Enhancement factor for the electron electric dipole moment in francium and gold atoms

T. M. R. Byrnes, V. A. Dzuba, V. V. Flambaum, and D. W. Murray
School of Physics, University of New South Wales, Sydney 2052, New South Wales, Australia
(Received 23 November 1998)

If electrons had an electric dipole moment (EDM) they would induce EDM's of atoms. The ratio of the atomic EDM to the electron EDM for a particular atom is called the enhancement factor *R*. We calculate the enhancement factor for the francium and gold atoms, with the results $910\pm\sim5\%$ for Fr and $260\pm\sim15\%$ for Au. The large values of these enhancement factors make these atoms attractive for electron EDM measurements, and hence the search for time-reversal invariance violation. [S1050-2947(99)06204-6]

PACS number(s): 32.10.Dk, 11.30.Er, 14.60.Cd

The existence of a nonzero electric dipole moment (EDM) of an atom, electron, or any quantum-mechanical system would imply that time-reversal invariance (T) and parity (P) are violated. To date, no nonzero EDM has been observed, though experimental limits on their magnitude have been obtained. The standard model predicts an upper limit on the electron EDM of the order of $10^{-40}e$ cm [1], while various alternative models predict values many orders of magnitude larger (for reviews of predicted values of the electron EDM see Refs. [2,3]). Measurements of the electron EDM are worthwhile as in the future they may be able to distinguish between these models. Direct measurements of the electron EDM are difficult due to the electron's charge (see, e.g., [4]), so results for the electron EDM are obtained from atomic EDM measurements instead. The present limit on the electron EDM is $|d_e|<4\times10^{-27}e$ cm, from an experiment on the EDM of the Tl atom [4]. A summary of the results of atomic EDM measurements can be found in Table 6.2 of Ref. [5].

An atomic EDM can be induced by the presence of an electron EDM (as well as by other mechanisms, such as T- and P-violating electron-nucleon or nucleon-nucleon interactions, and nucleon EDM's). This allows us to obtain experimental results for the electron EDM by measuring the atomic EDM. The atomic EDM (d_A) induced by the electron EDM (d_e) would be proportional to d_e, and the ratio $R=d_A/d_e$ for a particular atom is known as the enhancement factor. As was first noted by Sandars [6], the atomic EDM of a heavy atom can be many times larger than the electron EDM; in fact, R is of the order of $Z^3\alpha^2$ times a relativistic factor (~3 in heavy atoms), where Z is the atomic number and $\alpha=1/137$ (see, e.g., [7,8,5]). To convert experimental results for atomic EDM's to results for electron EDM's the value of the enhancement factor R is needed. Summaries of results for various enhancement factors can be found in Ref. [4] and Table 6.1 of Ref. [5]. In this work we do accurate calculations of R for the Fr and Au atoms.

The T- and P-odd interaction between the EDM of an electron and the electric field of the nucleus ($-d_e\gamma_0\boldsymbol{\Sigma}\cdot\mathbf{E}$) results in an admixture of the ground state of the electron with excited states of opposite parity, according to perturbation theory. On one side of the atom the ground-state and excited-state wave functions will have the same sign, while on the other side they will have opposite signs. Therefore the total wave function will be larger on one side of the atom, hence the electron will be more likely to be there and so the atom will have an EDM. An expression for this atomic EDM, and hence R, can be presented in the following form (see, e.g., Refs. [7,8,5]):

$$R=\frac{d_A}{d_e}=2e\sum_n \mathrm{Re}\frac{\langle0|z|n\rangle\langle n|(\gamma_0-1)\boldsymbol{\Sigma}\cdot\mathbf{E}|0\rangle}{E_0-E_n} \qquad (1)$$

(for an atom with one valence electron), where $|0\rangle$ is the unperturbed ground state, $\{|n\rangle\}$ is the set of states with which it is mixed (including unbound, continuum states for which the sum should be replaced by an integral), $-e$ is the charge on the electron, $\mathbf{E}$ is the electric field produced by the nucleus [$=Ze\mathbf{r}/r^3$; the main contribution to the second matrix element in Eq. (1) comes from short distances, where the electric field of the nucleus is unscreened], $z=\mathbf{r}_z$, and γ_0 and $\boldsymbol{\Sigma}$ are the normal matrices of relativistic quantum mechanics. The ground state of the valence electron in Fr is $7s$, while in Au it is $6s$. The operator $(\gamma_0-1)\boldsymbol{\Sigma}\cdot\mathbf{E}$ is a pseudoscalar and so it can only mix states having opposite parity and the same total angular momentum. Therefore the ground state is only mixed with $p_{1/2}$ states.

Equation (1) can be rewritten as

$$R=-\frac{4Z\alpha}{3}\mathrm{Re}\sum_n \frac{\int_0^\infty [f_s^*(r)rf_{np}(r)+g_s^*(r)rg_{np}(r)]r^2Q(r)\,dr\int_0^\infty g_{np}^*(r)r^{-2}g_s(r)r^2P(r)\,dr}{E_0-E_{np}} \qquad (2)$$

by using the following expression for the electron's relativistic wave function (see, e.g., [9]): $\psi_{nljm}=[f_{njl}(r)\Omega_{jlm}, -ig_{njl}(r)(\boldsymbol{\sigma}\cdot\mathbf{r}/r)\Omega_{jlm}]^T$, where f and g are radial wave functions (f_s refers to the ground state and f_{np} the $p_{1/2}$ excited states) and Ω_{jlm} is a spherical spinor (an eigenfunction of $\hat{j}^2$ and $\hat{j}_z$). Computer generated wave functions were used to calculate the integrals in Eq. (2) (where available, previously determined values were used). These wave functions were obtained using the relativistic Hartree-Fock method. The factors $P(r)$ and $Q(r)$ take into account the screening of the nuclear electric field by electrons and core polarization corrections (for the nondirect core polarization contribution these factors actually become nonlocal operators). We also took into account correlation corrections to the wave functions. The many-body perturbation theory methods that we used are described in Refs. [10–14]. As a test, we also performed calculations using a semiempirical method [7] that does not require computer calculations. The results were in good agreement with the numerical calculations.

