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AN OVERVIEW ON COLLISION PROCESSES OF HIGHLY CHARGED IONS WITH ATOMS

PRESENT STATUS AND PROBLEMS

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I. INTRODUCTION

The collision physics of highly charged ions is, at present, a significant part of many research fields, such as astrophysics, controlled thermonuclear synthesis, heavy ion physics, etc. The role of highly charged ions and their collision processes in modern astrophysical studies can hardly be overemphasized; most of our knowledge about the physical state of different astrophysical objects (particularly those containing hot plasmas) has been gained on the basis of understanding the structure and collision properties of highly charged ions. The same methodological approach is used in the investigations of hot laboratory plasmas, associated mainly with fusion research. The highly charged ions are also used for testing the quantum electrodynamics at supercritical fields and for studies of the structure of super heavy quasi-atoms ($Z \gtrsim 170$).

The first studies of collision processes of multiply charged ions with heavy atomic particles (atoms, ions, molecules) were done by Bohr in 1948, in the context of the stopping power problem. However, a strong motivation for a detailed investigation of these processes came in the fifties, when it was realized that highly charged impurites may significantly impair achievement of

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high temperatures in tokamak fusion plasmas. Later on, the detrimental (energy loss, instabilities, etc.) effects of impurities in tokamak plasmas were unambiguously demonstrated, which led to significant changes in the design concepts of present and future large scale fusion machines. Although within the new tokamak concepts the impurity problem seems to be satisfactorily solved, multiply charged ions continue to play an important role in magnetic fusion research (in several different contexts). Additional strong stimulae for the investigation of highly charged ion - atom collision processes have come in the sixties and seventies from the needs to develop adequate ion sources for the new generation of charged-particle accelerators (for heavy ion nuclear physics studies), to understand the physical processes associated with the inertial confinement (laser- and particle-beam) approach to fusion, search for VUV and X-ray lasers, etc. Starting from the mid-seventies both theoretical and experimental studies of the highly charged ion atom collision processes have marked an exponential growth, which is still continuing, and which have brought a wealth of quantitative information. The results of these studies are reviewed in several recent reviews.

This paper provides a brief discussion on the present status of the collision physics of highly charged ions with atoms. The emphasis is on the main achievements in understanding and describing the most important collision processes, and as charge transfer, ionization and Auger-type processes, and even more on those open problems which, due either to their scientific or practical importance, represent challenges to current research in this field. The paper concentrates on general ideas and problems whose development and solutions have advanced or will advance our basic understanding of the collision dynamics of multiply charged ions with atoms.

The most prominent feature of any inelastic collision process of a

multiply charged ion with atoms is the involvement of a large number of interacting states in the problem. Despite the fact that there exists a natural large parameter in the problem (the charge of the ion), the theoretical descriptions are not facilitated considerably, since the potential energy which the ion brings into the collision is so large that many reaction channels become open and since, in the case of a many-electron target atom, this energy can be disseminated by very complex electron rearrangement processes involving both discrete and continuum states. Furthermore, the strong, long-ranged Coulomb interaction of a highly charged ion with atomic electrons prevents the use of conventional perturbation-expansion methods to the collision energy regions where relativistic effects become important. Therefore, the description of any inelastic process in the nonrelativistic region has to incorporate the effects of the strong coupling of many electronic states, either by a coupled-channel formalism or by invoking a certain distorted-wave approach in which second- and higher-order dynamical effects are included. The inherent multistate interaction character of highly charged ion-atom collisions is also reflected in experimental studies, demanding application of coincidence techniques for resolving the reaction channels and for determining the states of reaction products. These studies have also been inhibited by the lack of suitable sources of low-energy highly charged ions.

After almost ten years of extensive experimental and theoretical investigations of the collision processes of highly charged ions with atoms, the status of our understanding of the underlying physics is, in general terms, the following. For the best studied (at least theoretically) and structurally the simplest hydrogen atom fully-stripped ion systems, the charge transfer problem is understood quite well, and a number of powerful

theoretical methods have been developed for calculating of the total cross section for any collision pair. However, only a limited number of these methods are capable of producing state-selective-capture cross sections with a high accuracy. The ionization problem in the same one-electron collision system has also been adequately understood, but the methods for cross-sectional calculations are less developed and usually coupled with significant computational difficulties. This particularly holds for the adiabatic energy region (which is, however, of lesser practical importance, since charge exchange here is the dominant process). While from a theoretical point of view the processes in a one-electron system are the most tractable, their experimental investigation encounters difficulties in preparing atomic hydrogen targets.

