Ab initio calculations of off-diagonal hyperfine interaction in cesium

A. Derevianko, M. S. Safronova, and W. R. Johnson
Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556

(Received 18 May 1999)

We have performed a relativistic many-body calculation of the off-diagonal hyperfine interaction mixing amplitude M_{hf} for the $6s$-$7s$ transition in atomic cesium. The *ab initio* result $M_{\mathrm{hf}}=0.8070(73)\times 10^{-5}|\mu_{\mathrm{B}}/c|$ is in excellent agreement with a previous semiempirical value $M_{\mathrm{hf}}=0.8094(20)\times 10^{-5}|\mu_{\mathrm{B}}/c|$. [S1050-2947(99)51509-6]

PACS number(s): PACS: 31.15.Ar, 32.80.Ys, 32.10.Fn

Recently, Bennett and Wieman [1] measured the ratio of the off-diagonal hyperfine amplitude to the tensor transition polarizability (M_{hf}/β) for the $6s$-$7s$ transition in atomic cesium. The value of β was then deduced using a *semiempirical* value of M_{hf} calculated by Bouchiat and Piketty [2]. Further, Bennett and Wieman combined the resulting value of β with a previous measurement of the parity-nonconserving (PNC) amplitude and with atomic structure calculations to determine a value of the weak charge Q_W. Their result differs from the prediction [3] of the standard model by 2.5σ. In light of this discrepancy and its dependence on the accuracy of the off-diagonal hyperfine amplitude M_{hf}, we perform an *ab initio* relativistic many-body calculation of M_{hf}. We find excellent agreement with the semiempirical value of Bouchiat and Piketty [2], providing a partial confirmation of the conclusion made by Bennett and Wieman [1].

The M_{hf} amplitude in conjunction with PNC in Cs was first discussed by Bouchiat and Bouchiat [4]. The magnetic-dipole transition amplitude between hyperfine levels F and F' of $6s$ and $7s$ states in cesium can be represented as

$$A_{M1}=M+(F-F')M_{\mathrm{hf}}.$$

The first term is the usual magnetic-dipole transition amplitude and is governed by relativistic many-body effects [5]. The second term arises because of hyperfine interaction mixing; in atomic units it is represented as

$$M_{\mathrm{hf}}=\frac{2}{\sqrt{6}}\frac{\langle 7s||t^1_{\mathrm{hf}}||6s\rangle}{E_{7s}-E_{6s}}(I+\tfrac{1}{2})g_I\mu_N\left|\frac{\mu_{\mathrm{B}}}{c}\right|,$$

where $I=7/2$ is the nuclear moment of ^{133}Cs, $g_I=0.737\,89$, and the reduced matrix element of the magnetic-dipole hyperfine interaction is given by

$$\langle i||t^1_{\mathrm{hf}}||j\rangle=(\kappa_i+\kappa_j)\langle -\kappa_i||C^1||\kappa_j\rangle \times\int_0^\infty \rho_\mu(r)\frac{dr}{r^2}\{G_i(r)F_j(r)+F_i(r)G_j(r)\}.$$

Here $G(F)$ are the large (small) component radial Dirac wave functions, $\rho_\mu(r)$ is the distribution of nuclear magnetization, $\kappa=(j+\frac{1}{2})(-1)^{j+l+1/2}$, and C^1 is a normalized spherical harmonic. In our calculations we model the nucleus as a uniformly magnetized ball of radius $R=5.6748$ fm.

In the nonrelativistic limit, the matrix element of the magnetic-dipole hyperfine interaction is proportional to the product of values of the wave functions at the origin. Therefore, in the one-particle approximation, the off-diagonal amplitude can be approximated as a geometric mean of hyperfine constants A_{6s} and A_{7s} [6],

$$M_{\mathrm{hf}}=(I+\tfrac{1}{2})\frac{\sqrt{A_{6s}A_{7s}}}{E_{7s}-E_{6s}}. \tag{1}$$

Two significant approximations—nonrelativistic and one-particle—were made in arriving at the above result. Contributions beyond this model have been considered by Bouchiat and Piketty [2]. They find corrections only at the level of 0.3%. The accuracy of the semiempirical value is assumed to be equal to the size of this correction [7] and

$$M^{\mathrm{s.e.}}_{\mathrm{hf}}=0.8094(20)\times 10^{-5}\left|\frac{\mu_{\mathrm{B}}}{c}\right|.$$

In our present calculations we employ the *ab initio* relativistic many-body method [8], which takes into account single and double excitations from the reference Dirac-Fock determinant. The method also includes the effect of triple excitations on the single excitation amplitudes. We direct the reader to Ref. [9] for a discussion of numerical calculations and an extensive comparison of theoretical results with experimental energies, electric-dipole matrix elements, and hyperfine-structure constants. In particular, the resulting correlated wave functions underestimate magnetic-dipole hyperfine constants for $6s$ and $7s$ states by 0.9%. Therefore, we expect to predict M_{hf} with an accuracy at a level of 1%.

In the lowest order we obtain $M_{\mathrm{hf}}=0.5379\times 10^{-5}|\mu_{\mathrm{B}}/c|$. Correlation corrections bring the amplitude to $0.7992\times 10^{-5}|\mu_{\mathrm{B}}/c|$. Finally, the Breit contribution estimated to second order in many-body perturbation theory and corrections for higher partial waves yield $M_{\mathrm{hf}}=0.7998\times 10^{-5}|\mu_{\mathrm{B}}/c|$. We estimate the omitted correlation corrections from the 0.9% difference of *ab initio* and experimental values for hyperfine-structure constants for $6s$ and $7s$ states and obtain

$$M_{\rm hf}=0.8070(73)\times10^{-5}\left|\frac{\mu_{\rm B}}{c}\right|.$$

This *ab initio* value is in excellent agreement with the semiempirical estimate [2] $M_{\rm hf}^{\rm s.e.}=0.8094(20)\times10^{-5}|\mu_{\rm B}/c|$ used by Bennett and Wieman [1] in their prediction of the weak charge.

[1] S. C. Bennett and C. E. Wieman, Phys. Rev. Lett. **82**, 2484 (1999).
[2] C. Bouchiat and C. A. Piketty, J. Phys. (France) **49**, 1851 (1988).
[3] W. J. Marciano and J. L. Rosner, Phys. Rev. Lett. **65**, 2963 (1990); **68**, 898(E) (1992).
[4] M. A. Bouchiat and C. Bouchiat, J. Phys. (France) **35**, 899 (1974).
[5] V. A. Dzuba, V. V. Flambaum, P. G. Silvestrov, and O. P. Sushkov, Phys. Scr. **31**, 275 (1985).
[6] J. Hoffnagle, Ph.D. thesis, Swiss Federal Institute of Technology, Zurich, 1982 (unpublished).
[7] M.-A. Bouchiat and J. Guéna, J. Phys. (France) **49**, 2037 (1988).
[8] S. A. Blundell, W. R. Johnson, and J. Sapirstein, Phys. Rev. A **43**, 3497 (191).
[9] M. S. Safronova, W. R. Johnson, and A. Derevianko (unpublished).