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PECULIARITIES OF EXCITED HELIUM PHOTOIONIZATION

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Лхагва О., Данзан С., Страхова С.И. E4-94-12
Особенности фотоионизации возбужденного гелия

Исследована физическая природа проявления закрытого канала при фотопроцессах с участием возбужденного гелия и формирования резонансной структуры в таких случаях. Показано, что в области энергии фотоэлектрона E > 0,5 а.е. конкуренция и интерференция ветвей прямого и через закрытый канал фотопереходов обуславливают особенности в энергетической зависимости различных характеристик фотопроцесса с участием возбужденного гелия, а также резонансных профилей АИС. Предлагается эффект закрытого канала и форму профилей резонансов, возбуждаемых при таких процессах, выявить путем измерения безразмерной характеристики — коэффициента угловой анизотропии вторичного фотона γ_2 в фото- и диэлектронной рекомбинации $He^+(1s) + e \Rightarrow He^{**} \Rightarrow \gamma_1 + (He(2^1P) \Rightarrow He(1^1S) + \gamma_2)$.

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Lhagva O., Danzan S., Strakhova S.I. E4-94-12
Peculiarities of Excited Helium Photoionization

The physical nature of the closed channel appearance in photoprocesses with the excited He is investigated. It is shown that in the photoelectron energy range E > 0.5 a.u. the competition and interference of the branches of the direct and via the closed channel phototransitions define the peculiarities in the energy dependence of different characteristics of the photoprocesses with the excited He as well as of autoionization resonance profiles. It is suggested revealing the closed channel effect and resonance profile peculiarities by measuring the dimensionless characteristics — angular anisotropy coefficient of secondary photons in the photo- and dielectronic recombination $He^+(1s) + e \Rightarrow He^{**} \Rightarrow \gamma_1 + (He(2^1P) \Rightarrow He(1^1S) + \gamma_2)$.

The investigation has been performed at the Bogoliubov Laboratory of Theoretical Physics, JINR.

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I. INTRODUCTION

Photoionization of the excited He is much less studied[1,2] than photoionization of He in the ground state. In the main, this is caused by technical difficulties in preparing excited He targets.

At present, a significant progress[3] is achieved in investigating photoionization of an excited atom, in particular, helium. This is favoured by the use[4,5] of laser and synchrotron sources for preparing targets of excited atoms and their photoionization, respectively. Thus, targets of the He($n^{1,3}$P) atoms (n=3,4,5) have been obtained by the laser pumping method[5,6]. In the mean time, substantially distinct features of direct and resonant branches of the excited He photoionization[2] and their interferences[7] as compared to the ground-state photoionization might allow a better understanding of the role of the electron correlations and also a resonance structure forming. So one may expect that with growing need to explore the actual problems, in the near future experiments on photoionization of the excited He would be realized in a wide range of its spectrum.

At the same time, a demand is growing for photoionization data of the excited He for fundamental and applied investigations. Thus, theoretical description of the problem of excited He photoionization needs to be developed.

At present, a number of questions related to the peculiarities[2] of the direct and resonance photoionization characteristics of the excited He are to be solved. In rather accurate calculations[2,8-10], a wide minimum in the cross section of the excited He photoionization has been detected in the range of the photoelectron spectra E> 0.5 a.u. Excitation of autoionization resonances (AIR) with a large profile index — q[2,15,16] in the excited He photoionization was observed as well. The "broadening" and "shift" phenomena in resonance profiles of dimensionless characteristics of the autoionization state (AIS), such as the angular anisotropy coefficients of the photoelectron in the atomic photoionization[9] and the secondary photon[15] in the dielectronic recombination: $He^{+}+e \rightarrow He^{**} \rightarrow \gamma_1 + [He(2^1P) \rightarrow He(1^1S)+\gamma_2]$ have also been reported.

The peculiarities mentioned above manifest themselves in the d-wave(also ^1D AIR) branch of photoprocesses with the He(2^1P) atom.

It is known that the AIS profile indices serve as a sensitive means to test the atomic structure model. The profile indices for the lowest resonances from the series of singlet and triplet S,P and D AIS produced from the excited helium $2^{1,3}S$ и $2^{1,3}P$ states have been calculated[8,9,17-21]. In the paper[2], a more complete set of estimates on the profile indices of the AIS excited from these states is given. The profile indices of these AIS have not yet been explored experimentally; moreover, the available theoretical estimations are often in disagreement.

The major point of the theory of the excited He photoionization is to build and to test a relatively simple and quite reliable structure model of the excited He for its photoionization. This problem has been considered in our previous work[2]. We have built the structure model that allows one to describe the excited He photoionization with the same accuracy as complicated calculations carried out by different methods[8-14]. Note, the majority of the computations[8-12] exploited the structure models in continuum wave functions in which the open and closed channels* were simultaneously taken into account, and for the initial states the multiparametric variational[8,9,13] and other complicated functions[10-12] were used.

In the work[2], the continuum wave function has been chosen within Balashov's diagonalization method[20] and it was represented in the form of a superposition of the function for the direct phototransition and the L^2-function for the " closed resonance" channel. Under this choice of the continuum

*) Under the channel of the reaction or scattering we mean a set of quantum numbers of a subsystem. The channels would be distinct if the set of quantum numbers differ at least by one figure. The channel is assumed to be closed if the channel function decays at infinity in all radial variables. If the channel function is nonzero at least along one radial variable at infinity, then the channel is open. For example, in He at photon energy E_γ=24.6 eV the channel $1sEd$ ^1D is open whereas the $2s3d$ ^1D channel is closed. It would be open only at $E_\gamma \cong$ 60.05 eV.

function, in contrast with other methods[8-10], one is able to separate explicitly the contributions of the open and closed resonance channels in the characteristics of the photoprocess. It should be noted that the closed channel problem is well known[23] in nuclear physics. But as far as we know, the problem has not yet been considered in atomic physics.

In our work[2], the wave functions of the He excited states have been calculated by the many- configuration Hartree-Fock method[22] which allows a flexible variation of electron correlation types. Similar computations may be standardized in comparison with calculations using variational functions.

