HIGH-MAGNETIC-FIELD CORRECTIONS TO CESIUM HYPERFINE STRUCTURE *

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Corrections to the Breit-Rabi formula for the ground state of ^{133}Cs are calculated. For a recently proposed high-magnetic-field frequency standard, the corrections amount to a few parts in 10^{12}.

De Marchi has proposed a cesium atomic-beam frequency standard based on the ($M_F = -1$, $\Delta M_F = 0$) transition, at the magnetic field ($B \approx 82$ mT) where the derivative of the frequency with respect to B is zero,[1] and has carried out preliminary experiments.[2] In order for this to be a *primary* frequency standard, it is necessary to relate the measured frequency to that of the zero-field transition frequency ν_0, which defines the SI unit of time. The Breit-Rabi formula predicts the frequency to be $\sqrt{15/16}\,\nu_0 = 8\,900\,727\,438.257$ Hz.[1] For higher accuracy, additional terms must be taken into account.

Three corrections to the Breit-Rabi formula have been measured for the ground-state hyperfine structure of rubidium by Larson and coworkers.[3–5] These are the dipole diamagnetic shift, the quadrupole diamagnetic shift, and the hyperfine-assisted Zeeman shift. These terms have not yet been measured for cesium.

The dipole diamagnetic shift results from a cross term between the contact hyperfine interaction and the atomic diamagnetic interaction in second-order perturbation theory. This leads to a shift, proportional to B^2, in the dipole hyperfine constant A. I evaluated the perturbation sum over states, including the continuum, by solving an inhomogeneous differential equation for the perturbed wavefunction. I used an empirical potential for the valence electron derived by Klapisch.[6] The result is $\delta A/A = 5.46 \times 10^{-10}\ B^2$, where B is expressed in teslas. This leads to an increase in the ($M_F = -1$) field-independent transition frequency of 33 mHz. Previous calculations have been reported by Bender[7] and by Ray *et al.*[8] In order to check the method, I used Klapisch's potential to calculate $\delta A/A$ for rubidium. The result is 10% below the experimental value. I estimate an accuracy of around 20% for the present calculation in cesium.

The quadrupole diamagnetic shift results from a cross term between the nuclear quadrupole hyperfine interaction and the electronic diamagnetic interaction in second-order perturbation theory. The interaction is diagonal in M_I and M_J. The perturbation sum over states is the same one that appears in the calculation of the quadrupole shielding factor γ_∞.[4] Using the value $\gamma_\infty(\mathrm{Cs}^+) = -86.8$,[9] I obtain the result

$$\langle M_I, M_J | H_{\mathrm{QD}} | M_I, M_J \rangle = -4.6 \times 10^{-5} B^2 \frac{[3M_I^2 - I(I+1)]}{I(2I-1)}. \qquad (1)$$

The result is in hertz if B is expressed in teslas. A similar calculation for rubidium yields a coefficient in good agreement with experiment.[4] For cesium, the estimate of the coefficient

for the shift is probably accurate within around 30%. However, for the special case of the $(M_F = -1)$ field-independent transition, the shift vanishes. The two states involved in the transition are $(|-1/2, -1/2\rangle \pm |-3/2, 1/2\rangle)/\sqrt{2}$, in the $|M_I, M_J\rangle$ basis, where + refers to the higher-energy state and − to the lower-energy state. Hence, the states are shifted by the same amount, since they have the same M_I-content.

The hyperfine-assisted Zeeman shift was explained by Fortson as a third-order perturbation, in which the contact hyperfine interaction acts twice and the electronic Zeeman interaction acts once.[10] Fortson gave diagonal matrix elements in the $|M_I, M_J\rangle$ basis. For the $(M_F = -1)$ field-independent transition, it is necessary to extend Fortson's calculation to include off-diagonal matrix elements. In the $|(IJ)F, M_F\rangle$ basis, the nonzero matrix elements for ^{133}Cs are

$$\langle 3, M_F | H_{\mathrm{HAZ}} | 4, M_F \rangle = 4h\beta B\sqrt{16 - M_F^2}. \tag{2}$$

Fortson used quantum-defect theory to make a semi-empirical estimate for β in rubidium; it agreed with experiment within 10%. The same method, applied to cesium, yields $\beta = 88$ mHz/T. For the $(M_F = -1)$ field-independent transition, the shift at $B = 82$ mT is $-2\sqrt{15}\beta B = -56$ mHz. This estimate of the shift is probably accurate within around 30%.

To achieve a theoretical error of 10^{-14} in the total frequency, which is the projected accuracy of the high-field frequency standard,[1] the larger shifts must be known within less than 1%. This could possibly be done by *ab initio* calculations or by experiments carried out at much higher magnetic field, similar to those of Larson and coworkers in rubidium.

Acknowledgments

This work was supported by the Office of Naval Research and the Army Research Office.

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