

The Method of Interacting Configurations in Complex Number Representation. Application for Calculations of Spectroscopic Characteristics of Quasi-Stationary States in Two Electron Systems

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Abstract

The method of interacting configurations in complex numbers representation is formulated on the basis of Siegert's complex energy formalism. The method is applied to the problem of electron impact ionization of atoms. The wave function of the atomic ground state is taken as multi-parametric variational one. The wave functions of the resonant electron-atom scattering are constructed. These functions take into account the excitation of arbitrary quantity of interacting quasi-stationary states of the "electron plus ion" system. Such states may decay into arbitrary number of open bound channels. Within the formulated method the curves of differential generalized oscillator's strengths are parameterized. The results of calculations of the positions, total and partial widths for the problem of helium atom ionization above the second ionization threshold of atom are presented.

Key Words: Method of Interacting Configurations, Helium Atom, Quasi-Stationary States, Positions and Widths.

Introduction

The resonant ionization is the multi-particle process in its nature. Its correct theoretical description needs taking into account the mixing of discrete and continuous spectrum configurations. Therefore, even in relatively simple cases of photoionization the corresponding mathematics is too much complicated. Despite the

existence of a large number of resonant photoionization calculations the number of papers on the problem of atom ionization by electron impact is rather small. The problem of electron-impact ionization of atoms in Born approximation is as follows.

Consider atom ionization by a fast electron with the momentum \vec{k}_0 , which is scattered to the angle χ with the momentum \vec{k} . Let the atom in the initial state be characterized by quantum numbers of total orbital angular momentum, spin and their projections L_0, S_0, M_0, M_{s_0} . The state of the system after interaction is determined by quantum numbers of residual ion L_f, S_f, M_f, M_{sf} and ejected electron, having the momentum \vec{k} and spin projection m_s . We use the atomic system of units and the energy is measured in Rydbergs (Ry).

In Born approximation, the amplitude of ionization is given by the expression:

$$T_{o \rightarrow f}^{L_f M_f S_f M_{sf} m_s}(\vec{k}, \vec{Q}) = \langle L_f M_f S_f M_{sf}; \vec{k} m_s | \sum_{j=1}^Z \hat{t}_j^b(\vec{Q}, \vec{r}_j) | L_0 M_0 S_0 M_{s_0} \rangle \quad (1)$$

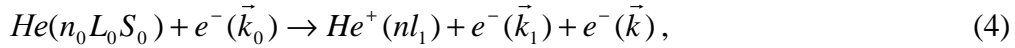
where

$$\hat{t}_j^b(\vec{Q}, \vec{r}_j) = -\frac{2a_0}{Q^2} \exp(i\vec{Q}\vec{r}_j), \quad (2)$$

and transferred momentum has the form

$$\vec{Q} = \vec{k}_0 - \vec{k}. \quad (3)$$

Denote the scheme of reaction under consideration for helium atom as



where $\vec{k}_0, \vec{k}_1, \vec{k}$ are the momenta of incident, ejected and scattered electrons, respectively. In Born approximation, the generalized oscillator strength for transition (GOS) has the form [1]:

$$\frac{\partial f_{nl_1}}{\partial E}(Q) = \frac{E}{Q^2} \sum_{lL} \left| \langle nl_1 l L | \sum_{j=1}^2 \exp(i\vec{Q}\vec{r}_j) | n_0 L_0 S_0 \rangle \right|^2. \quad (5)$$

In this formula, $E = k_0^2 - k^2$ is the energy loss; $\vec{Q} = \vec{k}_0 - \vec{k}$ is the transferred momentum; $|nl_1 l L : LS_0\rangle$ is the wave function of helium atom with total angular momentum L and spin S_0 .

Further, the electron with momentum l and the energy E is in the field of He^+ ion with electron having the quantum numbers $|nl\rangle$. The helium ground state wave function is $|n_0 LS_0\rangle$. The formulae for calculating GOS transitions in the continuous spectrum are given in the paper [2]. The ground state wave function was taken as the 41-parametric Tweed's wave function [3]. The summation over total angular momentum of helium was restricted by the contribution with $L \leq 3$.

Mathematical formulation

Usually the multi parametric wave function is taken for the description of helium atom ground state. It is due to the fact that the presence of only two electrons in only one atomic shell leads to the importance of correlations in the ground state. The criterion of choosing one or another wave function is the value of energy of the atomic ground state, which is obtained in the calculations on the basis of one or another wave function. Usually the Hylleraases multi-parametric wave functions (6-, 8- or 56-parametric) [4], Tweed's 41-parametric [3], or multi-configuration Hartree – Fock wave function [5] are used for systematic exact calculations. For simplified calculations the single configuration Hartree – Fock approximation, the Eccart's wave function, etc., are used.

We have take the 41-parametric Tweed's wave function for the description of He atom ground state. This wave function has the form:

$$F_l(r_1, r_2) = \sum_{m,n} A_{lmn} (r_1^m r_2^n + r_1^n r_2^m) \exp\{-\frac{1}{2}k(r_1 + r_2)\} \quad (6)$$

Here, according to [3], l, m, n, k are the parameters.

The four channels of direct ionization are opened in the region between the second and third thresholds. These channels are related to the electron over ground and first excited state of residual ion He^+ . The investigations of the processes of inelastic electron scattering on He ion [6,7] and photoionization processes [8-10] demonstrate that the coupling of these open channels is close. Therefore, the wave function of ionized helium is calculated within the framework of integral formulation of the open channel close coupling method in the description of direct ionization of helium by fast electrons in the region above the threshold of excited ions formation. In order to determine the K -matrix of the electron scattering on the ion He^+ the system of three integral equations is solved for $L=0$ and the system of four integral equations is solved for $L=1;2;3$. The explicit form of such equations is given in the paper [9]. In solving the system of equations for the K -matrix the solutions of single channel Schrödinger equation with shielded Coulomb potential are used as the basis functions for the description of electron in the continuous spectrum.

