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Effect of Breit interaction on resonant excitation of highly charged heavy ions*

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Abstract. Resonant excitation or resonant electron scattering is a two step process in which Auger rates are involved in both steps. First an electron is captured into a bound state and a bound electron is excited (inverse Auger effect). Then an Auger transition leads to the emission of the electron from the ion. The corresponding cross-sections are very sensitive to the Auger rates and allow a detailed study of the Breit interaction which is a current-current contribution to the static electron-electron interaction. The contribution of the Breit interaction to the cross-section of resonant excitation on hydrogen-like uranium ions is discussed and shown that it is roughly twice as large as in the case of dielectronic recombination.

PACS. 32.80.Hd Auger effect and inner-shell excitation or ionization – 32.80.Dz Autoionization

1 Introduction

Electron-ion recombination processes play an important role for highly charged heavy ions found in high-temperature plasmas or accelerators. These ions offer the opportunity to study relativistic and QED-effects because these effects grow proportionally to Z^4 whereas binding energies only increase with Z^2 [1]. Autoionizing states of highly charged heavy ions have to be considered because the cross-sections for excitation, ionization and recombination are strongly influenced by these states [2]. In the case of helium-like ions for instance excitation rates for the ground state are doubled when autoionizing states are included [3].

Here we consider electron-ion collisions with two-electron processes where a first electron is captured and a second electron is excited in the ion (inverse Auger process). Then the excited ion can be stabilized by Auger decay: resonant excitation (RE) or resonant electron scattering, or by emission of a photon: dielectronic recombination (DR). Both processes are resonant, this means they are possible only for certain energies of the free electron.

The Breit interaction [4,5] is a current-current correction to the static Coulomb interaction between electrons, caused by the interaction of electrons with the radiation field. It should be noted that the Breit interaction does not provide a testing of modern QED theory which involves the renormalization procedure, for example in the calculation of self-energy and vacuum polarization corrections. Our earlier studies of DR have shown that the Breit interaction considerably enhances the Auger rates in highly charged ions and thus the cross-sections [1,6–8]. Experimental studies have proven this effect [9]. In order to study the Breit interaction in greater detail, RE offers the advantage compared to DR that it depends on the sequence of an inverse and direct Auger transition in capture and emission of the electron, respectively.

The RE cross-section is very small compared with cross-sections of DR or other processes like direct scattering. Interference with the direct scattering process could therefore lead to terms of the same order as for RE itself. To make a better comparison with experiments one should develop a model that treats these processes together in a unified framework. In this paper, we only concentrate on KLL resonant processes where the electron scatters on a hydrogen-like uranium ion. In this case the effects of the Breit interaction are clearly present due to the relativistic velocities of the K-shell electrons. We leave out inelastic collisions since a double-excited LL-state can only decay back into the ground state. Measurements of RE in such systems are planned by Kozhuharov *et al.* [10] at the experimental storage ring (ESR) of the Gesellschaft für Schwerionenforschung (GSI) with a crossed-beam setup.

In the next section we present the formalism used for calculating the cross-section of the resonant excitation. We show the approximations made and the construction of the wave function of the free electron. Cross-sections for hydrogen-like systems and the influence of the Breit interaction in RE in comparison to DR and its dependence on Z are given in the following section. Finally, we present an outlook on further developments. The units used are atomic units: $\hbar = m_e = e = 1$.

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2 Theory

The Hamiltonian for N electrons and the radiation field consists of three parts

$$H = H_{\rm e} + H_{\rm r} + H_{\rm er} \tag{1}$$

with the electronic part

$$H_{\rm e} = \sum_{i=1}^{N}(c\boldsymbol{\alpha}_i\mathbf{p}_i + (\beta_i - 1)c^2 + V_{\rm nuc}(r_i)) + \sum_{i=1}^{N-1}\sum_{j=i+1}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}, \tag{2}$$

the energy of the radiation field

$$H_{\rm r} = \sum_{\mathbf{k}\lambda}\omega_k a^+_{\mathbf{k}\lambda}a_{\mathbf{k}\lambda}, \tag{3}$$

and the interaction between electrons and radiation field

$$H_{\rm er} = -\sum_{i=1}^{N}\sum_{\mathbf{k}\lambda}\sqrt{\frac{2\pi c^2}{V\omega_k}}\boldsymbol{\alpha}_i \times \left(\boldsymbol{\epsilon}^*_{\mathbf{k}\lambda}{\rm e}^{-{\rm i}\mathbf{k}\cdot\mathbf{r}_i}a^+_{\boldsymbol{\epsilon}_{\mathbf{k}\lambda}} + \boldsymbol{\epsilon}_{\mathbf{k}\lambda}{\rm e}^{{\rm i}\mathbf{k}\cdot\mathbf{r}_i}a_{\boldsymbol{\epsilon}_{\mathbf{k}\lambda}}\right). \tag{4}$$

