Progress Report

The research program of Winter and Alston addresses the fundamental processes of electron transfer, ionization, and excitation in ion-atom and ion-ion collisions. Attention is focussed on one- and two-electron systems and, more recently, quasi-one-electron systems whose electron-target-ion core 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 $p\text{-He}^+$ 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), where the coupling is weaker with, however, many more states being coupled together so that high-order perturbation theory is essential.

Recently, in a collaborative effort, Winter and Alston have applied both coupled-state and perturbative approaches to electron transfer and ionization in proton- He^+ collisions, and have shown that the two approaches are consistent and may be smoothly joined at high intermediate energies. This work has recently been published.¹

Secondly, Winter and Alston have applied the coupled-state and perturbative approaches to collisions between protons and neutral carbon atoms, considering the active electron to be initially in the K shell of carbon. This is a quasi-one-electron system for which the electron-carbon-ion core can be modeled by a one-electron, Hartree-Fock potential, such as that of Green, Sellin, and Zachor (GSZ).² Alston was the first to point out that neutral carbon targets 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 basis convergence of a few percent can be achieved, particularly with a suitably chosen Sturmian effective nuclear charge, and generally excellent agreement with experiment as well. This work will be published shortly.³

Alston has extended⁴ earlier work⁵ on the distorted strong-potential Born (DSPB) approximation for electron transfer from inner shells in asymmetric collisions at intermediate energies. Since the active-electron-target interaction in a multi-electron target can be described to good approximation by a local potential, the DSPB theory is

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first extended by incorporating the analytic, one-electron model potential noted above. The one-electron atomic potential is also used to obtain an initial-channel distortion potential, an important component of the DSPB amplitude. This potential primarily distinguishes the DSPB amplitude from the original undistorted SPB amplitude.⁶ In another extension of the earlier study, the amplitude is evaluated more accurately by employing a much less restrictive peaking approximation: only contributions to the final bound-state momentum integral (see below) arising from momentum components transverse to the incident projectile direction are neglected.⁷ Comparison with experiment for protons on carbon, neon, and argon shows excellent agreement.⁸ Remarkably good agreement with the coupled-Sturmian-pseudostate results³ of Winter is also obtained for the carbon case in the 0.2-0.6 MeV energy range. Compared to a strict impulse approximation, where the final bound-state momentum distribution is folded with the amplitude for ionization of the target electron in the projectile's outgoing direction, so-called off-shell effects in the intermediate-state scattering (which are so important for capture when Coulomb potentials are involved) are found to be generally much less important than in the undistorted SPB theory.⁷ Consistent with the increasing importance of target nuclear screening by the nonactive electrons, these effects increase uniformly as the impact energy decreases. This contrasts sharply with the SPB results which show different magnitude effects for different targets as well as strange oscillatory behavior not directly tied to any physical source. Moreover, the DSPB theory solves the nonintegrable singularity problem which plagues the undistorted theory. This work has been submitted for publication.⁴

Alston has compared the multiple-scattering approach in a second-order Faddeev approximation⁹ with the eikonal approximation for the contribution of the internuclear potential to the electron capture amplitude at forward scattering angles. At high, but nonrelativistic, impact velocities in the forward scattering direction, the second Born approximation, containing first- and second-order terms in the internuclear potential, gives no contribution due to the completely destructive interference of the partial amplitudes, even for the differential cross section.¹⁰ A contribution does appear, however, in the experimental differential cross section.¹¹ Generally, it can be represented by an eikonal version¹² of the amplitude obtained as a Bessel transform of the amplitude with the factor $b^{2i\nu}$, where b is the impact parameter and ν is the internuclear Sommerfeld parameter. In the Faddeev approximation, potentials are replaced by two-body transition matrices. Consequently, the internuclear contribution 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; that is, the slope of the cross section versus scattering angle is the same. Similar behavior is seen in proton-hydrogen and proton-helium collisions at impact velocities of 5 and 10 times the orbital velocity of the target electron. At the higher velocity for both systems, however, the magnitude of the eikonal differential cross section is a factor of 4 smaller than the Faddeev result. The source of this discrepancy is unknown, but it could be due to the inclusion in the Faddeev approach of extra contributions not present in the eikonal approximation. At the lower velocity, the results agree well. This work is being prepared for publication.

In a final project by Alston, the differential capture cross section for protons on helium at the intermediate energy of 293 keV has been calculated using a second-order Faddeev approximation.⁹ Generally quite good agreement with experiment¹³ has been found, although at larger angles (where the internuclear scattering contribution dominates) the calculated shape does not show quite the structure found in the experiment. In the electronic part of the full three-body amplitude, the interaction of the active electron with the target nucleus and other electron is represented by a potential which is the sum of a Coulomb part, derived from the long-range behavior of the electron's interaction with the residual target ion, and a short-range part representing the screening of the other electron. The corresponding two-body scattering amplitude appearing in the Faddeev amplitude is thus represented as the sum of Coulomb and short-range parts. A two-term Hartree-Fock wave function is used for the initial 1s state.¹⁴ The internuclear contribution to the amplitude is obtained by normalizing the internuclear contribution of the Faddeev amplitude at an angle of 1.4 mrad with a similar contribution obtained from the eikonal approximation.¹¹ The impact energy corresponds to a velocity of 3.43 au (roughly twice the characteristic velocity of the target electrons). Since this velocity is relatively low, the initial and final electronic scattering states are corrected for a loss of normalization arising from off-shell scattering effects.¹⁵ It is also shown that at this energy the amplitude representing the electron-target-ion scattering is not well approximated by an amplitude derived from a Coulomb potential with a screened charge. In the evaluation of the free Green function appearing in the amplitude, terms quadratic in the bound-state momentum variables are retained; 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 is being prepared for publication.

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