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SPECTROSCOPY OF MULTIELECTRON ATOM IN DC ELECTRIC FIELD: RELATIVISTIC OPERATOR PERTURBATION THEORY

We develop the theoretical basis of a new relativistic operator perturbation theory approach to multielectron atom in a DC electric field combined with a relativistic many-body perturbation theory formalism for a free multielectron atom. As illustration of application of the presented formalism, the results of energy and spectral parameters for a number of atoms are presented. The relativistic OPT method is tested for computing the Stark shifts of Rydberg states for a few the multielectron systems such as the sodium and rubidium. The approach allows an accurate and consistent treatment of a DC strong field Stark effect in multielectron atoms.

1. Introduction

An investigation of spectra, optical and spectral, radiative and autoionization characteristics for the rare-earth elements (isotopes) and corresponding ions in an external electric field is traditionally of a great interest for further development quantum optics and atomic spectroscopy and different applications in the plasma chemistry, astrophysics, laser physics, quantum and nano-electronics etc. (see Refs. [1–18]). At the present time it attracts a great interest especially for multielectron and Rydberg atoms that is stimulated by a whole range of interesting phenomena to be studied such as different processes in a laser plasma, astrophysical environments, quasi-discrete state mixing, a zoo of Landau-Zener anticrossings, autoionization in the multielectron atoms, the effects of potential barriers (shape resonances), new kinds of resonances above threshold etc [1-20]. There are many detailed reviews on the atomic Stark effect, including the DC strong field one (see, e.g., [1-11]).

The calculation difficulties in description of the multielectron atoms in electromagnetic (electric) field inherent to the standard quantum mechanical approach are well known. Here one should mention the well-known Dyson phenomenon for a Strong Filed 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. At the present time, the generalization of methods to account for the resonance interference, multielectron and relativistic effects is still an important problem, though here a definite progress has been reached too. Different calculational procedures are used in the Pade and then Borel summation of the divergent Rayleigh-Schrödinger perturbation theory series and in the sufficiently exact numerical solution of the difference equations following from expansion of the wave function over finite basis (see review in [2]). One should mention such approaches as a model potential method, quantum defect approximation, complex scaling plus B-spline methods (c.g., [1-19]) and effective operator perturbation theory (OPT) method [11-13]; the latter is taken as the basis for our approach.

In this paper we develop a new theoretical approach, namely, relativistic operator perturbation theory (ROPT) approach to multielectron atom in an electromagnetic field combined with a relativistic many-body perturbation theory (RMBPT) formalism for a free multielectron atom. The key advantage of such an approach that it can be applied to DC strong-field Stark effect problem for any multielectron system. As illustration here the approach is tested for the multielectron system such as rubidium Rb.

The relativistic density-functional approximation with the Kohn-Sham potential is taken as the zeroth approximation in the RMBPT formalism [20-29]. It allows to take into account the standard exchange-correlation corrections of the second order and dominated classes of the higher orders diagrams (polarization interaction, quasiparticles screening, etc.). The basis of our approach is an approach, developed in Refs. [17,18].

2. Relativistic operator perturbation theory for multielectron atoms in an electric field

As the principal ideas of the approach have been presented in Ref. [17,18], here we are limited to some key elements. As usually, we start from the Dirac Hamiltonian (in relativistic units):

$$H = \alpha p + \beta - \alpha Z / r_i + \sqrt{\alpha} \cdot \varepsilon \cdot z, \quad (1)$$

Here a field strength intensity ε is expressed in the relativistic units ($\varepsilon_{rel} = a^{5/2} \varepsilon_{at.un.}$; a is the fine structure constant). One could see that a relativistic wave function in the Hilbert space is a bi-spinor. In order to further diagonalize the Hamiltonian (1), we need to choose the correct basis of relativistic functions, in particular, by choosing the following functions as in Ref. [1313]. The corresponding matrix elements of the total Hamiltonian 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 standard 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. [8,14]. To simplify the calculational procedure, the uniform electric field ε should be substitute by the function (c.g. [12]:

$$e(t) = \frac{1}{t} e \left[(t - \tau) \frac{\tau^4}{\tau^4 + t^4} + \tau \right] \quad (2)$$

with sufficiently large t ($t=1.5t_2$). The motiva-

tion of a choice of the $\varepsilon(t)$ and some physical features of electron motion are presented in Refs. [56-58]. Here we only underline that the function $\varepsilon(t)$ practically coincides with the constant ε in the inner barrier motion region, i.e. $t < t_2$ and disappears at $t > t_2$. It is important that the final results do not depend on the parameter t . It is carefully checked in the numerical calculation. As usually (see [11-13]), the scattering states energy spectrum now spreads over the range $(-\varepsilon/2, +\infty)$, compared with $(-\infty, +\infty)$ in the uniform field. In contrast to the case of a free atom in scattering states in the presence of the uniform electric field remain quantified at any energy E , i.e. only definite values of β_1 are possible. The latter are determined by the confinement condition for the motion along the h -axis. The same is true in our case, but only for

$$E \subset \left(-\frac{1}{2} \varepsilon \tau, +\frac{1}{2} \varepsilon \tau \right).$$

Ultimately, such a procedure provides construction of realistic functions of the bound and scattering states. In a certain sense, this completely corresponds to the advantages of the distorted-wave approximation known in scattering theory [11].

