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Theory of hyperfine interactions in alkaline-earth ions isoelectronic with alkali-metal atoms: $^{25}\mathrm{Mg}^+$ ground state

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Relativistic many-body perturbation theory has been used to investigate the hyperfine structure of the singly ionized magnesium ion. These investigations were carried out to explain the recent experimental data in the ground state $3^2S_{1/2}$ of Mg^+ as well as to compare the hyperfine interaction results, both experimental and theoretical, in alkali-metal atoms with those in the corresponding isoelectronic alkaline-earth positive-ion series. The one-electron contribution to the hyperfine constant in $^{25}\mathrm{Mg}^+$ was found to be -553 MHz composed of the direct and exchange core-polarization contribution of -466 and -87 MHz, respectively, the many-electron correlation contribution being -48 MHz. The net theoretical hyperfine constant comes out to be $-(602 \pm 8)$ MHz, which agrees very well with the recent experimental value of -596.25 MHz obtained with the use of ion-storage techniques.

I. INTRODUCTION

While the hyperfine interactions in neutral alkali-metal atoms have been subject to a number of theoretical investigations,[1] including many-body effects in relativistic theory,[2] there have not been comparable efforts in the investigation of these interactions in the isoelectronic alkaline-earth positive ions. However, with the development of ion-storage techniques[3] and techniques involving beam laser analysis in accelerator experiments,[4] experimental data have started becoming available in the isoelectronic positive alkaline-earth ions. In particular, recently, experiments on $^{25}\mathrm{Mg}^+$ employing Penning-trap techniques[5] have been carried out and an accurate value of the hyperfine interaction constant has been obtained.[6]

There are several reasons which make first-principles theoretical investigations in the alkaline-earth series important.[7] First, such investigations can provide a quantitative understanding of the origin and trend of the hyperfine interactions in the ions of the series itself. Second, they allow one to obtain the trends of the direct, exchange core-polarization (ECP), and correlation contributions within the ion as well as the series as a whole. Finally, one can compare and correlate these contributions to their counterparts for the neutral alkali-metal series[2] where they are already available and reasonably well understood from recent investigations.

As part of a systematic investigation for the alkaline-earth positive-ion series, we have already investigated[7] the hyperfine interaction in the ground state of the relatively heavy ion Ba^+ by relativistic many-body perturbation theory and obtained good agreement with experiment. In the present work we have carried out a similar investigation on Mg^+, which is among the lighter members of the series and for which accurate experimental data have recently become available.[6]

In Sec. II we outline very briefly the relativistic many-body procedure employed in this work together with a few details of the potential and basis sets for the evaluation of the perturbation diagrams. Important diagrams describing the physical mechanisms contributing to the hyperfine interaction are also presented in this section. Section III presents the results for the contributions from various diagrams, with appropriate combinations of these to obtain the contributions associated with various physical mechanisms, namely, direct, ECP, consistency, and correlation effects. The results are discussed both with respect to comparison with experiment as well as correlation of results with corresponding results[7] in Ba^+ and in the neutral alkali-metal-atom series.[2] The main conclusions of the present work and its implications for other ions of the alkaline-earth series are also included in this section.

II. THEORY AND PROCEDURE

The relativistic many-body perturbation theory (RMBPT) adopted in the present work has been described in a number of papers.[1,2] For the sake of completeness, we present here only a brief résumé of the procedure, and some details specifically pertinent to Mg^+.

Using the terminology and notations adopted in recent work on alkali-metal atoms and in our recent work[7] on Ba^+, the linked-cluster-expansion expression for the hyperfine-interaction constant A in the spin Hamiltonian $\mathcal{H}_s = A\vec{I}\cdot\vec{J}$ can be written

$$A=\frac{1}{IJ}\sum_{m,n}^{L}\left\langle \Phi_J \left| \left[\frac{\mathcal{H}'}{E_0-\mathcal{H}_0}\right]^m \times \mathcal{H}_N \left[\frac{\mathcal{H}'}{E_0-\mathcal{H}_0}\right]^n \right| \Phi_J \right\rangle . \qquad (1)$$

The indices m and n appearing in expression (1) define the order of the perturbation diagrams contributing to A. Thus the lowest-order (zero-order) diagram resulting from $m=n=0$ is referred to as (0,0); the first-order diagrams are referred to as (0,1), while the second-order diagrams can be either of the form (1,1) or (0,2). For the evaluation of the diagrams, the basis set of bound and continuum states was generated in a V^{N-1} potential[8] with the self-Coulomb and self-exchange of the valence $3s_{1/2}$ states omitted.

