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Collision Cross Sections for Few Electron Systems

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An outline of the project

The purpose of this project was to produce accurate cross sections for collisionally induced reactions from the ground state and excited states of species of ions and atoms present in a hot fusion plasma. The collisional constituents may be divided into two categories for the purpose of calculations:-

Those in which a bare projectile excites a one electron or two electron ion or atom from its ground state, or excited states to higher excited states or ionized states.

Those in which the projectile has one or more electrons attached to it and excites a one electron or two electron ion or atom from its ground state, or excited states to higher excited states or ionized states. During the collision the projectile itself may change its state being simultaneously excited or ionized.

Cross sections are needed typically over the whole energy range from low velocities where molecular orbitals begin to form to high velocities where first Born or more sophisticated asymptotic theories can be used. These high energy cross sections are very useful for experimentalists to check the absolute normalization of their cross sections. The theoretical tools used were therefore both analytical and numerical in character. Numerical calculations were restricted to expansions of the wavefunctions in a set of finite hilbert basis states(FHBS).

The many body aspects of the problem, i.e. the important presence of the inter-electron force, or correlation, mandate a careful systematic approach. But this caution was tempered in our strategy by the fact that many of the cross sections needed, especially from excited states, have never been calculated or measured at all. Thus any information we can provide is useful even if later work may modify our results.

Six main results have been achieved :

A1. We have established that a single center expansion with an extended angular momentum range, is adequate, and may even be preferable, to accurately describe excitation and ionization of a target even when charge transfer plays an important role, R1-R4.

A2. We have established a basis which is numerically converged which simultaneously describes excitation of the $n=1$ and $n=2$ levels of a one electron atom by a bare projectile, R1-R4.

A3. We have completed a calculation in which correlation is included into the cross section for ionization using a many body perturbative approach. So far this has only been applied in the first Born approximation; but we have solved a long standing problem in the field, the Paul discrepancy. This promises to provide a definite prescription for the best IPM, R5. We have extended our FIM calculations with a larger basis to accurately reproduce cross sections for single and double ionization of helium by fast protons, R10.

A4. We have described a new asymptotic theory which allows an extension of analytical methods to lower energies for high energy neutral projectiles incident on ions and

atoms. The method, which we call Response Theory, is immediately applicable to many electron correlated targets. We have checked its efficacy on a simple solvable model as well as comparing to FHBS calculations, R6,T1.

A5. We have invented a simple independent particle model (IPM) to describe inclusive cross sections for collisions of ions each bearing one electron. We have reproduced for the first time the experimentally measured excitation of a helium ion by hydrogen, R7.

A6. We have successfully applied the new Response Theory to describe, over a wide energy range, the First Born approximation for ion-atom collisions taking fully into account the active role of electrons on the ion in exciting electrons on the target, T2, R8.

Detailed description of the progress

A1. A single centered basis approach

It has been an agreed fact since the preliminary work of Bates and McCarroll (1958) that charge transfer to the projectile is an important channel for flux loss from a target atom when the projectile and target nuclear charge are comparable. They pointed out the necessity of using two centered expansions in FHBS calculations, i.e. hilbert states centered on the target and the projectile. However, while this is true if one wishes to limit the calculation to a minimum number of states, the desire to simultaneously calculate cross sections to several excited Rydberg states of the system, as well as cross sections from the $n = 2$ level, mandates using a large number of basis states for the target. We postulated therefore that it should be possible to abandon the conventional two centered basis and return to a computationally simpler method of a target centered FHBS calculation as long as enough angular momentum was included in the target basis set. We have established the efficacy of this surprising result by repeating the standard proton hydrogen calculations (Ford *et al*, R1). We have demonstrated convergence with respect to the basis for $n = 1 \rightarrow 4$ transitions and for electron removal from the $n = 1$ initial state for the energy region from 15 keV to the energy where the cross sections merge to the first Born (around 500 keV).

A2. Excitation and ionization from the $n=2$ shell

Our numerical FHBS codes differ from most other authors in that they are based on a U-matrix approach. The reason for this is historical. Our interest in ion-atom collisions was initially sparked by the need for K-shell hole production cross sections in many electron atoms. We therefore had to deal with many electron targets from the very beginning. A U-matrix approach *simultaneously* calculates reaction cross sections for electrons in *all shells*. However in our study of K-shell ionization occurring at the same time as L-shell ionization we found that one has to be very careful with the choice of the FHBS to ensure convergence of all the cross sections. This had made us aware of the fact that reactions starting in the $n=2$ shell needed a very careful selection of the basis needed to establish convergence. Our second task, after A1, was to establish such a basis convergence in the proton-hydrogen system. We have done this (Ford *et al*, R2). We have applied this method to the study of proton impact with singly charged helium and doubly charged lithium (Hall *et al*, R3-R4).

