Z. Phys. D – Atoms, Molecules and Clusters 22, 407–409 (1991)

Atoms, Molecules
Zeitschrift für Physik D and Clusters

Influence of occupation number of single particle levels on K – K charge transfer in collisions of 90 keV – Ne^{9+} on Ne ⋆

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Received 17 May 1991; final version 24 June 1991

Abstract. The influence of the occupation of the single particle levels on the impact parameter dependent K – K charge transfer occuring in collisions of 90 keV Ne^{9+} on Ne was studied using coupled channel calculations. The energy eigenvalues and matrixelements for the single particle levels were taken from ab initio *self consistent* MO-LCAO-DIRAC-FOCK-SLATER calculations with occupation numbers corresponding to the single particle amplitudes given by the coupled channel calculations.

PACS: 34.10.+x; 31.20.

I. Introduction

To solve the time dependence of an ion-atom scattering problem within the independent particle model we expand the time dependent wavefunction in the DIRAC equation in a set of static molecular wavefunctions. The many particle Hamiltonian is approximated by a sum of single-particle Hamiltonians. The energy eigenvalues and matrixelements which show up in the resulting coupled channel equations [1] are taken from static *self consistent* DIRAC-FOCK-SLATER MO-LCAO calculations [2] for a large number of internuclear distances.

This procedure allows the study of inner shell charge transfer processes in heavy ion collisions. Recently we were able to present the first full ab initio results for a K–K charge transfer in S^{16+} on Ar [3]. As basis we used static molecular wavefunctions as discussed below. In this letter we discuss the first application of the method where we adapt the basis functions to the physical process in the collision via the change of the occupation numbers of the levels involved in the description. Instead of keeping the occupation numbers of the single particle levels at the asymptotic value for $t=-\infty$ we choose them according to the time dependent single particle amplitudes which we gain from the coupled channel calculations performed with fixed occupation numbers. A sensible change in the energy eigenvalues and matrixelements is observed and gives raise to a drastic increasing in the K – K charge transfer probability.

⋆ Dedicated to Prof. Dr. P. Armbruster on the occasion of his 60th birthday

II. Method

In the following we briefly present the formalism used. If the many-particle Hamiltonian $\hat{H}$ in the many-particle DIRAC equation is reduced within the independent particle model to a sum of single-particle hamiltonians $\hat{H}^{\mathrm{Eff}} = \sum \hat{h}^{\mathrm{Eff}}$ we get the set of coupled single-particle DIRAC equations

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

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

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

To solve (1) we expand the time dependent single-particle wavefunctions $\psi_i(t)$ in a set of M molecular wavefunctions $\{\varphi^{MO}\}$,

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

with $i=1,\ldots,N$. In our case the molecular basis states φ^{MO} are solutions from the static diatomic DIRAC-FOCK-SLATER (DFS) equation:

$$\hat{h}^{\mathrm{Eff}}(\mathbf{R})\,\varphi_m^{MO}(\mathbf{R})=\varepsilon_m(\mathbf{R})\,\varphi_m^{MO}(\mathbf{R}) \tag{4}$$

with $m=1,\ldots,M$. Inserting Ansatz 3 into (1) leads to the equivalent single-particle matrix coupled channel equations

$$i\hbar\frac{d}{dt}a_{il}=\sum_{m=1}^{M}a_{im}\left\langle\varphi_l^{MO}(R(t))\left|-i\hbar\frac{d}{dt}\right|\varphi_m^{MO}(R(t))\right\rangle \cdot e^{-\frac{i}{\hbar}\int^{t}(\varepsilon_m(\mathbf{R}(t'))-\varepsilon_l(\mathbf{R}(t')))\,dt'} \tag{5}$$

with $i=1, \ldots, N$.

On the other hand on could treat the collision problem by solving the many-particle time dependent DIRAC-FOCK-SLATER equation.

$$\hat{H}^{\mathrm{Eff}}\Psi_{el}(t)=i\hbar\frac{\partial}{\partial t}\Psi_{el}(t). \tag{6}$$

A solution of this equation is given by the SLATER-determinant

$$\Psi_{el}(t)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\psi_1(1) & \ldots & \psi_N(1)\\ \vdots & & \vdots\\ \psi_1(N) & \ldots & \psi_N(N)\end{vmatrix}. \tag{7}$$

where ψ_i are solutions of (1).

