THE EXCITED HELIUM PHOTOIONIZATION

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Abstract

The photoionization characteristic behaviour of the excited He atom has been studied by using the parametrical approach, and the physical nature of the processes is cleared up. It is shown that in the excited He photoionization, the profiles of the resonance structures appear far enough from the positions of autoionization states at energies comparable hundred times of their natural widths. The mentioned peculiarities in the recombination of the He^+ ion into excited states have been observed too.

It is also shown that such "extended" resonance structures are well described by "width" and "profile" functions of the energy. The competition and interference of phototransitions to open and closed (autoionization resonance) channels are found to be due to the broadening and shift in the resonance structure profile formed in the photoprocesses with the excited He.

The ways to reveal experimentally the influence of closed channels in the resonance structure forming the photoprocesses with excited He atoms are discussed.

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I. INTRODUCTION

At present, significant progress [1, 2] has been achieved in investigating excited atom photoionization , in particular, Helium. This is due to the use [2, 3, 4] of laser and synchrotron light 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].

Substantially distinct features of the excited He photoionization [7]-[12] as compared to the ground-state photoionization have been pointed out. At the same time, a demand is growing for photoionization data of the excited He for fundamental and different applied investigations. So it is believed that modern facilities come closely to carring out experiments on photoionization of an excited helium atom. In this respect, theoretical description of the excited He photoionization problem is also needed to be developed.

At present, in rather accurate calculations [8, 9, 10, 12], a wide minimum in the cross section of the excited He photoionization has been revealed in the range of the photoelectron spectra $E\rangle$ 0.5 a. u. Excitation of autoionization resonances (AIR) with a large profile index-q [8, 9], [12]-[15] in the excited He photoionization was noted as well.

The "broadening" and "shift" phenomena in profiles of dimensionless characteristics of the autoionization state (AIS), such as the angular anisotropy coefficients of the photoelectron in the excited He photoionization [9] and the secondary photon [15] in the dielectronic recombination: $He^+ + e \rightarrow He^{**}(^1D) \rightarrow \gamma_1 + [He(2^1P) \rightarrow He(1^1S) + \gamma_2]$ have also been reported. The latter phenomena have been observed [16, 17] in the photoionization processes of the heavier excited atoms too. The attempt was undertaken [17]

to describe the "broadening" and "shift" of the resonance profiles by introducing an effective width and shift. Note that the peculiarities mentioned above manifest themselves most strongly in the d-wave (also ^1D AIR) branch of photoprocesses with the He(2^1P) atom.

In the present paper, the characteristics of photoionization of the excited He atom are calculated. The recombination cross section and energy dependence of the angular distributions of secondary photons in the electron - ion recombination are evaluated as well. We demonstrate the role of the closed channel in forming a long "extended" profile of the resonance structure and clear up the physical nature of these processes.

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.

II. THE THEORETICAL FORMALISM

We will consider the photoionization from the He excited state $\mid 1sn_il_iS_iL_i >$ as a result of which the ion remains in its ground state 1s and the emitted electron moves away with the orbital quantum number l. Here $S_i and L_i$ are the spin and orbital quantum numbers of the excited state and n_i, l_i are the principal and orbital quantum numbers. 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;

In accordance with the diagonalization method [18, 19], the continuum wave function of the atom can be represented as a superposition of the wave functions $|1sEl{:}LS\rangle$, μ_L for open and closed channels, respectively. Here $|\mu_L LS\rangle$ is the wave function of the μ_L -th isolated autoionization state [18, 20].

The function $|1sEl:LS>$ can be written as .

$$|1sEl:LS>=i^l e^{-i\delta_l}\varphi_{1s}(r_1)f_{El}(r_2)Y_{lm}(\hat{r}_2)+(-1)^S(1\rightleftharpoons 2) \qquad (1)$$

Here $f_{El}(r)$ is the radial wave function, and S is the spin. The scattering phase is described by the following formula:

$$\delta_l=\eta_l+\sigma_l, \qquad \eta_l=\arg(L+1-i/k) \qquad (2)$$

The supplementary phase σ_l is due to the deviations from the pure Coulomb field; $\varphi_{1s}(r_1)$ is the ion ground state wave function.

