PROGRESS REPORT

For Grant No. DE-FG02-86ER13549:

Electron Transfer, Ionization, and Excitation in Atomic Collisions

Submitted by:

Thomas G. Winter, Professor
Steven G. Alston, Associate Professor
Department of Physics
Lehman, PA 18627

The Pennsylvania State University
University Park, PA 16802

Covering the Period June 15, 1992 to June 14, 1995

The research program of Winter and Alston addresses the fundamental processes of electron transfer, ionization, and excitation in ion-atom, ion-ion, and ion-molecule collisions. Attention is focussed on one- and two-electron systems and, more recently, quasi-one-electron systems whose electron–target-core interaction can be accurately modeled by one-electron potentials. The basic computational approaches can then be taken with few, if any, approximations, and the underlying collisional mechanisms can be more clearly revealed. Winter has focussed on intermediate collision energies (e.g., proton energies for p-He^+ collisions on the order of 100 kilo-electron volts), in which many electronic states are strongly coupled during the collision and a coupled-state approach, such as a coupled-Sturmian-pseudostate approach, is appropriate. Alston has concentrated on higher collision energies (million electron-volt energies), or asymmetric collision systems, for which the coupling with the projectile is weaker with, however, many more target states being coupled together so that high-order perturbation theory is essential. In the following paragraphs, several calculations by Winter and Alston are described, as set forth in the original proposal.

In two parallel calculations, Winter and Alston have applied the coupled-state and perturbative approaches to collisions between protons and neutral heavy atoms, considering the active electron to be initially in the K shell. These asymmetric systems are quasi-one-electron systems for which the electron–target-core interaction can be modeled by a one-electron, Hartree-Fock potential, such as that of Green, Sellin, and Zachor (GSZ).[1] The one-electron approximation is valid because for heavy targets the electron-nucleus interaction dominates the electron-electron interactions; the other electrons, for the most part, merely partially screen the nucleus from the projectile and the active electron.

In the calculation by Winter, the electronic wave function during the collision has been expressed in terms of a (double-center) coupled-Sturmian-pseudostate basis, as in previous work on purely one-electron systems.[2] This basis systematically approaches

completeness when enlarged, and accounts for the continuum intermediate states which are very important in asymmetric collisions. Alston was the first to point out that neutral targets such as carbon would be expected to be easier to treat in a coupled-state approach than ionic, C^{5+} targets, since the screening by the other electrons weakens the long-range potential and fewer basis functions would then be needed to represent the ionization and electron-transfer channels. Indeed, Winter has recently shown that for carbon targets basis convergence of a few percent can be achieved, particularly with a suitably chosen Sturmian effective nuclear charge, and generally excellent agreement with experiment[3] is obtained as well. This work has been published.[4]

The calculated ionization cross sections for neon targets also show little basis sensitivity, and agree extremely well with the experimental results of Rødbro *et al.*,[3] as for carbon targets. For electron transfer, the absolute basis sensitivity is also comparable to that for carbon targets, but the relative basis sensitivity is greater owing to the smaller cross section. There is generally very good agreement with the experimental results of Rødbro *et al.* for electron transfer from neon targets, as previously noted for carbon targets.[4] The agreement with the recently published perturbative results of Alston[5] is also very good for both targets. The coupled-state results for neon targets have also been published.[6]

In the parallel perturbative calculation, Alston has extended[5] the distorted strong-potential Born (DSPB) approximation[7] for inner-shell capture in asymmetric collisions at intermediate energies to incorporate an atomic model potential. Since the active-electron–target-core interaction in a multi-electron target can be described to good approximation by a local potential, the DSPB theory is first extended by incorporating the analytic, one-electron model potential noted above. The atomic potential is used further to obtain an initial-channel distortion potential which allows for the screening of the K shell by the outer shells and for the interplay of the projectile and the off-energy-shell electronic scattering motions. This distortion component is an essential ingredient

of the DSPB amplitude in comparison with the original, undistorted SPB amplitude.[8] Another extension of the initial study involved evaluating the amplitude more accurately using a less restrictive peaking approximation: in the integration over momentum of the product of the amplitude for virtual ionization of the electron and the final bound state, only components transverse to the projectile direction are neglected.[9] Comparison with experiment for protons on carbon, neon, and argon shows excellent agreement.[10] Very good agreement with the coupled-Sturmian-pseudostate results[4,6] of Winter is also obtained for the carbon and neon cases in the intermediate energy range.