The helium atom states in the region of continuous spectrum, where the autoionizing states (AIS) which converge to the third threshold are located, are described by some wave function. This wave function takes into account all inter-configuration interactions from finite number of basis configurations, which correspond to two electron excitations in the region between the second and third thresholds (closed channels) and the electron with positive value of energy above the ground and the first excited state of He^+ (open channels). The states with total angular momentum of the helium $L \leq 3$ are taken into account.

The subspace of closed channels is filled by twenty configurations for every angular momentum L and the Coulomb wave functions with the charge $z=2$ are used as the basis functions for their description. After that the subspace of these states is preliminary diagonalized. The subspace of open channels includes three configurations for $L=0$ and four configurations for other angular momenta L . It

corresponds to the inclusion into calculation of the channels, which are related to the ground and the first excited state of He^+ ion ($1s\epsilon L, 2s\epsilon L, 2p\epsilon(L-1), 2p\epsilon(L+1)$).

The problem of description and interpretation of cross section structure for the resonant processes is reduced to the determination of the curves of the corresponding cross sections and resonant-state characteristics. The estimation of contribution of each quasi-stationary state into the curve formation is the main problem in the atomic spectra interpretation in the region above the ionization threshold. The overlapping sets of resonances are found in the spectra of many atoms. Although the experimental resonant structure consists of separate asymmetric peaks, the identification of such peaks with the isolated resonances is sometimes not enough justified [10]. The parameters, which characterize the calculated resonant structure and which are obtained by the FUMILI fitting method, sometimes are not related to the real states of the given system.

Consider the description of the formalism of the method of interacting configurations in complex number representation for the problem of atom resonant ionization by electron impact.

We suppose that the state of the N-electron system in the field of the nucleus having the charge Z is described by the set of wave functions obeying the stationary Schrödinger equation:

$$\hat{H}\Psi_{jE}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n) = E\Psi_{jE}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_n). \quad (7)$$

In this formula, \hat{H} is the Hamiltonian of the system, which explicit form is determined by each particular physical problem, \vec{r}_i is the set of coordinates of i -marked electron, E is the total energy of the system.

In this section, we will find such solutions of the equation (7), which corresponds to the states of the atom with one electron in the continuous spectrum. Consider the Hamiltonian \hat{H} of the system as the sum of two operators \hat{H}_0 and \hat{V}^r . Let \hat{H}_0 be the model Hamiltonian of the system. The set of eigenfunctions of the operator \hat{H}_0 may be presented in a form of unification of two subspaces, which determine the sets of states of discrete and continuous spectra, respectively. Let us denote these subspaces as D and C . The matrix of the Hamiltonian \hat{H} in the representation of the \hat{H}_0 operator may be written in the following form:

$$\|\hat{H}\| = \begin{vmatrix} \|\hat{H}^{DD}\| & \|\hat{V}^{DC}\| \\ \|\hat{V}^{CD}\| & \|\hat{H}^{CC}\| \end{vmatrix}, \quad (8)$$

where \hat{H}^{DD} and \hat{H}^{CC} operators are the projections of the Hamiltonian \hat{H} on the subspaces D and C . The matrices of the operators \hat{V}^{DC} and \hat{V}^{CD} characterize the interaction between the subspaces of discrete and continuous states.

Denote the sets of the wave functions of discrete spectrum as $|n\rangle$ and as $|\lambda E\rangle$ that of the continuous spectrum as $|\lambda E\rangle$. Let these functions obey the following condition:

$$\langle n | \hat{H}^{DD} | n \rangle = E_n \delta_{nm}; \quad \langle \lambda' E' | \hat{H}^{CC} | \lambda E \rangle = E \delta_{\lambda\lambda'} \delta(E - E'). \quad (9)$$

Using the technique of Feshbach's projective operators [11,12] one may show that the solutions of the equation (9) have the following properties:

$$\langle n | \lambda E \rangle = 0; \quad \hat{H}^{CC} | n \rangle = 0; \quad \hat{H}^{DD} | \lambda E \rangle = 0; \quad (10a)$$

$$\langle n | m \rangle = \delta_{nm}; \quad (10b)$$

$$\langle \lambda E | \lambda' E' \rangle = \lambda_{\lambda\lambda'} \delta(E - E'). \quad (10c)$$

It follows from here that the set of the wave functions $|n\rangle \cup |\lambda E\rangle$ is the complete orthonormalized system and satisfies the Fano conditions [13,14]. In the representation of this basis the matrix of the Hamiltonian \hat{H} is written in the following form:

$$\|\hat{H}\| = \left\| \begin{array}{cc} E_n \delta_{nm} & \|\hat{V}^{DC}\| \\ \|\hat{V}^{CD}\| & E \delta_{\lambda\lambda'} \delta(E - E') \end{array} \right\|. \quad (11)$$

The comparison of this formula with (8) gives the possibility to separate the interaction in the form of the sum of model Hamiltonian \hat{H}_0^M and so-called residual interaction \hat{V}_M^r . Therefore one obtains

$$\|\hat{H}_0^M\| = \left\| \begin{array}{cc} \|\hat{H}^{DD}\| & 0 \\ 0 & \|\hat{H}^{CC}\| \end{array} \right\|, \quad (12a)$$

$$\|\hat{V}_M^r\| = \left\| \begin{array}{cc} 0 & \|\hat{V}^{DC}\| \\ \|\hat{V}^{CD}\| & 0 \end{array} \right\|. \quad (12b)$$

