ОПТИЧНІ, ОПТОЕЛЕКТРОННІ І РАДІАЦІЙНІ СЕНСОРИ

OPTICAL AND OPTOELECTRONIC AND RADIATION SENSORS

PACS 31.15.A-; UDC 539.184
DOI http://dx.doi.org/10.18524/1815-7459.2018.4.150501

OPTIMIZED RELATIVISTIC OPERATOR PERTURBATION THEORY IN SPECTROSCOPY OF MULTIELECTRON ATOM IN AN ELECTROMAGNETIC FIELD: SENSING SPECTRAL PARAMETERS

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OPTIMIZED RELATIVISTIC OPERATOR PERTURBATION THEORY IN SPECTROSCOPY OF MULTIELECTRON ATOM IN A DC ELECTRIC FIELD: SENSING SPECTRAL PARAMETERS

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Abstract. It is developed the optimized version of relativistic operator perturbation theory approach to calculation of the Stark resonances energies characteristics (energies and widths) for the multielectron atomic systems in an electromagnetic field. A new approach allows to perform an accurate, consistent treatment of a strong field DC(AC) Stark effect and includes the physically reasonable distorted-waves approximation in the frame of the formally exact relativistic quantum-mechanical procedure. As illustration, some test data for the Stark resonances energies and widths

in the heavy multielectron atoms (caesium, francium) are presented and compared with results of calculations within the alternative consistent sophisticated methods etc.

Keywords: multielectron atom in an electromagnetic field – modified relativistic operator perturbation theory – Stark resonances

ОПТИМІЗОВАНА РЕЛЯТИВІСТСЬКА ОПЕРАТОРНА ТЕОРІЯ ЗБУРЕНЬ В СПЕКТРОСКОПІЇ БАГАТОЕЛЕКТРОННОГО АТОМУ В ЕЛЕКТРОМАГНІТНОМУ ПОЛІ: ДЕТЕКТУВАННЯ СПЕКТРАЛЬНИХ ПАРАМЕТРІВ

Г. О. Кузнецова, А. В. Глушков, М. Ю. Гурська, А. А. Буяджи, В. Б. Терновський

Анотація. Розроблена оптимізована версія нового методу релятивістської операторної теорії збурень з метою обчислення характеристик штарківських резонансів (енергії і ширини) для багатоелектронних атомних систем в електромагнітному полі. Новий підхід дозволяє виконати кількісно прецизійний і теоретично послідовний опис сильно-польового (DC, AC) ефекту Штарка і включає в себе фізично обґрунтоване наближення перекручених хвиль в рамках формально точної релятивістської квантово-механічної процедури. В якості ілюстрації представлені деякі тестові дані для енергій і ширини штарківських резонансів у важких багатоелектронних атомах (цезій, францій), які порівнюються з результатами розрахунків в рамках альтернативних послідовних методів.

Ключові слова: багатоелектронний атом в електромагнітному полі - модифікована релятивістська операторна теорія збурень - штарківські резонанси

ОПТИМИЗИРОВАННАЯ РЕЛЯТИВИСТСКАЯ ОПЕРАТОРНАЯ ТЕОРИЯ ВОЗМУЩЕНИЙ В СПЕКТРОСКОПИИ МНОГОЭЛЕКТРОННОГО АТОМА В ЭЛЕКТРОМАГНИТНОМ ПОЛЕ: ДЕТЕКТИРОВАНИЕ СПЕКТРАЛЬНЫХ ПАРАМЕТРОВ

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Аннотация. Разработана оптимизированная версия нового метода релятивистской операторной теории возмущений с целью вычисления характеристик энергий штарковских резонансов (энергии и ширины) для многоэлектронных атомных систем в электромагнитном поле. Новый подход позволяет выполнить количественно прецизионное и теоретически последовательное описание сильнополевого (DC, AC) эффекта Штарка и включает в себя физически обоснованное приближение искаженных волн в рамках формально точной релятивистской квантово-механической процедуры. В качестве иллюстрации представлены некоторые тестовые данные для энергий и ширины штарковских резонансов в тяжелых многоэлектронных атомах (цезий, франций), которые сравниваются с результатами расчетов в рамках альтернативных последовательных методов.

