REALISTIC MANY ELECTRON COUPLED CHANNEL CALCULATIONS

IN HEAVY ION SCATTERING

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ABSTRACT

The time dependent Dirac equation which describes a heavy ion-atom collision system is solved via a set of coupled channnel equations with energy eigenvalues and matrix elements which are given by a selfconsistent field many electron calculation. After a brief discussion of the theoretical approximations and the connection of the many particle with the one particle interpretation we discuss first results for the systems F^{8+} - Ne and F^{6+} - Ne. The resulting P(b) curves for the creation of a Ne K-hole are in good agreement with the experimental results.

INTRODUCTION

The time dependence of a general quantum mechanical many electron system is correctly described by solving the time dependent Dirac equation. The best approximation which might be feasable for the description of a many electron ion-atom collision is the time dependent Hartree (Dirac) Fock equation but it is still not possible to solve it in practice. We instead try to solve the time dependent Dirac equation by approximating the Hamiltonian by a sum of one particle Hamiltonians and expanding the wavefunction in realistic molecular many electron Hartree-Fock wavefunctions as a basis and to solve a set of coupled channel equations instead. Up to now coupled channel calculations using the non-selfconsistent variable screening model[1] or AO+ calculations[2] are the best available.

In order to perform such many electron coupled channel calculations we have developed a static relativistic self-consistent field molecular Dirac-Fock-Slater code[3] which allows to calculate eigenvalues, wavefunctions and coupling matrix elements for diatomic quasi molecules as function of the internuclear distance. Using these values as input we are able to calculate the time dependence in a many body independent particle picture. We present here part of the theory and in addition results for the systems F^{3+} - Ne and F^{6+} - Ne.

THEORY

In the impact-parameter picture where the nuclear motion is treated classically and the electrons quantum mechanically the electronic wavefuction $|\Psi(t)\rangle$ of the collision system is given by the solution of the time dependent many electron Dirac equation

$$\hat{H}_e(\vec{R}(t))\ |\Psi(t)\rangle = i\hbar \frac{d}{dt}\ |\Psi(t)\rangle \tag{1}$$

subject to the appropriate initial condition

$$\lim_{t \to -\infty} [\ |\Psi(t)\rangle - |\Psi_{In}(t)\rangle\ ] = 0. \tag{2}$$

Collision exitation probability amplitudes are then given by the overlap of the scattering wave function $|\Psi(t \to +\infty)\rangle$ with the appropriate final states $|\Psi_{Fin}(t)\rangle$ defined by the experiment

$$f_{I \to F} = \lim_{t \to +\infty} \langle \Psi_{Fin}(t)|\Psi(t)\rangle. \tag{3}$$

The configuration space (N-electron) Dirac Hamiltonian

$$\hat{H}_e = \sum_{i=1}^{N} \hat{t}_i + \sum_{i=1}^{N} \hat{v}_i^{en} + \frac{1}{2} \sum_{i,j=1}^{N}{}' \hat{v}_{ij}^{ee} \tag{4}$$

is given by the kinetic energy operator

$$\hat{t}_i = c\,\hat{\vec{\alpha}}_i\ \hat{\vec{p}}_i + \hat{\beta}_i mc^2, \tag{5}$$

the implicit time dependent electron nuclear Coulomb potential

$$\hat{v}_i^{en}(\vec{R}(t)) = - Z_A/|\hat{\vec{r}}_i - \vec{R}_A(t)| - Z_B/|\hat{\vec{r}}_i - \vec{R}_B(t)| \tag{6}$$

and the electron-electron Coulomb potential

$$\hat{v}_{ij}^{ee} = 1/|\hat{\vec{r}}_i - \hat{\vec{r}}_j|. \tag{7}$$

Equ. (1) is solved by expanding the total scattering wavefunction in a complete set of time dependent many-electron (configuration space) wavefunctions[4]

$$|\Psi(t)\rangle = \sum_K |\phi_K(t)\rangle \cdot C_K(t). \tag{8}$$

Inserting this Ansatz into the Dirac equation (1) gives an equivalent matrix equation (coupled channel equations)

$$i\hbar\ \underline{\underline{S}}\ \frac{d}{dt}\ \underline{C} = \underline{\underline{M}}\ \underline{C} \tag{9}$$

for the column vector $\underline{C} = (C_K)$. The overlap matrix $\underline{\underline{S}} = (S_{LK})$ is defined by

$$S_{LK} = \langle \phi_L | \phi_K \rangle \tag{10}$$

and the coupling matrix $\underline{\underline{M}} = (M_{LK})$ by

$$M_{LK} = \langle \phi_L | \hat{H}_e - i\hbar \frac{d}{dt} | \phi_K \rangle . \tag{11}$$