Previous investigations on the alkali-metal-atom series and singly ionized alkaline-earth ion Ba^+ have shown that in all cases the (0,0), (0,1), and (0,2) diagrams shown in Figs. 1–3 make almost the entire contribution (more than 97%) to A. The (0,0) diagram represents the direct contribution from the valence $3s$ electron and is the only contribution that occurs in the restricted Hartree-Fock approximation where the core states differ only in spin. The (0,1) diagram represents the ECP effects where the core state with spin parallel to the valence electron experiences the exchange potential due to the latter while the antiparallel state does not. The core states being perturbed in the diagram of Fig. 2 can only be the s states in nonrelativistic theory, but in relativistic theory they can also[8] be p states. However, the latter have been found to contribute very little in alkali-metal atoms.[2] The (0,2) diagram represents the major correlation effect arising from the mutual dynamic excitations of the valence $3s$ electron and other core electrons. However, in alkali-metal atoms, the main correlation contribution has been found to arise[9] from only the outermost core electrons. In addition to the diagrams in Fig. 3 there are other second-order (1,1) and (0,2) diagrams as well as higher-order diagrams which are rather time consuming to evaluate and are also expected to be small. Such diagrams were explicitly evaluated in the case of alkali-metal atoms and were found to be very small. Therefore, rather than evaluating all these diagrams explicitly, we have considered only a few of them to verify their smallness, and an estimated value based on their sizes and on results of earlier work[7] on Ba^+ and alkali-metal atoms has been assumed in obtaining the final results.

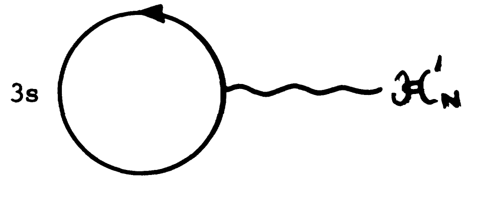

FIG. 1. (0,0) direct diagram.

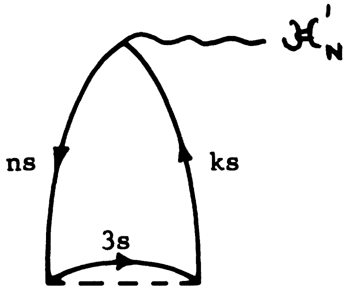

FIG. 2. Exchange core-polarization or (0,1) diagram. *ns* stands for 1*s* and 2*s* core electrons while *ks* stands for all excited *s* states including continuum.

III. RESULTS AND DISCUSSION

The results of the present calculation for $^{25}Mg^+$ which has a magnetic moment of -0.8551 nuclear

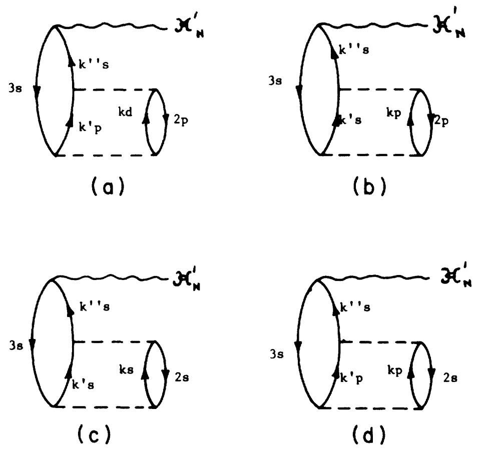

FIG. 3. Major (0,2) direct correlation diagrams.