The Schrödinger equation with the Hamiltonian \hat{H} in the representation (12) transforms into the system of integral-algebraic equations:

$$\left\{ \begin{array}{l} (E_n - E) a_{\lambda n}^{iE} + \sum_{\lambda'} \int_0^\infty b_{\lambda\lambda'}^{iE}(E') \cdot V_{n\lambda'}(E') dE' = 0 \\ \sum_m a_{\lambda m}^{iE} V_{m\lambda'}^*(E') + (E' - E) b_{\lambda\lambda'}^{iE}(E') = 0 \end{array} \right\}, \quad (13)$$

where i is the index of linearly independent solution of the system of equations (13); we will omit this index below. Index λ marks the channel of the scattering reaction and determines the asymptotic of the wave function and quantum numbers of the "ion + electron" system in the continuous spectrum. $a_{\lambda m}^E$ and $b_{\lambda\lambda'}^E(E')$ are the coefficients of the wave function $\Psi_\lambda^E(\vec{r}_1, \vec{r}_2)$ expansion in the basis of the states of the

discrete $|n\rangle$ and continuous $|\lambda E\rangle$ spectra. $V_{n\lambda}$ is the matrix element of \hat{V}^{CD} operator; $V_{n\lambda}(E) = V_{n\lambda}^*(E)$.

Recall that according to Fano [13,14]:

$$\Psi_{\lambda}^E(\vec{r}_1, \vec{r}_2) = \sum_m a_{\lambda m}^E |m\rangle + \sum_{\lambda'} \int_0^{\infty} b_{\lambda\lambda'}^E(E') |\lambda'E'\rangle dE'. \quad (14)$$

It is shown also in the well-known Fano's paper that the problem of finding the coefficients $a_{\lambda m}^E$ and $b_{\lambda\lambda'}^E(E')$ is solved analytically, if one restricts oneself to the single member in the expansion (14).

In order to provide the calculation of quasi-stationary states characteristics the fulfilling of the normalization condition for the function $\Psi_{\lambda}^E(\vec{r}_1, \vec{r}_2)$ on the δ -function over energy should be demanded. Moreover, the problem of description of the partial oscillator strengths of transition (or the ionization cross sections) needs taking into account the corresponding asymptotic boundary conditions. These conditions allowed putting into correspondence to the index of linearly independent solution of the system (13) such set of the quantum numbers, which characterizes the channel under consideration. According to the Burke's paper [15] the system of the wave functions in the representation of the total angular momentum, which have the following asymptotics

$$\begin{aligned} \Psi_{jL_f\lambda:LM}^E(\vec{r}_1, \dots, \vec{r}_N) &= \sum_{\vec{r}_N \rightarrow \infty} \sum_{j'L_f\lambda'\mu'M_f} \langle L_f M_f \lambda' \mu' | LM \rangle \times \\ \Psi_{jL_f M_f}(\vec{r}_1, \dots, \vec{r}_{N-1}) &\frac{1}{\vec{r}_N} Y_{\lambda'\mu'}(\theta_N, \varphi_N) \{ \delta_{\lambda\lambda'} \delta_{jj'} \delta_{L_f L_f'} \exp(i\theta_{jL_f'}(\vec{r}_N)) - \\ &[S_{jL_f\lambda:LM}^{j'L_f\lambda':LM}]^{\dagger} \exp(-i\theta_{jL_f'}(\vec{r}_N)) \}, \end{aligned} \quad (15)$$

corresponds to the ionization problem. Here j, L_f, M_f – are the quantum numbers, which characterized the ion; λ, μ – are the quantum numbers of the ejected electron;

$\Psi_{jL_f M_f}(\vec{r}_1, \dots, \vec{r}_{N-1})$ – is the wave function of ion; $S_{jL_f\lambda:LM}^{j'L_f\lambda':LM}$ is the scattering S -matrix,

$\theta_{jL_f}(\vec{r}_N) = k_{jL_f} \vec{r}_N + \frac{z'}{k_{jL_f}} \ln(k_{jL_f} \vec{r}_N)$; z' is the ion charge in the infinity.

In order to construct the set of the wave functions $\Psi_{\lambda}^E(\vec{r}_1, \vec{r}_2)$ with the asymptotic behavior (15) one has to determine the asymptotic properties of the basis $|\lambda E\rangle$ functions and to chose the corresponding method to go around the poles for the solutions of the system (13). It is known from the quantum scattering theory (see, e. g. [16]) that the method of going around the poles below corresponds to the set of wave functions with the asymptotics (15).

Using the formula for calculating the Cauchy type contour integral, we can present the formal solution of the system of equations (13) in the following form:

$$b_{\lambda\lambda'}^E(E') = P \frac{\sum_m a_{\lambda m}^E V_{m\lambda}(E)}{E - E'} + \left[A_{\lambda\lambda'} \pm i\pi \sum_m a_{\lambda m}^E V_{m\lambda'}(E) \right] \delta(E - E'). \quad (16)$$

The choice of the sign near $(\pm i\pi)$ determines the method of going around the poles “behind” or “below”. The matrix $A_{\lambda\lambda'}$ depends on the asymptotic properties of the basis $|\lambda E\rangle$ functions. The difference with Fano’s method is as follows. Fano put the real quantity instead of the square brackets.

