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SPECTROSCOPY OF THE COMPLEX AUTOIONIZATION RESONANCES IN SPECTRUM OF HELIUM: TEST AND NEW SPECTRAL DATA

We applied a generalized energy approach (Gell-Mann and Low S-matrix formalism) combined with the relativistic multi-quasiparticle (QP) perturbation theory (PT) with the Dirac-Kohn-Sham zeroth approximation and accounting for the exchange-correlation, relativistic corrections to studying autoionization resonances in the helium spectrum, in particular, we predicted the energies and widths of the number of the Rydberg resonances. There are presented the results of comparison of our theory data for the autoionization resonance 3s3p 1P0 with the available experimental data and those results of other theories, including, method of complex rotation by Ho, algebraic approach by Wakid-Callaway, diagonalization method by Senashenko-Wague etc.

1. Introduction

Here we continue our investigations of studying the autoionization state and AR in spectra of many electron complex atoms and ions. Let us note [1] that theoretical methods of calculation of the spectroscopic characteristics for heavy atoms and ions are usually divided into a few main groups [1-21]. At first, one should mention the well known, classical multi-configuration Hartree-Fock method (as a rule, the relativistic effects are taken into account in the Pauli approximation or Breit hamiltonian etc.) allowed to get a great number of the useful spectral information about light and not heavy atomic systems, but in fact it provides only qualitative description of spectra of the heavy atoms and ions. Another more consistent method is given by the known multi-configuration Dirac-Fock (MCDF) approach. In the MCDF calculations the one- and two-particle relativistic effects and important exchange-correlation corrections are usually taken into account practically, however the total accounting is not possible. In this essence it should be given special attention to very complex correlation effects, such as a continuum pressure and energy dependence of the inter electron interaction.

In this paper we applied a new relativistic approach [11-15] to relativistic studying the autoionization characteristics of the helium atom. The new elements of the approach include the combined the generalized energy approach and the gauge-invariant QED many-QP PT with the Dirac-Kohn-Sham (DKS) "0" approximation (optimized 1QP representation) and an accurate accounting for relativistic, correlation and others effects. The generalized gauge-invariant version of the energy approach has been further developed in Refs. [12,13]. Below we present new data on the energies and widths of the 2s,p, 3s,p ^{1}P, double excited AR for configurations ns^2 , np^2 , $3d^2\,{}^1$G, $4d^2\,{}^1$G, $5d^2\,{}^1$G, $4f^2\,{}^1$I , N snp $^{1,3}L^{\pi}$ and 3lnl′ $^{1,3}L^{\pi}$.

2. Relativistic approach in autoionization spectroscopy of heavy atoms

In refs. [11-15, 17-20] it has been in details presented, so here we give only the fundamental aspects. In relativistic case the Gell-Mann

and Low formula expressed an energy shift ΔE through the QED scattering matrix including the interaction with as the photon vacuum field as the laser field. The first case is corresponding to definition of the traditional radiative and autoionization characteristics of multielectron atom. The wave function zeroth basis is found from the Dirac-Kohn-Sham equation with a potential, which includes the ab initio (the optimized model potential or DF potentials, electric and polarization potentials of a nucleus; the Gaussian or Fermi forms of the charge distribution in a nucleus are usually used) [5]. Generally speaking, the majority of complex atomic systems possess a dense energy spectrum of interacting states with essentially relativistic properties. Further one should realize a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix *M* diagonalization [8-12]. The secular matrix elements are already complex in the second order of the PT. Their imaginary parts are connected with a decay possibility. A total energy shift of the state is presented in the standard form:

$$\Delta \mathrm{E} = \mathrm{Re}\,\Delta E + i\,\mathrm{Im}\,\Delta E \qquad \mathrm{Im}\,\Delta E = -\Gamma/2\,, \quad (1)$$