In the present paper, the appearance of a closed channel in the characteristics of the direct photoionization of the excited Helium is investigated. Moreover, we study the nature of forming the AIS with large q-indices in the excited He photoionization and the role of the closed channel in the radiation and dielectronic recombinations. The calculations have been performed using the above- mentioned structure model within the diagonalization method[20].

In the second part of the paper, the theoretical formalism is expounded. In the third and fourth subsections the computational procedure and results are considered; also the discussion is made.

2. THE THEORETICAL FORMALISM

a. Continuum wave function.

Let us represent the Helium continuum wave function under the n=2 threshold as a linear combination[20] of the function for direct phototransition and L^2-function for a branch photoprocess via the closed resonance channel(see appendix A.14):

$$\psi_E = a\Phi_o + \Sigma\, b_\mu\, \Phi_\mu , \qquad \Phi_o = \hat{A}[\varphi_o F_o^{(-)}]. \qquad (1)$$

Here the function $F_o^{(-)}(E)$ describes the photoelectron motion in the field of the ion $He^+(1s)$. The known functions Φ_μ represent the isolated autoionization levels (A.2-4) and are built to be orthogonal to the ground state wave function φ_0 of the $He^+(1s)$ ion(A.4). The configuration interaction coefficients $a(E)$ and $b_\mu(E)$ in (1) are described as (see (A.12) and (A.15)):

$$a(E) = 1 - \frac{E-E_\mu}{E-E_\mu - i/2\Gamma_\mu(E)} , \qquad (2)$$

$$b_\mu(E) = \frac{\langle \Phi_\mu | V_{12} | \Phi_o(E) \rangle}{E-E_\mu - i/2\Gamma_\mu(E)} . \qquad (3)$$

where

$$\Gamma_\mu(E) = 2\pi |\langle \Phi_o(E) | V_{12} | \phi_\mu \rangle|^2 \qquad (4)$$

is the probability for the electron to leave the channel μ via an interelectron Coulomb interaction V_{12} (see (A.8)). Using the function ψ_E in (1) one may write down the following expression for the phototransition amplitude:

$$T_{fi}(E) = \langle \psi^{(-)} | \hat{H}_\gamma | \Phi_i \rangle = \langle \Phi_o | \hat{H}_\gamma | \Phi_i \rangle \left\{ 1 + \sum_\mu \frac{q_\mu + i}{\varepsilon_\mu - i} \right\}, \qquad (5)$$

where

$$\varepsilon_\mu = 2 \frac{E - E_\mu}{\Gamma_\mu} . \qquad (6)$$

In (5) $\hat{H}_\gamma$ is the electron interaction operator with the photon. The profile parameter $q_\mu(E)$ in (5) will be given later (see (18)).

b. Formulae for the photoionization characteristics.

We will consider the photoionization of He excited state $|1sn_iS_iL_iM_i\rangle$ as a result of which the ion remains in its ground state φ_0, and the emitted electron moves away with the wave number $\mathbf{k}$. Here S_i, L_i, M_i are the spin and orbital also magnetic quantum numbers and n_i is the principal quantum number. Further, in the calculation we will neglect a spin-orbit interaction. It is suitable to use the LS representation in which the outgoing electron is described by the concrete angular momentum L, spin S and parity; so the continuum wave function in (1) can be written down in the following form:

$$\psi_E^{(-)}(\mathbf{k}, \mathbf{r}_1, \mathbf{r}_2) = \sum_{LM} Y^*_{LM}(\hat{k}) |EL:LSM\rangle \qquad (7)$$

where $Y^*_{LM}(\hat{k})$ is the spherical function of the ejected electron angle. The function $|EL:LSM\rangle$ in (7) is written as :

$$|1sEL:LSM\rangle = i^L e^{-i\delta_L} \left[\varphi_{1s}(\mathbf{r}_1) f_{EL}(\mathbf{r}_2) Y_{LM}(\hat{r}_2) + (-1)^s (1 \rightleftarrows 2) \right]. \qquad (8)$$

Here $f_{EL}(r)$ is the radial part of the function $F_o^{(-)}$. The scattering phase is described by the following formula:

$$\delta_L = \eta_L + \sigma_L, \eta_L = \arg(L+1-i/k), \qquad (9)$$

where the scattering phase δ_L is represented as

$$\delta_L = \eta_L + \sigma_L, \ \eta_L = \arg(L+1-i/k), \qquad (10)$$

and the supplementary phase σ_L is due to the deviations from the pure Coulomb field. We also use the notation $\Phi_\mu = |\mu LSM\rangle$.

In the case of the isolated resonance, using formula (5) and taking into account (7) one can write down the differential cross section as[24]

$$\frac{d\sigma}{d\Omega} = \frac{\sigma}{4\pi} \left[1 + \beta_2 P_2(\cos\theta) \right] \qquad (11)$$

where $P_2(\cos\theta)$ is the Legendre polynomial, θ is the angle of the outgoing photoelectron; β_2 is the angular anisotropy coefficient. The total cross section for the direct photoionization of the atom leaving the ion in its ground state (1s) is written down as

$$\sigma(E) = \sum_L \sigma_L . \qquad (12)$$

The partial cross section is defined by the following formula:

$$\sigma_L(E) = \sigma_L^{(0)}(E) + \sigma_L^{(0)}(E) \left[\frac{(q^i_{\mu L} + \varepsilon_\mu)^2}{1 + \varepsilon_\mu^2} - 1 \right]. \qquad (13)$$

The partial cross section for the direct phototransition into the open channel $\sigma_L^{(0)}$ is defined by the following formula:

$$\sigma_L^{(0)} = \frac{4\pi^2 \alpha \omega a_0^2}{3(2L_i+1)} |R_L|^2. \qquad (14)$$

Here α, ω и a_0 are the fine structure constant, photon frequency and the Bohr radius, respectively; R_L is the reduced matrix element

$$R_L = \langle 1sEL:LS \| \hat{D} \| n_i L_i \rangle, \qquad (15)$$

where

$$\hat{D} = \sum_k \mathbf{r}_k . \qquad (15a)$$

is the dipole transition operator. Let us introduce the quantity η

characterizing the ratio of the closed channel contribution to the partial cross section of the phototransition into the open channel

$$\eta(E) = \frac{\sigma_L}{\sigma_L^{(0)}(E)} \, 100\ \% \ , \tag{16}$$

where

$$\Delta\sigma_L = \sigma_L(E) - \sigma_L^{(o)} \ . \tag{17}$$

In formulae (13) the parameter $q_{\mu L}$ is determined as

$$q_{\mu L}(E) = \frac{\langle \mu SL \| \hat{D} \| 1sn\ L_i : L_i S_i \rangle}{\langle \mu LS | V_{12} | 1sESL:LS \rangle \langle 1sESL:LS \| \hat{D} \| 1sn_i L_i S:L_i S \rangle} \ . \tag{18}$$

Note that in the resonance approximation the parameters $\Gamma_\mu(E)$ and $q_{\mu L}(E)$ are determined at the AIS position $E=E_\mu$ and describe the width and the profile of the μ-th resonance curve, respectively.

