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EVALUATION OF THE USE OF FINITE ELEMENTS METHODS IN TIME DEPENDENT ATOMIC PHYSICS

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Abstract.

In this article we evaluate the use of finite elements methods in solving the time dependent Schrödinger equation (TDSE) for ion-atom collisions. While finite difference methods have been used for that for a while, finite elements have not been much used in atomic physics. There are mathematical reasons for that choice, but the impressive development that finite elements based codes and packages have had in recent years as well as the improvement in hardware mean that the implementation of finite elements code for realistic atomic systems are now straightforward. Adaptive mesh methods usually implemented in finite elements packages are particularly suitable for the study of atomic collisions. The accurate evaluation of collision process cross sections is probably still better achieved by the use of traditional methods, but the possibility of time evolution visualization of the collision process enhances the comprehension of the physics behind the quantum dynamics of electrons during atomic collisions.

1 INTRODUCTION

The study of electron capture, excitation and emission spectra in ion atom collisions has been a field of intense activity for years (Stolterfoht *et al* 1997). For intermediate to high energy single ionization there has been considerable theoretical efforts focused in the so-called two centre electron emission (TCEE) (Fainstein *et al* 1991, Pedersen *et al* 1990), Better description of the active electron moving in the presence of both residual target and projectile fields after the collision (final state) has been key for the improvement in the description of experimental data (Gulyás *et al* 1995). Except for classical models, like Classical Trajectory Monte Carlo, the description of Ion atom ionization, excitation and capture for intermediate and high impact energy, basically relies in approximate first order time independent perturbative methods, like Distorted Wave models, which are two state approximations. Moreover, heavy particle motion (projectile and target ions) are usually treated either in a first order quantum approximation or classically in a crude rectilinear trajectory impact parameter approximation. Within these approximations, it has been shown that, at least for high impact energy and multiply charged projectiles, Continuum Distorted Wave (CDW) theory of Belkić (1978) used together with an appropriate description of the initial bound and final continuum electron states, yields best results for ionization doubly differential cross sections (DDCSs) (Gulyás and Fainstein 1998, Ciappina *et al* 2003). However, when the projectile impact velocity decreases, the Continuum Distorted Wave – Eikonal initial state (CDW–EIS) theory of Crothers & McCann (1983) gives better results, its only difference being the choice of the initial state.

The field has experienced a renewed interest as a result of the development of the experimental technique known as COLTRIMS (cold-target recoil-ion momentum spectroscopy) (Moshammer *et al* 1994). With COLTRIMS, the projectile's tiny scattering angle can be obtained indirectly by measuring the ionized electron and recoil ion momenta. That means that kinematically complete measurement of the collision process is now possible. Fully differential cross sections (FDCS) for ion impact ionization can be measured now and this constitute a challenging ground for existing theories (Foster *et al* 2004). Good agreement between experiment and theory has been observed in the scattering plane for intermediate momentum transfer, but usual theories are not able to reproduce measurements for large values of momentum transfer and out of scattering plane. While most measurements are performed in multielectronic targets, most theories employed some form of one active electron approximation with hydrogenic wavefunctions for the initial and final electron states. Indeed, the simplest description for the He bound initial state is to assume it has one 'active' and one 'passive' electron and that the 'active' electron can be described as moving in the effective Coulomb field of the atomic core with an effective charge chosen either: (a) to reproduce the ionization energy or (b) so that the continuum wave is orthogonal to the initial state.

A more sophisticated description involves the use of full numerical Hartree–Fock wave functions for both initial and final states of the active electron (Gulyás *et al* 1995, Gulyás and Fainstein 1998, Foster *et al* 2004). Hartree–Fock description is based in one electron descriptions and does include radial correlations in the initial state.

Most finite element packages are suited for the solution of a partial derivatives equation like a one particle three dimensional (3D) time dependent Schrödinger equation (TDSE). One of the strengths of finite element methods lay in the handling of complex geometry boundary conditions, and while this might not the case in a simple ion atom collision process, it can be easily turned into one if, e.g., atomic processes in solids is considered where the ionized atom may be embedded in a complex environment. Another compelling feature of finite elements is

the advanced mesh algorithms that most packages possess, which is very well suited to the time dependent nature of the atomic collision process.