This relation between the single-particle and the many-particle description is discussed in [4, 5]. It allows us to treat many-particle collisions within the much more simple single-particle picture without loosing the many-particle aspect. Answers of experimental questions can be achieved by using inclusive probabilities discussed elsewhere [4, 5, 6, 7, 8].

III. Results and discussion

To study the influence of K−K charge transfer on the energy eigenvalues and matrixelements we took up the case of 90 keV Ne^{9+} on Ne where data from a coincidence measurement between charge state resolved projectile and target ions with respect to the projectile scattering angle θ are available in a range between $\theta=10$ mrad and $\theta=75$ mrad [9, 10]. The measurements show an impact parameter dependent oscillation in the probability of finding the target and the projectile in specific charge states. This oscillation was interpreted as an interference structure induced by the K-vacancy transfer between 1*s*-projectile and 1*s*-target states. Due to different autoionisation processes after the collision every measured combination of a projectile and target charge state is a superposition of states produced by different charge transfer processes during the collision. In the experiment [9] the case of finding the target in the charge state 7+ and the projectile in the charge state 5+ (target 7+/projectile 5+) after the collision has the most pronounced oscillatory structure. The origin of this structure very probably results from the K−K charge transfer process during the collision but it will be very much reduced from contributions of all other possible intermediate states after the collision. The fact that such a big structure remains in the experiment demonstrates that this channel is probably very dominant. In order to describe this structure we have performed a full scale ab initio calculation within this method with a static basis as described above. The final results is the dotted $P(b)$-curve in Fig. 2 which is much smaller than the experimental result. Of course in this calculation the basis was not adapted to the specific time dependent occupation of the single particle levels. In order to do this we have developed the following procedure:

In a first step we performed static DFS-calculations for a large number of internuclear distances keeping the occupation of the single particle levels according to the asymptotic occupation in the incoming channel for $t=-\infty$ i.e. $R=-\infty$. The 1(1/2) level which at $R=-\infty$ is the incoming 1*s* level of the projectile Ne^{9+} is occupied by one electron and the 2(1/2) level which corresponds to the Ne 1*s* level of the target atom is occupied by two electrons.

In a second step we performed coupled channel calculations for the 2 lowest levels (each doubly degenerate) with this set of energie eigenvalues and matrixelements as input values. These calculations produce a set of single particle amplitudes a_{ij} for all values of the internuclear distance ranging from $-\infty$ to $+\infty$.

In a third step we readjusted the occupation of the 2 lowest levels along the trajectory according to these single particle amplitudes a_{ij} taking $\sum_i |a_{ij}|^2$ as the new occupation numbers for the single particle levels j in the static DIRAC-FOCK-SLATER calculations. Tables 1, 2 show the occupation numbers choosen for the 2 lowest levels of the incoming and outgoing channel of the trajectory. The initial electronic configuration of 1 electron in the 1*s* shell of Ne^{9+} and 2 electrons in the 1*s* shell of the Ne target is mainly rearranged in the incoming channel at a internuclear distance between 0.90 and 0.40 a.u. In the outgoing channel this electronic configu-

Table 1. Electronic occupation of the single particle levels φ^{MO} in the static DFS-calculations performed for the incoming channel

	Incoming channel R/a.u.		
	$+\infty-0.90$	$0.90-0.40$	$0.40-0.00$
1(1/2) 1*s* Ne^{9+} ($R=-\infty$)	1.00	1.10−1.70	1.70
2(1/2) 1*s* Ne($R=-\infty$)	2.00	1.90−1.30	1.30

Table 2. Electronic occupation of the single particle levels φ^{MO} in the static DFS-calculations performed for the outgoing channel

	Outgoing channel R/a.u.		
	$0.00-0.40$	$0.40-0.90$	$0.90-+\infty$
1(1/2) 1*s* Ne^{9+} ($R=-\infty$)	1.70	1.70−1.61	1.61
2(1/2) 1*s* Ne($R=-\infty$)	1.30	1.30−1.39	1.39

