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LETTER TO THE EDITOR

Multiple vacancy inclusive probabilities for the scattering system 16 MeV S^{16+} on Ar*

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Abstract. To evaluate single and double K-shell inclusive charge transfer probabilities in ion-atom collisions we solve the time-dependent Dirac equation. By expanding the time-dependent wavefunction in a set of molecular basis states the time-dependent equation reduces to a set of coupled-channel equations. The energy eigenvalues and matrix elements are taken from *self-consistent relativistic* molecular many-electron Dirac-Fock-Slater calculations. We present many-electron inclusive probabilities for different final configurations as a function of impact parameter for single and double K-shell vacancy production in collisions of bare S on Ar.

In order to give a good description of the time-dependent relativistic many-electron ion-atom scattering problem for small and intermediate energies we have developed the following procedure. In a first step we solve the static molecular problem as a function of the internuclear distance with a relativistic *ab initio* self-consistent MO-LCAO Dirac-Fock-Slater code [1]. This program produces *ab initio* single particle MO energies as well as all the rotational and radial coupling matrix elements between the molecular levels. In a second step we solve the time-dependent scattering problem with the MO states as a basis by performing coupled-channel calculations for the considered static MO states [2]. This results in single-particle transition amplitudes of the electrons in the incoming and outgoing channels. The many-particle inclusive probabilities corresponding to the specific question being asked in the considered experiment are finally evaluated as complicated sums and products of the single-particle amplitudes [3-7]. This evaluation is an exact transformation from the single-particle to the many-particle interpretation in the framework of the independent particle model. It is the first time that such a *ab initio* procedure has been applied to a complicated many-electron scattering system.

As an example we deal with the case of 16 MeV S^{16+} on Ar. The method used is briefly given in the following formulae. The time-dependent single-particle equation to be solved reads

$$h^{\text{eff}}(\boldsymbol{R}(t))|\psi_n(t)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi_n(t)\rangle \tag{1}$$

where we expand the wavefunction $|\psi_n(t)\rangle$ in a (complete) set of single-particle molecular basis states

$$|\psi_n(t)\rangle = \sum_k |\phi_k(\boldsymbol{R}(t))\rangle c_{nk}(t). \tag{2}$$

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The molecular basis states $|\phi_k(\boldsymbol{R}(t))\rangle$ are the solutions from the static diatomic Dirac-Fock-Slater (DFS) calculations mentioned above [1]. Inserting expansion (2) in equation (1) leads to the equivalent single-particle matrix coupled channel equations

$$i\hbar \mathbf{s} \frac{d}{dt} c_{nk} = \mathbf{m} c_{nk} \qquad n = 1, 2, \ldots, N \tag{3}$$

for the single-particle amplitudes. $\mathbf{s} = (s_{lk})$ is the overlap matrix and $\mathbf{m} = (m_{lk})$ the coupling matrix. The matrix elements are taken from the static calculations performed at many internuclear distances. The wavefunctions $|\psi_n(t)\rangle$ have to satisfy the initial conditions

$$\lim_{t \to -\infty} (|\psi_i(t)\rangle - |\psi_i^0(t)\rangle) = 0 \qquad i = 1, 2, \ldots, N \tag{4}$$

where $|\psi_i^0(t)\rangle$ are the N orthogonal initial states. By solving separately the single-particle coupled-channel equations for each electron (or hole) involved in the collision system one gets N sets of transition amplitudes c_{kn}.

A solution of the many-particle time-dependent Dirac-Fock-Slater equation

$$H^{\text{eff}}(R(t))|\Psi(t)\rangle = i\hbar \frac{d}{dt} |\Psi(t)\rangle \tag{5}$$

with the independent-particle Hamiltonian

$$H^{\text{eff}}(R) = \sum_i^N h_i^{\text{eff}}(R) \tag{6}$$

is given by a time-dependent Slater determinant built up from the N single-particle wavefunctions $|\psi_n(t)\rangle$. In principle the many-particle equation (5) may also be solved by expanding the total wavefunction $|\Psi(t)\rangle$ in a (complete) set of time-dependent many-particle wavefunctions $|\Phi_k(t)\rangle$.

$$|\Psi(t)\rangle = \sum_k |\Phi_k(t)\rangle C_k(t). \tag{7}$$

Inserting the expansion (7) in equation (5) leads to a set of coupled-channel equations equivalent to (3) but for the many-particle amplitudes C_k. Both sets of amplitudes describe the same physics and thus a transformation from one to the other set is possible [3-7].

The system 16 MeV S^{16+} on Ar was chosen as a first example because detailed triple coincidence measurements for the following questions were available [8]. How large is the probability of finding:

(i) *one* hole in S 1s *and one* hole in Ar 1s (P_{SA})?

(ii) *two* holes in S 1s (P_{SS})?

(iii) *two* holes in Ar 1s (P_{AA})?