The total cross section for the photoionization of the atom from the initial state "i" with allowance for the influence of the first AIS of the angular momentun L can be written as

$$\sigma^i(E)=\sum_L \sigma^i_{\mu_L L}(E) \qquad (3)$$

The partial cross section $\sigma^i_{\mu_L L}(E)$ allowing for the first isolated μ_L resonance is determined by the following formula:

$$\sigma^i_{\mu_L L}(E)=\sigma^{i,(o)}_L(E)+\sigma^{i,(o)}_L\frac{[q^i_{\mu_L L}(E)+\epsilon_{\mu_L}(E)]^2}{1+\epsilon^2_{\mu_L}(E)} \qquad (4)$$

The partial cross section for the direct phototransition to the open channel $\sigma^{i,(o)}_L(E)$ is defined by the following formula :

$$\sigma_L^{i,(o)}(E) = \frac{4\pi^2\alpha a_o^2}{3(2L_i+1)} \mid R_L^i(E) \mid^2 \qquad (5)$$

Here α, ω I a_0 are the fine structure constant, photon frequency and the Bohr radius, respectively; $R_L^i(E)$ is the reduced matrix element

$$R_L^i(E) = < 1sEL : LS||\hat{D}||1sn_il_i : L_iS_i > \qquad (6)$$

where

$$\hat{D} = \sum_{k=1}^{2} r_k \qquad (7)$$

is the dipole transition operator.

$$\epsilon_{\mu_L} = 2(E - E_{\mu_L})/\Gamma_{\mu_L L}(E) \qquad (8)$$

$$\Gamma_{\mu_L L}(E) = 2\pi \mid < 1sEl : LS \mid V_{12} \mid \mu_L LS > \mid^2 \qquad (9)$$

In formula (4) the function $q_{\mu_L L}^i(E)$ is determined as

$$q_{\mu_L L}^i(E) = \frac{< \mu_L LS||\hat{D}||1sn_il_i : L_iS_i >}{< \mu_L LS \mid V_{12} \mid 1sEl : LS >< 1sEl : L||\hat{D}||1sn_il_i : L_iS_i >} \qquad (10)$$

Note that in the resonance approximation [18, 20] widely used for describing the photoionization from the atom ground state, the functions $\Gamma_{\mu_L}(E)$ and $q_{\mu_L L}(E)$ in (4) and (8) are constants determined at the AIS position $E = E_{\mu_L}$ and describe the width and the profile index of the μ_L-th resonance curve, respectively.

In the case of the isolated resonance one can write down the differential cross section as [21]

$$\frac{d\sigma}{d\Omega} = \frac{\sigma^i}{4\pi}[1 + \beta_2 P_2(\cos\theta)]$$

where $P_2(\cos\theta)$ is the Legendre polynomial, θ is the angle of the outgoing photoele

β_2 is the angular anisotropy coefficient.

Further, the cross section of dielectronic recombination will be used in our inves

tions . The total recombination cross section $\sigma^r(E)$ into the He excited state "i" ca

written in the following form [22]:

$$\sigma^r(E) = k_\gamma^2/k_e^2\sigma^i(E) \qquad (1$$

where k_γ and k_e are the photon and electron momenta, respectively, and the cross secti

$\sigma^i(E)$ is defined by formula (3). To calculate the β_γ coefficient for the secondary phot

in the recombination $He^+(1s) + e \to He^{**}((2p^2)^1D) \to \gamma_1 + (He(2^1P) \to He(1^1S) + \gamma$

, the formulae from our work [15] have been used.

Let us introduce the quantity characterizing the ratio of the closed channel contrib

tion to the partial cross section of photoionization into the open channel

$$\eta(E) = \frac{\Delta\sigma_L^i(E)}{\sigma_L^{i,(a)}(E)}100\%$$

where

$$\Delta\sigma_L^i(E) = \sigma_L^i(E) - \sigma_L^{i,(a)}(E)$$

III. THE COMPUTATIONAL MODEL

Let us introduce the abbreviation $F \mid I$ for the structure model which is the combin

tion 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
any- configuration Hartree-Fock method [23]. Denote these functions by MCHF. In the
CHF, the interaction of the following configurations is taken into account:

$$1s2s, 1s^2, 2s^2, 2p^2 \quad for \quad 2^1S \quad term$$

$$1s2s, 2s3s, 2p3p, 3d4d \quad for \quad 2^3S \quad term$$

$$1s2p, 2s2p, 2s3p, 2p3s, 2p3d \quad for \quad 2^1P \, and \, 2^3P \quad terms. \qquad (15)$$

