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On the Choice of the Wavefunction of the Ground State of He for Precision Calculations of Autoionization State Parameters above the Excited Ion Formation Threshold

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Abstract—The necessity of choosing multiparametric wavefunctions for describing the ground state of an atom in the problems of ionization of atoms by photons and electrons has been substantiated for the He atom as an example. Comparative analysis of application of different ground-state wavefunctions for this atom has been performed. The energies, widths, and partial widths of the lower autoionization state ^1P of the He atom above the excited ion formation threshold has been performed. It is shown that in contrast to total widths of quasi-stationary states, which differ insignificantly for different wavefunctions of the ground state, the partial widths are substantially different.

INTRODUCTION

In modern calculations of the cross sections of ionization of atoms by photons, electrons, and other particles, the wavefunction of the initial state is chosen as a rule in the same approximation as the wavefunction of the final state. This was demonstrated in the articles by Burke [1], Burke et al. [2], and Luke [3].

Fano [4] and Fano and Cooper [5] provided a grounded proof of the fact that in analysis of excitation of two-particle states for a large number of atoms of chemical elements in the ground state, multielectron correlations of type $(nl)^2$ must be taken into account above all. This is because the correlations in the ground state play an important role when the single shell of an atom contains only two electrons.

In calculations of the ionization cross sections of two-electron systems (e.g., the He atom above the threshold of formation of excited ions, namely, He^+ ($N = 2$)), this circumstance is of fundamental importance because along with one-particle channel $1s\varepsilon l$, the coupling with doubly excited channels $2s\varepsilon L$, $2p\varepsilon(L - 1)$, and $2p\varepsilon(L + 1)$ must be taken into account in this problem. The amplitude of excitation of these channels is determined by their coupling with channel $1s\varepsilon l$ in the final state as well as with multielectron correlations in the ground state.

The problem of calculation of the ground-state wavefunction for the model system considered here, which is described by the projection of the Hamilto-

nian on the subspaces of the $1s$, $2s$, and $2p$ states of the He^+ ion, corresponds to the problem of coupling of three closed channels. The system of equations of the coordinate representation of the method of strong coupling of channels in this case is transformed into the Hartree—Fock equation in the multiconfigurational approach [6—9].

The solution of this system of equations by the method of interacting configurations corresponds to the problem of determining the eigenvalues of the matrix of a real-valued infinite-rank symmetric operator. As regards two-electron systems, this corresponds to the solution of the multiconfigurational problem taking into account $(nl)^2$ configurations of the corresponding atom.

1. PROBLEM OF CHOOSING THE WAVEFUNCTION OF THE GROUND STATE OF THE HELIUM ATOM

The choice of the wavefunction of the ground state of an atom is an important step in the theoretical description of ionization of atoms. The criterion of the choice of the wavefunction of the ground state is the value of the ground-state energy of the atom, which is obtained in calculations based on the use of a certain wavefunction. The calculated value of the ground-state energy not always coincides with the experimental energy value. In precision calculations of autoionization state (AIS) parameters, this fact is of funda-

mental importance. For this reason, the wavefunction chosen for such calculations must exactly represent the experimental value of the ground-state energy. The most widely used class of the ground-state functions of a helium-like system is the class of wavefunctions represented in works by Hylleraas [10−12]:

$$\left(\Psi_0 = \sum_{n,l,m} C_{nlm}\psi_{nlm}, \ l = 0, 2, 4, ... \right), \quad (1)$$

where $\psi_{nlm} = s^n t^l w^m \exp(-s/2)/(n + l + m + 2)!$ Here, $s = r_1 + r_2$, $t = r_2 - r_1$, and $u = r_{12}$ are the independent variables determining the variational problem, and r_1, r_2, and r_3 are conventional notation for the mutual distances between the two electrons and the nucleus; n, l, and m are the quantum numbers (principal, orbital, and magnetic quantum numbers, respectively); C_{nlm} are the corresponding coefficients of the expansion in eigenfunctions ψ_{nlm} (see also, for example, formulas (10) and (10a) in [12] and comments to these formulas).

These functions successfully describe the ground-state energy of He; however, their applications in ionization problems is complicated by the method of calculation of amplitudes, the complexity of calculation of which is mainly due to the evaluation of the integrals containing a factor of the form $|r_1 - r_2|^m$. When the channel's strong coupling methods in the coordinate representation are used, the amplitudes are calculated at each point in energy.