We employ a formalism which has been used to calculate photo recombination cross-sections [11]. The Hilbert space is divided into three orthogonal spaces, for which projection operators [12,13] are introduced [7]:

$$P = \sum_{\alpha_i J_i M_i m_s}\int {\rm d}\Omega_p {\rm d}\epsilon_p |\alpha_i J_i M_i, \mathbf{p}m_s; 0\rangle\langle\alpha_i J_i M_i, \mathbf{p}m_s; 0|, \tag{5}$$

$$Q = \sum_{\alpha_d J_d M_d}|\alpha_d J_d M_d; 0\rangle\langle\alpha_d J_d M_d; 0|, \tag{6}$$

$$R = \sum_{\alpha_r J_r M_r}\sum_{\mathbf{k}\lambda}|\alpha_r J_r M_r; \mathbf{k}\lambda\rangle\langle\alpha_r J_r M_r; \mathbf{k}\lambda|. \tag{7}$$

The operator P projects on states consisting of a free electron with energy ϵ_p and $N-1$ bound electrons in an eigenstate with energy E_i. The wave function $\Psi(\alpha_i J_i M_i \mathbf{p} m_s)$ is an eigenfunction of the operator PHP with the energy $E_p = E_i + \epsilon_p$. The intermediate bound states lying in the Q space are described by the eigenfunctions $\Psi(\alpha_d J_d M_d)$ of QHQ with the energy E_d. Caused by the interaction with the radiation field, the R space contains bound electrons and a single photon with energy ω_k. The corresponding eigenfunctions to RHR are $\Psi(\alpha_r J_r M_r; \mathbf{k}\lambda)$ with the energy $E_k = E_r + \omega_k$. The parameters α contain all the remaining quantum numbers necessary to fully describe the corresponding states. Neglecting states with two or more photons we assume that $P + Q + R = 1$.

The normalizations for the functions are

$$\langle\alpha_i J_i M_i, \mathbf{p}m_s; 0|\alpha'_i J'_i M'_i, \mathbf{p}'m'_s; 0\rangle = \delta_{\alpha_i\alpha'_i}\delta_{J_i J'_i}\delta_{M_i M'_i}\delta_{m_s m'_s} \tag{8}$$

$$= \delta^{(1)}(\epsilon_p - \epsilon'_p)\delta^{(2)}(\hat{\mathbf{p}} - \hat{\mathbf{p}}'), \tag{9}$$

$$\langle\alpha_d J_d M_d; 0|\alpha'_d J'_d M'_d; 0\rangle = \delta_{\alpha_d\alpha'_d}\delta_{J_d J'_d}\delta_{M_d M'_d}, \tag{10}$$

$$\langle\alpha_r J_r M_r; \mathbf{k}\lambda|\alpha'_r J'_r M'_r; \mathbf{k}'\lambda'\rangle = \delta_{\alpha_r\alpha'_r}\delta_{J_r J'_r}\delta_{M_r M'_r}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\lambda\lambda'}. \tag{11}$$

The Hamiltonian can now be separated into

$$H = H_0 + V \tag{12}$$

with

$$H_0 = PHP + QHQ + RHR \tag{13}$$

and

$$V = PHQ + QHP + PHR + RHP + QHR + RHQ \tag{14}$$

where V is responsible for transitions between different spaces.

The cross-section for RE can be written in time-independent scattering theory [14]:

$${\rm d}\sigma_{if} = \frac{2\pi}{F_i}|\langle\alpha_f J_f M_f, \mathbf{p}_f m_{s_f}; 0|T|\alpha_i J_i M_i, \mathbf{p}_i m_{s_i}; 0\rangle|^2 \times \rho_f {\rm d}\Omega_f, \tag{15}$$

where F_i is the current of incoming electrons and ρ_f the density of the final states. The transition operator T is defined as in [15]:

$$T(z) = V + VG(z)V \tag{16}$$

where

$$G(z) = [z - H]^{-1} = [z - H_0 - V]^{-1}. \tag{17}$$

It can be shown, similar to [11], that

$$T(z) = \Lambda(z) + \Lambda(z)QG(z)Q\Lambda(z) \tag{18}$$

with the level shift operator

$$\Lambda(z) = V + VC[C(z - H)C]^{-1}CV \tag{19}$$

and $C = P + R$.

