SCA calculations of the proton induced alignment using relativistic Hartree-Fock wavefunctions

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Short Title: SCA calculations of proton induced alignment

Classification Numbers: 34.50, 31.20D

Received:

Abstract. Proton induced differential and total alignment is reviewed and some calculations presented. Density matrix formalism is employed as the theoretical framework and more efficient expansion into state multipoles used. The collision T-matrix elements entering the expression for the alignment tensor are calculated in the semiclassical approximation to first order. Coordinate space formulation including classical hyperbolic trajectories for the projectile path is adopted here, to take proper account of deflection. Relativistic Hartree-Fock orbital wave functions for bound and continuum electronic states in the partial wave expansion cover both screening and relativistic effects in the atom in a unifying scheme. The continuum orbitals are calculated iteratively until convergence in the frozen core $V^{N-1}$ potential.

1 Introduction

The information collected by simply measuring the cross-section averages over the degenerate initial states in ion-atom collisions is incomplete in the sense that, in general, there are different modes of populating the final (hole) states. For the particular subshell to be ionized, these substates have different magnetic quantum numbers $m_i$ (projections of the hole-state angular momentum on the quantization axis) and the transition probabilities for ionizing them are also different. The result is that our final state will in general be a mixture of the magnetic substates corresponding to the sharp angular momentum $j_i$.

Such a state can be described in terms of the reduced density matrix characterised by the number of independent parameters restricted by the symmetries relevant to the collision process (Blum 1981). The equivalent description of the excited state is obtained by taking linear combinations of the density matrix elements which behave as the components of the irreducible tensors under spatial rotations (Blum 1981, Berezhko and Kabachnik 1977). These so-called statistical tensors (or state multipoles) have the advantage that the symmetry properties of the collision system can be easily incorporated into the formalism since the geometric and dynamic properties separate
explicitly. In particular, the connection with the anisotropy and polarization properties of the radiation emitted from the atom after the hole was created is then more obvious (Berezhko and Kabachnik 1977, Berezhko et al 1978, Cleff and Mehlhorn 1974).

In this work we shall consider the projectile ion - target atom systems, both unpolarized in the initial state (before the scattering takes place), so that the resulting ensemble of ions is not oriented but is aligned (at least one component of the second-rank statistical tensor being different from zero). The interactions with any other open shells in the resulting ion will be neglected, which is a reasonable assumption since we will be concerned only with medium and heavy targets in this work. It will also be assumed that there is only one hole in the final state (our discussion is limited to asymmetric systems). The study of such systems provides an efficient tool for testing various theoretical models in the calculation of the collision processes. Some progress in this direction was made recently, starting with the plane wave Born approximation (PWBA) (McFarlane 1972, Berezhko and Kabachnik 1977, Berezhko et al 1978, Sizov and Kabachnik 1980). The semiclassical approximation (SCA) was also invoked, and the results for the integral alignment turned out to be close to the ones obtained with PWBA, except in the region of impact energies where the Coulomb deflection can be of importance (Rösel et al 1982, Kabachnik and Kondratyev 1988). Both theories closely follow the experimental data, except for small impact energies, in which case SCA provides better results. Therefore, the Coulomb deflection will be fully taken into account in this work by using correct hyperbolic trajectories.

The sensitivity of alignment parameters on the choice of the electronic wave functions was also investigated. Relativistic screened hydrogenic orbitals were often used as a good approximation (Rösel et al 1982), but for the more detailed comparison with experiments, a more sophisticated approach is necessary. Our approach to this problem is the use of relativistic Hartree-Fock wave functions for both bound and continuum states.

In section 2 we shall present a short review of the theory relevant to our treatment, and results of our calculations are dealt with in section 3.

2 Theory

The elements of the reduced density matrix describing the excited state can be written in terms of the scattering amplitudes. If the scattered projectile is observed, i.e. if we are interested in the impact parameter dependence, it reads

$$\rho_{m_i',m_i}(j,j';b) = \sum_{\tau_f} \int dE_e \int d\Omega_e \ f_{Q_i,q,Q_f}(m_i,\tau_f) \ f_{Q_f,q,Q_i}(m_i',\tau_f),$$

where $Q_i$ and $Q_f$ are the initial and final wave numbers of the projectile, respectively, and $b$ is the impact parameter corresponding to the projectile scattering angles $\Omega_p$. The summation (integration) in the expression above is extended over all the observables not observed in the experiment (energy $E_e$, helicity $\tau_f$ and angles $\Omega_e$ of the continuum electron). The scattering amplitude for ionization from the magnetic substate $m_i$ of the $(n_i,\kappa_i)$-shell is given in terms of the T-matrix element

$$f_{Q_i,q,Q_f}(m_i,\tau_f) = \left( \frac{1}{2\pi} \frac{m_p^*}{(2\pi\hbar)^4} \frac{E_e}{(\hbar c)^2 q Q_f}{Q_i} \right)^{1/2} T_{Q_f,q,Q_i}(m_i,\tau_f),$$