Detailed analysis of parameters using the Hylleraas method is given in [13] taking into account the Fock modification [14]. It was shown in [13] that even in the sixth approximation, we have

$$\Psi^{(6)} = \Psi^{(4)} + [c_5 u^5 r^{-2} + c_6(5s + t^2/s)r^3]\exp(-zS), \quad (2)$$

where

$$\Psi^{(4)} = \exp(-zS)\{1 + u/2 + (1 + u/2)R_1 \\ \times [c_1 r^{-1} + c_2 + c_3 r] + c_4 u^2 R_1 r^{-3}\}.$$

Such a ground-state function gives an energy value close to the experimental value, namely, $E = 2.903557$ a.u. In calculations, multiparametrical Hylleraas wavefunctions (containing 6, 8, or even 56 parameters) are used as a rule.

In contrast to such a type of variational functions, the wavefunctions obtained in the multiconfigurational Hartree−Fock approximation fail to give the values of the ground-state energy for helium, which are close to the experimental value (see, for example, [8, 9, 15]. In our opinion, the most accurate analysis of multiparametrical variational wavefunctions for the helium atom was performed by Pekeris [16, 17]. However, the application of such functions in serial calculations is complicated and cumbersome.

It is more convenient to seek the solution to the Schrödinger equation for the ground state of He in the class of functions with inseparable variables. The most widely used among them is the analytic form of the Hartree−Fock wavefunction in the single-configurational approximation

$$\chi(r) = N_r(\exp(-\xi r) + 0.6\exp(-\zeta r)) \quad (3)$$

and the Eckart correlation function

$$\chi(\alpha r) = N_a(\exp(-\alpha r)), \quad \alpha = 2/a_0, \quad (4)$$

where a_0 is the Bohr radius and letters ξ and ζ in expression (3) denote the numerical parameters that are explained, for example, in [18, 19]. Coefficients N_r and N_a in these functions are chosen from the condition of normalization of wavefunction $\Psi_0(r_1, r_2)$ to unity. However, functions of this form are used only for obtaining rough estimates.

According to [20], the ground-state wavefunction can be written in the form

$$\Psi_0(r_1, r_2) = \sum_l B_l Y_l^{00}(r_{12})F_l(r_1 r_2), \quad (5)$$

where Y_l^{00} can be represented in the form $Y_l^{00} = \sum_\mu Y_{l\mu}(\theta_1, \varphi_1)C_{l\mu l-\mu}^{00}Y_{l\mu}(\theta_2, \varphi_2)$; B_l is the expansion coefficient, r_i is the radius vector of the ith electron, r_i is the corresponding modulus, $C_{l\mu l-\mu}^{LM} \equiv \langle l\mu l - \mu|LM\rangle$ are the coefficients of vector summation, and $F_l(r_1, r_2)$ are the radial functions describing the contribution of $(nl)^2$ configurations to the ground state. The choice of trial functions $F_l(r_1, r_2)$ is arbitrary in the general case. Only linear independence of the set and a correct asymptotic form of the solution are required. In such a case, functions $F_l(r_1, r_2)$ can be written in the form

$$F_l(r_1, r_2) = \sum_{mn} A_{mn}^l \left[\chi_m^\alpha(r_1)\chi_n^\beta(r_2) + \chi_n^\alpha(r_2)\chi_m^\beta(r_1) \right], \quad (6)$$

where χ_n^α are arbitrary sets of the continuous function of one variable, and α and β are parameters that are chosen from the variational principle.

Generally speaking, one can avoid using the variational principle for calculating functions $F_l(r_1, r_2)$ and choose functions χ_n^α in the form of the Coulomb basis. However, the expansion of type (5), (6) in this case converges very slowly, and a very large number of expansion terms must be taken into account for obtaining the required accuracy. The application of the variational principle for choosing parameters α and β noticeably accelerates the convergence of expansion (6). Tweed [20] formulated the one-parametric variational problem for the expansion considered here. He proposed that functions $\chi_n^\alpha(r)$ be sought in the form

$$\chi_n^\alpha(r) = r^n \exp\left(-\frac{\alpha}{2}r\right); \quad \alpha = \beta, \quad (7)$$

