Spin-flip process in radiative recombination of an electron with H- and Li-like uranium

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The radiative recombination of an electron with H- and Li-like ^{238}U in its ground state is studied. An experiment is proposed in which both the electron and the ion are polarized in the same direction, along or opposite to the initial electron momentum. Since, owing to the Pauli principle, the electron can be captured into the ground state of He- and Be-like uranium, respectively, only via a spin-flip transition, one may uniquely identify spin-flip transitions for arbitrary photon emission angles. The cross section of the process is calculated for a wide range of initial electron energies.

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I. INTRODUCTION

Radiative recombination (RR) is one of the basic processes occurring in electron–heavy-ion collisions. This process is closely related to radiative electron capture (REC) occuring in an energetic collision between a high-Z ion and a low-Z target atom. Because a loosely bound target electron can be considered as quasifree, REC is essentially equivalent to RR, or its time-reversed process, the photoelectric effect. During the last decade, reactions of this type have been the subject of continued interest and they have been broadly investigated both theoretically in a fully relativistic framework [1–8] and experimentally at ion-projectile energies up to 300 MeV/u [9–17]. One of the main goals of these investigations consists in studying relativistic and quantum electrodynamical (QED) effects in RR and REC caused by the strong electric field felt by the electron in the vicinity of a heavy nucleus. In particular, the spin-flip contribution to REC [2], which is of pure relativistic origin, was recently identified in angular-differential measurements at the forward direction of the emitted photon [15] where the nonrelativistic contribution to the cross section vanishes.

In the present paper we consider the radiative recombination of a polarized electron with polarized H- and Li-like ^{238}U in its ground state as a tool to study the spin-flip contribution to RR for arbitrary angles of the emitted photon. Neglecting interelectronic interactions which are of the order $1/Z$ compared to the electron-nucleus interaction, the process is equivalent to recombination with a bare nucleus into the $1s$ or $2s$ state with one substate being blocked by the Pauli principle. If both the electron and ion are polarized in the same direction, along or opposite to the initial electron momentum, the cross section of the process is completely defined by the spin-flip contribution. For the case of opposite polarization of the two particles, only the non-spin-flip process contributes to the cross section. Therefore, an appropriate investigation with both the highly charged ion and the electron being polarized would allow for a separation of spin-flip and non-spin-flip contributions by experiment. We evaluate the cross sections of both processes for various initial electron energies and for various angles of the emitted photon. The experimental precision is by far not sensitive to any minor effects [15] and in our theoretical evaluation we neglect marginal effects like the recoil effect caused by the finite mass of the ion, compared to the electron. At the kinetic energies of the electron under consideration here, up to about $4\, m_e c^2$, they are much less important than other neglected contributions like the electron-electron interaction. Relativistic units ($\hbar = m_e = c = 1$) are used in the paper.

II. BASIC FORMULAS

To zeroth order in $1/Z$, in the ion-rest frame the differential cross section of the process under consideration is given by (see, e.g., [18])

$$\frac{d\sigma}{d\Omega_f} = \frac{(2\pi)^4}{v_i}\mathbf{k}_f^2 |\langle b| e\alpha_\nu A_f^{\nu *}|p_i\mu_i\rangle|^2, \tag{1}$$

where $\mathbf{k}_f$ and v_i are the photon momentum and the incident electron velocity, respectively, $\alpha^\nu = (1,\boldsymbol{\alpha})$, and $\boldsymbol{\alpha}$ is the vector of Dirac matrices,

$$|b\rangle = \begin{pmatrix} g_b(r)\Omega_{\kappa_b\mu_b}(\hat{\mathbf{r}}) \\ i f_b(r)\Omega_{-\kappa_b\mu_b}(\hat{\mathbf{r}}) \end{pmatrix} \tag{2}$$

denotes the wave function of the bound electron, $\kappa = (-1)^{j+l+1/2}(j+1/2)$ is the quantum number determined by angular momentum and parity of the state, $\hat{\mathbf{r}} = \mathbf{r}/|\mathbf{r}|$,

$$A_f^\nu(\mathbf{x}) = \frac{\epsilon_f^\nu \exp(i\mathbf{k}_f\cdot\mathbf{x})}{\sqrt{2k_f^0(2\pi)^3}} \tag{3}$$

