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SPECTROSCOPY OF THE COMPLEX AUTOIONIZATION RESONANCES IN SPECTRUM OF BERYLLIUM

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 beryllium Be spectrum, in particular, we predicted the energies and widths of the number of the 2pns resonances. There are presented the results of comparison of our theory data for the autoionization resonances 2pnl with the available experimental data and those results of other theories, including, methods by Greene, by Tully-Seaton-Berrington and by Kim-Tayal-Zhou-Manson etc.

1. Introduction

Here we continue our investigations of studying the autoionization state and AR in spectra of a few electron complex atoms and ions. Let us note [1-5] that theoretical methods of calculation of the spectroscopic characteristics for heavy atoms and ions are usually divided into a few main groups [1-21]. Let us remind 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. Besides, different methods such as various forms of the *R*-matrix method, the multiconfiguration Tamm-Dancoff approximation, the hyperspherical method, a hyperspherical close-coupling calculation, and a multiconfiguration relativistic random-phase approximation have been employed [3].

In this paper we applied a new relativistic approach [11-15] to relativistic studying the autoionization characteristics of the beryllium atom. The method wich has been used is in details presented in our prwvius papers (see, for example, [4]). LHere we remind that 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].

2. Relativistic approach in autoionization spectroscopy of beryllium atom

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 character-

istics of multielectron atom. The wave function zeroth basis is found from the Dirac equation with a potential, which includes the ab initio (the optimized model potential or DF potentials, electric and polarization potentials of a nucleus) [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:

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

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 complex secular matrix *M* is represented in the form [9,10]:

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

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. 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 studied 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:

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

where the coefficients C are determined in [4].

The matrix element of the relativistic interparticle interaction

$$V(r_i r_j) = exp(i\omega_{ij} r_{ij}) \cdot (1 - \alpha_i \alpha)/r_{ij} \tag{4}$$

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

$$V_{\beta_1\beta_2;\beta_4\beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \times$$
$$\times (-1)^{j1+j2+j3+j4+m1+m2} \times$$
$$\times \sum_{a\mu} (-1)^{\mu} \begin{pmatrix} j_1 & j_3 & a \\ m_1 & -m_3 & \mu \end{pmatrix} \begin{pmatrix} j_2 & j_4 & a \\ m_2 & -m_4 & \mu \end{pmatrix} \times \tag{5}$$
$$\times Q_a(n_1 l_1 j_1 n_2 l_2 j_2; n_4 l_4 j_4 n_3 l_3 j_3),$$

$$Q_a = Q_a^{\mathrm{Qul}} + Q_a^{\mathrm{B}} \quad . \tag{6}$$

Here Q_a^{Qul} and Q_a^{B} is corresponding to the Coulomb and Breit parts of the interlparticle interaction (6). The Coulomb part Q_λ^{Qul} is expressed in the radial integrals R_λ, angular coefficients S_λ as follows:

$$\begin{aligned} Q_\lambda^{\mathrm{Qul}} \sim \{ & R_l(1243) S_\lambda(1243) + \\ & + R_\lambda(\tilde{1}24\tilde{3}) S_\lambda(\tilde{1}24\tilde{3}) + \\ & + R_\lambda(\tilde{1}\tilde{2}\tilde{4}3) S_\lambda(\tilde{1}\tilde{2}\tilde{4}3) + \\ & + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3}) \} \end{aligned} \tag{7}$$

The calculation of radial integrals $\mathbf{Re}R_\lambda(1243)$ is reduced to the solution of a system of differential equations:

$$\left.\begin{aligned} y_1' &= f_1 f_3 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_2' &= f_2 f_4 Z_\lambda^{(1)}(\alpha|\omega|r) r^{2+\lambda}, \\ y_3' &= [y_1 f_2 f_4 + y_2 f_1 f_3] Z_\lambda^{(2)}(\alpha|\omega|r) r^{1-\lambda}. \end{aligned}\right\} \tag{8}$$