The substitution of the expression (16) into the system of equations (13) leads to the system of inhomogeneous algebraic equations with the complex matrix of coefficients:

$$(E_n - E)a_{\lambda n}^E + \sum_m [F_{nm}(E) - i\gamma_{nm}(E)]a_{\lambda m}^E = -\sum_{\lambda'} A_{\lambda\lambda'} V_{\lambda n}(E); \quad (17a)$$

$$\gamma_{nm}(E) = \pi \sum_{\lambda} V_{n\lambda}(E) \cdot V_{\lambda m}(E); \quad F_{nm}(E) = \frac{1}{\pi} \int_0^\infty \frac{\gamma_{nm}(E')}{E - E'} dE'. \quad (17b)$$

The procedure of solving this system is as follows. First we determine the eigenvectors and eigenvalues of the symmetrical complex matrix, which belongs to the left-hand part of the system (17). We denote this matrix as $W_{nm}(E)$.

$$W_{nm}(E) = E_n \delta_{nm} + F_{nm}(E) - i\gamma_{nm}(E). \quad (18)$$

Since the elements of the matrix $W_{nm}(E)$ are the functions of the total energy E , its eigenvalues and eigenvectors also depend on E . Let $B_{nm}(E)$ be the matrix of eigenvectors and $\eta_n(E)$ be the vector of eigenvalues of the matrix $W_{nm}(E)$. The matrix (18) is not Hermitian. Therefore, $B_{nm}(E)$ and $\eta_n(E)$ are the complex values. Denote:

$$\eta_n(E) = E_n(E) + i\tilde{\gamma}_n(E), \quad (19)$$

where $\tilde{\gamma}_n = \frac{\Gamma_n(E)}{2}$.

It is known from the theory [17] that the following relation is valid for the eigenvectors of the symmetrical complex matrix:

$$\sum_k B_{ik}(E) \cdot B_{jk}(E) = \delta_{ij} \beta_j(E), \quad (20)$$

where $\beta_j(E)$ – is the complex vector, which depends on the normalization condition for the eigenvectors. Further we shall suppose that normalization for $B_{ik}(E)$ is such that $\beta_j(E) = 1$.

The next step after determining the eigenvectors and eigenvalues for the matrix $W_{nm}(E)$ is as follows. We shall find the coefficients $a_{\lambda m}^E$ of expansion and the

solution of the system of equations (17) in the form of linear combination of eigenvectors $B_{nm}(E)$. Thus,

$$a_{\lambda m}^E = \sum_{m'} B_{m'm}(E) \cdot \tilde{M}_{\lambda m'}(E). \quad (21)$$

Substituting (21) into the system (17), together with taking into account that $B_{nm}(E)$ are eigenvectors of the matrix $W_{nm}(E)$, we determine the system of linear equations with respect to the coefficients of linear combination (21). Therefore,

$$\sum_{m'} B_{m'm}(E) \cdot \tilde{M}_{\lambda m'} [E - E_{m'}(E) + i\Gamma_{m'}(E)/2] = \sum_{\lambda'} A_{\lambda\lambda'} V_{\lambda'm}(E). \quad (22)$$

Multiplying left and right sides of the system (22) by matrix $B_{nm}(E)$ and taking into account the property (20), we find the expression for $\tilde{M}_{\lambda m}(E)$:

$$\tilde{M}_{\lambda m}(E) = \frac{\sum_{k\lambda'} B_{nk}(E) V_{k\lambda'}(E) A_{\lambda\lambda'}}{E - E_m(E) + i\Gamma_m(E)/2} = \frac{\sum_{\lambda'} \tilde{V}_{m\lambda'} A_{\lambda\lambda'}}{E - E_m(E) + i\Gamma_m(E)/2}, \quad (23)$$

where $\tilde{V}_{m\lambda'}(E) = \sum_{m'} B_{m'm}(E) \cdot V_{m'\lambda'}(E)$. solution (23) determines the coefficients of the expansion with the accuracy to the matrix $A_{\lambda\lambda}$. Further, the properties of the matrix $A_{\lambda\lambda}$ depend on the asymptotic properties of the functions of the basis $|\lambda E\rangle$. The expressions for the coefficients of the expansion have the following form:

$$a_{\lambda m}^E = \sum_{m'} B_{m'm}(E) \frac{\sum_{\lambda'} A_{\lambda\lambda'} \tilde{V}_{\lambda'm'}(E)}{E - E_{m'}(E) + i\Gamma_{m'}(E)/2}. \quad (24a)$$

Taking into account (23), we have:

$$a_{\lambda m}^E = \sum_{m'} \tilde{M}_{\lambda m'}(E) \cdot B_{m'm}(E). \quad (24b)$$

It is convenient to introduce the matrix $M_{\lambda m}(E)$, which is related to the matrix $\tilde{M}_{\lambda m}(E)$ by the relationship:

$$M_{\lambda m}(E) = \tilde{M}_{\lambda m}(E) \times [E - E_m(E) + i\Gamma_m(E)/2]. \quad (24c)$$

Thus, the link between the matrix $M_{\lambda m}(E)$ and matrices $A_{\lambda\lambda}$, $B_{nm}(E)$, $V_{n\lambda}(E)$ will be presented by the formula:

$$M_{n\lambda}(E) = \sum_k \sum_{\lambda'} B_{nk}(E) \cdot V_{k\lambda'} \cdot A_{\lambda\lambda}. \quad (25)$$

Moreover,

$$[M_{n\lambda}(E)]^* = M_{\lambda n}(E), \quad (26)$$

which is not valid for the matrix $\tilde{M}_{\lambda m}(E)$.