For Fr, we used the experimental value of the $7s$-$7p_{1/2}$ radial integral of r [the first integral in Eq. (2)] that was determined in [15]: $-5.238(10)$, in units of the Bohr radius (this compares well with the calculated value in [14]: -5.241). For the $7s$-$8p_{1/2}$ radial integral of r we used the value calculated in [14] (we used the most complete many-body calculation value denoted by ''Brueckner plus non-Brueckner'' in Table IV of this work), with an estimated accuracy of 3%. The $7s$-$9p_{1/2}$ and $7s$-$10p_{1/2}$ radial integrals of r were calculated by us, as were the $7s$-$np_{1/2}$ values of the second integral in Eq. (2) (all with an estimated accuracy of 3%). We used the values of the $7s, 7p_{1/2}$, $8p_{1/2}$, and $9p_{1/2}$ energy levels listed in [16], while we calculated the $10p_{1/2}$ energy level ourselves. We truncated the summation in Eq. (2) for the discrete states at the $10p_{1/2}$ state, as the remainder of this series is very small (it gives a contribution to the enhancement factor ~ 3, i.e., 0.3%). For the unbound, continuum states all integrals were calculated in the present work. For these we did not take into account screening, core polarization or correlation corrections, and so the errors for these integrals are larger (we estimate a 50% error for the whole continuum contribution), though this does not have an excessively large effect on the final error as the contribution of the continuum states to the enhancement factor is small ($=30$). The final value of the enhancement factor for Fr is 910, with an estimated 5% error.

For Au, we used the energy levels listed in [17]. Using the experimental result for the oscillator strength for the $6s$-$6p_{1/2}$ transition in [18], we obtained the value of the $6s$-$6p_{1/2}$ radial integral of r: $-2.16(2)$. All of the other radial integrals were calculated in the present work, with an estimated accuracy of 10% for the discrete states. Once again, we estimate the error for the continuum contribution as 50% [the continuum contribution was again small ($=20$)]. We truncated the summation over discrete states at the $8p_{1/2}$ state, with the remainder of the series giving a contribution ~ 1 (0.3%) to the enhancement factor. The final value of the enhancement factor for Au is 260, with an estimated 15% error.

These results are in reasonable agreement with the previously determined estimates of the enhancement factors: ≈ 1150 for Fr [19] and ≈ 250 for Au [20].

[1] M.E. Pospelov and I.B. Khriplovich, Yad. Fiz. **53**, 1030 (1991) [Sov. J. Nucl. Phys. **53**, 638 (1991)].

[2] W. Bernreuther and M. Suzuki, Rev. Mod. Phys. **63**, 313 (1991).

[3] S.M. Barr, Int. J. Mod. Phys. A **8**, 209 (1993).

[4] E.D. Commins, S.B. Ross, D. DeMille, and B.C. Regan, Phys. Rev. A **50**, 2960 (1994).

[5] I.B. Khriplovich and S.K. Lamoreaux, *CP Violation Without Strangeness* (Springer-Verlag, Berlin, 1997).

[6] P.G.H. Sandars, Phys. Lett. **14**, 194 (1965).

[7] V.V. Flambaum, Yad. Fiz. **24**, 383 (1976) [Sov. J. Nucl. Phys. **24**, 199 (1976)].

[8] I.B. Khriplovich, *Parity Nonconservation in Atomic Phenomena* (Gordon and Breach, Philadelphia, 1991).

[9] V.B. Berestetskiĭ, E.M. Lifshitz, and L.P. Pitaevskiĭ, *Relativistic Quantum Theory* (Pergamon Press, Oxford, 1971).

[10] V.A. Dzuba, V.V. Flambaum, P.G. Silvestrov, and O.P. Sushkov, J. Phys. B **20**, 1399 (1987).

[11] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Lett. A **140**, 493 (1989).

[12] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Lett. A **141**, 147 (1989).

[13] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Lett. A **142**, 373 (1989).

[14] V.A. Dzuba, V.V. Flambaum, and O.P. Sushkov, Phys. Rev. A **51**, 3454 (1995).

[15] J.E. Simsarian, L.A. Orozco, G.D. Sprouse, and W.Z. Zhao, Phys. Rev. A **57**, 2448 (1998).

[16] Reference [14] and references therein.

[17] C.E. Moore, *Atomic Energy Levels*, Natl. Bur. Stand. Ref. Data. Ser., Natl. Bur. Stand. (U.S.) Circ. No. 35 (U.S. GPO, Washington, D.C., 1971), Vol. III.

[18] P. Hannaford, P.L. Larkins, and R.M. Lowe, J. Phys. B **14**, 2321 (1981).

[19] P.G.H. Sandars, Phys. Lett. **22**, 290 (1966).

[20] W.R. Johnson, D.S. Guo, M. Idrees, and J. Sapirstein, Phys. Rev. A **34**, 1043 (1986).