Calculation of strongly forbidden $M1$ transitions and g-factor anomalies in atoms considered for parity-nonconservation measurements

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We calculate magnetic dipole transition amplitudes in $s-s$ and $s-d$ transitions of Rb, Cs, Ba^+, Fr, Ra^+, Yb^+, Ac^{2+} and Th^{3+}. These transitions were used or considered to be used for parity-nonconservation (PNC) measurements. We also calculate the magnetic g-factor anomalies for a selection of states, along with electric quadrupole transition amplitudes for $s-d$ transitions in these systems.

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I. INTRODUCTION

Currently the interest to study parity-nonconservation (PNC) in atoms remains high due to its status as the best low-energy test of the standard model. There is interest in obtaining important information by improving the accuracy of the measurements and their interpretation, studying PNC in a chain of isotopes, and measuring nuclear P-odd anapole moments (see, e.g., review [1]). The most accurate test of the standard model in atomic PNC comes from the study of the $6s-7s$ PNC transition amplitude in cesium [2]. This is due to the extremely high accuracy of measurements [2] and calculations [3–5]. The $6s-7s$ transition in cesium is a strongly forbidden magnetic dipole (M1) transition. Using the strongly forbidden M1 transitions for PNC measurements was first suggested by Bouchiat and Bouchiat [6]. More recent proposals to use M1 transitions for PNC measurements include $s-s$ and $s-d$ transitions in Ba^+ [7,8], Ra^+ [9], Yb^+ [10], Fr [11], Rb [12], and Fr-like ions [13] (see also Refs. [14–16]).

The experimental data on the values of the M1 transition amplitudes is poor. Among the mentioned atoms there are only experimental data for the $6s-7s$ transition in cesium [17–19] and plans to measure the $6s-5d_{3/2}$ M1 amplitude in Ba^+ [20]. Knowing the value of this M1 amplitude is important when planning and interpreting the measurements and for testing atomic theory [20].

In this work we present theoretical calculations of M1 transition amplitudes in a variety of systems considered for PNC measurements [12–14]. These amplitudes are calculated in the relativistic Hartree-Fock approximation with contributions from core polarization and the Breit interaction included to all orders.

We also calculate magnetic g-factor anomalies, which are produced by the same mechanisms as the strongly forbidden M1 transitions, and provide a good test of the accuracy. There are two main mechanisms (see, e.g., [21]). The first one is due to the relativistic corrections to the magnetic moment operator [$\sim -\alpha^2 = -(1/137)^2$] and dominates in light atoms. The second mechanism is due to the combined action of the exchange core polarization and the spin-orbit interaction. It increases very fast with the nuclear charge ($\sim Z^4\alpha^4$) and dominates in heavy atoms [21]. In the present work we use the relativistic magnetic moment operator; therefore the relativistic corrections (the first mechanism) are included at the Hartree-Fock level. The second mechanism is included in the calculation of the core polarization effects. In many cases the core polarization is essentially the sole contributor to the M1 amplitudes and g-factor anomalies (compared with Hartree-Fock and Breit alone). Comparison of the calculated M1 amplitude may be made with experiment in the case of cesium, for which there is good agreement. We also present results for other systems, including Ba^+ (for which PNC measurements are being considered [7]) and Ra^+ and Fr, for which PNC measurements are underway [11,22]). Also presented are calculations of $s-d$ electric quadrupole (E2) transition amplitudes, including both core polarization and electron correlation effects. Calculated E2 values are compared with previous calculations for Ba^+, Ra^+, and Ac^{2+}. Experimental E2 data exists for Cs and Ba^+, and comparing with our calculated values shows good agreement for Ba^+; however, the Cs data has poor experimental accuracy.

