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RELATIVISTIC METHOD OF DESCRIPTION OF THE COMPLEX AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA: REVIEW OF METHOD AND NEW SPECTRAL DATA

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In the paper we give a review of a new 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 complex atomic spectra. As application, we list the energies and widths of the number of the Rydberg resonances in helium. There are presented the results of comparison of our theory data for some helium autoionization resonances 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. Besides, we present new data on the energies of the configurations 1s5s, 1s5p, 1s5d, 1s5f, 1s5g terms in the spectrum of the ion Kr XXXV, as well as the corresponding values of the lifetimes of these states, calculated on the basis of the relativistic energy approach

Keywords spectroscopy of autoionization resonances, relativistic energy approach, new spectral data

1. INTRODUCTION

In the last decade it is intensively developed spectroscopy of multiply charged ions covering UV and X-ray spectrum. Significant progress in experimental research methods, including a substantial increase in the intensity and quality of laser radiation, the use of accelerators, heavy ion collider, sources of synchrotron radiation and as a result, the possibility of more precise study of energy processes, stimulates further development of theory of heavy atoms and new theoretical methods of calculation of their characteristics, including radiation and autoionization widths [1-20]. It is known that autoionization states (AS) play a significant role in various elementary atomic processes such as autoionization, selective photoionization, electron scattering on atoms, the atom - and ion - atomic collisions, etc. The presence of AS of different ions significantly affect on the nature of high radiation spectrum of laboratory and astrophysical plasmas. Their radioactive decay is accompanied by the formation of the most complex spectra dielectronic satellites to the resonance lines of ions subsequent ionization multiplicity, which contain information on the state of plasma, used for its diagnosis and the study of physical conditions in the solar corona and other astrophysical objects.

There appear also new classes of problems such as the study of Bose condensate in the vapor of alkali atoms, "radiation" working substance in atomic Carnot machines, theory of the atomic clock, finally, a new physics Rydberg state of matter. Knowledge of the properties of the AS is also very important to understand the processes, e.g. in laser plasma. Their collapse can greatly affect on kinetics of population of the excited levels and emission intensity of spectral lines. Fundamentally new directions should be considered related to the study of dynamic of the AS collapse in external electromagnetic fields, especially high-intensive ones and the impact of the collision effects, for example, in a plasma medium.

In the paper we give a review of a new 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 complex atomic spectra, following to our papers [12-20]. As application, we list the energies and widths of the number of the Rydberg resonances in helium. There are presented the results of comparison of our theory data for some helium autoionization resonances 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. Besides, we present new data on the energies of the configurations 1s5s, 1s5p, 1s5d, 1s5f, 1s5g terms in the spectrum of the ion Kr XXXV, as well as the corresponding values of the lifetimes of these states, calculated on the basis of the relativistic energy approach

2. RELATIVISTIC APPROACH IN AUTOIONIZATION SPECTROSCOPY OF HEAVY ATOMS

In refs. [8-21] there are in details described all aspects of the method, so below we are shortly limited only by 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 [12]

$$\Delta E = Re\Delta E + iIm\Delta E \quad Im\Delta E = -\Gamma/2 \qquad (1)$$

where Γ is interpreted as the level width, and the decay possibility $P = \Gamma$. 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

$$\Gamma\left(n_1^0 j_1^0, n_2^0 j_2^0; J\right) = \frac{2\pi\varepsilon}{K_0}\sum_{\beta_1\beta_2}\sum_{\beta_1'\beta_2'} C^J\left(\beta_1\beta_2\right)\times$$
$$\times C^J(\beta_1'\beta_2')\sum_{\beta\beta_K} V_{\beta_1\beta_2;\beta\beta_K} V_{\beta_K\beta;\beta_1'\beta_2'} \qquad (3)$$

where the coefficients *C* can be determined as follows:

$$C^J\left(\beta_1\beta_2\right) = C^J\left(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0\right)\times$$
$$\times A\left(j_1 m_1; j_2 m_2; JM\right), \qquad (4a)$$

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

$$C^J\left(n_1 j_1 n_1^0 j_1^0; n_2 j_2 n_2^0 j_2^0\right) = N\left(n_1^0 j_1^0, n_2^0 j_2^0\right)\times$$
$$\times[\delta\left(n_1^0 j_1^0 n_1 j_1\right)\delta\left(n_2^0 j_2^0 n_2 j_2\right) + (-1)^{j_1 - j_2 + M}\times \qquad (4c)$$
$$\times\delta\left(n_1^0 j_1^0 n_2 j_2\right)\delta\left(n_2^0 j_2^0 n_1 j_1\right)],$$