Regarding the collision processes involving many-electron targets or projectiles, the situation is rather different. Although for charge exchange and ionization one can identify the basic transition mechanism in many particular collision systems, and in certain energy regions even formulate the corresponding scattering equations in general form, there is still a lack of well-elaborated theoretical methods for description of these processes which are able to provide sufficiently accurate cross sections. For many processes involving two- (or more-) electron transitions even the underlying dynamic picture is not yet clarified. This is particularly pertinent to the multiple Auger processes with strongly correlated electron transitions. A more detailed analysis of these classes of processes and a discussion of the main achievements and issues in their current investigations follow.

II. CHARGE EXCHANGE PROCESSES

One of the most studied processes between highly charged ions and atoms is the single electron transfer process

$$A^{Z+} + B \rightarrow A^{(Z-1)} + B^{+},$$

which is at the same time also the most important from a practical point of view. The following three groups of theoretical methods have been developed (or have been extensively used) in the past for description of this process:

(a) close-coupling methods, based either on a molecular or atomic basis set expansion. In certain limiting cases these methods allow formulation of simple analytical models for the process;

(b) higher-order perturbational methods, including distorted wave treatments and eikonal expansions;

(c) classical methods.

Within each of these approaches different versions have been used, depending on the complexity of the collision system, collision energy, and strength of the ionic field (the value of Z). Some of these methods are applicable only to a one-electron collision system. The best description of the process at low and intermediate collision velocities v ($v \ll v_o$, and $v \sim v_o$, respectively, where v_o is the classical velocity of bound electron) can be provided by the coupled-channel formalism. The major progress in the theoretical description of the low-to-medium energy range in the last several years has been in understanding the crucial role of the electron momentum transfer and in devising methods for its adequate inclusion in theoretical treatments. Although a uniquely accepted prescription of how to deal with the electron momentum transfer problem in the velocity region $0.1\ v_o \lesssim v \lesssim 1\ v_o$ is

still lacking, several practical alternatives have been proposed with well-established merits and limitations. The relationships of this problem to the boundary conditions for the charge exchange process, the size of molecular basis set, etc., have also been established. Many large-size, molecular-basis, close-coupling calculations have been performed for the electron capture problem in the hydrogen atom fully-stripped ion system with appropriate treatment of the electron translational motion. The most elaborate ones have been made for the C^{6+} + H and O^{8+} + H with 33 basis states.

In the region $v \gtrsim v_o$, appropriate expansion basis for coupled channel calculations is the orthogonalized two-center, atomic orbital basis. However, due to the increasing role of the continuum states in the capture process with increasing collision velocity, an adequate description can be achieved only if a very large number of states are included in the expansion. In order to reduce the basis and still retain the effects of high lying and continuum states, expansions over pseudostates have been employed with considerable success. The pseudostates are usually chosen to represent adequately the continuum at higher collision energies and/or the quasimolecular effects at lower energies. Suitably chosen pseudostate expansions have proved to be capable of giving a good description of the capture process within a close-coupling scheme, even using a moderate-size basis.

Since the numerical treatments of coupled-channel equations using either a molecular or atomic (implemented by pseudostates) basis are difficult to handle (particularly for many-electron collision systems) and are not able to provide insight into the general dependences of the cross sections upon dynamic parameters, analytical approaches to the multistate coupling problem have been developed using certain simplifying assumptions. Starting with

conceptually simple models, such as the absorbing sphere and decay models, this approach has recently led to an approximate analytical solution of the system of close-coupled equations, containing the multistate Landau-Zener theory and the decay model as limiting cases.

In the high energy collision region ($v >> v_o$), significant achievements have been made in summing parts of the pertubational expansion (the so-called strong potential Born theory), in obtaining a closed-form solution for the one-electron system within the eikonal-Brinkman-Kramers approximation, and in devising practical schemes to estimate the second term on the Born expansion for the T-matrix. Also, more convenient schemes have been developed to estimate the continuum distorted wave reaction amplitude.

