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OPTIMAL TWO RYDBERG ATOM PAIR FOR NONSYMMETRIC PENNING IONIZATION: ALKALI CASE

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ABSTRACT

The paper studies the processes of Penning ionization (PI) involving Rydberg states of alkali atoms in cold gas media. Within the binary model framework, PI analysis has been performed in terms of the autoionization widths of a quasi-molecule formed by an atomic pair of collision partners. The obtained data on the PI cross-sections σ_i revealed interesting and structurally diverse features of σ_i behavior depending on the quantum numbers of the Rydberg states of the atomic pair subjected to a long-range dipole-dipole interaction. In contrast to previous works, which focused mainly on the hydrogen atoms case, a strong instability of σ_i with respect to the variations of orbital quantum numbers was observed.

1. INTRODUCTION.

In the physics of atomic collisions, relative energies of heavy particles in the interval from thermal to ultracold are conventionally divided into several ranges. They include: (i) (10^{-3} – 1) eV – the range of thermal and subthermal collisions in low-temperature plasmas; (ii) (10^{-6} – 10^{-3}) eV – the range of cold collisions in ionized gas; and (iii) (10^{-9} – 10^{-6}) eV – the range that is characteristic for ultracold gases and plasmas. Cold media are currently seen as promising physical objects in connection with a number of interdisciplinary applied problems, including both the issues of quantum information processing [1] and the physics of the unique ultracold plasma creation [2].

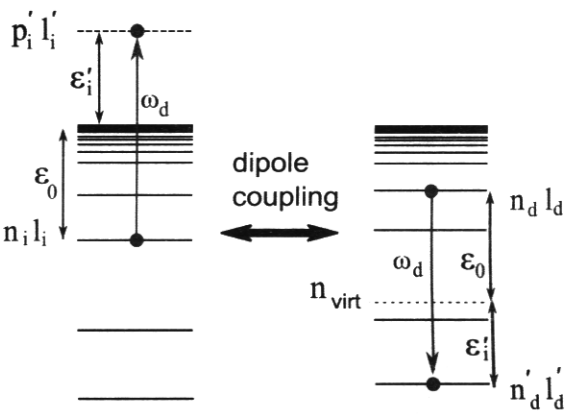

Fig. 1 Auger resonance process resulting in PI

Ultracold plasma is formed at times of the order 150 ns in the "frozen" Rydberg gas of alkali atoms placed in an magneto-optical trap and excited into the initial states with the principal quantum number of $n \sim 50$ and concentration $\rho_0 > 5 \cdot 10^{10}$ cm^{-3}. Under these conditions Penning ionization should be considered to be the most important type of collision processes that create primary charged particles in cold media:

$$A(n_d l_d) + A(n_i l_i) = A(n'_d l'_d) + A^+ + e(p'_i l'_i) \quad (1)$$

Long-distance dipole-dipole interaction between two alkali Rydberg atoms results in a free electron escaping due to the Auger process (see Figure 1): one of the atoms (d) undergoes a transition from state $n_d l_d$ to a deeper bound state $n_d' l_d'$, while the other atom (i) gains the released energy and jumps from state $n_i l_i$ to the continuum state $\varepsilon_i' l_i'$. Here n and l are the principal and orbital quantum numbers respectively.

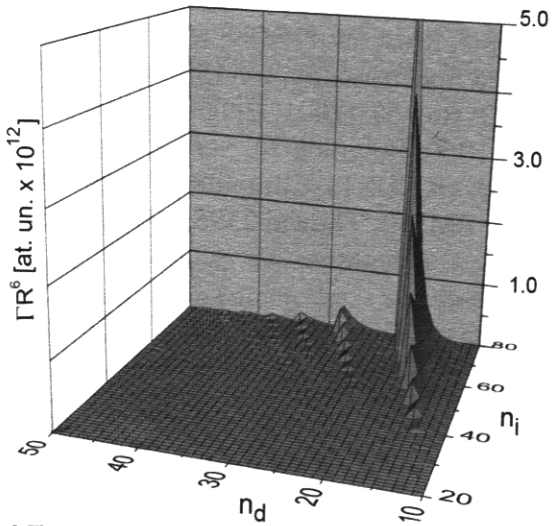

Fig. 2 The reduced PI width of a two-atom system as a function of the principal quantum numbers. The case of the s-p pair of Na atoms.

