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Use of the Operator Approach in the Collisions of Highly-Charged Ions with Few-Electron Atoms

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Abstract

The probabilities and cross sections for the $1s^2{}^1S \to 2s^2{}^1S$ and $1s^2{}^1S \to 2s2p^1P$ transitions induced in collisions of fast charged projectiles with helium atoms have been investigated in the framework of the operator approach to the few-body problem (V. A. Sidorovich, Physica Scripta, accepted for publication). Calculations have been performed for the case of the $2s^2{}^1S$ excitation of helium by projectiles with Z_p varying from 3 to 9 at collision energy $E_p = 1.5$ MeV/u. The calculated cross sections are in satisfactory agreement with the available experimental data. The cross section dependence upon the projectile charge is established. The wavefunctions for few-electron atom, satisfying the boundary condition $U = 0$ (U is the interconfiguration interaction potential) in the past or in the future, and the closure relation for joint system functions are presented.

1. Introduction

Here we study the $1s^2{}^1S \to 2s^2{}^1S$ and $1s^2{}^1S \to 2s2p^1P$ transitions induced in fast collisions of multicharged ions with helium atoms on the basis of the operator method of solution of the non-relativistic Schrödinger equation for few-body systems with a pair-wise interaction, worked out in Ref. [1]. The study of double-electron transitions in collisions of structureless charged particles with helium atoms is especially urgent as in such collisions an insight into the physical nature of multi-electron processes is accessible. The present paper continues the theoretical investigations of multi- electron processes in atomic particle collisions (see, e.g., [2–6]).

2. Closure relation for joint system functions and structure of the multi-electron transition amplitude

The scattering problem is solved in the impact parameter treatment. During collision the charged particle moves along a straight line $\mathbf{R}(t) = \mathbf{b} + \mathbf{v}t$ (where $\mathbf{b}$ is the impact parameter and $\mathbf{v}$ is the ion velocity relative to the nucleus of the target atom), and the electron wavefunction Ψ of the target atom is determined by the non-relativistic Schrödinger equation, which in the interaction picture has the form

$$\mathrm{i}\frac{\partial}{\partial t}\Psi^{\mathrm{int}}(t) = \tilde{V}(t)\Psi^{\mathrm{int}}(t) \quad \text{with} \quad \Psi^{\mathrm{int}}(t) \mid_{t\to\pm\infty} = \Psi_{\{I,F\}}(\mathbf{r}). \tag{1}$$

$\tilde{V}(t)$ is the operator of the fast ion-target atom interaction in the interaction picture and $\mathbf{r}$ denotes a set of all electron coordinates of the atomic system relative to the atomic nucleus. The wavefunction $\Psi_{\{\gamma\}}(\mathbf{r})$ is an eigenfunction of the atomic Hamiltonian $\hat{H}_a$ with an eigenvalue $E_{\{\gamma\}}$

$$\hat{H}_a \Psi_{\{\gamma\}}(\mathbf{r}) = E_{\{\gamma\}}\Psi_{\{\gamma\}}(\mathbf{r}). \tag{2}$$

In the framework of the operator approach to the many body problem [1] the solution of the Schrödinger equation for few-electron atomic system has been expressed in terms of the wavefunctions, determined in the framework of the isolated configuration approximation (ICA). The relationship between the CI-wavefunction $\Psi_{\{\gamma\}}$ of the atomic system and the wavefunction ϕ_γ of its ICA-analogue (which we shall call the basic ICA-state) is established by means of some configuration mixing operator $\mathcal{M}_{(\pm)}$

$$\Psi_{\{\gamma\}} \equiv \mid \{\gamma\}^{(\pm)} > = \mathcal{M}_{(\pm)}\phi_\gamma \equiv \mathcal{M}_{(\pm)} \mid \gamma > . \tag{3}$$

Different signs with the $\mathcal{M}_{(\pm)}$-operator correspond to different ways of moving the pole off the real axis. Each of the ICA-wavefunctions ϕ_γ is represented by an antisymmetrical product of the single-electron wavefunctions [1]. The Schrödinger equation (2) has two sets of eigenfunctions of operator $\hat{H}_a$ [1]: $\{\mid \{\gamma\}^{(+)} >\}$ and $\{\mid \{\gamma\}^{(-)} >\}$. As will be shown in further publications, $\mid \{\gamma\}^{(+)} >$ ($\mid \{\gamma\}^{(-)} >$) represents the electron wavefunction of an atom (the positron wavefunction of an antiatom) when the boundary condition $U = 0$ is satisfied in the past (here U is the interconfiguration interaction potential). When the boundary condition $U = 0$ is satisfied in the future the opposite is true.