the continuum wave function the function $| 1sEl : LS >$ for the direct phototransition
denoted by PS and the function of the final state is also called PS for brevity. Thus, our
culations have been performed in the structure model PS |MCHF. The wave function
the direct phototransition $f_{El}(r)$ in (1) was taken to be the solution of the radial
rödinger equation in the following central parametric potential[24]

$$V(\alpha, r) = -\frac{1}{r}\{e^{-\alpha_1 r} + \alpha_2 r e^{-\alpha_3 r} + 1\} \qquad (16)$$

16), for the singlet state the parameters α_1, α_2,α_3 take the values 8.90663, 16.38067
9.82222, and the values 33.46494, 7.91893 I 3.27399 for the triplet state, respectively.
s function satisfies the following asymptotic and normalization conditions :

$$f_{EL}(r) = \sqrt{\frac{2}{\pi k}}\frac{1}{r}\sin(kr - \frac{L\pi}{2} - \frac{1}{k}ln(2kr) + \delta_L), r \to \infty, \qquad (17)$$

$$< f_{EL} \mid f_{E'L'} >= \delta(E - E')\delta_{LL'} \qquad (18)$$

estimates and analysis show that the latter function (PS) and the solution of the
—dinger 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 la enough energy interval. On the other hand, the function PS is very simple, and moreo as the calculations [24] and our test show, it appears quite reliable in describing differ photoprocesses.

The wave function of the AIS $| \mu_L LS >$ has been computed by the diagonalizati of the He atom Hamiltonian in the closed channel subspace under the second thresh of the ionization by using the Coulomb basis function with the charge Z=2. For t $^{1,3}S$, AIS have been mixed configurations 2sns,2pnp,3sns,3pnp,3dnd and 2snp,2pns,2p for the $^{1,3}P$ states as well as confgurations 2pnp,2snd,2pnf for the $^{1,3}D$ AIS, respectiv ($n \leq 5$). In the matrix diagonalzation, the convergence was checked by enlarging the ba dimension up to 20, and our data, obtained with the Coulomb function in the continuu (in place of the PS), have reproduced the estimates on the profile index $-q$ and widt [18, 19] up to three significant figures.

We introduce also abbreviations for the structure models in the calculations of oth authors. The Hylleraas-type variational function containing 56 parameters, is denoted b 56H and the function obtained by the close coupling method [8, 9] is denoted by CC.

IV. THE RESULTS AND DISCUSSIONS

We have calculated the energy dependence of the functions $\Gamma_{\mu_L L}(E)$ and $q^i_{\mu_L,L}(E)$ fo the He photoionization from the $(2^{1,3}S)$ and $(2^{1,3}P)$ states in a wide range of photoelectro spectrum including the resonance region (Figs.1 and 2). Figs. 1 and 2 demonstrate tha

The functions $\Gamma_{\mu_L,L}(E)$ and $q^i_{\mu_L L}(E)$ are already not constants even in the vicinity of the AIS positions, as it is demanded in accordance with the resonance approximation, but on the contrary they change drastically in a very large interval. It is also seen that the functions $q^i_{\mu_L L}(E)$ take large absolute values as compared with the profile- index value (q = - 2.75)[27] for the resonance excited in the photoionization from the He ground state (Fig. 2). So we find out that to describe the excited He photoionization it is necessary to extend the parametric theory[18] introducing the width and profile functions of energy. This the is main qualitative distinction between the descriptions of the He ground state and excited state photoionizations with the use of the diagonalization method.

The partial cross section for the He photoionization from the 2^1P state with excitation of the ^1D AIS evaluated in the resonance approximation (full line) and with the $\Gamma_{\mu_L,L}(E)$ and $q^i_{\mu_L L}(E)$ functions (dotted line) are shown in Fig.3. The difference between these cross sections are obviously significant. At the same time, our estimates on the total cross section for the photoionization He($2^{1,3}S$) of the He($2^{1,3}P$) atoms are in good agreement with available calculations[8]-[12],[24, 25], for example see Fig. 4. In Fig.4, we also see a wide minimum mentioned above.

