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Resonant channel coupling at electron transitions to the continuum

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Abstract

The process of simultaneous ionization and excitation of helium by proton impact, $p + He(1s^2\,{}^1S) \rightarrow p + e + He^+(nl\,{}^2L)$, is investigated using perturbation theory alllowing for the configuration interaction. It is shown that the resonant channel coupling causes sudden drops at electron energies $E_e = E_{n_1 l_1\,{}^2L_1} - E_{nl\,{}^2L}$ in the ejected electron energy spectrum (here, $E_{nl\,{}^2L}$ is the energy of the $nl\,{}^2L$ state of the He^+ ion; n_1, l_1 and L_1 are the principal and orbital quantum numbers and the orbital angular momentum for the states of the He^+ ion above the $nl\,{}^2L$ state). The drops in the energy spectrum of electrons ejected at the $1s^2\,{}^1S \rightarrow nl\boldsymbol{\kappa}$ transition are located in the range of electron energies $0 < E_e \leqslant -E_{nl\,{}^2L}$.

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1. Introduction

The investigation of electron transitions in fast collisions of structureless charged particles with few-electron atomic systems yields information on the dynamics of the electron–electron interaction. Two-electron transitions in atoms with transference of one of the atomic electrons into the continuum are of fundamental importance to the understanding of electron correlation effects in few-body Coulomb systems. Helium presents the simplest object for investigation of two-electron transitions and so the simultaneous ionization and excitation of helium by electron and proton impact have been studied by many authors both theoretically [1–8] and experimentally [9–13]. The main subjects of almost all these investigations are the cross sections and mechanisms of two-electron transitions in the simultaneous ionization and excitation processes.

In the present work we shall consider the normalization of the helium continuous state wave function determined allowing for the configuration interaction and investigate the influence of the channel coupling upon the form of the ejected electron energy spectrum. To do this we must have a pure electron energy spectrum. We shall consider a specific process,

$$p + He(1s^2\,{}^1S) \rightarrow p + e + He^+(2s\,{}^2S). \qquad (1)$$

We choose the ionization–excitation process, because in this case the states of both helium electrons are determined and there is no superposition of different energy spectra due to the excitation of different states of the He^+ ion. Although there are the $n_1 l_1 n_2 l_2\,{}^1L$ au-

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toionizing states with energies satisfying the condition

$$E_{n_1l_1n_2l_2\,{}^1L} = E_{2s\,{}^2S} + \tfrac{1}{2}\kappa^2, \tag{2}$$

in reality, the autoionizing peaks in the energy spectrum also must not be observed, because the Auger decay of the helium autoionizing state takes place only when one of the helium electrons goes to the ground state of the ion.

2. General statements

Let us consider the scattering of a fast proton by the helium atom in the impact parameter representation. It is assumed that the projectile moves along a straight line $\boldsymbol{R}(t) = \boldsymbol{\rho} + \boldsymbol{v}t$ (where $\boldsymbol{\rho}$ is the impact vector and $\boldsymbol{v}$ is the velocity of the projectile relative to the atomic nucleus), while the electron wave function is independent of the relative distance between the colliding particles and is given by the Schrödinger equation which in the interaction picture has the form

$$\mathrm{i}\frac{\partial \Psi(t)}{\partial t} = \tilde{V}(t)\Psi(t),$$
$$\Psi(t)|_{t\to\pm\infty} = \Psi_{\mathrm{I,F}}(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{3}$$

where

$$\tilde{V}(t) = \exp(\mathrm{i}\hat{H}_0 t)\left(-\sum_{j=1}^{2}\frac{1}{|\boldsymbol{R}(t) - \boldsymbol{r}_j|}\right)\exp(-\mathrm{i}\hat{H}_0 t) \tag{4}$$

is the interaction operator in the interaction picture. The wave function $\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the eigenfunction of the atomic Hamiltonian $\hat{H}_a$ with the eigenvalue E,

$$\hat{H}_a\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = E\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2). \tag{5}$$

