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Relativistic calculation of dielectronic recombination for He-like krypton*

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Dielectronic recombination (DR) cross sections and rate coefficients of He-like Kr are calculated employing the relativistic flexible atomic code, in which autoionization rates are calculated based on the relativistic distorted-wave approximation and the configuration interaction is considered. The Auger and total radiative rates of some strong resonances are listed and compared with the results from multiconfiguration Dirac–Fock and Hebrew University Lawrence Livermore Atomic Code methods. The n^{-3} scaling law is checked and used to extrapolate rate coefficients. We also show the variation of DR branching ratio with different DR resonances or atomic number Z. The effect of radiative cascades on DR cross sections are studied.

Keywords: dielectronic recombination, rate coefficients, radiative cascade, n^{-3} scaling law
PACC: 3480L

1. Introduction

Dielectronic recombination (DR) is an important atomic process contributing to ion balance in high-temperature laboratory and astrophysical plasmas.[1−3] It is a two-step resonant process. When a free electron collides with an ion, it may be captured nonradiatively and transfer energy to a bound electron to form a doubly excited state. Subsequently, the state decays into a nonautoionizing state through radiative transition processes. These reactions have the form

$$\left(1s^2\right) + e^- \rightarrow \left(1snln'l'\right) \rightarrow \left(1s^2n''l''\right) + h\upsilon.$$

We choose krypton for a detailed study in this paper since it has recently been proposed as a coolant for the plasma edge regions of future tokamaks.[4] Several measurements and calculations on DR of He-like Kr have been reported. Chen[5] calculated the DR rate coefficients for the He isoelectronic sequence from C^{4+} to Mo^{40+} using multiconfiguration Dirac–Fock (MCDF) method. Fuchs *et al*[4] reported the measurement of DR cross sections for highly charged He-like, Li-like, Be-like, B-like, C-like Krypton ions, and also gave theoretical results employing the Hebrew University Lawrence Livermore Atomic Code (HULLAC).

The flexible atomic code (FAC), recently developed by one of the authors, has been successfully used to calculate indirect x-ray line formation process in Fe L-shell ions,[6] radiative recombination rate coefficients for bare through F-like isosequences of Mg, Si, S, Ar, Ca, Fe and Ni,[7] and dielectronic recombination rate coefficients for H-like through Ne-like isosequences of these elements.[8] In this paper, we calculate the DR cross sections and rate coefficients for Kr^{34+} ion using FAC. Our results are shown in good agreement with other calculations. Also we study the effects of configuration interaction and radiative cascades on DR cross sections, give the variation of DR branching ratio with different DR resonance and atomic number Z, and discuss the validation of n^{-3} scaling law for the extrapolation in the calculation of rate coefficients. In Section 2, we give the outline of the theoretical method. In Section 3, we give the results and discussion.

2. Outline of the theory

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The DR strength can be written as

$$S_{ij} = \frac{\pi^2\hbar^3}{m_e E_{ij}} \frac{g_j}{2g_i} A^a (j \to i)\, B_j^r, \qquad (1)$$

where j represents a doubly excited intermediate state, i represents the initial ground state. E_{ij} is the resonant energy, g_i and g_j are the statistical weights of states i and j. $A^a (j \to i)$ is the autoionization rate from level j to level i. The radiative branching ratio B_j^r can be written as

$$B_j^r = \frac{\sum_f A^r (j \to f)}{\sum_f A^r (j \to f) + \sum_k A^a (j \to k)}. \qquad (2)$$

$\sum_k A^a (j \to k)$and $\sum_f A^r (j \to f)$ are total Auger and radiative rates of state j. f represents a non-autoionizing state. Ignoring the detailed structure of the resonance profiles, the DR cross section is written as

$$\sigma_{ij}(E) = S_{ij}\delta (E - E_{ij}). \qquad (3)$$

To compare with experimental measurement, we convolve the above cross section with a Gaussian profile for the electron energy distribution.