Let us determine the matrix $A_{\lambda\lambda'}$. Substitute (23) and (24) into the expansion (14) for this purpose. In this case the explicit form of the solution of the Schrödinger equation is as follows:

$$\begin{aligned} \Psi_{\lambda}^{E(-)}(\vec{r}_1, \vec{r}_2) = & \sum_{\lambda'} A_{\lambda\lambda'} |\lambda'E\rangle + \sum_m \frac{M_{\lambda m}(E)}{E - E_m(E) + i\Gamma_m(E)/2} \times \\ & \times \left[\sum_n B_{mn}(E) |n\rangle + \sum_{\lambda'} \left(\int_0^{\infty} \frac{\tilde{M}_{\lambda m}(E')}{E - E'} \right) \sum_{\lambda} A_{\lambda\lambda'} |\lambda E'\rangle dE' - i\pi \tilde{M}_{\lambda m} \sum_{\lambda'} A_{\lambda'\lambda} |\lambda'E\rangle \right] \end{aligned} \quad (27)$$

If we consider now more convenient basis of the wave functions

$$\varphi_{\lambda}^E(\vec{r}_1, \vec{r}_2) = \sum_{\lambda'} A_{\lambda\lambda'} |\lambda'E\rangle \quad \text{ta} \quad \tilde{\varphi}_m^E(\vec{r}_1, \vec{r}_2) = \sum_n B_{mn}(E) \cdot |n\rangle, \quad (28)$$

then we get the expression (27) in the form:

$$\begin{aligned} \Psi_{\lambda}^{E(-)}(\vec{r}_1, \vec{r}_2) = & \varphi_{\lambda}^E(\vec{r}_1, \vec{r}_2) + \sum_m \frac{M_{\lambda m}(E)}{E - E_m(E) + i\Gamma_m(E)/2} \times \\ & \times \left[\tilde{\varphi}_{\lambda}^E(\vec{r}_1, \vec{r}_2) + \sum_{\lambda'} \left(\int_0^{\infty} \frac{M_{\lambda m}(E')}{E - E'} \tilde{\varphi}_{\lambda'}^{E'}(\vec{r}_1, \vec{r}_2) dE' - i\pi M_{\lambda m}(E) \varphi_{\lambda'}^E(\vec{r}_1, \vec{r}_2) \right) \right]. \end{aligned} \quad (29)$$

The wave functions $|\lambda E\rangle$ and, therefore, $\varphi_{\lambda}^E(\vec{r}_1, \vec{r}_2) = \sum_{\lambda'} A_{\lambda\lambda'} |\lambda'E\rangle$, are the multi-channel functions, so the expression for their asymptotics may be presented in the form

$$|\lambda E\rangle_{r_n \rightarrow \infty} \rightarrow \sum_j \frac{\Psi_j(\vec{r}_1, \dots, \vec{r}_{n-1})}{\vec{r}_n} [\tilde{b}_{\lambda j} \cos(\theta_j(\vec{r}_n) + \xi_j) + \tilde{a}_{\lambda j} \sin(\theta_j(\vec{r}_n) + \xi_j)]. \quad (30)$$

The matrices $\|\tilde{a}\|$ and $\|\tilde{b}\|$ are determined from the normalization condition for the function $|\lambda E\rangle$ on the δ -function over energy. With respect to these matrices the normalization condition will have the following form:

$$\|\tilde{a}\|^2 + \|\tilde{b}\|^2 = 1, \quad (31)$$

therefore

$$\|A\| = \|\tilde{a} + i\tilde{b}\|^{-1}. \quad (32)$$

If the wave functions $|\lambda E\rangle$ obey the condition (14), the matrix $A_{i\lambda}$ will have the following form $A_{i\lambda} = \delta_{i\lambda}$. Therefore, the wave function $\Psi_{\lambda}^{E(-)}(\vec{r}_1, \vec{r}_2)$ has the form:

$$|\Psi_{\lambda}^{E(-)}(\vec{r}_1, \vec{r}_2)\rangle = |\lambda E\rangle + \sum_m \frac{\tilde{V}_{m\lambda}(E)}{E - E_m(E) + i\Gamma_m(E)/2} (|\tilde{\Phi}_m^E\rangle - i|\chi_m^E\rangle), \quad (33)$$

$$|\tilde{\Phi}_m^E\rangle = |\varphi_m^c\rangle + \frac{1}{\pi} \int_0^\infty \frac{|\chi_m^{E'}\rangle}{E - E'} dE' \quad i |\chi_m^{E'}\rangle = \pi \sum_\lambda \tilde{V}_{m\lambda}(E) |\lambda E\rangle \quad (34)$$

Here the set of quantum numbers, which is determined by the relation (15), is put into correspondence to the λ index. In order to calculate the oscillator's strength (or cross section) for ionization the amplitude of ionization should be determined. As it is known the amplitude of ionization may be written in general case in the following form:

$$T_{|0\rangle \rightarrow |\lambda E\rangle} = \sqrt{C(E)} \langle \Psi_\lambda^{E(-)} | \hat{t} | 0 \rangle, \quad (35)$$

where

$$|0\rangle \equiv |n_0 L_0 S_0\rangle, \quad (36)$$

which determines the wave function of atom in the initial state, $C(E)$ is the kinematic factor.

The substitution of expressions (33)-(34) into (35) determines the partial amplitudes of resonant ionization:

$$T_{|0\rangle \rightarrow |\lambda E\rangle} = t_\lambda^{dir}(E) + \sum_m \frac{H_{m\lambda}(E)}{\varepsilon_m(E) + 1}. \quad (37)$$

The following relations determine the quantities, which are written in (37):

$$t_\lambda^{dir}(E) = \sqrt{C(E)} \langle \lambda E | \hat{t} | 0 \rangle; H_{m\lambda}(E) = 2\tilde{V}_{m\lambda}(E) [t_m(E) - i\tau_m(E)] G_m^{-1}(E), \quad (38)$$

$$t_m(E) = \sqrt{C(E)} \langle \tilde{\Phi}_m^E | \hat{t} | 0 \rangle; \tau_m(E) = \sqrt{C(E)} \langle \chi_m^E | \hat{t} | 0 \rangle. \quad (39)$$

