Abstract for the DOE/BES Research Meeting on High Energy Atomic Physics, April 5-7, 1979

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THEORY OF ELECTRON TRANSFER AND IONIZATION

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A small atomic theory group in the Physics Division of ORNL, formed in 1977 with BES support, has had the part-time participation of staff members J. B. McGrory, C. Bottcher, and the author, together with the collaboration of several visitors: C. Feuillade (U. Manchester), B. R. Junker (Office of Naval Research), K. C. Kulander (Daresbury Res. Estab.), A. D. MacKellar (U. Kentucky), and A. L. Ford and J. F. Reading (Texas A & M Univ.). At present our research is motivated primarily by (1) needs of the magnetic fusion energy program for cross sections for collision processes in plasmas and for the spectroscopy of highly stripped heavy ions, and (2) needs of developing areas of atomic physics studied experimentally with charged-particle accelerators.

In the area of spectroscopy, Joe McGrory has spent some time converting existing nuclear shell model computer programs to a form suitable for configuration mixing calculations of the structure of heavy ions. Because of commitments in nuclear theory, he will probably not find much time to donate to atomic theory this year, and the project does not have the funding now to support a structure theorist. We would like very much to find a way to use these very powerful codes for complicated atomic structure calculations.

Chris Bottcher has spent part of his time in the area of chemical physics and lasers, continuing work begun at the Univ. of Manchester.[1-3]

The main effort of the group has been directed toward charge transfer and ionization in high energy atomic collisions. The research may be divided into classical trajectory calculations, quantum-mechanical collision theory, and phenomenological treatments of quantal interference effects in heavy ion collisions.

Beginning in 1964, Percival and collaborators[4] found that the method of "molecular dynamics" (i.e. following classical trajectories starting with initial conditions obtained by Monte-Carlo sampling) extended to electronic transitions in p+H and e+H collisions, gave results much better than those of the binary encounter approximation and, indeed, in good agreement with experiment at high impact velocities. A decade later, because of the growing availability of multiply-charged ions, Olson and Salop[5] did extensive Percival-type calculations for bare nuclei with $Z \leq 36$ incident on atomic hydrogen at velocities of about 1 to 3 Bohr velocities. Partially stripped projectile ions were also treated, in the approximation that the remaining electrons were ignorable, by assuming a fractional effective nuclear charge. The results have been very useful, and in many cases gave good fits to experiments such as the ORNL charge transfer data of Phaneuf et al.[6] A generalization of the calculation to treat two active electrons has been made by MacKellar and Becker. Results for H+H collisions have been reported,[7] and calculations are in progress for He^{+} and Li^{2+} projectiles. Initial conditions for He and He-like ions are being sought by Becker in collaboration with Don Noid of the Chemistry Division. Calculations for targets in Rydberg states are also being done.

Two forms of quantum mechanical theory for high energy atomic collisions are being pursued. A modification of the Born approximation which properly takes into account the non-orthogonality of atomic orbitals centered on different nuclei (projectile and target) was given by Bates in 1958. The few calculations done so far have been rather approximate and have been restricted by the availability of only a few two-center matrix elements containing translational factors. B. R. Junker, who spent the summers of 1976 and 1978 at ORNL, has recently completed a paper[8] on the calculation of general matrix elements of this kind and has performed some accurate Bates-Born calculations of electron transfer. Junker and Becker are planning multi-state Bates-Born and coupled two-center calculations.

An extensive set of codes for single-center, coupled-channels calculations of inner-shell vacancy production, which has been developed and used at Texas A & M University over the past several years, has been further refined at ORNL. The codes were originally designed for direct ionization of a heavy target by a light projectile ($Z_T >> Z_P$), but charge transfer to a hydrogenic ground state has been included recently. The full Hartree-Fock potential of the target is employed and resonant virtual excitation of the continuum of the target (the dominant second order process) is included. A recent calculation[9] gives a good account of K-shell electron capture and vacancy production data of Macdonald et al. (Kansas State U.) for high energy protons on Ar, and preliminary calculations[10] for O^{q+} + H(q = 3 and 6) gave good agreement with ORNL electron capture data[6] on absolute cross sections and variation with ionic charge. Work in progress involves increasing the intermediate-state basis from s and p only, to s, p, and d; and incorporating antisymmetry effects.

Recent electron transfer cross sections[11] taken at the ORNL model EN tandem Van de Graaff accelerator with heavy projectiles, ${}_{73}Ta^{q+}$, ${}_{74}W^{q+}$, and ${}_{79}Au^{q+}$ (q = 5 to 18), incident on H atoms showed an unexpected oscillation superimposed on the monotonic increase with q. While we hope to account for such oscillations in coupled-channels calculations later, at present a simple physical explanation is called for. Bottcher has proposed (see Ref. 11) a "transition state" model of capture by a highly stripped projectile at high energies in which: first the projectile transfers energy greater than the ionization potential to the electron; then the electron moves classically to the saddle point of the electrostatic potential where it is either captured by the heavy ion or escapes, depending on its kinetic energy. If σ_L is the electron-loss cross section of binary encounter theory and σ_c is the capture cross section, then the ratio σ_c/σ_L given by classical transition state theory is $\exp(-2v/q^{1/2})$. The oscillations in σ_c vs. q for $Z \approx 75$ are thought to result from an f-wave resonance in σ_L. Bottcher also is working on simple treatments of the ratio of cross sections for molecular vs. atomic targets (e.g. H_2/H) and for the forward peak in ORNL-U. Tn. data on projectile ionization.[12]

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