Off-shell effects in the intermediate-state scattering, which are crucial in a strong-potential approximation and are neglected entirely in the impulse approximation, are found to be much smaller than in the undistorted SPB theory.[9] Moreover, the SPB results show different magnitude effects for different targets as well as strange oscillatory behavior not tied directly to any physical source. Consistent with the increasing importance of target nuclear screening by the nonactive electrons, the screening effects in the DSPB results increase uniformly as the impact energy decreases. Finally, the DSPB amplitude, in its use of distorted waves and short-range interactions and unlike the undistorted version, is formally well behaved, thus validating approximate evaluation of it. This work has been published.[5]

Thirdly, Winter has considered the simpler (i.e., purely one-electron) collisional system p-He^+ in greater detail. Previously, he and others had determined only integrated cross sections for electron transfer.[2,11] The coupled-state results of Winter were noted to be stable with respect to basis size to within 10%, and there was general agreement of the coupled-state cross sections with the experimental results. A more exacting test of theory is therefore appropriate. Cross sections differential in scattering angle are now being determined experimentally for the first time at the University of Giessen by Salzborn and co-workers.[12] To test theory against these anticipated experimental results, differential cross sections have been calculated in the eikonal

approach using two independent methods: First, as described in the original proposal, a Sturmian-pseudostate basis has been used to determine the transition coefficients in the eikonal expression for the scattering amplitude—the same basis was used previously to obtain the integrated cross section.[2] Secondly, in a calculation which goes beyond the original proposal,[13] a triple-center, atomic-state basis[11] has also been used. The agreement between the resulting two sets of differential cross sections is remarkably good, generally to within 10% or better, over the range of (center-of-mass) energies considered from 4 to 25 keV for forward scattering angles. This work has been published.[14]

The fourth calculation goes beyond the original proposal to determine cross sections for electron-transfer in collisions between protons and alkali atoms such as Na or K. It is a collaboration of Winter and Ashok Jain, who has recently joined our group here at Penn State. For Na targets, not only have electron transfer cross sections been determined, but also cross sections for target excitation and ionization. The present study is partly in response to a surge of experimental interest[15] in the $H^+ + Na$ system. The goal of the present theoretical study is to understand fully the collisional dynamics of the $H^+ + Na$ ($3s$ or $3p$) system in the low-to-intermediate-energy regime. We have employed the two-center coupled-Sturmian-pseudostate approach recently developed and applied to several quasi-one-electron systems by Winter[4,6] (the first calculation described in this progress report). A total of 70 states (43 on Na and 27 on H) are included in the treatment of charge-transfer (up to $n=4$, $l=2$), target excitation (up to $n=4$, $l=2$), and ionization (direct and capture to the continuum) channels. In the present energy regime, all three channels (capture, excitation and ionization) are strongly coupled; therefore, a careful choice of the Sturmian basis set and analytic Hartree-Fock potential is important. Convergence tests at various stages of the calculation were carried out in order to estimate the accuracy of the final cross sections (10% for capture and excitation, 25% for ionization). From the initial analysis of

calculated amplitudes, it was found that the present integral cross sections $\left(\sigma_{cap}^{tot}, \sigma_{cap}^{H(n=2)}, \sigma_{cap}^{H(2S)}, \sigma_{cap}^{H(2P)}, \sigma_{exc}^{Na(3S\to3P)}, \sigma_{exc}^{Na(3S\to3D)}, \sigma_{ion}^{tot}\right)$ and the A_{20} alignment parameter for Na($3S \to 3P$) compare very well with the available experimental data, as well as with previous theoretical results. For all of the above quantities, comparison between theory and experiment shows as good or better agreement than the earlier coupled-state calculations.[16,17] There are no measurements available for $\sigma_{\rm ion}$ in the lower energy (1-20 keV) region, where $\sigma_{\rm ion}$ may be characterized by resonance behavior. However, a comparison with the corresponding electron-Na ionization measurements, plotted with respect to projectile (electron and proton) velocity, reveals that the present $\sigma_{\rm ion}$ results are in good agreement with experiment. This p-Na work has been submitted for publication.[18]

An additional coupled-state calculation has just been completed for the related He^{2+} + Na collisional system. This collision is more difficult to treat, since more highly excited projectile-centered states are degenerate with the initial state. A 74-state calculation has been found satisfactory. The results of this calculation for electron transfer, target excitation, and ionization have been found to agree well with experimental results,[19] and will shortly be written up for publication.