The indices S and A denote a hole measured in the 1s shell of sulphur and argon respectively. The correlation diagram from the static DFS molecular calculations for the system S^{16+}-Ar is presented in figure 1. The simplest way to describe the K-K charge transfer is to use the two lowest levels (each doubly degenerate) as a basis which can be attributed asymptotically ($R = +\infty$) to S 1s and Ar 1s. Because this procedure does not allow a description of exchange with higher lying levels we increased the basis by choosing the first 20 relativistic one-particle channels $1\frac{1}{2}\pm$ to $8\frac{1}{2}\pm$ and $1\frac{3}{2}\pm$ to $2\frac{3}{2}\pm$. The initial occupation of these 20 levels was chosen according to the asymptotic occupation of the separated atoms at $t = -\infty$.

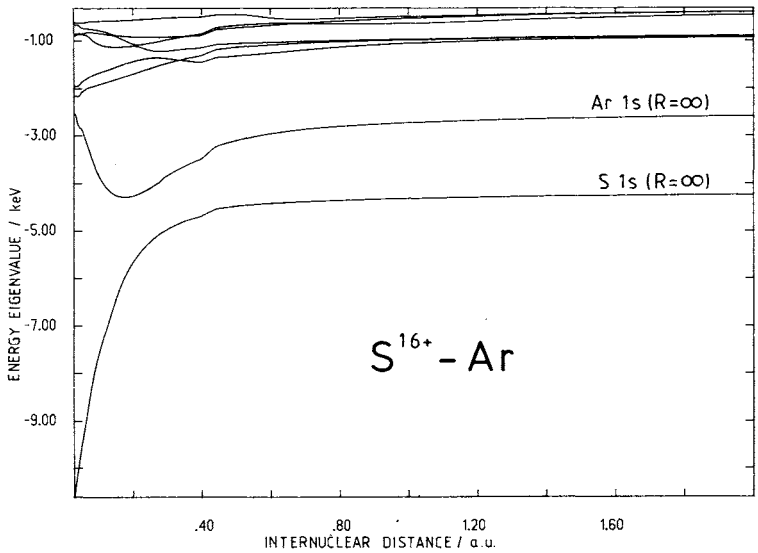

Figure 1. Correlation diagram of the system S^{16+}–Ar.

Table 1. The 16 possible ways of putting 0, 1, 2, 3 or 4 electrons into four levels: ●, occupied; ○, unoccupied. On the right-hand side we mark the contribution to the probabilities P_{SS}, P_{AA} and P_{SA}. The last column gives the corresponding curve in figures 2 and 3.

Occupation				Contribution			
S 1s+	S 1s−	Ar 1s+	Ar 1s−	P_{SA}	P_{AA}	P_{SS}	Figure
○	○	○	○	◇	◇	◇	2(*a*)
●	○	○	○	◇	◇		2(*b*)
○	●	○	○	◇	◇		2(*b*)
○	○	●	○	◇		◇	2(*c*)
○	○	○	●	◇		◇	2(*c*)
○	○	●	●			◇	3
●	●	○	○		◇		2(*d*)
○	●	●	○	◇			2(*e*)
●	○	○	●	◇			2(*e*)
○	●	○	●	◇			2(*f*)
●	○	●	○	◇			2(*f*)
●	●	●	○				
○	●	●	●				
●	○	●	●				
●	●	○	●				
●	●	●	●				

The probabilities P_{SS}, P_{AA} and P_{SA} cannot be directly expressed in terms of simple inclusive probabilities. In a first step the probabilities of the 16 combinations given in table 1 were calculated. Eleven of the 16 combinations can contribute to one or more of the probabilities P_{SS}, P_{AA} and P_{SA}. All 16 probabilities are exclusive within the four lowest channels but inclusive with respect to the other channels. Figures 2(*a*)-(*f*) and figure 3 show the probabilities of the 11 combinations presented in table 1 which contribute to the probabilities P_{SS}, P_{AA} and P_{SA}. Because we do not take spin polarization into account by degeneracy the 11 contributions reduce to seven different figures. The incoming channel (figure 3: two electrons in Ar and two holes in S) stays dominant over a wide range of values of the impact parameter *b*. Only for small values of *b* does its value reduce to a few per cent while the combination corresponding to four holes in the four lowest levels (figure 2(*a*)) rises to about 25%. Figures 2(*e*) and 2(*f*) show the K-K charge transfer probability while figure 2(*c*) gives the probability of one electron from Ar 1s being transferred to higher levels. The probabilities P_{SS}, P_{AA} and P_{SA} can be evaluated by summing the contributions which are given in figures

