Interference effects in the recombination process of hydrogenlike lead

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We have calculated the total cross section of the recombination of an electron with hydrogenlike lead in the vicinity of the *KLL* resonances. The effects, including both the radiative overlap of identical levels and coupling between the different channels of the process, are taken into account in the frames of QED. The numerical results show the existence of noticeable interference effects in the cross section and may be of interest for the near future storage-ring experimental studies of recombination.

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I. INTRODUCTION

In the last years, the great advances have been achieved in the direct observations of electron recombination with multicharged heavy ions, carried out using a wide range of technologies. The experimental investigations provide a promising perspective for both high-precision measurements of electron-ion collision cross sections and sensitive tests of QED theory of the processes. Theoretically, the general description of electron recombination has first to go beyond the independent-process approximation to take into account the different channel-coupling effects. The radiative-recombination (RR) and dielectronic-recombination (DR) channels were considered from the unified quantum-mechanical point of view, for example, in Refs. [1–5]. Then the total cross section of the recombination process includes DR and RR cross sections, and a term that describes the interference between DR and RR. Effects of the DR-RR interference are also known to be most important for individual transitions involving the low-lying levels. The second point that has to be taken into account in the theory is the inclusion of the interference effects due to the radiative overlap of identical DR resonances with the same parity and total angular momentum. This phenomenon was first discussed for the radiative decay process of the doubly-excited levels [6–9]. Note that because the radiative overlap of the low-lying DR resonances is the pure relativistic effect, it can be accurately treated within the QED approach only. Recombination process with hydrogenlike multicharged ion is, probably, the simplest one for investigation of the interference effects. The expression for the cross section of recombination with hydrogenlike heavy ion was obtained in Ref. [10] using the Green function method [11]. Numerical calculations of the process with U^{91+} performed in Ref. [10] found the existence of the radiative and DR-RR interference effects which are strong enough to be measurable. Recombination cross sections, but for heliumlike uranium, were calculated in the frames of the projection-operator formalism [3–5] with using of a multiconfiguration Dirac-Fock (MCDF) approximation for the required energies and rates (see Refs. [12,13]). The DR-RR interference effect in the latter case is similar to that obtained in Ref. [10]. But, the interference due to radiative overlap turned out to be somewhat small there. Note that the size of summarized effects also depends on whether one is looking at discussed effects on the whole *KLL* spectrum or just individual transitions. However, as for the energy-averaged recombination cross sections, with current experimental capabilities these effects lead to too small corrections to be seen [12,13]. Double radiative-interference effects in DR with hydrogenlike uranium were recently discussed in Ref. [14].

The purpose of the present work is to investigate the interference effects in the recombination process with Pb^{81+} ion that seems most promising from the experimental observation point of view. As overlapping DR resonances, the doubly-excited states $[2s_{1/2}^2]_0$ and $[2p_{1/2}^2]_0$ have been considered. The relativistic calculations of the DR process for hydrogenlike Pb ion with estimations of the RR background were made in Ref. [15]. In contrast to the latter paper, we emphasize, namely, those interference terms in the total cross section of the process that have been omitted there. The working formulas are given in Sec. II. Our numerical results for the recombination cross section are then presented and discussed in Sec. III. Relativistic units $\hbar = c = 1$ with the fine-structure constant $\alpha = e^2$ are used.

II. THEORY

We shall consider the recombination process of an electron with hydrogenlike multicharged ion A^{q+} in its ground state, which may be schematically represented as

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DR: $A^{q+}(1s_{1/2})+e^- \rightarrow A^{(q-1)+}(d)^{**} \rightarrow A^{(q-1)+}(r)^*+\gamma$

and

RR: $A^{q+}(1s_{1/2}) + e^- \rightarrow A^{(q-1)+}(r)^* + \gamma,$

where e^- denotes the incident electron with energy ε and momentum $\mathbf{p}$, and γ is the emitted photon with frequency ω. The intermediate single-excited state r decays radiatively up to the ground one. As doubly-excited states d we choose the group of mutually overlapping levels. Then the resonance condition is $\varepsilon + \varepsilon_{1s} \approx E_d$, where E_d is the energy of the heliumlike ion. Besides, it is supposed that only the photons in the frequency region of $\omega \approx E_d - E_r$ are measured in the experiment.