Fig.5 illustrates that the partial cross sections for the direct photoionization of the excited He atoms are smaller than the cross section for the ground state approximately one up to few orders of magnitude . These cross sections decrease very fast as increases the photoelectron energy. Note that a particular fast falling down appears in the case of the $He(2^1P) + \gamma = He^+(1s) + e(Ed)$ process (Figs.5, full line).

In such conditions far enough from the AIS region the contribution of the phototransition to the closed resonace channel (formulae (13, 14)) turned out to be noticeable and

its amount grows as increases the energy (Fig. 4, Tabl. 1). As a result of the competitio and interference of the amplitudes of these two phototransition branches, the resonanc structure appears at distances comparable hundred times of natural widths far from th AIS region. It should be noted that an "extended" structure is just the major physica nature which leads to broadening and shift of resonance profile curves. (Figs. 3, 4 an Tabl. 1). The mentioned effect manifests itself much stronger in the process $He(2^1P) + 1$ $= He^+(1s) + e$ as well. In tabl. 1 we see that the quantity η at energy $E = 1$ a.u. (at th distances 6.1 and 8.24 eV from the first ^1S, ^1D resonance positions) amounts to 75.6 % for the ^1S wave and 91.2 % for the ^1D wave. The interference of the transition amplitude to the open and closed channels may lead to the difference $\Delta\sigma$ of the distinct signs a well (Tabl. 1).

In the energy dependence of dimensionless quantities, such as the coefficient of th photoelectron angular anisotropy β_e, the closed channel manifests itself much stronge than in the cross section of the photoionization. Our calculations show that in the cas of ionization from the 2^1P state at energy 0.9 a. u., the closed channel contributio to the β_e coefficient amounts to 131.7%. Figure 6 shows the energy dependence of th coefficient β_e for photoionization of the $He(2^1P)$ atom. The estimates obtained in th resonance approximation (full line 1) and with allowance for the energy dependence of th resonance profile and width parameters (curve 2) differ from each other significantly. A far enough distance from the resonance position, the behaviours of the coefficient obtaine with allowing for the closed resonace channel (curves 1, 2, 4) and without it (line 3) an compared. The curves 3 and 4 are the close coupling estamates [9](Jacobs, CC | 56E model). So we see that a rather strong appearance of the resonance profiles very far from

the resonance positions ($E(E_{\mu_L})$ is due to the influence of the closed resonace channel (let call it shortly the closed channel effect).

The closed channel effect also appears in the characteristics of ion- electron recombination into the He excited state which is the inverse process of the excited He photoionization. In table 2, the dependence of the closed channel contribution to the total photorecombination cross section upon the electron energy is given. A stronger effect is observed in the angular anisotropy coefficient [15] β_γ of the secondary photon γ_2 in the photorecombination process: $He^+(1s) + e \to \gamma_1 + (He(2^1P) \to He(1^1S) + \gamma_2)$ (Fig.7). In the nonresonant ($E(E_{\mu_L})$ region, the curve β_γ obtained by allowing for the closed channel (Fig. 7, dotted line 2) essentially differs from the curve calculated without taking it into account (Fig. 7, dashed line 3). Here, it is easy to note a large difference between the curves evaluated in the resonance approximation (full line 1) and with allowance for the energy dependence of the resonance profile and width functions (dotted line 2).

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 on the profile function ($q^i_{\mu_L L}(E)$) sign too. Thus, the results of our investigations (Figs. 1-7 and Tabl. 1-2) on the whole demonstrate the fact that the resonance struture formed in the photoprocess with the $He(2^1P)$ atom manifests itself essentially, far enough from the ^1D resonance position, at energies comparable hundred times of its natural width. Under similar physical circumstances the resonance structure with a large, in absolute value, profile function $q^i_{\mu_L L}(E)$ (Fig. 1) is formed.

In general, resonance structures formed in the photoionization of heavier atoms from loosely bound excited states might appear to be extended also in wide enough energy

interval[16, 17].

It seems interesting and expedient to explore experimentally the resonance pro behaviour considered in this work. We think that observing the fluorescence of the s ondary emission following the photo- and dielectronic recombination of the He^+ ion mig be more convenient to reveal experimentally the "broadening" and "shift" phenomena the excited atom photoionization. At present, direct measurements of an elementary pr cess cross section for the electron- ion recombination are performed[28]. We would like draw attention to a possibility to measure in principle, energy dependences of the wid and profile functions by using the polarized targets of He atoms[5, 6].