Each of the sets of orthonormal eigenfunctions $\{\mid \overline{\{\gamma\}}^{(\pm)} >\}$ of $\hat{H}_a$ is closed

$$\sum_{\{\gamma\}} \mid \overline{\{\gamma\}}^{(\pm)} >< \overline{\{\gamma\}}^{(\pm)} \mid = \mathbf{E}, \tag{4}$$

where $\mathbf{E}$ is the unit operator. The use of the last relation gives rise to matrix elements of the form $< \overline{\{\gamma_K\}}^{(\pm)} \mid (-Z_p/\mid \mathbf{R}(t) - \mathbf{r}_j \mid) \mid \overline{\{\gamma_L\}}^{(\pm)} >$ in higher order terms of the scattering amplitude (here $\mathbf{r}_j$ is the jth atomic electron radial vector; Z_p is the ion charge) . In such matrix elements the ways of moving the pole off the real axis are different for the states before and after scattering. If instead we use the relation

$$\sum_{\{\gamma\},\{\beta\}} \mid \overline{\{\gamma\}}^{(+)} >< \overline{\{\gamma\}}^{(+)} \mid \overline{\{\beta\}}^{(-)} >< \overline{\{\beta\}}^{(-)} \mid = \mathbf{E} \tag{5}$$

we come to matrix elements $< \overline{\{\gamma_K\}}^{(-)} \mid (-Z_p/\mid \mathbf{R}(t) - \mathbf{r}_j \mid) \mid \overline{\{\gamma_L\}}^{(+)} >$ in which the ways of moving the pole off the real axis are the same for the states before and after scattering.

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As a solution of equation (2) we use the normalized CI-wavefunction of the form

$$| \overline{\{\gamma^{(I)}\}}^{(\pm)} > \equiv \frac{1}{N} | \{\gamma^{(I)}\}^{(\pm)} > = \frac{\pm i}{N} \Big[| \gamma > + \Big(\sum_{v} + \int \mathrm{d}v \Big) | v > \frac{< v | U | \gamma >}{E - E_v^{(L)} \pm \mathrm{i}\varepsilon} \Big]. \quad (6)$$

Here N is the normalizing factor and $E_v^{(L)}$ is the v-state energy of atomic system determined in ICA. It represents the first order term in the power series expansion of the exact CI-wavefunction $| \overline{\{\gamma\}}^{(\pm)} >$ in terms of U [1]. Up to a phase multiplier this function coincides with that from Ref. [4], determined in the diagonalization approximation. It can be shown that the functions $| \{\gamma^{(I)}\}^{(+)} >$ and $| \{\beta^{(I)}\}^{(-)} >$ (with $\gamma \neq \beta$) are orthogonal to each other, at least accurate up to the first order in the potential U. So the relation (5) may be rewritten in the form of approximate equality

$$\sum_{\{\gamma\}} \frac{1}{N_{\{\gamma\}}^4} | \{\gamma^{(I)}\}^{(+)} > < \{\gamma^{(I)}\}^{(-)} | \approx \mathbf{E}, \quad (7)$$

which we shall call *the closure property for joint system functions*. Then the scattering amplitude A has the form

$$\begin{aligned} A(\{F\} \leftarrow \{I\}; \mathbf{b}) &= \frac{-\mathrm{i}}{N_{\{I\}} N_{\{F\}}} \int_{-\infty}^{+\infty} \mathrm{d}t \exp[\mathrm{i}(E_{\{F\}} - E_{\{I\}})t] \\ &\times < \{\gamma_F^{(I)}\}^{(-)} | \sum_{j=1}^{n} \frac{-Z_\mathrm{p}}{| \mathbf{R}(t) - \mathbf{r}_j |} | \{\gamma_I^{(I)}\}^{(+)} > \\ &+ \frac{(-\mathrm{i})^2}{N_{\{I\}} N_{\{F\}}} \Big(\sum_{\{K\}} + \int \mathrm{d}\{K\} \Big) \frac{1}{N_{\{K\}}^4} \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \\ &\times \exp[\mathrm{i}(E_{\{F\}} - E_{\{K\}})t_1] \exp[\mathrm{i}(E_{\{K\}} - E_{\{I\}})t_2] \\ &\times < \{\gamma_F^{(I)}\}^{(-)} | \sum_{j=1}^{n} \frac{-Z_\mathrm{p}}{| \mathbf{R}(t_1) - \mathbf{r}_j |} | \{\gamma_K^{(I)}\}^{(+)} > \\ &\times < \{\gamma_K^{(I)}\}^{(-)} | \sum_{l=1}^{n} \frac{-Z_\mathrm{p}}{| \mathbf{R}(t_2) - \mathbf{r}_j |} | \{\gamma_I^{(I)}\}^{(+)} > + \ldots . \end{aligned} \quad (8)$$