where α is determined from the conditions of the ground-state energy minimum. Coefficients A_{nm}^l are calculated by diagonalization of the matrix of the corresponding Hamiltonian. Depending on the numbers taken into account in expansion (6) of multiplets, the class of the Tweed wavefunctions includes 21-, 31-, and 41-parameter functions containing the $(np)^2$, $(nd)^2$, and $(nf)^2$ configurations, respectively. For the computational procedure, we can use the following formula:

$$F_l(r_1, r_2) = \sum_{m,n} A_{lmn}(r_1^n r_2^m + r_1^m r_2^n) \exp\left\{-\frac{1}{2}k(r_1 + r_2)\right\}. \quad (8)$$

Concluding the brief review, we note that analysis of the wavefunctions of the ground state with an essentially different approach can be carried out using the Monte Carlo method. In [21], this is done, for example, for a function of the form

$$\Psi_{49} = (1 + P_{12})\exp\left(\frac{\sum_{k=0} a_k r_1^n r_2^l r_{12}^m}{\sum_{k=0} b_k r_1^n r_2^l r_{12}^m}\right. \\ \left. + c(r_1^2 + r_2^2 - r_{12}^2)\ln[r_1^2 + r_2^2] - \alpha r_1 - \beta r_2\right). \quad (9)$$

The value of the ground-state energy of helium obtained in this approximation is the closest to the experimental value.

Wavefunction (8) will be used in further analysis.

2. CALCULATION OF PARTIAL SPECTROSCOPIC CHARACTERISTICS OF AUTOIONIZATION STATES IN THE REGION BETWEEN THE SECOND AND THIRD THRESHOLDS OF THE He ATOM

The diagonalization approximation [22, 23] makes it possible to trace the channels into which the autoionization states existing in the region above the threshold of formation of excited He$^+$ ions decay and in which ratio this process occurs. This question is especially topical because it reveals the resonances that decay into a certain channel (in this case, we can disregard the coupling of channels for such states), as well as the resonances decaying into several channels, for which the channel coupling must necessarily be taken into account. Such information can generally be obtained from analysis of data by comparing the values of positions and resonances in different approximations. However, this information is insufficient without the data on the particle decay widths.

For calculating the transition oscillator strength (or the ionization cross section), we must determine the

ionization amplitude, which can be presented in the general case in the form

$$T_{|0\rangle \to |\lambda E\rangle} = \sqrt{C(E)}\langle \Psi_\lambda^{E(-)}|\hat{t}|0\rangle, \quad (10)$$

where $|0\rangle \equiv |n_0 L_0 S_0\rangle$ is the wavefunction of the initial state of the atom and $C(E)$ is the kinematic factor.

Let us suppose that wavefunctions $|\lambda E\rangle$ in relation (10) satisfies the asymptotic conditions [1, 2]. As shown in [24, 25], the matrix of the eigenstates of the energy operator of the system is $A_{i\lambda} = \delta_{i\lambda}$ in this case. Then, we can write wavefunction $\Psi_\lambda^{E(-)}(r_1, r_2)$ in expression (10) in the form

$$|\Psi_\lambda^{E(-)}(\mathbf{r_1 r_2})\rangle = |\lambda E\rangle \\ + \sum_m \frac{\tilde{V}_{m\lambda}(E)}{E - E_m(E) + i\Gamma_m(E)/2}(|\tilde{\Phi}_m^E\rangle - i|\chi_m^E\rangle), \quad (11)$$

where

$$|\tilde{\Phi}_m^E\rangle = |\varphi_m^c\rangle + \frac{1}{\pi}\int_0^\infty \frac{|\chi_m^{E'}\rangle}{E - E'}dE', \\ |\chi_m^{E'}\rangle = \pi\sum_\lambda \tilde{V}_{m\lambda}(E)|\lambda E\rangle, \quad (12)$$

and we put in correspondence to index λ a set of quantum numbers, which is defined by the relation for the asymptotic form of wavefunctions [1].

