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Effects of Configuration Interaction on the Alignment of Beryllium-Like Ions

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Effects of configuration interaction on the alignment of beryllium–like ions

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Abstract. The radiative electron capture into (initially) lithium–like ions is studied within the framework of the density matrix approach. Special attention is paid to the magnetic sublevel population of the residual ionic states which is described by a set of alignment parameters. Detailed calculations of these parameters have been performed for the capture into the $1s^2\, 2s\, 3d_{3/2}\ J_f = 2$ level of high–Z ions along the beryllium isoelectronic sequence. We devote special attention to the modifications in the many–electron case as opposed to single-electron systems. The electron correlation leads to an enhancement of the alignment, which becomes more pronounced as the nuclear charge decreases and the electron-electron interaction gains in strength as compared to the electron-nucleus interaction.

1. Introduction

Experimental studies on relativistic ion–atom collisions have a long tradition at the GSI accelerator and storage ring facility in Darmstadt [1, 2]. Among other topics, these experiments have focused on the *transfer* of an electron from the atomic or electronic target into a bound state of highly–charged projectiles. If such a transfer is accompanied by the emission of photon which carries away the excess energy and momentum, it is usually denoted as the radiative electron capture (REC). In the past, most of the REC studies were performed for the electron capture into highly–charged, bare ions, including measurements on the total and angle–differential cross sections, the alignment of the residual ions as well as on the polarization of the emitted (recombination) photons. Apart from the REC by bare ions, recent interest has been focused also on the *few–electron*, heavy ions, for which the angular distributions of the recombination as well as the subsequent decay photons were measured for the capture into either the ground or some excited states of the ions. Theoretically, the (measured) angular distributions from few–electron, high–Z ions can be understood within the effective "one–particle" calculations if the Pauli principle is properly taken into account. For the recombination of few–electron, heavy ions, in fact, the one–electron model is still well justified because the interelectronic effects are much weaker in the high–Z domain than the electron–nucleus interaction and, hence, should not (strongly) affect the properties of the emitted radiation.

Despite the good applicability of effective one–electron calculations, we have recently reported two case studies in which the many–electron effects beyond the Pauli principle and momenta coupling became (relatively) important [3, 4]. These studies concerned: (i) the REC by decelerated ions with energies $T_p \leq 5$ MeV/u and (ii) the electron recombination into the

highly–excited ionic states. For the latter case, in particular, we showed that the alignment of the (excited) beryllium–like uranium ions U^{88+} following REC may be influenced by the interelectronic interactions [4]. Since the effects of the electron–electron correlations are known to enhance if the nuclear charge decreases, here we continue and extend our investigations towards the REC into lighter few–electron ions. Again, we will focus on the beryllium isoelectronic sequence, whose ions are known to be sensitive to many–particle effects. In the next section, therefore, we will briefly discuss the basic formulas, which are applied later in section 3 to calculate the alignment parameters of the $1s^2\,2s\,3d_{3/2}$ $J_f = 2$ state of (finally) beryllium–like europium Eu^{59+}, gold Au^{75+} and uranium U^{88+} ions following REC for a wide range of projectile energies.

2. Theory

Since the density matrix approach has been applied very frequently for studying the polarization and correlation phenomena in the radiative electron capture, we will restrict ourselves to a rather short account of its basic expressions and refer for all further details to the Refs. [3, 4, 5]. Within the density matrix formalism, the magnetic sublevel population of the residual ion $|\alpha_f J_f\rangle$ following electron capture is described in terms of the so–called statistical tensors $\rho_{k0}(\alpha_f J_f)$. Of course, the form of these tensors depends on the choice of the quantization axis of the overall system (which is, by convention, the z axis) as well as on the "set–up" of a particular experiment. By adopting, for example, a quantization axis along the incoming ion momentum and by assuming that the recombination x–ray photons remain unobserved we obtain the following expression for the statistical tensors [see, e.g., Eq. (2) in Ref. [4]]:

$$
\begin{aligned}
\rho_{k0}(\alpha_f J_f) &= \frac{32\pi^3}{2J_i + 1} \sum_{Lp} \sum_{JJ'\kappa\kappa'} [l, l', j, j', J, J']^{1/2}\,(-1)^{J_i + L - J_f + J - J' - 1/2}\,\langle l0l'0 \,|\, k0\rangle \\
&\times \left\{ \begin{array}{ccc} j & j' & k \\ l' & l & 1/2 \end{array} \right\} \left\{ \begin{array}{ccc} j & j' & k \\ J' & J & J_i \end{array} \right\} \left\{ \begin{array}{ccc} J & J' & k \\ J_f & J_f & L \end{array} \right\} \\
&\times \langle(\alpha_i J_i, \epsilon l j)J\,||H_\gamma(pL)||\,\alpha_f J_f\rangle \langle(\alpha_i J_i, \epsilon l' j')J'\,||H_\gamma(pL)||\,\alpha_f J_f\rangle^* .
\end{aligned}
\tag{1}
$$

