Relativistic ab initio calculations for ion–atom collisions

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*Within the independent particle model we solve the time-dependent single-particle equation using ab initio SCF-*DIRAC–FOCK–SLATER *wavefunctions as a basis. To reinstate the many-particle aspect of the collision system we use the inclusive probability formalism to answer experimental questions. As an example we show an application to the case of* S^{15+} *on Ar where experimental data on the K-K charge transfer are available for a wide range of impact energies from 4.7 to 90 MeV. Our molecular adiabatic calculations and the evaluation using the inclusive probability formalism show good results in the low energy range from 4.7 to 16 MeV impact energy.*

In order to solve the time dependent many-particle behaviour of an ion-atom system during a collision we start with the semi-classical approximation for the nuclear motion. Thus the time-dependent many-particle DIRAC equation for the electrons involved in the collision system has to be solved. As an approximation we use an effective many-particle Hamiltonian given as a sum of DIRAC–FOCK–SLATER single-particle Hamiltonians. This leads to a set of time-dependent single-particle equations

$$\left(\hat{h}_i^{\mathrm{DFS}} - i\hbar\frac{\partial}{\partial t}\right)\psi_i(t) = 0 \qquad \text{with} \quad i = 1,\ldots,N. \tag{1}$$

The wavefunctions $\psi_i(t)$ have to satisfy the initial conditions for the N electrons

$$\lim_{t\to-\infty}(\psi_i(t) - \psi_i^0(t)) = 0 \qquad \text{with} \quad i = 1,\cdots,N. \tag{2}$$

The solution of the electronic many-particle equation is given as a determinant built-up from the single-particle wavefunctions $\psi_i(t)$.

We use a basis-set method to solve equation 1. The time-dependent single-particle wavefunctions $\psi_i(t)$ are expanded in a set of M molecular wavefunctions $\left\{\varphi^{MO}\right\}$

$$\psi_i(t) = \sum_{m=1}^{M} a_{im}(t)\varphi_m^{MO}(\vec{R}(t))e^{-\frac{i}{\hbar}\int^t \varepsilon_m(\vec{R}(t'))dt'} \tag{3}$$

with $i = 1, \ldots, N$. The set of molecular wavefunctions $\left\{\varphi^{MO}\right\}$ is taken as the solutions from the static DFS equation

$$\hat{h}^{\mathrm{DFS}}(\vec{R})\varphi_m^{MO}(\vec{R}) = \varepsilon_m(\vec{R})\varphi_m^{MO}(\vec{R}). \tag{4}$$

with $m = 1, \ldots, M$[1].

We solve equation 4 by expanding the molecular orbitals $\varphi_m^{MO}(\vec{R})$ in a set of numerical atomic orbitals from static atomic DFS calculations.

$$\varphi_i^{MO}(\mid \vec{R} \mid) = \sum_{k=1}^{\mathbf{K}} d_{\lambda k}\xi_k^{AO}(\vec{r}, s). \tag{5}$$

Using the time dependent molecular basis (5) the problem of solving the time–dependent single–particle equations 1 is equivalent to solving the single–particle matrix coupled–channel equations

$$i\hbar\frac{d}{dt}a_{il} = \sum_{m=1}^{\mathbf{M}} a_{im}\langle\varphi_l^{MO} \mid -i\hbar\frac{d}{dt} \mid \varphi_m^{MO}\rangle e^{-\frac{i}{\hbar}\int^t(\varepsilon_m(\vec{R}(t'))-\varepsilon_l(\vec{R}(t')))dt'} \tag{6}$$

with $i = 1, \ldots, N$ for the single particle amplitudes a_{il}[2,3].

During the solution of the static DFS equation the matrix elements are also calculated in an ab initio way. Each of the N electrons in the collision system defines a new initial value problem for the M coupled channels taken into account in equation 6. Solving the coupled channel equations one ends up with N sets of single–particle amplitudes $\left\{a_{ij}\right\}$ with $i = 1, \cdots, N$ and $j = 1, \cdots, M$.

To match the many–particle aspect of the collision system and take the antisymmetry of the many–particle wavefunction into account one has to formulate the experimental questions as inclusive probabilities given in terms of single–particle amplitudes[4,5,6,7,8,9].

Schuch et al.[10] have measured the impact parameter dependent probability to find at least one vacancy in the K–shell of the Ar–target in collisions of S^{15+} on Ar. The measurements were done for a wide impact energies range from 4.7 to 90 MeV. We are interested in understanding the low energy collisions from 4.7 to 16 MeV where our LCAO–MO description of the collision problem should be good. We performed a 20 channel calculation taking all the channels into account that are shown in Fig.1 . Figs. 2 to 4 show the experimental P_{KK} values versus different theoretical approaches our results being the full curves.