When the initial state of the atom and incoming photon are unpolarized for the isolated closed channel, the coefficient of the angular anisotropy β_2 can be represented as[15,24]:

$$\beta_2 = \frac{A\varepsilon^2 + B\varepsilon + C}{X\varepsilon^2 + Y\varepsilon + z} \ , \tag{19}$$

where

$$A = f \sum_{LL'} S(LL'LL') R_L R_{L'} \cos(\delta_L - \delta_{L'}), \tag{20}$$

$$B = 2f \sum_L S(LL_\mu LL_\mu) R_L R_{L_\mu} \left[q_{L_\mu} (\cos(\delta_{L_\mu} - \delta_L) + \sin(\delta_{L_\mu} - \delta_L) \right], \tag{21}$$

$$C = A - 2f \sum_L S(LL_\mu LL_\mu) R_L R_{L_\mu} \left[\cos(\delta_{L_\mu} - \delta_L) - q_{L_\mu} \sin(\delta_{L_\mu} - \delta_L) \right] + (1+q_{L_\mu}^2) f R_{L_\mu}^2 S(L_\mu L_\mu L_\mu L_\mu), \tag{22}$$

$$X = \sum_L R_L^2 \ ; \quad Y = 2qR_{L_\mu}^2 \ ; \quad Z = X - R_{L_\mu}^2 (1 - q_{L_\mu}^2), \tag{23}$$

where

$$S(L'LLL') = \frac{1}{\sqrt{6}} (-1)^{L+L'} [LL'] \langle L0L'0|20 \rangle \times \begin{Bmatrix} 1 & L & L_i \\ L' & 1 & 2 \end{Bmatrix}, \tag{24}$$

$f = 3(-1)^{L_i}$, $\begin{Bmatrix} a, & b, & c \\ d, & e, & f \end{Bmatrix}$ is Wigner's 6j symbol.

The formula (19) shows that far from the closed channel ($\varepsilon \to \pm\infty$) where its influence is negligible the asymmetry coefficient β_2 tends to A/X.

In the case of several overlapping closed channels with angular momentum L_j ($j=1,\ldots,N$) the formula for the β_2 coefficient turns out into a more cumbersome one[15,24]. Below we shall write down it for a particular case of two closed (autoionization) ^1S and ^1D channels for the photoionization of the $He(2^1P)$ atom.

$$\beta_2(E) = -2 \frac{\sqrt{2}[(\varepsilon_o \varepsilon_2 + 1)\cos\Delta - (\varepsilon_2 - \varepsilon_o)\sin\Delta] C_{o2} R_o R_2 - D_{2o} R_2^2 / 2}{R_o^2 D_{o2} + R_2^2 D_{2o}} \ , \tag{25}$$

where

$\Delta = \delta_0 - \delta_2$, $C_{o2} = (q_o + \varepsilon_o)(q_2 + \varepsilon_2)$, $D_{ij} = (q_i + \varepsilon_i)^2 (\varepsilon_j^2 + 1)$, i and j = 0,2.

Further, in our investigations the cross section of dielectronic recombination, which is the inverse process with respect to the photoionization, will be used. The total dielectronic recombination cross section $\sigma^r(E)$ can be obtained from the photoionization cross section (12) and (13) by using the so-called "time inverse" theorem

$$\sigma^r(E) = q^2/k^2 \, \sigma(E) \ , \tag{26}$$

where q and r are the photon and electron momenta, respectively. It ought to be stressed that to calculate the β_2 coefficient for the secondary photon in the dielectronic recombination $He^+(1s) + e \to He^{**}(2p^2\ ^1D) \Rightarrow \gamma_1 + (He(2^1P) \Rightarrow He(2^1S) + \gamma_2)$ the formulae have been used from our work[15].

III. THE COMPUTATIONAL MODEL

Let us introduce the abbreviation F|I for the structure model which is the combination of the wave functions of atomic initial I and final F states.

The wave functions of the He discrete excited states have been computed by using the many- configuration Hartree-Fock method[21]. Denote these functions as MCHF. In the MCHF, the interaction of the following configurations is taken into account:

$$\begin{array}{lll} 1s2s,\ 1s^2,\ 2s^2,\ 2p^2 - & \text{for } 2^1S \text{ term}, & \\ 1s2s,\ 2s3s,\ 2p3p,\ 3d4d & \text{for } 2^3S \text{ term}, & (27) \\ 1s2p,\ 2s2p,\ 2s3p,\ 2p3s,\ 2p3d & \text{for } 2^1P \text{ and } 2^3P \text{ terms}. & \end{array}$$

In the continuum wave function (1), the function Φ_0 for the direct phototransition is denoted by PS and the function of the final state is also called PS for brevity. Thus, our calculations have been performed in the structure model PS|MCHF. The wave function for the direct phototransition $f_{EL}(r)$ in (7,8) was taken to be the solution of the radial Schrödinger equation in the following central parametric potential[14]

$$V(\alpha,r) = -\frac{1}{r}\left[e^{-\alpha_1 r} + \alpha_2 r e^{-\alpha_3 r} + 1\right]. \qquad (28)$$

In (28), in the case of a singlet state the parameters $\alpha_1,\alpha_2,\alpha_3$ take the values 8.90663, 16.38067 and 9.82222, and the values 33.46494, 7.91893 and 3.27399 for the triplet state, respectively. This function satisfies the following asymptotic and normalization conditions :

$$f_{EL}(r) \sim \sqrt{\frac{2}{\pi k}}\,\frac{1}{r}\,\mathrm{Sin}\left(kr - \frac{L\pi}{2} - \frac{1}{k}\ln(2kr_1) + \delta_L\right),\ r \to \infty\ , \qquad (29)$$

and

$$\langle f_{EL}|f_{E'L'}\rangle = \delta(E-E')\delta_{LL'}\,. \qquad (29a)$$

Our estimations and analysis[2] show that the latter function (PS) and the solution of the Schrödinger equation in the potential with allowance for the exchange term (Hartree-Fock potential) in the combination with the MCHF lead to very close results in a large enough energy interval. On the other hand, the function PS is very simple, and moreover, as the calculations[14] and our test show, it appears quite reliable in describing different photoprocesses.

