PHYSICS OF HIGHLY IONIZED IONS
PRODUCED IN HEAVY ION COLLISIONS

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PROGRAM AND ABSTRACTS

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jointly administered by

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Progress in Numerical Calculations of Ion-Atom Collisions

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Introduction

An ion-atom collision produces a time dependent perturbation of a many fermion system. In this collision excitation, ionisation and charge transfer can occur. The driving mechanism for these processes may be thought of as the potentials seen by individual electrons at any given separation of the projectile and target nuclei. If we think of these potentials as belonging to the target (a nucleus and electrons) and the projectile (another nucleus and electrons) then as detected by an electron the potentials change because: (a) the target and projectile change position, and (b) electrons on the target and projectile change states.

The great exciting challenge of the next decade is to accurately describe (b). We have perhaps seen some start with this with the work of Devi and Garcia,¹ and from the point of view of some new ideas on two body correlations the work of Macek and Lin¹ looks promising. In any case the difficulties clearly intersect with the nucleus-nucleus problem and one can expect fruitful interplay between the two fields. We are still at the beginning stages in atomic physics because the target and projectile potentials are often dominated by the nuclear potentials which do not change in the collision. This coupled with the modest strength of the Coulomb force means electron-electron correlations are not dominant. Apart from taking proper account of the exclusion principle correlations may be neglected to a good approximation. Thus most work in the past fifty years has concentrated on solving the independent particle model (IPM). Cracks are beginning to appear in this model which only allows for type (a) changes in the potential. But in a short review we shall have quite enough to do in understanding the progress made in the last decade on the IPM.

The rest of this paper is divided into three parts. The first deals with how to reduce the IPM to the single electron model (SEM). The second is on a new method where charge transfer is important. The third confronts some standard models with modern calculations.

CESIME Processes: IPM to SEM

In the IPM we determine some standard potentials with which to describe the average (assumed moving but time independent) potentials, e.g. the Hartree-Fock potentials of the target, V_T , and projectile, V_p , ground states. The wave function is initially a single determinant and remains a single determinant throughout the collision. The single electron wave functions all satisfy

$$[-\nabla_r^2/2m_e + V_p + V_T]\psi = i \frac{\partial}{\partial t}\psi. \quad (1)$$

Because of this it is possible to prove a basic theorem for an inclusive probability p_1 for producing a hole (in a single particle state), labelled by 1, on the projectile or target, i.e.

$$p_1 = \sum_b |a_{b1}|^2 = 1 - \sum_\lambda |a_{\lambda 1}|^2. \quad (2)$$

Here b designates a sum over initially unoccupied states, and λ a sum over initially occupied states. The amplitudes a_{ij} describe single electron transitions between the states i and j with no regard to any other electrons in the problem. Thus eq (2) connects the IPM and SEM. The many electron nature of problem only manifests itself here in the restriction of the states λ and the determination of the potentials.

The probability p_{12} for two holes to be produced is given by the determinant

$$p_{12} = \begin{vmatrix} 1 - \sum_\lambda |a_{\lambda 1}|^2 & - \sum_\lambda a_{\lambda 1}^* a_{\lambda 2} \\ - \sum_\lambda a_{\lambda 2}^* a_{\lambda 1} & 1 - \sum_\lambda |a_{\lambda 2}|^2 \end{vmatrix} \leq p_1 p_2 \quad (3)$$

The off-diagonal terms if coherent in phase can give a noticeable suppression of single electron probabilities. Sometimes an enhancement results so we call such events CESIME processes: the coherent enhancement or suppression of independent-particle model events. These have been observed by the Frankfurt group.¹ They are a phenomena unique to atomic physics because as two body correlations are weak inclusive cross sections have experimental significance.

How though are we to solve eq (1) to accurately describe such processes?

The one and a half centered expansion (OHCE)

When the target and projectile are of comparable charge flux loss due to charge transfer may be important. The conventional way to deal with this is to include target, χ_n , and projectile, ϕ_m , centered states in the basis, i.e. a two centered expansion (TCE).

$$\psi(\text{TCE}) = \sum_{n=1}^N a_n(t) \chi_n(\vec{r}, t) + \sum_{m=1}^M b_m(t) \phi_m(\vec{r}, t). \quad (4)$$

If only a few states χ_n , ϕ_m are needed this provides an excellent algorithm. But in a many electron atom we need to calculate all $a_{\lambda\lambda'}$ and often for ionisation $a_{b\lambda}$ also. Thus perforce $(N+M)$ is a large number. Two difficulties now arise:

a) As χ_n and ϕ_m are not mutually orthogonal coupled equations have to be solved at each time step;

b) At convergence as χ_n and ϕ_m are linearly dependent these equations for $a_n(t)$ and $b_m(t)$ are linearly dependent.

Both these problems are solved by the OHCE. Here the algorithm is

$$\psi(\text{OHCE}) = \sum_{n=1}^N a_n(t) \chi_n(\vec{r}, t) + \sum_{m=1}^M b_m(\infty) \phi_m(t) \phi_m(\vec{r}, t) \quad (5)$$

Here $\theta_m(t)$ is preset subject to the boundary conditions at $t = \pm\infty$,
 e.g. $\theta_m(-\infty)=0$, $\theta_m(\infty)=1$.
 Equations for $a_n(t)$ are found by imposing

$$\langle \chi_n | i \frac{\partial}{\partial t} - H | \psi(\text{OHCE}) \rangle = 0 \quad (6)$$

and the subsidiary condition

$$b_m(\infty) = i \int_{-\infty}^{+\infty} \langle \phi_n | i \frac{\partial}{\partial t} - H | \psi(\text{OHCE}) \rangle dt \quad (7)$$

gives the b_m 's. The equations have to be uncoupled once by a single algebraic inversion making the OHCE an important practical method for performing calculations.

Comparison with standard approximations

The speed and accuracy of these modern numerical methods provides a benchmark against which standard approximations such as the Born, the PSS, Glauber, Magnus, etc. can be tested. Perhaps the most easily realisable test is provided by asking for comparisons between different schemes when V_p is changed in sign. This test is not completely silly as though anti-proton beams are not available, pion beams are, and we have positrons and electrons already. For weak perturbations the PSS is excellent and the Glauber and Magnus fail. For strong perturbations the Glauber and Magnus are good for dipole allowed transitions but fail for forbidden transitions.

Conclusion

The single electron problem is far from played out. Just recently for example, we discovered the sensitivity of ionisation by a slow projectile to the slope of the positive energy wave function. This means that convergence is extremely poor. We solved this by diagonalizing powers of H_T instead of H_T itself. Nevertheless many of the pernicious problems have at last been solved.

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