Ключевые слова: многоэлектронный атом в электромагнитном поле - модифицированная релятивистская операторная теория возмущений - штарковские резонансы

1. Introduction

Studying optical and spectral, radiative and autoionization characteristics of the multielectron atomic systems in a electromagnetic fields is traditionally of a great importance and actuality for further development quantum optics and atomic spectroscopy, quantum and nano-and sensor electronics and different applications in the plasma chemistry, astrophysics, laser physics etc. (see Refs. [1–17]). The calculational difficulties of the standard theoretical quantum mechanical approaches to the multielectron atoms in a strong electromagnetic (electric) field are well known. Here one should remember about such phenomenon as the well-known Dyson one for a strong field AC, DC Stark effect. Besides, in contrast to the hydrogen atom, the non-relativistic Schrödinger and relativistic Dirac equations for an electron moving in the field of the atomic core in many-electron atom and a uniform external electric field does not allow separation of variables in the parabolic coordinates. The known quasiclassical (WKB) approximation overcomes these difficulties for the states lying far from the " new continuum" boundary. The detailed review of a modern states of art for spectroscopy of multielectron atoms in an electric (laser) field is presented in Refs. [16-19].

In this paper we present the theoretical basis of the optimized version of relativistic operator perturbation theory (ROPT) approach to calculation of the Stark resonances energies characteristics (energies and widths) for the multielectron atomic systems in an electromagnetic field. A new approach allows to perform an accurate, consistent treatment of a strong field DC(AC) Stark effect and includes the physically reasonable distorted-waves approximation in the frame of the formally exact relativistic quantum-mechanical procedure. The relativistic density-functional approximation with the Kohn-Sham potential is taken as the zeroth approximation in the relativistic many-body perturbation theory (RMBPT) formalism. There have taken into account all exchange-correlation corrections of the second order and dominated classes of the higher orders diagrams (polarization interaction, quasiparticles screening, etc.). New form of the multi-electron polarization functional has been used. As illustration of application of the presented formalism, new data on the energy and spectral parameters for heavy alkali atoms in an electric (electromagnetic) field are presented.

2. Relativistic operator and many-body perturbation theory for multielectron atoms in an electromagnetic field

Here we present a new relativistic quantum approach to modelling the chaotic dynamics of atomic systems in a dc electric and ac electromagnetic fields, based on the theory of quasi-stationary quasi-energy states, optimized operator perturbation theory, method of model-potential, a complex rotation coordinates algorithm method [16,17]. The universal chaos-geometric block will be used further to treat the chaotic ionization characteristics for a number of heavy atomic systems.

Let us remind that in the case of the electromagnetic field atomic Hamiltonian is usually as follows:

$$H = \frac{1}{2} p^2 + V_{at}(r) + zF_0 \cos(\omega t). \qquad (1)$$

The field is periodic, of course one should use the Floquet theorem; then the eigen-Floquet states $|\Psi_{E_j}(r,t)>$ and quasi-energies E_j are defined as the eigen-functions and eigen-values of the Floquet Hamiltonian $H_F = H - i\partial_t$. In the general form with using the method of complex coordinates the problem reduces to the solution of stationary Schrödinger equation, which is as follows in the model potential approximation:

$$(-1/2 \cdot \nabla^2 + V_{at}(r) + \omega L_z + F_o z)\Psi_E(r) = E\Psi_E(r), \qquad (2)$$

i.e. to the stationary eigen-values and eigen-vectors task for some matrix A (with the consideration of several Floquet zones): $(A - E_j B)|E_j>=0$. As a decomposition basis, system of the Sturm functions of the operator perturbation theory basis is used. In relativistic theory one should start from the Dirac Hamiltonian (in relativistic units):

$$H = \alpha p + \beta - \alpha Z / r_i + \sqrt{\alpha} Fz. \qquad (3)$$

Here a field strength intensity is expressed in the relativistic units (F_{rel}= $a^{5/2}F_{at.un.}$; a is the fine structure constant). One could see that a relativistic wave function in the Hilbert space is a bi-spinor. Using the formal transformation of co-ordinates $r \to r\exp(i\theta$ in the Hamiltonian (3), one could get:

$$H(\theta) = (\alpha cp - Z/r)\exp(-i\theta) + \beta - \sqrt{\alpha}Fz\exp(i\theta) \quad . (4)$$