Here, J_i and J_f are the total angular momenta of the ion before and after electron recombination, and $\langle(\alpha_i J_i, \epsilon l j)J\,||H_\gamma(pL)||\,\alpha_f J_f\rangle$ denotes the (reduced) transition amplitude for the capture of a free electron with kinetic energy ϵ under the simultaneous emission of a photon with angular momentum L and parity $(-1)^{L+p}$. In Eq. (1), moreover, κ denotes Dirac's angular momentum quantum number of the initial, free electron: $\kappa = \pm(j + 1/2)$ for $l = j \pm 1/2$, and $[l_a, l_b, ...] = (2l_a + 1)(2l_b + 1)....$

The statistical tensors (1) contain the complete information about the population of the magnetic sublevels $|\alpha_f J_f, M_f\rangle$ as produced by the REC. They can be utilized, therefore, in order to explore the angular and polarization properties of the subsequent radiative decay if the electron is initially captured into an excited ionic state. For such an analysis of the decay radiation, however, it is often more convenient to re–normalize the statistical tensors $\rho_{k0}(\alpha_f J_f)$ with respect to the zero–rank tensor [6]:

$$
\mathcal{A}_{k0}(\alpha_f J_f) = \frac{\rho_{k0}(\alpha_f J_f)}{\rho_{00}(\alpha_f J_f)} .
\tag{2}
$$

For the case of the capture of an unpolarized electron into the bound state of the unpolarized ion, these renormalized (or, so–called reduced) tensors describe the *alignment* of the residual ions and are are known to have several properties. In particular, the parameter $\mathcal{A}_{k0}(\alpha_f J_f)$ is nonvanishing only if k is even and satisfies the condition $k \leq 2J_f$. This implies that, for the ionic level with $J_f = 2$, for example, only two parameters $\mathcal{A}_{20}(\alpha_f J_f = 2)$ and $\mathcal{A}_{40}(\alpha_f J_f = 2)$

are required to describe the alignment produced by the electron recombination. In section 3, we calculate these two parameters for the REC into $1s^2 2s 3d_{3/2}$ $J_f = 2$ state of the (finally) beryllium–like europium Eu^{59+}, gold Au^{75+} and uranium U^{88+} ions.

Before the discussion of our results, a few words have to be said, however, about the theoretical model which is used in the computations. To calculate the transition amplitudes $\langle (\alpha_i J_i, \epsilon l j) J \, || H_\gamma(pL) || \, \alpha_f J_f \rangle$ in Eq. (1), the multiconfiguration Dirac–Fock (MCDF) method has been applied to generate the bound–state wave functions. In this model, both the initial $\langle \boldsymbol{r}_1, ... \boldsymbol{r}_{N-1} \, | \, \alpha_i J_i \rangle$ and the final $\langle \boldsymbol{r}_1, ... \boldsymbol{r}_N \, | \, \alpha_f J_f \rangle$ ionic wavefunctions are represented as a linear combination of configuration state functions (CSF) and optimized on the basis of the Dirac–Coulomb Hamiltonian. Further relativistic contributions were added by diagonalizing the Dirac–Coulomb–Breit Hamiltonian matrix. The REC amplitudes were obtained by using the REC of the RATIP program [7], which now facilitates the computation of the REC cross sections and alignment parameters within a distorted–wave approximation.

3. Results and discussions

Motivated by a large set of available experimental data [1, 8], extensive calculations have been performed for the alignment of hydrogen–like heavy ions, following the radiative capture of an electron [5]. Apart from the L–shell REC, special attention has been paid to the $3d$ levels which can decay subsequently into the $1s_{1/2}$ ground state due to the leading electric quadrupole transition. For the electron capture into $3d_{3/2}$ state, for example, the second–rank parameter was found to change in the range $-0.9 \leq \mathcal{A}_{20} \leq -0.6$ depending on the nuclear charge Z and the energy T_p of the projectile ions [5]. In contrast to $\mathcal{A}_{20}$, the fourth–rank alignment parameter $\mathcal{A}_{40}$ vanished identically for hydrogen–like ions as it follows from the selection rule $k \leq 2J_f = 3$.