where $m_p^*$ is the reduced mass of the projectile-target system and $q$ is the wave number
of the ejected electron. The normalization constant was chosen according to

\[
Tr \rho(j, j; b) = \sum_{m_i} \frac{d\sigma(m_i)}{d\Omega_p},
\]

so that the diagonal components are the ionization cross sections \(\sigma(m_i)\) from the particular magnetic substates \(m_i\). Detailed description of the T-matrix in the SCA approximation was given previously (Pauli \textit{et al.} 1978, Trautmann and Rösel 1980, Halabuka \textit{et al.} 1994).

The (\(k, \kappa\)) component of the statistical tensor is given by

\[
\rho_{kk}(j, j; b) = (2k + 1)^{1/2} \sum_{m_im_i'} (-1)^{j_i-m_i} \binom{j_i}{m_i} \binom{j_i'}{-m_i'} \binom{k}{-\kappa} \rho_{m_im_i}(j, j; b).
\]

Inserting the SCA T-matrix elements into the expression above, we can write for the tensor component, differential in the scattering angle

\[
\rho_{kk}(j, j; b) = \left(\frac{me}{\hbar}\right)^2 \left(\frac{4m_p^*}{me}\right)^2 (Z_p\alpha)^2 \int dE_e \left(\frac{d\sigma}{d\Omega_p}\right)_{\text{Ruth}} \frac{4\pi^2 Q_f}{Q^2} (2k + 1)^{1/2}
\]

\[
\times \sum_{m_im_i'} (-1)^{j_i-m_i} \binom{j_i}{m_i} \binom{j_i'}{-m_i'} \sum_{\kappa f m_f \ell ml' m'} C_{lm}(\kappa_i, m_i, \kappa_f m_f) C_{lm}^*(\kappa_i, m_i', \kappa_f m_f)
\]

\[
\times J_{\kappa_i \kappa_f}^{lm}(\epsilon, \xi, a_c) J_{\kappa_i \kappa_f}^{lm*}(\epsilon, \xi, a_c),
\]

where \(C_{lm}\) are the angular coefficients defined in terms of the Wigner 3j symbols by

\[
C_{lm}(\kappa_i, m_i, \kappa_f m_f) = (-1)^{m_f+\frac{1}{2}}\left(1 + (-1)^{l_f+l_i}\right) \left(\frac{(2j_f + 1)(2l + 1)(2j_i + 1)}{4\pi}\right)^{1/2}
\]

\[
\times \begin{pmatrix}
\frac{j_f}{l/2} & 0 & -1/2 \\
1/2 & l & j_i \\
0 & -m_f & m_i
\end{pmatrix}.
\]

The last expression in eq. 5 ("rotated" semiclassical integral) is given by

\[
J_{\kappa_i \kappa_f}^{lm}(\epsilon, \xi, a_c) = \frac{e^{izm}}{2l+1} \sum_{m\bar{m}} d_{m\bar{m}}^{l} \left(\frac{\pi}{2}\right) Y_{l\bar{m}} \left(\frac{\pi}{2}, \frac{\pi + \theta_p}{2}\right) I_{\kappa_i \kappa_f}^{lm}(\epsilon, \xi, a_c),
\]

where \(d_{m\bar{m}}^{l}\) are the elements of the rotation matrix in the notation of Edmonds (1960). For detailed description of the semiclassical integrals \(I_{\kappa_i \kappa_f}^{lm}\) and the electronic radial form factor, we point to the same reference as for the T-matrix description. The quantization axis in all the expressions above points in the direction of the incident beam. Further on we will use the dimensionless alignment parameters defined by

\[
A_{kk}(j, j; b) = \frac{\rho_{kk}(j, j; b)}{\rho_{00}(j, j; b)}.
\]

The total alignment parameters (when the scattered projectile is not observed) are obtained from the expressions above by integrating over the projectile angles (Rösel
In that case the number of independent parameters is further reduced for axially symmetric systems, and we can write

$$\rho_{kn} = \int d\Omega_p \rho_{kn}(j, j; b) = \rho_{k0}\delta_{k0}.$$  \hspace{1cm} (9)

3 Results and discussion

All calculations were performed with SCA code IONHYD developed by the Basel group and recently extended for Dirac-Fock electronic form factors (Halabuka et al 1994). The calculations with the relativistic screened hydrogen-like orbitals (screening numbers are chosen according to Slater rules in this work) are also repeated here for convenience of comparison with the previous work. To determine the Dirac-Fock form factors, we have calculated numerically the overlap matrix elements between the bound and continuum orbitals. All bound states were generated with the GRASP code (Dyall 1989) in a self-consistent run for the neutral atom in the ground state. The continuum partial waves of the ejected electron were calculated as the excited states in the field of the frozen ionic core with the hole in the ionized subshell. The procedure adopted here is to iterate the exchange potential until convergence is achieved (Perger et al 1991, 1993).