2. CROSS SECTION OF PI

Our method for calculating PI (1) cross section is based on the Katsuura-Smirnov model [3, 4], in which the main dynamic variable is the autoionization width $\Gamma_N = \Gamma_N^{\%} / R^6$ of a pair of colliding atoms. If atoms are in quantum states $N \equiv \{N_d = n_d l_d, N_i = n_i l_i\}$ at fixed internuclear distance R, the reduced Penning width $\Gamma_N^{\%}$ consists of partial widths $\Gamma_{NN'}^{\%}$, corresponding to individual bound-free atoms transitions $N \to N'$ (see Figure 1): $\Gamma_N^{\%} = \sum_{N'} \Gamma_{NN'}^{\%}$. Partial widths (the atomic system of units are used in what follows)

$$\Gamma_{NN'}^{\%} = | D_{N_D' N_D} |^2 \frac{c\sigma_{ph}}{\pi | \omega_d |} \qquad (2)$$

include dipole matrix elements $D_{N_D' N_D}$ for the bound d-atom transitions and the photoionization cross section σ_{ph} for the i-atom, in accordance with its transition into continuum. Frequency ω_d of partial atomic transitions determines the energy that the d-atom transfers to the i-atom (see Figure 1) upon the dipole-dipole interaction. The ionization condition means $\omega_d \geq \varepsilon_0$, where ε_0 is the i-atom binding energy. The dotted line n_{vir} in Figure 1 shows the position of an imaginary level that lies below the $n_d l_d$ state by ε_0 value and, therefore, determines the position of the ionization limit: $n_d' < n_{vir}$.

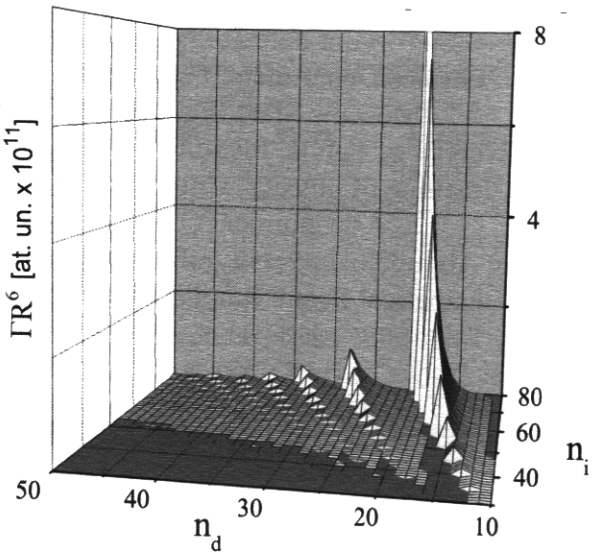

Fig. 3 The same as for Fig. 2 in the case of the s-s pair of Na atoms.

In Katsuura-Smirnov model, the cross-section σ_i of PI, subject to the long-range dipole-dipole interaction, is determined directly by width $\Gamma_N^{\%}$

$$\sigma_i = 3.37 \times \Gamma_N^{\%/5} / v^{2.5}, \qquad (3)$$

where v is the relative velocity of colliding Rydberg particles. Thus, the identification of PI features is associated with the analysis of $\Gamma_N^{\%}$ behavior for different quantum configurations of atomic pairs.

Paper [5] suggests simple quasi-classical formulas for calculating radiation constants of optical transitions in alkali atoms. Those formulas were used in the investigations of PI involving rubidium atoms for symmetric pairs ($n_d = n_i$) [6]. A detailed analysis of PI for asymmetric collisions ($n_d \neq n_i$) of hydrogen atoms was carried out in [7].

