UDC 539.182

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# ADVANCED RELATIVISTIC APPROACH IN SPECTROSCOPY OF COMPLEX AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA

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

The knowledge of autoionization states properties of atomic systems is of a great importance note for many applications in atomic and molecular physics, plasma chemistry and physics, laser physics and quantum electronics etc. [1-52]. In this paper, which goes on our studying autoionization phenomena in different atomic systems, we present an advanced new relativistic approach [11-15] to relativistic calculating autoionization resonances (AR) characteristics of the helium atom. The new elements of the approach include the combined the generalized energy approach and the gauge-invariant relativistic many-body perturbation theory (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].

## 2. Relativistic perturbation theory approach in spectroscopy of autoionization states

In refs. [11-15, 17-20] the fundamentals of the relativistic many-body PT formalism have been in details presented, so further we are limited only by the novel elements. Let us remind that the majority of complex atomic systems possess a dense energy spectrum of interacting states. In refs. [11-15, 17-20] it is realized a field procedure for calculating the energy shifts ΔE of degenerate states, which is connected with the secular matrix *M* diagonalization [8-12]. 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 complex secular matrix *M* is represented in the form [9,10]:

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

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. The diagonal matrix $M^{(1)}$ can be presented as a sum of the independent 1QP contributions. 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.

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:

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

$$\times C^J(\beta_1'\beta_2') \sum_{\beta\ \beta_K} V_{\beta_1\beta_2;\beta\ \beta_K} V_{\beta_K\beta\ ;\beta_1'\beta_2'} \qquad (2)$$

where the coefficients C are in details described, for example, in Refs. [1-5]. The matrix element of the relativistic inter-particle interaction

$$V(r_i r_j) = exp(i\omega_j r_j) \cdot (1 - \alpha_i \alpha_i) / r_j \qquad (3)$$

(here $\alpha_I$ –the Dirac matrices) in (3) is determined as follows:

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

$$\times (-1)^{j1+j2+j3+j4+m1+m2} \times \qquad (4)$$

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

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

$$Q_a = Q_a^{\mathrm{Qul}} + Q_a^{\mathrm{B}} \ . \qquad (5)$$

Here $Q_a^{\mathrm{Qul}}$ and $Q_a^{\mathrm{B}}$ is corresponding to the Coulomb and Breit parts of the interparticle interaction (5). The calculating of all matrix elements, wave functions, Bessel functions etc is reduced to solving the system of differential equations. 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 wave functions is very important, namely, they should have the following asymptotic at $r \to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{-1/2} sin(kr + \delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{-1/2} cos(kr + \delta). \end{cases} \qquad (6)$$

The important aspect of the whole procedure is an accurate accounting for the exchange-correlation effects. We have used the generalized relativistic Kohn-Sham density functional [33-35] in the zeroth approximation of relativistic PT; naturally, the perturbation operator contents the operator (3) minus the cited Kohn-Sham density functional. Further the wave functions are corrected by accounting of the first order PT contribution. Besides, we realize the procedure of optimization of relativistic orbitals base. The main idea is based on using ab initio optimization procedure, which is reduced to minimization of the gauge dependent multielectron contribution $Im\delta E_{ninv}$ of the lowest QED PT corrections to the radiation widths of atomic levels. According to [35-37], "in the fourth order of QED PT (the second order of the atomic PT) there appear the diagrams, whose contribution to the $Im\delta E_{ninv}$ accounts for correlation effects and this contribution is determined by the electromagnetic potential gauge (the gauge dependent contribution)". The accurate procedure for minimization of the functional $Im\delta E_{ninv}$ leads to the Dirac-Kohn-Sham-like equations for the electron density that are numerically solved by the Runge-Cutta standard method It is very important to known that the regular realization of the total scheme allow to get an optimal set of the 1QP functions and more correct results in comparison with so called simplified one, which has been used in Refs. [34-34] and reduced to the functional minimization using the variation of the correlation potential parameter *b*. Other details can be found in refs.[10-13,16-20,41-74] as well as description of the "Superatom" and Cowan PC codes, used in all computing.

**3. Results and conclusion**

In the Table 1 we present the comparison of our advanced 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 Senashen-

ko-Wague, relativistic Hartree-Fock (RHF) method 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].

Table 1a

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

| Method/Data | Er (eB) | Γ/2 (eB) |
|---|---|---|
| Our | 69.9113 | 0.1912 |
| ACC | 69.8892 | 0.1891 |
| Diagon. method | 69.9096 | 0.1491 |
| RHF | 69.8703 | - |
| APC1 | 69.8103 | - |
| $L^2$ tech. | 69.8737 | 0.1915 |
| Feshbach th. | 69.8991 | 0.1143 |
| K-matrix $L^2$ | 69.8788 | 0.1839 |
| PT- Svin | 69.9055 | 0.1854 |
| CR method | 69.8722 | 0.1911 |
| MC HF | 69.8703 | - |
| R-matrix | 69.8797 | 0.1796 |
| E:Wisconsin | 69.917±0.012 | 0.178±0.012 |
| E: SSRL-1987 | 69.917±0.012 | 0.178±0.012 |
| E: BESSY | 69.914±0.015 | 0.200±0.020 |
| E: DSRS | 69.880±0.022 | 0.180±0.015 |

Note: ACC- Algebraic close coupling; APC - Adiabatic potential curves; CR method-method of complex rotation; DM method – Diagonalization method

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. In Table 2 we present the resonance energies and widths for the 2p3s,2p3p resonances in the beryllium spectrum.