The partial differential oscillator strength of the transition to the channel of ionization λ is proportional to the square of the module of the expression (37). The summing all partial contributions over the index λ fulfills the calculation of the total ionization cross section λ . We select some group of channels among all the channels taken into account in the problem. Let Δ be the set of the channels of the reaction, and α be some subset of the set Δ , so that $\alpha \in \Delta$. Differential oscillator's strengths for transition with excitation of channels, which are characterized by $\lambda \in \alpha$ index, are written as follows:

$$\frac{\partial f_\alpha(E)}{\partial E} = G(E) \sum_{\lambda \in \alpha} \left| t_\lambda^{dir}(E) + \sum_m \frac{H_{m\lambda}(E)}{\varepsilon_m(E) + 1} \right|^2 \quad (40)$$

where $G(E)$ is the normalization factor, linking the cross section with the differential oscillator's strength for transition in the following way:

$$\sigma_\alpha(E) = \frac{1}{G(E)} \frac{\partial f_\alpha(E)}{\partial E}, \quad (41)$$

or

$$\sigma_{\alpha}(E) = \sigma_{\alpha}^{dir}(E) + \sum_{\lambda \in \alpha} \left\{ \sum_m \left[\frac{t_{\lambda}^{dir*}(E)H_{m\lambda}(E)}{(\varepsilon_m(E) + i)(\varepsilon_n(E) - i)} + \frac{t_{\lambda}^{dir}(E)H_{m\lambda}^*(E)}{\varepsilon_m(E) - i} \right] + \sum_{nm} \frac{H_{m\lambda}(E)H_{n\lambda}^*(E)}{(\varepsilon_m(E) + i)(\varepsilon_n(E) - i)} \right\}. \quad (42)$$

Further, we transform the expression (42) to the form, which is similar to Shore's parametric formulae [18] in the non-overlapping resonance approximation

$$\sigma_{\lambda}(E) = \sigma_{\lambda}^{dir}(E) + \sum_m \frac{\Gamma_m(E)P_{m\lambda}(E) + \varepsilon_m(E)Q_{m\lambda}(E)}{\varepsilon_m^2(E) + 1}. \quad (43)$$

The real functions of the total energy $P_{m\lambda}(E)$ and $Q_{m\lambda}(E)$ are the double parts of the real and complex parts of the complex function $N_{m\lambda}(E)$, where the last one has the following form:

$$N_{om}(E) = \sum_{\lambda \in \alpha} H_{m\lambda}(E)(t_{\lambda}^{dir}(E) + \sum_n \frac{H_{m\lambda}(E)}{\varepsilon_n(E) - \varepsilon_m(E) + 2i})^*. \quad (44)$$

Therefore, the resonant ionization cross section is determined by the set of the following functions of the total energy: $\sigma_{\lambda}^{dir}(E); N_{om}(E); \varepsilon_m(E); \Gamma_m(E)$.

the basis of the formula (43) one may come to the system of characteristics of interacting AIS, which are similar to the parameters introduced by Fano [13,14] for a single isolated resonance, i. e.:

$$q_{m\alpha}(E) = \text{tg}(\beta_{m\alpha}(E)); \sigma_{m\alpha}(E) = |N_{m\alpha}(E)|^2 \cos(\beta_{m\alpha}(E)), \quad (45)$$

$$\rho_{m\alpha}^2(E) = \frac{\sigma_{m\alpha}(E)}{\sigma_{\alpha}^{dir}(E)}; \beta_{m\alpha}(E) = \frac{1}{2} \text{Arg}(N_{m\alpha}E) + \frac{k\pi}{2}; (k \in N). \quad (46)$$

Thus, the argument of the complex function $N_{m\alpha}(E)$ is determined in different ways, with the accuracy to $k\pi$ (where k is integer real number, $k > 0$). Therefore, two sets of characteristics given by relations (45), (46) correspond to each value of the function $N_{m\alpha}(E)$. The functions (45), (46) may be easily presented over $N_{m\alpha}(E) = 2(P_{m\alpha}(E) + Q_{m\alpha}(E))$. Then the parameters will have the following form:

$$\rho_{m\alpha}^{2(\pm)}(E) = \frac{P_{m\alpha}(E) \pm \sqrt{P_{m\alpha}^2(E) + Q_{m\alpha}^2(E)}}{\sigma_{\alpha}^{dir}(E)}, \quad (47)$$

$$q_{m\alpha}^{(\pm)}(E) = \frac{Q_{m\alpha}(E)}{P_{m\alpha}(E) \pm \sqrt{P_{m\alpha}^2(E) + Q_{m\alpha}^2(E)}}. \quad (48)$$

In the case of isolated resonance both systems of functions $q_{m\alpha}^{(\pm)}(E)$ and $\rho_{m\alpha}^{2(\pm)}(E)$ have a simple geometric sense. The quantities $q_{m\alpha}^{(\pm)}(E)$ determine the distance

between the extremums of the resonant curve and the resonance position $E_m(\tilde{E}_m)$. The quantities $\rho_{m\alpha}^{2(\pm)}(E)$ are determined with respect to background of the amplitude of extremums. In the case of few interacting autoionizing states such interpretation of the functions (47), (48) is approximate. The set of functions (47), (48) in Fano's theory is determined exactly from the condition $\rho^2 > 0$, which in our notation corresponds to the choice (+) of the sign. Therefore, the expression for the calculation of cross sections will have the following form:

$$\sigma_{\alpha}(E) = \sigma_{\alpha}^{dir}(E) \left[1 + \sum_m \left(\frac{[\varepsilon_m(E) + q_{m\alpha}(E)]^2}{\varepsilon_m^2(E) + 1} \rho_{m\alpha}^2(E) - \rho_{m\alpha}^2(E) \right) \right]. \quad (49)$$

Dependent of the definition of the subset of the channels α the formula (49) will describe either total or partial characteristics of excitation of atomic quasi-stationary states.