3. RESULTS AND DISCUSSION

Figures 2 and 3 show the calculations of the reduced autoionization width $\Gamma_N^{\%}$. for a pair of

Rydberg sodium atoms which form different states of a quasimolecule in relation to the orbital quantum numbers l. The surface in Figure 2 represents the dependence of $\Gamma_N^{\%}$ on the atomic pair principal quantum numbers n_d, n_i for the s-p pairs configuration ($l_d = 0, l_i = 1$). Figure 3 corresponds to s-s pairs ($l_d = 0, l_i = 0$). Figures 2 and 3 demonstrate the strong $\Gamma_N^{\%}$ dependence (by an order of magnitude) on the orbital quantum numbers. This property is inherent only in alkali atoms and is not observed in the case of hydrogen atoms [7].

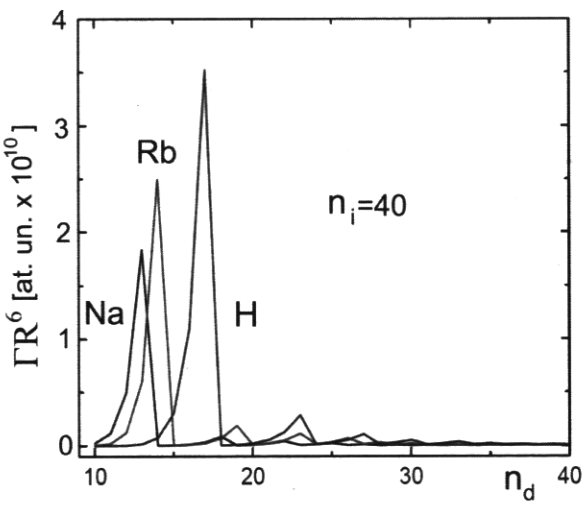

Fig. 4 The reduced PI width as a function of the d-atom principal quantum number while the i-atom one is fixed. The case of s-s pairs.

Noteworthy is a well-observed oscillatory structure of $\Gamma_N^{\%}$ with variations of both n_d and n_i, which is expressed in a mountain-like form of surfaces $\Gamma_N^{\%}$: a chain of ridges (peaks) separated by deep valleys (minima). These oscillations are among PI characteristic features. They are caused by the nonlinear dependence of the optical transitions parameters entered into the relation (2) on the atomic pair quantum numbers [6, 7]. A widely known property of both dipole matrix elements $D_{N_D' N_D}$ (ω_d) [7] and photoionization cross-sections $\sigma_{ph}(\varepsilon_i')$ [8] is their rapid decrease when arguments increase. Therefore, the appearance of $\Gamma_N^{\%}$ peaks corresponds to the realization of the photoionization threshold values $\varepsilon_i' = 0$, which in Figure 1 means superimposition of the real state $n_d' l_d'$ on the virtual level n_{virt}. Their divergence leads to the decrease of $\Gamma_N^{\%}$, while the convergence results in $\Gamma_N^{\%}$ growth, i.e. in oscillations.

The nature of the curves in Figures 2, 3 indicates the emergence of a paradoxical phenomenon that contradicts the classical intuitive notions of quantum states. The larger the atom sizes ($\sim n^2$), the larger the dipole moments associated with them should be. And the more effective the processes stimulated by dipole-dipole interaction should be, in particular ionization process. For almost symmetric ($n_d \approx n_i$) collisions these expectations are fulfilled, and the simultaneous growth of the principal quantum numbers of atomic pairs is accompanied by $\Gamma_N^{\%}$ growth.