So the collision of a projectile with an atom proceeds as follows: as a result of the first scattering the atom goes from its initial state $| \overline{\{\gamma_I^{(I)}\}}^{(+)} >$, satisfying the boundary condition $U = 0$ in the past, to the intermediate state $| \overline{\{\gamma_K^{(I)}\}}^{(-)} >$, satisfying the boundary condition $U = 0$ in the future. Between two sequential scatterings the atom goes from the state $| \overline{\{\gamma_K^{(I)}\}}^{(-)} >$, satisfying the boundary condition $U = 0$ in the future, to the state $| \overline{\{\gamma_K^{(I)}\}}^{(+)} >$, satisfying the boundary condition $U = 0$ in the past, and so on. After the whole collision process the atom is registered by the apparatus in the state, satisfying the boundary condition $U = 0$ in the future.

3. Results and discussion

Examining the two-electron transitions in helium we can restrict ourselves for the terms of the perturbation series up to the second order in the potential $\tilde{V}(t)$ and the approximation (6) for the CI-wavefunctions. The wavefunctions for $1s^2\,{}^1S$, $2s^2\,{}^1S$ and $2s2p\,{}^1P$ states of helium are determined with allowance for orbitals $1s^2$, 1s2s, 1s2p, $1s\vec{\kappa}$, $2s^2$, 2s2p, $2p^2$, $2s\vec{\kappa}$, $2p\vec{\kappa}$ only. The normalizing factor $N_{\{K\}}$ for the intermediate state wavefunction $| \{\gamma_{\{K\}}^{(I)}\}^{(\pm)} >$ is equal to 1.04 because we take into account only the orbitals $1s^2$, 1s2s, $2s^2$, $2p^2$.

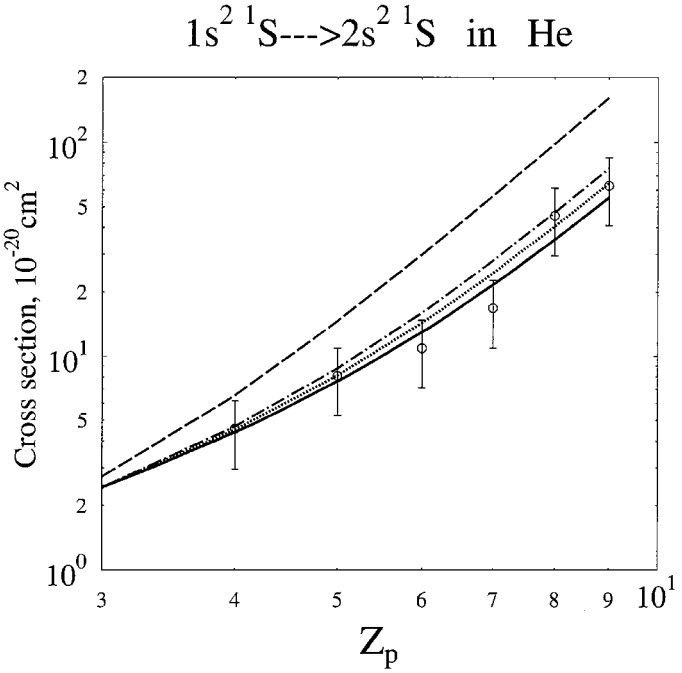

Fig. 1. The helium $1s^{21}S \rightarrow 2s^{21}S$ excitation cross section at collision energy $E = 1.5$ MeV/u as a function of the projectile charge. Full curve presents the results using relation (7); dotted curve, the results using relation (4) and CI-wavefunctions (6); dash-dotted curve, the results using the IPM-wavefunctions in the intermediate states; dashed curve, the results using the independent electron approximation for the second term of amplitude (8). The experimental results are from Ref. [7].

The cross sections of the $1s^{21}S \rightarrow 2s^{21}S$ excitation of helium induced in collisions of charged projectiles with helium at collision energy $E = 1.5$ MeV/u are presented in Fig. 1 versus the projectile charge Z_p ranging from 3 to 9. The results which use relation (7) are in a better agreement with the experimental data than others.

4. Empirical analysis

The calculated cross sections, with a higher degree of accuracy, may be approached by the function

$$\sigma = \sigma_0 Z_\mathrm{p}^{a \ln Z_p + b}. \quad (9)$$

The parameters σ_0, a, b depend on the scattering energy E. For the present case we have: $\sigma_0 = 1.385 \times 10^{-20}\mathrm{cm}^2$, $a = 1.057$ and $b = -0.645$. The present cross sections are in good agreement with the measured ones [7], but the Z-dependence of the cross section (relation (9)) differs from that presented in Ref. [7] (in Ref. [7]: $\sigma = A Z_\mathrm{p}^B$ and $B = 3$).

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