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May 24, 1990

Annual Report
Covering the Period June 1, 1989 to May 31, 1990

COLLISIONAL PROCESSES OF INTEREST
IN MFE PLASMA RESEARCH

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ABSTRACT

Research on this grant is devoted to the calculation of heavy particle collision cross sections needed for diagnostic studies of magnetic fusion plasmas. This work requires the development and testing of new theoretical methods, with the implementation of benchmarked techniques to collisions pertinent to fusion reactors. Within the last context, we have provided charge-exchange-recombination cross sections to specific n, l -levels for diagnostic studies on TFTR and for a major compilation for IAEA. We have also completed a cross section study related to the planned neutral beam current drive for ITER. In addition, calculations were completed to assess the use of He neutral atom angular scattering measurements for JT-60. Also, new theoretical methods have been developed to more accurately calculate cross sections involving either He or H_2 targets and partially stripped multiply-charged ions.

PROGRESS REPORT

Our research accomplishments for the period June 1, 1989 to May 31, 1990 are reported below. The papers published on the various topics during the last year are listed at the end of each subsection.

A. IMPURITY ION CHARGE-EXCHANGE-RECOMBINATION

We completed a large series of calculations to determine the n, l product distributions for collisions of

and

at energies from 40 keV/u to 140 keV/u. This work was published in tabulation form by an IAEA sponsored publication in Physica Scripta.

A complementary series of calculations for the n, l charge-exchange-recombination cross sections were made for the $He^{++} + H$ and $N^{7+} + H$ reactions. These data, and the C^{6+} and O^{8+} results, were transmitted via floppy disk to Ron Phaneuf at the Oak Ridge and Ranko Janev at IAEA Data Centers for inclusion in their fusion energy cross section data bases.

Physica Scripta, Vol. T28, 71-76, 1989.

n, l Distributions for Electron-Capture from H(1s) by C^{6+} and O^{8+}

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Received September 21, 1988, accepted October 16, 1988

Abstract

Total cross sections for electron-capture from the ground state of hydrogen by C^{6+} (40, 50, 60, 80, 100 and 120 keV/u) and O^{8+} (40, 50, 60, 80, 100, 120 and 140 keV/u) have been calculated using the classical-trajectory Monte Carlo (CTMC) technique. We tabulate these cross sections as a function of projectile energy for (i) capture to all product states, (ii) capture to product n -levels, and (iii) capture to product n, l -levels. The results of these calculations agree with and extend previous CTMC n, l distribution results [1].

B. ITER NEUTRAL BEAM CURRENT DRIVE

We have completed a series of cross section calculations central to the determination of a neutral beam penetration in an ITER plasma for assessing the feasibility of current drive. For the dense, high density ITER plasma, a D^0 beam energy of 1 MeV/u to 2 MeV/u is anticipated. However, the ionization efficiency of H^0 by the plasma from not only one-step impact ionization

but via multi-step ionization

followed by

or

had to be determined for the main plasma constituents of $Aq^+ = H^+, He^{++}, C^{6+}, O^{8+},$ and Fe^{26+} .

We used a combination of classical-trajectory Monte Carlo, symmetric Eikonal, and atomic orbital coupled-state calculations to provide reliable cross sections for the above reactions. This work, which combines our expertise with that of Wolfgang Fritsch at the Hahn Meitner Institute in Berlin, provides the cross sections over the energy range of 0.25 MeV/u to 2 MeV/u. The paper describing the theoretical methods and the results has just recently been accepted for publication by Physical Review A.

A modeling study of the ITER neutral beam penetration has been published in Nuclear Instruments and Methods. In this paper the magnetic field ionization of the highly excited deuterium components has been considered along with the "ladder walking" collisional ionization processes described above.

*Nuclear Instruments and Methods in Physics Research B42 (1989) 479-484
North-Holland, Amsterdam*

PENETRATION OF AN ENERGETIC D⁰ BEAM INTO AN ETR PLASMA *

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A beam of energetic D⁰ atoms can be injected into a thermonuclear reactor plasma for heating, fuelling or current drive. A computer code has been written to determine the penetration of the D⁰ beam into a steady-state tokamak Engineering Test Reactor (ETR) such as the proposed International Thermonuclear Experimental Reactor (ITER). The code includes multistep processes, and uses a combination of experimental and theoretical cross sections and scalings for the relevant atomic processes.

C. H⁻ BEAM STUDIES

We joined in an experimental-theoretical effort to determine the cross sections for electron removal from H⁻ by collisions with singly and multiply-charged ions

for charge states q=1 to q=8. The original work covered the energy range from 3 keV/u to 100 keV/u, but now it has been extended to 500 keV/u.