In comparison with an analogous non-relativistic theory, here there is arisen a technical problem. In formulae (4) there is term β, which can not be simply transformed. One of the solving receptions os a limitation of a sub-space of the Hamiltonian eigen-functions by states of the definite symmetry (momentum J and parity P). These states can be described by the following functions:

$$\Psi_{PJ}^{M} = 1/r\begin{pmatrix} f(r)\mathrm{Y}_{lJ}^{M}(n,\sigma) \\ g(r)\mathrm{Y}_{l'J}^{M}(n,\sigma) \end{pmatrix}. \qquad (5)$$

Here l (l') and spin ½ in the coupling scheme give a state with the total momentum J and its projection M_J=M. Action of the Hamiltonian on the functions (5) with definite J results in:

$$\hat{H}(\theta)\Psi_{PJ}^{M} = \alpha_r(\hat{p}_r - \frac{i\omega(J+1/2)}{r}\beta)\exp(-i\theta)\Psi_{PJ}^{M} + \\ + (\beta - \frac{\alpha Z}{r}\exp(-i\theta) - \sqrt{\alpha}Fz\exp(-i\theta))\Psi_{PJ}^{M} \quad , (6)$$

where $\alpha_r \begin{pmatrix} 0....\sigma n \\ \sigma n... \end{pmatrix}$, $\beta \begin{pmatrix} 1....0 \\ 0. \end{pmatrix}$,

$p_r = -i(1/r)(d/dr)r$, $\vec{n} = \vec{r}/r$, σ - the Pauli matrices; parameter ω=-1, if l=J-1/2 and ω=1, if l=J+1/2. In order to further diagonalize the Hamiltonian (6), we need to choose the correct basis of functions in the subspace (5), in particular, by choosing the following functions (the sitter or water-like type):

$$\Psi_{PJ}^{a,M} = 1/r\begin{pmatrix} F(r)\mathrm{Y}_{lJ}^{M}(n,\sigma) \\ 0 \end{pmatrix} \qquad (7)$$

$$\Psi_{PJ}^{b,M} = 1/r\begin{pmatrix} 0 \\ iG(r)\mathrm{Y}_{l'J}^{M}(n,\sigma) \end{pmatrix}. \qquad (8)$$

It is easy to see that the matrix elements (6) will be no-zeroth only between the states with the same M_J. In fact this moment is a single limitation of the whole approach. Transformation of co-ordinates in the Pauli Hamiltonian (in comparison with the Schrodinger equation Hamiltonian it contents additional potential term of a magnetic dipole in an external field) can be performed by the analogous way. However, procedure in this case is significantly simplified. They can be expressed through the set of one-dimensional integrals, described in details in Refs. [14-17]. In Ref. [17] it is presented an effective scheme, which provides a general receipt to combine the OPT method with the RMBPT in spherical coordinates for a free atom. The details of the used method can be found in the references [17].

In Ref [17,20] it is presented our version of the RMBPT approach to calculation of spectra and spectral parameters of the multielectron atoms. It is clear that the spectra of multielectron heavy atoms have essentially relativistic properties. So, correct theoretical method of their studying can be based on the convenient field procedure, which includes computing the energy shifts ΔE of the degenerate electron states. More exactly, speech is about constructing secular matrix M (with using the Gell-Mann and Low adiabatic formula for ΔE), which is already complex in the relativistic theory, and its further diagonalization [21,22]. In result one could compute the energies and decay probabilities of a non-degenerate excited state for a complex atomic system. The secular matrix elements can be further expanded into a PT series on the inter-electron interaction. Here the standard Feynman diagrammatic technique is usually used. Generally speaking, the secular matrix M can be represented as follows:

$$M = M^{(0)} + M^{(1)} + M^{(2)} + M^{(3)} + ... + M^{(k)} \quad , (9)$$

where $M^{(0)}$ is the contribution of the vacuum diagrams of all PT orders (this contribution determines only the general levels spectrum shift); $M^{(1)}$, $M^{(2)}$, $M^{(3)}$ are contributions of the 1-, 2- and 3- quasiparticle (QP) diagrams respectively. The matrix $M^{(1)}$ can be presented as a sum of the independent one-QP contributions. Substituting these quantities into (9) one could have sum-

marized all the one-QP diagrams contributions. In the empirical methods here one could use the experimental values of one-electron energies, however, the necessary experimental quantities (especially for the rare-earth and other elements) are not often available. The detailed procedure for computing $\mathrm{Re}\,M^{(2)}$ is presented, for example, in Ref. [21,22].

We will describe an atomic multielectron system by the relativistic Dirac Hamiltonian (the atomic units are used) as follows [20,23-25]:

$$H = \sum_i \{\alpha c p_i - \beta c^2 - Z/r_i\} + \sum_{i>j} \exp(i\,|\,\omega\,|\,r_{ij})(1-\alpha_i\alpha_j)/r_{ij}, \quad (11)$$

where Z is a charge of nucleus, a_i, a_j are the Dirac matrices, ω_{ij} is the transition frequency, c – the velocity of light. The interelectron interaction potential (second term in (3)) takes into account the retarding effect and magnetic interaction in the lowest order on parameter of the fine structure constant. In the PT zeroth approximation it is used ab initio mean-field potential:

$$V^{DKS}(r) = [V^D_{Coul}(r) + V_X(r) + V_C(r\,|\,a)], \quad (12)$$

with the standard Coulomb, exchange Kohn-Sham V_X and correlation Lundqvist-Gunnarsson Vc potentials (look details in Refs. [18-20]). An effective approach to accounting the multielectron polarization contributions is described earlier and based on using the effective two-QP polarizable operator, which is included into the PT first order matrix elements.

3. Some results and conclusions

As illustration od the possibilities of the presented approach we carried out computing a dependence of the Stark components energies $(j,|m_j|)$ upon electric field strength F_0 for the Rydberg states $nD_{3/2,5/2}$ (n=39-46) of the Cs and Fr atoms (look figure 1) and compared the obtained results with the empirical perturbation theory calculation results by by Zhao et al [4].

Analysis of the data shows that the positions (energies) of the Stark resonances in the present calculation are in a physically reasonable agreement with theoretical data obtained by Zhao et al and experimental results. However, it should be noted that the results for the width of resonance could differ more significantly from each other. As it has been underlined in [40], in the case of a weak electric field (naturally the widths of resonances became very small), the methods have difficulties in obtaining a stable value of a width. In order to obtain the well-converged results, it is necessary to use larger basis size. Naturally, in a limit of a weak electric field the well-known quasiclassical WKB approximation and standard PT calculation will be more appropriate. One of the serious advantages of the modified ROPT method is that an increasing a field strength does not lead to an increase of computational effort and there is no a convergence problem [17].

