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Magnetic dipole hyperfine interactions in $^{137}Ba^{+}$ and the accuracies of the neutral weak interaction matrix elements

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The relativistic coupled-cluster method is applied to calculate the magnetic dipole hyperfine constant "A" of the $6s_{1/2}$, $6p_{1/2}$, $6p_{3/2}$, and $5d_{3/2}$ states of singly ionized barium. After the inclusion of two-body correlation effects into the computation of the hyperfine matrix elements, the accuracy of the obtained values was significantly increased compared to earlier computations. Based on these numbers and earlier calculations of the electric dipole transitions and excitation energies, an estimate for the accuracy of the $|[5p^6]6s_{1/2}\rangle \rightarrow |[5p^6]5d_{3/2}\rangle$ parity-nonconserving electric dipole transition amplitude is carried out. The results suggest that for the first time, to our knowledge, a precision of better than 1% is feasible for this transition amplitude.

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An experiment to observe parity nonconservation (PNC) in a single trapped and laser cooled ion was proposed by Fortson about a decade ago [1]. Initial steps towards the realization of such an experiment on Ba^{+} have been taken and the results were reported recently [2].

Relativistic many-body calculations have been performed for the parity-nonconserving electric dipole amplitude for the $|[5p^6]6s_{1/2}\rangle \rightarrow |[5p^6]5d_{3/2}\rangle$ transition in $^{137}Ba^{+}$ [3,4]. However, it is not clear how accurate these calculations are as the uncertainties of the matrix elements of the parity-nonconserving neutral weak interactions have not been estimated. It is not possible to determine the accuracies of these matrix elements by comparing directly with experimental data, but it is indeed possible to estimate them by comparing the results of the relativistic many-body calculations of the magnetic dipole hyperfine constant (A) with those of experiments. Although the origins of the neutral weak and hyperfine interactions are fundamentally very different, the matrix elements of both these interactions depend on the overlap of single-particle wave functions in or close to the nuclear region.

In this Rapid Communication, we present the results of our relativistic coupled-cluster calculations of A for the ground and excited states of $^{137}Ba^{+}$ that are relevant in estimating the accuracies of the neutral weak interaction matrix elements associated with the $|[5p^6]6s_{1/2}\rangle \rightarrow |[5p^6]5d_{3/2}\rangle$ parity-nonconserving transition in that ion. These quantities have not been calculated earlier except for the ground state.

The relativistic hyperfine Hamiltonian is given by

$$H_{hfs} = \sum_k M^{(k)} \cdot T^{(k)}, \tag{1}$$

where $M^{(k)}$ and $T^{(k)}$ are spherical tensor operators of rank k, representing the nuclear and electronic parts, respectively. In the case of the magnetic dipole hyperfine constant $k=1$, the magnetic dipole hyperfine interaction constant [5] is defined as

$$\langle H_{hfs} \rangle = A \langle \mathbf{I} \cdot \mathbf{J} \rangle. \tag{2}$$

Explicitly given by

$$A = \mu_N \left[\frac{\mu_I}{I} \right] \frac{\langle J || T^{(1)} || J \rangle}{\sqrt{J(J+1)(2J+1)}}, \tag{3}$$

where $\mathbf{I}, \mu_N, \mu_I$, and $\mathbf{J}$ are the nuclear spin, nuclear magnetic moment, nuclear-spin magnetic moment, and total angular momentum of the electrons, respectively. The expression for $T^{(1)}$ is given by

$$T^{(1)} = \sum t_q^{(1)} = \sum_j -ie\sqrt{8\pi/3 r_j^2}\, \alpha_j Y_{1q}^{(0)}. \tag{4}$$

The single-particle reduced matrix element can be written as

$$\langle \kappa || t_q^{(1)} || \kappa' \rangle = -\langle -\kappa || C_q^{(1)} || \kappa' \rangle (\kappa + \kappa') \times \int dr \frac{(P_\kappa Q_{\kappa'} + Q_\kappa P_{\kappa'})}{r^2}.$$

P_κ and $Q_{\kappa'}$ are the large and small radial components of the Dirac-Fock single particle wave functions and

$$\langle \kappa || C_q^{(1)} || \kappa' \rangle = (-1)^{(j+1/2)} \sqrt{j+1/2} \sqrt{j'+1/2} \begin{pmatrix} j & 1 & j' \\ 1/2 & 0 & -1/2 \end{pmatrix}. \tag{5}$$

The Dirac-Coulomb Hamiltonian for an atomic system is given by

$$H=\sum_{i=1}^{N}\left[c\alpha_i p_i+(\beta_i-1)mc^2+V_{nuc}\right]+\sum_{i>j}\frac{1}{r_{ij}}, \quad (6)$$

where atomic units (a.u.) have been used in the above expression.