In the intermediate energy region ($v \sim v_o$), the classical description of the electron capture process in atom highly charged ion systems has proved to be unexpectedly successful. For the hydrogen atom fully-stripped ion system two approaches have been developed: numerical solution of the Hamilton equations and analytical treatments based on the separability of the problem in the prolate spheroidal coordinates and the use of some statistical arguments. The success of classical descriptions probably originates from the high symmetry properties of the Coulomb field (one- and two-center Coulomb problem), reflected for the hydrogen atom, among others, in the equivalence of the groundstate electron momentum distributions in both classical and quantum mechanics.

In the theoretical treatments of the charge exchange processes, two aspects are always involved: an electronic-structure aspect, which defines the interacting states and the interaction potentials, and a dynamical aspect formulated in terms of the scattering equations or another equivalent form. The dynamical part of the collision problem is the same for any collision

system. However, the electronic-structure part is, in practice, considerably different for the one-electron and many-electron systems. The one-electron two-Coulomb center system at the present time may be considered as solved, whereas the generation of the electronic basis and the corresponding potentials and coupling interactions in many-electron colliding systems is a complex quantum-mechanical problem. Therefore, most of the charge exchange cross-sectional calculations have been performed for the hydrogen atom fully-stripped ion case.

The extensive theoretical and experimental investigations of the charge-exchange process have yielded abundant information about the total cross sections for different systems and a global picture of their general features. However, in order to get a more refined insight into the collision dynamics, as well as to meet the needs in some applied research fields, the investigations of the charge-exchange process are presently oriented toward the following problems: (i) capture into specific final states; (ii) scaling properties of the total and partial cross sections; (iii) clarification of some anomalies in the cross-sectional behavior.

The most important aspect of the state-selective-capture problem is the distribution of captured electrons over the final state quantum number. It is evident that the resonant (or quasiresonant) condition for the process at a given energy will lead to preferential population of one state (or a relatively small group of states). For $v \ll v_o$, the principal quantum number n_m of a preferentially populated final level is given approximately by $n_m \approx Z^{3/4} I_o^{-1}$, where $-I_o$ is the binding energy of the initial electron state. For $v \lesssim v_o$, the resonance condition gives $n_m = (Z/\sqrt{2I_o})\ f(v,v_o)$, where $f(v,v^o) \to 1$, for $v \sim v_o$, and $f(v,v_o) \to 0$ at $v \to \infty$. Thus, in the limit of high energies, the n-distributions are peaked at $n_m = 1$. Athough numerous

calculations of the partial cross sections $\sigma_n = f(n,v)$ exist, no analytical dependences of σ_n on n or v have so far been derived. Most of the calculations have been made for the hydrogen atom fully-stripped ion for which experimental measurements of the state selective capture are difficult. For many electron collision partners there are a few measurements of the partial cross sections, but only in the Li + He^{2+} case has a fair agreement with the theoretical predictions been obtained. The distribution of captured electrons over the angular momentum quantum numbers has been calculated for the one-electron system using different methods. Some insight has been obtained in the general behavior of these distributions with variation of the collision energy, but no decisive conclusions can be drawn. Experimental data are lacking to decide between widely dispersed theoretical results. The clarification of the problem of state selective capture remains one of the most challenging problems for both the theory and the experiment.

For practical applications it is important to know the scaling properties of total charge transfer cross section with respect to the charge Z of the projectile ion and the initial state electron binding energy. The investigations have shown that, generally speaking, in the region $v \lesssim v_o$, the cross section scales linearly with Z, whereas in the region of asymptotically high velocities it scales like Z^5. There is a large velocity domain ($2v_o \lesssim v \lesssim 20\ v_o$) in which the Z-scaling is not certain. Only in the region $2.5\ v_o \lesssim v \lesssim (3.5\text{-}4)\ v_o$ has a Z^3-scaling been demonstrated both theoretically and experimentally. The dependence of the Z-scaling on the atomic and dynamic parameters of the collision system in this wide velocity region has not yet been investigated. The cross-sectional dependence on the initial state electron binding energy, I_o, is a rather controversial matter, and insufficient experimental data are available, at present, to decide between

different alternatives. The structure of the colliding system has an essential, but still not clarified, influence on the form of I_o-scaling.

