this case in the matrix element (1) it is sufficient to take into account the ket or bra the admixture by the exchange Coulomb interaction of the states with an excited inner-shell electron. The corresponding correction to the g factor is equal to

\[ \Delta g = \sum_{n', l', j', \text{subshell}} \int \left\langle \phi_{n'lj'} | \hat{\mu}^e \right| \phi_{nlj} \right\rangle, \]

where \( n, l, j \), and \( j' \) respectively denote the principle quantum number, the orbital quantum number, the total angular momentum of the electron. The states \( |nlj\rangle \) lie below the \( \text{ff} \) state, while the states \( |n'l'j'\rangle \) lie above it (naturally, the continuous spectrum should be included here).

The matrix element \( \left\langle n'l'j' | \hat{\mu}^e | nlj \right\rangle \) for \( n' \neq n \) is equal to zero if \( j' \neq j \), but is nonzero in first order in the spin-orbit interaction for \( j' = j = 2 \) (the fact that it is not too much suppressed in heavy atoms was earlier discovered by means of a numerical computation by Neuffer and Commins\(^2\)).

\[ \left\langle n'l'j' | \hat{\mu}^e | nlj \right\rangle = \frac{e}{2m_0c} \alpha(n'lj; nlj), \]

where \( \alpha(n'lj; nlj) \) is the overlap integral of the corresponding radial wave functions. In first order in the spin-orbit interaction \( \alpha(n'lj; nlj) \rightarrow \alpha(n'l'j'; nlj) \). From this it is very easy to verify that (2) in fact, a quantity that is of second order in the spin-orbit interaction.

The thus found correction to the g factor of the ground state of cesium is equal to

\[ \Delta g = \frac{a}{g_u} \left\langle \phi_{nlj} | | \phi_{nlj} \right\rangle \]

Here \( G^e \) is the exchange Coulomb integral. It should be noted that in the formula (4) the dependence of the \( G^e \) on \( j \) and \( j' \) (i.e., on the spin-orbit interaction) is not of less importance than the dependence on their energy denominator. A numerical computation in the effective-potential approximation (see the Appendix) on the basis of the formula (4) yields \( \Delta g = 3.66 \times 10^{-4} \).

Let us consider the other mechanisms that contribute to the correction to the g factor. These are, first, the relativistic corrections to the magnetic-moment operator of the outer electron; second, the magnetic interaction of the outer electron with the inner-shell electron; and, finally, the above-mentioned contribution, connected with configuration mixing, of fourth-order perturbation theory. The relativistic wave function of the outer electron has the form

\[ \psi_{nlj} = \frac{1}{(2\pi)^3} \int d\mathbf{r} \phi_{nlj}(\mathbf{r}) \]

With the aid of the Dirac equation, the exact relativistic expression for the magnetic-moment operator of the outer electron can be reduced to a form in which the small corrections (\( a^2 \)) are explicitly separated out (we set \( \hbar = c = 1 \));

\[ \Delta g_{\text{rel}} = -\frac{a}{g_u} \left\langle \phi_{nlj} | \hat{\mu}^e \right| \phi_{nlj} \right\rangle \]

Here \( a \) is the energy, \( V(r) \) is the effective potential, \( \nu = (-1)^{j} \nu_{l} / \nu_{l+1} \). A numerical computation for cesium \( (\nu = -1) \) on the basis of this formula yields \( \Delta g_{\text{rel}} = -0.38 \times 10^{-5} \).

A correction to the g factor, due to the magnetic interaction of the outer electron with the inner-shell electrons, arises in the Coulomb gauge \( (\text{div} A = 0) \) from the diamagnetic term \( e^2A^2 / 2m^2c^2 \) in the Hamiltonian. In the present case \( A = A_x + A_y \), where \( A_x, A_y \) are the vector potentials of the external field and the outer electron. The corresponding correction to the magnetic moment can be reduced to the form

\[ \Delta g_{\text{magn}} = \frac{a}{g_u} \left\langle \phi_{nlj} | \hat{\mu}^m \right| \phi_{nlj} \right\rangle \]

Here \( \nu(r) \) is the core-electron density and \( a_0 \) is the Bohr radius. The matrix element in (7) is evaluated, using the wave functions of the outer electron. In cesium \( (\nu = -1) \) the numerical computation based on this formula yields \( \Delta g_{\text{magn}} = 0.12 \times 10^{-4} \). The same result can be obtained on the basis of the Breit Hamiltonian for the interaction of two electrons\(^1\) after making the substitution \( p \rightarrow p - eA / c \) in it.

Besides the direct magnetic interaction, the exchange magnetic interaction, as well as the exchange spin-orbit interaction, contributes to the correction to the g factor. The computation of their contribution for cesium yields \( \Delta g_{\text{exch}}(\text{Si}) = 0.38 \times 10^{-5} \).