Table 2

**The energy position E, width Γof the Be 2p3s, 2p3p resonances (see text)**

| nl | Exp, WLB | Exp, (EMR) (ME) | Th, TSB | Th, CHC | Th, KTZM | Our data |
|---|---|---|---|---|---|---|
| 3s | 10.889 | 10.93<br>10.71 | 10.915 | 10.63 | 10.910 | 10.903 |
| 3p | 531(10) | - | 606 | - | 473 | 478 |

The experimental (by Wehlitz-Lukic-Bluett, WLB; by Mehlman-Balloffet-Esteva, ME; by Esteva-Mehlman-Balloffet-Romand, EMR) and alternative theoretical data by Chi-Huang- Cheng (CHC), Tully-Seaton-Berrington (TSB) and by Kim- Tayal-Zhou-Manson (KTZM) are taken from Ref. [4].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 (different degree of the gauge invariance performance), degree of accounting for the exchange-correlation effects and some other additional computing approximations.

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UDC 539.183

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## ADVANCED RELATIVISTIC APPROACH IN SPECTROSCOPY OF COMPLEX AUTOIONIZATION RESONANCES IN ATOMIC SPECTRA

**Abstract**

We present an advanced relativistic approach to to studying autoionization resonances parameters in the atomic systems, which is based on an generalized energy approach (Gell-Mann and Low S-matrix formalism) combined with the relativistic multi-quasiparticle perturbation theory with the Dirac-Kohn-Sham zeroth approximation and accurate accounting for the exchange-correlation, relativistic corrections. The optimization of relativistic orbitals base is reduced to minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels, which in their turn leads to the Dirac-Kohn-Sham-like equations for the electron

density. As illustration of an advanced approach application there are presented the results on energy and width for the autoionization resonance 3s3p $^1P_0$ in helium He atom spectrum, namely, 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.

**Key words:** spectroscopy of autoionization resonances, advanced relativistic approach, helium

УДК 539.183

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## УСОВЕРШЕНСТВОВАННЫЙ РЕЛЯТИВИСТСКИЙ ПОДХОД В СПЕКТРОСКОПИИ СЛОЖНЫХ АВТОИОНИЗАЦИОННЫХ РЕЗОНАНСОВ В АТОМНЫХ СПЕКТРАХ

**Резюме**

В работе развивается усовершенствованный релятивистский подход к изучению параметров автоионизационных резонансов в атомных системах, который основывается на обобщенном энергетическом подходе (S-матричный формализм Гелл-Манна и Лоу) и релятивистской многочастичной теорией возмущений с нулевым приближением Дирака-Кона-Шэма и аккуратным учетом обменно-корреляционных, релятивистских эффектов. Оптимизация базиса релятивистских орбиталей сводится к минимизации калибровочно-зависимого многоэлектронного вклада от обменно-корреляционных поправок КЭД теории возмущений в радиационные ширины атомных уровней, что в свою очередь, сводится к решению системы уравнений типа Дирака-Кона-Шэма для электронной плотности. В качестве иллюстрации возможностей предлагаемого подхода приведены данные по энергии и ширине автоионизационного резонанса 3s3p $^1P_0$ в спектре атома гелия и проведено сравнение 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, усовершенствованный релятивистский подход, гелий

УДК 539.183

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## УДОСКОНАЛЕНИЙ РЕЛЯТИВІСТСЬКИЙ ПІДХІД В СПЕКТРОСКОПІЇ СКЛАДНИХ АВТОІОНІЗАЦІЙНИХ РЕЗОНАНСІВ В АТОМНИХ СПЕКТРАХ

**Резюме**

В роботі розвивається вдосконалений релятивістський підхід до вивчення параметрів автоіонізаціонних резонансів в атомних системах, який ґрунтується на узагальненому енергетичному підході (S-матричний формалізм Гелл-Манна і Лоу) і релятивістської багаточастинковій теорії

збурень з нульовим наближенням Дірака-Кона-Шема і акуратним урахуванням обмінно- кореляційних, релятивістських ефектів. Оптимізація базису релятивістських орбіталей зводиться до мінімізації калібрувально-залежного багатоелектронного вкладу від обмінно-кореляційних поправок КЕД теорії збурень в радіаційні ширини атомних рівнів, що в свою чергу, зводиться до вирішення системи рівнянь типу Дірака-Кона-Шема для електронної густини. В якості ілюстрації можливостей запропонованого підходу наведені дані по енергії і ширині автоіонізаційного резонансу $3s3p\ ^1P_0$ в спектрі атома гелію і проведено порівняння з наявними експериментальними даними і результатами інших теорій, в тому числі, методом комплексного обертання Хо, алгебраїчного підходу Wakid-Callaway, методу діагоналізації Senashenko-Wague і т.і.

**Ключові слова:** спектроскопія автоіонізаційних резонансів, удосконалений релятивістський підхід, гелій