Cross section for the recombination is given by the sum of the following terms [10]

$$\sigma_{DR}(\varepsilon) = \frac{\pi^2}{2p^2} \sum_{j,l,J,M} \sum_d \frac{W_{dd} |\langle d_L|\hat{I}|i\rangle|^2}{\xi_d^2 + \Gamma_d^2/4}, \qquad (1)$$

$$\sigma_{DR}^{int}(\varepsilon) = \frac{\pi^2}{p^2} \sum_{j,l,J,M} \mathrm{Re}\left(\sum_{\substack{d,d'\\ d<d'}} \frac{W_{dd'} \langle d_L|\hat{I}|i\rangle \langle d'_L|\hat{I}|i\rangle^*}{(\xi_d + i\Gamma_d/2)(\xi_{d'} - i\Gamma_{d'}/2)} \right), \qquad (2)$$

$$\sigma_{DR-RR}^{int}(\varepsilon) = \frac{\pi^2}{p^2} \sum_{j,l,J,M} \mathrm{Re}\left(\sum_d \frac{W_{di} \langle d_L|\hat{I}|i\rangle}{\xi_d + i\Gamma_d/2} \right), \qquad (3)$$

$$\sigma_{RR}(\varepsilon) = \frac{\pi^2}{2p^2} \sum_{j,l,J,M} W_i. \qquad (4)$$

Here $p^2 = \varepsilon^2 - m^2$ and state $|i\rangle$ depends on the set of quantum numbers $|1s_{1/2}\varepsilon jlJM\rangle$, where J is the total angular momentum of the system, M is the projection of J, and j,l are the total and orbital angular momenta of the incoming electron. The magnitude $\xi_d \equiv \varepsilon + \varepsilon_{1s} - E_d$ denotes the disorder from the resonance d. The continuum wave functions are normalized on the energy scale. The complex eigenvalues $\mathcal{E}_d \equiv E_d - i\Gamma_d/2$ of the non-Hermitian operator $\hat{H}$ are defined with taking into account the electron self-energy, vacuum polarization, and interelectron interaction corrections in the first order of the $1/Z$ expansion. The right $|d_R\rangle$ and left $\langle d_L|$ eigenvectors of $\hat{H}$ introduced in Ref. [11] are normalized by the condition $\langle d_L \mid d'_R \rangle = \delta_{dd'}$. Due to T invariance the components of the left eigenvector $\langle d_L|$ are equal to the corresponding components of the right vector $|d_R\rangle$. We define the operator for the emission of a photon with the polarization $\mathbf{e}$ and the momentum $\mathbf{k}$ as

$$\hat{R}_\omega = e\sqrt{\frac{2\pi}{\omega}} \sum_{n=1}^{2} (\boldsymbol{\alpha} \cdot \boldsymbol{e}^*) e^{-i\mathbf{k}\cdot\mathbf{x}_n}, \qquad (5)$$

where $\boldsymbol{\alpha}$ is the Dirac matrix. Then the expressions for widths are given by multipolar expansions of

$$W_{dd'} = \sum_r W_{dd',r} = 2\pi\omega^2 \sum_{r,\mathbf{e}} \int \frac{d\Omega}{(2\pi)^3} \langle r|\hat{R}_\omega|d_R\rangle \langle r|\hat{R}_\omega|d'_R\rangle^*, \qquad (6)$$

$$W_{di} = 2\pi\omega^2 \sum_{r,\mathbf{e}} \int \frac{d\Omega}{(2\pi)^3} \langle r|\hat{R}_\omega|d_R\rangle \langle r|\hat{R}_\omega|i\rangle^*, \qquad (7)$$

$$W_i = 2\pi\omega^2 \sum_{r,\mathbf{e}} \int \frac{d\Omega}{(2\pi)^3} |\langle r|\hat{R}_\omega|i\rangle|^2, \qquad (8)$$

where $d\Omega$ means the integration over the directions of the photon emission. The matrix elements of the operator

$$\hat{I} = \alpha(1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) \frac{\exp(i|\omega|r_{12})}{r_{12}} \qquad (9)$$

describe the excitation process of the states d by radiationless capture with taking into account the retardation effect.