The estimation of the above-mentioned contribution of fourth-order perturbation theory in the case when the closed shells are opened by the Coulomb interaction with the outer electron shows that \( \Delta g_4 \sim 10^{-4} \).

Let us note that there arises in the formal computation of the fourth-order multipole order (it is precisely such a correction, with the difference between the Coulomb integrals for the \( p_x \) and \( p_y \) electrons neglected, that has been considered before\(^2\))(\nu_{l} \nu_{l+1} \text{subshell})\). It is clear, however, that this term need not be taken into account, since the \( F^e \) integrals they are matrix elements of the centrally symmetric self-consistent field, which has already been taken into account in the wave functions in the solution of the Dirac equation. It is not difficult to verify by means of a direct calculation that the indicated correction is already contained in the formula.
Adding all the calculated contributions, we obtain
\[ \delta g = \delta g_6 + \delta g_7 + \delta g_{\text{em}} \times 3.2 \times 10^{-4}. \]

(8)

Allowing for the fact that our computation of the Coulomb integrals in one and the same—for all the electrons—effective potential constitutes a very rough approximation, the agreement with the experimental value of \( \delta g = 2.18 \times 10^{-4} \) (Ref. 11) is quite satisfactory.

3. THE AMPLITUDE OF THE STRONGLY FORBIDDEN \( 6s_{1/2} \rightarrow 7p_{1/2} \)

The amplitude of the \( M1 \) transition \( 6s_{1/2} \rightarrow 7p_{1/2} \)
\[ M_{\text{(1)}} = (9/11)(2/1), L_{\text{(1)}} = (1/1), \]

can be computed in exactly the same way as the correction to the \( g \) factor.\(^{11}\) The contribution due to the mixing of the configurations is equal to (cf. (4)):
\[ M_{\text{mix}} = \frac{2}{3}(\delta g_6 + \delta g_7 + \delta g_{\text{em}}) \times 3.2 \times 10^{-4} \]

(9)

The relativistic correction to the amplitude of the \( 1s(6s) \rightarrow 2p(7p) \) \( M1 \) transition of the outer electron has the form (cf. (6)):
\[ M_{\text{rel}} = \frac{1}{3} \left[ \left( \lambda_0 + \frac{1}{\alpha} \right) \delta g_6 + \left( \lambda_0 - \frac{1}{\alpha} \right) \delta g_7 + \delta g_{\text{em}} \right] \times 3.2 \times 10^{-4} \]

(10)

where \( \lambda_0 = \lambda_1 = \lambda_2 = 1 \) (Ref. 11). The second term in the curly brackets arose from the expansion of the exponential function in the photon wave function. For the \( 6s_{1/2} \rightarrow 7p_{1/2} \) transition in cesium (\( \lambda = -1 \)), \( M_{\text{rel}} = 0.010 \times 10^{-4} \). The contribution of the magnetic corrections is computed with the aid of the formula (7), and is equal to \( M_{\text{mag}} = 0.03 \times 10^{-4} \). The relativistic and magnetic corrections are equal to \( \delta g = 0.172 \times 10^{-4} \). The total correction to the \( g \) factor of the \( 6s_{1/2} \) state is \( \delta g = \delta g_6 + \delta g_7 + \delta g_{\text{em}} = \approx 0.3 \times 10^{-4} \). This number coincides with the number obtained by Ref. 19. The computation from the formula (7) of the magnetic interaction of the outer electron with the inner-shell electrons yields \( \delta g_{\text{em}} = -1.23 \times 10^{-4} \). Notice that the formula (7) does not agree with the analogous expression obtained in Ref. 19. However, numerically, this discrepancy does not turn out to be very important. The calculation of the contribution of the exchange magnetic and spin-orbit interactions in thallium turns out to be significantly more tedious than the calculation in cesium. Its numerical value is equal to \( \delta g_{\text{em}} = 0.19 \times 10^{-4} \). As for the correction of fourth-order perturbation theory, in this case it turns out to be less than \( 2 \times 10^{-5} \). The total correction to the \( g \) factor of the \( 6p_{1/2} \) state
\[ \delta g = \delta g_6 + \delta g_7 + \delta g_{\text{em}} = \approx 2 \times 10^{-4}. \]

(12)

The quantity \( \delta g \) computed by us is in good agreement with the experimental value \( \delta g = -2.012(18) \times 10^{-4} \) (Ref. 23), and numerically close to the result of the calculation in Ref. 19.