V. CONCLUSION

In this work, the photoionization of the excited He atom is studied in a wide rang of the spectrum. According to the diagonalizatioin approach [18], the atomic continuum structure has been described by the function which is a superposition of the function for the direct phototransition and of the L^2- function for the closed resonance channel The initial state wave functions have been calculated by using the many-configuration Hartree-Fock method.

Our estimates 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. 5) the resonance struture profiles noticeably manifest themselves (Figs. 3, 4, 6; Tabls. 1) The competition and interference of the phototransition amplitudes to open and closed

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Captions

Fig.1. Energy dependence of the parameter $\Gamma_{\mu_L,L}(E)$. Figures 1 ,2, 3 and 4 correspond to the $He(2^1P)+\gamma \rightarrow He^+(1s) + E(Es)$, $He(2^1P)+\gamma \rightarrow He^+(1s) + E(Ed)$, $He(2^1S)+\gamma \rightarrow He^+(1s) + E(Ep)$, $He(2^3S)+\gamma \rightarrow He^+(1s) + E(Ep)$ proceesses, respectively. In the brackets the AIS formed in these processes are indicated. The symbols show the experimental points: ◇, X and △ - Gelebart et al. (1976), ref.[26], + - Kossmann et al. (1988), ref.[27].

Fig.2. Energy dependence of the the parameter $q^i_{\mu_L L}(E)$. Figures 1, 2, 3 and 4 correspond to the same processes as Fig. 1. The curves 1 and 4 correspond to the values $[-q^i_{\mu_L L}(E)]$.

Fig.3. Cross section of the $He(2^1p) + \gamma \rightarrow He^{**}(^1D) \rightarrow He^+(1s)$ + E(d) process as a function of photoelectron energy; 2 is the estimates obtained in the resonance approximation $q_{res}(E) = 471.9$; 1 is the calculation with the functions $q^i_{\mu_L L}(E)$ and $\Gamma_{\mu_L,L}(E)$, L = 2.

Fig.4. Total cross section σ^i(E) of the $He(2^1p)$ atom photoionization as a function of the photoelectron energy.

Fig.5. The direct partial cross sections $\sigma^{(o)}_L(E)$ as a function of the energy in comparison with the cross section of the ground state photoionization (curve 0). Figures correspond to the same processes as in Fig. 1.

Fig.6. Energy dependence of the angular anisotropy coefficient of the photoelectron β_e(e
in the $He(2^1P) + \gamma \rightarrow He^+(1s) + e$ process taking into account both the ^1D and ^1S
resonances, is shown. Here 1 is the result in the resonance approximation , 2 is th
calculation with the functions $q^i_{\mu_L L}(E)$ and $\Gamma_{\mu_L L}(E)$. Far from the resonance region, th
behaviours of the coefficient obtained allowing for the closed channel influence (curves 2
4) and without it (line 3) are also compared. The curves 3 and 4 are taken from ref.[5
(Jacobs, CC|56H).

Fig.7. Energy dependence of the angular anisotropy coefficient of the secondary photon
$\beta_1(E)$(we use this notation in place of $\beta_2(E)$) from the $He(2^1P)$ atom following the re
combination ($e + He^+$). Curves 1 ,2 and 3 correspond to the same approximations as i
figure 6.

able I. Contributions of the first ^1D and ^1S closed channels to the partial cross section of the $He(2^1P)$ atom photoionization. In tabl. a^{-b} means $ax10^{-b}$.

	^1D			^1S		
E (a.u)	$\sigma_2^{(o)}$ mb	$\Delta\sigma$ Mb	$\eta(\%)$	$\sigma_0^{(o)}$ mb	$\Delta\sigma$ Mb	$\eta(\%)$
0.5	3.7^{-2}	-8.1^{-3}	21.9	2.8^{-2}	2.6^{-3}	9.3
0.6	2.0^{-2}	-6.8^{-3}	34.0	2.0^{-2}	2.7^{-3}	13.4
0.7	1.1^{-2}	-5.8^{-3}	51.3	1.5^{-2}	3.0^{-3}	19.4
0.8	6.8^{-3}	-4.9^{-3}	72.8	1.2^{-2}	3.5^{-3}	28.4
0.9	4.3^{-3}	-4.0^{-3}	93.8	9.9^{-3}	4.3^{-3}	43.4
1.0	2.8^{-3}	-2.6^{-3}	91.2	8.2^{-3}	6.2^{-3}	75.6