Using the projection operator P for the initial and final state we have

$$PT(z)P = P\Lambda(z)P + P\Lambda(z)QG(z)Q\Lambda(z)P = PVR[C(z - H)C]^{-1}RVP + P\Lambda(z)QG(z)Q\Lambda(z)P. \tag{20}$$

The first term is a radiative correction of the continuum states which we neglect here. The second term we approximate [7] by

$$PT(z)P \approx P(V + VRG_0(z)RV)QG(z) \times Q\,(V + VRG_0(z)RV)P \tag{21}$$

$$= PV_{\rm el}\,QG(z)Q\,V_{\rm el}P \tag{22}$$

with

$$G_0(z) = [z - H_0]^{-1} \tag{23}$$

$$V_{\rm el} = H_{\rm e} + H_{\rm er} R G_0(E) R H_{\rm er}, \tag{24}$$

where we have substituted the operator PVR with $H_{\rm er}$.

The second term in $V_{\rm el}$ describes the interaction of electrons through the exchange of a virtual photon creating a quantum electrodynamical correction of the instantaneous Coulomb interaction. The imaginary parts of the corresponding matrix elements are neglected in our calculations and the real parts can be described by the Breit interaction, where ω is the energy of the exchanged virtual photon:

$$V_{\rm Breit} = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \left[-\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j \frac{\cos(\omega r_{ij})}{r_{ij}} + (\boldsymbol{\alpha}_i \cdot \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \cdot \boldsymbol{\nabla}_j) \frac{\cos(\omega r_{ij}) - 1}{\omega^2 r_{ij}} \right]. \tag{25}$$

Let us assume an isolated resonant state d with energy E_d (isolated resonance approximation). In reality the resonances can overlap due to the rather large decay widths of the examined levels. A discussion of the interference of overlapping resonances is given in Section 4. For a single resonant state we can write

$$QG(z)Q = Q[Q(z - H_0 - \Lambda(z))Q]^{-1}Q \tag{26}$$

$$= \sum_{M_d} \frac{|\alpha_d J_d M_d; 0\rangle\langle\alpha_d J_d M_d; 0|}{z - E_d - \Delta E_d + {\rm i}\Gamma_d/2}, \tag{27}$$

where ΔE_d is the shift of the resonance energy and Γ_d the sum of the widths of radiative and Auger decays.

For the total cross-section of RE we have to sum (15) over the quantum numbers of the final and resonant states and to average over those of the initial state. Additionally, we have to carry out integrals over the scattering angles of the electron:

$$\sigma^{\rm RE}_{i\to f} = \sum_d \frac{2\pi^2}{p^2} \frac{A_a(d \to f)}{\Gamma_d} L_d(E)\, V_a(i \to d) \tag{28}$$

with

$$A_a(d \to f) = \frac{2\pi}{2J_d + 1} \times \sum_{M_f, M_d, m_{s_f}} \int {\rm d}\Omega_e |\langle \alpha_f J_f M_f, \mathbf{p}_f m_{s_f}; 0 | V_{\rm el} | \alpha_d J_d M_d; 0\rangle|^2 \rho_f \tag{29}$$

$$L_d(E) = \frac{\Gamma_d/2\pi}{(E - E_d - \Delta E_d)^2 + \Gamma_d^2/4}, \tag{30}$$

$$V_a(i \to d) = \frac{2\pi}{2(2J_i + 1)} \times \sum_{M_i, M_d, m_{s_i}} \int {\rm d}\Omega_p |\langle \alpha_d J_d M_d; 0 | V_{\rm el} | \alpha_i J_i M_i, \mathbf{p}_i m_{s_i}; 0\rangle|^2 \rho_i. \tag{31}$$

$A_a(d \to f)$ is the rate for the Auger decay of the intermediate resonant state d. It is related to the capture rate $V_a(f \to d)$ of the electron from the continuum state f to the resonant state d by the theorem of detailed balance

$$A_a(d \to f) = \frac{2(2J_f + 1)}{2J_d + 1} V_a(f \to d). \tag{32}$$

The wave functions of bound states are described by relativistic multiconfiguration state functions. They are calculated with a multiconfiguration Dirac Fock method implemented in the MCDF module provided by the GRASP package [16]. For very heavy systems as heliumlike uranium, the Coulomb interaction corrections are so small that hydrogenlike Dirac wave functions could also be applied instead of the Dirac-Fock wave functions. The GRASP program is also used for the computation of the radiative widths needed for the calculation of the total width Γ_d of the resonant states. The energy shifts ΔE_d in (27) contain corrections due to the Breit interaction and radiative effects (self-energy and vacuum polarization) which are included in a perturbation approximation.