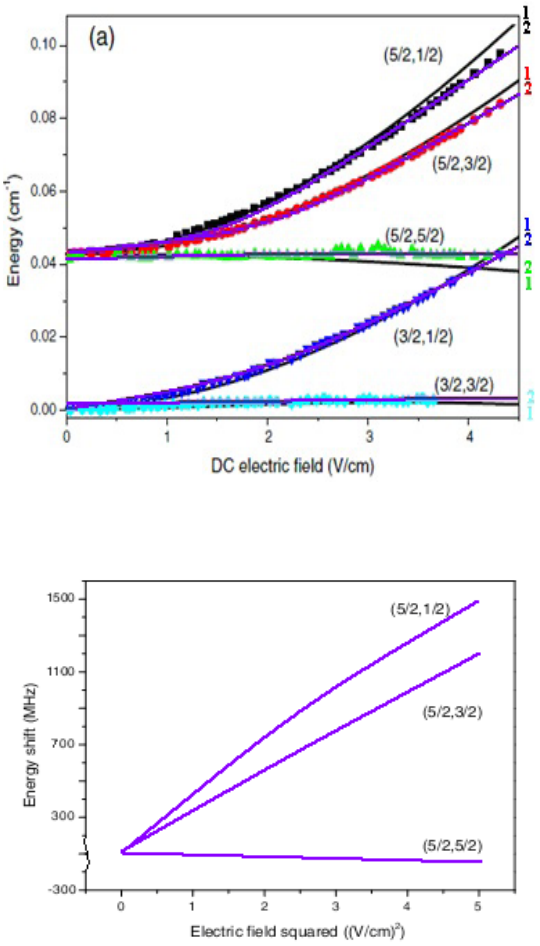

Figure 1 (a) – Dependence of energy (cm $^{-1}$; the energy of the level for F_0=0 is accepted as zero) of the Stark components $(j,|m_j|)$ for the state 39D Cs upon the electric field strength F_0 (Experiment-□,o,Δ◊); Theory: 1 – empirical perturbation theory (on F_0) data by Zhao et al; 2 – our data; (b) – the Stark shift (MHz) for different $(j,|m_j|)$ for the state 44D Fr upon F_0^2 (our data)

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Стаття надійшла до редакції 16.10.2018 р.

PACS 31.15.A-; UDC 539.184
DOI http://dx.doi.org/10.18524/1815-7459.2018.4.150501

OPTIMIZED RELATIVISTIC OPERATOR PERTURBATION THEORY IN SPECTROSCOPY OF MULTIELECTRON ATOM IN AN ELECTROMAGNETIC FIELD: SENSING SPECTRAL PARAMETERS

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Summary

The aim of the work is to develop and present a new effective approach to analysis and calculation of the energy and spectral parameters of heavy multielectron atoms in an electromagnetic field, which are of a great importance for different applications in quantum optics and atomic spectroscopy, quantum and nano-and sensor electronics, plasma chemistry, astrophysics, laser physics etc.

It is developed the optimized version of relativistic operator perturbation theory approach to calculation of the Stark resonances energies characteristics (energies and widths) for the multielectron atomic systems in an electromagnetic field. A new approach allows to perform an accurate, consistent treatment of a strong field DC(AC) Stark effect and includes the physically reasonable distorted-waves approximation in the frame of the formally exact relativistic quantum-mechanical procedure. As illustration, some test data for the Stark resonances energies and widths in the heavy

multielectron atoms (caesium, francium) are presented and compared with results of calculations within the alternative consistent sophisticated methods etc

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ОПТИМІЗОВАНА РЕЛЯТИВІСТСЬКА ОПЕРАТОРНА ТЕОРІЯ ЗБУРЕНЬ В СПЕКТРОСКОПІЇ БАГАТОЕЛЕКТРОННОГО АТОМУ В ЕЛЕКТРОМАГНІТНОМУ ПОЛІ: ДЕТЕКТУВАННЯ СПЕКТРАЛЬНИХ ПАРАМЕТРІВ

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Реферат

Метою роботи є розробка та обґрунтування нового ефективного підходу до аналізу та розрахунку енергетичних та спектральних параметрів важких багатоелектронних атомів в електромагнітному полі, чисельні величини яких мають велике значення для різних застосувань у квантовій оптиці та атомній спектроскопії, квантовій, нано-і сенсорній електроніці, хімії плазми, астрофізиці, лазерній фізиці тощо.

Розроблена оптимізована версія нового методу релятивістської операторної теорії збурень з метою обчислення характеристик штарківських резонансів (енергії і ширини) для багатоелектронних атомних систем в електромагнітному полі. Новий підхід дозволяє виконати кількісно прецизійний і теоретично послідовний опис сильнопольового (DC, AC) ефекту Штарка і включає в себе фізично обґрунтоване наближення перекручених хвиль в рамках формально точної релятивістської квантово-механічної процедури. В якості ілюстрації представлені деякі тестові дані для енергій і ширин штарківських резонансів у важких багатоелектронних атомах (цезій, францій), які порівнюються з результатами розрахунків в рамках альтернативних теоретичних методів.

Ключові слова: багатоелектронний атом в електромагнітному полі - модифікована релятивістська операторна теорія збурень - штарківські резонанси