In the low energy region, the Z-dependence of the total cross section exhibits oscillations connected with the selectivity of the electron capture process. This connection, demonstrated both experimentally and theoretically, has not yet been elucidated. Even more puzzling are the experimentally observed oscillations in the Z-dependence of the total cross section at high collision velocities. There are some indications that these anomalies might be connected with the electronic structure of the projectile ion. However, the true physical origin of these oscillations is still unknown.

From a purely theoretical point of view, the problem of description of the electron momentum transfer in the charge exchange process (or the foundation and the best choice of the electron translational factors in the basis-set functions) is still unsatisfactorily settled and is probably one of the most challenging problems for the theory. Another group of problems is associated with the description of double and multiple electron transfer. Although some elements of the theory of two-electron capture have been formulated and important results on the coupling interactions obtained, many dynamical problems are still unresolved.

III. IONIZATION

The ionization processes in atom highly charged ion collisions are much less investigated than the electron capture ones. Due to the long-ranged character of the Coulomb field of a highly charged ion, the first term of the Born expansion becomes an accurate representation of transition amplitude only at extremely high collision velocities, where relativistic effects begin to be important. At lower energies, where the experiments are usually performed, an

adequate treatment of the intermediate and continuum states is required. Thus any coupled-channel description of the ionization process must represent the continuum by a number of suitably chosen pseudostates. Distortion of the continuum final electronic states by the target atom ionic core is also a strong effect which has to be incorporated in theoretical treatments.

The most important achievements in the description of the ionization process have been made in the last several years for the collision system of hydrogen atoms and fully-stripped ions. These achievements have been made within the close-coupling method using continuum pseudostates, the unitarized distorted wave approximation, and the classical trajectory Monte Carlo method. The developed close-coupling method uses only two discrete states (ground and resonant) and two continuum pseudo-states chosen in such a way as to reproduce the effective oscillator strength of the atom for ionization. Within the dipole approximation, the close-coupled equations can be solved aproximately, and the cross section is obtained in closed form. The dipole-approximation close-coupling method has revealed that the ionization cross section scales linearly with Z in the region around the cross-sectional maximum. The energy at which the cross-sectional maximum takes place also scales linearly with the projectile charge. Below the cross-sectional maximum, where the cross section exponentially decreases with the decreasing energy, the Z-scaling is a complex function of Z, while at energies above the maximum, the cross section obeys the Bethe-Born Z^2-scaling. We note that the linear Z-scaling of the ionization cross section in the region of its maximum differs from the predictions of the perturbation or impulse-type approximations, but it is consistent with the classical trajectory Monte Carlo calculations.

As for the cross-sectional scaling with respect to the initial state electron binding energy, I_o, the existing theoretical models for the process give different predictions. The dipole-approximation close-coupling theory predicts an $I_o^{-3/2}$ scaling in the region of cross-sectional maximum and an $\sim I_o^{-1} \ln I_o$ dependence in the Born region. For energies below the cross-sectional maximum, the I_o-scaling of the ionization cross section is more complex. The $I_o^{-3/2}$ scaling at moderate collision energies is also predicted by the classical model of Bohr, while at high energies the classical impulse approximation predicts an I_o^{-1} dependence of the cross section.

The significant differences in the Z- and I_o-dependences of the ionization cross section predicted by various models of the process and the absence of sufficiently accurate and broad-range experimental data to select between the theoretical predictions illustrate the present status of the ionization problem. Evidently new efforts, both experimental and theoretical, are needed to make an advancement in our understanding of the dynamics of the ionization process. As it concerns the theory, one of the possible approaches is to undertake elaborate close-coupling, large-size pseudostate expansion calculations for the intermediate- and low-energy regions. In the high energy region, improvements over the first-order perturbation theory may be achieved by more accurate treatment of distortion effects. In the case of complex atoms, correlation effects may play a significant role in ionization, as well as different electron correlated-type processes. The experimental investigations of these processes require multiple coincidence techniques, while theoretical studies may rely only on very extensive coupled-channel calculations or on some sophisticated models.