The term $|\mu LSM\rangle$ of the final state wave function has been computed[2] by the diagonalization of the atomic Hamiltonian in the closed channel subspace using the Coulomb basis function with the charge Z=2. For the $^{1,3}S$ states in the continuum there have been mixed configurations 2sns,2pnp,3sns,3pnp,3dnd and 2snp,2pns,2pnd for the $^{1,3}P$ states as well as 2pnp,2snd,2pnf configurations for the $^{1,3}D$ states, respectively ($n \leq 5$). In the matrix diagonalzation, the convergence was checked by enlarging the basis dimension up to 20, and our data, obtained with the Coulomb function in the continuum (in place of the PS), have

reproduced the estimates on the profile index-q and width[20,21] up to three significant figures.

We introduce also abbreviations for the structure models in the calculations of other authors. The Hylleraas-type variational function containing 56 parameters, is denoted by 56H, and the frozen core Hartree-Fock function[8,13] and the function obtained by the close coupling method[8,9] are denoted by FCHF and CC, respectively.

IV. THE RESULTS AND DISCUSSIONS

Our calculations show[2] that in the photoelectron energy range E<0.5 a.u. the closed channel contributions in the characteristics of the excited He photoionization are negligible. But at energies E>0.5 a.u. the square of the absolute value of the coefficient $b_\mu(E)$ in (1) characterizing the probability to find the electron in the closed channel μ appears to be noticeable (Fig.1).

The appearance of the closed channel in the direct photoprocess with the excited He is illustrated in Figs.2-6 and Tabls.1-3. Figure 2 depicts the cross sections which we have evaluated allowing for only the open channel for the photoionization $He(2^{1,3}S)$ and $He(2^{1,3}P)$ atoms. The cross sections obtained in different quite reliable calculations[2,8-12], in which both the open and closed channels have been taken into account except the works[13,14], are represented in Fig.3. It is seen that at E>0.5 a.u. with increasing electron energy the cross section of the direct phototransition decreases (Figs.2 and 3) and a particular quick falling down appears in the case of the $He(2^1P)+\gamma = He^+(1s)+e(Ed)$ process (Figs.2 and 3b). At the same time, in the direct photoionization cross section the contribution of the phototransition via the closed channel (formula (16)) turned out to be noticeable and its amount grows with increased energy (Figs.3b,c and Tabl.1).

The competition and interference of the amplitudes of these two phototransition branches are due to the peculiarities in the energy dependence of different characteristics of the photoprocess (Figs.3,4 and Tabls.1,2). In the considered energy range, the influence of the closed channel is noticeable

Tabl.1. The contributions of the first ^1D and ^1S closed channels to the partial cross section of the $He(2^1P)$ atom photoionization. In the tabl. a^{-b} means $a\times10^{-b}$

		^1D				^1S		
E au	Γ(E) eV	σ_0 Mb	Δσ Mb	η(%)	Γ(E) eV	σ_0 Mb	Δσ Mb	η(%)
.5	.15	3.7^{-2}	-8.1^{-3}	21.9	.23	2.8^{-2}	2.6^{-3}	9.3
.6	.14	2.0^{-2}	-6.8^{-3}	34.0	.22	2.0^{-2}	2.7^{-3}	13.4
.7	.13	1.1^{-2}	-5.8^{-3}	51.3	.21	1.5^{-2}	3.0^{-3}	19.4
.8	.12	6.8^{-3}	-4.9^{-3}	72.8	.20	1.2^{-2}	3.5^{-3}	28.4
.9	.11	4.3^{-3}	-4.0^{-3}	93.8	.19	9.9^{-3}	4.3^{-3}	43.4
1.0	.10	2.8^{-3}	-2.6^{-3}	91.2	.19	8.2^{-3}	6.2^{-3}	75.6
1.1	.09	1.8^{-3}	1.4^{-3}	80.2				

Tabl.2. The contributions of the second ^1D and ^1S closed channels to the partial cross section of the $He(2^1P)$ atom photoionization. In the tabl. a^{-b} means $a\times10^{-b}$

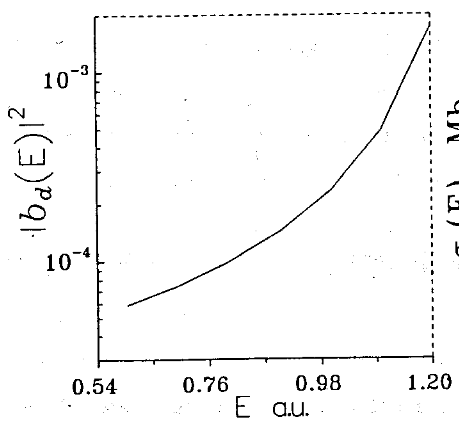
		^1D				^1S		
E au	Γ(E) eV	σ_0 Mb	Δσ Mb	η(%)	Γ(E) eV	σ_0 Mb	Δσ Mb	η(%)
.5	.032	3.7^{-2}	2.6^{-4}	0.7	.013	2.8^{-2}	7.6^{-4}	2.7
.6	.031	2.0^{-2}	2.2^{-4}	1.1	.012	2.0^{-2}	7.2^{-4}	3.6
.7	.029	1.1^{-2}	1.9^{-4}	1.7	.010	1.5^{-2}	7.1^{-4}	4.7
.8	.027	6.8^{-3}	1.8^{-4}	2.6	8.8^{-3}	1.2^{-2}	7.3^{-4}	6.1
.9	.026	4.3^{-3}	1.7^{-4}	4.0	7.7^{-3}	9.9^{-3}	8.0^{-4}	8.1
1.0	.024	2.8^{-3}	1.8^{-4}	6.3	6.8^{-3}	8.2^{-3}	9.1^{-4}	11.1
1.1	.023	1.8^{-3}	1.8^{-4}	10.2				