We have not considered the Breit interaction as its contribution to the properties (particularly for the $[5p^6]5d_{3/2}$ state), we are interested in the present work, is well below 1%. This is evident from the work of Derevianko and others [6–9].

We assume the Dirac-Fock state ($|\Phi_0\rangle$) as our reference state for the closed-shell atomic system (Ba^{2+} in the present case). The exact atomic state of a single-valence system in the framework of coupled-cluster theory can be expressed [10] as

$$|\Psi\rangle=e^T\{1+S_v\}|\Phi_v\rangle$$
$$=e^T\{1+S_v\}a_v^\dagger|\Phi_0\rangle, \quad (7)$$

where T- and S_v- are the closed- and open-shell excitation operators, respectively. In the present work, we have considered only single and double excitations; keeping in mind the computational cost involved in coupled-cluster calculation and the rather small contributions of the higher-order excitations. Therefore, we can write

$$T=T_1+T_2 \quad \text{and} \quad S_v=S_{1v}+S_{2v}.$$

In the second quantized notation they can be represented as

$$T_1=\sum_{a,p}a_p^\dagger a_a t_a^p, \quad T_2=\frac{1}{2}\sum_{ab,pq}a_p^\dagger a_q^\dagger a_b a_a t_{ab}^{pq}$$

and

$$S_{1v}=\sum_{p\neq v}a_p^\dagger a_v s_v^p, \quad S_{2v}=\frac{1}{2}\sum_{a,pq}a_p^\dagger a_q^\dagger a_a a_v s_{va}^{pq}.$$

The method employed in the computation of the cluster amplitudes t_a^p, t_{ab}^{pq}, s_v^p, and s_{va}^{pq} has been described in some of our group's earlier papers [11,12]. If "O" is a general single-particle physical operator, then the expectation value of this operator in coupled-cluster theory can be expressed as

$$\langle O\rangle=\frac{\langle\Psi_v|O|\Psi_v\rangle}{\langle\Psi_v|\Psi_v\rangle}$$
$$=\frac{\langle\Phi_v|\{1+S_v^\dagger\}e^{T^\dagger}Oe^T\{1+S_v\}|\Phi_v\rangle}{\langle\Phi_v|\{1+S_v^\dagger\}e^{T^\dagger}e^T\{1+S_v\}|\Phi_v\rangle}. \quad (8)$$

We define $\overline{O}=e^{T^\dagger}Oe^T$ and using Wick's theorem we carry out the following expression:

$$\overline{O}=(e^{T^\dagger}Oe^T)_{fc}+(e^{T^\dagger}Oe^T)_{ob}+(e^{T^\dagger}Oe^T)_{tb}+\cdots$$

TABLE I. Hyperfine constant for different states of Ba^+.

States	Present (MHz)	Geetha [a] (MHz)	Others (MHz)	Expt. (MHz)
$[5p^6]6s_{1/2}$	4072.83	4193.02	4208 200 [b]	4018 [c]
$[5p^6]6p_{1/2}$	736.98	783.335		742.04 [c]
$[5p^6]6p_{3/2}$	130.94	134.079		125.9 [c]
$[5p^6]5d_{3/2}$	188.76	198.759		191.2(6) [d]

[a]Reference [4].
[b]Reference [13].
[c]Reference [14].
[d]Reference [15].

up to five-body terms. We have used the abbreviation fc, ob, and tb for fully contracted, one body, and two body, respectively. The truncated $\overline{O}$ used in our calculations contains the dominant terms given by

$$\overline{O}=O+T^\dagger O+OT+T^\dagger OT. \quad (9)$$

The contributions from the three-body and higher-order terms for the property calculation are negligible and hence they are not considered in the present work. The largest contribution comes from the one-body terms. We have also taken into account the two-body terms which are most important. They possess the following structure:

$$(e^{T^\dagger}Oe^T)_{two\text{-}body}=OT_1+T_1^\dagger O+OT_2+T_2^\dagger O. \quad (10)$$