The initial boundary condition for $\underline{C}(t)$ is given by the asymptotic relation

$$\lim_{t \to -\infty} [\langle \phi_L | \Psi_{in} \rangle - \sum_K S_{LK} C_K] = 0; \quad L = 1,2,3,\ldots \tag{12}$$

For practical reasons the basis should be as small as possible and well adapted to the problem. Static molecular wavefunctions of Hartree-Fock type probably fullfill these conditions quite well[5].

Having this in mind we define time dependent single particle collision states $|\Psi(t)\rangle$ as the solutions of the single particle time dependent Dirac equation

$$\hat{h}^{eff}(\vec{R}(t)) \, |\psi(t)\rangle = i\hbar \frac{d}{dt} \, |\psi(t)\rangle \tag{13}$$

where $\hat{h}^{eff}$ is defined as the Hartree-Fock Hamiltonian

$$\hat{h}^{eff}(\vec{R}) = \hat{t} + \hat{v}^{en}(\vec{R}) + \hat{v}^{eff}(\vec{R}) . \tag{14}$$

Equ. (13) will be solved by an analog method as described above for the many particle equation (1), the details of the solution will be discussed later. At the moment we asume that we have a set $|\psi_n(t)\rangle$ of solutions of equ. (14) to N mutual orthogonal initial conditions

$$\lim_{t \to -\infty} [|\psi_n(t)\rangle - |\psi_n^{in}(t)\rangle] = 0; \quad n=1,2,\ldots N. \tag{15}$$

Then the Slater determinant

$$| \Psi^{eff}(t)\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |\psi_1(t)\rangle^1 & \cdots & |\psi_1(t)\rangle^N \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ |\psi_N(t)\rangle^1 & \cdots & |\psi_N(t)\rangle^N \end{vmatrix} \tag{16}$$

is a solution of the many particle time dependent Dirac equation

$$\hat{H}^{eff}(\vec{R}(t)) \, | \Psi^{eff}(t)\rangle = i\hbar \frac{d}{dt} \, | \Psi^{eff}(t)\rangle \tag{17}$$

with the effective many particle Hamiltonian

$$\hat{H}^{eff}(\vec{R}) = \sum_{i=1}^{N} \hat{h}_i^{eff}(\vec{R}).$$ (18)

Equ. (17) differs from the original equ. (1) by the replacement of the exact Hamiltonian $\hat{H}_e$ with the effective Hamiltonian $\hat{H}^{eff}$ which defines the independent particle model within the Hartree-Fock scheme.

METHOD OF SOLUTION

First we expand the single particle scattering wavefunctions $|\psi_n(t)\rangle$ in a (complete) set of single particle basis states

$$|\psi_n(t)\rangle = \sum_k |\varphi_k^{eff}(\vec{R}(t))\rangle \cdot c_{kn}$$ (19)

For $|\varphi_k^{eff}(\vec{R})$ we use the single particle wavefunctions from static diatomic selfconsistent relativistic Dirac-Fock-Slater calculations as a basis. Inserting this into equ. (13) gives the equivalent single particle matrix (coupled channel) equations

$$i\hbar \; \underline{\underline{s}} \; \frac{d}{dt} \; \underline{c}_n = \underline{\underline{m}} \; \underline{c}_n; \quad n=1,2,\ldots,N$$ (20)