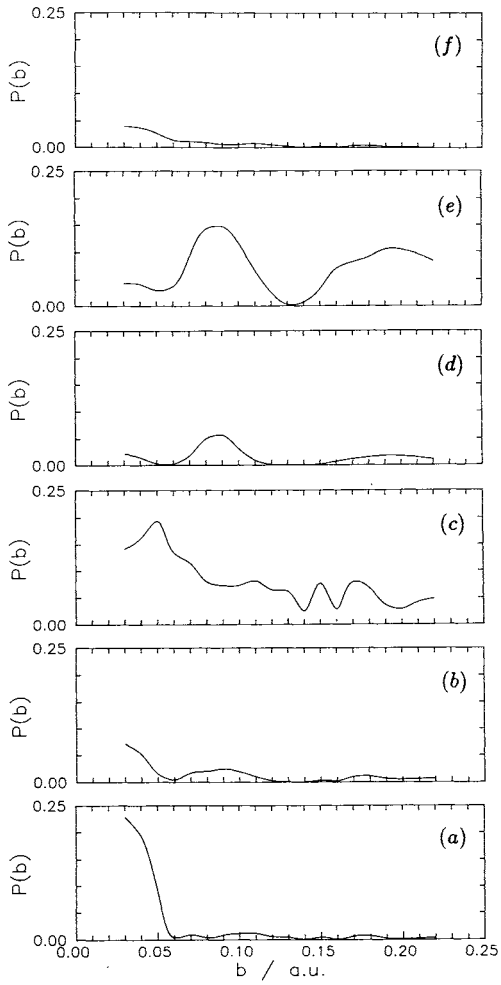

Figure 2. $P(b)$ curves for the combinations given in table 1.

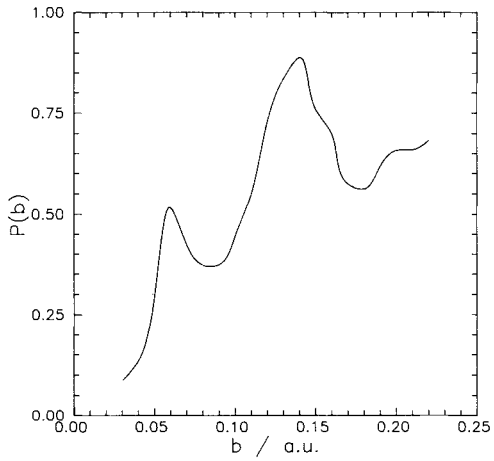

Figure 3. $P(b)$ curves for the combination of two electrons in Ar and two holes in S.

2 and 3. P_{SS} is given by one sixth of the result of figure 2(a) plus two thirds of figure 2(c) plus figure 3. P_{AA} and P_{SA} are given analogously in table 1. Figures 4 and 5 show the probabilities P_{SS}, P_{AA} and P_{SA}. The qualitative agreement with the experimental results is good. Especially for the probabilities P_{SS} and P_{AA} the position and even the amplitudes for P_{AA} are well reproduced. The agreement for the probability P_{SA} where a sum over nine contributions has to be performed is not as good as for the two others but the structure and order of magnitude is good. In addition the result strongly depends on the weight attributed to each contribution in the partial summation of the nine probabilities which in reality may be other than statistical.

We have shown here that it is possible to study complex many-particle collision systems with *ab initio* Dirac–Fock–Slater calculations in combination with coupled-channel calculations of a reasonable small number of basis functions. Although the energy of the collision in our case is so high that an adiabatic picture is only partially valid the 20 lowest channels are nevertheless able to lead to a reasonably good

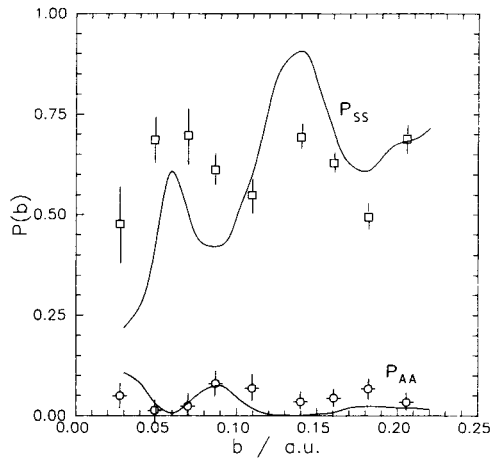

Figure 4. P_{AA} and P_{SS}.

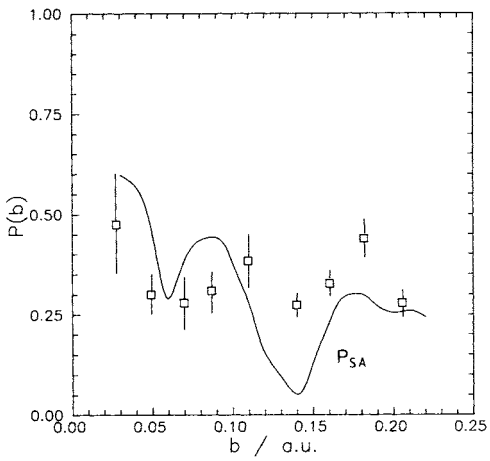

Figure 5. P_{SA}.

reproduction of the experimental results. The formalism of inclusive probabilities allows the answering of complicated questions such as occupation numbers or anisotropies in the final configuration of a many-electron collision system.

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