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

The matrix element of the relativistic inter-particle interaction

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

Here α_i –the Dirac matrices in (3) is determined as follows:

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)}\times$$
$$\times\sum_{a\mu}(-1)^{\mu}\begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix}\begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & \mu \end{pmatrix}\times \qquad (6)$$
$$\times Q_a(n_1 l_1 j_1 n_2 l_2 j_2; n_4 l_4 j_4 n_3 l_3 j_3),$$

$$Q_a = Q_a^{Qul} + Q_a^{\mathrm{Br}} \tag{7}$$

Here Q_a^{Qul} and Q_a^{Br} is corresponding to the Coulomb and Breit parts of the interparticle 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]

$$\frac{\cos|\omega|r_{12}}{r_{12}} = \frac{\pi}{2\sqrt{r_1 r_2}} \sum_{\lambda=0} (\lambda) J_{\lambda+\frac{1}{2}}(|\omega| r_<) \times \\ \times J_{-\lambda-\frac{1}{2}}(|\omega| r_>) P_\lambda(cosr_1 r_2). \tag{8}$$

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

$$ReQ_\lambda^{Qul} \sim Re\{R_l(1243) S_\lambda(1243) + \\ + R_\lambda(\tilde{1}24\tilde{3}) S_\lambda(\tilde{1}24\tilde{3}) + \\ + R_\lambda(\tilde{1}\tilde{2}43) S_\lambda(\tilde{1}\tilde{2}43) + \\ + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\} \tag{9}$$

where, for example, ReQ_λ(1243) is as follows

$$ReR_\lambda(1243) = \iint dr_1 r_1^2 r_2^2 f_1(r_1) f_3(r_1) f_2(r_2) \times \\ \times f_4(r_2) Z_\lambda^{(1)}(r_<) Z_\lambda^{(1)}(r_>). \tag{10}$$

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

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

The angular coefficient is defined by standard way as above [3]. The calculation of radial integrals **Re**R_λ(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, $y_3(\infty)$=**Re**R_λ(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 integral, the correct normalization of the function Ψ_k is a problem. The correctly normalized function should have the following asymptotic at $r\to 0$

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

When integrating the master system, the function is calculated simultaneously

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

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 (24.58 eV) [18].

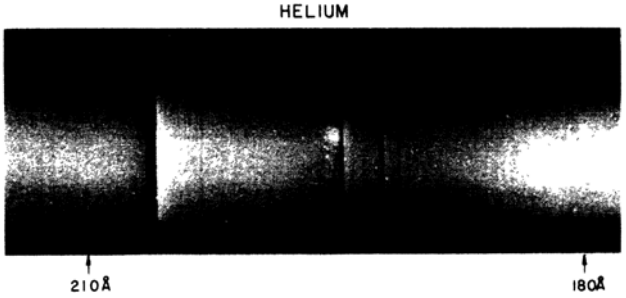

Fig. 1 - The fragment of the experimental He photoionization spectrum (210-180A).

In the Tables 1(a, b) and 2 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) [1,3,5,18,22-24].

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 = 13.603876 eV.

Table 1a - Theoretical data for energy of the AR 3s3p $^1P_0$ (our data with those of other theories [18])

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	- 0.67139
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	-0.66927
K-matrix L^2 basis-set	Moccia-Spizzo	-0.67077

Table 1b - Theoretical data for width of the AR 3s3p $^1P_0$ (our data 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	-
Feshbach method	Wu-Xi	0.00704
K-matrix L^2 basis-set	Moccia-Spizzo	0.00420 0.00676

Table 2 - 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		
REA-PT	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 = 13.603876 eV.

An interesting and valuable renewed data on Rydberg AR energies (in atomic units) of the double excited states are listed in Table 3 for He-like ion of the krypton.