Knowing the alignment of the $3d_{3/2}$ level for the REC into bare ions, here we address the questions of how the presence of (a few) additional "spectator" electrons affects the behaviour of the parameters $\mathcal{A}_{20}$ and $\mathcal{A}_{40}$ for many–particle systems. As an example, we analyze the capture into the $1s^2 \, 2s \, 3d_{3/2}$ $J_f = 2$ level of beryllium–like heavy ions. Due to the coupling of the electron momenta to the total angular momentum $J_f = 2$, both, the second– and the fourth–rank parameters are required to describe the alignment of these ions. The $\mathcal{A}_{20}$ and $\mathcal{A}_{40}$ parameters are displayed in Fig. 1 as a function of projectile energy and for the REC by initially lithium–like europium Eu^{60+} (left panel), gold Au^{76+} (middle panel) and uranium U^{89+} (right panel) ions. Results from MCDF calculations in Coulomb and Babushkin gauges are compared with the data from an independent–particle approximation (IPA), in which a proper set of Slater determinants with hydrogen–like orbitals has been applied to account for the Pauli principle. As seen from the Figure, the IPA calculations predict the large negative alignment parameter $\mathcal{A}_{20}$ while, again, the fourth–rank parameter $\mathcal{A}_{40}$ is zero over all the energy range in accord with the one–electron picture. A *qualitatively* different behaviour of the $\mathcal{A}_{40}$ has been obtained by means of the MCDF approach. The MCDF calculations show that REC into the $1s^2 \, 2s \, 3d_{3/2}$ $J_f = 2$ state of (finally) beryllium–like ions results in relatively large alignment $\mathcal{A}_{40}$, which is almost 0.17 and 0.06 for Eu^{59+} and U^{88+} at a projectile energy of $T_p = 10$ MeV/u and slightly decreases to 0.002 and 0.013 for higher energies. Such a—nonvanishing—parameter arises mainly due to the mixture of the $1s^2 \, 2s \, 3d_{3/2}$ $J_f = 2$ level with other levels having a strong alignment. From our calculations, in particular, we found a (relatively) large admixture of the $1s^2 \, 2s \, 3d_{5/2}$ $J_f = 2$ level for which a large positive parameter $\mathcal{A}_{40}$ has been predicted before [5]. This admixture increases from 0.5% for U^{88+} to almost 5% for lower nuclear charges as expected from the $1/Z$ scaling law for the electromagnetic interaction between the electrons. As seen from Fig. 1, besides the non–zero parameter $\mathcal{A}_{40}$, the configuration interaction effects also lead to an enhancement (of the absolute value) of the alignment parameter $\mathcal{A}_{20}$. This enhancement becomes most pronounced for europium ions, for which the degree of alignment $\mathcal{A}_{20}$ level is increased by almost 10% due to the mixing between the $1s^2 \, 2s \, 3d_{3/2}$ $J_f = 2$ and
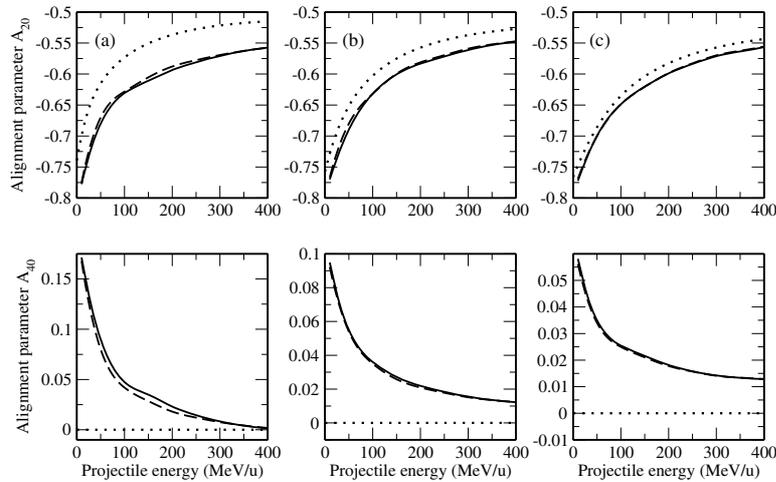
Figure 1. Alignment parameters $\mathcal{A}_{20}$ and $\mathcal{A}_{40}$ of the $1s^2\,2s\,3d_{3/2}$ $J_f = 2$ state of beryllium–like ions following REC by europium (a), gold (b) and uranium (c) projectiles. Results from an independent particle model $(\cdots\cdots)$ are compared with those from MCDF calculations in Coulomb $(---)$ and Babushkin (———) gauge.

$1s^2\,2s\,3d_{5/2}$ $J_f = 2$ states.

4. Summary

In conclusion, we have investigated the effects of electron–electron interaction on the alignment of heavy, few–electron ions following electron capture process. For the particular case of REC into the $1s^2\,2s\,3d_{3/2}$ $J_f = 2$ state of (initially) europium, gold and uranium ions, detailed calculations have been performed within the multiconfiguration Dirac–Fock approach as well as the independent–particle approximation. Both these approximations yield almost identical results for the alignment parameter $\mathcal{A}_{20}$ but predict a *qualitatively* different behaviour of the degree of alignment $\mathcal{A}_{40}$. Namely, while this fourth–rank parameter obtained from the IPA is identical to zero (in full agreement with the "one–electron picture"), the configuration interaction effects taken into account within the MCDF approach result in additional alignment of the $1s^2\,2s\,3d_{3/2}$ $J_f = 2$ level and, hence, in $\mathcal{A}_{40}$ being relatively large for the projectile energies $10 \leq T_p \leq 400$ MeV/u. Such a discrepancy between two theoretical approaches clearly indicates that apart from the momentum coupling and the Pauli principle, the interelectronic interaction effects may play a very important role, even in relativistic heavy ion collisions.

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