Tabl.3. The contributions of the closed channel to the total cross section of the recombination $He^+(1s)+e \Rightarrow He(2^1P) + \gamma_1$

E au	$\sigma^r\times10^{-5}$ Mb	Δσ Mb	η(%)
.4	0.20	-0.007	6.1
.5	0.12	-0.005	7.8
.6	0.08	-0.004	10.0
.7	0.06	-0.003	11.0
.8	0.05	-0.001	5.2
.9	0.04	0.0003	2.1
1.0	0.05	0.004	32.7
1.1	0.08	0013	154.0

in all cases except for the photoprocess $He(2^3P)+\gamma \Rightarrow He^+(1s)+e$ (Fig.3). We see that most strongly this effect manifests itself in the process $He(2^1P)+\gamma = He^+(1s)+e$ (Fig.3c). Tabls. 1 and 2 demonstrate the partial cross section contribution of the photoionization from the 2^1P state for the S and D waves which is due to the influence of the closed channel (Δσ, formula (17)) and its amount η in per cent with respect to the cross section of the direct phototransition into the open channel at different photoelectron energies. The quantity η at energy E=1 a.u. (at the distances 6.1 and 8.24 eV from the first ^1S и ^1D resonance positions) amounts to 75.6 % for the ^1S wave and 91.2 % for the ^1D wave (Tabl.1).

Fig.1. Probability for the electron (d-wave) to be in the closed channel $|b_d(E)|^2$ as a function of the photoelectron energy



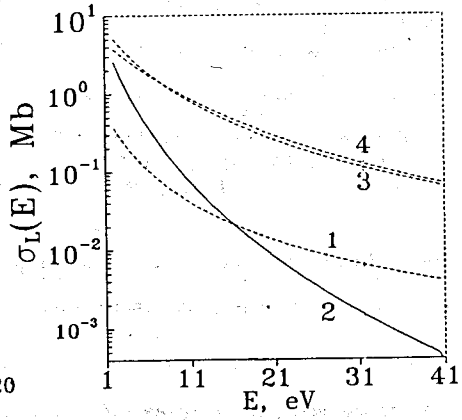


Fig.2. Energy dependence of the partial cross sections $\sigma_L(E)$. Figures 1 ,2, 3 and 4 correspond to $He(2^1P) + \gamma \Rightarrow He^+(1s) + e(Es)$, $He(2^1P) + \gamma \Rightarrow He^+(1s) + e(Ed)$ and $He(2^1S) + \gamma \Rightarrow He^+(1s) + e(Ep)$ $He(2^3S) + \gamma \Rightarrow He^+(1s) + e(Ep)$ processes, respectively

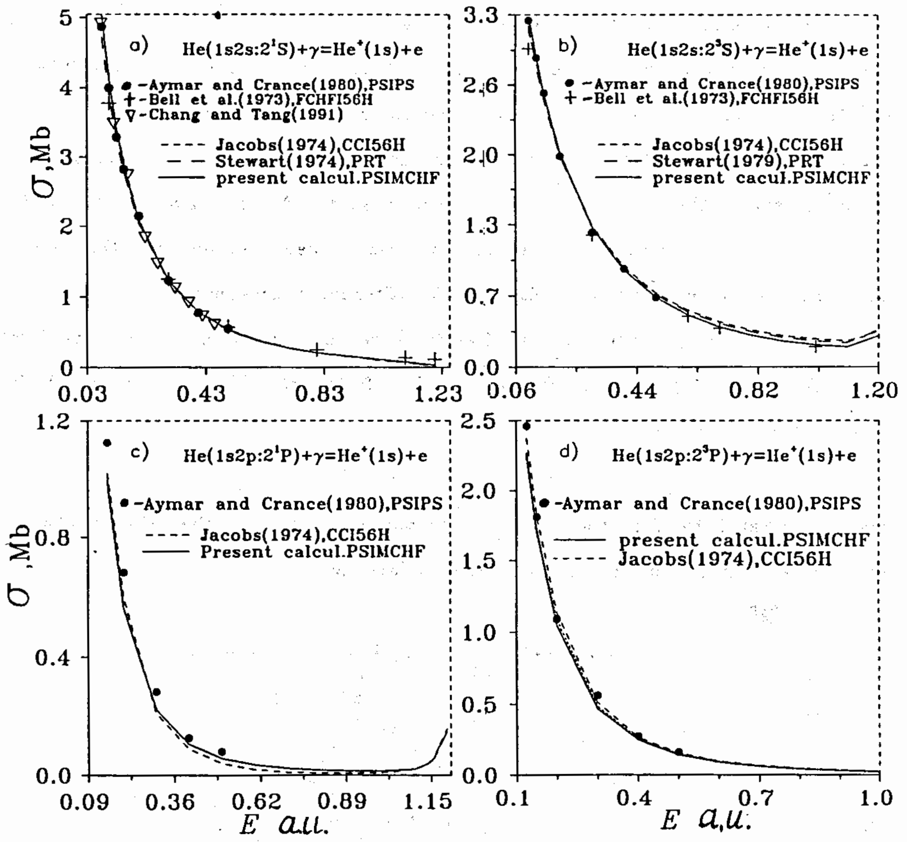


Fig.3. Total cross sections of the $He(2^{1,3}S)$ and $He(2^{1,3}P)$ atom photoionization as a function of the photoelectron energy

As we see, at energies 0.5<E<1 a.u. for the d wave the difference $\Delta\sigma$ has negative but at 1.1 a.u. positive signs whereas for the S wave the difference $\Delta\sigma$ is positive (Tabl.1). So the interference of the terms of the transition amplitudes to the open and via the closed channels may lead to the difference $\Delta\sigma$ of the distinct signs depending on the transition nature (Tabl.1).