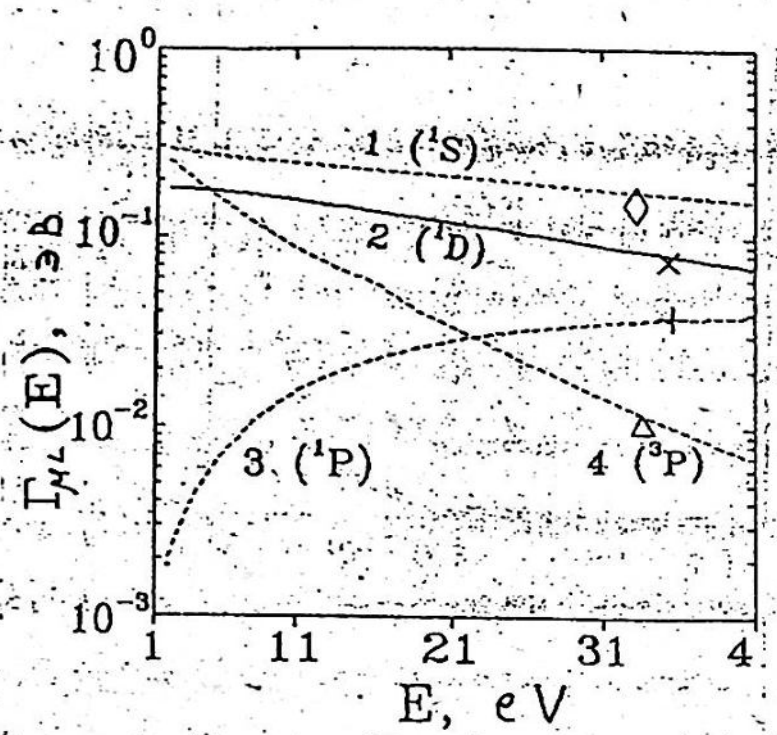
10^0
10^{-1}
10^{-2}
10^{-3}
$\Gamma_{\mu L}(E)$, эВ
1 (^{1}S)
2 (^{1}D)
3 (^{1}P)
4 (^{3}P)
1
11
21
31
4
E, eV

Fig. 1

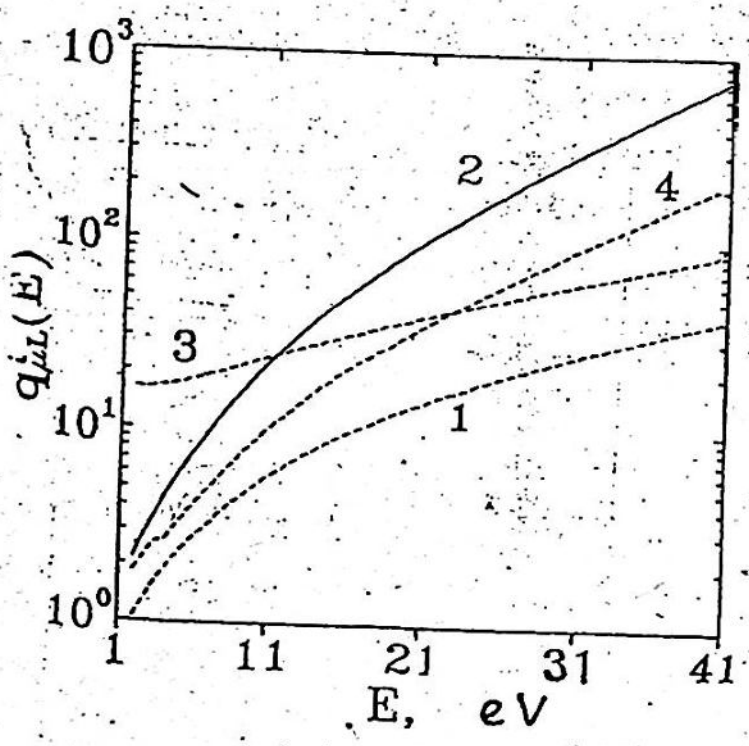
10^3
10^2
10^1
10^0
$q^i_{\mu L}(E)$
2
4
3
1
1
11
21
31
41
E, eV