magneton[10] and nuclear spin $\frac{5}{2}$, have been presented in Table I. The (0,0) diagram shown in Fig. 1 represents the direct contribution from the $3s_{1/2}$ electron. The contribution of -466.4 MHz by this mechanism to the hyperfine constant A constitutes about 78% of the experimental value. One expects the remainder to arise from the unsymmetric interaction between the spin-up valence electron and the spin-up and spin-down core electrons. This unsymmetric interaction is composed of exchange core-polarization and correlation effects. The (0,1) diagram given in Fig. 2 describes the exchange core polarization of the core s electrons by the valence $3s_{1/2}$ electron. This diagram yields a value of -68.6 MHz. However, because of the use of a V^{N-1} potential mentioned earlier, ladder corrections similar to those described elsewhere,[8] have to be applied to this diagram. As is shown in Table I, after applying the hole-hole and hole-particle ladder corrections the net contribution to A from the ECP mechanism is found to be -87.1 MHz. This result is in good agreement with an earlier result of -90 MHz obtained[11] by a different procedure. Turning next to correlation effects, the major (0,2) direct diagrams are given by Fig. 3 while Fig. 4 presents some of the important exchange counterparts of Fig. 3. Evaluation of the important (0,2) diagrams, both direct and exchange, provides a value of -50.0 MHz, with diagram 3(a) providing the dominant contribution followed by the exchange diagram 3(b), a feature in common with that observed[7] in Ba$^+$ and in the alkali-metal-atom series.[9]

TABLE I. Contributions from different mechanisms to the hyperfine constant A.

Mechanism	Contribution (MHz)
Zero-order (Fig. 1)	-466.4[a]
ECP (Fig. 2)	-68.6
Ladder correction to ECP	-18.5
ECP with ladder corrections	-87.1[a]
Major (0,2) correlation (Figs. 3 and 4)	-50.0
Estimated (1,1) correlation	-4.1
Estimated other second-order and higher-order correlation	$+5.9$
Net correlation	-48.2
Total	$-(602\pm 8)$
Experimental[b]	$-596.2544(5)$

[a] Our direct and ECP contributions compare very well with the corresponding values of -463 and -90 MHz, respectively, of Lindgren (Ref. 11).

[b] Reference 6.

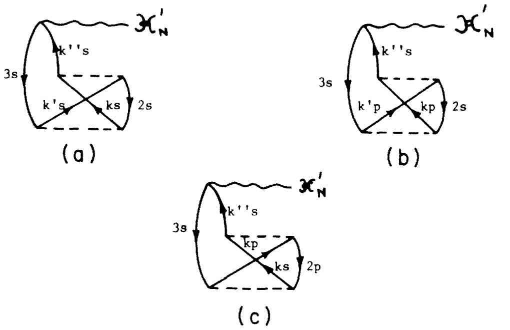

FIG. 4. Major (0,2) exchange correlation diagrams.

Table I also contains values of -4.1 MHz for (1,1) diagrams and $+5.9$ MHz for other (0,2) and higher-order diagrams. These values are obtained from estimates based on results for similar small diagrams in the case of sodium atom[12] where they were calculated explicitly. In making these estimates, we have taken account of the observation that the major (0,2) diagrams for Mg$^+$ were found to be related by a reasonably constant factor to their counterparts in the sodium atom, a feature found[7] also for the isoelectronic Ba$^+$ and Cs.

Combining the various contributions in Table I, a total contribution of $-(602\pm 8)$ MHz to the hyperfine constant A has been obtained in the present investigation. This sum includes contributions from all the mechanisms that have been found to be important in the present system and the related alkali-metal-atom systems[9] and[7] Ba$^+$. In arriving at the confidence limit of our result we note that the total value of -602 MHz is composed of a value of -585.0 MHz which we have obtained by explicit evaluations of important diagrams and a value of -16.6 MHz that we have estimated for the remaining ones. The confidence limit of 8 MHz for the present calculation takes into account the possible uncertainties associated with the estimations for the small contributions, and the accuracy of our computational procedures. Within this confidence limit, the agreement with the experimental result[6] is found to be good.

Table II lists the breakdown of important contributions from major correlation diagrams.