The aim of this paper is to present preliminary 3D finite element solutions for the 3D TDSE for ion atom collisions. Atomic units are used throughout unless otherwise stated.

2 THEORIES

Let us consider the single ionization of an active electron initially bound to a target ion representing the rest of the atom (*T*) with mass M_T and charge Z_T by the impact of an ion (*P*) of mass M_P and charge Z_P, expressed as the following reaction:

$$P^{Z_P} + T^{Z_T} \longrightarrow P^{Z_P} + T^{Z_T+} + e \tag{1}$$

This system description can be given in any Jacobi coordinates pair, defined as $(\mathbf{r}_T, \mathbf{R}_T)$, $(\mathbf{r}_P, \mathbf{R}_P)$, $(\mathbf{r}, \mathbf{R})$, as can be seen in figure 1. We assume that (i) the initial state for the 'active' electron is described by a hydrogenic wave function (this scheme could be trivially enhanced by the use of an analytical Rothan–Hartree–Fock scheme (Clemente and Roetti 1974)) and (ii) in the final state the 'active' target electron moves in the combined Coulomb field of the target core with an effective charge.

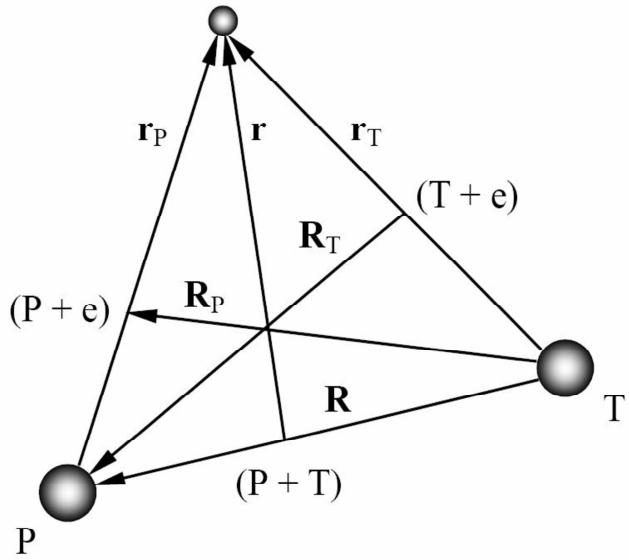

Figure 1: Figure 1: Jacobi coordinates describing the three particle system

The hamiltonian describing the dynamics for the active electron wave function is:

$$H = [H_0 + V_T(r_T)] + [V_P(r_P) + V_{PT}(R)] \tag{2}$$

where H_0 corresponds to the free particle hamiltonian and the interaction potentials are given by:

$$V_T(r_T) = -\frac{Z_T}{r_T} \quad V_P(r_P) = -\frac{Z_P}{r_P} \quad V_{PT}(R) = \frac{Z_P Z_T}{R} \tag{3}$$

The time dependent Schrödinger equation (TDSE) that describes the electron wave function dynamics reads

$$i\hbar\frac{\partial\Psi}{\partial t} = H\,|\Psi\rangle \tag{4}$$

subjected to the initial condition

$$\Psi(t=0) = \Phi_i \tag{5}$$

where Φ_i is the unperturbed electron initial bound state. We will be interested in the wave function itself as well as on the probability density, defined as

$$\delta(\vec{r},t) = (\Psi(\vec{r},t))^2 \tag{6}$$

We solve the TDSE using Flex-PDE finite element solver. FlexPDE is a fully integrated PDE solver, combining several modules. FlexPDE uses a Galerkin finite element method, with quadratic and cubic basis functions. Petrov-Galerkin weighting is used in advection terms.