The wave function for the initial state is constructed as an antisymmetrized product of a multiconfiguration function for the bound electrons and a continuum function for the free electron:

$$\Psi(\alpha_i J_i M_i \mathbf{p} m_s) = \mathcal{A}\left(\Psi(\alpha_i J_i M_i) \cdot \psi(\mathbf{p} m_s)\right). \tag{33}$$

For the continuum function solving the Dirac equation with a screened Coulomb potential, a partial wave expansion is necessary to obtain the momentum $\mathbf{p}$ and spin projection m_s [17]

$$\psi(\mathbf{p} m_s) = \sum_{\kappa\mu} {\rm i}^l {\rm e}^{{\rm i}\Delta_\kappa} \sum_{m_l} Y^*_{lm_l}(\hat{p}) C(l \tfrac{1}{2} j | m_l m_s \mu) \psi_{p\kappa\mu}(\mathbf{r}). \tag{34}$$

Δ_κ are phase shifts which have to be chosen in a way that the wave function satisfies the boundary condition for a plane wave in the direction of $\mathbf{p}$ and an outgoing scattered wave. $\psi_{p\kappa\mu}(\mathbf{r})$ has the form of a single particle wave function

$$\psi_{p\kappa\mu}(\mathbf{r}) = \frac{1}{r} \begin{pmatrix} P_{p\kappa}(r) & \chi_{\kappa\mu}(\hat{r}) \\ {\rm i} Q_{p\kappa}(r) & \chi_{-\kappa\mu}(\hat{r}) \end{pmatrix}, \tag{35}$$

$$\chi_{\kappa\mu} = \sum_{m_s} C(l\, \tfrac{1}{2}\, j | m_l m_s \mu) Y_{lm_l}(\hat{r}) \phi_{m_s}. \tag{36}$$

The normalizations are

$$\int \psi^*(\mathbf{p} m_s) \psi(\mathbf{p}' m'_s) {\rm d}V = \delta_{m_s m'_s} \delta(\epsilon_p - \epsilon'_p) \delta(\hat{p} - \hat{p}'), \tag{37}$$

$$\int \psi^*_{p\kappa\mu}(\mathbf{r}) \psi_{p'\kappa'\mu'}(\mathbf{r}) {\rm d}V = \delta_{\kappa\kappa'} \delta_{\mu\mu'} \delta(\epsilon_p - \epsilon'_p). \tag{38}$$

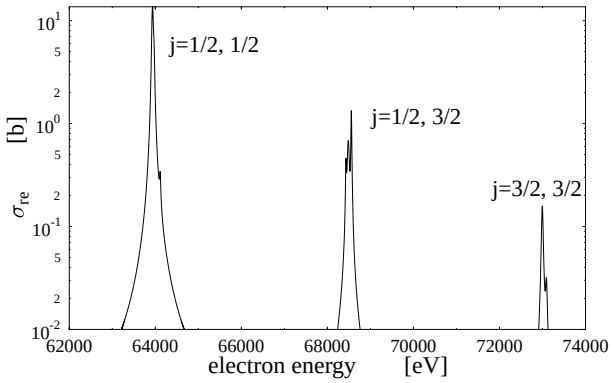

Fig. 1. Total cross-section for KLL-RE on hydrogen-like uranium as a function of the energy of the continuum electron.

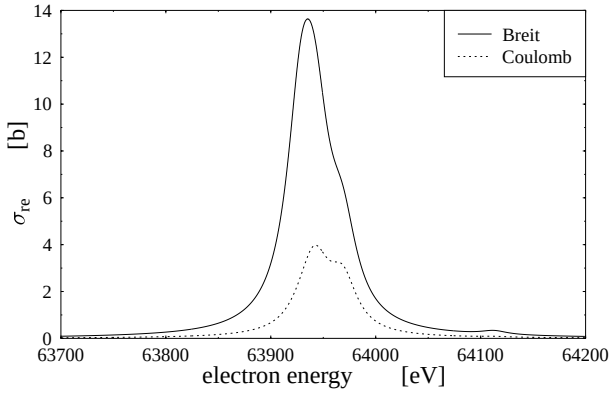

Fig. 2. The effects of the Breit interaction on the $KL_{1/2}L_{1/2}$ resonance group for KLL-RE on hydrogen-like uranium. The solid and dotted curves are calculated with and without the Breit interaction in the Auger matrix elements.

