

Scientific report of Dr. Duran's Stay as a Short Term Scientific Mission within the COST Scientific programme on Electron Controlled Chemical Lithography (ECCL)

1 Introduction.

The stay of Dr. Durán working with Prof. Gianturco has been from 12/01/09 to 13/03/09. The motivation of this stay was the interest in the scattering of electrons from molecular gases in the presence of electromagnetic fields.

Prof. Gianturco has a long-standing experience in this topic in the free case, i. e. without external fields. It was planned that under the supervision of Prof. Gianturco Dr. Durán could work on this problem.

Taking into account that the closed problem of the atom-molecule scattering is well known by Prof. Gianturco and Dr. Durán, it was thought to first add the electromagnetic fields to this kind of systems as they are more general. The experience gained here will then be applied later to the electronic problem.

In order to do so we took as starting point the code ASPIN [1]. It has been recently developed by Dr. Durán, Dr. Bodo, and Prof. Gianturco, and published in Computer Physics Communications, which means that will be free to be used by any interested scientist. ASPIN carries out the calculation of state-to-state integral cross sections and their sums over final states for atom-molecule (linear) scattering processes. The atom is taken to be structureless while the molecule can be in its singlet, doublet, or triplet spin states and can be treated as either a rigid rotor or a rovibrational target. Our main objective is the building of a new code which includes the presence of external electromagnetic fields. From now on, we will call it "FIELDSPIN".

The main difference between problems without external fields (ASPIN) and those with external fields (FIELDSPIN) is that in the latter case the total angular momentum J is not conserved. In both cases the problem is reduced to solving the *coupled channel* (CC) equations and obtain the radial coefficients of the wavefunction, and then, the scattering observables. In the field-free case J is conserved and we can solve the CC equations for a given value of it. On the contrary, in the non-free problem, J is not conserved anymore but its component along one axis of the space fixed reference system M is conserved. Thus we

can solve the CC equations for a given value of M instead of a given value of J. Therefore, the general scheme of work is the same in both cases.

However, it is clear that the physical problem is different and it is reflected in the way in which we are constructing FIELDSPIN. The main difference with respect to the field free case is the diagonalization of the isolated diatomic part and the subsequent transformation of the interatomic potential of the system.

2 Theory.

The Hamiltonian for an structureless atom A colliding with a diatomic molecule BC in presence of a magnetic \vec{B} and electric \vec{E} field can be written in the form

$$H = -\frac{\hbar^2}{2\mu} \nabla_R^2 + H_{BC}(\vec{r}) + V(r, R, \theta), \quad (1)$$

with $H_{BC}(\vec{r})$ the Hamiltonian corresponding to the diatomic molecule:

$$H_{BC}(\vec{r}) = -\frac{\hbar^2}{2\mu_{BC}} \nabla_r^2 + V_{BC}(r) + \gamma \vec{N} \vec{S} + 2\mu_0 \vec{B} \vec{S} - \vec{E} \vec{d} \quad (2)$$

and $V(r, R, \theta)$ the intermolecular BC-A potential.

The total scattering wavefunction for the full system is

$$\Psi_{vNsL}^{JM}(\vec{r}, \vec{R}, \hat{r}_s) = \sum_{v'} \sum_{N'} \sum_{s'} \sum_{L'} \chi_{v'N'}(r) \frac{G_{v'N's'L'}^{JvNsL}(R)}{R} \Upsilon_{N's'L'}^{JM}(\hat{r}, \hat{R}, \hat{r}_s), \quad (3)$$

being $G_{v'N's'L'}^{JvNsL}(R)$ the as yet unknown radial coefficients and $\Upsilon_{N's'L'}^{JM}(\hat{r}, \hat{R}, \hat{r}_s)$ the angular part of the wavefunction obtained employing an *uncoupled representation*.

The Schrödinger equation for the whole system can then be written as follows:

$$\left\{ -\frac{\hbar^2}{2\mu} \frac{1}{R^2} \frac{\partial}{\partial R} d^2 \frac{\partial}{\partial R} - \frac{\vec{L}^2}{2\mu R^2} + H_{BC}(\vec{r}) + V(r, R, \theta) - E \right\} \quad (4)$$

$$\left\{ \sum_{v'} \sum_{N'} \sum_{s'} \sum_{L'} \chi_{v'N'}(r) \frac{G_{v'N's'L'}^{JvNsL}(R)}{R} \Upsilon_{N's'L'}^{JM}(\hat{r}, \hat{R}, \hat{r}_s) \right\} = 0. \quad (5)$$

After a little of algebra we obtain the new set of CC equations, in which $G_{v'N's'L'}^{JvNsL}(R)$ are the functions we are trying to obtain and V^{trans} is the transformed intermolecular potential:

$$\left\{ \frac{d^2}{dR^2} - \frac{L'(L'+1)}{R^2} + k_{v'N'}^2 \right\} G_{v'N's'L'}^{JvNsL}(R) = \quad (6)$$

$$\frac{2\mu}{\hbar^2} \sum_{v''} \sum_{N''} \sum_{s''} \sum_{L''} \langle v' N' s' L' J | V^{trans} | v'' N'' s'' L'' J \rangle G_{v''N''s''L''}^{JvNsL}(R). \quad (7)$$

Eq. (7) is usually written in a matrix form:

$$\left\{ 1 \frac{d^2}{dR^2} - \frac{L^2(R)}{R^2} + K^2 - V^{trans}(R) \right\} G(R) = O. \quad (8)$$

$L^2(R)$ is the matrix representation of the square of the orbital angular momentum L , K^2 is the diagonal matrix of the asymptotic squared wavenumbers, $V^{trans}(R)$ is the potential coupling matrix, and $G(R)$ is the vector matrix.