The amplitude of the \( M1 \) transition \( 6p_{1/2} \rightarrow 7p_{1/2} \) is also due largely to the relativistic and diamagnetic corrections, the contribution of which is computed from the formulas (6) and (7): \( M_{\text{rel}} = 0.172 \times 10^{-4} \), \( M_{\text{mag}} = 0.17 \times 10^{-4} \), \( M_{\text{em}} = -0.18 \times 10^{-4} \). However, here an appreciable role is played by the configuration-mixing effects arising in fourth-order perturbation theory. In this case the contribution of the \( \delta g_{\text{em}} \) term is replaced by the configuration-mixing effect. With allowance for the above-indicated uncertainty in the magnitude of the Coulomb integrals, we obtained for the estimate \( M_{\text{rel}} = 0.3 \times 10^{-4} \). Thus, the calculated value of the transition amplitude is close to \( M_{\text{cal}} = M_{\text{rel}} + M_{\text{mag}} = 2.9 \times 10^{-4} \).

(13)

This value of \( \delta g \) differs in sign from both the experimental value, \( 2.7 \times 10^{-4} \times 10^{-4} \), and the earlier computed value, \( M_{\text{cal}} = 3.3 \times 10^{-4} \). It is possible that the difference in sign is connected with the inconsistency of the definitions of the magnetic moment (for our definition of \( M_{\text{mag}} \) see the footnote, 3, to the formula (9)). Unfortunately, we were not able to establish unequivocally the sign with which the \( M_{\text{cal}} \) is defined in Refs. 8 and 19.

A similar computation for the amplitudes of the \( M1 \) transitions \( 6s_{1/2} \rightarrow 6p_{1/2}, 6p_{3/2} \) yields
\[ M_{\text{rel}}(6p_{1/2} \rightarrow 6s_{1/2}) = 1.8 \times 10^{-4} \], \( M_{\text{rel}}(6p_{3/2} \rightarrow 6s_{1/2}) = 1.2 \times 10^{-4} \). (14)

As for the contribution to the \( g \) factor of the \( 6p_{1/2} \) state, the contribution made to it by the third-order mechanism considered in Sec. 2 is equal to
\[ M_{\text{rel}} = -\frac{1}{2} \sum_{x=1}^{3} \left( \frac{1}{\alpha} \right) \delta g_6 + \left( \frac{1}{\alpha} \right) \delta g_7 + \delta g_{\text{em}} \times 3.2 \times 10^{-4} \]

(15)

\[ \delta g = \delta g_6 + \delta g_7 + \delta g_{\text{em}} = 2.6 \times 10^{-4}. \]

The relativistic and magnetic corrections are computed from the formulas (6) and (7) with \( \alpha = 2 \).

Sushkov et al. 39

Sov. Phys. JETP 48(1), July 1978
We do not know the experimental value of this quantity. We do not know the experimental value of this quantity.

\[
\Delta q \approx 10^{-4}.
\]

(10)

[APPENDIX]

For all the computations in cesium we used the effective potential

\[
V'(r) = \frac{(Z-1)}{r} \left( \frac{\alpha^2}{4\pi^2} + \frac{1}{r} \right).
\]

(1.1)

Actually, this is the Tietz potential\(^{25}\) truncated at large distances. For \(r > \mu\), this potential is well approximated by the Thomas-Fermi potential. The potential (1.1) reproduces the experimental energies and the fine structure of all the states (including the inner-shell ones) with an error not worse than a few percent.

In thallium we used the potential proposed in Ref. 19:

\[
V'(r) = \frac{(Z-1)}{r} \left( \frac{\alpha^2}{4\pi^2} \right) 1_{\text{eff}}^2.
\]

(2.1)

The error in the energy and fine-structure fits here is also not worse than a few percent.

\(^{1}\)V. G. Zheludevskii has drawn our attention to the fact that this circumstance leads to the appearance of a paramagnetic correction, \(\sim 1.2\alpha^2\),\(^{32}\) to the diamagnetic susceptibility of an inert gas. The magnitude of this correction can easily be computed with the aid of the formula (1.3).

\(^{2}\)One of the present authors S. B. Khraplovich takes the opportunity to note that in an error in the preprint of his work published in Ref. 8 was corrected after he had become acquainted with M. and C. Bouchiat's paper.\(^{33}\)

\(^{3}\)We define \(\Delta q\) in such a way that \(\Delta Q = -\Delta q \left( I_2 + 2 \Delta \right)\) in the nonrelativistic limit. All the radial wave functions used by us are positive in the \(r = 0\) limit.


\(^{5}\)Kusch and H. Tash, Phys. Rev. 75, 1477 (1949).


\(^{11}\)Sushkov, V. V. Flambaum, and I. B. Khriplovich, Yad. Fiz. 21, 1046 (1975) [Sov. J. Nucl. Phys. 22, 538 (1976)].

\(^{12}\)A. K. Agret, Translated by A. K. Agret.