One of the motivations behind this study was to assess the feasibility of using a plasma neutralizer for H⁻ to increase the neutral H⁰ yield from about 55% for gas strippers to around 85% for a plasma stripper.

Our modeling studies do indeed indicate an 85% yield for the plasma stripper when using the newly measured and calculated cross sections. However, even at 500 keV/u, the stripping cross sections do not scale as q^2 , but rather as $q^{1.3}$, which translates to an unacceptable path length for a plasma stripper configuration. This work was published in Europhysics Letters.

EUROPHYSICS LETTERS

1 July 1989

Europhys. Lett., 9 (5), pp. 433-439 (1989)

Single- and Double-Electron Removal from H^- in Energetic Collisions with Multiply-Charged Argon Ions.

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(received 22 March 1989; accepted 20 April 1989)

PACS. 34.70 - Charge transfer.

PACS. 52.20H - Atomic, molecular, ion and heavy particle collisions.

Abstract. - Absolute cross-sections have been measured and compared to CTMC-calculations for single- and double-electron removal from H^- in collisions with Ar^{q+} ions ($q \leq 8$) at $E_{lab} = 50$ keV. The single-electron removal cross-sections are found to scale with $q^{1.3}$, and for the $H^- + Ar^{q+}$ system, this cross-section is found to have a weak energy dependence from 8 keV to 100 keV. A major implication of our measurements is that plasma neutralizers based on multiply charged ions for high-efficiency conversion of intense H^- beams into H^0 gain little in expected reduced length due to the inapplicability of q^2 -scaling in the H^- single-electron removal cross-section.

D. He ATOM AND ION ANGULAR SCATTERING

We have collaborated with Tony Donné at the FOM Institute for Plasma Physics in Amsterdam on the interpretation of using a neutral He atom probe for measuring ion temperatures in a fusion plasma. We provided the angular scattering cross sections and neutral atom survival probabilities required to analyze data taken at JT-60 and make predictions for applications to future tokamak fusion devices. Within this study, we investigated single and

double ionization and charge exchange in small impact parameter collisions with H^+ , C^{6+} , and O^{8+} ions in the range from 25 keV/u to 100 keV/u. Good agreement was realized for the comparison of this technique to other methods for giving the impurity ion concentration in the JT-60 plasma, indicating the feasibility of future applications. At present, we are continuing to provide cross sections for this modeling effort.

In order to have confidence in the cross sections we are providing for the fusion effort, we continue to benchmark our calculations against fundamental atomic physics data. In the three studies listed below, we have been able to successfully predict the complete three-body transverse momentum spectra for ionizing collisions between H^+ and He. This bodes well for our collaboration with Donné in providing the atomic physics data for neutral beam ion probes. Also, we have demonstrated that our theoretical methods predict the angular, and energy, profiles of the electrons ejected in collisions between H^+ , He^{++} and He in the energy range of 50 keV/u to 500 keV/u.

The role of small-impact-parameter electron-loss processes on ion temperatures measured by active-beam plasma diagnostics

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(Received 19 May 1988; accepted for publication 6 September 1988)

The shape of the energy distribution of scattered particles in an active-beam scattering experiment can be influenced considerably by the presence of highly charged impurity ions in the plasma. In this work it is shown theoretically that multiply charged impurities have only a small effect on the scattering distribution at low energies (< 10 keV/amu) and at high energies (> 75 keV/amu). The effect of the impurities is the most pronounced for energies close to 30 keV/amu. The results of the calculations are in good agreement with experimental results at various energies. Extrapolation to higher beam energies leads to the conclusion that the active-beam scattering diagnostics can be applied also in future fusion devices for measuring the local ion temperature.

Three-Body Interactions in Proton-Helium Angular Scattering

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(Received 23 February 1989)

$H^+ + He$ scattering at 0.5 MeV has been investigated using a coincidence technique that completely determines the three-body transverse momentum exchange in single-ionization collisions. Three scattering regions could be distinctly recognized that are dominated by proton-helium-nucleus, proton-electron, or electron-helium-nucleus interactions. Calculations and the experimental data show that the coupling between the electronic and nuclear degrees of freedom is required to understand the dynamics for more than 97% of the ionizing collisions.