In thermal plasmas, the rate coefficient is defined as

$$\alpha_i (T) = \sum_j \int_0^\infty v f(v,T)\, \sigma_{ij}(v)\, dv, \qquad (4)$$

where $f(v,T)$ is the Maxwellian distribution of electron velocities. Thus, using Eqs.(1), (3) and (4) we have

$$\alpha_i (T) = \frac{h^3}{(2\pi m_e kT)^{3/2}} \sum_j \frac{g_j}{2g_i} A^a (j \to i)\, B_j^r \times \exp(-E_{ij}/kT). \qquad (5)$$

In the present paper we employ FAC to calculate all the basic atomic data including energy levels, Auger and radiative transition rates.[8] FAC uses a relativistic configuration interaction approximation to calculate bound–bound processes of atomic systems. Autoionization processes are treated in the first-order perturbation theory using distorted-wave approximation for the continuum electrons. Such a treatment ignores the coupling between resonances and the continuum background, and assumes no overlap between different resonances. These approximations are expected to give accurate results for highly charged ions, such as He-like Kr.

3. Results and discussion

3.1. Auger and radiative transition rates

As the first step, the Auger and total radiative transition rates of some intermediate doubly excited states are calculated by FAC, and compared with the MCDF results of Chen[5] and the HULLAC results of Fuchs *et al.*[4] In Table 1, the autoionization and total radiative transition rates of some strongest 1s2l2l′ DR resonances calculated in the present work and those of MCDF and HULLAC are listed. The deviations between MCDF and FAC results are less than 7% in most cases.

Table 1. The autoionization and total radiative transition rates of some strongest 1s2l2l′ DR resonances calculated using MCDF,[5] HULLAC[4] and FAC.

Config. and term	$A_{ji}^a(s^{-1})$			$\sum A_{jf}^r + \sum A_{jd}^r(s^{-1})$		
	HULLAC	MCDF	FAC	HULLAC	MCDF	FAC $\left(\sum A_{jf}^r\right)$
$1s2s^2\ ^2S_{1/2}$	1.46×10^{14}	1.59×10^{14}	1.50×10^{14}	5.05×10^{13}	5.11×10^{13}	5.47×10^{13}
$1s2s(^3S)2p\ ^2P_{1/2}$	7.85×10^{13}	9.74×10^{13}	7.51×10^{13}	6.80×10^{14}	7.40×10^{14}	7.71×10^{14}
$1s2p^2\ ^4P_{5/2}$	7.11×10^{13}	7.08×10^{13}	7.24×10^{13}	3.50×10^{14}	3.87×10^{14}	3.91×10^{14}
$1s2p^2\ ^2D_{3/2}$	1.23×10^{14}	1.19×10^{14}	1.24×10^{14}	1.45×10^{15}	1.46×10^{15}	1.54×10^{15}
$1s2p^2\ ^2D_{5/2}$	9.91×10^{13}	9.89×10^{13}	9.78×10^{13}	5.26×10^{14}	5.09×10^{14}	5.44×10^{14}

3.2. The effect of configuration interaction

Configuration interaction (CI) can change the energy levels and transition rates, so it should be considered in calculation. In the present work, we only consider the DR from intermediate states n=2 ($\Delta n = 1$), so we make mixtures between all possible states of 1s2ln'l′ and 1s2l$(n'+1)$l′ configurations for n'=3, 4, 5; 1s2ln'l′ and 1s2l$(n'-1)$l′, 1s2l$(n'+1)$l′ configurations for n'=6, 7, 8, 9, 10.

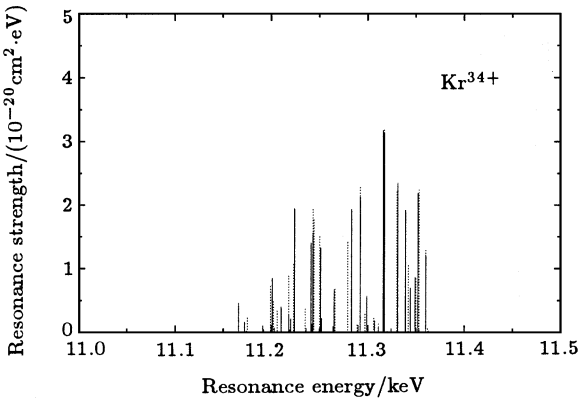


Fig.1. DR strengths of KLM resonance; solid lines are configuration-mixed values, and dotted lines are single configuration values.

From Fig.1 we can find that the energies and strengths of most DR resonances do change if CI is included. For some specific resonances, strengths may increase by a factor of 2 or decrease by a factor 3. But the calculation shows that the effect of CI on the total cross sections is minimal.

3.3. Radiative cascades

In many published theoretical work,[9,10] radiative cascades are not considered. It means that the radiative decays of intermediates state to doubly excited low-lying levels are not included in our calculation as show in Eq.(2), since these decays are usually weak radiative transitions and probably autoionize subsequently.[11] Here, we will discuss the effect of radiative cascades on the DR cross sections in detail.