Fig. 2

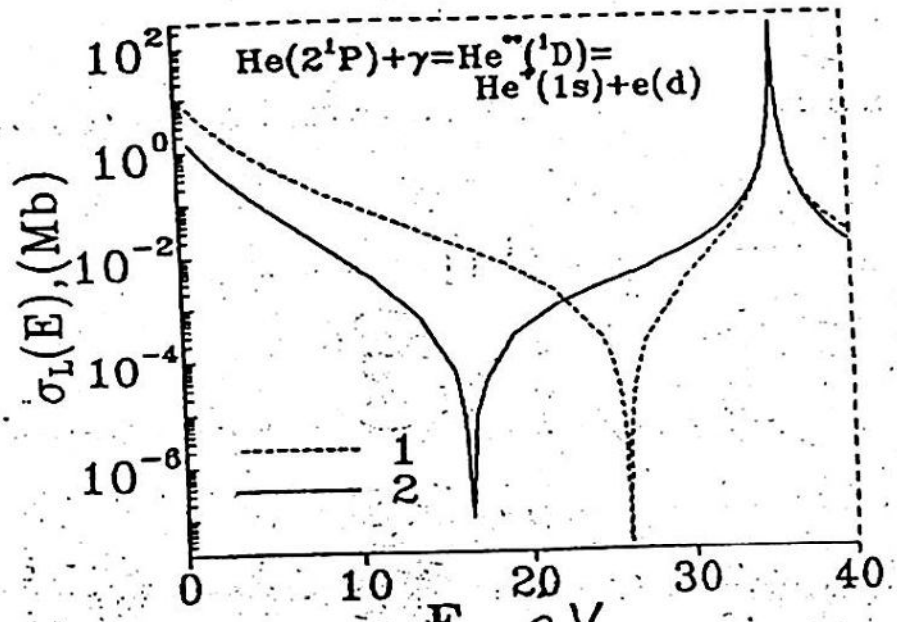
10^2
10^0
10^{-2}
10^{-4}
10^{-6}
$\sigma_L(E)$,(Mb)
$He(2^1P)+\gamma=He^{**}(^1D)=$
$He^+(1s)+e(d)$
1
2
0
10
20
30
40
E, eV

Fig.3

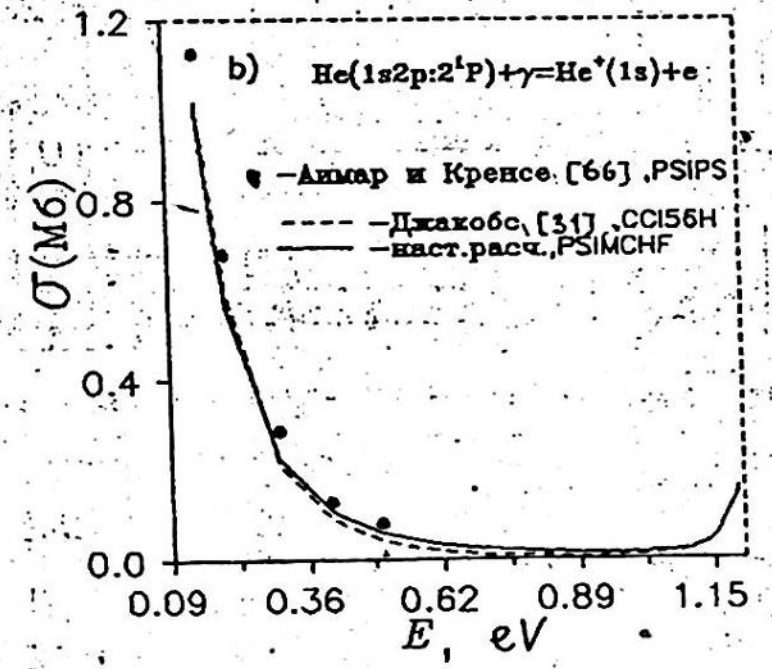
1.2
0.8
0.4
0.0
σ(Мб)
b) $He(1s2p:2^1P)+\gamma=He^+(1s)+e$
–Аммар и Кренсе [66] ,PSIPS
–Джакобс [31] ,CCI56H
–наст.расч.,PSIMCHF
0.09
0.36
0.62
0.89
1.15
E, eV

Fig.4