Substituting expressions (11) and (12) into (10), we define the resonant ionization partial amplitudes as

$$T_{|0\rangle \to |\lambda E\rangle} = t_\lambda^{dir}(E) + \sum_m \frac{H_{m\lambda}(E)}{\varepsilon_m(E) + 1}. \quad (13)$$

In this expression, $\varepsilon_m(E) = 2[E - E_m(\tilde{E}_m)]/\Gamma_m(\tilde{E}_m)$ and $\Gamma_m(\tilde{E}_m)$ is the AIS width. This transition splits the amplitude into two terms; the first term fixes the contribution of the direct process, while the second term, the contribution of the resonant process. The remaining quantities appearing in formula (13) are defined by the relations

$$t_\lambda^{dir}(E) = \sqrt{C(E)}\langle \lambda E|\hat{t}|0\rangle, \\ H_{m\lambda}(E) = 2\tilde{V}_{m\lambda}(E)[t_m(E) - i\tau_m(E)]\Gamma_m^{-1}(E), \quad (14) \\ t_m(E) = \sqrt{C(E)}\langle \tilde{\Phi}_m^E|\hat{t}|0\rangle, \quad \tau_m(E) = \sqrt{C(E)}\langle \chi_m^E|\hat{t}|0\rangle.$$

The partial differential oscillator strength λ of the operator of transition to ionization channel is proportional to the squared modulus of expression (13). The total ionization cross section is calculated by summing all partial contributions over index λ. Then, the expression for the cross section is parametrized as follows:

$$\sigma_\lambda(E) = \sigma_\lambda^{dir}(E) + \sum_m \frac{\Gamma_m(E)P_{m\lambda}(E) + \varepsilon_m(E)Q_{m\lambda}(E)}{\varepsilon_m^2(E) + 1}. \quad (15)$$

The real-valued functions of total energy $P_{m\lambda}(E)$ and $Q_{m\lambda}(E)$ are doubled real and complex parts of complex function $N_{m\lambda}(E)$, which has the form

$$N_{\alpha m}(E)$$
$$= \sum_{\lambda c\alpha} H_{m\lambda}(E)\left(t_\lambda^{\text{dir}}(E) + \sum_n \frac{H_{m\lambda}(E)}{\varepsilon_n(E) - \varepsilon_m(E) + 2i}\right)^*. \quad (16)$$

Thus, the resonant ionization cross section can be determined by a set of total energy functions: $\sigma_\lambda^{\text{dir}}(E)$, $N_{\alpha m}(E)$, $\varepsilon_m(E)$, and $\Gamma_m(E)$.

Proceeding from the above arguments, we can pass to a system of characteristics of interacting AISs analogous to those introduced by Fano in [4] for an isolated resonance using functions $P_{m\alpha}(E)$ and $Q_{m\alpha}(E)$. Then, the parameters assume the form

$$\rho_{m\alpha}^{2(\pm)}(E) = \frac{P_{m\alpha}(E) \pm \sqrt{P_{m\alpha}^2(E) + Q_{m\alpha}^2(E)}}{\sigma_\alpha^{\text{dir}}(E)},$$
$$q_{m\alpha}^{(\pm)}(E) = \frac{Q_{m\alpha}(E)}{P_{m\alpha}(E) \pm \sqrt{P_{m\alpha}^2(E) + Q_{m\alpha}^2(E)}}. \quad (17)$$

In the case of an isolated resonance, both systems of functions $q_{m\alpha}^{(\pm)}(E)$ and $\rho_{m\alpha}^{2(\pm)}(E)$ have a simple geometrical meaning. Quantities $q_{m\alpha}^{(\pm)}(E)$ define the distance between the extrema of the resonance curve and the position of resonance $E_m(\tilde{E}_m)$, while functions $\rho_{m\alpha}^{2(\pm)}(E)$ are defined relative to the background of the amplitude of the extrema. In the presence of several interacting AISs, such an interpretation of functions (17) is approximate. Set of functions (17) in the Fano theory is determined unambiguously from the condition $\rho^2 > 0$, which corresponds to the choice of the plus sign in the notation adopted here. Therefore, the expression for calculating the cross sections has the form

$$\sigma_\alpha(E) = \sigma_\alpha^{\text{dir}}(E)$$
$$\times \left[1 + \sum_m \left(\frac{[\varepsilon_m(E) + q_{m\alpha}(E)]^2}{\varepsilon_m^2(E) + 1}\rho_{m\alpha}^2(E) - \rho_{m\alpha}^2(E)\right)\right]. \quad (18)$$

Depending on the definition of the subset of channels α, this expression describes either total or partial characteristics of excitation of the quasi-stationary states of atoms.