where Γ is interpreted as the level width, and the decay possibility $\mathrm{P} = \Gamma$. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to the calculation and diagonalization of the *M*. The *jj*-coupling scheme is usually used. The complex secular matrix *M* is represented in the form [9,10]:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)}. \qquad (2)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all order of PT, and $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ those of the one-, two- and three-QP diagrams respectively. $M^{(0)}$ is a real matrix, proportional to the unit matrix. It determines only the general level shift. We have assumed $M^{(0)} = 0$. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. For simple systems (such as alkali atoms and ions) the 1QP energies can be taken from the experiment. Substituting these quantities into (2) one could have summarized all the contributions of the 1QP diagrams of all orders of the formally exact QED PT. The optimized 1-QP representation is the best one to determine the zeroth approximation. In the second order, there is important kind of diagrams: the ladder ones. These contributions have been summarized by a modification of the central potential, which must now include the screening (anti-screening) effect of each particle by two others. The additional potential modifies the 1QP orbitals and energies. Let us remind that in the QED theory, the photon propagator D(12) plays the role of this interaction. Naturally, an analytical form of D depends on the gauge, in which the electrodynamic potentials are written. In general, the results of all approximate calculations depended on the gauge. Naturally the correct result must be gauge invariant. The gauge dependence of the amplitudes of the photoprocesses in the approximate calculations is a well known fact and is in details investigated by Grant, Armstrong, Aymar-Luc-Koenig, Glushkov-Ivanov [1,2,5,9]. Grant has investigated the gauge connection with the limiting non-relativistic form of the transition operator and has formulated the conditions for approximate functions of the states, in which the amplitudes are gauge invariant (so called Grant's theorem). These results remain true in an energy approach as the final formulae for the probabilities coincide in both approaches. In ref. [16] it has been developed a new version of the approach to conserve gauge invariance. Here we applied it to get the gauge-invariant procedure for generating the relativistic DKS orbital bases (abbreviator of our method: GIRPT).

A width of a state associated with the decay of the AR is determined by square of the matrix element of the interparticle interaction $\Gamma \infty |V(\beta_1\beta_2, \beta_3 k)|^2$. The total width is given by the expression:

$$\Gamma(n_1^0 j_1^0, n_2^0 j_2^0; J) = \frac{2\pi\varepsilon}{K_0} \sum_{\beta_1\beta_2} \sum_{\beta_1'\beta_2'} C^J(\beta_1\beta_2) \times$$

$$\times C^J(\beta_1'\beta_2') \sum_{\beta\,\beta_K} V_{\beta_1\beta_2;\beta\,\beta_K} V_{\beta_K\beta\,;\beta_1'\beta_2'} \qquad (3)$$

where the coefficients C can be determined bas follows:

$$C^J(\beta_1\beta_2) = C^J(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0)\times$$

$$\times A(j_1 m_1; j_2 m_2; JM) \tag{4a}$$

$$A(j_1 m_1, j_2 m_2 JM) = (-1)^{j_1 - j_2 + M}\begin{pmatrix} j_1 & j_2 & J \\ m_1 & m_2 & -M \end{pmatrix}\sqrt{2J+1} \tag{4b}$$

$$C^J(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0) = N(n_1^0 j_1^0, n_2^0 j_2^0)\times$$

$$\times[\delta(n_1^0 j_1^0 n_1 j_1)\delta(n_2^0 j_2^0 n_2 j_2) + \tag{4c}$$

$$+(-1)^{j_1+j_2+J+1}\delta(n_1^0 j_1^0 n_2 j_2)\delta(n_2^0 j_2^0 n_1 j_1)]$$

$$N(n_1^0 j_1^0; n_2^0 j_2^0) = \begin{cases} \frac{1}{\sqrt{2}} & n_1^0 j_1^0 = n_2^0 j_2^0 \\ 1 & n_1^0 j_1^0 \neq n_2^0 j_2^0 \end{cases} \tag{4d}$$

The matrix element of the relativistic interparticle interaction

$$V(r_i r_j) = exp(i\omega_{ij} r_{ij})\cdot(1-\alpha_i\alpha)/r_{ij} \tag{5}$$

(here α_1 –the Dirac matrices) in (3) is determined as follows:

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\times$$

$$\times(-1)^{j1+j2+j3+j4+m1+m2}\times$$

$$\times\sum_{a\mu}(-1)^{\mu}\begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix}\begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & \mu \end{pmatrix}\times \tag{6}$$

$$\times Q_a(n_1 l_1 j_1 n_2 l_2 j_2; n_4 l_4 j_4 n_3 l_3 j_3),$$

$$Q_a = Q_a^{\text{Qul}} + Q_a^{\text{B}}\ . \tag{7}$$

Here Q_a^{Qul} and Q_a^{B} is corresponding to the Coulomb and Breit parts of the interlparticle interaction (5). It is worth to remind that the real part of the interaction matrix element can be expanded in terms of Bessel functions [5,8]:

