Interference between dielectronic and radiative recombination of Be-like highly charged ions

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We perform a systematical study for the polarization of x rays emitted when a free electron is captured by Be-like highly charged ions theoretically. We focus on the dielectronic recombination of the $J = 1/2 \rightarrow J = 1/2$ transition and its polarization is zero due to axial symmetry. Including the interference between the dielectronic and radiative recombinations, the polarization changes dramatically when the electron energy crosses the resonant energy. By comparing the simulations with or without certain interactions, we found that the Breit interaction is not important even for very high-Z ions. For low-Z ions, the configuration interaction of the dielectronic recombination states affects the polarization greatly, while for high-Z ions the configuration interaction of the ground state of Be-like ions plays an important role.

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I. INTRODUCTION

Interference between the same initial and final states via different paths is the core of quantum mechanics. The phenomenon, like one bound state embedded into a continuum background, covers broad research fields, from atomic physics [1] to solid-state physics [2]. The interference was observed between both the same partial waves [3] and different partial waves [4]. The dielectronic recombination (DR) (bound state) embedded into the radiative recombination (RR) when a free electron is captured by a highly charged ion (HCI) is a typical example. The x ray can be emitted directly from the RR (nonresonant) or DR (resonant) state. The interference between DR and RR results in the Fano profile [1]—an asymmetric distribution of the total capture cross section as a function of photon energies.

Since the emitted x ray from HCI can be used for the diagnostics of plasma [5,6] and astrophysics [5,7,8], the HCIs created in an electron-beam ion trap (EBIT) have been a hot topic for atomic and plasma physics. Such a study provides a unique way to study many fundamental processes, like electron-ion collision as well as the fundamental interactions, like the Breit interaction [9], quantum electrodynamics effects, and nuclear size. By analyzing the emitted x-ray energy distribution and its polarization, one can identify the role of different interactions, which cannot be easily observed in neutral atoms. With the newly developed Compton polarimeter [10], the observation of RR polarization in Tokyo-EBIT [11] was reported [12].

We are more interested in the DR emission since it is a resonant process and both its energy and polarization depend sensitively on the specified transitions and atomic ion species. The DR emission contains more information than the RR emission so it provides a good playground to study high-order interactions, like Breit interaction [13]. Since the DR is a resonant process and it is orders of magnitude stronger than the RR, the interference between the dielectronic and radiative recombinations in HCIs was ignored in most of the polarization studies. For the Be-like $J = 1/2 \rightarrow J = 1/2$ DR transition, the polarization is zero since the initial state is isotropic, and most existing experiments [14–16] focused on the $J = 3/2$ and $5/2$ DR states. Note that there are different name conventions, and we use the name of the ion states in the initial state, not the photoionization initial state. There were also some reports on the polarization of $J = 3/2$ and $5/2$ DR states named B-like ions [17–19]. In all those studies, no one studied the polarization of the $J = 1/2$ DR state and no one studied the interference between DR and RR either. Recently, a strong polarization has been observed from a $J = 1/2$ to $1/2$ Be-like Pb DR transition, which should be zero due to axial symmetry. The unexpectedly large polarization is attributed to the quantum interference between the DR and RR transitions [20].

Conceptually, it is difficult to distinguish the DR and RR contributions separately since there are three terms involved, DR only, RR only, and the interference between the two. When one process is dominant, like DR at the resonant energy, RR contribution can be neglected. This is the case for the x-ray emission from DR at the resonant energy since the DR yields are two to four orders larger than the ones from RR, so in almost all theoretical studies the interference between DR and RR was ignored, yet the calculated polarizations [21,22] were still in reasonable agreement with the measurements [23,24]. When the RR and DR polarizations differ significantly, we will ask how the polarization changes from RR dominant to DR dominant and then back

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TABLE I. Configurations used in the simulation. In the following discussion, sc stands for single configuration simulations in which only the configurations set in bold are used, and mc stands for multiconfiguration simulations, in which all the configurations in the table are used.