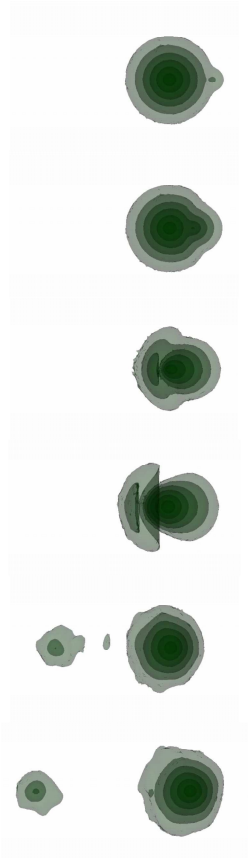

Figure 2: Figure 2: electron probability density evolution at $t = -1$, -0.5,1,2,3 and $4au$, for 100keV proton hidrogen collisionn. Electron capture by the projectile ion, as well as target excitation are clearly seen.

The mesh generation module constructs a triangular or tetrahedral finite element mesh over a two or three-dimensional problem domain. In three-dimensional problems, an arbitrary two-dimensional domain is extruded into a the third dimension and cut by arbitrary dividing surfaces. The resulting three-dimensional figure is filled with an unstructured tetrahedral mesh. An adaptive mesh refinement procedure measures the adequacy of the mesh and refines the

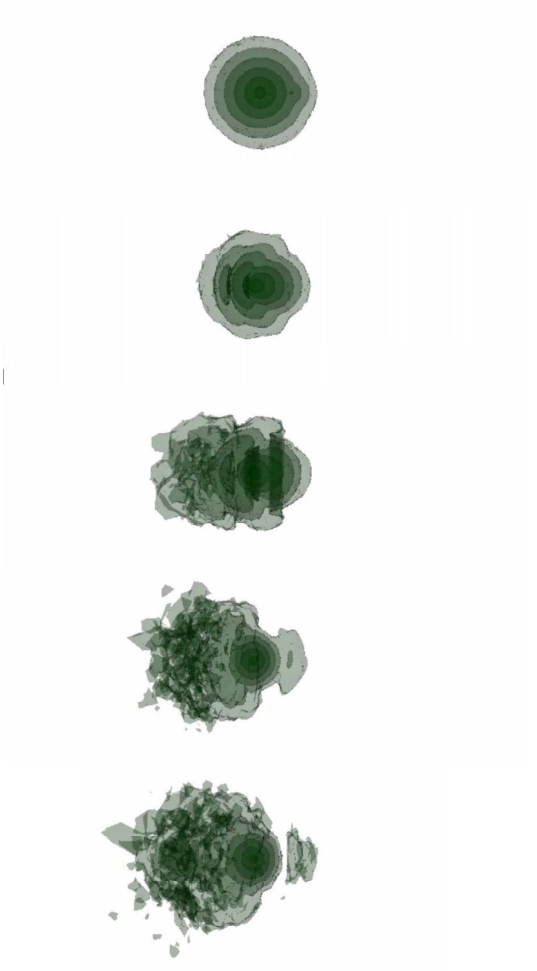

Figure 3: Figura 3: Idem Figure 2 for $t = -0.5$,1,2,3 and $4au$, showing the electron ionization. Note the backward low energy emission probability.

mesh wherever the error is large. The system iterates the mesh refinement and solution until a user-defined error tolerance is achieved. Integrals in FlexPDE are formed by Gaussian quadrature rules of varying number of points, depending on the particular geometry and basis. In the present work we analyze the feasibility of using FEM in order to visualize general collision dynamics in a qualitative way. This task can be carried out in a personal computer, which is a requirement if it is to be used as a qualitative tool in order to understand the physics beneath the different approximations employed.

More rigorous calculations for specific processes are currently being carried out, but these require powerful computational resources, in order to extract useful cross sections.