To estimate the accuracy of the M1 amplitude calculations, we present calculations of the g-factor anomalies in the same atoms and ions, as well as a comparison with the available experimental data. The deviation of the g factor of s states of single-valence-electron atoms from the g factor of a free electron, known as the g-factor anomaly, has been considered in many atomic systems [21,23–30]. However, the behavior of this discrepancy is not uniform across the periodic table: for light atoms δg is almost constant, whereas in heavy atoms it changes its sign and increases rapidly with Z, suggesting two different underlying mechanisms. In Refs. [21,23] the authors showed how relativistic corrections and the effect of core polarization account for the behavior of δg in heavy atoms such as cesium. Experimental data is available for Cs, Fr, and Rb, and comparison with our results for Cs and Fr yields good agreement. (In Rb there is a cancellation of two contributions which increases the relative error.)

II. METHOD

To calculate transition amplitudes and g factors, we utilize the relativistic Hartree-Fock (Dirac-Fock) approximation in a V^{N-1} potential. Core polarization and core-valence correlations are included by means of the time-dependent Hartree-Fock (TDHF) and correlation potential methods [31]. The TDHF method is equivalent to the well-known random-phase approximation (RPA).

The Hartree-Fock Hamiltonian has the form

$$\hat{H}_0 = c\alpha\cdot\hat{\mathbf{p}} + (\beta-1)mc^2 - \frac{Ze^2}{r} + \hat{V}, \qquad (1)$$

where $\hat{V}$ is the self-consistent potential created by electrons from the core. In addition to the Coulomb interaction, we include the effect of magnetic interactions and retardation via the Breit interaction, the details of which are given in [32].

In the TDHF calculations every single electron wave function of the atom is presented in the form

$$\tilde{\psi}_n = \psi_n + X_a e^{-i\omega t} + Y_n e^{i\omega t}, \tag{2}$$

where index n enumerates single-electron states, ψ_n is the unperturbed wave function for state n, which is an eigenstate of the Hartree-Fock Hamiltonian (1), and X_n and Y_n are corrections due to the magnetic field of an external photon with frequency ω.

These corrections, applicable to all atomic states, are found by self-consistent iteration of the TDHF equations:

$$\begin{aligned}(\hat{H}_0 - \epsilon_n - \omega)X_n &= -(\hat{H}_{M1} + \delta\hat{V}_{M1})\psi_n,\\ (\hat{H}_0 - \epsilon_n + \omega)Y_n &= -(\hat{H}^\dagger_{M1} + \delta\hat{V}^\dagger_{M1})\psi_n.\end{aligned} \tag{3}$$

Here $\delta\hat{V}$ is the correction to the self-consistent Hartree-Fock potential $\hat{V}$ due to the external dipole magnetic (M1) field. The equations in (3) are first solved self-consistently for all states in the core. Then corrections to valence states are calculated in the field of frozen core.

In the relativistic case the matrix elements for the operator $\hat{H}_{M1} = \vec{\mu}\cdot\vec{B}$ and wave functions

$$\psi(r) = \frac{1}{r}\begin{pmatrix} f(r)\Omega_{\kappa m} \\ i\alpha g(r)\Omega_{-\kappa m}\end{pmatrix} \tag{4}$$

are given by

$$\begin{aligned}\langle\psi_a|\hat{H}_{M1}|\psi_b\rangle &= (\kappa_a + \kappa_b)\langle -\kappa_a||C^1||\kappa_b\rangle\\ &\times \int 3\,(f_a g_b + g_a f_b)\, j_1(kr)dr,\end{aligned} \tag{5}$$

where $\kappa = l$ for $j = l - 1/2, \kappa = -l - 1$ for $j = l + 1/2$, C^1 is a normalized spherical harmonic, wave vector $k = \omega/c$, and $j_l(kr)$ is the spherical Bessel function.

When core polarization is included the matrix element $\langle a||M1||b\rangle$ becomes $\langle a||M1 + \delta V_{M1}||b\rangle$. Calculations of these latter matrix elements with RPA included are given in Table I.

III. RESULTS

Tables I, II, and III contain a summary of our results for all elements considered. In all cases the transition energy is taken as the experimental value [33,35], except for Ac^{2+} $7s \to 8s$, where the transition energy is taken from calculation [36]. Table I clearly illustrates the importance of core polarization for M1 amplitudes. Indeed, in almost all systems the RPA value is several orders of magnitude larger than that given by Hartree-Fock calculations alone.