is the wave function of the emitted photon, $k_f^0 = |\mathbf{k}_f| \equiv \omega$ is the photon energy, $\epsilon_f = (0,\mathbf{e}_f)$ is the photon polarization, $p_i = (\varepsilon_i, \mathbf{p}_i)$, and $|p_i\mu_i\rangle = \psi_{p_i,\mu_i(+)}(\mathbf{x})$ indicates the wave function of the incoming electron with a defined asymptotic momentum and a spin projection with respect to the direction of the electron momentum. Introducing a current vector by

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$$\mathbf{j}(\mathbf{k}_f)=\langle b|\boldsymbol{\alpha}\exp(-i\mathbf{k}_f\cdot\mathbf{r})|p_i\mu_i\rangle, \tag{4}$$

the differential cross section (1) can be represented as

$$\frac{d\sigma}{d\Omega_f}=\frac{4\pi^2\varepsilon_i\alpha\omega}{p_i}|\mathbf{e}_f^*\cdot\mathbf{j}|^2, \tag{5}$$

where α denotes the fine-structure constant.

The calculation of Eq. (5) can be performed in two different ways. The first one is to consider the incident electron propagating along the z axis. In this case the partial-wave expansion of the wave function of the incident electron which propagates in the positive z direction takes the form (cf., e.g., [1])

$$|p_i\mu_i\rangle=\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{\varepsilon_i p_i}}\sum_{\kappa} i^l e^{i\Delta_\kappa}\sqrt{2l+1}C^{j\mu_i}_{l0,(1/2)\mu_i}|\varepsilon_i\kappa\mu_i\rangle, \tag{6}$$

where $C^{j_3m_3}_{j_1m_1,j_2m_2}=\langle j_1m_1j_2m_2|j_3m_3\rangle$ denotes a Clebsch-Gordan coefficient and $|\varepsilon_i\kappa\mu_i\rangle$ is the electron wave function of a continuum state with the energy ε_i, the quantum number κ, and the angular momentum projection μ_i on the z axis:

$$|\varepsilon_i\kappa\mu_i\rangle=\begin{pmatrix} g_{\varepsilon_i\kappa}(r)\Omega_{\kappa\mu_i}(\hat{\mathbf{r}}) \\ if_{\varepsilon_i\kappa}(r)\Omega_{-\kappa\mu_i}(\hat{\mathbf{r}})\end{pmatrix}. \tag{7}$$

Summing the differential cross section (5) over the polarizations $\lambda=\pm1$ of the emitted photon and employing (e.g., [19])

$$\sum_\lambda(\mathbf{a}\cdot\mathbf{e}_\lambda)(\mathbf{b}\cdot\mathbf{e}^*_\lambda)=[\mathbf{a}\times\mathbf{n}]\cdot[\mathbf{b}\times\mathbf{n}], \tag{8}$$

we obtain

$$\frac{d\sigma}{d\Omega_f}=\frac{4\pi^2\varepsilon_i\alpha\omega}{p_i}|\mathbf{n}\times\mathbf{j}(\mathbf{k}_f)|^2, \tag{9}$$

where $\mathbf{n}\equiv\hat{\mathbf{k}}=\mathbf{k}_f/|\mathbf{k}_f|$. Utilizing the standard expansion of the exponent in the current vector,

$$\exp(-i\mathbf{k}_f\cdot\mathbf{r})=4\pi\sum_{L,M} i^{-L}j_L(\omega r)Y_{LM}(\hat{\mathbf{k}}_f)Y^*_{LM}(\hat{\mathbf{r}})$$

(cf., e.g., [20]), where $j_L(x)$ is a spherical Bessel function, and performing the angular integration, we find

$$\frac{d\sigma}{d\Omega_f}=\frac{32\pi^3\omega\alpha}{3p_i^2}\sum_t\Bigg|\sum_{\kappa LJmq} i^{l-L}e^{i\Delta_\kappa}\sqrt{2l+1}\times C^{j\mu_i}_{l0,(1/2)\mu_i}C^{J(\mu_i-\mu_b)}_{j\mu_i,j_b-\mu_b}C^{J(\mu_i-\mu_b)}_{Lm,1q}C^{1t}_{1(t-q),1q}\times P_{JL}(\omega;(\varepsilon_i\kappa\mu_i)b)Y_{Lm}(\hat{\mathbf{k}}_f)Y_{1(t-q)}(\hat{\mathbf{k}}_f)\Bigg|^2. \tag{10}$$

For an explicit form of the functions P_{JL}, we refer to [6].