Inserting the partial wave expansion into (33) we can write

$$\Psi(\alpha_i J_i M_i \mathbf{p} m_s) = \sum_{\kappa\mu} \mathrm{i}^l \mathrm{e}^{\mathrm{i}\Delta_\kappa} \sum_{m_l} Y^*_{lm_l}(\hat{p}) C(l\frac{1}{2}j|m_l m_s \mu) \times \sum_{JM} C(J_i j J|M_i \mu M) \times \sum_r c_r(\alpha_i J_i) \Phi(\gamma_r J_i; p\kappa; JM) \quad (39)$$

where the antisymmetrized wave function Φ contains a single continuum orbital. The orthogonality of the continuum orbital to the other states is achieved by using a Schmidt orthogonalization procedure.

The functions $\psi_{p\kappa\mu}$ are calculated by numerically solving the Dirac Fock equations containing the direct potential caused by the nucleus and the bound electrons. The effects of the exchange potential can be neglected as earlier calculations have shown. The difference method used by GRASP for calculating bound states leads to unsatisfying results for continuum functions at distances far from the nucleus. Therefore, we made use of another program DE [18] for the numerical integration of the radial equation for the continuum states.

For the calculation of the normalization and the phase shifts Δ_κ we employ a method by Müller *et al.* [19]. Here, an analytical solution of the Dirac equation for a screened Coulomb potential with charge $Z - N + 1$ is used to describe the continuum function far away from the ion. At a matching radius r_m the ratios of the large and small components of this outer function and of the numerically obtained inner solution have to be equal

$$\frac{P^{(i)}_{p\kappa}(r_m)}{Q^{(i)}_{p\kappa}(r_m)} = \frac{P^{(o)}_{p\kappa}(r_m)}{Q^{(o)}_{p\kappa}(r_m)} \,. \quad (40)$$

From this condition one can derive equations for the phase shifts Δ_κ.

3 Results

In Figure 1 we present results of our calculations for the total cross-section of RE on hydrogen-like uranium. In this case, we consider a bound $1s$ and a free electron in the initial and final states. Because of the fine structure of the L shell we get three distinct resonance groups at 64, 68.5 and 73 keV. The widths of the resonances lie in the range of 30 to 56 eV and are nearly independent of the Breit interaction since the major contributions come from the radiative decay.

One typical behaviour of RE is the strong decrease of the cross-section for the energetically higher resonances which can not be found for the corresponding DR processes. The largest contributions of the Breit interaction to the Auger rates of highly charged heavy ions occur in the energetically lower resonances, whereas smaller Auger rates are found for higher resonances. Combined with the fact that RE depends on the square of the Auger rate A_a^2 and DR only linearly, the cross-sections for RE decrease faster with the electron energy than those for DR. Since double excited resonant states in helium-like uranium preferably decay through photon emission, the cross-section for RE is about 70 times smaller than the one for DR.

For a more detailed study of the effect of the Breit interaction on the cross-section we show the RE cross-section for the first resonance group in Figure 2. In this group the first two of four resonances lie very close (13 eV) giving rise to one single peak. The second peak resulting from the third resonance is also visible in the dotted curve which is calculated with the Coulomb interaction only. After inclusion of the Breit interaction (full curve) the first two resonances are much more enlarged and dominate the whole resonance group. Only the right shoulder is slighty affected by the third resonance.

The influence of the Breit interaction on all resonances is depicted in Figure 3 where the energy-integrated cross-sections for KLL-RE on hydrogen-like uranium for all 10 LL-resonant states are presented. The lowest two resonances contribute most (about three quarters) to the total cross-section. The Breit interaction is responsible for a large part of these cross-sections, especially in the case

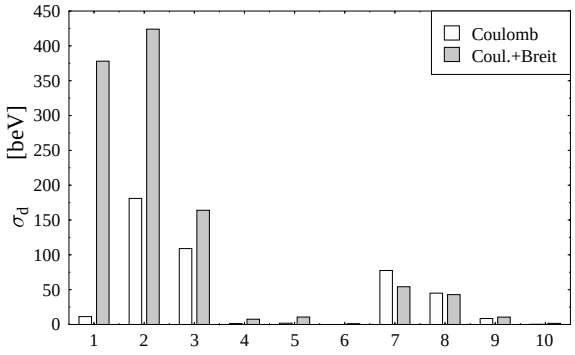

Fig. 3. The effects of the Breit interaction on the energy-integrated cross-section for KLL-RE on hydrogen-like uranium. Grey and dark bars are obtained without and with the Breit interaction, respectively.