The most well-studied system in Table I is cesium. Experimental values of the reduced $6s - 7s$ M1 amplitude are the following:

$$\begin{aligned}M &= (9.04 \pm 0.588) \times 10^{-5}|\mu_B|\ [16]\\ M &= (10.1 \pm 0.441) \times 10^{-5}|\mu_B|\ [17]\\ M &= (10.3 \pm 0.196) \times 10^{-5}|\mu_B|\ [18]\end{aligned} \tag{6}$$

TABLE I. Magnetic dipole transition amplitudes.

		M1 ($\lvert\mu_B\rvert \times 10^{-5}$)		
Element	Transition	HF	RPA	Total
Rb	$5s - 6s$	−1.473	2.689	1.216
	$5s - 4d$	0.2447	0.744	1.019
Cs	$6s - 7s$	−1.652	15.79	14.13
	$6s - 5d$	0.5662	11.42	11.98
Ba^+	$6s - 7s$	−4.050	17.58	13.53
	$6s - 5d$	2.006	20.05	22.06
Fr	$7s - 8s$	−2.491	179.0	176.5
	$7s - 6d$	0.7374	126.2	126.9
Ra^+	$7s - 8s$	−5.744	190.8	185.1
	$7s - 6d$	2.401	207.9	210.3
Yb^+	$6s - 7s$	−5.536	48.71	43.17
	$6s - 5d$	2.166	50.25	52.42
Ac^{2+}	$7s - 8s$	−8.911	−2382	−2390
	$7s - 6d$	3.510	210.1	213.6
Th^{3+}	$7s - 8s$	−13.23	−2536	−2549
	$7s - 6d$	4.432	207.8	212.2

compared with the value presented here of $M = 14.13 \times 10^{-5}|\mu_B|$.

There is another contribution to the M1 amplitude—the nuclear-spin-dependent (NSD) amplitude induced by the hyperfine interaction. It can be separated experimentally due to its dependence on the hyperfine component of the M1 transition. In $s - s$ transitions the hyperfine induced amplitude is an order of magnitude smaller than the nuclear-spin-independent (NSI) amplitude (see, e.g., [47]). In the $s - d$ transitions the NSD amplitude is even smaller, since the nondiagonal $s - d$ hyperfine interaction matrix elements are smaller.

In addition to M1 amplitudes, we present the E2 $s - d$ transition amplitudes given in Table II. In these calculations we have included the effect of correlations using the all-order correlation potential $\hat{\Sigma}$ method (see, e.g., [31]). Applying this method to M1 amplitudes makes little difference, as $\hat{\Sigma}$ changes only the radial wave function, which M1 transitions are not sensitive to.

The forbidden M1 amplitudes are very small and sensitive to different corrections. Matrix elements of the M1 operator

TABLE II. Electric quadrupole transition amplitudes in units of a_0^2.

Element	Transition	This work	Other calculations	Experiment
Rb	$5s - 4d$	33.42		
Cs	$6s - 5d$	33.60		35 ± 3.5 [37]
Ba^+	$6s - 5d$	12.69	12.734 [39]	12.74 ± 0.37 [43]
			12.63 [40]	
			12.625 [41]	
			12.74 [42]	
Fr	$7s - 6d$	33.59		
Ra^+	$7s - 6d$	14.77	14.59 [38]	
Yb^+	$6s - 5d$	12.19		
Ac^{2+}	$7s - 6d$	9.58	9.52 [38]	
Th^{3+}	$7s - 6d$	7.10		

TABLE III. g-factor anomaly δg ($\times 10^{-5}$) for $s_{1/2}$, $d_{3/2}$, and $d_{5/2}$ states. The g_j-factor may be recovered using $g_{1/2} = \delta g_{1/2} + g_{\rm free}$, $g_{3/2} = \delta g_{3/2} + (6 - g_{\rm free})/5$, and $g_{5/2} = \delta g_{5/2} + (g_{\rm free} + 4)/5$, respectively, for the three states considered. Here $g_{\rm free} = 2.002\,319\,304$ is the measured free electron g factor [34].