The fifth calculation, as described in the original proposal, extends the previous calculation by Winter of the excitation of helium by high-energy protons (and anti-protons).[20] Due to programming limitations, that calculation treated only the excitation of the lowest doubly excited state $(2s^2)^1S$, the lowest singly excited states 2^1S and 2^1P, the ^1S and ^1P ionization channels, and the coupling among these states and channels using Sturmian bases which discretize the ionization continuum. The omitted doubly excited state $(2s2p)^1P$ is now being included; this state has the largest double excitation cross section, and a comparison with experimental results[21] for this state should be less ambiguous. [This state may also have some effect on the $(2s^2)^1S$ cross section.[22]] Tests show that a (symmetrized) $(nsn'p_{0,1})^1P$ Sturmian basis with $n, n' \leq 8$

(and a Sturmian effective charge $Z=2$) yields a value of -0.66 a.u. for the $(2s2p)^1P$ energy, not far from the exact value -0.69 quoted in Ref. 22. The scattering program is now being modified to include this doubly excited state. At least preliminary scattering results will be obtained by the end of this contract year. Due to possible ambiguity in the integrated experimental cross sections,[23] as noted in the original proposal, it may be necessary to make a comparison between theory and experiment at the level of cross sections differential in electronic energy. On the other hand, a comparison among integrated theoretical cross sections[22,24,25] is meaningful, since the lifetimes of the doubly excited states greatly exceed the collision time.

In a project on the contribution of the internuclear potential to electron capture at forward scattering angles, Alston has compared the multiple-scattering approach within a second-order Faddeev approximation[26] with the eikonal approach.[27] At high impact velocities in the forward scattering direction, the Born approximation, including terms through the second-order in the internuclear potential, gives no such contribution, due to the destructive interference of the partial amplitudes, even for the differential cross section.[28] However, a contribution of the internuclear potential does appear in the experimental differential cross sections.[29] Generally, it is thought that this contribution can be included using an eikonal version of the amplitude obtained by a Bessel transform of the electronic amplitude with the phase factor $b^{2iZ_PZ_T/v}$ included, where b is the impact parameter, v is the velocity, and Z_P and Z_T are the projectile and target nuclear charges.

The Faddeev approximation effectively replaces two-body potentials with transition matrices. Consequently, the internuclear contribution arising from the representation of the generalized Thomas mechanisms does not vanish and indeed agrees with experiment quite well at high energies. Relative to the eikonally transformed cross section, the Faddeev result gives the proper momentum transfer dependence at large scattering angles. Comparisons have been made between the Faddeev and eikonal approaches for

proton-hydrogen and proton-helium collisions at impact velocities of 5 and 10 times the respective orbital velocities of the target electron. These velocities correspond approximately to the intermediate- and high-velocity collision regimes. The significant finding in the high velocity case for both systems is that the magnitude of the eikonal differential cross section beyond 0.8 mrad is, to good precision, a factor of 4 smaller than the Faddeev result (which implies a factor of two difference in the amplitudes). The source of this discrepancy apparently derives from the Faddeev approach including *two* separate, constructively interfering channels corresponding to the two generalized Thomas mechanisms (where, in one, an electron-projectile collision is followed by a projectile-target nucleus collision and, in the other, a projectile-target nucleus collision is followed by an electron-target nucleus collision). The eikonal approach contains only the single standard two-step mechanism. At the lower velocity, the results agree fairly well, although there are significant unexplained differences in the 0.3-0.7 mrad region where, however, there is appreciable cancelation between the first-order Born term and the second-order term. This work has been submitted for publication.[30]