Including all possible transitions, the radiative branching ratio has the exact form[12]

$$B_{\rm j}^{\rm r} = \frac{1}{\Gamma_{\rm j}} \sum_{\rm f} \left[A^{\rm r}({\rm j} \to {\rm f}) + \sum_{\rm d} \frac{A^{\rm r}({\rm j} \to {\rm d})}{\Gamma_{\rm d}} A^{\rm r}({\rm d} \to {\rm f}) \right], \qquad (6)$$

with

$$\Gamma_{\rm j} = \sum_{\rm f,d} A^{\rm r}({\rm j} \to {\rm f,d}) + \sum_{\rm k} A^{\rm a}({\rm j} \to {\rm k}), \qquad (7)$$

where intermediate state d is an autoionizing doubly excited state. $\Gamma_{\rm d}$ is the total decay rate of state d similar to $\Gamma_{\rm j}$.

In Ref.[11], the effect of radiative cascades was checked for $(2s2p)^7 3l3l'$ complex of Ne-like W and found to be less than 3%. So Behar suggested that the radiative cascades could be neglected for higher complexes. We find similar results for simple configurations $1s2ln'l'$ of He-like Kr. Figure 2 shows the calculated DR cross sections with and without cascades. The deviation between these two cross sections is less than 3%. Based on the analysis for the values of A^r, we find that $\sum_{\rm f} A^{\rm r}({\rm j} \to {\rm f})$ are mostly more than one order larger than $\sum_{\rm d} A^{\rm r}({\rm j} \to {\rm d})$ in strong resonances, and it results in the little effect of radiative cascade on total cross sections. So we can conclude that the calculation without radiative decays to autoionizing states is a quite good approximation and it will save a great deal of computation time.

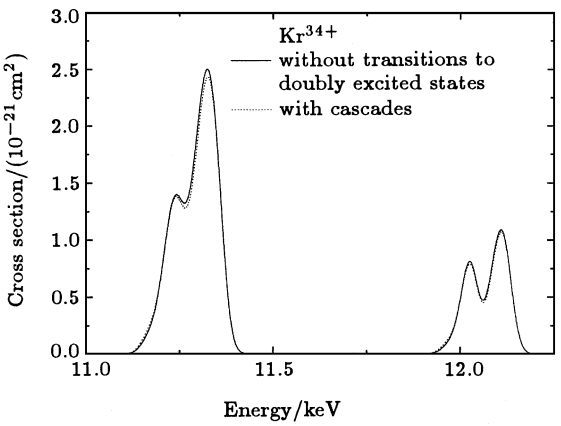


Fig.2. DR cross sections with and without radiative cascades, obtained by applying a 50eV FWHM Gaussian to the resonance strengths $S_{\rm ij}$.

3.4. DR cross sections

The calculated DR cross sections with $1s2ln'l'$ ($n' = 2 - 12$) intermediate states are shown in Fig.3. We compare the KLL resonances with the HULLAC calculation of Fuchs *et al*[4] in Fig.4 and find that the deviation between these two results is within 5%.

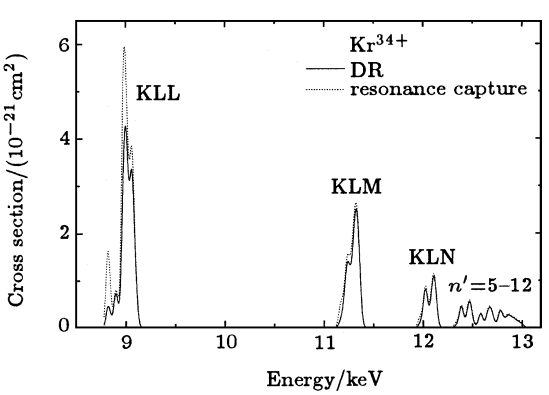


Fig.3. DR and resonance capture cross sections for Kr^{35+}, by applying a 50eV FWHM Gaussian to the resonance strengths $S_{\rm ij}$.