State	Configuration	J	State	Configuration	J
$\Psi_{\rm F}$	$1s^22s^22p_{1/2}$	1/2			
				$\mathbf{1s^22s^2\epsilon s}$	**1/2**
$\Psi_{\rm DR}$	$\mathbf{1s2s^22p_{1/2}^2}$	**1/2**	Ψ_s	$1s^22p_{1/2}^2\epsilon s$	1/2
	$1s2s^22p_{1/2}2p_{3/2}$	1/2		$1s^22p_{3/2}^2\epsilon s$	1/2
	$1s2s^22p_{3/2}^2$	1/2			
				$\mathbf{1s^22s^2\epsilon d_{3/2}}$	**3/2**
$\Psi_{\rm A}$	$1s^22s2p_{1/2}\epsilon p_{1/2}$	1/2	Ψ_d	$1s^22p_{1/2}^2\epsilon d_{3/2}$	3/2
	$1s^22s2p_{3/2}\epsilon p_{1/2}$	1/2		$1s^22p_{3/2}^2\epsilon d_{3/2}$	3/2

to RR dominant again when the electron energy crosses the resonance.

Meanwhile, early studies [21,22] showed that DR polarization is sensitive to the Breit interaction for Li-like ions. Without considering the Breit interaction, none of the measured DR polarization agrees with the Coulomb interaction-only simulation. For most of the DR emissions, the experiments are in reasonable agreement with the simulations without the interference between DR and RR [14,15]. Therefore, we have to answer under which conditions the interference between DR and RR is important. In this paper, we present our systematical studies of the polarization of DR transitions of Be-like ions. The polarization changes from RR dominant to DR dominant, then back to RR dominant again. Such prediction can be verified by future experiments.

II. THEORETICAL METHOD

In the radiative capture process, we fix the electron beam direction and investigate the polarization of the x ray emitted perpendicular to the electron beam. If we reversed the time, it is equivalent to the photoionization of the target by a linearly polarized x ray. Therefore, the DR and RR processes are the inverse processes of photoabsorption involving an autoionization state, which has been studied extensively for neutral atoms. Thus we start with the photoabsorption processes. Within the dipole approximation, the photoionization cross section by a linearly polarized light can be expressed as [25]

$$\frac{d\sigma}{d\Omega} = \frac{\sigma_T}{4\pi}[1 + \beta P_2(\cos\theta)], \tag{1}$$

with σ_T the total photoionization cross section, β the asymmetry parameter, and θ the angle between the ejected electron momentum and the electric field of the incident light. The detailed expressions of σ_T and β depend on the target and the initial and final states. The general expression of the photoionization is given in Ref. [26] and the general form of DR polarization is given in Ref. [27]. For the present paper, all states involved are listed in Table I as four groups: the final state ($\Psi_{\rm F}$), initial states with s (Ψ_s) or $d_{3/2}$ (Ψ_d) continuum waves, DR states ($\Psi_{\rm DR}$) with $J = 1/2$, and the Auger states ($\Psi_{\rm A}$) after the nonradiative decay of the DR states. The Auger states are used to calculate the nonradiative lifetime of the DR states. The total cross-section and asymmetry parameters for Be-like ions are expressed as [28,29] (atomic units $m_e = \hbar = e = 1$ are used unless otherwise stated)

$$\sigma_T = \frac{8\pi^2}{3c\omega}(|a|^2 + |b|^2), \quad \beta = \frac{|b|^2 + 2\sqrt{2}\mathrm{Re}(a^*b)}{|a|^2 + |b|^2}, \tag{2}$$

with the reduced transition matrix elements

$$a = \langle\Psi_{\rm F}||T^k||\Psi_s\rangle, \quad b = \langle\Psi_{\rm F}||T^k||\Psi_d\rangle, \tag{3}$$

c the velocity of light in vacuum, and ω the x-ray energy. Here the transition initial states can be written as

$$\begin{aligned}|\Psi_c\rangle &= C_1|1s^22s^2\rangle + C_2\big|1s^22p_{1/2}^2\big\rangle + C_3\big|1s^22p_{3/2}^2\big\rangle,\\ |\Psi_s\rangle &= |\Psi_c\ \epsilon s\rangle, \quad |\Psi_d\rangle = |\Psi_c\ \epsilon d_{3/2}\rangle.\end{aligned} \tag{4}$$

The DR state can be expressed as

$$\begin{aligned}|\Psi_{\rm DR}\rangle = {}& D_1\big|1s2s^22p_{1/2}^2\big\rangle + D_2|1s2s^22p_{1/2}2p_{3/2}\rangle\\ &+ D_3\big|1s2s^22p_{3/2}^2\big\rangle.\end{aligned} \tag{5}$$

