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Kinetic and spectral descriptions for atomic processes involving autoionizing resonances in high-temperature plasmas

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ABSTRACT

An investigation has been in progress on the influence of autoionizing resonances on atomic processes in high-temperature plasmas, particularly those encountered in magnetic- and laser-fusion research and in astrophysics. In the kinetic-theory description, account is taken of the indirect contributions of autoionizing resonances to the effective rates for excitation, de-excitation, ionization, and recombination. A microscopic kinetic-theory foundation is employed for the systematic reduction to the macroscopic radiation-hydrodynamics description. From the spectral perspective, particular emphasis has been directed at radiative emission processes from autoionizing resonances. These processes can give rise to resolvable dielectronic-recombination satellite features, which have been analyzed to determine plasma temperatures, densities, electric and magnetic-field distributions, and charge-state distributions. We also investigate radiative absorption processes, which play important roles in the denser plasmas encountered in laser–matter interactions. Particular emphasis is directed at radiative excitation processes involving autoionizing resonances, which can provide significant contributions to the non-equilibrium ionization structures and to the radiative absorption and emission spectra in the presence of intense electromagnetic fields. A reduced-density-matrix formulation has been under development for the microscopic description of the electromagnetic interactions of many-electron atomic systems in the presence of collisional and radiative decoherence and relaxation processes. A central objective is to develop a fundamental quantum-statistical formulation, in which bound-state and autoionization-resonance phenomena can be treated on an equal footing. An ultimate goal is to provide a comprehensive framework for a systematic and self-consistent treatment of non-equilibrium (possibly coherent) atomic-state kinetics and high-resolution (possibly overlapping) spectral-line shapes. This should enable a unified treatment for a broad class of atomic processes in laboratory and astrophysical plasmas covering extensive density and field regimes.

1. Introduction

Elementary transitions involving autoionizing resonances of many-electron atomic systems (in various stages of ionization) are known to play important roles in the determination of the atomic-state populations and the spectral intensities of radiative absorption and emission processes in high-temperature laboratory and astrophysical plasmas. We will be primarily concerned with the elementary atomic transitions that are illustrated in the energy-level diagram shown in Fig. 1. In this diagram, we indicate elementary transitions that can influence the atomic-state population densities of the bound states b and i, of the z- and $(z+1)$-times ionized atomic systems X^{+z} and $X^{+(z+1)}$, respectively. These transitions involve the autoionizing states a and a' of the atomic system X^{+z}, which is assumed to have at least two bound electrons.

The transitions between the autoionizing state a and the ionization continuum associated with the bound state i can occur by means of the radiationless electron-capture and inverse autoionization processes:

$$X^{+(z+1)}(i) + e^{-}(\varepsilon_i) \leftrightarrow X^{+z}(a). \quad (1)$$

At low densities, the initial atomic systems can be assumed to be predominantly in their ground states. Autoionization processes leading to the formation of an excited state j following radiationless electron capture can provide a resonant contribution to the rate for the electron-impact excitation of the transition $i \rightarrow j$. As a preliminary approximation, we will neglect the direct transitions between these states which involve three-body electron-capture and collisionally-induced autoionization processes, as well as the corresponding photon induced processes. At very high electron

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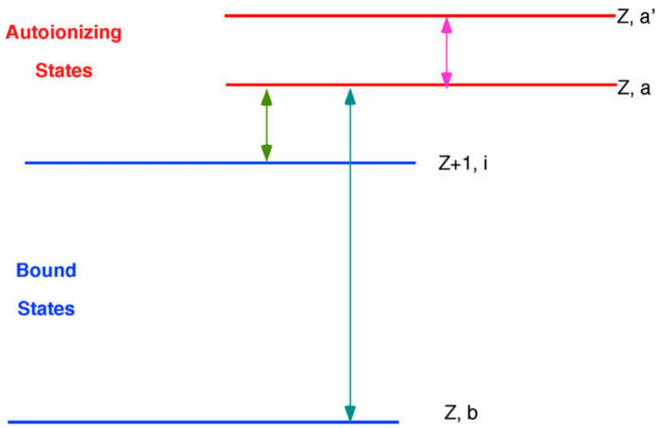

Fig. 1. Elementary transitions involving autoionizing states of many-electron atomic systems.

densities or for suitably intense electromagnetic radiation fields, these additional transitions must be taken into account. Although the autoionization rates decrease as n^{-3}, where n denotes the principal quantum number of the outer electron of the autoionizing state, the transitions involving large values of n can provide the dominant contributions to the rate for the two-step (resonant) dielectronic-recombination process [1].