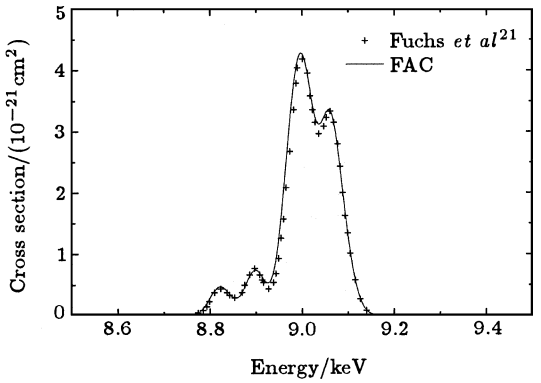


Fig.4. DR cross section of KLL resonance of our calculation compared with values obtained by Fuchs *et al* using HULLAC[4].

Figure 3 shows the variation of DR branching ratio with respect to n'. In the KLL resonances ($n' = 2$), the average DR branching ratio is about 0.72, and in KLM resonances ($n' = 3$), the average branching ratio is about 0.95. When $n' \geq 4$, the branching ratios are approximately equal to 1. Evidently, DR branching ratio increases as n' increases.

In order to find the dependence of DR branching ratio on atomic number Z, we have also calculated the DR cross sections for He-like Argon. Figure 5 shows the resonance capture and DR cross sections for Ar^{16+}. From Fig.5, we can see that the average DR branching ratio is about 0.26 in KLL resonances, and about 0.69 in KLM resonances. It is obvious that the DR branching ratio increases as Z increases.

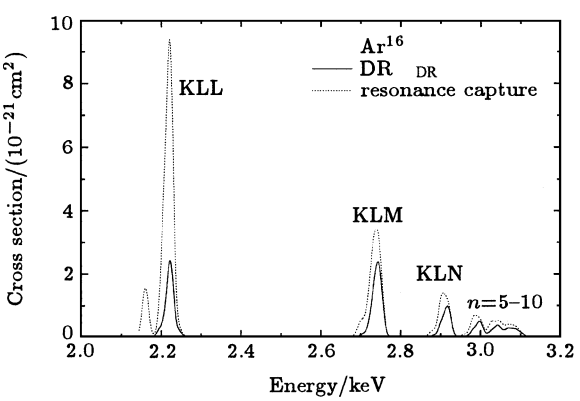


Fig.5. DR and resonance capture cross sections for Ar^{17+}, by applying a 50eV FWHM Gaussian to the resonance strengths S_{ij}.

3.5. n^{-3} scaling law

In the present work we only calculated the $\Delta n = 1$ DR resonances up to $n' = 12$. But the calculation of rate coefficient should include all intermediate levels $1s2ln'l'$ with $n' \to \infty$. We can extrapolate the DR rate coefficients based on the n'^{-3} scaling law of autoionization rates.[10,13] The reason for this extrapolation can be explained as follows.

For intermediate and high Z ions, the radiative branching ratio B_j^r approximately equals 1 when n' is larger. Thus, in these cases we can conclude from Eq.(1) that the resonance strength S_{ij} depends only on the autoionization rate A_{ij}^a. Since $A_{ij}^a \propto 1/n'^3$,[13] the resonance strength also goes as

$$S_{ij} \propto 1/n'^3. \tag{8}$$

From Fig.3 we can find that the difference of resonant energies E_{ij} is very small when $n' \geq 12$, so based on Eq.(5) the total DR rate coefficient of a KLn' resonance also goes approximately as

$$\alpha_i(T, n') \propto 1/n'^3. \tag{9}$$

Figures 6 and 7 show the variation of total strengths and rate coefficients of KLn' resonances as a function of n'. From the figures we can find that the n^{-3} scaling law is valid for both cases when $n' \geq 12$.

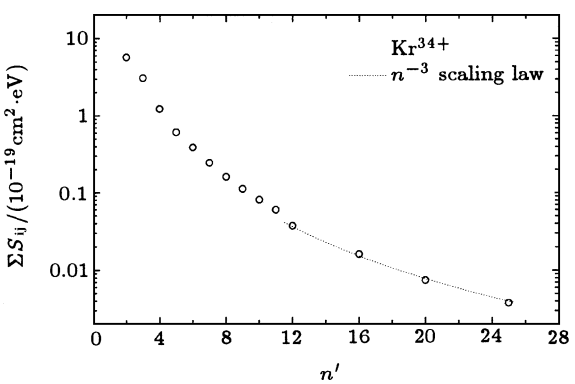


Fig.6. Total DR strength summed over intermediate states with the same principle quantum number.