Here, $\hat{H}_0 = \hat{H}_a + \hat{K}$ is the free-motion Hamiltonian; $\hat{K} = \hat{\boldsymbol{P}}^2/2M$ and M are the kinetic energy operator and the reduced mass of colliding particles; $\hat{\boldsymbol{P}}$ is the relative motion momentum operator; $\boldsymbol{R}(t)$ and $\boldsymbol{r}_j$ are the radius vectors of the projectile and of the jth atomic electron relative to the target atom nucleus.

The electron wave function of the helium atom μ-state $\Psi_\mu(\boldsymbol{r}_1, \boldsymbol{r}_2)$ determined alllowing for the configuration interaction has the form [14]

$$\Psi_\mu(\boldsymbol{r}_1, \boldsymbol{r}_2) = \Phi_\mu(\boldsymbol{r}_1, \boldsymbol{r}_2) + \left(\sum_\nu{}' + \int \mathrm{d}\nu\right)\lambda_\nu\,\Phi_\nu(\boldsymbol{r}_1, \boldsymbol{r}_2), \tag{6}$$

where

$$\lambda_\nu = \frac{\langle\Phi_\nu|W^{\mathrm{c}}|\Phi_\mu\rangle}{E_\mu - E_\nu - \mathrm{i}0} \tag{7}$$

Here, $\Phi_\mu(\boldsymbol{r}_1, \boldsymbol{r}_2)$ is the electron wave function of the helium atom in the self-consistent field approximation; E_L is the energy of the L-state of the helium atom determined alllowing for the electron correlations; $W^{\mathrm{c}} = V^{\mathrm{c}} = 1/r_{12}$ is the operator of the correlation interaction of the electrons of the helium atom. The prime on the summation sign denotes the summation does not include states that can lead to self-mixing. The imaginary part i0 in the energy denominator in expression (7) has the effect of moving the pole off the real axis when Φ_ν describes a state in the continuous spectrum. Concerning the choice of W^{c} and of the sign of the imaginary part in the energy denominator, see Ref. [15].

For what follows it is convenient to introduce some definitions. States Φ_γ with two electrons in the discrete spectrum we call helium discrete states; states Φ_γ in which one or two helium electrons are in the continuous spectrum we call helium continuous states. The first term in the right-hand side of (6) we call the basic state (configuration). All states entering in the last term in the right-hand side of (6) we call included states (configurations). As

$$\frac{1}{E_\mu - E_\nu - \mathrm{i}0} = \mathrm{i}\pi\delta(E_\mu - E_\nu) + \frac{P}{E_\mu - E_\nu}, \tag{8}$$

in the sum over the different electron states in (6) there are states which possess the same energy as the basic state. Such states we call the resonant included states (configurations); the rest of the included states we call nonresonant included states (configurations). The appropriate reaction channel corresponds to each state in the right-hand side of (6). We call them, respectively, basic channel, resonant included channels, and nonresonant included channels. Accordingly, the coupling of the basic channel with the resonant or nonresonant included channels we call, respectively, the resonant or nonresonant channel coupling.

From expressions (6) and (8) it follows that the states belonging to the continuous spectrum can be both resonant and nonresonant included states; but the states belonging to the discrete spectrum can be nonresonant included states only.

The helium normalized wave functions $\tilde{\Psi}$ for the initial $1s^2\ ^1S$ and final $2s\boldsymbol{\kappa}$ states are determined by the expressions

$$\tilde{\Psi}_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{N_i}\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2) \tag{9}$$

and

$$\tilde{\Psi}_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{N_f(\boldsymbol{\kappa})}\Big(\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2) - \frac{1}{N_i^2}\langle\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle \times \Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)\Big). \tag{10}$$

Here, N_i and $N_f(\boldsymbol{\kappa})$ are normalizing factors for the initial and final state wave functions, respectively. The wave function $\tilde{\Psi}_\gamma$ is normalized to unity for the states of discrete spectrum and to a δ-function of the momentum for the states of the continuous spectrum (or to the product of two δ-functions in the case of the states with two electrons in the continuum).