The stabilizing transition from the autoionizing state a to the bound state b can occur by means of the spontaneous radiative-decay process:

$$X^{+z}(a) \rightarrow X^{+z}(b) + \hbar\omega. \tag{2}$$

The two-step dielectronic-recombination process [1] is accomplished through these stabilizing radiative transitions following radiationless electron captures. These radiative transitions appear in the emission spectra as satellites in the vicinity of a resonance line of the recombining atomic system. When the satellite features are resolvable from the associated resonance line, an analysis of the satellite and resonance line spectra can provide information on the physical properties within the emitting region, such as temperatures, densities, and charge-state distributions [2,3]. When the satellite features cannot be resolved, their contribution to the resonance line intensity must be taken into account as an effective contribution to the intensity of the associated resonance line. In the presence of a sufficiently intense electromagnetic radiation field at the angular frequency ω, it would be necessary to allow for the inverse photo-excitation process leading to the formation of the autoionizing state a, together with the stimulated radiatively stabilizing transition.

In order to evaluate the resonant contributions to the electron-impact ionization rates, which arise from autoionization following inner-shell-electron collisional excitation [4], it is necessary to take into account the inner-shell-electron-impact excitation and de-excitation processes:

$$X^{+z}(b) + e^{-}(\varepsilon_b) \leftrightarrow X^{+z}(a) + e^{-}(\varepsilon_a). \tag{3}$$

The inner-shell-electron collisional-excitation process is also an important mechanism for the formation of the dielectronic satellite lines [2,3], in addition to the radiationless electron-capture process. The collisional de-excitation process becomes competitive with the radiative stabilization process only at very high electron densities, which are encountered in laser-produced plasmas [5].

With increasing electron density, substantial modifications to the low-density corona-model expressions for the atomic-state population densities can occur due to the electron-induced collisional transitions between autoionizing states, corresponding to the elementary excitation and de-excitation processes:

$$X^{+z}(a) + e^{-}(\varepsilon_a) \leftrightarrow X^{+z}(a') + e^{-}(\varepsilon_{a'}). \tag{4}$$

Due to the greater spatial extent of the doubly-excited autoionizing states, especially with increasing value of the outer-electron principal quantum number n, the electron-induced collisional transitions can become competitive with autoionization and spontaneous radiative decay at much lower densities than in the case for the collisionally-induced stabilization process described by Eq. (3) [3,6]. Transitions between autoionizing states can also be induced by ion collisions. The effects of the plasma ions on spectral-line shapes have been traditionally described by invoking the quasi-static approximation in the general theory of line broadening by plasmas and introducing an electric microfield distribution function that must be determined from statistical mechanics [7]. The effects of stimulated radiative transitions between autoionization states can also play an important role in the presence of intense electromagnetic radiation fields.

The remainder of this paper has been organized in the following manner: In Section 2, we present a brief discussion of the analysis based on atomic and plasma kinetic theory, which leads to a reduced statistical description involving a limited number of atomic bound or autoionizing states and to the introduction of effective transition rates connecting these states in the set of equations for the atomic-state population densities. In Section 3, we discuss the simulation of the dielectronic satellite spectra for both the low-density and high-density regimes. A discussion of the determination of the charge-state distributions, which is based on the evaluation of effective ionization and recombination rates, is presented in Section 4. In Section 5, the evaluation of the radiative energy exchange rate is described, with consideration given to the radiative emission processes associated with bound–bound, free–bound, and free–free atomic transitions in plasmas. In Section 6, we discuss work in progress based on a reduced-density-matrix approach, utilizing Liouville-space projection-operator techniques. The objective of this approach is to provide a framework for a self-consistent determination of the non-equilibrium atomic-state population densities and the spectral-line shapes, and also a unified treatment of coherent atomic phenomena and environmental collisional and radiative decoherence and relaxation processes. Finally, our conclusions are presented in Section 7.

2. Indirect contributions to kinetic-theory transition rates

The kinetic-theory analysis of plasma processes is based on the partial-differential equations for the position and velocity distribution functions representing the various plasma particles and the photons. For atomic systems with bound electrons, it is necessary to consider the position and velocity distribution function for each atomic state. The fundamental many-body kinetic-theory formulation [8,9] is usually reduced to a one-body kinetic-theory description [10,11], with is based on a set of partial-differential equations for single-atom, single-electron, and single-photon distribution functions obtained by introducing suitable approximations for the many-body correlation (or collision) terms. This reduction procedure can be carried out within the framework of either classical statistical mechanics [12] or quantum-statistical mechanics (and quantum electrodynamics) [13]. However, the quantum-statistical approach is necessary for the precise treatment of bound atomic states. The single-body kinetic-theory equations are further reduced to hydrodynamics or radiation-hydrodynamics equations [11,14] by taking various velocity moments. On the left-hand side of the kinetic-theory equation for the single-body