Consider the spectroscopic characteristics of interacting quasi-stationary states in total and partial differential oscillator's strength for transition. It follows from the expressions (40), (41) i (49) that the excitation and decay of m -number quasi-stationary state over the group of channels $\alpha \in \Delta$ is characterized by two complex functions: $N_{\alpha m}(E)$ i $\eta_m(E) = E_m(E) - \frac{i}{2} \Gamma_m(E)$. The functions $\eta_m(E)$ enter the expression for the S matrix of resonant scattering. The zeros of these functions on the complex energy plane determines the poles of the scattering S -matrix, which correspond to the excitation of the quasi-stationary states of scattering matrix corresponding to the quasi-stationary state excitation. According to the results of Siegert's paper [19], the real part of the complex energy pole determines the position of the resonance and the complex part determines its width. Hence, the problem of finding the positions and widths of resonances is reduced to finding the solutions of the system of non-linked complex equations:

$$E - E_m(E) + \frac{i}{2} \Gamma_m(E) = 0. \quad (50)$$

The equality (50) is valid only for the complex energy values E . Solving the equations (50) needs analytical extension in the problem of construction of eigenvectors and eigenvalues of the complex matrix $W_{nm}(E)$ (18) with the complex values of the energy E . The real and imaginary parts of this matrix are linked between each other by the Gilbert transformation. Therefore, the following matrix

$$W_{nm}^z(E) = E_n \delta_{nm} + \int_{-\infty}^{\infty} \frac{\gamma_{nm}(E')}{E_1 + iE_2 - E'} dE' \quad (51)$$

will be the analytical extension of $W_{nm}(E)$ on the whole complex plane of the energy $E = E_1 + iE_2$.

Using the relations for the closed path integral of Cauchy type we show that

$$W_{nm}^z(E) \rightarrow_{E_2 \rightarrow \pm 0} \delta_{nm} E_n + F_{nm}(E_1) \pm i\gamma_{nm}(E). \quad (52)$$

The positions of the poles are determined by the values E_1 and E_2 , at which the matrix $\delta_{nm}(E_1 + iE_2) - W_{nm}^z(E_1 + iE_2)$ degenerates.

The condition of the matrix degeneration is the equality to zero of its determinant. From this condition the system of equations for determining the complex energies of quasi-stationary states follows.

$$\begin{cases} \operatorname{Re}[\det\|(E_1 + iE_2)\delta_{nm} - W_{nm}^z(E_1 + iE_2)\|] = 0, \\ \operatorname{Im}[\det\|(E_1 + iE_2)\delta_{nm} - W_{nm}^z(E_1 + iE_2)\|] = 0. \end{cases} \quad (53)$$

Hence, the system of equations (53) must be solved in order to determine the position and width of m -resonance.

As it was mentioned above introduction of the system of spectroscopic parameters, which characterize the profiles of autoionizing states in the ionization cross section, corresponds to the possibility of using the resonant approximation in the formulae (42) - (48).

In the case when this approximation may be used, the positions and widths of the resonant states may be found from (53) in the first order of perturbation theory. Let us find the solutions of the following equations:

$$E_m(\tilde{E}_m) - \tilde{E}_m = 0. \quad (54)$$

We consider the solutions of these equations as the positions of the autoionizing states. The widths are determined as the value of the function $\Gamma_m(E)$ with $E = \tilde{E}_m$. The parameterization of the functions $N_{m\alpha}(E)$ is also fulfilled at $E = \tilde{E}_m$. From here we find the expressions

$$\frac{\partial f_\alpha(E)}{\partial E} = \frac{\partial f_\alpha^{dir}(E)}{\partial E} \left[1 + \sum_m \rho_{m\alpha}^2(E) \left[\frac{(\varepsilon_m(E) + q_{m\alpha})^2}{\varepsilon_m^2(E) + 1} - 1 \right] \right], \quad (55)$$

$$\varepsilon_m(E) = \frac{2[E - E_m(\tilde{E}_m)]}{\Gamma_m(\tilde{E}_m)}; \quad q_{m\alpha}(\tilde{E}_m) = \operatorname{ctg} \left[\frac{1}{2} \operatorname{Arg}[N_{m\alpha}(\tilde{E}_m)] \right], \quad (56)$$

$$\rho_{m\alpha}^2 = \frac{|N_{m\alpha}(\tilde{E}_m)|^2 \sin(\frac{1}{2} \operatorname{Arg}(N_{m\alpha}(\tilde{E}_m)))}{\sigma_\alpha^{dir}(E)}, \quad (57)$$

for the differential oscillator's strengths.

The validity of parameterization introduction should be analyzed in each particular physical problem by exact calculation of the functions $N_{m\alpha}(E)$ and $\eta_m(E)$. It is often necessary to determine the partial widths of quasi-stationary states decay via few decay channels in the calculation of autoionizing states excitation differential characteristics.

In diagonalizing approximation the partial width is introduced over the matrix element of decay in the following way:

$$\tilde{\Gamma}_{m\alpha}(E) = 2\pi \sum_{\lambda \in \alpha} |\langle m | \widehat{V} | \lambda \mathcal{E} \rangle|. \quad (58)$$

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 similarly to the diagonalizing approximation (58), i. e.:

$$\tilde{\Gamma}_{m\alpha}(E) = 2\pi \sum_{\lambda \in \alpha} \tilde{V}_{m\alpha}(E) \tilde{V}_{m\lambda}^*(E). \quad (59)$$

The above- formalism is realized in the special program complex using the programming language FORTRAN-77. It consists of the following parts.

1. The programs of calculations of the matrix elements $V_{mm}(E)$, $V_{n\lambda}(E)$ and $V_{\lambda\lambda'}(E)$ are created and used. The Coulomb and Hartree – Fock functions may be chosen in these programs as the wave functions for the calculation of the matrix elements. The functions of the continuous spectrum are calculated in the shielding potential.