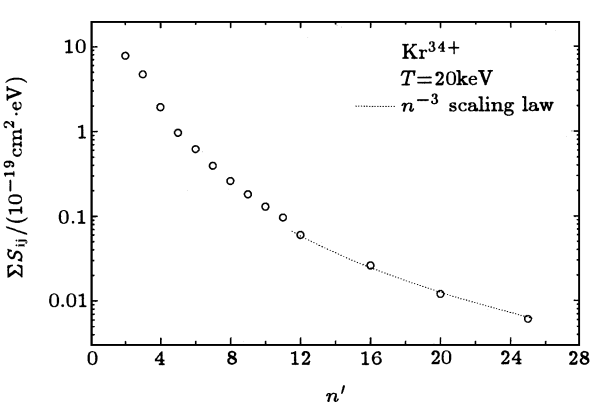


Fig.7. Total DR rate coefficient summed over intermediate states with the same principle quantum number.

Thus, the total DR rate coefficient can be approximated as

$$\alpha^{\rm tot}(T) = \sum_{n'=2}^{n'_{\rm s}} \alpha_{\rm i}(T, n') + \sum_{n'=n'_{\rm s}+1}^{\infty} (n'_{\rm s}/n')^3 \alpha_{\rm i}(T, n'_{\rm s}), \tag{10}$$

when $n' > n'_{\rm s}$, the n'^{-3} scaling law will become quite appropriate. Exactly, $n'_{\rm s}$ is not the same at different electronic temperature.[14] But since the error is quite small, we chose a unique $n'_{\rm max}$ as n'. Now Eq.(10) has the form[12]

$$\alpha^{\rm tot}(T) = \sum_{n'_{\rm calc}=2}^{n'_{\rm max}} \alpha_{\rm i}(T, n'_{\rm calc}) + \sum_{n'_{\rm ex}=n'_{\rm max}+1}^{\infty} (n'_{\rm max}/n'_{\rm ex})^3 \alpha_{\rm i}(T, n'_{\rm max}), \tag{11}$$

where $n'_{\rm calc}$ runs over all explicitly calculated DR resonances with intermediate state 1s2ln'l$'$ ($n' \leq n'_{\rm max}$, in the present work, we choose $n'_{\rm max} = 12$) and the second term is the contribution from all remaining levels.

Our calculation shows that when $n' \geq 12$ $n'^3\alpha_{\rm i}(T, n')$ becomes constant, so we use the average of $n'^3\alpha_{\rm i}(T, n')$ (n=12, 16, 20, 25) as $n'^3_{\rm max}\alpha_{\rm i}(T, n'_{\rm max})$. The contribution from the levels with $n' > 12$ is about 1.5% of total rate coefficient at T=7keV, and about 3% at T=25keV.

3.6. DR rate coefficients

Figure 8 shows the DR rate coefficients with some intermediate state ($n' = 2 - 6$) and total DR rate coefficient. Total rate coefficient evaluated using MCDF method by Chen[5] is also shown in Fig.8. Our total rate coefficient is larger than Chen's result by 9%.

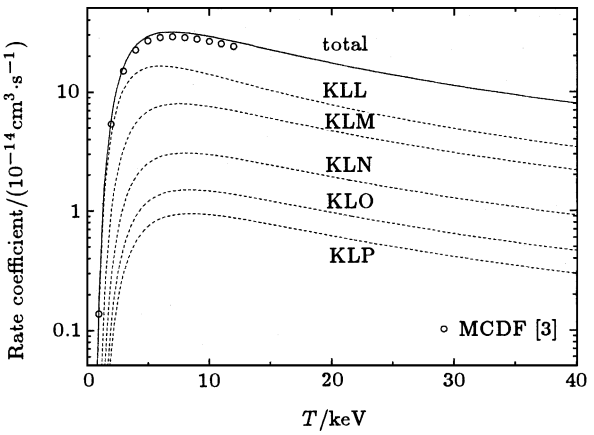


Fig.8. Detailed and total DR rate coefficients for Kr^{35+}, compared with total rate coefficient by Chen[5].

4. Conclusion

In this paper, we calculate the detailed autoionization and radiative rates of He-like Kr using a recently developed relativistic atomic code FAC, the results agree well with the values obtained using MCDF and HULLAC codes. The n^{-3} scaling law is shown to be valid in our calculation and is used to extrapolate the rate coefficient up to $n' \to \infty$. The DR branching ratio is shown to increase as n' of intermediate states and the atomic number Z increase. We also find that the effect of radiative cascades to the DR cross sections is less than 3% in the present case, therefore, ignoring the radiative decays to autoionizing levels in the calculation is a good approximation.

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