In the DSPB theory, the exact scattering state is approximated by the product of a distorted-wave projectile scattering state, based on the projectile–target-core Coulomb interaction and the short-range (screened) interaction of the passive electrons, and a wave packet of electronic off-energy-shell scattering states in the strong target field (representing the virtual ionization of the electron).[5] Whether this DSPB scattering state retains the normalization of its exact counterpart bears generally on the validity of the approximation itself, for it has been shown in the undistorted version of the theory (SPB) that the large modification of the impulse approximation cross section by the so-called off-shell factor results directly, also, in a concomitant loss of scattering state normalization—the theory needs to be renormalized. In a near-the-energy-shell approximation, the off-shell states in the wave packet are approximated by continuum states with momenta centered about the outgoing projectile's momentum and with a

distribution determined by the final bound state. In this approximation, which is the same as was used in the SPB analysis, it is found that the loss of normalization in the DSPB theory is very slight: on average, 0.1 percent for Ar, 3 percent for Ne, and 4 percent for C over the whole applicable intermediate energy range. Only at very small velocities at the limit of applicability of the perturbative approach does the normalization correction become appreciable. For example, for protons on carbon at 200 keV (i.e., at a velocity of 2.8 a.u.), the correction is 7.5%. Thus, the DSPB approximation retains, effectively, the exact-state normalization; there is minimal need for renormalization. The similar SPB loss of normalization is roughly an order of magnitude larger, up to 70% for protons on C at the low-energy side of the peak in the capture cross section.[31] This work has been submitted for publication.[32]

Alston's study of inner-shell capture by a light projectile at intermediate energies has continued with an investigation, using the DSPB approximation, of the effect on K-shell capture of screening from the outer atomic shells (outer-shell screening). Using the above-noted model potential[1] and K-shell energies calculated from it using Winter's Sturmian program, a series of calculations for second-row atoms was performed to compare capture cross sections for targets along isoelectronic sequences (e.g., for the $1s^2 2s^2$ configuration, from Be through Ne^{6+}) and sequences involving various stages of ionization of a species (e.g., Ne through Ne^{9+}). Scaling the capture cross sections and impact energy using the known plane-wave Born approximation scaling relationship for ionization[33] allows factoring of the virtual ionization component of inner-shell capture, thereby revealing the changes in the process along a sequence due to outer-shell screening. For the isoelectronic sequences, the K-shell Slater-screened charge[34] is used and, for the ionization-state sequences, the initial-final bound-state energy difference is used. Generally, it is found that the scaled capture cross section decreases when the outer screening is less diffuse, i.e., when the outer orbitals are more tightly bound. A mapping of the capture cross section is important in the modeling of fusion plasmas.

This work, a collaboration of Alston and Morris, has been submitted for publication.[35]

A further study of outer-shell screening for boron through fluorine atoms comprising calculations of capture from the positive-ion, neutral, and negative-ion forms of a given species (e.g., C^+, C, and C^-) is in progress. The surprising finding is that from just above the high energy side of the peak in the capture cross section down through the low energy side, the negative-ion cross section, although somewhat shifted from the positive-ion cross section, is almost of the same magnitude. There is a need for experimental data on these systems.

In another project, Alston has developed a modified second-order Faddeev approximation for application to electron capture at *lower* impact velocities. The modified amplitude has been applied to protons on helium at the intermediate energy of 293 keV, corresponding to a velocity of 3.43 au (roughly twice the characteristic velocity of the target electrons). Quite good agreement with experiment[36] and with the results of the two-state atomic expansion[37] of Lin and Soong has been found. A wave function close to the converged Hartree-Fock level (near HF) is used for the initial $1s$ state of helium.[38] Consistent with this, in the electronic part of the full amplitude, the interaction of the active electron with the target nucleus and the other electron is represented by a sum of potentials which derives from the electron-nucleus attraction and the screening of the other electron. The corresponding two-body scattering amplitude used in the Faddeev amplitude is represented as the sum of Coulomb and short-range parts. Since the energy is rather low, making the more approximately evaluated internuclear contribution to the amplitude less accurate, this part is normalized to the corresponding eikonal amplitude at a large angle (2.5 mrad), where only the internuclear amplitude contributes.[27] Also, because the impact velocity is relatively low, the initial and final electronic scattering states are corrected for a loss of normalization arising from off-shell scattering effects.[31] It is shown that at this energy the amplitude representing the electron–target-ion scattering is not approximated well

by an amplitude derived from a Coulomb potential with an effective (screened) charge. In the evaluation of the free Green function appearing in the amplitude, terms quadratic in the bound-state momentum variables are retained[39]; since the Thomas double scattering mechanism plays a negligible role at 293 keV, a linear approximation in the momentum variables, valid for this mechanism, is inadequate here. This work has been submitted for publication.[40]