A3. IPM study for reactions involving neutral atoms

The previous studies eradicated all serious numerical difficulties associated with calculating cross sections for the reactions of interest for a *one electron* system, or a many electron system in which the electrons are moving independently, i.e. an IPM.

In an effort to answer what is the best IPM we returned to an old problem, to wit :- the fact that IPM calculations of K-shell hole production (Ford *et al* 1977, 1979, 1981) are not in agreement with experiment (Paul *et al* 1989); the so called Paul discrepancy (Idrees *et al*, 1991). The original theoretical calculations were performed using the ground state single particle Hartree-Fock potential of the target atom in an IPM approximation. We shall call this the Hartree-Fock independent particle model. In this work, R5, we re-examined this choice of the static mean field used, with respect to the many body corrections to the cross section that apply to the IPM assumption. We discussed a different choice for the mean field. We showed that with either choice a simple correlation correction gives a satisfactorily converged answer for an exclusive first Born K-shell vacancy cross section. *The correlation correction however is much smaller for our new choice of mean field.* The new correlated cross section differs from the old in such a way as to substantially reduce the Paul discrepancy, R5.

A4. An asymptotic theory of reaction cross sections for ion-atom collisions: short range forces

The purpose of this work is try to determine *analytically* the asymptotic high energy form of a direct reaction cross section when the Second Born term is important. Thus if we write the cross section, σ , as

$$\sigma = Z_p^2 \sigma_B (1 + \alpha Z_p + \dots), \quad (1.1)$$

we are concerned with determining α . In eq(1.1) Z_p is the coupling constant of the potential, V_p , between a projectile and a struck target electron. The electron is assumed to be bound initially to some fixed heavy nucleus. When Z_p is small, and the excitation energy is held fixed, the asymptotic reaction cross section is given by the first term in eq(1.1), the First Born approximation. To determine α we will need to calculate the interference between the First Born amplitude and the Second Born amplitude.

The intellectual imperative for producing such a theory is to develop approximations for reaction cross sections to energies lower than those at which the First Born approximation is accurate. Generally we seek to develop a Response Theory with which to calculate accurately the way a correlated many electron system responds to these probes; this theory can then be used to complement elaborate numerical calculations using expansions in a finite Hilbert basis set (FHBS) (Epstein, 1926; Bates and McCarroll, 1958; Wilets and Gallaher, 1966). Those calculations have been successful in explaining the low energy sector of ejected electrons which often dominate total cross sections (Reading and Ford, 1990). However FHBS methods are not directly useful in explaining the high energy sector needed for differential cross sections (Olson *et al*, 1989) because of the practical difficulty of accurately describing an electron with high energy and high angular momentum with a modestly sized basis set (Fang and Reading, 1991).

In this opening investigation we limit ourselves to the much simpler system of one electron being perturbed by a short ranged potential. Guided by comparison with FHBS calculations we demonstrate the efficacy of this new theory, and hence motivate the unfortunate necessity for the more complicated developments needed to address systems with long range Coulomb interactions; these we plan to tackle in subsequent work.

At sufficiently high projectile velocities, v_p is large compared to the speed of the struck circulating electron; further we shall assume that the time, τ_c taken for the interaction, measured by $\frac{1}{v_p \gamma}$, is short compared to the period of the orbiting electron. Clearly this condition is never satisfied for an unscreened Coulomb potential. Never-the-less there are important systems which can be approximated by this model. For example the collision of a helium atom with a helium ion.

There are several asymptotic theories extant in the literature that were designed to calculate higher order Born terms in such a collision. We mention four types. The Glauber approximation (Glauber, 1958) treats the struck electron as if it were frozen in position during the collision. The Cheshire approximation (Cheshire, 1964) treats the struck electron as if it were at rest in the target and able to freely scatter from the projectile. The impulse approximation (Reisenfeld and Watson, 1956) assumes a distribution of momenta for the electron which is assumed to recoil freely when interacting with the projectile. Lastly there are numerical FHBS expansion methods already alluded to, though we are unaware of any calculations performed hither-to for short range potentials.

