Quantum Geometry: New approach to quantization of quasi-stationary states of Dirac equation for relativistic many-body system and calculating some spectral parameters

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Abstract New advanced approach to calculating spectra of the relativistic many-body atomic system with an account of radiative corrections is presented. The approach is based on the formalism of the gauge-invariant quantum-electrodynamical many-body perturbation theory. An advanced procedure for quantization of the quasi-stationary states of the Dirac equation for relativistic many-body atomic system is presented. The numerical illustrations for some heavy multicharged ions are listed.

Keywords Relativistic many-body Dirac equation · quantization of quasi-stationary states · Eigen functions and energy eigen values

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1 Introduction

A development of the consistent methods of calculating a spectra of energy eigen values for relativistic Hamiltonian of the many-body systems with account of the nuclear and radiative corrections is still actual and fundamentally important problem of the modern quantum geometry and relativistic quantum theory of the many-fermion systems (see, for example, [1]–[8]). Theoretical methods used to calculate the energy parameters of the heavy finite many-body fermi-systems are traditionally divided into a few groups (see, for example, [1]–[12]). The relativistic Hartree-Fock (RHF) and Dirac-Fock (DF) approaches are the most popular ones and often used to determine an energy spectrum and

different spectral parameters of the relativistic many-body systems. The one- and two-body relativistic effects are taken into account practically precisely in the RHF and DF calculation schemes. One could remind a few very general and important computer codes for relativistic and quantum-electrodynamical (QED) calculations of spectra for multi-electron systems developed in the Oxford, German-Russian and Odessa groups etc ("GRASP", "Dirac"; "BERTHA", "QED", "Dirac"; "Superatom-Odessa") (see, for example, [1]–[12] and references there). The useful overview of the relativistic electronic structure theory is presented in refs. (see, for example, [1], [2], [5]–[10]). from the QED point of view. Further, in the study of lower states for multielectron systems with $Z \leq 40$ an expansion into double series of the PT on the parameters $1/Z$, αZ (α is the fine structure constant) turned out to be quite useful. It allows to determine contributions of the different expansion terms: relativistic, QED contributions as the functions of Z. A great interest attracts developing the high precise methods of account for the radiative and nuclear effects in a case of the heavy quantum systems to calculate adequately their energy spectra. Speech is about the radiative or QED effects, in particular, the vacuum polarization (VP) contribution, correction on the nuclear finite size for heavy elements and its account for different spectral properties of these systems etc ([1]–[14]). In Refs. [2]–[6] it has been presented a new advanced approach to calculating spectra of the relativistic many-body atomic system with an account of electroweak and hyperfine interactions, which is based on the QED perturbation theory and generalized relativistic mean field nuclear approach. In a case of the relativistic one-electron systems the one-particle Dirac equation can be naturally considered as the most exact and correct. A consistent treating relativistic many-body systems requires a development of the corresponding approximate methods and its correctness should be provided as by the basic fundamental properties as the direct numerical calculation and comparison with empirical data. In this paper, which goes on our previous works ([3]–[6]), we present a new, advanced ab initio approach to relativistic calculation of the spectra for heavy many-body ions with an account of relativistic, nuclear, QED effects. Within it an advanced procedure for quantization of the quasi-stationary states of the Dirac equation is proposed. The numerical illustrations of for a number of the heavy lithium-like multicharged ions are listed.

2 Quantization of states of the relativistic many-body Dirac equation with advanced nuclear and vacuum-polarization potentials

In this section we describe the key moments of our approach to description of the relativistic heavy many-body atomic systems with account of the relativistic and nuclear effects. The corresponding procedure for quantization of the quasi-stationary (stationary) states of the relativistic Dirac equation with an account of the cited effects by means of the advanced potentials is briefly described too. Foe definiteness let us consider a heavy lithium-like ion. The relativistic wave function zeroth basis is found from the Dirac equation with the total potential, which must include the electric and vacuum-polarization potentials of a nucleus and a self-consistent potential of electron subsystem. Surely, an effect of the finite nuclear size should be accounted for (see below). The standard relativistic Dirac equation for the large F and small G components can be represented as follows (see details, for example, in [5]):

$$f' = -(\chi + |\chi|)\frac{f}{r} - \alpha Z V g - \left(\alpha Z E_{n\chi} + \frac{2}{\alpha Z}\right) g,$$
$$g' = (\chi - |\chi|)\frac{g}{r} - \alpha Z V f + \alpha Z E_{n\chi} f. \qquad (1)$$

where α is the fine structure constant, $E_{n\chi}$ is one-electron energy without the rest energy and the moment number is as follows:

$$\chi = \begin{cases} -(1+1), & j > 1 \\ 1, & J < 1 \end{cases} \qquad (2)$$

Here we have used the Coulomb units (C.u.) are used; 1 C.u. of length = 1 a.u. Z; 1 C.u. of energy = 1 a.u. Z^2. The total potential V in Eq. (1) consist of the electric and vacuum-polarization potentials of a nucleus and a self-consistent potential of electron subsystem. The local DF potential is chosen as the electron subsystem potential [5]). In order to take into account a finite nuclear size effect we use the well-known Fermi-model for the distribution of the charge in a nucleus ([3]– [5]). As the detailed description of physical essence for the main radiative effects, namely self-energy part of the Lamb shift, vacuum polarization (VP) contribution, is presented in ([3]- [6]), here we are limited by a original description. The vacuum-polarization effect is taken into account by means of the generalized Uehling-Serber potential with an effective account of the Källen-Sabry and Wichmann-Kroll high-order corrections on the parameter $\alpha^k(\alpha)^n$. The cited potential can be written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp\left(-\frac{2rt}{\alpha Z}\right)\left(1+\frac{1}{2t^2}\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \qquad (3)$$

where $g = \frac{r}{\alpha Z}$. In our theory we use more exact approach, proposed in ([5]). The Uehling-Serber potential, determined as a quadrature 3, may be approximated with high precision by a simple analytical function. The use of new approximation of the Uehling-Serber potential permits one to decrease the calculation errors for this term down to $0.5 \div 1\%$. Besides, using such a simple analytical function form for approximating the polarization potential allows its easy inclusion into the general system of differential equations. This system includes also the Dirac equations and the equations for matrix elements.

The system of equations (1) has two fundamental, solutions. Naturally one should be interested in the solution regular at $r \to 0$. The boundary values of the correct solution are found by the first term s of the expansion into the Taylor series (see details in [1]):

$$\begin{aligned} g &= \frac{(V(0) - E_{n\chi})r\alpha Z}{2\chi + 1}; \qquad f = 1 \quad \text{at} \quad \chi < 0, \\ f &= \left(V(0) - E_{n\chi} - \frac{2}{\alpha^2 Z^2}\right)\alpha Z; \qquad g = 1 \quad \text{at} \quad \chi > 0. \end{aligned} \tag{4}$$

The condition $f, g \to 0$ at $r \to \infty$ determines the quantified energies of the state $E_{n\chi}$. As usually (see details in [1]) Eq. (1) can be solved by the standard Runge-Kutta method. The initial integration point $r = R/10^7$, where R is the nucleus radius, the end of the integration interval is determined as $r_k \approx 50n^*$.

3 Definition of the hyperfine structure parameters

The formulas for determination of the hyperfine structure parameters and the expressions for the energy of the quadruple (W_q) and magnetic dipole (W_μ) interactions, which define a hyperfine structure, are given in Refs. (c.f. [5],[14]), namely:

$$\begin{aligned} W_q &= [\Delta + c(C+1)]B; \\ W_\mu &= 0.5AC; \\ \Delta &= -\frac{4}{3}\frac{(4\chi - 1)(I+1)}{I - (I-1)(2I-1)}; \\ C &= F(F+1) - J(J+1) - (I+1). \end{aligned} \tag{5}$$

Here I is a spin of nucleus, F is a full momentum of system, J is a full electron momentum. Constants of the hyperfine splitting are expressed through the

standard radial integrals:

$$A = \frac{4.32587 \cdot 10^{-4} Z^2 \chi g_I}{4\chi^2 - 1}(RA)_{-2};$$
$$B = \frac{7.2878 \cdot 10^{-7} Z^3 Q}{(4\chi^2 - 1)I(I-1)}(RA)_{-3}. \quad (6)$$

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (in Barn); radial integrals are defined as follows ([3], [11]):

$$(RA)_{-2} = \int_0^\infty drr^2 F(r)G(r)U(1/r^2, R);$$
$$(RA)_{-3} = \int_0^\infty drr^2 [F^2(r) + G^(r)U(1/r^2, R)] \quad (7)$$

and calculated in the Coulomb units ($= 3.57 \cdot 10^{20} Z^2$ m^{-2}; $= 6.174 \cdot 10^{30} Z^3$ m^{-3} for valuables of the corresponding dimension). The radial parts F and G of two components of the Dirac function for electron, which moves in the potential $V(r,R)+U(r,R)$, are determined by solution of the Dirac equations (see above; (1)). For calculation of potentials of the hyperfine interaction $U(1/r^n, R)$, we solve the following differential equations:

$$U(1/r^n, R) = -\frac{ny(r,R)}{r^{n+1}}$$

The functions $dU(1/r^n, R)/dR$ are calculated within the analogous procedure.