for the column vectors $\underline{c}_n = (c_{kn})$. Eigenvalues and radial as well as rotational coupling matrix elements are taken from the static calculations for a large number of internuclear distances. These are full scale Dirac-Fock-Slater calculations taking into account all electrons and a large number of unoccupied states[3]. The results are written on disk so that in the coupled channel calulations the physically relevant channels can be choosen acording to the physical question of interest. In addition the initial condition prescribing how many electrons are in which channels has to be chosen according to the experiment. For each state n in which an electron is present a separate coupled channel calculation has to be performed. As result one gets N sets of amplitudes c_{kn} where k marks the final states. These c_{kn} are then used for the interpretation in the many particle picture i.e. the C_K from equ. (8). Both sets of $\underline{c}$ and $\underline{C}$ are absolutely equivalent and contain the same physical information. These amplitudes now allow us to answer different questions. For example one may ask how large is the chance of finding one hole in a certain atomic level, or two, or at least one hole in the Ne 1s shell. The experiment[6] is performed with the last question how large is the chance of finding at least one hole in the Ne 1s shell in the outgoing scattering system.

RESULTS

We are interested in understanding the systems F^{3+} - Ne and F^{6+} - Ne as first examples because a large number of experimental results are available for these systems[6]. They are already complicated many electron systems although with small Z which means that a non-relativistic calculation should be sufficient. But this relativistic version which we use here directly allows us to proceed to heavier systems where the relativistic effects become stronger or even dominant.

In Fig. 1 we present the correlation diagram of the system F^{3+} - Ne where the lowest level can be attributed to the F 1s state and the second to Ne 1s. This interchange is due to the high ionization of the Fluorine. Because we are interested in the creation of holes in the Ne 1s shell we choose only those levels which are directly connected with this level or which are very near it. Thus the minimum number of levels which have to be taken into account as channels in the coupled channel calculations are the 1(1/2), 3(1/2), 4(1/2) and 1(3/2) levels. With this selection the number of one-particle channels in equ. (19) is 8 because each level can carry two electrons with an angular momentum projection on the internuclear axis of + or -. As initial condition we know that there is only one electron in the two 1(1/2) states and that both 3(1/2) states are occupied. Although we also know the initial occupation of the higher levels in Fluorine and Neon at infinity we do not know the exact occupation of the 4(1/2) and 1(3/2) levels because electrons are transfered from higher states into these levels in the incoming part of the collision via dynamical couplings which are not included in our 8 level calculations. To take these couplings into account in a pragmatic way we assumed that the 4(1/2) and 1(3/2) states are initially occupied with a number of electrons which we use in these calculations as a parameter which allows us to improve the agreement with the experimental results. The results of the coupled channel calculations are given in Fig. 2 for the three impact energies 0.13 MeV/u, 0.23 MeV/u and 0.5 MeV/u. In this figure the experimental values as well as theoretical values from an AO+ calculation of Fritsch and Lin[2] are presented as well. In our calculation the electrons (or holes) which come into the Ne 1s shell via the 'normal 2pπ-2pσ coupling' are also included because we have included in the calculation electrons in the upper levels. In the case of the three energies discussed here no electron, two electrons and three electrons respectively were taken into account for the three energies presented in Fig. 2.
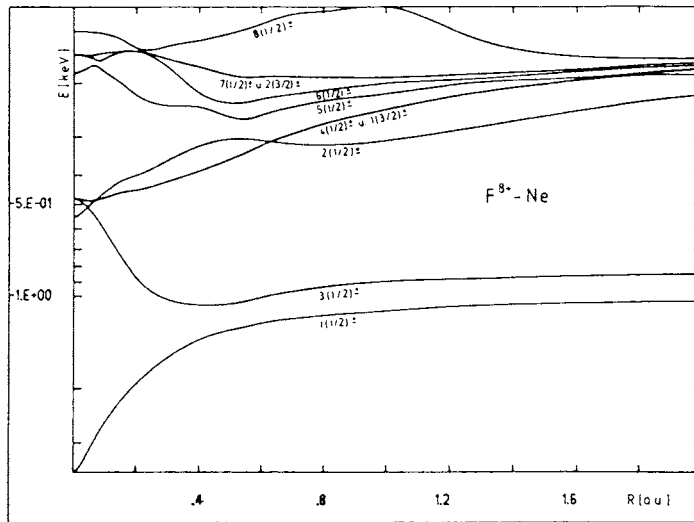
FIG. 1: Correlation diagram for the system F^{8+} - Ne. Due to diabatization the second level is called 3(1/2) because it correlates with the third level at R = 0.