In whole a 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 - Energies of the terms of configurations 1s5s, 1s5p, 1s5d, 1s5f, 1s5g in spectrum of the ion Kr XXXV, as well as the corresponding values of the lifetimes of these states (our theory)

Conf.	Term	Energy	τ(s)
1s5s	$^3S_1$	1221.43148	2.024–13
1s5p	$^3P_0$	1221.61042	8.469–14
1s5s	$^1S_0$	1221.62768	1.684–13
1s5p	$^3P_1$	1221.63328	2.981–14
1s5p	$^3P_2$	1221.93725	8.902–14
1s5d	$^3D_1$	1222.02199	4.456–14
1s5d	$^3D_2$	1222.03178	4.392–14
1s5p	$^1P_1$	1222.03285	1.048–14
1s5d	$^3D_3$	1222.12328	4.587–14
1s5d	$^1D_2$	1222.13420	4.462–14
1s5f	$^3F_2$	1222.13486	9.180–14
1s5f	$^3F_3$	1222.13462	9.186–14
1s5f	$^3F_4$	1222.18624	9.262–14
1s5f	$^1F_3$	1222.19322	9.265–14
1s5g	$^3G_3$	1222.19314	1.540–13
1s5g	$^3G_4$	1222.18708	1.541–13
1s5g	$^3G_5$	1222.21015	1.552–13
1s5g	$^1G_4$	1222.21160	1.549–13

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 [18] 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 [18] 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 final estimates have indicated on the absence of the width giant broadening effect for the helium case, except for the minor standard classical spectroscopic changes of the corresponding widths.

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РЕЛЯТИВИСТСКИЙ МЕТОД ОПИСАНИЯ СЛОЖНЫХ АВТОИОНИЗАЦИОННЫХ РЕЗОНАНСОВ В АТОМНЫХ СПЕКТРАХ: ОБЗОР МЕТОДА И НОВЫЕ СПЕКТРАЛЬНЫЕ ДАННЫЕ

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В работе представлен обзор обобщенного энергетического подхода (S-матричный формализм Гелл-Мана и Лоу) в комбинации с релятивистской теорией возмущений с дирак-кон-шэмовским нулевым приближением и учетом обменно-корреляционных и релятивистских поправок, применяемого к изучению автоионизационных резонансов в спектрах сложных атомов, в частности, приведены энергии и ширины ряда ридберговых резонансов. Представлены результаты сравнения данных нашей теории, в частности, для ряда автоионизационных резонансов в спектре гелия с имеющимися экспериментальными данными и результатами других теорий, в том числе, теории комплексного вращения Хо алгебраического подхода Wakid-Callaway, метода диагонализации Senashenko-Wague и т.д. Кроме того, мы представляем новые данные по энергиям термов конфигураций 1s5s, 1s5p, 1s5d, 1s5f, 1s5g в спектре иона Kr XXXV, а также соответствующих значений времени жизни этих состояний, вычисленные на основе релятивистского энергетического подхода.

Ключевые слова: спектроскопия автоионизационных резонансов, релятивистский энергетический подход, новые спектральные данные

РЕЛЯТИВІСТСЬКИЙ МЕТОД ОПИСУ СКЛАДНИХ АВТОІОНІЗАЦІОНИХ РЕЗОНАНСІВ В АТОМНИХ СПЕКТРАХ: ОГЛЯД МЕТОДУ І НОВІ СПЕКТРАЛЬНІ ДАНІ

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В роботі наведено огляд узагальненого енергетичного підходу (S-матричний формалізм Гелл-Мана та Лоу) в комбінації із релятивістською теорією збурень з дірак-кон-шемівським нульовим наближенням та урахуванням обмінно-кореляційних і релятивістських поправок, застосованого до вивчення автоіонізаційних резонансів у спектрах складних атомів, зокрема, наведені енергії та ширини ряду рідбергових резонансів. Представлені результати порівняння даних нашої теорії, зокрема, для ряду автоіонізаційних резонансів в спектрі атому гелію з наявними експериментальними даними і результатами інших теорій, у тому числі, теорії комплексного обертання Хо, алгебраїчного підходу W-akid-Callaway, методу діагоналізації Senashenko-Wague і т.д. Крім того, представлені нові дані по енергіях термів конфігурацій 1s5s, 1s5p, 1s5d, 1s5f, 1s5g в спектрі іону Kr XXXV, а також відповідні значення часу життя для цих станів, обчислені на основі релятивістського енергетичного підходу.

Ключові слова: спектроскопія автоіонізаційних резонансів, релятивістський енергетичний підхід, нові спектральні дані

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