Another way to evaluate (5) is to consider the final photon propagating in the positive z direction. In this case the polarization vectors of the photon coincide with the unit vectors $\mathbf{e}_{\pm1}$ of the spherical coordinate system. The partial-wave expansion of the incident electron wave function takes the form

$$|p_i\mu_i\rangle=\frac{1}{\sqrt{4\pi}}\frac{1}{\sqrt{\varepsilon_i p_i}}\sum_{\kappa,m_i} i^l e^{i\Delta_\kappa}\sqrt{2l+1}C^{j\mu_i}_{l0,(1/2)\mu_i}\times D^j_{m_i\mu_i}(\hat{\mathbf{z}}\to\hat{\mathbf{p}}_i)|\varepsilon_i\kappa\mu_i\rangle, \tag{11}$$

where $D^j_{m_i\mu_i}(\hat{\mathbf{z}}\to\hat{\mathbf{p}}_i)$ is a Wigner rotation matrix (see, e.g., [21]), which rotates the $\hat{\mathbf{z}}$ direction into the $\hat{\mathbf{p}}_i$ direction. The bound electron wave function should also be transformed to make the angular momentum of the bound electron quantized along $\hat{\mathbf{p}}_i$ instead of $\hat{\mathbf{z}}$:

$$|b\mu_b\rangle_{\hat{\mathbf{p}}_i}=\sum_{m_b} D^{j_b}_{m_b\mu_b}(\hat{\mathbf{z}}\to\hat{\mathbf{p}}_i)|bm_b\rangle_{\hat{\mathbf{z}}}, \tag{12}$$

where the wave functions on the left-hand side and the right-hand side have the angular momentum quantized along the vectors $\hat{\mathbf{p}}_i$ and $\hat{\mathbf{z}}$, respectively. Finally, we obtain for the process under consideration

$$\frac{d\sigma}{d\Omega_f}=\frac{\pi\alpha\omega}{p_i^2}\sum_{t\neq0}\Bigg|\sum_{\kappa,L,J,m_i,m_b} i^{(l-L+1)}e^{(i\Delta_\kappa)}\sqrt{(2l+1)(2L+1)}\times C^{j\mu_i}_{l0(1/2)\mu_i}C^{Jt}_{L01t}C^{J(m_i-m_b)}_{jm_i,j_b-m_b}P_{JL}(\omega;(\varepsilon_i\kappa m_i)(bm_b))\times D^{j_b}_{m_b\mu_b}(\hat{\mathbf{z}}\to\hat{\mathbf{p}}_i)D^j_{m_i\mu_i}(\hat{\mathbf{z}}\to\hat{\mathbf{p}}_i)\Bigg|^2. \tag{13}$$

Formulas (10) and (13) determine the spin-flip (with $\mu_i=-\mu_b$) and non-spin-flip (with $\mu_i=\mu_b$) contributions to the radiative recombination of an electron with a bare nucleus. If radiative recombination of a polarized electron takes place with a polarized H(Li)-like ion in its ground state, and the electron is captured into the ground state of the He(Be)-like ion, the cross section is completely defined by the spin-flip or non-spin-flip contribution, depending on the directions of the polarizations with respect to the initial electron momentum. If both polarizations have the same direction, only the spin-flip process contributes to the cross section. In the opposite case, only the non-spin-flip process must be considered.