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 integral, the correct normalization of the function Ψ_k requires the attention. The correctly normalized function should have the following asymptotic at $r \to 0$:

$$\left.\begin{matrix} f \\ g \end{matrix}\right\} \to (\lambda\omega)^{-1/2} \begin{cases} \left[\omega + (\alpha Z)^{-2}\right]^{1/2} \sin(kr+\delta), \\ \left[\omega - (\alpha Z)^{-2}\right]^{1/2} \cos(kr+\delta). \end{cases} \tag{9}$$

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

$$N(r) = \left\{ \pi\omega_k \left[f_k^2 \left[\omega_k + (\alpha Z)^{-2} \right] + g_k^2 \left[\omega_k + (\alpha Z^{-2}) \right] \right] \right\}^{1/2} \tag{10}$$

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 Be+ ion-yield scan across the 2*pns* and 2*pnd* resonances (circles connected by a black line) and a least-squares fit curve of Fano profiles (gray curve) [3]. In Fig.2 there are presented The Be+ ion-yield scan across the 2*pns* and 2*pnd* resonances (solid line) together with calculated cross sections by Green (dash-dotted line), by Tully-Seaton-Berrington (gray solid line), and by Kim- Tayal-Zhou-Manson (dotted line). The experimental data [3] were scaled to match the theoretical cross section (from Ref.[3]).

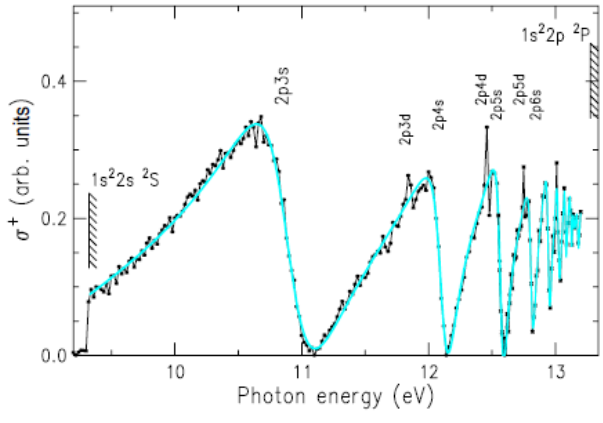

Figure 1. Be+ ion-yield scan across the 2pns and 2pnd resonances (circles connected by a black line) and a least-squares fit curve of Fano profiles (gray curve) [3]

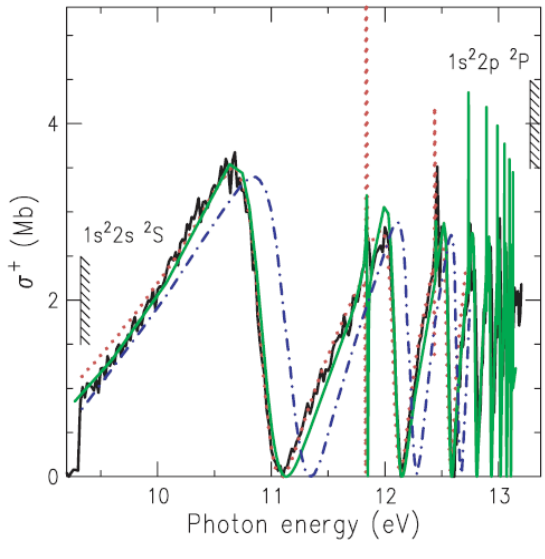

Figure 2. The Be+ ion-yield scan across the 2pns and 2pnd resonances (solid line) together with calculated cross sections by Green (dash-dotted line), by Tully-Seaton-Berrington (gray solid line), and by Kim- Tayal-Zhou-Manson (dotted line). The experimental data [3] were scaled to match the theoretical cross section.

In Tables 1 we present the resonance energies and widths for the 2pns resonances in the beryllium spectrum. 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. [3].