The coefficients C_i and D_i are obtained by the configuration interaction. The transition operator T^k including autoionization is written as [30]

$$T^k = \hat{d} + \hat{d}\frac{|\Psi_{\rm DR}\rangle\langle\Psi_{\rm DR}|}{\epsilon - \epsilon_r + i\Gamma/2}V_{ee}, \tag{6}$$

with $\hat{d}$ the dipole operator in velocity form [31,32], and ϵ and ϵ_r the electron energy and the resonant energy. V_{ee} is the electron-electron interaction including the Coulomb interaction as well as the generalized Breit interaction (GBI) [33], which is expressed as

$$\begin{aligned}V_{ee}(\mathbf{r}_i, \mathbf{r}_j) = {}& \frac{1}{r_{ij}} - \boldsymbol{\alpha}_i\cdot\alpha_j\frac{\cos(\nu r_{ij})}{r_{ij}}\\ &+ (\boldsymbol{\alpha}_i\cdot\boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j\cdot\boldsymbol{\nabla}_j)\frac{\cos(\nu r_{ij}) - 1}{\nu^2 r_{ij}},\end{aligned} \tag{7}$$

with ν the virtual photon energy between the two electrons. If we set $\nu = 0$, we call it the Breit interaction in the zero-frequency limit (BI0). If we only consider the electron-electron Coulomb interaction, we notate it as C only. The reduced transition matrix elements in Eq. (3) can be recast as

$$\begin{aligned}a &= \langle\Psi_{\rm F}||\hat{d}||\Psi_s\rangle + \frac{\langle\Psi_{\rm F}||\hat{d}||\Psi_{\rm DR}\rangle\langle\Psi_{\rm DR}||V_{ee}||\Psi_s\rangle}{\epsilon - \epsilon_r + i\Gamma/2}\\ &= a_{\rm RR} + a_{\rm DR},\end{aligned} \tag{8}$$

$$b = \langle\Psi_{\rm F}||\hat{d}||\Psi_d\rangle = b_{\rm RR}. \tag{9}$$

Evaluation of the reduced matrix elements in Eq. (3) needs the coupling coefficients of the angular momenta, which are calculated by the ANCO package [34] and the radial wave functions, which are obtained by a relativistic density-functional theory [35]. The free-electron wave function is calculated numerically from the optimized effective potential [30] and the phase shift is obtained by matching the numerical wave function to the asymptotic form of the relativistic Coulomb wave functions. .

The first term $a_{\rm RR}$ in Eq. (8) stands for the radiative recombination, the second term $a_{\rm DR}$ stands for the dielectronic recombination, and Γ is the total lifetime of the DR state, including radiative and nonradiative ones. For the inverse process, the radiative capture cross section is expressed as [36]

$$\sigma_T^r(\epsilon) = \frac{g_f}{g_i}\frac{\omega^2}{\epsilon^2 + 2\epsilon c^2}\sigma_T(\omega). \tag{10}$$

Here g_i and g_f are the multiplicities of the transition initial and final states. The polarization of the emitted x ray at 90° to the electron beam direction is related to the asymmetry parameter as

$$P(\epsilon) = \frac{3\beta}{4+\beta}, \tag{11}$$

which is a function of the incident electron energy. We rewrite β in Eq. (2) explicitly as

$$\beta = \frac{|b_{\rm RR}|^2 + 2\sqrt{2}{\rm Re}[(a^*_{\rm RR} + a^*_{\rm DR})b_{\rm RR}]}{|a_{\rm RR} + a_{\rm DR}|^2 + |b_{\rm RR}|^2}. \tag{12}$$

If we set $a_{\rm DR} = 0$, we get

$$\beta_{\rm RR} = \frac{|b_{\rm RR}|^2 + 2\sqrt{2}{\rm Re}[a^*_{\rm RR} b_{\rm RR}]}{|a_{\rm RR}|^2 + |b_{\rm RR}|^2}. \tag{13}$$

