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PROGRESS REPORT

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Electron Transfer, Ionization, and Excitation in Atomic Collisions

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The research being carried out at Penn State by Winter and Alston addresses the fundamental processes of electron transfer, ionization, and excitation in ion-atom (and ion-ion) collisions. The focus is on intermediate- and higher-energy collisions, corresponding to proton energies of about 25 kilo-electron-volts (keV) or larger. At intermediate energies, where the transition probabilities are not small, many states must be coupled in a large calculation, while at higher energies, perturbative approaches may be used. Several studies have been carried out in the current three-year period; most of these treat systems with only one or two electrons, so that fewer approximations need be made and the basic collisional mechanisms can be more clearly described.

The first calculation, carried out by Winter, treats electron transfer and ionization in collisions between protons and helium atoms at the intermediate proton energies from 50 to 200 keV. This work has been published.¹ Cross sections have been determined for electron transfer into each individual state of hydrogen from 1s to 3d₂; the sensitive dipole moments and Runge-Lenz vectors for the 2nd and 3rd principal quantum levels have also been determined. The coupled-Sturmian-pseudostate approach previously applied by Winter² to several one-electron systems has here been extended to the prototype, two-electron system p-He. Detailed convergence tests show that the dominant cross sections—those for ionization and capture into lower-lying s states—are stable with respect to basis size and agree well with experimental results at higher intermediate energies;

specifically, a long-standing discrepancy between theory and experiment³ has been removed. Cross sections and other quantities depending on higher angular-momentum states display larger basis sensitivity to ionization channels, but are consistent with experimental results and are within the spread of coupled-state results of others.^{4,5} The only approximation made in the present calculation has been to neglect interatomic exchange, which is valid at higher intermediate energies; the basis sensitivity to ionization channels, which has been demonstrated here for the first time, generally exceeds the sensitivity to interatomic exchange.

The second calculation carried out by Winter treats excitation and ionization in high-energy collisions between protons and helium atoms; this work has also been published.⁶ It is an outgrowth of the intermediate-energy calculation previously described, but focuses on the excitation of the helium atom rather than on electron transfer to the proton: At million-electron-volt (MeV) energies, electron transfer is much less likely than ionization, and so transfer channels may be neglected as far as excitation is concerned. Ionization, on the other hand, is the dominant process at MeV energies, and it is the inclusion of potentially important ionization channels which distinguishes the present calculation from other recent coupled-state^{7,8} and perturbative approaches.⁹ (It is a matter of convenience to use existing coupled-state programs, which include perturbations to all orders; the excitation processes are probably at most second order.) Of the several doubly excited

states considered experimentally¹⁰ and theoretically⁷⁻⁹ by others, only the lowest state $(2s^2)^1S$ has been considered here due to the limitations of the present coupled-Sturmian program. For this state, ionization channels have been found to be important, not only to define the state (since it is embedded in the ionization continuum), but also to provide second-order coupling. The present results (for anti-protons as well as protons) agree better with the experimental results than do the other coupled-state results. The attached proposal will describe extensions of the present calculations.

The third calculation, a collaboration of Winter with Stodden and Monkhorst of the University of Florida and Szalewicz of the University of Delaware, treated muon-catalyzed d-t fusion based on accurately calculated $p\text{-He}^+$ stripping and excitation cross sections; this work has been published.¹¹ Winter's role in this work was primarily to provide the coupled-Sturmian computer program for calculating the $p\text{-He}^+$ cross sections and to instruct in its use.

The fourth calculation, carried out jointly by Winter and Alston, treated electron transfer and ionization in high-energy $p\text{-He}^+$ collisions; this work has been accepted for publication.¹² The $p\text{-He}^+$ system is a prototype, asymmetric one-electron system. The present work extends the previous coupled-state calculations by Winter² and Stodden, Monkhorst, Szalewicz, and Winter¹¹ to MeV energies. A numerical connection is made both with first-order perturbative results for ionization and second-order perturbative results for electron transfer. Improved perturbative results for

electron transfer have here been determined¹² by Alston using an impulse version of the distorted strong-potential Born approximation;¹³ the agreement between perturbative and coupled-state results for electron transfer is now comparable to that for ionization down to intermediate energies as low as 30 keV.

The fifth calculation, a collaboration of Winter with McLaughlin of the Harvard-Smithsonian Center for Astrophysics, treats direct excitation of the $n=3$ levels of hydrogen in intermediate-energy proton-hydrogen-atom collisions. This work is an extension of the coupled-state, triple-center calculation by Winter and Lin¹⁴ on direct excitation of and electron transfer to the $n=2$ levels of hydrogen. The third-center functions partly allow for ionization channels. Preliminary results¹⁵ for the Balmer- α cross section agree well with recent experimental results obtained at the Queen's University of Belfast.¹⁶