From (9), (10) it follows that the normalizing factors for the $1s^2\ ^1S$ and $2s\boldsymbol{\kappa}$ state wave functions must be determined from the relations

$$N_i^2 = \langle\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle \tag{11}$$

and

$$N_f^2(\boldsymbol{\kappa}) = \langle\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle - \frac{1}{N_i^2}|\langle\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)|\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle|^2. \tag{12}$$

From expressions (6)–(10) we can see that the normalizing factors for discrete state wave functions are constants, and they are functions of the electron momentum for continuum state wave functions.

3. The two-electron transition amplitude

The amplitude of the two-electron transition $1s^2\ ^1S \rightarrow 2s\boldsymbol{\kappa}$ induced in a collision of a fast structureless charged particle with helium as a function of the impact parameter $\rho = |\boldsymbol{\rho}|$, is

$$A(2s\boldsymbol{\kappa} \leftarrow 1s^2\ ^1S;\rho) = \frac{1}{N_i N_f(\boldsymbol{\kappa})} \times \langle\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)|S(+\infty,-\infty)|\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)\rangle, \tag{13}$$

where $S(+\infty,-\infty)$ is the scattering S-matrix. Using the results of Ref. [14] and restricting ourselves to the second order of the perturbation theory series in the interaction potential, we can write the amplitude (13) in the form

$$A(2s\boldsymbol{\kappa} \leftarrow 1s^2\ ^1S;\rho) = \frac{1}{N_i N_f(\boldsymbol{\kappa})}[a_{on}^{c1}(2s\boldsymbol{\kappa};\rho) + a_{off}^{c1}(2s\boldsymbol{\kappa};\rho) + a^{12}(2s\boldsymbol{\kappa};\rho) + a^{c2}(2s\boldsymbol{\kappa};\rho)]. \tag{14}$$

Here, a_{on}^{c1} and a_{off}^{c1} are the amplitudes of two-electron transitions occurring as a result of a single scattering of a projectile by the helium atom and the correlation interaction of atomic electrons, a_{on}^{c1} describes the on-energy shell transitions and a_{off}^{c1} describes the off-energy shell ones; a^{12} is the amplitude of a transition of two helium electrons as a result of a single interaction of each of them with the projectile; a^{c2} is the amplitude of a two-electron transition occurring as a result of the double scattering of a projectile on helium and the correlation interaction of the atomic electrons.

Expressions for the amplitudes a_{on}^{c1}, a_{off}^{c1}, a^{12} and a^{c2} for the considered two-electron transition may be obtained from the results presented in Ref. [14].

4. Results and discussion

Calculation results of the single differential cross section (SDCS) for the process of ionization of the helium atom with simultaneous excitation of the atomic residual to the 2s state, induced in collisions of protons with helium atoms, are presented in Fig. 1 for three values of the proton energy, E_p = 0.5, 1.5 and 5.0 MeV, versus the ejected electron energy E_e. In the calculations the term a^{c2} in the ionization–excitation amplitude (14) was not taken into account as it is much smaller than the other terms of the amplitude