For the same partial phototransition there strongly manifests itself the closed channel, corresponding to the level, for which the quantity $\Gamma_\mu(E)$ has

relatively large values. When Γ_μ is small, the effect turns out to be weaker. This is well seen from the contributions of the first (Tabl.1) and second (Tabl.2) ^1D and ^1S closed channels in the energy dependence of the quantities $\Delta\sigma$ and Γ_μ for the ionization of the $He(2^1P)$ atom. The physical meaning of this phenomenon is probably that the greater the quantity Γ_μ the more intensive is entering of an electron into the closed channel and also its leaving off the open channel through the interelectron correlation.

In the energy dependence of dimensionless quantities, such as the coefficient of the photoelectron angular anisotropy β_2 ((19), further denote it as β_e), the closed channel manifests itself much stronger than in the cross section of the photoionization. Our calculations show that in the case of ionization from the 2^1P state at energy 0.9 a.u., the closed channel contribution to the β_e coefficient amounts to 131.7% and in the total cross section it is equal to 2.1%. Figure 4 shows the energy dependence of the coefficient β_e for photoionization of the $He(2^1P)$ atom in comparison with the estimates[9] obtained in the close coupling method in combination with the 56 parametric variational function (the CC|56H model, curve 4). In the case of ionization of the $He(2^1P)$ atom, we see that in the far enough region from the resonance position ($E<E_\mu$) the behaviours of the β_e coefficient evaluated with allowing for the closed channel (curve 2) and without it (dashed line 3) differ significantly from each other. This strong difference in the behaviour as a rule is essentially due to changing of the d wave branch (Tabl.1).

The closed channel also appears in the characteristics of the photorecombination which is the inverse process of the photoionization at energies below the resonance region. In table 3, the dependence of the closed channel contribution to the photorecombination cross section upon the electron energy is given. The effect is stronger in the angular anisotropy coefficient[15] β_γ (we use β_γ in place of β_2) of the secondary photon γ_2 in the photorecombination process: $He^+(1s)+ e \rightarrow \gamma_1 +$ ($He(2^1P) \Rightarrow He(2^1S) + \gamma_2$) (Fig.5).

Fig.4. Energy dependence of the angular anisotropy coefficient of the photoelectron $\beta_e(E)$ in the $He(2^{1,3}P)+\gamma \Rightarrow He^+(1s)+e$ process

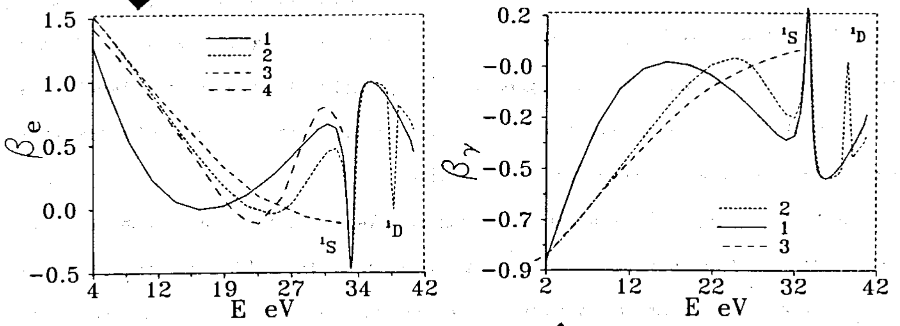


Fig.5. Energy dependence of the angular anisotropy coefficient of the secondary photons $\beta_\gamma(E)$ from the $He(2^1P)$ atom following the recombination $(e + He^+)$

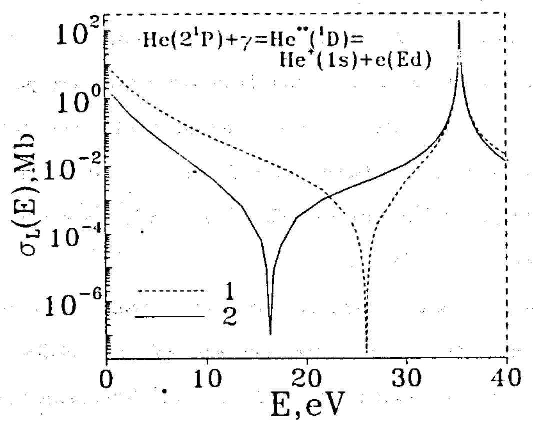
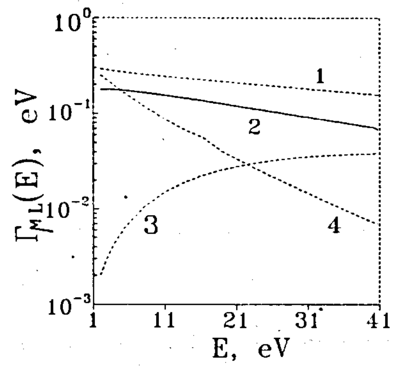


Fig.6. Cross section of $He(2^1P) + \gamma \Rightarrow He^{**}(^1D) \Rightarrow He^+(1s) + e(d)$ process as a function of the emitted electron energy E. 2 is the estimates obtained in the resonance approximation. 1 is the calculation allowing for the closed channel

Fig.7. Energy dependence of the quantity $\Gamma_{\mu L}(E_b)$; figures 1 ,2, 3 and 4 correspond to the same processes as in Fig.2



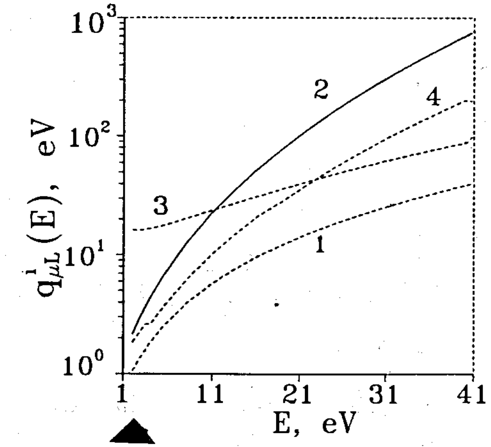


Fig.8. Energy dependence of the quantity $q^i_{\mu L}(E_b)$. Figures 1, 2, 3 and 4 correspond to the same processes as in fig.2. The curves 1 and 3 correspond to the values $-q^i_{\mu L}(E_b)$

In the nonresonant ($E<E_\mu$) region, the curve β_γ obtained by allowing for the closed channel (Fig.4, dashed line 2) noticeably differs from the curve calculated without taking it into account (Fig.4, dashed line 3).