If we remove the RR part by setting $a_{\rm RR} = 0, b_{\rm RR} = 0$, we get $\beta_{\rm DR} = 0$ since it is a $J = 1/2 \rightarrow 1/2$ DR transition. In most experiments [14,15], the DR polarization is measured by removing the RR background while the interference with RR is still included. In such a case, we define the DR asymmetry parameter including the interference with RR as

$$\beta_{\rm DR/w} = \frac{2\sqrt{2}{\rm Re}[a^*_{\rm DR} b_{\rm RR}]}{|a_{\rm RR} + a_{\rm DR}|^2 - |a_{\rm RR}|^2}. \tag{14}$$

Note that this definition is only valid around the resonant energy. In Eqs. (12)–(14), we can calculate the polarization of the DR only, which is zero, or RR only ($\beta_{\rm RR}$), the total one including the interference between the two (β), as well as the one by removing the RR background ($\beta_{\rm DR/w}$). Meanwhile, we can use the initial state and DR state of a single configuration (set in bold in Table I) or multiconfiguration from the mixed one including all the initial and RR states listed in Table I. Comparing the results with or without the Breit interaction, or configuration interaction, we can investigate their contributions to the DR polarization.

III. RESULTS AND DISCUSSION

Since the total radiative capture cross section $\sigma_T^r(\epsilon)$ and the polarization $P(\epsilon)$ of the emitted x rays are the two essential quantities to describe the process, we first analyze $\sigma_T^r(\epsilon)$ and $P(\epsilon)$ as shown in Fig. 1. The results in Fig. 1 are obtained by including the GBI and all the configurations listed in Table I. For the polarization, the upper panel of Fig. 1 shows that the polarizations at the two sides far away from the resonant energy are dominated by RR emission with positive values. This means that the polarization is mainly along the electron-beam direction. When the electron energy approaches the resonant energy, the polarization changes to zero, almost isotropic distribution, especially for low-Z ions. The minimum polarization starts at the resonant energy for low-Z ions and then moves to the low-energy side as atomic number Z increases (green dashed line). The minimum polarization also increases from 0.04 to 0.38 as Z increases from 30 to 95.

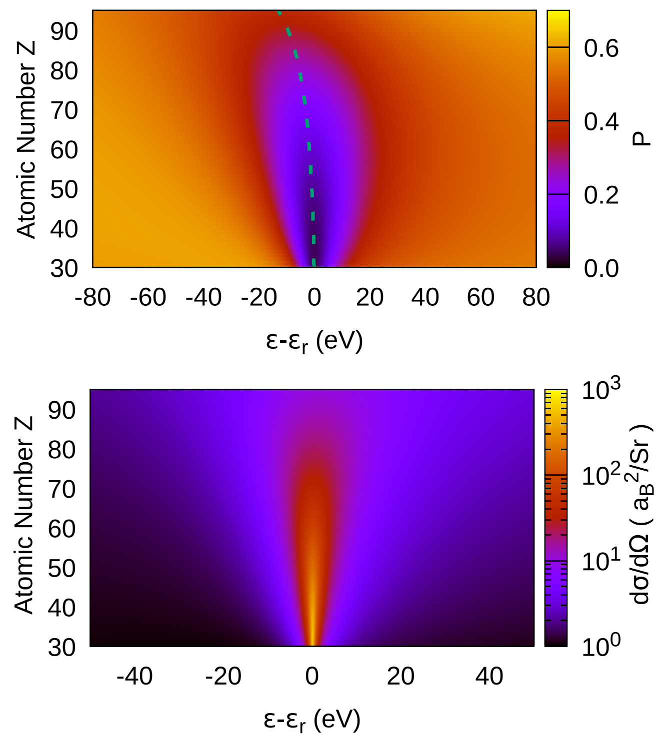

FIG. 1. Polarization (upper panel) and differential capture cross section (lower panel) of x rays emitted perpendicular to the electron beam by DR of Be-like ions around the autoionization energy of the $1s2s^22p^2_{1/2}$ $J = 1/2$ state. The green dashed line in the upper panel shows the position of the minimum polarization as a function of Z. $a_B = 5.29 \times 10^{-9}$ cm is the Bohr radius.