The first three methods are analytical; they are based on approximations which are believed to be reliably accurate when the conditions outlined above are met. The Glauber and Cheshire approximations are particularly simple as they involve no convolution integral over the momenta of the target wave functions, and it is this type of approximation that we shall be concerned with here.

For example if we set γ to zero one version of the approximations (Binstock and Reading, 1975) leads to the result that

$$\sigma_{Glauber} = Z_p^2 \sigma_B |\Gamma(1 + in)|^2 e^{n\pi}, \quad (1.2)$$

and

$$\sigma_{Cheshire} = Z_p^2 \sigma_B |\Gamma(1 + in)|^2 e^{\pm n\pi}, \quad (1.3)$$

where $n = -Z_p/v_p$. In eq(B1.3) the sign of the exponent is determined by the momentum transfer. This type of result is so simple it offers the hope of being practical enough to address correlated systems if only the approximation can be made reliably accurate.

The results just described represent only one version of the approximations. Many variations of the basic ideas have been used to successfully confront experimental data, e.g. CDWA-EIS Crothers and McCann, 1983, and Ishii *et al*, 1982. Not just the Second Born term is considered in these approaches. An approximation is developed for all terms in the Born series.

The aim of this work is, in this context, modest. We seek to develop a simple method of finding the correction to the First Born approximation due to the interference of the First and Second Born amplitudes. If we cannot get this right there seems little point in worrying about higher order terms. In the same vein, comparison with experiment is,

we believe, premature at this stage. We test our new method to be described against an FHBS calculation. Further we will consider only the most basic of reactions, the $1s - 2s$ excitation of a hydrogen-like atom. We will give two versions of the theory: a simple high energy result based upon the Response Theorem, and a slightly more complicated version which allows an estimate of the error in the method. We believe this feature, of a built in check to the accuracy of the approximation, is its great virtue.

Figure 1. The interference term between the First and Second Born amplitudes for the reaction cross section $1s - 2s$ is plotted as a function of the reduced projectile velocity, v_p . The screening parameter, γ , is 0.1. The zeroth order term of the response theory developed in this paper is the solid line; the dashed curve includes an error estimate due to the variance term. The dotted lines are versions of the Cheshire and Glauber approximations as described by Binstock and Reading. Another version of the Glauber approximation, the long dashed line, would give zero for α (McGuire et al, 1973). The filled circles are numerical results obtained from an FHBS calculation.

We show that the new method proposed here is an improvement on some versions of the Glauber and Cheshire approximations, while retaining the essential simplicity of those approaches. Our new method is a natural extension of the work of Reading and MacKellar, 1968, first performed in a nuclear physics context for elastic collisions. The method relies on a new theorem of scattering from bound systems that we have invented:-it is called the Response Theorem. It connects the scattering of a bound electron to an *on shell* projectile-electron t-matrix element chosen in such a way that the first order correction to the theory is guaranteed to be zero. The only knowledge of the atomic system needed is two form factors; the usual scalar form factor and a linear, vector form factor connecting the initial and final states. We call this the zeroth order theory. The theory is immediately applicable to correlated many electron systems. We illustrate the results in fig.1.

A5. A static mean field model for inclusive cross sections involving collision of ions each bearing an electron

Figure 2. The total cross section for the $1s - 2s$ excitation of He^+ by H is plotted as a function of incident projectile energy E_p . The filled circles are the experimental results of Shah and Gilbody, 1978. The solid curve is the present static mean field model result; the dashed curve is the two electron FHBS calculation of Bell and Kingston, 1978; the dotted curve is the two electron Born result of Bell and Kingston, 1978; and the long dashed curve is the single electron result obtained using an unshielded proton as the projectile.

The results we obtain using our single electron model but with, in our judgement, an insufficient number of basis states are given by the open circles.

In this work we introduce a very simple static mean field model for the calculation of cross sections involving collisions between ions each bearing an electron. The model is designed primarily for calculating exclusive target excitations accompanied by inclusive projectile reactions. This implies the measurement is specific with respect to the final target state occupancy. We assume that no information is available as to the deposition of the projectile electron. The model is anticipated to be most accurate when the target nuclear charge, Z_T , is much greater than the projectile nuclear charge, Z_P . Explicit expressions are given for corrections to the model but they will be evaluated in subsequent work.