Finally, all these operators are connected with at most one S- and/or one $S^\dagger$ operator for the calculation of the expectation value of the hyperfine interaction operator. A similar approach has been followed to evaluate the normalization constant. A detailed account of the computational approach is given by Gopakumar *et al.* [12]. The single-particle orbitals used in our calculations are partly numerical and partly analytical. Such an approach has been explained in detail by Majumder *et al.* [16]. The analytical orbitals are Gaussian-type orbitals (GTOs) having the form

$$G_{i,k}(r)=r^{k_i}e^{-\alpha_i r^2}, \quad (11)$$

where $k=0,1,\ldots$ for $s,p,\ldots$ functions. We have used the even tempering condition, i.e., different α_i for orbitals of different symmetries. The large and small components of the GTOs satisfy the kinetic balance condition [17].

In this calculation we have used $17s$, $17p$, $15d$, and $5f$ orbitals out of which seven s, five p, and three d orbitals are numerical and the rest are analytical. The magnetic dipole hyperfine constants A for different low-lying states for Ba^+ are given in Table I. Table II contains a breakup into contributions from one-body terms (part I), two-body terms (part II), and one-body terms without core correlations (part III). It is evident from Table II that the dominant contribution to electron correlation comes from the OS_1 and OS_2 with their adjoints which are shown in Figs. 1 and 2, respectively. It is

TABLE II. Contributions from some of the important terms of the present calculation in MHz.

Terms	$6s_{1/2}$	$6p_{1/2}$	$6p_{3/2}$	$5d_{3/2}$
(I) Contribution from one-body terms				
$\overline{O}$	2860.75	488.52	72.09	134.53
$S_{1v}^{\dagger}\overline{O}+\overline{O}S_{1v}$	650.24	125.63	17.68	9.21
$S_{2v}^{\dagger}\overline{O}+\overline{O}S_{2v}$	553.004	112.31	34.32	37.47
$S_{1v}^{\dagger}\overline{O}S_{1v}$	36.93	8.09	1.08	0.16
$S_{1v}^{\dagger}\overline{O}S_{2v}+S_{2v}^{\dagger}\overline{O}S_{1v}$	44.63	9.42	2.75	1.01
$S_{2v}^{\dagger}\overline{O}S_{2v}$	73.27	7.24	3.63	9.09
Norm.	−71.94	−9.05	0.18	−2.39
(II) Contribution from two-body terms				
$S_{2v}^{\dagger}OT_1+T_1^{\dagger}OS_{2v}$	−3.46	−0.38	−0.052	−0.32
$S_{2v}^{\dagger}OT_2+T_2^{\dagger}OS_{2v}$	−57.89	−5.14	−0.87	0.67
$S_{1v}^{\dagger}T_2^{\dagger}OS_{2v}+S_{2v}^{\dagger}OT_2S_{1v}$	−6.55	−0.13	−0.027	0.00
(IA) Important contributions from the one-body part in the individual form				
Dirac-Fock	2929.41	492.74	71.84	128.17
$S_{1v}^{\dagger}O+OS_{1v}$	663.20	126.53	17.65	8.92
$S_{2v}^{\dagger}O+OS_{2v}$	465.91	98.98	28.64	25.23
$S_{1v}^{\dagger}OS_{1v}$	93.84	−12.24	1.63	−0.078

interesting to note that the former is larger than the latter for $6s$ and $6p_{1/2}$ states, but this trend is reversed for the $6p_{3/2}$ and $5d_{3/2}$ states. This can be explained by probing carefully the interplay of the hyperfine and the residual electron-electron interaction. To be specific, OS_1 involves the hyperfine interaction of a valence electron, which is highly significant for s and $p_{1/2}$ electrons, because these electrons have an overlap with the nuclear region where the hyperfine operator is active. On the other hand, the OS_2 term represents the hyperfine interaction of a polarized core electron, and here no preference is given to any specific orbital.