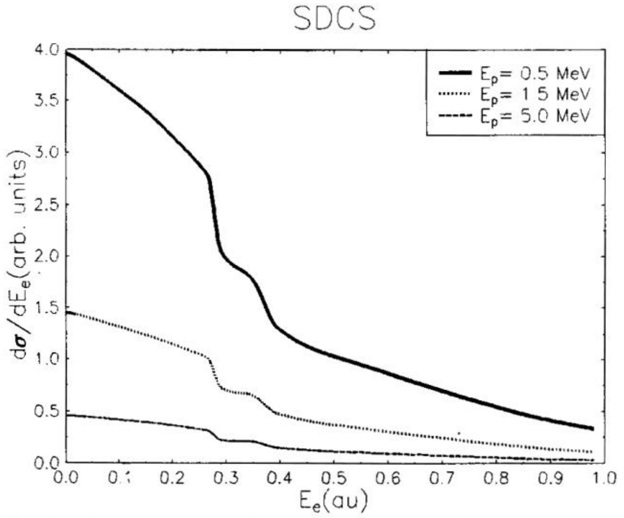

Fig. 1. The value of $d\sigma/dE_e$ as a function of E_e, the ejected electron energy, for the $p + He(1s^2\,^1S) \rightarrow p + e + He^+(2s\,^2S)$ transition at three different proton energies.

[14]. Calculating the amplitude (14) we also took into account the on-energy shell transitions only. So

$$A(2s\boldsymbol{\kappa} \leftarrow 1s^2\,^1S;\rho) = \frac{1}{N_i N_f(\boldsymbol{\kappa})}[a_{on}^{cl}(2s\boldsymbol{\kappa};\rho) + a^{12}(2s\boldsymbol{\kappa};\rho)] \quad (15)$$

was used as the amplitude of the two-electron transition.

The present calculations give 1.08 for the normalizing factor N_i of the $\tilde{\Psi}_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ wave function. Determining the normalizing factor $N_f(\boldsymbol{\kappa})$ we assumed that the states described by the $\Psi_{1s^2\,^1S}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ and $\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ wave functions are weakly coupled with each other. We took into account only the $ns\boldsymbol{\kappa}$ resonant included states in the expansion of $\Psi_{2s\boldsymbol{\kappa}}(\boldsymbol{r}_1,\boldsymbol{r}_2)$ over the self- consistent field states. Contributions from states with $n > 4$ are determined as $1/n^3$.

The calculation results show that at ejected electron energies $E_e = E_{nl\,^2L} - E_{2s\,^2S}$ (where $E_{nl\,^2L}$ is the energy of the $nl\,^2L$ state of the He^+ ion; n, l and L are the principal and orbital quantum numbers and the orbital angular momentum for the states of the He^+ ion lying higher than the $2s\,^2S$ one) there are sudden drops in the SDCS. The appearance of these drops is due to the opening of new resonant channels. Actually, as for resonant included states

$$E_{2s\,^2S} + E_e = E_{nl\,^2L} + E'_e, \quad (16)$$

taking into account that $E'_e = 0$ in the threshold, for the electron energy we obtain the values mentioned above. So, at electron energies $E_e = E_{nl\,^2L} - E_{2s\,^2S}$ there is a possibility of electron transfer to the new resonant included state. The sudden drops in the energy spectrum of the ejected electrons are due to the resonant channel coupling effect. The uppermost resonant included state is the helium atom state with two electrons in the continuous spectrum. So, all drops in the ejected electron energy spectrum are located in the range of electron energies $0 < E_e \leqslant -E_{2s\,^2S}$.

A similar situation occurs in two-electron transitions in helium to any $nl\boldsymbol{\kappa}$ state. In these cases the drops in the electron energy spectra are located in the range of electron energies $0 < E_e \leqslant -E_{nl\,^2L}$. In the case of two-electron ionization of helium by protons or by any structureless charged particles the electron energy spectrum has no sudden drops due to the resonant channel coupling because in this case the thresholds for all resonant states are below the basic state threshold.

In the present calculations we did not take into account the nonresonant channel coupling. Nonresonant channel coupling exists at any energy of the ejected electrons and it gives rise to a fair change of the electron energy spectrum only. The sudden drops in the electron energy spectrum can be observed at energies of ejected electrons corresponding to the threshold energies. Exactly at these energies the opening of new ways of a transference of the electrons from the basic state to the other ones occurs.

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