We stress that in the above evaluations, the term "spin-flip" strictly refers to $\mu_b=-\mu_i$ with $\mu_i=\pm1/2$ being the helicity of the initially free electron and μ_b denoting the projection of the bound electron's angular momentum on the collision direction. This is in agreement with the terminology employed in [1,2] only if forward or backward emission of the photon is considered, $\hat{\mathbf{k}}_f=\pm\hat{\mathbf{p}}_i$. In those works, the direction of the spin quantization was chosen to be $\hat{\mathbf{k}}_f$ in accordance with the nonrelativistic limit for the photoelectric effect, and the term "spin-flip" was employed for $\mu_b=$

TABLE I. The spin-flip σ_{sf}, non-spin-flip σ_{nsf}, and total cross section σ for radiative recombination of an electron with bare uranium, $Z=92$, in barns. The electron is captured into the 1s state. T_e is the kinetic energy of the incoming electron in the ion-rest frame; T_p is the corresponding ion kinetic energy per atomic-mass unit in the electron-rest frame. The numbers in the column marked T_p are rounded off. The σ_{sf} term determines the total cross section for RR of an electron with H-like uranium into the ground state, if both electron and ion are polarized in the same direction, along or opposite to the initial electron momentum.

T_e(keV)	T_p(MeV/u)	σ_{sf} (b)	σ_{nsf} (b)	σ (b)
5	9.114	173.19	3242.8	3416.0
30	54.69	29.34	478.98	508.32
50	91.14	18.11	262.72	280.83
100	182.3	9.77	107.71	117.48
200	364.6	5.465	39.563	45.027
300	546.9	3.893	21.009	24.902
400	729.2	3.031	13.224	16.256
500	911.4	2.474	9.200	11.673
600	1094	2.079	6.836	8.915
800	1458	1.555	4.291	5.846
1000	1823	1.224	3.005	4.229
1500	2734	0.770	1.602	2.372
2000	3646	0.545	1.045	1.590

TABLE II. The spin-flip σ_{sf}, non-spin-flip σ_{nsf}, and total cross section σ for radiative recombination of an electron with bare uranium, $Z=92$, in barns. The electron is captured into the 2s state. T_e is the kinetic energy of the incoming electron in the ion-rest frame; T_p is the corresponding ion kinetic energy per atomic-mass unit in the electron-rest frame. The numbers in the column marked T_p are rounded off. The σ_{sf} term determines the total cross section for RR of an electron with Li-like uranium into the ground state, if both electron and ion are polarized in the same direction, along or opposite to the initial electron momentum.

T_e (keV)	T_p (MeV/u)	σ_{sf} (b)	σ_{nsf} (b)	σ (b)
5	9.114	25.45	528.83	554.28
30	54.69	3.979	80.303	84.282
50	91.14	2.369	43.838	46.206
100	182.3	1.216	17.482	18.698
200	364.6	0.660	6.120	6.780
300	546.9	0.469	3.148	3.617
400	729.2	0.368	1.938	2.305
500	911.4	0.302	1.326	1.628
600	1094	0.256	0.973	1.229
800	1458	0.194	0.599	0.794
1000	1823	0.155	0.414	0.569
1500	2734	0.099	0.216	0.315
2000	3646	0.071	0.139	0.210

$-\mu_i$ with respect to that direction. However, since for relativistic continuum electrons, the spin projection has a sharp value only in the direction of propagation, the quantization in the photon direction is only meaningful if forward or backward emission of the photon is considered. If the spin state is not measured directly [15] (and hence one takes a sum over spin projections), the cross section at forward angles provides a unique signature [2] for spin-flip processes, irrespective of the quantization axis. We stress, however, that only quantization in the direction of the electron propagation, as performed in the present work, yields the proper spin-flip contribution for an arbitrary angle of the emitted photon.

III. NUMERICAL RESULTS AND DISCUSSION

The spin-flip and non-spin-flip differential cross sections have been numerically calculated by both methods described above [Eqs. (10) and (13)]. Perfect agreement in all results has been found. The computer code developed in [2] and modified in [6] has been adapted for evaluating the spin-flip and non-spin-flip RR cross sections. The angular integrations have been carried out analytically. The RADIAL package from [22] has been employed to calculate the exact bound and continuum state wave functions for extended nuclei. To achieve the desired accuracy, partial waves with $|\kappa|$ up to 50 have been taken into account.