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}}\sum_{\lambda=0}(\lambda)J_{\lambda+1/2}(|\omega|r_<)\times$$

$$\times J_{-\lambda-1/2}(|\omega|r_>)P_\lambda(\cos\mathbf{r}_1\mathbf{r}_2) \tag{8}$$

The Coulomb part Q_λ^{Qul} is expressed in the radial integrals R_λ, angular coefficients S_λ as follows:

$$\text{Re}\,Q_\lambda^{\text{Qul}} \sim \text{Re}\{R_l(1243)S_\lambda(1243)+$$

$$+R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3})+$$

$$+R_\lambda(1\tilde{2}4\tilde{3})S_\lambda(1\tilde{2}4\tilde{3})+$$

$$+R_\lambda(\tilde{1}\tilde{2}4\tilde{3})S_\lambda(\tilde{1}\tilde{2}4\tilde{3})\} \tag{9}$$

where, for example, $\text{Re}Q_\lambda(1243)$ is as follows:

$$\text{Re}\,R_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) f_2(r_2)\times$$

$$\times f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>) \tag{10}$$

Here f is the large component of radial part of the 1QP state Dirac function and function Z is :

$$Z_\lambda^{(1)} = [2/|\omega_{13}|\alpha Z]^{\lambda+1/2} J_{\lambda+1/2}(\alpha|\omega_{13}|r)/[r^\lambda\Gamma(\lambda+3/2)] \tag{11}$$

The angular coefficient is defined by standard way as above [3]. The calculation of radial integrals $\mathbf{Re}R_\lambda(1243)$ is reduced to the solution of a system of differential equations:

$$\left.\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_3' &= [y_1 f_2 f_4 + y_2 f_1 f_3] Z_\lambda^{(2)}(\alpha|\omega|r) r^{1-\lambda}. \end{aligned}\right\} \tag{12}$$

In addition, $y_3(\infty)=\mathbf{Re}R_\lambda(1243)$, $y_1(\infty)=X_\lambda(13)$. The system of differential equations includes also equations for functions $f/r^{|æ|-1}$, $g/r^{|æ|-1}$, $Z_\lambda^{(1)}$, $Z_\lambda^{(2)}$. The formulas for the autoionization (Auger) decay probability include the radial integrals $R_\alpha(\alpha k\gamma\beta)$, where one of the functions describes electron in the continuum state. When calculating this inte-

gral, the correct normalization of the function ψ_k is a problem. The correctly normalized function should have the following asymptotic at $r \to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} sin(kr+\delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} cos(kr+\delta). \end{cases} \quad (13)$$

When integrating the master system, the function is calculated simultaneously:

$$N(r) = \left\{\pi\omega_k \left[f_k^2 \left[\omega_k + (\alpha Z)^{-2}\right] + g_k^2 \left[\omega_k + (\alpha Z^{-2})\right]\right]\right\}^{-1/2} \quad (14)$$

It can be shown that at $r \to \infty$, $N(r) \to N_k$, where N_k is the normalization of functions f_k, g_k of continuous spectrum satisfying the condition (9). Other details can be found in refs.[10-13,16-20] as well as description of the "Superatom" and Cowan PC codes, used in all computing.

3. Results and conclusions

In figure 1 there are presented the fragments of the He photoionization spectrum plus absorption (due to the data by NIST [22]). Spectral range includes the ARs, which are on average 35-40 eV above the first ionization potential (24.58eV).

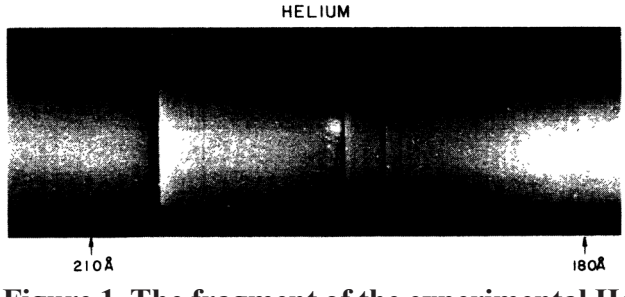

Figure 1. The fragment of the experimental He photoionization spectrum (210-180A)

One of the first members of the AR series is associated with the transition to double the permitted level excited 2s2p $^1P_1^0$. Generally there are identified two series of the resonances namely 2snp, 2pns, and both have a first member 2s2p and converge to 189.6A). In Table 1 we list the experimental data on energy and width (NBS, National Bureau of Standards) $^1P_0$, lying below the ionization threshold n=2, and theoretical results - one of the most accurate theory type Fano (Bhatia-Temkin: Th1) and our theory (Th2)[1,3], which shows the comparison is quite acceptable accuracy of our theory. Another important test of any theory - calculation parameters AS 3s3p $^1P_0$.