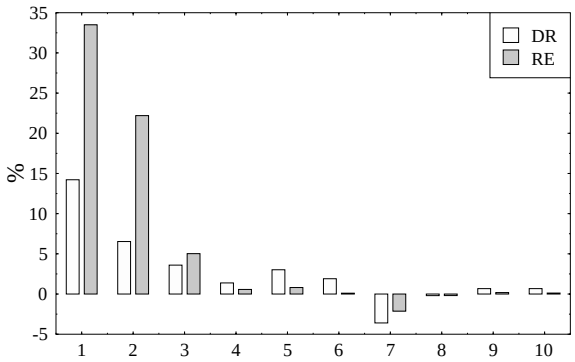

Fig. 4. Percentage of the Breit contribution of each LL-resonance to the total cross-section for DR (grey bars) and RE (dark bars) on hydrogen-like uranium.

of the first resonance because the corresponding transition is nonrelativistically forbidden.

Figure 4 compares the percentage of the Breit interaction of each LL-resonance on the total DR and RE cross-sections for hydrogen-like uranium. The percentage for RE of the first three levels is much larger than for DR. The Breit term of the first resonance even contributes about one third to the total cross-section for RE, but only 15% for DR. It seems that for levels where the inclusion of the Breit interaction is absolutely necessary the percentage of the Breit term is larger for RE than for DR. For other levels (levels 4–7 or levels in systems with more electrons) the percentage of the Breit term is smaller, but also the cross-sections are smaller (see Fig. 3, levels 4–7). Summing up all contributions we find that 60% of the RE cross-section is caused by Breit interaction, twice as much as for DR.

Since the Breit interaction is a relativistic effect, this effect should have a strong dependence on the charge of the ion. Figure 5 gives the percentage of the Breit contribution to the KLL cross-section on hydrogen-like ions of the first and second resonance as a function of the ion charge Z. Since the first resonance (full curve) is non-relativistically forbidden, even small Breit matrix elements can lead to a high percentage for small values of Z. The Breit contribution in the case of the second resonance (dotted curve) continues to rise slowly with Z until

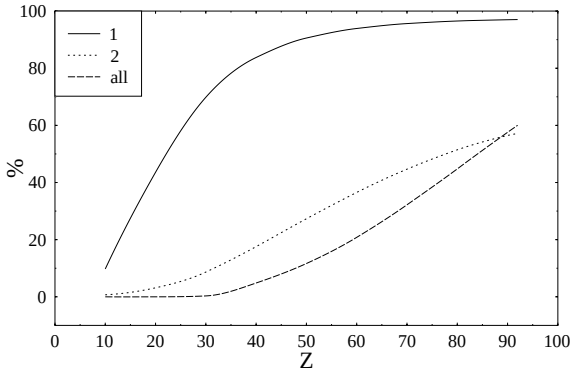

Fig. 5. Percentage of the contribution of Breit interaction to the KLL cross-section for RE energy-integrated over the first and second resonances (full and dotted curves) and over all resonances (broken curve) for hydrogen-like ions.

it reaches its maximum value for uranium. The same behaviour can be seen for the Breit contribution to the total KLL cross-section (broken curve).

4 Summary and outlook

The Breit interaction is very important for resonant excitation or resonant scattering of electrons on highly charged heavy ions. KLL-Auger rates and, therefore, cross-sections are appreciably increased by this interaction. A drawback for experimental studies of this effect in RE might be that the total cross-sections are very small due to the small Auger widths in comparison to the radiative widths.

As can be seen in Figure 2 the use of the isolated resonance approximation is not fully justified. Further calculations could study the effects of overlapping resonances on the cross-sections. Karasiov *et al.* [20] have done this for DR and radiative recombination (RR) and found that the overlapping resonance effect is comparable with the DR-RR interference effect and reaches about 30% for uranium in the region between two resonances in the KLL transition. According to Shabaev [21] the effect of the overlapping resonances gives a dominant contribution to the asymmetry parameter characterizing a deviation of the resonance line shape from the Lorentz-type form. Also it might be prospective to calculate interferences between RE and direct scattering. Since the cross-sections for direct electron scattering on heavy ions are orders of magnitude larger, the interference term might even be greater than the RE cross-section.

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