We illustrate the model with a calculation of the 1s-2s excitation by a hydrogen atom of a helium ion. The cross section is inclusive in the exit channel of the hydrogen atom. Comparison with measurements (Shah and Gilbody, 1978) for the helium system shows a *dramatic improvement* in agreement of theory and experiment over previous calculations (Bell and Kingston, 1978; Wada and Fujimoto, 1987).

We illustrate the efficacy of the new method which has no adjustable parameters in fig.2.

A6. The response theory result for asymptotic cross section for collisions of single electron ions with hydrogen atoms

Fig.3. Comparison of First Born inclusive cross sections (10^{-18} cm^2) for excitation of $\text{He}^+(1s \rightarrow 2s)$ by neutral Hydrogen. Points:- accurate results of Bates and Griffing; broken line:- closure approximation; solid curve:- Response Theory.

We applied the Response Theory to address the problem of how to accurately calculate First Born cross sections for excitation of a single electron ion by a neutral Hydrogen atom. The method is analytical and so simple to apply we expect to be able to use it for correlated many electron systems. We compare the Response Theory with accurate results by Bates and Griffin, and a simple closure approximation of Anholt in fig.3. We note the Response Theory, when compared to the closure approximation, is accurate in reproducing the exact answer to much lower projectile energies.

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Papers resulting from this Contract

R1. A. L. Ford, K. Hall K, and J. F. Reading *Single-Centered Calculations of Excitation and Electron Removal in Intermediate Energy Proton-Hydrogen Collisions*, J.Phys.B:At.Mol.Phys. 26, 4537-4551.

R2. A. L. Ford, J. F. Reading and K. A. Hall *Single-Centered Calculations in Intermediate Energy $p + H(n = 2)$ Collisions*, J.Phys.B:At.Mol.Opt. Phys. 26, 4553-4560(1993).

R3. K.A. Hall, J. F. Reading and A.L. Ford *Single-Centered Independent Particle Model Calculations for Excitation and Electron Removal in $p + He^+$ Collisions*, J.Phys.B:At.Mol.Opt. Phys. 27, 5257-5270(1994).

R4. K.A. Hall, J. F. Reading and A.L. Ford *Single-Centered Independent Particle Model Calculations for Excitation and Electron Removal in $p + Li^+$ Collisions*, Submitted to J.Phys.B:At.Mol.Opt. Phys.

R5. E. Lindroth, J.F. Reading, A. L. Ford and M. Idrees. *Dynamic Correlation effects in K-shell hole production by fast protons*, J.Phys.B:At.Mol.Opt. Phys. 26, 4584-4598(1993)

R6. K.A. Hall, J.F. Reading and A. L. Ford *An Asymptotic Theory of Reaction Cross Sections for Ion-Atom Collisions: Short Range Forces*, J.Phys.B:At.Mol.Opt. Phys. 26, 1697-1710(1993).

R7. J.F. Reading, K.A. Hall and A.L. Ford *A Static Mean Field Model for Inclusive Cross Sections Involving Collision of Ions Each Bearing One Electron*. J.Phys.B:At.Mol. Opt. Phys. 26, 3549-3558(1993).

R8. J.F. Reading, K.A. Hall, A. Neves and A.L. Ford, *The Response Theory Approximation to the First Born Cross Section for the Excitation of a Single Electron Highly Charged Projectile by a Neutral Hydrogen Atom*. To be submitted to J.Phys.B:At.Mol.Opt. Phys.

R9. J.F. Reading, A.L. Ford, K.A. Hall and E. Lindroth *A Review of Some Selected Two Electron Processes in Ion-Atom Collisions* Nucl.Instr.Meth.B. 86, 38-44(1994).

R10. A.L. Ford and J.F. Reading, *Improved Forced Impulse Method Calculations of Single and Double Ionization of Helium by Collision with High Energy Protons and Antiprotons*, J.Phys.B:At.Mol.Opt.Phys. 27, 4215-4227 (1994)

Theses resulting from this Contract

T1. Mathew Fitzpatrick. Masters Thesis, *Comparison of an Exact Analytical Second Born Term with its Asymptotic Approximations*

T2. Andrea Neves, Masters Thesis, *Asymptotic Cross Sections for Composite Projectile Reactions*