Now we proceed to consider the features of the resonance structure formed under the above-mentioned physical conditions for the photoprocesses. The profile behaviour of the AIS formed in the photoprocesses with the excited He is shown in Figs.3,4 and 6. For the photoprocess, whose direct transition cross section decreases very quickly with energy (Fig.2, line 2), the resonant branch turns out to be dominant over the direct photoionization. For a rather small width Γ_μ these photoprocesses lead to the forming of the resonance structure with a large value of the profile index[2] (fig.8, line 2, formula 18). We see that this pattern is clearly seen from the first ^1D AIS excited from the Helium 2^1P state (Fig.9).

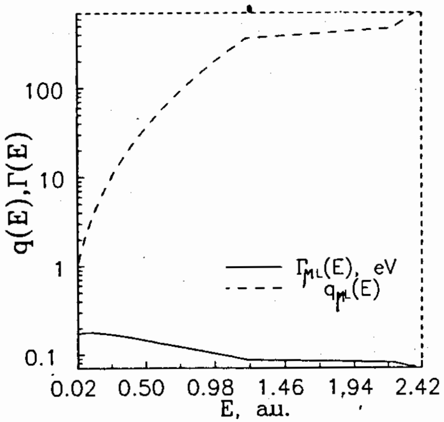


Fig.9. Energy dependence of the quantities $q^{i}_{\mu L}(E_b)$ and $\Gamma_{\mu L}(E_b)$ for the $He(2^1P)$ + $\gamma \Rightarrow He^{**}(^1D) \Rightarrow He^{+}(1s) + e(Ed)$ process

An important feature of the photoprocess with the excited He, as our results show, is that the profile curves of the characteristics of the processes depend not only on the quantities Γ_{μ} and q_{μ}, but on the q-index sign too: for the positive q the resonance is displaced far beyond its own width (^1D AIS, Figs.4,5,6) to the left and for q<0 some shift occurs to the right. Fig.6 shows the cross section of photoionization from He 2^1P state calculated in the resonance approximation (q_{μ} and Γ_{μ} are constants, solid line) and with allowance for closed channels ($q_{\mu}(E)$ and $\Gamma_{\mu}(E)$ are functions of E, dashed line). The cross section of the phototransition exciting the ^1D AIS in the resonance approximation at the distance ≅19 eV from its position E_{μ} has the "zero" minimum, whereas the calculations including the closed channel reach their local minimum at the distance ≅ 9.3 eV. Similar pictures are also observed in the energy dependence of the angular anisotropy coefficients of the photoelectron β_e and the secondary photon β_{γ} in dielectronic recombination (Figs.4 and 5). It should be noted that in the case of the resonance approximation, the peak corresponding to the ^1D AIS disappears washing off to the right far enough beyond the resonance range (Figs.4 and 5, solid lines). At the same time, in the calculations allowing for the closed channel the peaks of the ^1D resonance in

the coefficients β_e and β_{γ} appear at their own positions (Figs.4 and 5, dashed lines). Thus, the results of our investigations (Figs. 2-9 and Tabl.1-3) on the whole demonstrate the fact that at the photoelectron energies E>0,5 a.u., where the cross section of the direct phototransition is substantially small, the closed channel contribution to the characteristics of the photoprocess with the $He(2^1P)$ atom becomes noticeable.

In similar physical conditions, the interference and competition of these branches define the peculiarities in the energy dependence of characteristics of the photoprocess, especially of the dimensionless quantities such as the coefficients β_e and β_{γ} (Figs.4 , 5 and 6) and lead to the formation of the AIS with a large, in absolute value, profile index q (Figs.8 and 9).

Our investigations, we think, clear up the physical nature of the known problems such as a resonance form in the d-wave and phenomenon of the shift and broadening of the ^1D AIS[15,16] in the photoprocess with excited He (Figs.4 and 5) and other heavier atoms[16] arising in their description in the resonance approximation. In this regard, it seems to us that in the case of the $(2p^2)^1D$ AIS the automatical continuation of the resonance approximation into the energy range at distances (below) from the resonance position E_{μ}, exceeding hundred times its own width ($E_{\mu}-E \gg \Gamma(E_{\mu})$), contradicts the energy conservation law because in this situation the ^1D resonance is deeply located in the closed channel. Moreover, at these energies the closed channel naturally manifests itself as a virtually excited "resonance" in the open channel region (Fig.9) which leads to the peculiarities in the characteristics of the photoprocess with the $He(2^1P)$ atom.

We think that observing of the fluorescence of the secondary emission following the photo-and dielectronic recombination has some priority in the sense of being experimentally realized as compared to the direct measuring of the excited He photoionization characteristics.

A task of prime importance in our opinion is the experimental study of the closed channel appearance and peculiarities of the resonance structure formation in photoprocesses with the excited He by measuring the energy dependence of the angular anisotropy coefficients for the secondary photons γ_2 in the process $He^+(1s) + e \rightarrow He^{**}(2p^2\ {}^1D) \Rightarrow \gamma_1 + (He(2^1P) \Rightarrow He(2^1S) + \gamma_2)$ at energies E> 0,5 a.u. including the resonance region.

V. CONCLUSION

In this work, the closed channel appearance and the peculiarities of the AIR structure formation in the photoprocesses with the excited He are investigated in a wide range of the spectrum. The atomic continuum structure has been described by the function which is the superposition of the Schrödinger equation with the effective central potential[14] for the direct phototransition and of the L^2-function for the closed channel (and resonance branch) in the diagonalization approximation[20]. The initial state wave functions have been calculated using the many-configuration Hartree-Fock method. Such an approach to the problem allows one to separate explicitly the contributions of the closed and open channels to the characteristics of the photoprocess.

Our investigations show that in the energy range E>0,5 a.u.where the cross sections of the direct photoprocess from the He excited states are substantially small (Figs.2 and 3), the closed channels noticeably manifest themselves (Figs.3-5, Tabls.1-3). At the energy E=1 a.u., the contributions via the closed channels to the cross section of the photoionization from the He 2^1P state at the distance 6.1 and 8.2 eV from the positions of the first ^1S and ^1D resonance levels amount to 75,6 and 91,2% with respect to the corresponding partial cross sections without the closed channels taken into account.