In figure 1 the total alignment parameter $A_{20}$ for the ionization of the $L_3$ subshell of silver bombarded by protons is plotted as a function of the squared reduced velocity $V^2$ defined by

$$V^2 = \frac{m_e m_p^*}{E_p E_{L_3}},$$  \hspace{1cm} (10)

where $E_p$ and $E_{L_3}$ are impact energy and binding energy of the $L_3$ subshell, respectively. In this case the expression for $A_{20}$ can be written more explicitly as

$$A_{20} = \frac{\sigma(\frac{3}{2}) - \sigma(\frac{1}{2})}{\sigma(\frac{3}{2}) + \sigma(\frac{1}{2})},$$  \hspace{1cm} (11)

where $\sigma(m_i)$ now denotes the total cross section. The agreement with the experiment is very good for $V^2 \gtrsim 0.04$, showing that quite precise description is possible in this region of impact energies, if screening effects are treated properly. For the values $V^2 \lesssim 0.04$ there is still some discrepancy when compared with experiment and the influence of screening and relativistic effects does not improve the situation, as seen in figure 1. Going beyond first-order perturbation theory as, for example, in the coupled-channel formalism (Mehler 1987), or using the two-center expansions could possibly tell us more about the nature of the disagreement.

From the computational point of view, in our approach to SCA, it was found necessary to take into account enough terms in the multipole expansion of the Coulomb interaction to obtain convergence. The results proved to be much more sensitive on this point in regions where the reduced velocity takes the value $\approx 1$, and also when $V^2 \lesssim 0.01$. Even the multipole terms of the order higher than 6 can modify the results by about 10 percent. For practical reasons we have done all calculations with 6 multipoles.

The same formalism was applied for the calculation of differential alignment parameters. In this way a more detailed study of the atomic properties and collision processes...
is possible when the predictions of the various theoretical models are compared with the results of experiments performed by the coincidence method. In figure 2 the impact parameter dependence of $A_{20}$ for the p-Sm system is shown. The convergence was found to be satisfactory at smaller impact parameters $b$, but getting worse with increasing value of $b$ (in this case at about 8000 fm). The position of the curve maximum shifts to the larger values of impact parameters when more multipole terms are taken into account, and its height increases in magnitude. At first sight, this increases the disagreement when compared with the experimental values plotted, and the improvement achieved by taking into account the Hartree-Fock description of screening improves the situation only slightly. On the other side, the experimental error is greater in that region. It should also be mentioned that the curves in figure 2 are actually flatter at the right flank, as the result of the residual contribution arising from higher-order multipole terms, leading to somewhat better agreement. It can be concluded that the first-order perturbation theory works very well in this case, as can be seen from the comparison of our results with the ones of Mehler et al. (1987), where the more general coupled-state formalism was used.

We have also plotted the alignment parameters for the $M_3$ subshell of gold in figures 3, 4 and 5. The situation in this case is somewhat more complicated, arising from the more complex nodal structure of the radial wave functions. For the larger impact parameter values, the screening effects become more pronounced. By varying the impact energy, the behaviour of the parameters can differ to a large extent (Kabachnik and Kondratyev 1988, Kabachnik 1988), exhibiting the influence of projectile-target interactions. It is tempting to investigate these features, in the framework of SCA combined with relativistic Hartree-Fock electronic orbitals, in more detail.

4 Acknowledgments

WFP gratefully acknowledges the support of the US National Science Foundation for a travel grant, NSF INT-9214087, which supported this work.
5 References

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FIG. 1
Integral $L_3$ -subshell alignment parameter $A_{20}$ for the system p+Ag as a function of the squared reduced velocity $V^2$. Dashed line - with hydrogen-like orbitals screened according to the Slater rules. Full line - with Dirac-Fock orbitals. Data from Richter et al (1981).

FIG. 2
Differential $L_3$ -subshell alignment parameter $A_{20}$ for the system p+Sm as a function of the impact parameter $b$ at the constant projectile energy $E_p=4$ MeV. Dashed line - with hydrogen-like orbitals (Slater screening). Full line - with Dirac Fock orbitals. Data from Zehender (1985).

FIG. 3
Differential $M_3$ -subshell alignment parameter $A_{20}$ for the system p+Au as a function of the impact parameter $b$ at the constant projectile energy $E_p=0.3138$ MeV. Dashed line - with hydrogen-like orbitals (Slater screening). Full line - with Dirac Fock orbitals.

FIG. 4
The same as in figure 3 for the alignment parameter $A_{21}$.

FIG. 5
The same as in figure 3 for the alignment parameter $A_{22}$.