The first two terms of the cross section for recombination [see Eqs. (1),(2)] correspond to the DR channel, the third term given by Eq. (3) describes the interference between the DR and RR channels, and the fourth one σ_{RR} contributes only to the RR background. The term σ_{DR}^{int} is caused by the radiative interference of DR amplitudes for the identical levels. Note that such separation of the total cross section is somewhat artificial since the separate terms of the sum written in different representations involve the interference effects differently. The magnitude of the radiative interference effect is defined by the nonorthogonality integral $\langle d'_R|d_R \rangle$, which is connected with nondiagonal width $W_{dd'}$ by the Bell-Steinberger equality [16]

$$W_{dd'} = i(\mathcal{E}_d - \mathcal{E}_{d'}^*) \langle d'_R|d_R\rangle. \qquad (10)$$

Equations (1)–(3) are transformed by Eq. (10) and the equality

$$W_{di} = i\langle i|(\hat{I} - \hat{I}^\dagger)|d_R\rangle \qquad (11)$$

to the form convenient for numerical calculations [17]

$$\tilde{\sigma}_{DR}(\varepsilon) = \frac{\pi^2}{2p^2} \sum_{j,l,J,M} \sum_d \Gamma_d \frac{\mathrm{Re}\left(\langle i|\hat{I}|d_R\rangle \langle d_L|\hat{I}|i\rangle \right)}{\xi_d^2 + \Gamma_d^2/4}, \qquad (12)$$

$$\tilde{\sigma}^{int}(\varepsilon) = -\frac{\pi^2}{p^2} \sum_{j,l,J,M} \sum_d \xi_d \frac{\mathrm{Im}\left(\langle i|\hat{I}|d_R\rangle \langle d_L|\hat{I}|i\rangle \right)}{\xi_d^2 + \Gamma_d^2/4}. \qquad (13)$$

In this representation, the term $\tilde{\sigma}^{int}(\varepsilon)$ includes the radiative and DR-RR interferences, which lead to the asymmetry of the summarized shape. In addition, we note that a small part of the interference contributions is involved yet in the superposition of the Lorentz resonances $\tilde{\sigma}_{DR}(\varepsilon)$. It should also be stressed that Eqs. (1)–(4) [as

TABLE I. Listed are the intermediate doubly-excited states d, their binding energies E_d, total radiative widths Γ_d, resonance energies ε of the incoming free electron, the Auger widths $\mathcal{A}_d$ of the states d, the final single-excited states r, the energies E_{dr} of the emitted photons, and the partial radiative widths $W_{dd,r}$ for the decays of the intermediate states d to the final states r. All quantities were calculated in the biorthogonal basis. Only the dipole-transition contributions were taken into account in the rates.

d	E_d (keV)	Γ_d (eV)	ε (keV)	$\mathcal{A}_d$ (eV)	r	E_{dr} (keV)	$W_{dd,r}$ (eV)
$[2s_{1/2}2p_{1/2}]_0$	-51.707	19.385	49.630	0.402	$[2s_{1/2}1s_{1/2}]_1$	75.150	19.351
					$[2p_{1/2}1s_{1/2}]_1$	75.017	0.035
$[2s^2_{1/2}]_0$	-51.697	15.868	49.640	0.508	$[2s_{1/2}1s_{1/2}]_1$	75.160	0.042
					$[2p_{1/2}1s_{1/2}]_1$	75.027	15.954
$[2s_{1/2}2p_{1/2}]_1$	-51.670	19.377	49.667	0.171	$[2s_{1/2}1s_{1/2}]_1$	75.188	12.907
					$[2p_{1/2}1s_{1/2}]_1$	75.055	0.023
					$[2s_{1/2}1s_{1/2}]_0$	74.991	6.435
					$[2p_{1/2}1s_{1/2}]_0$	74.988	0.012
$[2p^2_{1/2}]_0$	-51.547	22.916	49.790	0.097	$[2s_{1/2}1s_{1/2}]_1$	75.311	0.029
					$[2p_{1/2}1s_{1/2}]_1$	75.178	23.072

well as Eqs. (12),(13)] were derived within the resonance approximation. According to our knowledge, no relativistic expressions for the recombination cross section obtained out of this approximation are published in the literature. The problem, concerning a possible distortion of the shape due to the nonresonant corrections, requires further nontrivial efforts.