2. The program of constructing the previous diagonalizing states of the continuous spectrum of the atom is realized. The working algorithm of this program is based on the solution of the system of integral equations like (13) by means of the successive approximation method or on the reduction of this system to the system of algebraic equations. We have found the amplitudes describing the direct process of atom (or ion) excitation with the inclusion of the coupling of the channels, see (38). (39).

3. The next block of programs consists of the algorithms of calculation of the energy dependence of the parameters of $E_n(E)$, $\Gamma_n(E)$, $N_{m\lambda}(E)$, $H_{m\lambda}(E)$. Further, Fano's and Shore's parameters are calculated for any AIS, the GOS are found and the cross sections in the resonant approximation are obtained.

The connection between the programs is provided via the database, which is located on the hard disk with direct access and is specified for the work with such complex of programs.

Results of calculations

Below we demonstrate that this formalism enabled us to fulfill precise calculations of the positions (as well as of the total and partial widths) of AIS in the problem of electron-impact ionization of atoms and ions.

For example, we present the calculated positions, total and partial widths for the problem of helium atom ionization above the second ionization threshold, i. e. between the second and the third helium ionization thresholds. In this region, the AIS are located, which decay into three open channels for the S-terms and into four open channels for the P, D, F- terms.

The numerical values of calculated quantities are presented in tables 1 – 4.

Table: 1

N π/π	E_r , eV	Γ_r , eV	1ses	2ses	2p ϵ p
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
6	72.24057	0.01974	0.00002	0.00038	0.00006
7	72.33661	0.01643	0.00117	0.00487	0.01038
8	72.40086	0.01048	0.00087	0.00926	0.00035
9	72.48489	0.00058	0.00001	0.00047	0.00010
10	72.54845	0.00812	0.00067	0.00259	0.00486

Positions, total and partial widths of ten lowest ^1S resonances.

Table: 2

N π/π	E_r , eV	Γ_r , eV	1s ϵ p	2s ϵ p	2p ϵ s	2p ϵ d
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
6	71.02307	0.00070	0.000001	0.00042	0.00023	0.00005
7	72.20032	0.02446	0.0000001	0.0000001	0.00543	0.01903
8	72.25068	0.03066	0.00025	0.00937	0.01938	0.00166
9	72.26011	0.00040	0.0000001	0.00006	0.00006	0.00028
10	72.37193	0.00046	0.000001	0.00006	0.00017	0.00023

Positions, total and partial widths of ten lowest ^1P resonances.

Table: 3

N π/π	E_r , eV	Γ_r , eV	1s ϵ d	2s ϵ d	2p ϵ p	2p ϵ f
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
6	71.91431	0.02680	0.00111	0.00740	0.01595	0.00234
7	72.12195	0.02845	0.00445	0.01443	0.00679	0.00278
8	72.14948	0.06274	0.0000004	0.00327	0.05909	0.00038
9	72.18266	0.00749	0.0000003	0.00111	0.00631	0.00007
10	72.25821	0.04451	0.00032	0.00012	0.04336	0.00071

Positions, total and partial widths of ten lowest ^1D resonances.

Table: 4

N π/π	E _r , eV	Γ _r , eV	1sεf	2sεf	2pεd	2pεg
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
6	72.37193	0.01244	0.00001	0.00334	0.00594	0.00314
7	72.43971	0.00085	0.0000003	0.00075	0.000001	0.00011
8	72.44394	0.00182	0.0000006	0.00070	0.00066	0.00046
9	72.47220	0.00001	0.000003	0.00001	0.000001	10 ⁻⁸
10	72.59225	0.00862	0.00001	0.00168	0.00559	0.00134

Positions, total and partial widths of ten lowest ¹F resonances.

Conclusions

1. The method of interacting configurations in the complex number representation is formulated. The basis Fano's general assertions [13,14] and complex energies formalism of Siegert's [19] are used in the development of the method. The method is applied to the description of the total and partial differential oscillator's strengths of the transitions into the continuous spectrum in the problem of electron impact ionization of atoms. The method is formulated without any appealing to the particular form of inter-particle interaction operator. Therefore, this method may be applied to other problems, e. g., to the nuclear physics and quantum chromodynamics problems.

2. The choice of the helium atom ground state function is substantiated, its particular form is verified. The proof of necessity of using in calculations the multi-parametric class of Tweed's [3], Hylleraases [4], etc, wave functions is given.

3. The method of the wave function construction, which diagonalizes the state subset of the continuous spectrum of the considering system Hamiltonian in the wide energy range including single particle decay thresholds, is developed and realized.

4. The parametric expressions for GOS of transition into the continuous spectrum of an atom in the energy range above the threshold of the excited ion generation are found. Hence, the calculation of cross sections in the problem of electron impact ionization of atoms is essentially simplified. In particular, the dependence of resonance parameters from the transferred momentum in the spectra of losses are analyzed.

5. The method of interacting configurations in the complex number/energy representation has a high precision in the problem of determination of positions and widths of AIS in the processes of ionization of the atoms by photons, electrons and other particles. Nevertheless, the precision of the calculations depends on the choice of the wave function of the ground state of the target. As the analyses of the results of

the calculations demonstrates the wave function of the ground state of the target should reproduce with the high precision the energy of the ground state of the target.

The method of interacting configurations in the complex number representation is the further development and generalization of the method of interacting configurations in the real number representation. The advantages of this method in comparison with hyperspherical coordinates (HSC), closed coupling approximation (CCA), R-matrix and some other methods are as follows. First it is the absence of difficulties with the identification of resonances (of AIS), further we may mark the possibility of finding here the widths of quasi-stationary states, which is a problematical task in such methods as HSC, CCA and others.

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