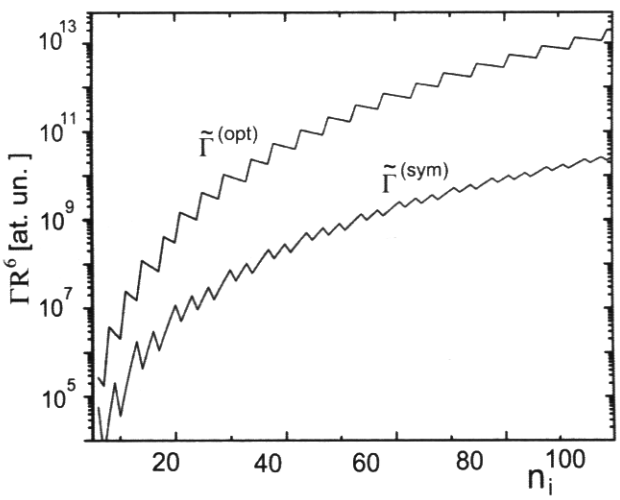

Fig. 5 Comparison of reduced widths values for symmetrical (sim) and optimal (opt) s-p pairs of Li atoms.

For fixed sizes of an i-atom, the situation, however, changes drastically, as illustrated in Figure 4. It shows the growth of $\Gamma_N^{\%}$ when the size of the de-excited d-atom for s-s pairs of H, Na and Rb atoms collapses. This is a purely quantum effect [7], caused by a decrease "on average" of arguments ω_d and ε_i' for radiation constants in Eq. (2) as the values of n_d decrease. For each atom type, the existence of $n_d^{(opt)}$ value, which is optimal for an i-atom ionization, can be seen. For this value $n_d^{(opt)}$ the maximum peak $\Gamma_{(opt)}^{\%}(n_i)$ of the reduced width of the pair arises. The realization of the optimal pair ($n_d^{(opt)}$, n_i) corresponds to the coincidence of the energy of the virtual level n_{virt} and the energy of $n_d' l_d'$ state, which is nearest from below to the initial $n_d l_d$ state (see Figure 1):

$$\gamma_d^{(min)} \left(n_d^{(opt)} - \delta_{l_d} \right)^{-3} = \left(n_i - \delta_{l_i} \right)^{-2} / 2 \quad (4)$$

Here, δ_l is the quantum defect of the l-atomic series. The positive parameter $\gamma_d^{(min)} > 0$ assumes

a minimum value for the effective quantum numbers difference Δn^* between the l_d- and l_d'-series ($n^* = n - \delta_l$).

Relation (4) describes well the position of $n_d^{(opt)}$ for all three atoms shown in Figure 4. The question by how many times the PI efficiency jumps when the symmetric pair ($n_d = n_i$, n_i) is replaced by the optimal one ($n_d^{(opt)}$, n_i) was considered in [7] for the case of a hydrogen atom. The obtained relation

$$\Lambda(n_i) = \Gamma^{(opt)}(n_i) / \Gamma^{(sym)}(n_i) = n_i \quad (5)$$

for the corresponding widths predicts a possible increase of PI by orders of magnitude for the asymmetric collisions of Rydberg atoms. Penning ionization intensification for asymmetric pairs of alkali atoms is clearly seen in the case of lithium atoms (Figure 5). The corresponding gain Λ turns out to be higher than for hydrogen atoms, and at $n_i \sim 100$ reaches three orders of magnitude.

As a reference, we give the conversion factor from the atomic system of units in SI for the PI reduced width $\Gamma_N^{(opt)}$: 1 at. un. = $0.906 \cdot 10^{-45} m^6 s^{-1}$.

4. CONCLUSION

The paper studies the features of Penning ionization in cold gas media of alkali atoms. In contrast to the case of hydrogen atoms, the corresponding autoionization widths show a drastic dependence (by an order of magnitude) on the orbital quantum numbers of Rydberg atoms, a subject to a long-range dipole-dipole interaction. An important feature of the PI is the nontrivial dependence of its efficiency on the size of colliding particles. We have found optimal, highly asymmetric configurations of Rydberg pairs, which lead to explosive intensification (by several orders of magnitude) of free electron escaping due to PI processes. This property makes Penning ionization an important source of primary charged particles when a cold Rydberg medium evolves into a cold plasma.

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