It can be seen from expressions (15) and (18) that the excitation and the decay of the mth quasi-stationary state in the group of channels $\alpha \in \Delta$ is characterized by two complex-valued functions $N_{\alpha m}(E)$ and $\eta_m(E) = E_m(E) - i\Gamma_m(E)/2$. Functions $\eta_m(E)$ appear in expression (11). Zeros of these functions on the complex plane determine the poles of the S scattering matrix, which correspond to excitation of quasi-stationary states. According to the concepts formulated by Siegert [26], the real part of the complex energy of a pole determines the position of a resonance, while

the imaginary part determines its width. Therefore, the problem of determining the positions and widths of resonances involves the solution of the system of uncoupled complex equations

$$E - E_m(E) + i\tilde{A}_m(E)/2 = 0. \quad (19)$$

This equality holds only for complex values of energy E. The solution of Eq. (19) requires analytic continuation in the problem of determining the eigenvectors and eigenvalues of complex matrix $W_{nm}(E)$:

$$W_{nm}(E) = E_n\delta_{nm} + F_{nm}(E) - i\gamma_{nm}(E). \quad (20)$$

Since the elements of matrix $W_{nm}(E)$ are functions of total energy E, its eigenvalues and eigenvectors also depend on E. Since the imaginary and real parts of this matrix are connected by the Hilbert transform, the analytic continuation of $W_{nm}(E)$ onto the entire complex plane of energy $E = E_1 + iE_2$ is a matrix of the form

$$W_{nm}^z(E) = E_n\delta_{nm} + \int_{-\infty}^{\infty} \frac{\gamma_{nm}(E')}{E_1 + iE_2 - E'}dE'. \quad (21)$$

Using the relations for the Cauchy-type contour integral, we can show that

$$W_{nm}^z(E) \to {}_{E_2 \to \pm 0}\delta_{nm}E_n + F_{nm}(E_1) \pm i\gamma_{nm}(E_1). \quad (22)$$

The positions of the poles are determined by values of E_1 and E_2 for which matrix $\delta_{nm}(E_1 + iE_2) - W_{nm}^z(E_1 + iE_2)$ degenerates. The degeneracy condition for the matrix is the equality of its determinant to zero, which gives the following set of equations for determining the complex energies of quasi-stationary states:

$$\begin{cases} \text{Re}[\det \|(E_1 + iE_2)\delta_{nm} - W_{nm}^z(E_1 + iE_2)\|] = 0, \\ \text{Im}[\det \|(E_1 + iE_2)\delta_{nm} - W_{nm}^z(E_1 + iE_2)\|] = 0. \end{cases} \quad (23)$$

Thus, for determining the position and width of the mth resonance, we must solve system of equations (23). As shown above, the introduction of spectroscopic parameters characterizing the AIS profiles in the ionization cross sections is associated with the possibility of using the resonance approximation in formulas (11)−(18). In the case when this approximation can be used, the positions and widths of the resonance states can be determined from Eq. (23) in the first order of perturbation theory.

Let us find the solutions to the following equations:

$$E_m(\tilde{E}_m) - \tilde{E}_m = 0. \quad (24)$$

We assume that the roots of these equations are the positions of AISs and define the width as the values of functions $\Gamma_m(E)$ for $E = \tilde{E}_m$. In the problems of calculation of the differential characteristics of AIS excitation, it is often necessary to determine the partial widths of the decay of quasi-stationary states into a few decay channels. In the diagonalization approxima-

tion, the partial width is introduced in terms of the matrix element of the decay:

$$\tilde{\Gamma}_m(E) = 2\pi \sum_\lambda |\langle m|\hat{V}|\lambda\varepsilon\rangle|^2, \quad \lambda \in \alpha. \quad (25)$$

The total width corresponds to $\alpha = \Delta(\tilde{\Gamma}_m(E)) = \Gamma_{m\Delta}(E)$. In the case of interacting quasi-stationary states, we introduce the partial widths analogously to the procedure in diagonalization approximation (25), namely,

$$\tilde{\Gamma}_j(E) = 2\pi \sum_\lambda \tilde{V}_{m\alpha}(E)\tilde{V}_{m\lambda}^*(E), \quad (26)$$

where j is the partial channel index. However, total width $\Gamma_m(E)$ in this case, which is determined by the diagonalization of the complex matrix, does not coincide with the sum of partial widths as for expression (25).