We now turn to the estimation of the error for the neutral weak interaction matrix elements. The parity-nonconserving electric dipole transition amplitude for $|[5p^6]6s_{1/2}\rangle \rightarrow |[5p^6]5d_{3/2}\rangle$ in Ba^+ is given by

$$\mathcal{A}(E1)_{PNC}=\sum_{I\neq 6s_{1/2}}\frac{\langle 5d_{3/2}|D|I\rangle\langle I|H_{PNC}|6s_{1/2}\rangle}{E_{6s_{1/2}}-E_I}+\sum_{I\neq 5d_{3/2}}\frac{\langle 6s_{1/2}|D|I\rangle\langle I|H_{PNC}|5d_{3/2}\rangle}{E_{5d_{3/2}}-E_I}, \tag{12}$$

where I stands for the intermediate states. It has been recently shown that the largest contribution to the above expression comes from the intermediate states $[5p^6]6p_{1/2}$ (90%) and $[5p^6]6p_{3/2}$ (8%) [4]. The accuracies of the electric dipole matrix elements and the excitation energies corresponding to these intermediate states have been determined earlier and found to be better than 1% [11,12]. However, the accuracies of the two involved weak interaction matrix elements $\langle[5p^6]6p_{3/2}|H_{PNC}|[5p^6]5d_{3/2}\rangle$ and $\langle[5p^6]6p_{1/2}|H_{PNC}|[5p^6]6s_{1/2}\rangle$ cannot be determined by comparison with the experimental data. Instead, it has been

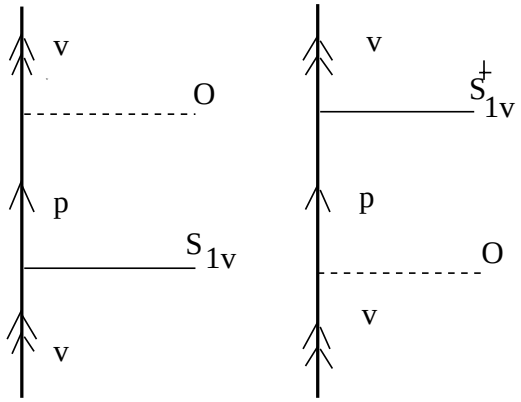

FIG. 1. OS_{1v} and $S_{1v}^{\dagger}O$ diagrams.

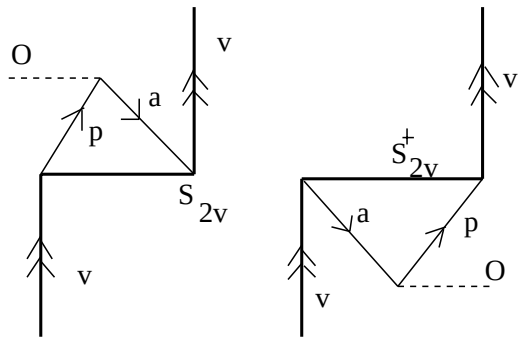

FIG. 2. OS_{2v} and $S_{2v}^{\dagger}O$ diagrams.

TABLE III. Square root of the products of relevant hyperfine dipole matrix elements in calculation and experiment and their deviation.

	Present work	Experiment	Deviation (in %)
$\sqrt{A_{6s_{1/2}}A_{6p_{1/2}}}$	1732.5	1726.7	0.3
$\sqrt{A_{6p_{3/2}}A_{5d_{3/2}}}$	157.2	155.2	1.3

proposed to estimate the errors with the help of the appropriate magnetic dipole hyperfine constants [18]. The reason for this is related to the fact that both, the weak interaction and the magnetic dipole hyperfine matrix elements, depend critically on the behavior of the wave functions in the nuclear region. As a consequence, the errors in the weak interaction matrix elements are estimated from the errors in $\sqrt{A_{6p_{3/2}}A_{5d_{3/2}}}$ and $\sqrt{A_{6s_{1/2}}A_{6p_{1/2}}}$, for which experimental values are available. Table III compares our computed results for these quantities with the corresponding experimental values. When transferring the accuracies to the weak interaction matrix elements, the results are very encouraging. If we take into account the different relative weights of the intermediate states contributing to the $\mathcal{A}(E1)_{PNC}$ matrix elements, the overall estimated error is about 0.4%. It therefore appears that $\mathcal{A}(E1)_{PNC}$ for the transition of experimental interest in Ba^+ can be calculated to an accuracy of better than 1%.

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