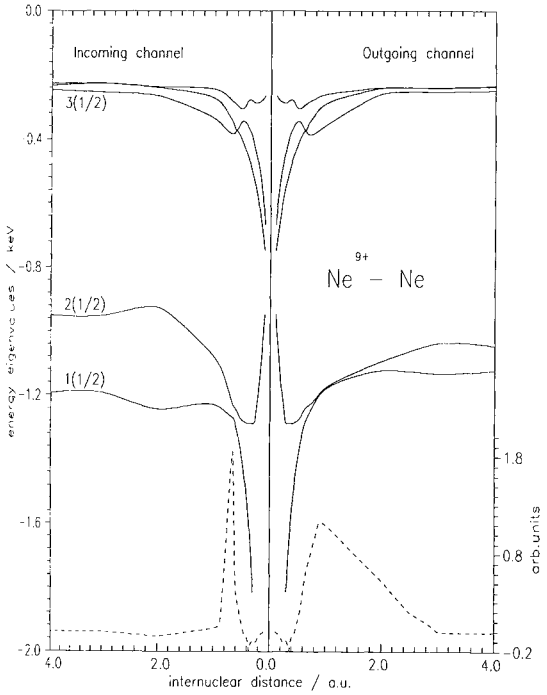

Fig. 1. *Full curves:* Correlation diagram for the system Ne^{9+} on Ne. The symmetry between incoming and outgoing channel is broken by K – K charge transfer. *Dotted curves:* Radial coupling matrixelement between 1(1/2) and 2(1/2) level

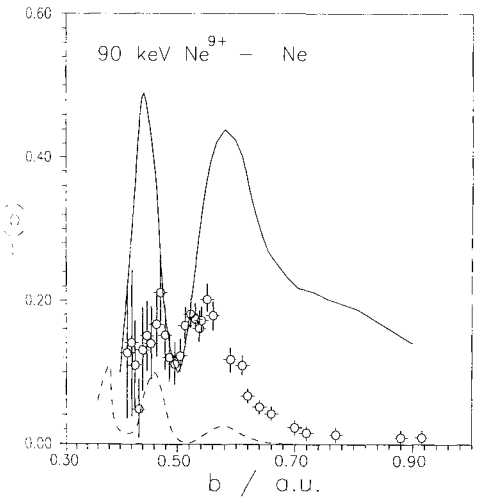

Fig. 2. Measured Data: target 7+/projectile 5+ [9]. *Full curve:* $P(b)$-curve for K – K charge transfer with dynamically adapted occupation numbers. *Dotted curve:* $P(b)$-curve for K – K charge transfer with static occupation numbers

ration is only slightly changed keeping its main shape from the rearrangement in the incoming channel. The resulting correlation diagram and the radial coupling matrixelement between 1(1/2) and 2(1/2) level are presented in Fig. 1. The incoming and outgoing channels are no longer symmetric. In the incoming channels the energy eigenvalues of 1(1/2) and 2(1/2) levels show a gap of nearly 200 eV at large internuclear distance R. This gap is reduced to 70–90 eV by K – K charge transfer in the outgoing channel.

In a fourth step we redid a coupled channel calculation with this corrected set of energy eigenvalues and matrixelements.

Finally we calculated the probability for this specific experiment within the framework of inclusive probabilities [8, 3].

The inclusive probability for a transfer of a hole initially in the projectile $1s$ level of Ne^{9+} to the $1s$ level of the Ne target at $t = +\infty$ is presented in Fig. 2. The shape of the curve is in good agreement with the experimental values. In this procedure the amplitude of the curve is now bigger than the measured values of the final combination (target 7+/projectile 5+) and much bigger than the calculation with the static basis (dotted line). This remaining discripancy between the full curve and the experiment may now easily be explained by the superposition of several intermediate states [9, 10] involved in the inclusive probability of this final combination. The main shape is quite well reproduced.

IV. Conclusion

Choosing the occupation of the single particle levels along the trajectory according to their single particle amplitudes is one way of giving a first order approximation to the fully time dependent DIRAC-FOCK-SLATER description of a collision system. With this method we are able to study complex many-particle collision systems and it allows us to give the main shape of complex impact parameter dependent probabilities of the final configuration and charge states of projectile and target.

This work is partially supported by the Deutsche Forschungsgemeinschaft (DFG) and the Gesellschaft für Schwerionenforschung, Darmstadt (GSI).

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