In actual calculations using the strong channel coupling method (see, for example, [27]), the position of a resonance is determined by the energy value for which the proper phase of the corresponding channel is equal to $\pi/2$. The determination of this quantity is reduced to the solution of the following equations:

$$\text{Arg}[\eta_i(E)] = \pi/2, \quad (27)$$

where $\eta_i(E)$ is the eigenvalue of the S matrix, which corresponds to the ith channel. The set of the widths can also be determined in terms of the value of function $\Gamma_m(E)$ at points $\tilde{E}_m$ satisfying condition (24). However, such a method for determining the positions and widths has a considerable disadvantage: the set of the solutions to Eq. (24) also contains the roots associated with so-called shape resonances in the continuous spectrum of the atom. The identification of AISs in this case involves direct analysis of the poles of the S scattering matrix. With such a method of determining the positions of resonant states, each reaction channel has its own set of solutions of the relevant equation [6, 27]. As it regards the widths, these quantities are determined by fitting of function $\eta_i(E)$ when the apparatus of the strong coupling method is employed [6].

The states of helium in the region of the continuum containing AISs converging to the third threshold were described by the wavefunction [24] taking into account all interconfigurational interactions of a finite number of basis configurations corresponding to two-electron excitations in the region between the second and third thresholds (closed channels), and an electron with a positive value of energy above the ground and first excited states of the He$^+$ ion (open channels). In our calculations, the states with the total angular momentum $L \leq 3$ of the helium atom were taken into account.

For each angular momentum L, the subspace of closed channels was filled by 20 configurations, and the Coulomb wavefunctions with charge $z = 2$ were used as the basis functions. Then, the subspace of

Table 1. Partial widths of lower five ^1S resonances obtained in the diagonalization approximation in the representation of real numbers

No.	E, eV	Γ, eV	$1s\varepsilon s$, eV	$2s\varepsilon s$, eV	$1p\varepsilon p$, eV
1	69.39400	0.08235	0.00264	0.07904	0.00067
2	70.48503	0.17282	0.00659	0.04469	0.12154
3	71.40519	0.04091	0.00269	0.03755	0.00067
4	71.91078	0.04045	0.00226	0.01187	0.02632
5	72.07814	0.01973	0.00155	0.01767	0.00053

Table 2. Partial widths of lower five ^1P resonances obtained in the diagonalization approximation in the representation of real numbers

No.	E, eV	Γ, eV	$1s\varepsilon p$, eV	$2s\varepsilon p$, eV	$2p\varepsilon s$, eV	$2p\varepsilon d$, eV
1	69.91937	0.16584	0.00033	0.03206	0.09450	0.03899
2	71.24768	0.00101	0.00001	0.00063	0.00027	0.00011
3	71.47437	0.06436	0.00011	0.00240	0.00368	0.05817
4	71.66483	0.06522	0.00033	0.01596	0.04076	0.00818
5	71.78036	0.00066	0.00001	0.00007	0.00003	0.00057

these states was diagonalized preliminarily. The subspace of open channels included three configurations for $L = 0$ and four configurations for other angular momenta L. This corresponds to taking into account the channels corresponding to the ground and first excited state of the He$^+$ ion ($1s\varepsilon L$, $2s\varepsilon L$, $2p\varepsilon(L-1)$, and $2p\varepsilon(L+1)$).

3. RESULTS OF CALCULATIONS

For describing the ground state of the He atom, one of the authors of this work and his colleagues in [24, 25] used the 41-parameter Tweed wavefunction [20] and obtained the exact values of the AIS parameters for the helium atom, which lie in the region above the excited ion formation threshold. It would be interesting to analyze the effect of the choice of the ground-state function on the partial characteristics of AISs. The partial AIS widths in the helium photoionization problem were calculated in [28] using the 6-parameter Hylleraas function in the diagonalization approximation. Along with this approximation, the method of interacting configurations in the representation of complex numbers was used in [24, 25], and the results were given in all approximations following from this method; however, the 41-parameter Tweed function was used as the ground-state function of the helium atom in all variants of calculations [20]. On the other hand, the concept of partial width makes sense only in the diagonalization approximation [22–25]. Tables 1–4 contain, in particular, the resultant partial widths of lower AISs.

