

MANY ELECTRON COUPLED CHANNEL CALCULATIONS FOR THE SYSTEM $F^{8+} - Ne$

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Abstract - To describe the time dependence of an atomic collision system the Dirac equation usually is rewritten in a coupled channel equation. We first discuss part of the approximation used in this approach and the connection of the many particle with the one particle interpretation. The coupled channel equations are solved for the system $F^{8+} - Ne$ using static selfconsistent many electron Dirac-Fock-Slater wavefunctions as basis. The resulting $P(b)$ curves for the creation of a Ne K-hole are in reasonable agreement with the experimental results.

Introduction

In general the calculation of realistic complicated many electron low energetic ion-atom collisions is still not possible. Coupled channel calculations using the non-selfconsistent variable screening model /1/ or $A0+$ calculations /2/ are the best available up to now. The results reproduce partially the gross structure but not the details.

In recent years 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 internuclear distance. Using these values as input in coupled channel calculations we are able to calculate the time dependence in a many body independent particle picture. We first present here part of the theory and in addition results for the system $F^{8+} - Ne$.

Theory

In the impact-parameter picture the electronic wavefunction $|\Psi(t)\rangle$ of the collision system is given by the solution of the time dependent many electron Dirac equation

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

subject to the appropriate initial condition

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

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

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

The configuration space (N-electron) Dirac Hamiltonian

$$\hat{H}_e = \sum_{i=1}^N \hat{t}_i + \sum_{i=1}^N \hat{v}_i^{en} + 1/2 \sum_{i,j=1}^N \hat{v}_{ij}^{ee} \quad (4)$$

is given by the kinetic energy operator

$$\hat{t}_i = c \hat{\alpha}_i \cdot \hat{p}_i + \hat{\beta}_i mc^2, \quad (5)$$

the implicit time dependent electron nuclear Coulomb potential

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

and the electron-electron Coulomb potential

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

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

$$|\Psi(t)\rangle = \sum_K |\Phi_K(t)\rangle c_K(t). \quad (8)$$

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

$$i\hbar \underline{S} \frac{d}{dt} \underline{C} = \underline{M} \underline{C} \quad (9)$$

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

$$(S_{KL}) = \langle \Phi_K | \Phi_L \rangle \quad (10)$$

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

$$(M_{KL}) = \langle \Phi_K | \hat{H}_e - i\hbar \frac{d}{dt} | \Phi_L \rangle. \quad (11)$$

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

$$\lim_{t \rightarrow -\infty} [\langle \Phi_K | \Psi_{in} \rangle - \sum_L S_{KL} C_L] = 0; \quad K = 1, 2, 3, \dots \quad (12)$$

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 fulfill these conditions quite well /5/.

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

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

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

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

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 assume that we have a set $|\Psi_i(t)\rangle$ of solutions of equ. (14) to N mutual orthogonal initial condition

$$\lim_{t \rightarrow -\infty} [|\Psi_i(t)\rangle - |\Psi_i^{\text{in}}(t)\rangle] = 0; \quad i=1,2,\dots,N \quad (15)$$

Then the Slater determinant

$$|\Psi(t)\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |\Psi_1(t)\rangle^1 & \dots & |\Psi_1(t)\rangle^N \\ \vdots & & \vdots \\ |\Psi_N(t)\rangle^1 & \dots & |\Psi_N(t)\rangle^N \end{vmatrix} \quad (16)$$

is a solution of the many particle time dependent Dirac equation

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

with the effective many particle Hamiltonian

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

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

Computational method

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

$$|\Psi_i(t)\rangle = \sum_k |\varphi_k(t)\rangle c_{ki}. \quad (19)$$

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

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

for the column vectors $\underline{c}_i = (c_{ki})$. Eigenvalues and radial as well rotational coupling matrix elements are taken from the static calculations for a large number of internuclear distances. These are usually 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 calculations the physical relevant channels can be chosen according to the physical question

of interest. In addition the initial condition how many electrons are in which channels has to be chosen according to the experiment. For each state i where an electron is present a separate coupled channel calculation has to be performed. As result one gets i sets of amplitudes c_{ki} where k marks the final state. These c_{ki} 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 absolute equivalent and contain the same physical information.

Results and discussion

We are interested to understand the system $F^{8+} - Ne$ as a first example because a large number of experimental results are available for this system /6/. It is already a complicated many electron system although with small Z which means that a non-relativistic calculation should be sufficient. In fig. 1 we present the correlation diagram of this system 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 Fluor. Because we are interested in the creation of holes in the $Ne 1s$