The good agreement obtained between the theoretical and experimental[6] hyperfine constant provides confidence in the accuracy of the individual ECP and correlation contributions, which were substantial and rather important for the explanation of the experimental result. It is interesting to compare these contributions especially as fractions of the direct contribution with the results for the

TABLE II. Individual contributions from major correlation diagrams.

Mechanism	Contribution (MHz)
Diagram 3(a)	−28.3
Diagram 3(b)	−18.5
Diagram 3(c)	−3.5
Diagram 3(d)	−0.7
Diagram 4(a)	+1.6
Diagram 4(b)	−0.2
Diagram 4(c)	−0.4
Total (0,2) major correlation contribution	−50.0

TABLE III. Comparison of ECP and correlation contributions in Mg^+ with similar results in other available isoelectronic systems.

Contribution	Na[a] (%)	Mg^+ (%)	Cs[b] (%)	Ba^+[c] (%)
ECP:direct	22.4	18.7	17.0	13.8
Correlation:direct	15.3	10.3	37.1	23.8

[a] T. Lee *et al.* in Ref. 1. The ratios listed in sodium are close to the corresponding ratios of 23.1%, and 16.5% obtained in a later work by H. Lindberg, A. M. Martensson, and S. Svanberg (Ref. 13) by a different many-body procedure.

[b] B. P. Das *et al.* in Ref. 2.

[c] Reference 7.

heavier alkaline-earth ion Ba^+ that has been studied by both theory[7] and experiment, and also with the isoelectronic atom, sodium. A comparison between these fractional contributions is presented in Table III which also includes the cesium atom which is isoelectronic with Ba^+.

Comparing the results for the two alkaline-earth ions, the ECP contribution is seen to decrease in going from Mg^+ and Ba^+, while the correlation contribution increases, the latter change being much more rapid than the former, a feature similar to that observed in the corresponding isoelectronic neutral alkali-metal atoms sodium and cesium. These trends can be physically understood in terms of deformabilities of the core and valence electrons and the average separations between them in going from the lighter atom to the heavier one. Thus, the trend in the ECP effect indicates that as one goes to the heavier ion, the core states become more tightly bound and thus less susceptible to deformation through exchange interaction with the unpaired spin valence electron. The valence electron, on the other hand, is expected to become more deformable in heavier atoms, because of the more tightly bound core electrons which shield the nuclear charge more effectively compared to those in lighter atoms. The correlation effect which arises because of mutual polarization of valence and core electrons, is expected to increase in importance as the valence electron gets more loosely bound. However, there is a competing effect as well. A more loosely bound valence electron would have larger separation with respect to the core electrons which then would be expected to lead to an opposite trend in the correlation effect. The substantial increase in the correlation contribution observed in going from sodium to cesium and from Mg^+ to Ba^+ indicates that the distance effect is overwhelmed by the increased deformability of the valence electron.

A comparison between sodium and Mg^+ in Table III indicates that the ECP and correlation contributions in sodium are substantially larger than those in Mg^+. The results in sodium[12] listed in Table III are obtained by the nonrelativistic counterpart of the procedure used here and are in good agreement with results[13] of later work by a different procedure. The influence of relativistic effects on the contributions to the hyperfine interaction involve the combination of relativistic effects on the hyperfine-interaction and electron-electron interaction matrix elements as well as energy denominators involved in the corresponding diagrams. These effects are discussed in various places[14–16] in the literature, the most pertinent one for the present case being that in the recent[14] calculation on rubidium. In the latter work it was shown that the relativistic and nonrelativistic ratios $A_{\mathrm{ECP}}/A_{\mathrm{direct}}$ and $A_{\mathrm{cor}}/A_{\mathrm{direct}}$ do not differ significantly, a result that should be applicable to sodium, where relativistic effects are expected to be significantly less important than in rubidium. The smaller values of the ratios for Mg^+ as compared to Na are expected because of the greater polarizability of the neutral alkali-metal atom, analogous to the corresponding situation[7] between Cs and Ba^+. It is hoped that similar theoretical analysis as carried out in the present work and experimental data for other alkaline-earth ions will become available in the future and a systematic study of the continuous trends over the entire series as well as their comparison with the trends already available[9] in the alkali-metal atom series will become possible.

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