IV. TRANSFER IONIZATION

In slow collisions of multiply charged ions with a many-electron atom, the whole collision system can be mediated as a super-excited complex with the lower states vacant. Such a system can relax by a reorganization of the outer electronic shells and emission of electrons (to conserve the total electronic energy). The most characteristic process which can occur in the course of such a collision is the transfer-ionization process: a number of electrons are captured by the ion while other target electrons are ejected into the continuum. Multiple electron transition processes of this type have been observed recently and show very specific features: a pronounced collective character of the process, energy independence of the number of released electrons, very weak dependence on the electronic structure of the target, etc. These features indicate that the process is analogous to the potential electron emission from a metal when it is bombarded by slow ions. Some statistical arguments may also be invoked in describing the collective transfer-ionization phenomenon.

When only two electrons are involved in the transfer-ionization (one captured and one ejected), the mechanisms which may govern the process are the following: a double electron capture, followed by Auger relaxation of doubly excited projectile ion product, quasiresonant capture of one electron into an excited state, followed by its deexcitation with simultaneous emission of another target electron and, finally, direct electron capture into a low-lying projectile state with simultaneous ejection of another target electron. A phenomenological theory of these processes can be constructed by considering the initial states as quasistationary and adopting a nonadiabatic character during the evolution of the system. However, due to the problem of normalization of quasistationary states, consistent models for the transfer-

ionization process in its simplest form have not yet been developed. Some particular results, however, have been obtained in a few very simplified approaches. Thus, the process of transfer-ionization when either two or more electrons are involved is a great theoretical challenge. More experimental data are needed to clear up the main features of the process and its correlation with different atomic or collisional parameters.

V. OTHER PROCESSES

The charge transfer, ionization, and transfer-ionization processes are only the most investigated ones of a much broader spectrum of processes which may occur in atom highly charged ion collisions. The attention paid to them so far is connected with their role in various practical applications. Other processes have also recently attracted the interest of atomic physicists. For example, the conceptually relatively simple process of excitation has been investigated theoretically by the dipole-approximation close-coupling method and the unitarized distorted wave approximation. No experimental data have so far been reported for excitation with multiply charged ions ($Z > 3$). The electron-loss process (combined charge exchange and ionization) has also received in the past considerable attention both theoretically and experimentally. The problems associated with the low-energy charge exchange and high-energy ionization are equally pertinent to the electron loss process. Studies of the collision processes of high- and low-charged ions have also begun. All the above discussed processes have been studied also with molecular targets.

Particular attention has been given in the past several years to the processes associated with close, violent collisions of the partners in the multi-MeV energy region. The goal of these studies, performed with heavy

highly charged ions, is to reach the conditions where specific effects due to transient quasiatom (or relativistic quasimolecule) formations are expected. Some of these effects are the continuum X-ray radiation (already observed), charged vacuum polarization, dynamically induced and spontaneous (for Z of the quasi-atom higher than ~ 170) electron-position pair formation, etc. The last issue has been extensively investigated in particular. While dynamically induced positron emission has recently been observed, the attempts to observe spontaneous pair creation have failed (although the re n of critical combined charge of collision partners, $Z_c \sim 170$, has been reached).

VI. CONCLUSIONS

The above brief presentation of the current status of the collision processes between highly charged ions and atoms has shown that:

(a) Of all the possible processes that may occur in these collisions, the single electron transfer process has been the most investigated, and its dynamics are the best understood. Especially abundant is the theoretical information for the electron transfer in one-electron systems.

(b) The most challenging problems for present and future investigations of the charge exchange process are the state selective capture, the scaling laws in the intermediate energy range, and the Z-oscillations of total cross sections. The understanding of two- and more-electron capture processes is rather incomplete, and more investigations are expected.

(c) The single electron ionization and excitation processes are also relatively little investigated. The general methods of atomic collision theory when applied to these processes either are too cumbersome or oversimplify the dynamics. There is a need for developing specific theoretical methods which will reflect the physical conditions involved in

these processes (the large projectile charge, etc.) in a more direct way.

(d) Transfer-ionization and other Auger-type processes are presently only in their initial stages of investigation. New ideas are required for an adequate description of these processes, especially when multi-electron transitions are involved.

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