PACS numbers: 34.10.+x, 34.50.Fa

RAPID COMMUNICATIONS

PHYSICAL REVIEW A

VOLUME 40, NUMBER 5

SEPTEMBER 1, 1989

Single- and double-ionization cross sections for angular scattering of fast protons by helium

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(Received 27 March 1989; revised manuscript received 14 July 1989)*

The angular scattering of H^+ by He has been investigated for single ionization at energies of 0.5, 1.0, and 3.0 MeV; and for double ionization at 1.0 MeV. The classical-trajectory Monte Carlo method has been used within one- and two-electron models to illustrate the collision dynamics. The angular differential single-ionization cross sections are in good agreement with experiment, and display the combined effects of proton scattering from the He nucleus and its electrons. The relative fraction of double ionization, as a function of scattering angle, shows a maximum at ~ 0.9 mrad that is in agreement with the experiments of Giese and Horsdal [Phys. Rev. Lett. 60, 2018 (1988)]. This maximum is found to be due to two uncorrelated scattering events between the H^+ and the He atom's two electrons in the double-ionization reaction from impact parameters different than that for the single-ionization reaction.

J. Phys. B: At. Mol. Opt. Phys. 22 (1989) L39-L43. Printed in the UK

LETTER TO THE EDITOR

Study of the dependence of the electron emission spectra on the projectile charge in H^+ , $He^{2+} + He$ collisions

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Received 18 October 1988

Abstract. The classical trajectory Monte Carlo method (CTMC) has been used to calculate doubly differential ionized-electron cross sections for the impact of He^{2+} and H^+ on He at collision energies of 50 and 100 keV amu $^{-1}$. The results exhibit the capture to the continuum peak and agree in both shape and magnitude with experimental data. The dependence of the cross sections on the projectile charge Z_p is analysed and it is found to be very asymmetric with regard to the capture to the continuum peak. This behaviour is in agreement with very recent experimental data. Large deviations from the Z_p^2 scaling predicted by first-order theories are found at large ejection angles.

E. DEVELOPMENTS IN DESCRIBING MANY-ELECTRON TARGETS

One of our goals over the last several years has been to develop theoretical methods applicable to partially-stripped ions like Fe^{10+} and many-electron targets such as He and H_2 . Accurate methods are increasingly needed for our cross section studies for fusion modeling efforts.

Along these lines, we have finally successfully developed a model potential method that accurately incorporates the screening of the nucleus by the other $N-1$ electrons in our calculations. Basic to this development was the use of a momentum distribution description similar to the microcanonical distribution we use for hydrogenic targets in our classical-trajectory Monte Carlo calculations. The procedure uses Thomas-Fermi-Dirac tabulations of the atomic, or ionic, species and now allows us to investigate any ion or atom for nuclear charges from $Z=1$ (hydrogen) to $Z=54$ (xenon).

To investigate the sensitivity of the method, we have performed calculations for not only H^+ , but also e^- and their anti-particles, on He and Kr. Existing experimental data verified our procedure.

Along these same lines, we have developed a classical phase-space model for H_2 . This method has been successfully applied to electron capture and ionization in collisions with ions in charge states $q=1$ to $q=10$ at energies from 25 keV/u to 500 keV/u. The calculations clearly show the nonequivalence of the cross sections for H_2 with those of doubled H^0 .

values. Molecular orientation effects were also investigated to further probe the collision dynamics.

PHYSICAL REVIEW A

VOLUME 40, NUMBER 7

OCTOBER 1, 1989

Electron removal from molecular hydrogen by fully stripped ions at intermediate energies

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(Received 19 May 1989)

A classical phase-space model of the hydrogen molecule is presented and applied to the study of the electron-capture and -ionization processes in collisions of fully stripped ions with H_2 at intermediate impact energies and charge states from 1 to 10. The model is based on the independent-electron and the impact-parameter approximations. The electron-impinging-ion and electron-target-nuclei interactions are exactly taken into account. The interaction between the electrons is approximated by model potentials. The calculated total cross sections for production of free electrons and capture of one electron are in good agreement with different experimental data. The ratio between the capture cross sections from molecular and atomic hydrogen targets is also analyzed and compared with available empirical scalings. It is found that this ratio varies from a value less than 1 at low impact energy to 4 at higher energies. The reasons for these differences are discussed. A comparison is made between the capture cross sections for different orientations of the hydrogen molecule.

Nuclear Instruments and Methods in Physics Research B42 (1989) 527-535
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DYNAMICS OF MATTER-, ANTIMATTER-ATOM COLLISIONS

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Dynamical effects which lead to differences in the cross sections for single- or multi-electron removal from atoms by singly-charged particles, (e, $\bar{e}$, p, $\bar{p}$) impact are caused by the differences in mass and sign of the charge of the projectile. This fact, often masked by simple first order theories, has now been demonstrated both experimentally and by more appropriate and sophisticated theoretical methods. Here we summarize our recent work elucidating these effects using the classical trajectory Monte Carlo technique to examine the total cross sections, and various cross sections differential in angle and energy, for electron removal. These cross sections have been calculated for intermediate velocity (1 to 6 a.u.) collisions of e, $\bar{e}$, p and $\bar{p}$ with H and He, and have been compared with other theoretical results and experimental measurements.