Table 1

The energy and width of the AR He $^1P_0$ (see text)

	Th.1	Th.2 (our data)	Exp. (NBS, NIST)
E	60.1444	60.1392	60.133±0.015 60.151±0.0103
Γ	0.0369	0.0374	0.038±0.004 0.038±0.002

In the Tables 2 and 3 we present the comparison of our data for the AR 3s3p $^1P_0$ with those of other theories, including, method of complex rotation by Ho, algebraic approach by Wakid-Callaway, diagonalization method by Senashenko-Wague, relativistic Hartree-Fock (RHF) methid by Nicolaides-Komninos, R-matrix method by Hayes-Scott, method of the adiabatic potential curves by Koyoma-Takafuji-Matsuzawa and Sadeghpour, L^2 technique with the Sturm decomposition by Broad- Gershacher and Moccia-Spizzo, the Feshbach method by Wu-Xi) and data measurements in laboratories: NIST (NBS; 2SO-MeV electron synchrotron storage ring (SURF-II)), Wisconsin Laboratory (Wisconsin Tantalus storage ring), Stanford Synchrotron Radiation Laboratory (SSRL), Berlin electron storage ring (BESSY), Daresbury Synchrotron Radiation Source (DSRS) [1,3,5,22-24].

On the one hand, there is sufficiently good accuracy of our theory, the secondly (bearing in mind that most of the listed methods are developed specifically for the study helium and can not be easily generalized to the case of the heavy multi-electron atoms) the definite advantage of the presented approach. Note that during translation for the units "Ry-eV" there was used the He ground-state energy value: E=- 5.80744875 Ry and the reduced Rydberg constant 1Ry = 13.603 876 eV.

Table 2a

Theoretical data for energy of the AR 3s3p $^1P_0$ (our data with those of other theories)

Method	Authors	E_r (Ry)
PT-REA	Our theory	-0.668802
Complex-rotation	Ho	-0.671252
Algebraic close coupling	Wakid-Callaway	-0.670
Diagonalization method	Senashenko-Wague	-0.6685
RHF	Nicolaides-Komninos	- 0.671388
R-matrix calculation	Hayes-Scott	-0.6707
Adiabatic potential curves	Koyoma etal	-0.6758
Adiabatic potential	Sadeghpour	-0.67558
L^2 tech.+Sturm	Broad-Gershacher	-0.67114
Feshbach method	Wu-Xi	-0.669 27
K-matrix L^2 basis-set	Moccia-Spizzo	-0.670 766

Table 2b

Theoretical data for width of the AR 3s3p $^1P_0$ (our data with with those of other theories)

Method	Authors	Γ/2 (Ry)
PT-REA	Our theory	0.006814
Complex-rotation	Ho	0.007024
Algebraic close coupling	Wakid-Callaway	0.00695
Diagonalization method	Senashenko-Wague	0.00548
RHF	Nicolaides-Komninos	-
R-matrix calculation	Hayes-Scott	0.00660
Adiabatic curves	Koyoma etal	-
Adiabatic potential	Sadeghpour	-
L^2 tech.+Sturm	Broad-Gershacher	0.00704
Feshbach method	Wu-Xi	0.00420
K-matrix L^2 basis-set	Moccia-Spizzo	0.00676

An interesting and valuable renewed data on Rydberg AR energies (in atomic units) of the double excited states $ns^2\ ^1S$ are listed in Table 4.

In whole an detailed analysis shows quite physically reasonable agreement between the presented theoretical and experimental results. But some difference, in our opinion, can be explained by different accuracy of estimates of the radial integrals, using the different type basis's (gauge invariance conservation or a degree of accounting for the exchange-correlation effects) and some other additional computing approximations.