The total Hamiltonian does not possess the bound stationary states. According to Ref. [12,13], one has to define the zero order Hamiltonian H_0 , so that its spectrum reproduces qualitatively that of the initial one. To calculate the width G of the concrete quasistationary state in the lowest PT order one needs only two zeroth-order EF of H_0 : bound state function Ψ_b and scattering state function Ψ_s . There can be solved a more general problem: a construction of the bound state function along with its complete orthogonal complementary of scattering functions Ψ_E with

$$E \subset \left(-\frac{1}{2} \varepsilon \tau, +\infty \right).$$

The imaginary part of state energy (the resonance width) in the lowest PT order is determined by the standard way:

$$\text{Im}E = G/2 = p | \langle Y_{Eb} | H | Y_{Es} \rangle |^2 \quad (3)$$

with the total Hamiltonian H . The state functions $\Psi_{\mathbf{E}}$ and $\Psi_{\mathbf{E}'}$ are assumed to be normalized to 1 and by the $\delta(k-k')$ condition, accordingly. The matrix elements $\langle \Psi_{\mathbf{E}} | H | \Psi_{\mathbf{E}'} \rangle$ entering the high-order PT corrections can be determined in the same way. They can be expressed through the set of one-dimensional integrals, described in details in Refs. [2,12].

Further the ROPT scheme is combined with the RMBPT in spherical coordinates for a free atom. The details of this procedure can be found in the references [17,18]. The RMBPT formalism is constructed following to Refs. [2,23,26]. We will describe an atomic multielectron system by the relativistic Dirac Hamiltonian (the atomic units are used) as follows:

$$H = \sum_i \{ \alpha c p_i - \beta c^2 - Z / r_i \} + \sum_{i>j} \exp(i | \omega | r_{ij}) (1 - \alpha_i \alpha_j) / r_{ij} \quad (4)$$

where Z is a charge of nucleus, a_i, a_j are the Dirac matrices, w_{ij} is the transition frequency, c – the velocity of light. The interelectron interaction potential (second term in (4)) 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:

$$V^{DKS}(r) = [V_{Coul}^D(r) + V_X(r) + V_C(r|a)] \quad (5)$$

with the standard Coulomb (or some model potential analog), exchange Kohn-Sham V_X and correlation V_C potentials (look details in Refs. [19,20]). An effective approach to accounting the multi-electron 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. In order to calculate the decay (transition) probabilities and widths an effective relativistic energy approach (version [19-21]) is used. In particular, a width of the state, connected with an autoionization decay, is determined by a coupling with the continuum states and calculated as square of the matrix element [19]:

$$V_{\beta_1 \beta_2; \beta_4 \beta_3} = \sqrt{(2j_1+1)(2j_2+1)(2j_3+1)(2j_4+1)} \quad (-1)^{j_1+j_2+j_3+j_4+m_1+m_2} \quad \times$$

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

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

Here $Q_a = Q_a^{\text{Coul}} + Q_a^{\text{B}}$, where Q_a^{Coul} , and Q_a^{B} correspond to the Coulomb and Breit parts of the interelectron potential and express through Slater-like radial integrals and standard angle coefficients. Other details can be found in Refs. [2,23,26]. The most complicated problem of the relativistic PT computing the complex multi-electron elements spectra is in an accurate, precise accounting for the multi-electron exchange-correlation effects (including polarization and screening effects, a continuum pressure etc), which can be treated as the effects of the PT second and higher orders.

The detailed description of the polarization diagrams and the corresponding analytical expressions for matrix elements of the polarization QPs interaction (through the polarizable core) potential is presented in Refs. [2,19,20,26].

3. Results and Conclusions

In the framework of the development of spectroscopy of the heavy atoms in the external field, a quantitative study of the electric field effect on the energy levels in the spectra of the some alkali atoms was performed.

In Table 1 we present the calculation results for the Stark resonance energies for some Rydberg states of the Na atom in an electric field with the strength 3.59 kV/cm.

Table 1.
The energies (in cm^{-1}) of the Stark resonances for Na atom ($e=3.59$ kV/cm).