The sixth calculation, carried out by Alston and now published,¹⁷ dealt with charge transfer in proton-helium and proton-hydrogen collisions at MeV energies. A Faddeev approach to the three-body scattering problem was employed within a second-order approximation incorporating near-the-energy-shell evaluations of the exact two-body transition matrices which appear in the transfer amplitude. For capture at scattering angles of the projectile of less than 1 mrad, four separate regions can be identified with different scattering effects playing major roles in each one: first, the extreme forward region of less than 0.2 mrad where the first Born term is the major contribution (reflecting the dominance of three-body

scattering); second, an interference region between 0.2 and 0.4 mrad where large cancellations occur between the various partial amplitudes; third, the Thomas peak region between 0.4 and 0.7 mrad where a double-scattering mechanism dominates; and fourth, the region of greater than 0.7 mrad in which the nuclear scattering takes over. The second-order Faddeev theory not only reproduces the data¹⁸ quite well over the whole 1 mrad region (when the cross sections are properly folded with the experimental beam profile), but it also clearly isolates the separate aspects of the scattering in its partial amplitudes.

Over this same range of forward scattering angles, it has been recognized for some time that in the second Born approximation the first- and second-order terms containing the internuclear potential interfere destructively to the order of the ratios of the nuclear charges to the impact velocity, which are small for large velocities.¹⁹ That is, essentially no internuclear contribution to capture occurs at all, even in the differential cross section. One knows, however, that such a contribution exists in the experimental differential cross section and that the eikonal amplitude (Bessel transform of the amplitude with $b^{2i\mu}$, with b the impact parameter and μ the internuclear Sommerfeld parameter) represents it well.²⁰ The second-order Faddeev approximation¹⁷ was shown to reproduce the internuclear contribution in the data very well and to agree with the eikonal form of the continuum distorted-wave theory beyond 0.7 mrad.²¹ Thus, the level of approximation in a multiple-scattering theory beyond the second Born necessary to give this

contribution is established. Other work directly comparing the Faddeev multiple-scattering and eikonal approaches to the contribution of the internuclear potential at forward scattering angles will be submitted for publication shortly.²² The coherent contributions of the generalized Thomas mechanisms¹⁷ represented in the Faddeev approximation are shown numerically to reproduce the effects of the eikonal phase factor.

In another published work²³ by Alston within the Faddeev framework, it was shown for symmetric collisions (with a common nuclear charge Z) using an analytic evaluation of the amplitude through second order with a linearized propagator approximation that the magnitude of the double-scattering contribution is increased by a factor of $e^{2\pi Z/v}$, with v the impact velocity, over the second Born result. This increase agrees with experiment¹⁸ and results from a better treatment of each Coulomb scattering.

In the seventh completed project, Alston formally generalized²⁴ the distorted-wave Born approximation to the exact electron capture amplitude of Taulbjerg and Briggs²⁵ (which has been shown¹⁷ to be equivalent to the electronic part of the Faddeev amplitude at forward projectile scattering angles) to the case of ion-ion collisions by incorporating scattering states, similar to those of the distorted strong-potential Born approximation of Macek and Taulbjerg,²⁶ that contain the proper (logarithmic) Coulomb phase factors. This generalized distorted-wave Born (GDWB) amplitude contains other capture amplitudes which have been discussed recently in the literature as approximations to it, including the first- and second-order

boundary-corrected Born (B1B, B2B0),^{27,28} the Coulomb Born (CB),²⁹ and the distorted strong-potential Born (DSPB) approximations.¹³ These more approximate amplitudes are obtained by introducing simplified forms for the initial and (or) final GDWB scattering states, for example, by neglecting second-order scattering contributions.

In the eighth project, Alston presented a simple study of the effects of screening of the target nucleus by nonactive electrons on the charge-transfer cross section; this work is also published.³⁰ For protons incident on helium at collision energies of 10^2 - 10^4 keV, use of a single-parameter screening potential in the boundary-corrected first Born approximation²⁷ showed in a straightforward manner how the screened cross section decreases by more than 60% with respect to the unscreened one as a result of the projectile's increasing penetration of the target-electron charge cloud with increasing impact energy. This work showed the sensitivity of the B1B approximation to the treatment of the internuclear potential.

Recent work by Alston has centered on the development of a program for the calculation of transfer-excitation (simultaneous projectile excitation and charge transfer) cross sections for hydrogenlike projectile ions incident on loosely bound targets.³¹ An impulse version of the distorted strong-potential Born approximation is being used which incorporates both correlated and uncorrelated (or resonant and nonresonant) mechanisms as well as a correlated final two-electron projectile state, calculated by means of the truncated diagonalization

procedure.^{32,33} Some allowance is made for cascading from intermediate excited projectile states. The required single-electron capture, excitation, radiative-decay and two-electron correlated-excitation amplitudes are all evaluated using partial-wave analyses and radial, high-order Gauss-Laguerre quadrature.³⁴ Asymmetric collisions, such as O^{7+} ions incident on He atoms, will be the main application; the change in the relative importance of and interference between the resonant and nonresonant amplitudes as the asymmetry varies is of particular importance, and work on these points has been limited.

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