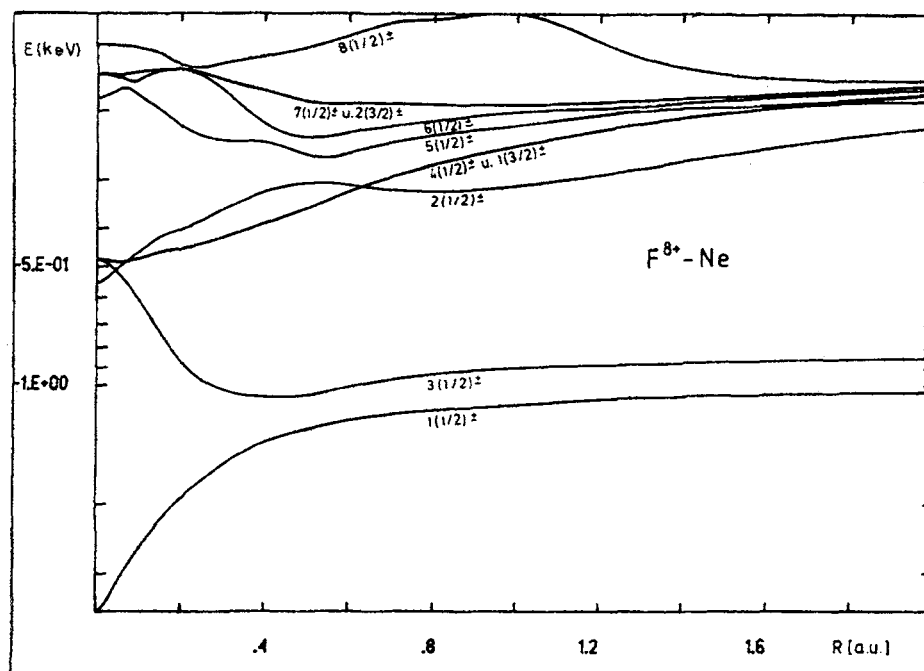


Fig. 1: Correlation diagram for the system $F^{8+} - Ne$. Due to diabaticization the second level is called $3(1/2)$ because it correlates with the third level at $R = 0$.

shell we choose only those levels which are directly connected with this level or which are very near. Thus the minimum number of levels which have to be taken into account 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. For the incoming state we know that there is only one electron in the two $1(1/2)$ states and that both $3(1/2)$ states are occupied. The $4(1/2)$ and $1(3/2)$ levels correlate to the $2p$ shell of F. But we do not know the exact occupation of these states in the incoming part of the collision because we do not include higher initially occupied states which couple to these four states at large internuclear distances. To take these couplings into account we assumed that the $4(1/2)$ and $1(3/2)$ states are initially occupied with about 2 electrons. This number can be used in these calculations as a parameter which allows to improve the agreement with the experimental results.

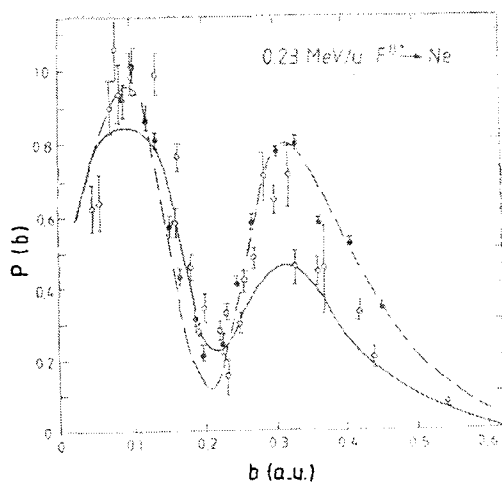


Fig. 2: $P(b)$ curves for the Ne K electron excitation for $0.23 \text{ MeV/u } F^{8+} - \text{Ne}$ collision. Experimental values: Ref. 6. Dashed line: Ref. 2. Full line: This work.

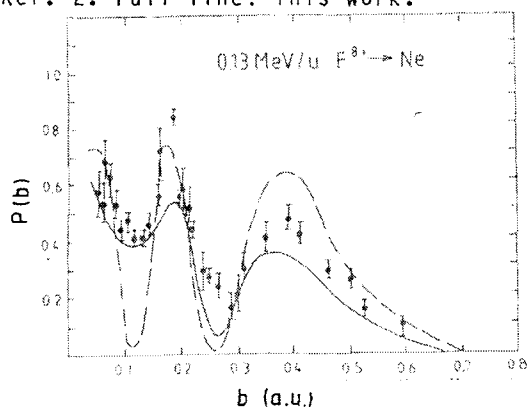


Fig. 3: $P(b)$ curves for the Ne K electron excitation for $0.13 \text{ MeV/u } F^{8+} - \text{Ne}$ collision. Experimental values: Ref. 6. Dashed line: Ref. 2. Full line: This work.

The results of the coupled channel calculations are given in fig. 2 and fig. 3 for the two impact energies 0.23 MeV/u and 0.13 MeV/u respectively. In these figures the experimental values as well as theoretical values from an A0+ calculation of Fritsch and Lin are presented as well. In our calculation the electrons (or holes) which come into the Ne 1s shell via the "normal 2p -2p coupling" are also included because we have also included calculations with holes in the upper levels. In the case of the higher energy only one electron and for the lower energy two electrons were taken into account.

The interpretation of the resulting amplitudes is performed for the question how large is the chance to find at least one hole in the Ne 1s shell. The agreement between the experimental P(b) curves and our result is relatively good whereas the A0+ calculations of Fritsch and Lin give a good qualitative picture but no detailed agreement.

Of course we have to increase the number of states in the coupled channel calculations in order to also calculate the filling of the $4(1/2)$ and $1(3/2)$ levels from the incoming Ne levels.

Acknowledgement

This work has been supported by Gesellschaft für Schwerionenforschung (GSI) Darmstadt and Deutsche Forschungsgemeinschaft.

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