The numerical results for the spin-flip, non-spin-flip, and total RR cross sections for uranium are presented in Tables I and II. The calculations are carried out in the nucleus-rest frame for recombination into the 1s and 2s states and kinetic electron energies in the range 5–2000 keV. The spin-flip contribution determines the complete differential cross section for the radiative recombination of an electron with H(or Li)-like uranium, if both the electron and the ion are polarized in the same direction, along or opposite the initial electron momentum (the cross section is the same for both directions). The non-spin-flip contribution gives the cross section of the

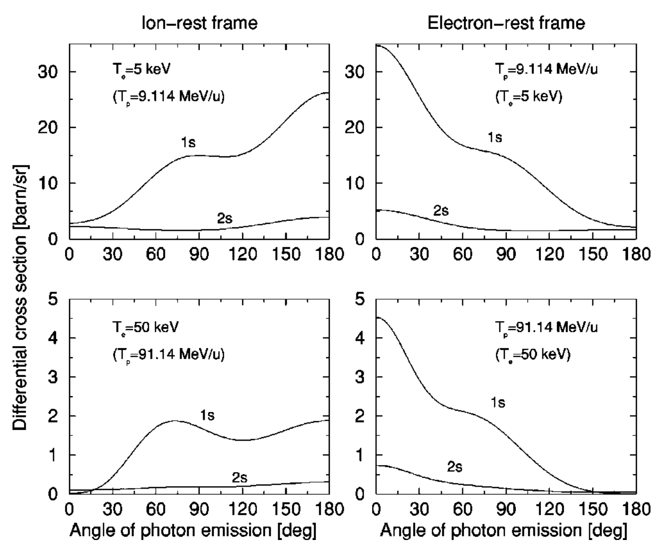

FIG. 1. The spin-flip differential cross section of radiative recombination into the 1s and 2s states of bare uranium. The results are shown in the ion and the electron-rest frames at kinetic electron energies of 5 and 50 keV, corresponding to ion-projectile energies of 9.114 MeV/u and 91.14 MeV/u, respectively. In the ion-rest frame, the angles are defined with respect to the electron-motion direction, and in the electron-rest frame, the angles are defined with respect to the ion-motion direction.

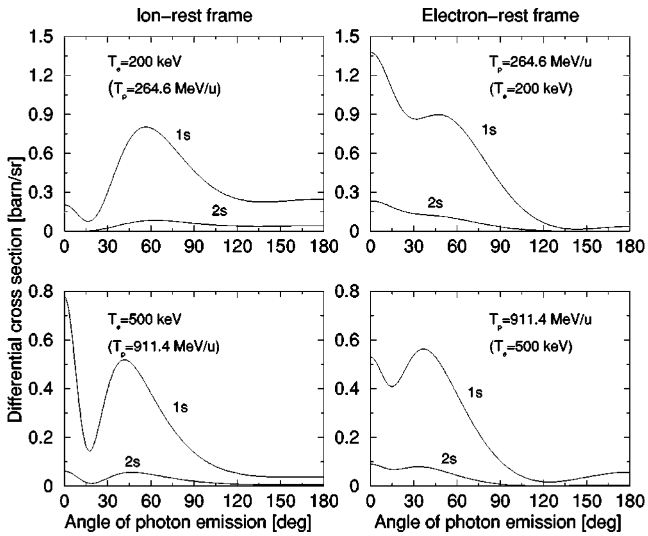

FIG. 2. The same as Fig. 1 but for kinetic electron energies of 200 and 500 keV, corresponding to ion-projectile energies of 264.6 MeV/u and 911.4 MeV/u, respectively.

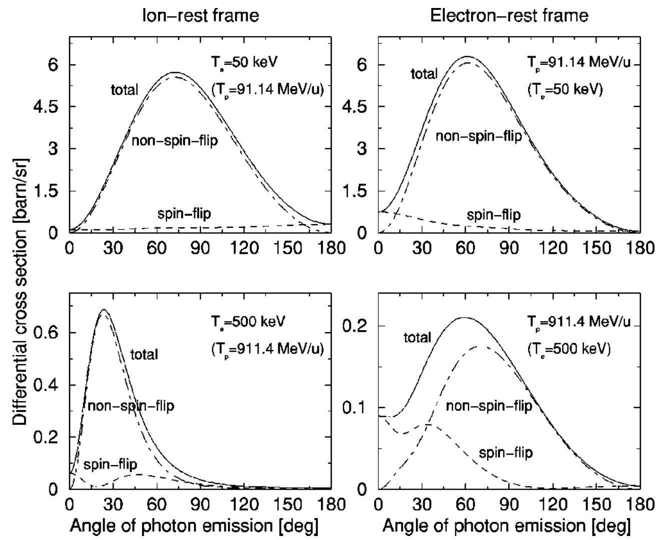

FIG. 4. The same as Fig. 3 but for radiative recombination into the $2s$ state.