III. RESULTS

The energies and rates of the heliumlike lead were calculated in the frames of $1/Z$ expansion. The results we obtained are given in Table I. For convenience the identical states are classified according to the LS limit. The energies of the levels have the radiative [18–20] (electron self-energy and vacuum polarization) and the exact one-photon interelectron interaction corrections included. The finite nucleus size was taken into account directly in the Dirac wave functions. The effects of configuration interaction on the energies and rates are not significant for very high-Z ions, and have been neglected. Our results given in Table I are in good agreement with those previously obtained within the MCDF approximation in Ref. [15]. The parameters of identical levels calculated in the biorthogonal basis are listed in Table II.

The recombination cross section associated with the $2s, 2p - 1s$ stabilizing radiative transitions of the Pb^{80+} was computed using its different representations presented in Sec. II. Note that all summations in Eqs. (1)–(4) as well as in Eqs. (12),(13) are finite. In the expressions for widths [see Eqs. (6)–(8)], only the dipole-transition contributions were taken into account. The total cross section depending on the incident electron energy is shown in Fig. 1 by the solid line. The level of accuracy of the calculations, which is assumed to be mainly connected with the uncertainties in the computation of widths for low-lying resonances, can be estimated as about 5%. The dashed curve corresponds to the cross section without the interference terms $\tilde{\sigma}^{int}(\varepsilon)$. As can be seen, the most promising candidate for an observation of the interference effects in the recombination of Pb^{81+} is the $[2p^2_{1/2}]_0$ resonance. At the disorder of the resonance around its half width, the extent of asymmetry of the line (see Ref. [21]) turns out to be about -0.14, and agrees with the magnitude of the nonorthogonality inte-

TABLE II. Parameters of the identical levels $d = [2s^2_{1/2}]_0$ and $d' = [2p^2_{1/2}]_0$ obtained in the biorthogonal basis.

r	$W_{dd',r}$ (eV)
$[2s_{1/2}1s_{1/2}]_1$	$0.034 - i0.004$
$[2p_{1/2}1s_{1/2}]_1$	$-19.028 - i2.460$
$\langle d_R \vert d'_R \rangle = \langle d'_R \vert d_R \rangle^* = i0.127$	

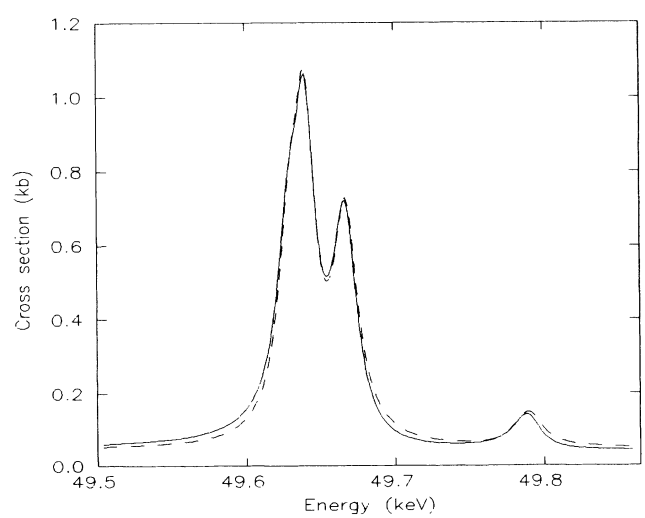

FIG. 1. Total cross section for the recombination with Pb^{81+} as a function of the incident electron energy (solid curve). The dashed curve corresponds to the calculation without taking into account the interference terms $\tilde{\sigma}^{int}$.

gral given in Table II. This size of effect is likely to be measured in the near future storage-ring experiments.

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