Element	State	$\delta g_{\rm HF}$	$\delta g_{\rm RPA}$	$\delta g_{\rm total}$	$\delta g_{\rm expt}$
Rb	$5s_{1/2}$	−2.6	4.9	2.3	1.18 ± 0.2 [28]
	$4d_{3/2}$	−0.4	−0.9	−1.3	–
	$4d_{5/2}$	−0.6	0.0	−0.6	–
Cs	$6s_{1/2}$	−2.9	28.4	25.5	22.1 ± 0.2 [28]
	$5d_{3/2}$	−0.7	−4.8	−5.5	–
	$5d_{5/2}$	−1.3	1.2	−0.1	–
Ba^+	$6s_{1/2}$	−6.4	31.6	25.2	17.13 ± 0.11 [44]
					17.29 ± 0.1 [45]
	$5d_{3/2}$	−4.7	−16.7	−21.4	-20.8 ± 0.03 [45]
	$5d_{5/2}$	−7.3	1	−6.3	-9.29 ± 0.7 [46]
Fr	$7s_{1/2}$	−4.3	335.7	331.4	265.1 ± 9 [27]
	$6d_{3/2}$	−0.7	−26.7	−27.4	–
	$6d_{5/2}$	−1.2	12.2	11.0	–
Ra^+	$7s_{1/2}$	−8.8	356.2	347.4	–
	$6d_{3/2}$	−4.7	−73.4	−78.1	–
	$6d_{5/2}$	−6.6	29.6	23.0	–
Yb^+	$6s_{1/2}$	−8.6	88.4	79.8	–
	$5d_{3/2}$	−5.7	−23.6	−29.3	–
	$5d_{5/2}$	−8.2	12.5	4.3	–
Ac^{2+}	$7s_{1/2}$	−13.3	342	328.7	–
	$6d_{3/2}$	−9.0	−78.4	−87.4	–
	$6d_{5/2}$	−11.7	28.0	16.3	–
Th^{3+}	$7s_{1/2}$	−18	326.5	308.5	–
	$6d_{3/2}$	−13.5	−78.4	−91.9	–
	$6d_{5/2}$	−16.7	24.4	7.7	–

are very sensitive to the frequency of the laser field ω. All g factors are calculated at $\omega = 0$. This is why they are similar. In contrast, each M1 amplitude is calculated at the frequency of this transition, and frequencies grow rapidly with the degree of ionization. This is why the amplitudes are different. For example, the frequency of the $7s - 8s$ transition in Ac^{2+} is about 2 times larger than in Ra^+. If we calculate the M1 amplitude for Ac^2+ at the same frequency as in Ra^+, we get an answer very close to that of Ra^+.

Our method to estimate the higher-order corrections to M1 amplitudes that are omitted is based on the calculations of the g-factor anomalies which have similar mechanisms. Results of our calculations for the g-factor anomalies due to the relativistic and many-body corrections are presented in Table III. Comparison with the experimental data for the g-factor anomalies (and $6s - 7s$ M1 amplitude in Cs) indicates that the theoretical error in our calculation is from 10% to 40%.

Previous calculations for $s - d$ M1 transitions exist for some systems: $80 \times 10^{-5}|\mu_B|$ [39] for Ba^+, and $140 \times 10^{-5}|\mu_B|$ and $130 \times 10^{-5}|\mu_B|$ for Ra^+ and Ac^{2+}, respectively [38]. The values for Ra^+ and Ac^{2+}, while differing from our calculations given in Table I, are nevertheless consistent with our values given the error estimates discussed previously. In the case of Ba^+ the difference is too large and should be treated as a disagreement between present calculations and those of Ref. [39]. Additionally, the calculations of the E2 transition amplitudes for these ions have also been performed previously. In the case of Ba^+, experimental data for E2 exists and a comparison with our result indicates an accuracy of better than 1%. Comparison may also be made with previous calculations, the results of which are given in Table II, which are consistent with this level of accuracy.

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