3 RESULTS

As an application example, we have simulated the collision of a 100 keV ($v = 2$ a.u.) proton against an hydrogen atom. The ”box” in which the simulation takes place, and wich defines the size of the mesh is a sphere of 30a.u. diameter. The mesh is adaptive so the number of elements and its concentration depends on the evolution of the electron wave function. Simulation time is restricted by the size of the box, and the collision parameters. Total electron probability (which

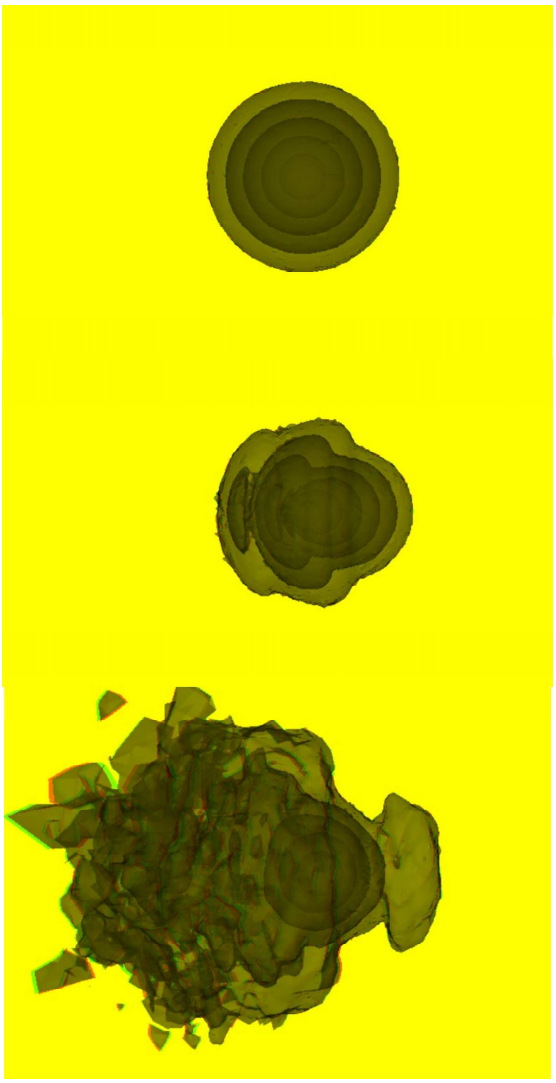

Figure 4: Figura 4: Idem Figure 3, shown in 3D graphics for $t = 0$,1, and $3au$.

is bound to be unity, since the probability of finding the electron inthe wholespace should be equal to 1) is controled and found to be stable throughout the simulation. In figures 2 and 3 we show snapshots for the evolution of the probability density $\delta(\vec{r}, t)$ as a function of time for small impact parameter. As we solve the full TDSE, all processes are taken into account. In figure 2, we see that electron distortion in the entrance channel is not important until the ion is very close to the atom. On the way out we see how the projectile takes part of the probability with it, meaning that the process of electron capture (and capture to the continuum) by the projectile is the dominant process at this impact energy, while there is appreciable probability for the target atom to became excited. However if we look at smaller probabilities, showed in figure 3, we see for the same collision that also ionization does take place. In particular the low energy backscattered portion of the electron wave function is clearly seen. Forward emission characteristics are not as clearly seen in this type of figure. We can consider our simulation as a 'true' 3D, so a 3D visualization can be helpful.

We include such a picture in Figure 4, which is to be watched with the aid of 3D glasses. In this way, the ionization dynamics can be better seen. Simulations would take an average of 10 hours in a single 2GHz Athlon processor. In order to calculate different cross sections (e.g.,capture, excitation, ionization), detailed simulations have to be calculated for several (more than 10) different impact parameters. Preliminary results indicate that capture and excitation

cross sections are relatively easy to calculate, while ionization cross sections are more difficult to extract, since they involve the projection of the final state into a continuum momentum or energy base.

The main limitation of the present scheme is at the moment the physical memory, which restricts the size of the box in which the collision takes place.

4 CONCLUSIONS

We have solved the time dependent Schrödinger equation (TDSE) in three spatial dimensions applied to ion-atom collision processes by using a standard finite element solver. Qualitative first results are encouraging, since they reveal well known features of intermediate energy ion atom collisions, for capture, ionization and excitation processes. The required simulation parameters for qualitative calculations are easily achieved by present multiple core personal computers. Quantitative calculations for excitation, capture, and ionization cross sections will now being carried out in order to compare this method with traditional perturbative solutions, and experimental data.

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