PHYSICAL REVIEW A

VOLUME 40, NUMBER 9

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Large-angle scattering in positron-helium and positron-krypton collisions

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(Received 7 June 1989)

We have calculated differential cross sections as a function of the projectile scattering angle for positron-helium and positron-krypton collisions using the classical-trajectory Monte Carlo technique. These intermediate-velocity collisions have been simulated by various independent-electron and n -electron models, using both screened Coulomb and quantum model potentials to approximate the effects of electron-electron interactions. These several models all indicate that scattering of positrons to large angles in ionizing collisions persists to high impact velocities. In a previous work [Phys. Rev. A 38, 1866 (1988)] we proposed that the recent experiments that have measured the total cross section for positronium formation could be affected by the loss of positron flux due to incomplete confinement after large-angle scattering. Here, utilizing these newly calculated differential-scattering cross sections, adjustments are computed that account for the difference between the experimental and theoretical behaviors of the positronium formation cross section. Further, it is demonstrated that large-angle scattering in the elastic channel is important for one of the experiments. We have also computed total cross sections for ionization and charge transfer for collisions of protons with krypton. Good agreement is obtained in these cases with experimental measurements.

F. ALPHA PARTICLE DIAGNOSTICS

A major fraction of our effort was spent collaborating with Ray Fisher and Art Howald at General Atomics on carbon pellet alpha particle diagnostics. The basic idea behind the use of the ablation cloud from a carbon pellet is to provide a medium for double electron capture for the alpha particle born at 3.5 MeV by the D-T reaction via the double charge exchange reaction:

Such an idea is intriguing in that electron capture proceeds most readily when there is a velocity match between the projectile velocity and the captured electrons. For carbon, the inherent velocity of the K-shell electrons closely matches that of a 3.5 MeV He^{++} . Thus, it is not necessary to accelerate a neutral beam such as Li^0 to 6 MeV, a costly proposition, when the atomic properties of the target can be used.

Originally, the carbon pellet scheme looked extremely promising, as the electron capture primarily proceeds from the K-shell of the carbon, so that partially-stripped C^q+ in the ablation cloud with $q=0$ to $q=4$ would all yield the same result.

Our involvement in the project is to provide the cross sections necessary to accurately estimate the neutralized fraction of He^0 produced when an He^{++} traverses a carbon pellet plasma. The needed cross sections are not only the

double electron capture values for the reaction given above, but also the sequential one-electron capture cross sections for the reactions

and the competing ionization cross sections for the He^{+} and He° on the carbon plasma constituents. It was also necessary to calculate the K-shell capture relative to L- and higher shells in order to predict the equilibrium fractions.

We used the classical-trajectory Monte Carlo method with the newly developed model potentials described in the previous section to estimate the ionization cross sections. Then an atomic orbital calculation was used to obtain the single and double electron K- to K-shell transfer. These values were then used as input by Art Howald at GA to compute the neutral equilibrium fraction which was compared to Japanese CH_4 gas target data. Good agreement was found at 3.5 MeV, but serious differences occurred at lower energies.

We then reassessed our assumption of only K- to K-shell capture and provided another series of calculated cross sections for L- to K-shell capture from carbon to the alpha particle. At first light, this inclusion appears to remove the discrepancy. However, we will only be able to quantitatively confirm, or reject, our recent insight into the collision mechanisms when Art returns from Japan and includes our new values in his equilibrium code.

If this modeling study is successful, we will have generated the atomic physics data base needed for the carbon pellet diagnostic. The uncertainty for the project, however, is that it may now be necessary to know precisely the charge state distribution of the carbon ablation cloud in order to predict the He^0 neutral yield.

Along these same lines, we have been concerned about the energy and position (i.e., stopping power) for the alpha particle in the carbon plasma. Original estimates of the slowing down of the alpha by the carbon plasma diagnostic were based on solid targets, not a plasma with long-range coulomb interactions. To investigate this problem more fully, we have developed the capability to calculate stopping powers for ions in gases and solids at MeV energies. These calculations have been benchmarked against existing data and appear appropriate for a future application to the carbon pellet problem.

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ENERGY DEPOSITION BY ENERGETIC HEAVY-IONS IN MATTER

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A direct calculation of heavy-ion stopping powers has not been possible until the development of the n-body Classical Trajectory Monte-Carlo (nCTMC) method¹. This theoretical procedure explicitly follows the motion of the projectile ion, target nucleus, and target electrons through an ensemble of scattering events. It provides, for the first time, a method for simultaneously determining the angular distributions and energies of the recoil target ion, the projectile ion, and the ejected electrons. Post collision interactions are included in the method, along with the coupling between electronic and nuclear degrees of freedom.

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