4 Some numerical results and conclusion

We have carried out the calculation of constants of the hyperfine interaction: the electric quadruple constant B, the magnetic dipole constant A with inclusion of nuclear finiteness and the Uehling-Serber potential for Li-like ions. Analogous calculations of the constant A for ns states of lithium- like ions were performed in Refs. [3], [10]– [15]. In these papers other basis's of the relativistic orbitals were used. Besides, another model for the charge distribution in the nucleus and treating the QED corrections was used. In Table 1 the calculation results for the constants of the hyperfine splitting for the lowest excited states of Li-like ions are presented. In Table 2 we present the numerical values of derivatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2l, 3l, 4l (l = 0, 1) states of the Li-like ions with minimally possible values of j:

$$\frac{\partial\langle|V|\rangle}{\partial R} = Z^3 DV, \quad (\text{cm}^{-1}/\text{cm});$$
$$\frac{\partial\langle|U|\rangle}{\partial R} = Z^5 DU, \quad (\text{cm}^{-1}/\text{cm});$$

Table 1 Constants of the hyperfine electron-nuclear interaction: $A = Z^3 g_I \bar{A}$ cm^{-1}, $B = \frac{Z^3 Q}{I(2I-1)} \bar{B}$ cm^{-1}

nlj	Z	20	69	79	92
2s	$\bar{A}$	93 −03	176 −02	215 −02	314 −02
3s	$\bar{A}$	26 −03	51 −03	63 −03	90 −03
3s	$\bar{A}$	15 −03	19 −03	24 −03	36 −03
$2p_{1/2}$	$\bar{A}$	25 −03	56 −03	71 −03	105 −02
$3p_{1/2}$	$\bar{A}$	81 −04	16 −03	20 −03	31 −03
$4p_{1/2}$	$\bar{A}$	32 −04	72 −04	91 −04	11 −03
$2p_{3/2}$	$\bar{A}$	50 −04	67 −04	71 −04	72 −04
	$\bar{B}$	9 −04	13 −04	15 −04	17 −04
$3p_{3/2}$	$\bar{A}$	13 −04	19 −04	21 −04	22 −04
	$\bar{B}$	31 −05	51 −05	55 −05	65 −05
$3d_{3/2}$	$\bar{A}$	88 −05	10 −04	11 −04	12 −04
	$\bar{B}$	51 −06	9 −05	10 −05	11 −05
$4d_{3/2}$	$\bar{A}$	35 −05	51 −05	55 −05	58 −05
	$\bar{B}$	12 −06	44 −06	50 −06	56 −06
$3d_{5/2}$	$\bar{A}$	36 −05	48 −05	50 −05	52 −05
	$\bar{B}$	21 −06	38 −06	39 −06	40 −06
$4d_{5/2}$	$\bar{A}$	15 −05	19 −05	20 −05	21 −05
	$\bar{B}$	59 −07	15 −06	16 −06	17 −06

Table 2 Deriviatives of the one-electron characteristics on nuclear radius (in cm^{-1}/cm) for 2s, 3s, 4s states of the Li-like ions

nlj Z		20	30	41	59	69	79	92
$2s_{1/2}$	DV	10 +11	20 +11	41 +11	121 +12	223 +12	415 +12	967 +12
	DU	15 +06	14 +06	16 +06	20 +06	25 +06	36 +06	64 +06
	DA	15 +06	19 +06	24 +06	44 +06	63 +06	101 +07	197 +07
$3s_{1/2}$	DV	28 +10	60 +10	12 +11	35 +11	65 +11	122 +12	293 +12
	DU	45 +05	42 +05	44 +05	60 +05	81 +05	10 +06	18 +06
	DA	44 +05	56 +05	74 +05	12 +06	18 +06	29 +06	57 +06
$4s_{1/2}$	DV	11 +10	24 +10	51 +10	13 +11	26 +11	50 +11	121 +12
	DU	18 +05	17 +05	18 +05	24 +05	32 +05	47 +05	80 +05
	DA	18 +05	23 +05	30 +05	55 +05	81 +05	11 +05	23 +05

$$\frac{\partial A}{\partial R} = Z^4 g_I D A, \quad (\text{cm}^{-1}/\text{cm}).$$

Here 1 cm^{-1} is an energy unit and 1 cm is a length unit. Let us remember that here V is a potential of the electron-nuclear interaction and U is the Uehling-Serber vacuum-polarization potential.

Analysis of our data and comparison with available point-like theoretical data ([3], [10]– [12], [15]) shows that our approach provides a high-precise determination of the corresponding spectral parameters for heavy three-electron ions. It allows to believe that this approach to determination of the eigen values spectra for the heavy atomic systems with an account of relativistic, nuclear and radiative corrections can be used in a precise studying the energy parameters for

more complicated systems. Correspondingly, a procedure for quantization of the stationary (quasistationary) states of the relativistic Dirac equation is naturally correct in these cases too.

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