Table 3

Theoretical and experimental data for energy and width of the AR 3s3p $^1P_0$ (our data with those of other best theories)

Method	E_r (eV)	Γ/2 (eV)
Theories		
Our data	69.9055	0.1854
Complex-rotation	69.8722	0.1911
MCHF	69.8703	-
R-matrix	69.8797	0.1796
Exp.		
NBS-I (1973)	69.919±0.007	0.132±0.014
Wisconsin(1982)	69.917±0.012	0.178±0.012
SSRL (1987)	69.917±0.012	0.178±0.012
BESSY (1988)	69.914±0.015	0.200±0.020
DSRS (2009)	69.880±0.022	0.180±0.015

Note: the He ground-state energy value: E=-5.80744875 Ry and the reduced Rydberg constant 1Ry = 13.603 876 eV.

Table 4

Predicted data for Rydberg AR energies (in atomic units) of the He double excited states $ns^2\ ^1S$ (our theory)

State	Energy	State	Energy
$6s^2$	0.08697	$10s^2$	0.03002
$7s^2$	0.06288	$11s^2$	0.02468
$8s^2$	0.04467	$12s^2$	0.01998
$9s^2$	0.03697	$13s^2$	0.01923
$14s^2$	0.01596	$18s^2$	0.00928
$15s^2$	0.01370	$19s^2$	0.00832
$16s^2$	0.01198	$20s^2$	0.00746
$17s^2$	0.01042	$21s^2$	0.00507

In our theory there are used gauge-optimized basis's of the relativistic and such basis has advantage in comparison with the standard DF type basis's.

In conclusion let us remind that in ref. [14] (see also [5,12]) it had been predicted a new optics and spectroscopy effect of the giant changing of the AS width in a sufficiently weak electric field (for two pairs of the Tm, Gd AR). Naturally any two states of different parity can be mixed by the external electric field. The mixing leads to redistribution of the autoionization widths. In a case of the heavy elements such as lanthanide and actinide atoms the respective redistribution has a giant effect. In the case of degenerate or near-degenerate resonances this effect becomes observable even at a moderately weak field.

We have tried to discover the same new spectral effect in a case of the He Rydberg autoionization states spectrum using the simplified version of the known strong-field operator PT formalism [5,14]. However, the preliminary estimates have indicated on the absence of the width giant broadening effect for the helium case, except for minor changes of the corresponding widths, which are well known in the standard atomic spectroscopy.

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Abstract.

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Key words: spectroscopy of autoionization resonances, relativistic energy approach, helium

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СПЕКТРОСКОПИЯ СЛОЖНЫХ АВТОИОНИЗАЦИОННЫХ РЕЗОНАНСОВ В СПЕКТРЕ ГЕЛИЯ: ТЕСТ И НОВЫЕ СПЕКТРАЛЬНЫЕ ДАННЫЕ

Резюме.

Обобщенный энергетический подход (S-матричный формализм Гелл-Мана и Лоу) и релятивистская теория возмущений с дирак-кон-шэмовским нулевым приближением и учетом обменно-корреляционных и релятивистских поправок применены к изучению автоионизационных резонансов в атоме гелия, в частности, предсказаны энергии и ширины ряда ридберговых резонансов. Представлены результаты сравнения данных нашей теории, в частности, для автоионизацийного резонанса 3s3p $^1P_0$ с имеющимися экспериментальными данными и результатами других теорий, в том числе, методом комплексного вращения Хо алгебраического подхода Wakid-Callaway, метода диагонализации Senashenko-Wague и т.д.

Ключевые слова: спектроскопия автоионизационных резонансов, релятивистский энергетический подход, гелий

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СПЕКТРОСКОПІЯ СКЛАДНИХ АВТОІОНІЗАЦІЙНИХ РЕЗОНАНСІВ В СПЕКТРІ ГЕЛІЮ: ТЕСТ І НОВІ СПЕКТРАЛЬНІ ДАНІ

Резюме.

Узагальнений енергетичний підхід (S-матричний формалізм Гелл-Мана та Лоу) и релятивістська теорія збурень з дірак-кон-шемівським нульовим наближенням та урахуванням обмінно-кореляційних і релятивістських поправок застосований до вивчення автоіонізаційних резонансів у атомі гелію, зокрема, передбачені енергії та ширини ряду рідбергових резонансів. Представлені результати порівняння даних нашої теорії, зокрема, для автоіонізаційного резонансу $3s3p\ ^1P_0$ з наявними експериментальними даними і результатами інших теорій, у тому числі, методом комплексного обертання Хо, алгебраїчного підходу Wakid-Callaway, методу діагоналізації Senashenko-Wague і т.д.

Ключові слова: спектроскопія автоіонізаційних резонансів, релятивістський енергетичний підхід, гелій