For the differential capture cross section when the photon is emitted perpendicular to the electron-beam direction, the lower panel in Fig. 1 shows that the cross section peaks at the resonant energy with a yield two or three orders stronger than the values at two sides. The peak is very narrow and shows almost no shift from the resonant energy. The low- and high-energy sides are not symmetric due to the interference between RR and DR, which results in the Fano profile [1]. The lifetime or the width of the DR looks broader in the figure since it is plotted on a log scale. The lifetime of the DR for $Z = 30$ is 0.6 eV and the value increases to 34.2 eV for $Z = 95$, roughly scaled by Z^4, dominated by the radiative decay.

Although Fig. 1 contains all the essential information, it is difficult to get detailed information quantitatively. To look for more details, we choose Be-Like Pb ($Z = 82$) ions as an example. The polarization and capture cross sections are shown in Fig. 2. Since the resonant energy calculated with GBI is 73.70 keV, different from the C-only value, which is 73.94 keV, we plot the polarization as a function of the energy difference between the emitted x-ray energy and the resonant energy. The resonant width for including the GBI is 18.83 eV and the value changes to 18.97 for C-only simulation. The polarization in Fig. 2 includes both the RR and DR contributions as well as the interference between the two. First we see that the dip of polarization has a broader distribution than

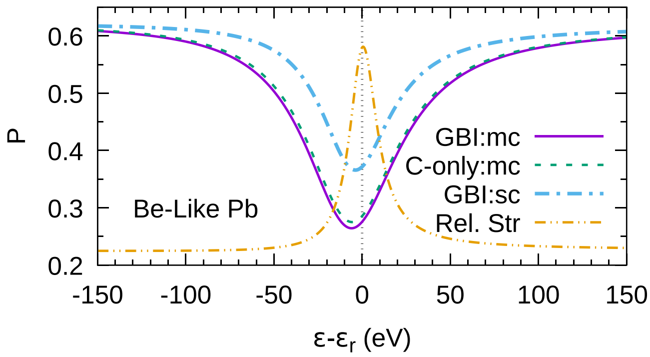

FIG. 2. Polarizations of Be-like Pb ions as a function of electron energy around the resonance of the $1s2s^22p_{1/2}^2$ $J = 1/2$ DR state calculated with various methods. The relative strength of the capture cross section is also plotted (dash-dotted curve).

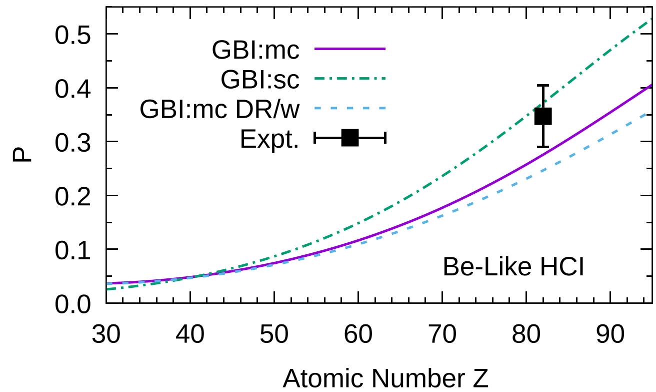

FIG. 4. Polarization of Be-like atomic ions for atomic number $Z = 30$–95 at the resonant energy. The experimental data for Pb ions [20] are also plotted.

the total cross section. Secondly, the configuration interactions affect the polarization greatly while the GBI is negligibly small. There is almost no difference between the results of GBI and BI0 so we only plot the results of the GBI. For the single configuration's results, we set $C_1 = 1.0$, $D_1 = 1.0$, and other coefficients are zero. Different from the Li-Like DR case [21–23], in which the GBI is important, the GBI effect can be neglected completely for Be-like ions, even for a very high-Z ion.