same process but for an electron and an ion having opposite polarizations. Finally, the sum of the spin-flip and non-spin-flip contributions for the $1s$ and $2s$ states defines the complete differential cross section for the radiative recombination of an electron with bare uranium into the $1s$ and $2s$ states, respectively. Our values from Tables I and II agree with the recent evaluation in Ref. [4], where the cross section divided by the number of vacancies, $(2j_b+1)$, was tabulated.

The spin-flip RR differential cross section for various kinetic energies of the incident electron between 5 and 500 keV is presented in Figs. 1 and 2 both for the ion-rest frame and the electron-rest frame. In the ion-rest frame, the angles are defined with respect to the electron-motion direction, and in the electron-rest frame, the angles are defined with respect to the ion-motion direction. The differential cross section in the electron-rest frame is obtained from the differential cross section in the ion-rest frame by employing the transformation rules given in [1]. In order to display the relative magnitude of the spin-flip effect on RR with bare uranium, the spin-flip, non-spin-flip, and total differential cross sections are presented in Figs. 3 and 4. From these figures it can be seen that in that case the non-spin-flip part gives the dominant contribution to the total differential cross section, except for the forward direction in the electron-rest frame or at energies not yet accessible experimentally. Therefore, the only way to identify the spin-flip contribution in RR processes with a bare nucleus is to measure the differential cross section in the forward direction [2,15]. However, if one wants to identify spin-flip contributions to RR at arbitrary angles, one needs an experiment in which a polarized electron recombines with an H- or Li-like heavy ion polarized in the same direction. In this work we have presented numerical results for uranium only. Of course, the arguments given above are also valid for all other H- and Li-like ions. However, in the case of lighter ions the electron-electron interaction becomes more important.

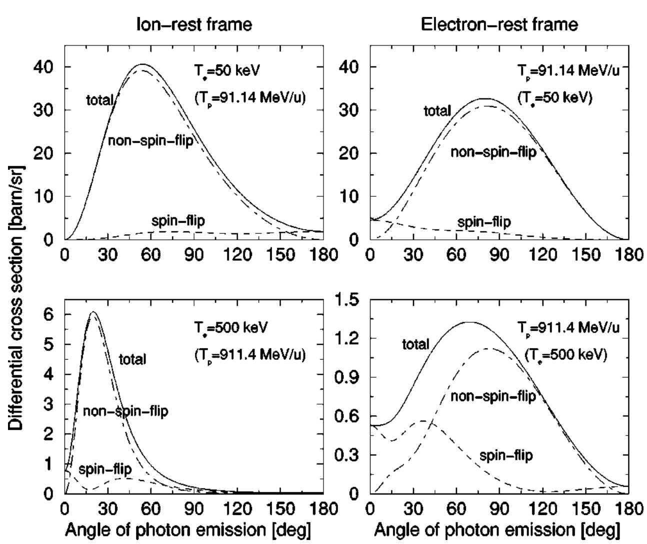

FIG. 3. The spin-flip, non-spin-flip, and total differential cross section for radiative recombination into the $1s$ state of bare uranium. The results are shown in the ion and the electron-rest frames at kinetic electron energies of 50 and 500 keV, corresponding to ion-projectile energies of 91.14 MeV/u and 911.4 MeV/u, respectively. In the ion-rest frame, the angles are defined with respect to the electron-motion direction, and in the electron-rest frame, the angles are defined with respect to the ion-motion direction.

We expect that the spin-flip RR cross section evaluated in the present work will be available for experimental investigations at GSI in the near future [23]. It will provide an excellent possibility for testing relativistic effects in electron–heavy-ion collisions.

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