The solution vectors form a matrix solution Ψ and then the LogDerivative matrix is defined:

$$Y \equiv \frac{\Psi'}{\Psi}. \quad (9)$$

Y satisfies the Riccati matrix equation

$$\frac{dY}{dR} + W + Y^2 = O, \quad (10)$$

with

$$W = K^2 - V^{trans}(R) - \frac{L^2(R)}{R^2}. \quad (11)$$

Eq. (10) is solved for Y , beginning with the condition $Y^{-1} = O$ instead of solving eq. (8) for the solution matrix Ψ .

3 Results and Conclusions.

As an example of the work developed during the stay, we show two plots in which the results from FIELDSPIN are compared with Ref. [2]. We can see that FIELDSPIN has reached a promising level, and although does not reproduce accurately as yet the results of Ref. [2] this is a preliminary version of the code and we expect that the definitive one will be able to be used shortly.

The work developed during this period did not yet produce any publication, but we expect to get results in the next months. Systems like He-NH [3] or Rb-OH [4] have already been studied. We plan to apply FIELDSPIN in systems still unknown, for instance, Rb-NH or Cs-NH, for which we already know the interaction.

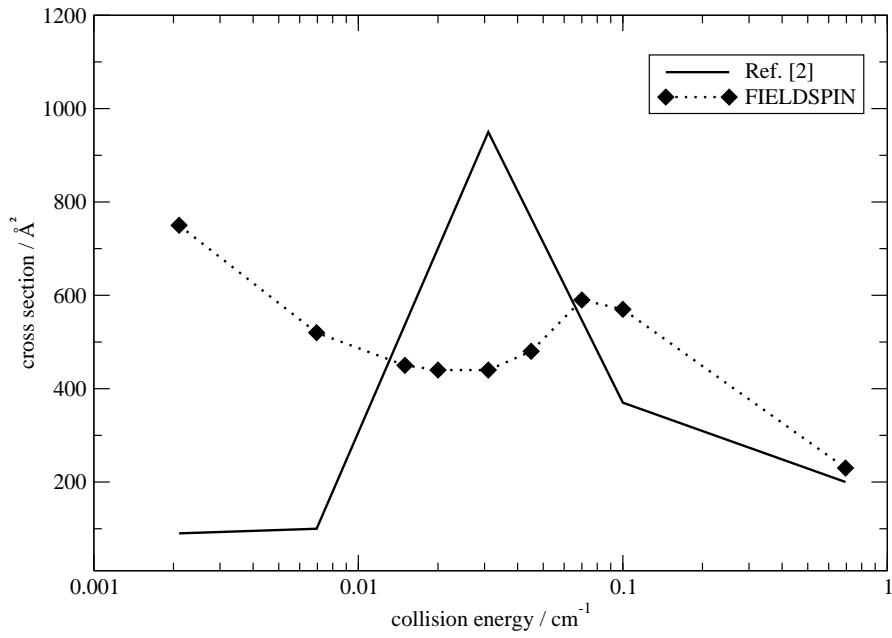
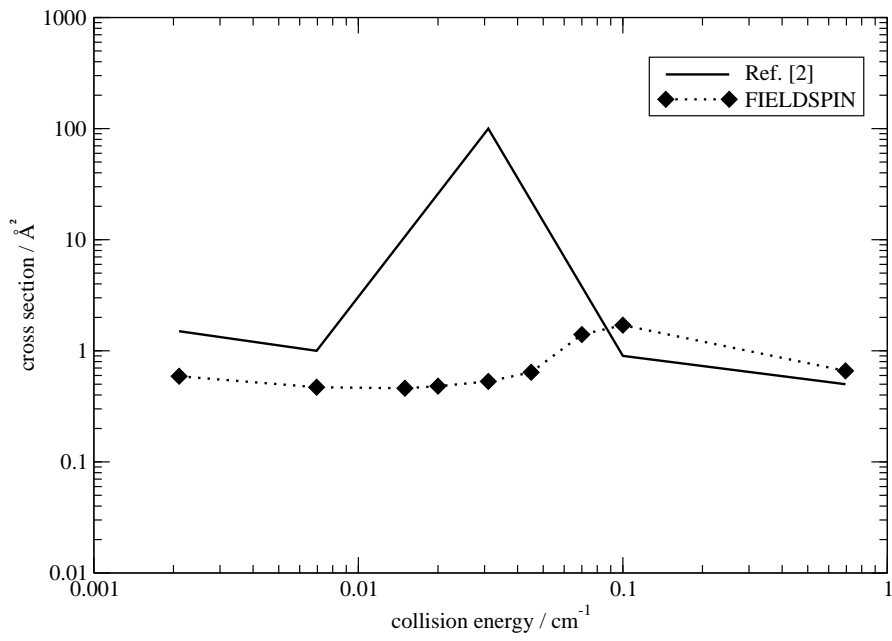


Figure 1: Current state of FIELDSPIN with respect to known results.

References:

- [1] D. López-Durán, E. Bodo, and F. A. Gianturco, *Comp. Phys. Comm.* **179**, 821 (2008).
- [2] T. V. Tscherbul and R. V. Krems, *J. Chem. Phys.* **125**, 194311 (2006).
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- [4] Manuel Lara, John L. Bonn, Daniel Potter, Pavel Soldan and Jeremy M. Hutson, *Phys. Rev. Lett.* **97**, 183201 (2006).