Table 1a.

The energy position E, width Γof the Be 2pns resonances (see text)

The energy position E (eV)						
n	Exp, WLB	Exp, (EMR) (ME)	Th, (TSB)	Th, (CHC)	Th, KTZM	Our data
3	10.889	10.933 10.71	10.915	10.63	10.910	10.903
4	12.112	12.096 11.97	12.102	12.09	12.092	12.098
5	12.571	12.572 12.53	12.571	12.64	12.558	12.570
6	12.812	12.811 12.78	12.800	12.91	12.791	12.806
7	12.944	12.945 12.92	12.932	13.06	12.924	12.952
8	13.022	13.029 13.01	-	13.15	13.007	13.028
9	13.078	13.083	-	13.21	13.062	13.092
10	13.123	13.121	-	13.25	13.101	13.130
11	13.143	13.152	-	-	13.129	13.152
12	13.178	13.170	-	-	-	13.180
13	-	-	-	-	-	13.213
14	-	-	-	-	-	13.248

Table 1b.

The energy position E, width Γof the Be 2pns resonances (see text)

The width Γof the resonance (meV)					
n	Exp, WLB	Th, (TSB)	Th, Green	Th, KTZM	Our data
3	531. (10)	606	530	473	473
4	174. (10)	180	168	162	176
5	77.(10)	78	76	73	78
6	47.(3)	42	-	-	51
7	29.(3)	22	-	-	33
8	16.(3)	-	-	-	18
9	3(5)	-	-	-	5
10	3(5)	-	-	-	4
11		-	-	-	4
12		-	-	-	3

In the Table 2 we present the comparison of our data on the the resonance energies and widths for the AR 2pnd resonances in the beryllium spectrum.

Table 2.

Theoretical data for positions (eV) of the Be 2pnd resonances compared to previously published resonance positions (see text)

The energy position E (eV)						
n	Exp, WLB	Exp, (EMR) (ME)	Th, (TSB)	Th, (CHC)	Th, KTZM	Our data
3	11.840 (6)	11.855 11.862	11.840	12.03	12.831	11.848
4	12.460 (6)	12.503 12.466	12.448	12.61	12.437	12.458
5	12.742 (6)	12.789 12.757	12.735	12.89	12.727	12.746
6	-	12.952 12.919	12.893	13.05	12.886	12.908
7	-	-	-	-	-	13.092
8	-	-	-	-	-	13.262

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. Let us note 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 Be 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. 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. 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.

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Abstract

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 beryllium Be 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 $3s3p\ ^1P_0$ with the available experimental data and those results of other theories, including, method Greene, by Tully-Seaton-Berrington and by Kim- Tayal-Zhou-Manson etc

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

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СПЕКТРОСКОПИЯ СЛОЖНЫХ АВТОИОНИЗАЦИОННЫХ РЕЗОНАНСОВ В СПЕКТРЕ БЕРИЛЛИЯ

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 бериллия, в частности, предсказаны энергии и ширины ряда ридберговых резонансов. Представлены результаты сравнения данных нашей теории, в частности, для автоионизацийного резонанса 2pnl с имеющимися экспериментальными данными и результатами других теорий, в том числе, теорий Greene, Tully-Seaton-Berrington, Kim-Tayal-Zhou-Manson и т.д.

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

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СПЕКТРОСКОПІЯ СКЛАДНИХ АВТОІОНІЗАЦІЙНИХ РЕЗОНАНСІВ В СПЕКТРІ БЕРИЛІЮ

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 берилію, зокрема, передбачені енергії та ширини ряду рідбергових резонансів. Представлені результати порівняння даних нашої теорії, зокрема, для автоіонізаційного резонансу 2pnl з наявними експериментальними даними і результатами інших теорій, у тому числі, теорій Greene, Tully-Seaton-Berrington, Kim-Tayal-Zhou-Manson і т.д.

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