DISCUSSION

The agreement between the experimental P(b) curves and our result is good whereas the AO+ calculations of Fritsch and Lin give a good qualitative picture but no detailed agreement. For all three calculations the number of electrons in the 4 upper channels is used as a parameter in order to get optimal agreement with the experiment. The number of electrons which we find are 3, 2 and 0 respectively for the three energies in increasing order. This result seems to be very plausible from a physical point of view because for the higher energies the electrons in the higher levels will probably be more and more ionized during the incomming part of the collission.

For the case F^{6+} - Ne the lowest two levels in the correlation diagram are in normal order again due to the stronger shielding of the Fluorine nucleus. But both levels are filled with two electrons each in the experiment. Thus we perform the calculations for 0.23 MeV/u with the two electrons which we have learned are needed from the calculations discussed above, plus one electron which comes from the F 2s shell. The result of this calculation is the dashed line in the lower left of Fig. 2b. Again we find a
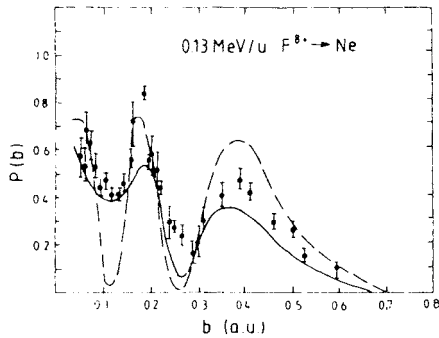
Fig. 2a:
P(b) curves for the Ne
K electron excitation for
0.13 MeV/u   F3+ - Ne
collision.
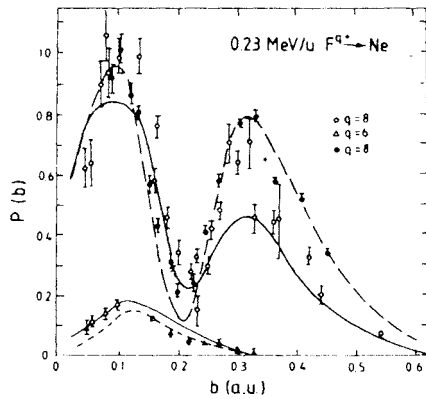Experimental values: Ref. 6
Dashed line: Ref. 2
Full line: This work.

Fig. 2b:
P(b) curves for the Ne
K electron excitation for
0.23 MeV/u   F8+ - Ne and
F5+ - Ne collisions.
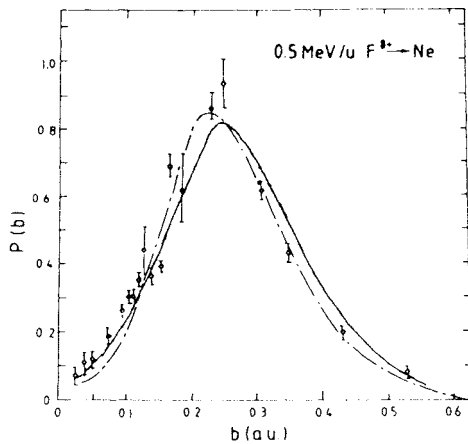Experimental values: Ref. 6
Dashed line: Ref. 2
Full line: This work.

Fig 2c
P(b) curves for the Ne
K electron excitation for
0.50 MeV/u   F3+ - Ne
collisions.
Experimental values: Ref. 6
Dashed line: Ref. 2
Full line: This work.

good agreement with the experimental results. In order to understand also the filling of the 4(1/2) and 1(3/2) levels from the incoming Ne or/and F levels we have to increase in future calculations the number of states in the coupled channel calculations.

As final statement we can say that a calculation with 8 levels (which are only 3 non-relativistic levels) for such a complicated many electron system is sufficient in order to get a good agreement. This is possible because we use a very sophisticated procedure to generate the channels where most of the many particle interaction already is included. The advantage of this effort is that the physical interpretation in terms of molecular states is easily possible. In this way the physics is much clearer to understand than in any other method.

ACKNOWLEDGEMENT

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