As we see in Table I, there are two kinds of configuration mixing in the simulation. One is the configuration interaction of DR states in Eq. (5), and the other is the configuration interaction of the initial core states in Eq. (4). Figure 3 shows the coefficients $C_{2,3}$ and $D_{2,3}$. We see that the configuration mixing of the initial core state is important for high-Z ions while the $1s2s^22p_{1/2}^2$ DR state is the dominant one. For low-Z ions, the configuration mixing of the three DR states is more important than the core state mixing. The two kinds of coefficients cross roughly about $Z = 40$. This can be easily understood since for low-Z ions the fine-structure splitting is smaller so the three DR states are close to each other in the energy domain, which results in a large configuration mixing for the DR states. As Z increases, the fine-structure splitting also increases and this reduces the configuration mixing of the DR states, while the configuration mixing of the initial core states $1s^22s^2$ and $1s^22p_{1/2}^2$ is relatively stable. Therefore, we concluded that the configuration mixing of the initial core states is important for high-Z ions as the energies of $2s$ and $2p_{1/2}$ are degenerate, while the configuration mixing of the DR states is important for low-Z ions, which is consistent with previous work [37,38], and $|C_2|$ and $|D_2|$ cross over at $Z > 40$. For even lower-Z ions, the LS coupling takes over the jj coupling and it is difficult to distinguish the DR states with $J = 1/2, 3/2$, and $5/2$. So DR spectra of low-Z ions were assigned with LS coupling.

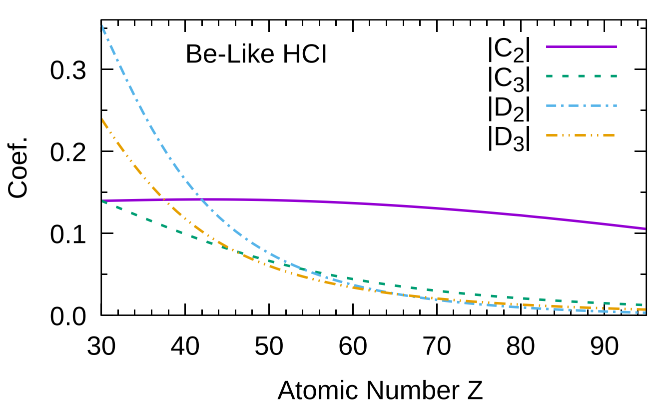

FIG. 3. CI coefficients (C_i, D_i) of initial and DR states as a function of atomic number Z.

Figure 4 shows the polarization of Be-like ions for atomic number $Z = 30$–95 with and without configuration interaction and the GBI term at the resonant energies. Since we already know that the GBI effect is negligibly small even for very high-Z ions, we skip the discussion about the GBI effect. It is interesting to see that the configuration interactions change the order of polarization. For low-Z (<40) ions, the polarization with the configuration interaction is larger than the one of the single configuration, while for high-Z (>40) ions the polarization with the configuration interaction is smaller than the one of the single configuration. Although in the figure, the polarization at $Z = 30$ does not change dramatically with or without the configuration interaction, the numerical value drops from 0.041 for multiconfiguration to 0.028 for single configuration, more than 50%.

The interference between RR and DR comes from $a_{\rm DR}$ and $b_{\rm RR}$. The phase difference between $a_{\rm DR}$ and $b_{\rm RR}$ is $\pi/2$ at the resonant energy [Eq. (6)]. Thus the interference can be enhanced when the phase difference between ϵs and $\epsilon d_{3/2}$ can compensate $\pi/2$ and also the relative strengths between $a_{\rm DR}$ and $b_{\rm RR}$ should be comparable. Those data were already shown in recent work [20] so we do not repeat the plot here. Indeed, we see that the ratio of $|a_{\rm DR}/b_{\rm RR}|$ decreases as Z increases. This results in a large polarization at the resonant energy as Z increases. The result is against our intuition that the DR is stronger for high-Z ions. Indeed the DR strength increases as Z increases. The decreases of the ratio mainly are due to the increase of the lifetime being faster as Z increases. We also see that the phase difference between ϵ_s and $\epsilon_{d_{3/2}}$ of the Pb ion is also around $\pi/2$. All these explain why the large polarization was observed in the DR $J = 1/2 \rightarrow J = 1/2$ transition for Be-like ions.

In summary, we have studied the x-ray polarization of dielectronic recombination embedded into radiative recombination when an electron is radiatively captured by a highly charged ion. The polarization changes from RR dominant to DR dominant, then back to RR dominant again. For the DR transition of Be-like ions, the generalized Breit interaction is negligibly small while the configuration mixing is important. Upon further analysis, we find the configuration mixing of the DR states is important for low-Z ions while the configuration mixing of the core states is important for high-Z ions. The crossover is at $Z = 40$. The interference between DR and RR may also affect other DR transitions and its contribution should be larger for high-Z ions. The present paper can be verified by future experiments.

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