In a separate project, Alston has made an initial study of electron capture in ion-molecule collisions at high impact velocities using protons incident on molecular hydrogen as the prototype.[41] This type of collision introduces significantly more detail into the capture process because the molecule can assume various orientations. At the high energies considered (2.5 and 10 MeV), owing to the short collision times involved, the internuclear coordinate's orientation and magnitude do not have time to vary appreciably and can be assumed fixed. The Thomas double-scattering mechanism in proton-atom collisions[42] appears as a secondary maximum in the differential cross section at 0.054°. Since this angle is determined by the first collision with the projectile, the peak location is not altered when a hydrogen molecule is the target. In the second collision, however, the electron can scatter off either molecular nucleus, resulting in an interference of amplitudes, with the orientation of the molecule playing, possibly, an important role. How the Thomas mechanism is modified in collisions of protons with spatially oriented hydrogen molecules, as opposed to hydrogen atoms, is of particular interest because the signature of this mechanism is a secondary maximum in the cross section—since a prominent feature of the cross section can be tied to a specific mechanism, the interplay of this mechanism with the diffraction effects due to scattering from the two nuclei of the molecule can be more cleanly investigated.

The second-order Born calculation employs a near Hartree-Fock wave function[43] for the initial bound state of the molecule. Consistent with this wave function and derived from it, a screened electron–target-core (two-center) potential is employed. A

free propagator which is linearized in the bound-state momentum variables is also used.[44] The use of a near Hartree-Fock wave function in the molecular case leads to more significant changes in the cross section than in the (united-atom) p-He case. In the calculated cross sections, the diffraction effects are very apparent when the molecule is oriented at a nonzero angle to the incident direction in the plane including the transverse component of the projectile momentum transfer vector. If the molecule is oriented perpendicularly to this vector, then the atomic-like Thomas peak is recovered as it is when the molecule is oriented parallel to the incident projectile direction.

A more approximate, but more intuitive, evaluation of the second-order Born amplitude (relying on the momentum transfer being much greater than R) effectively separates the diffraction aspect of the collision from the Thomas mechanism. It is shown, however, that this approximate amplitude gives a poor representation of the cross section, being a factor of two to three too low in the forward peak and too high in the Thomas peak region. A separation of the two principal aspects of the capture event gives an inadequate picture of the process—they do not work independently. Experimental detection of collisions from oriented molecules is under development by two groups.[45]

The cross section obtained from a beam of protons incident on a gas of hydrogen molecules will consist of a suitable average of fixed R cross sections over the orientation and magnitude of R. In its simplest form, a uniform average over all orientations of a cross section calculated at the equilibrium value R_e can be performed. The calculated, averaged cross section at 10 MeV is found to be very similar to the cross section for the molecule oriented along the incident projectile direction and, at 2.5 MeV, to be of the same shape but 20-30% lower. Finally, it is to be noted that a higher-order theory than the second-order Born approximation (e.g., the Faddeev approximation) will likely be necessary to obtain agreement with experiment. The second-order Born theory provides the conceptual framework but is not adequate for quantitative comparison. This work

has been submitted for publication.[46]

In another project, Alston is studying transfer ionization in ion-atom collisions at high impact velocities using the second-order Born approximation.[47] The effect on the double collision mechanism, where the ultimately captured electron scatters off the projectile and then another target electron, of describing the ejected electron by means of a Coulomb wave rather than a plane wave is being considered. The amplitude is being evaluated using adaptive multi-dimensional Monte-Carlo quadrature.[48] In order to verify the feasibility of the method, the exact second-order Born amplitude for simple electron capture in p-H collisions has been evaluated using this technique and the results compared with previously reported exact results.[49] It has proved possible to obtain the differential cross section to an accuracy of ± 10 percent, even at a velocity of 10 a.u. and in the Thomas peak region. This work is in progress.

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