It is found that the contribution of the closed channel in the ionization cross section strongly depends upon the value of the probability of the electron transition ($\Gamma_\mu(E)$) from the closed channel to the open channel via the electron correlation (Tabls.1,2). The larger this probability $\Gamma_\mu(E)$, the stronger the contribution of the closed channel to the photoionization cross section. In the energy range $E \sim E_\mu$, the smallness of direct phototransition cross section serves as one of the main reasons which lead to forming of the AIS with a large, in absolute value, profile index q (Figs.2 and 8).

The competition and interference of the direct phototransition amplitudes into the open and through the closed channels determine the substantial peculiarities in the energy dependence of the dimensionless characteristics such as angular anisotropy coefficients of the photoelectron β_e and the secondary photon in the photo- and dielectronic recombination β_γ (Figs.4 and 5). In similar physical conditions there occurs a remarkable shift and broadening of the ^1D AIS profile in the photoprocess characteristics (Figs.4, 5 and 6).

We think that modern experimental equipment used to investigate the recombination characteristics is able to reveal the closed channel appearance and peculiarities of the ^1D AIR profile by measuring the angular anisotropy coefficient of the secondary photon in the photo- and dielectronic recombination $He^+(1s) + e \Rightarrow He^{**}({}^1D) \Rightarrow \gamma_1 + (He(2^1P) \Rightarrow He(1^1S) + \gamma_2)$ in a wide spectrum range. The peculiarities of the closed channel appearance and the AIR structure formation in the photoprocesses with the excited He may play an important role in heavier atoms. Thus, clarification of these problems may be of major significance for atomic physics.

We would like to thank Professor V.V.Balashov from the Institute of Nuclear Physics, Moscow State University for his continuous interest and support and useful discussions.

Appendix *A*

Following Balashov et al.[20] we shall represent the He continuum wave function under n=2 threshold as

$$\psi_E(\mathbf{r},\mathbf{r}') = \hat{A}[\varphi_o(\mathbf{r})X_o(E,\mathbf{r}')] + \sum_\mu b_\mu \Phi_\mu . \qquad (A.1)$$

Here, the function $X_o(E,r')$ describes electron motion in the $He^+(1S)$ ion field. Known functions Φ_μ are obtained by the unitary transformation diagonalizing the He hamiltonian in the subspace of closed channels which are constituted by the states of the two- electron excitation[20] :

$$\Phi_\mu = \hat{A} \sum_{n,m} c_\mu(n,m)\varphi_n(r)\varphi_m(r'), \qquad (A.2)$$

and satisfy the property:

$$\langle\Phi_\mu|\hat{H}|\Phi_{\mu'}\rangle = E_\mu \delta_{\mu\mu'} \qquad (A.3)$$

where $\hat{H}$ is He hamiltonian, $\varphi_n(r)$ is the $He^+(1S)$ ion wave function; $\hat{A}$ is the operator of antisymmetrization. It is obvious that the functions Φ_μ in (A.1) satisfy the following condition

$$\langle\Phi_\mu| \varphi_0\rangle = 0. \qquad (A.4)$$

To find the function ψ_E in (A.1) it is needed to calculate the function $X_o(E,r')$ and coefficients b_μ satisfying the equations:

$$b_\mu(E-E_\mu)=\langle\Phi_\mu|V|\hat{A}[\varphi_o X_o(E)]\rangle, \qquad (A.5)$$

$$(\hat{H}_o-E)X_o(E) = -\sqrt{2}\sum_\mu b_\mu\langle\varphi_o|V|\Phi_\mu\rangle. \qquad (A.6)$$

Here, the hamiltonian $\hat{H}_o$ for the ejected electron is written as

$$\hat{H}_o X(E,r')=(-\tfrac{1}{2}\Delta_{r'} + \langle\varphi_o|V|\varphi_o\rangle)X_o(E,r')+\varphi_o(r')\langle\varphi_o|V|X_o\rangle, \qquad (A.7)$$

where $\qquad V = 1/|r - r'|$. (A.8)

Using the Green function one may represent the solution of the inhomogeneous equation (A.6) in the following form:

$$X_o = F_o^{(-)} + \sum_\mu b_\mu \frac{1}{E^{(-)} - \hat{H}_o}\langle\varphi_0|V|\Phi_\mu\rangle. \qquad (A.9)$$

Here $F_o^{(-)}$ is the solution of the equation $(\hat{H}_o - E)X_o=0$ satisfying the incoming boundary conditions in the asymptotic region. Substituting (A.9) into (A.5) and using the following identities

$$\frac{1}{E^{(-)} - \hat{H}_o} = \frac{P}{E^{(-)} - \hat{H}_o} - i\pi\delta(E - \hat{H}_0), \qquad (A.10)$$

$$\delta(E - \hat{H}_0) = |F_o^{(-)}\rangle\langle F_o^{(-)}|, \qquad (A.11)$$

we may get a system of algebraical equations for b_μ. In this system, ignoring the indirect coupling between the μ and μ' closed channels through the direct phototransition [20], one may get separate equations which can result in the following expression for b_μ

$$b_\mu(E-E_\mu) = \frac{\langle\Phi_\mu|V|\Phi_o\rangle}{E - E_\mu + \frac{i}{2}\Gamma_\mu} ; \qquad (A.12)$$

where $\qquad \Gamma_\mu(E) = 2\pi|\langle\Phi_o|V|\Phi_\mu\rangle|^2 \qquad$ (A.13)

is the probability for the electron to leave the channel μ via an electrostatic interaction V. Note that to obtain (A.11) we ignore the contribution of the first term in (A.10) for the principal value integral. By introducing (9) into (1) and taking into account the relations (10,11) and (12) the continuum wave function of the helium can be written as

$$\psi_E = a\Phi_o + \Sigma\, b_\mu \Phi_\mu , \qquad \Phi_o=\hat{A}[\varphi_o F_o^{(-)}], \qquad (A.14)$$

where

$$a(E) = 1 - \frac{i}{2}\sum_\mu \frac{\Gamma_\mu}{E-E_\mu-i/2\Gamma_\mu} . \qquad (A.15)$$

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