Analysis of the application of various wavefunctions was carried out for the lower ^1P state described in Table 2. The results of this analysis are given in Table 5.

Table 3. Partial widths of lower five ^1D resonances obtained in the diagonalization approximation in the representation of real numbers

No.	E, eV	Γ, eV	$1s\varepsilon d$, eV	$2s\varepsilon d$, eV	$2p\varepsilon p$, eV	$2p\varepsilon f$, eV
1	69.66939	0.15198	0.00001	0.00342	0.14499	0.00356
2	70.50481	0.12298	0.00076	0.00837	0.11141	0.00244
3	71.22368	0.01108	0.00227	0.00306	0.00332	0.00244
4	71.54640	0.21438	0.00571	0.00076	0.20598	0.00193
5	71.56122	0.03308	0.00018	0.00776	0.02507	0.00008

Table 4. Partial widths of lower five ^1P resonances obtained in the diagonalization approximation in the representation of real numbers

No.	E, eV	Γ, eV	$1s\varepsilon f$, eV	$2s\varepsilon f$, eV	$2p\varepsilon d$, eV	$2p\varepsilon g$, eV
1	70.88120	0.08686	0.00006	0.03679	0.02921	0.02079
2	71.48071	0.00495	0.0000001	0.00185	0.00244	0.00065
3	71.99411	0.02403	0.00002	0.00749	0.01043	0.00608
4	72.13817	0.00074	0.0000004	0.00054	0.00016	0.00004
5	72.13959	0.00347	0.000002	0.00160	0.00128	0.00058

Table 5. Parameters of the lower ^1P autoionization state of the He atom in the energy range above the excited ion formation threshold, obtained using different wavefunctions of the ground state

Functions	E, eV	Γ, eV	$1s\varepsilon s$, eV	$2s\varepsilon p$, eV	$2p\varepsilon p$, eV	$2p\varepsilon d$, eV
6-parameter Hylleraas function [28]	69.89	0.150	0.893(−3)	0.918(−1)	0.313(−1)	0.257(−1)
41-parameter Tweed function	69.92	0.165	0.312(−3)	0.945(−1)	0.320(−1)	0.389(−1)
6-parameter Hylleraas function	69.90	0.154	0.871(−3)	0.814(−1)	0.315(−1)	0.407(−1)
8-parameter Hylleraas function	69.81	0.158	0.852(−3)	0.836(−1)	0.310(−1)	0.425(−1)
Monte Carlo function [21]	69.91	0.159	0.476(−3)	0.991(−1)	0.235(−1)	0.359(−1)

Table 5 contains the parameters of the lower ^1P state in the problem of photoionization of the helium atom above the excited ion formation threshold. The calculations were performed for different wavefunctions of the ground states. Analysis shows that the parameters of the quasi-stationary states depend on the choice of the wavefunction of the ground state.

CONCLUSIONS

The calculations of resonant cross sections in the photoionization problems and analysis of resonant profiles provide information on the structure of atomic systems and make it possible to choose the theoretical models more correctly; the choice of the ground-state wavefunction affects the values of the corresponding resonance parameters.

Investigations in the excitation energy range above the second ionization threshold (or above the threshold of formation of excited He$^+$ ions) are similar in many respects to earlier investigations carried out in the energy range between the first and second ionization thresholds but are much more effective. The spectrum of the characteristics in question is richer. This is due to the possibility of population of the ground state as well as excited state of the residual ions that subsequently pass to the ground state by emitting a photon during direct as well as resonant ionization by photons and electrons. This makes it possible to investigate the profiles of resonances converging to the threshold $N = 3$ of the He atom both in total and partial ionization cross sections; the coupling of channels in these processes must necessarily be taken into account. The choice of the ground-state wavefunction directly affects the values of the corresponding matrix elements appearing in the ionization cross section.

The results of calculations demonstrate that in contrast to total AIS widths, the partial widths are substantially different for different wavefunctions of the ground state. It can be seen from Table 5 that the total widths are also different when they are calculated on the basis of different wavefunction in the same approach; however, the difference in partial widths is larger in this case. This could be explained by the difference in the ground-state wavefunctions. However, further investigations are required for detailed analysis of the reasons for these effects.

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