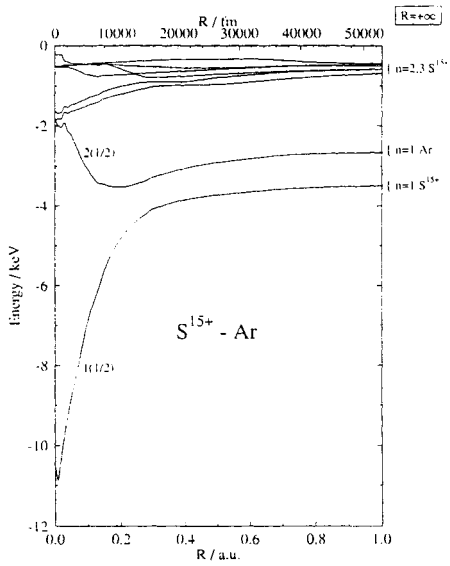

Fig.1 : Correlation diagram for S^{15+}-Ar

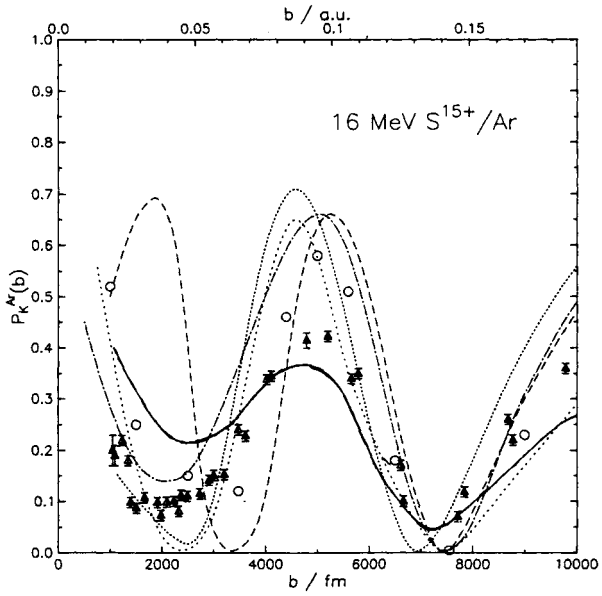

Fig.2 : Experimental values : $P_K^{Ar}(b)$ in collision of 16 MeV S^{15+} on Ar. Broken curve : Stolterfoht et al.[15,16]. Narrow dotted curve : Lin and Tunnell[11]. Chained curve : Fritsch and Lin[12] Open circle : Grün et al.[14]. Wide dotted curve : Schuch et al.[10]. Full curve : our inclusive probability

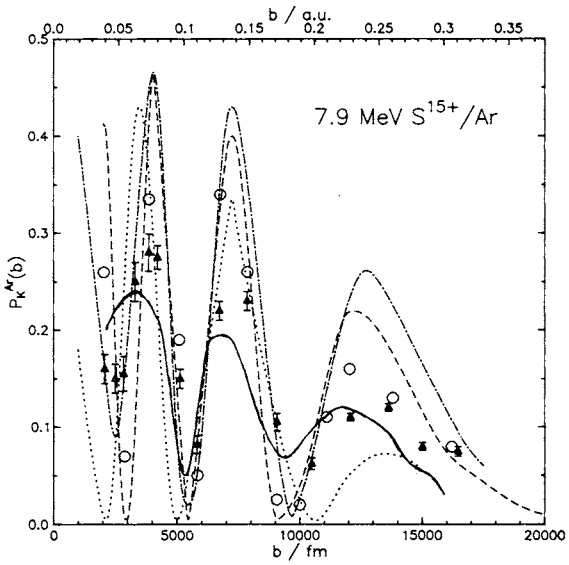

Fig.3 : Experimental values : $P_K^{Ar}(b)$ in collision of 7.9 MeV S^{15+} on Ar. Broken curve : Stolterfoht et al.[15,16]. Chained curve : Fritsch and Lin[12] Open circle : Grün et al.[14]. Wide dotted curve : Schuch et al.[10]. Full curve : our inclusive probability

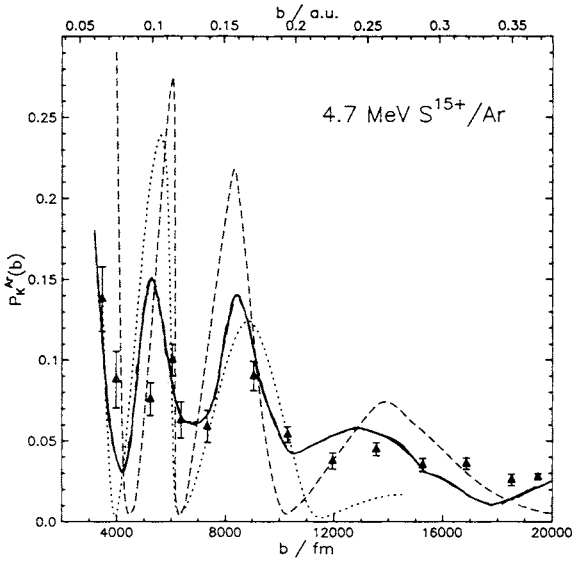

Fig.4 : Experimental values : $P_K^{Ar}(b)$ in collision of 4.7 MeV S^{15+} on Ar. Broken curve : Stolterfoht et al.[15,16]. Wide dotted curve : Schuch et al.[10]. Full curve : our inclusive probability

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