State: ($n_1 n_2 m$)	Exp.	[4]	[7]	This work
26,0,0	15.5	15.5	15.5	15.4
25,0,1	21.1	21.1	21.1	20.9
25,0,0	35.5	35.5	35.5	35.3
24,0,1	41.1	40.4	41.0	40.9
24,1,0	50.5	50.3	50.5	50.4
24,0,0	56.5	57.0	56.5	56.3

23,0,1	61.2	60.7	61.1	61.0
23,0,0	79.3	80.3	79.4	79.2
22,0,1	84.1	83.1	83.9	83.5
22,1,1	75.0	74.9	75.1	74.9

For comparison, we also list the experimental data, the results of calculation within the $1/n$ -expansion and model PT version (c.g.[4,6,7, 10]). Agreement between both the theory and the experiment is quite satisfactory. Our results are obtained in the first PT order, i.e., the first PT order provides physically reasonable results. In Table 2 we present the calculation results for the Stark resonance energies for some Rydberg states of the Rb atom in an electric field with the strength 2.189 kV/cm. For comparison there are also presented the results of calculation in the framework of $1/n$ -approximation (taking into account the permeability of the barrier), the method of summation of the PT series and experimental data (c.g.[4,6,7, 10]). There is physically reasonable agreement between theory and experiment.

Note that our results are obtained in the first PT order, i.e. already the first PT order

Table 2.

The energies (in cm^{-1}) of the Stark resonances for Rb atom ($e=2.189$ kV/cm).

n_1, n_2, m	Exp. [6]	$1/n$ [4]	PT [7]	This work
23,0,0	133.1	132.8	132.9	133.0
22,0,0	157.0	157.1	157.2	157.1
21,1,0	161.1	159.5	160.6	160.9
20,2,0	163.9	163.2	163.7	163.9
21,0,0	185.2	184.2	184.8	185.1
20,1,0	186.3	185.4	185.8	186.2
20,0,0	217.2	214.6	214.9	216.9
18,1,0	248.4	247.2	247.3	248.2
16,2,0	284.7	284.0	284.1	285.5
18,0,0	289.5	288.6	289.0	289.3

provides the physically reasonable results. Naturally its accuracy can be increased by an account of the next PT order. The ROPT approach can be used in calculating the Stark resonance param-

eters in a case of the strong electric fields and it is of a great interest for many modern atomic, molecular, plasmas and semiconductors physics applications (see Refs. [31-39]).

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SPECTROSCOPY OF MULTIELECTRON ATOM IN DC ELECTRIC FIELD: RELATIVISTIC OPERATOR PERTURBATION THEORY

Summary. We develop the theoretical basis of a new relativistic operator perturbation theory approach to multielectron atom in a DC electric field combined with a relativistic many-body perturbation theory formalism for a free multielectron atom. As illustration of application of the presented formalism, the results of energy and spectral parameters for a number of atoms are presented. The relativistic OPT method is tested for computing the Stark shifts of Rydberg states for a few the multielectron systems such as the sodium and rubidium. The approach allows an accurate and consistent treatment of a DC strong field Stark effect in multielectron atoms.

Keywords: multielectron atom, electric field, relativistic operator perturbation theory, Rydberg states

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СПЕКТРОСКОПИЯ МНОГОЭЛЕКТРОННОГО АТОМА В ЭЛЕКТРИЧЕСКОМ ПОЛЕ: РЕЛЯТИВИСТСКАЯ ОПЕРАТОРНАЯ ТЕОРИЯ ВОЗМУЩЕНИЙ

Резюме. Изложены теоретические основы нового аппарата релятивистской операторной теории возмущений в спектроскопии многоэлектронного атома в электрическом поле, объединенного с формализмом релятивистской многочастичной теории возмущений для свободного многоэлектронного атома. В качестве иллюстрации применения представленного формализма приведены результаты энергетических и спектральных параметров для ряда атомов. Релятивистский метод ОРТ тестируется для вычисления штарковских сдвигов ридберговских состояний для нескольких многоэлектронных систем, в частности, для натрия и рубидия. Новый подход разработан для последовательного описания эффекта Штарка в многоэлектронных атомах в сильном внешнем электрическом поле.

Ключевые слова: Многоэлектронные атом, электрическое поле, релятивистская операторная теория возмущений оператора, ридберговские состояния

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СПЕКТРОСКОПІЯ БАГАТОЕЛЕКТРОННОГО АТОМА В ЕЛЕКТРИЧНОМУ ПОЛІ: РЕЛЯТИВІСТСЬКА ОПЕРАТОРНА ТЕОРІЯ ЗБУРЕНЬ

Резюме. Викладено теоретичні основи нового апарату релятивістської операторної теорії збурень в спектроскопії багатоелектронного атома в електричному полі, об'єднаного з формалізмом релятивістської багаточастинкової теорії збурень для вільного багатоелектронного атома. В якості ілюстрації застосування представленого формалізму наведені результати обчислення енергетичних і спектральних параметрів для ряду атомів. Релятивістський метод ОРТ тестується для обчислення штарківських зсувів рідбергівських станів для декількох багатоелектронних систем, зокрема, для натрію і рубідію. Новий підхід розроблений для послідовного опису ефекту Штарка в багатоелектронних атомах в сильному зовнішньому електричному полі.

Ключові слова: багатоелектронний атом, електричне поле, релятивістська операторна теорія збурень оператора, рідбергівські стани