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# Quantum Geometry: New approach to quantization of quasistationary states of Dirac equation for superheavy ion and calculating hyperfine structure parameters

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**Abstract** New advanced approach to calculating spectra of the superheavy quantum (atomic) systems with an account of relativistic and radiative corrections is proposed and based on the formalism of the gauge-invariant quantum electrodynamical many-body perturbation theory ([1]-[4]).An advanced numerical procedure for quantization of the quasistationary states of the relativistic Dirac equation for superheavy relativistic ions is presented. The results of relativistic calculation of the eigen values of energy, hyperfine structure parameters, the derivatives of the one-electron characteristics on nuclear radius for hydrogen atom and superheavy hydrogen-like multicharged ions with account of relativistic, nuclear and radiative effects are presented.

**Keywords** Relativistic Dirac equation · Hyperfine structure · Eigen functions and eigen values of energy

**Mathematics Subject Classification (2000)** 55R05 · 53B05

## 1 Introduction

In the modern quantum geometry and relativistic quantum theory of the many-fermion systems there is a number of very complex problems, connected with a development of the consistent methods of calculating a spectra of eigen values of energy for the relativistic Hamiltonians of the many-body systems with account of the exchange-correlation, nuclear and radiative corrections. Theoretical meth-

ods used to calculate the energy parameters heavy and superheavy fermi-systems are traditionally divided into a few main groups (see, for example, [1]–[12]). The multi-configuration relativistic Hartree-Fock (RHF) and Dirac-Fock (DF) approaches are the most used methods of calculation for multi-electron systems with a large nuclear charge. Usually, in these calculations the one- and two-body relativistic effects are taken into account practically precisely. It should be given the special attention to three very general and important computer systems for relativistic and QED calculations of atomic and molecular properties developed in the Oxford and German-Russian groups etc ("GRASP", "Dirac"; "BERTHA", "QED", "Dirac") (see, for example, [1]–[12] and references there). For example, the BERTHA program embodies a new formulation of relativistic atomic and molecular structure theory within the framework of relativistic QED. This leads to a simple and transparent formulation of the Dirac-Hartree-Fock-Breit self-consistent field equations, electron correlation, and higher order QED effects. These equations are solved by a direct method based on a relativistic generalization of the McMurchie-Davidson algorithm for corresponding integrals that economizes memory requirements and is not significantly more expensive computationally than comparable nonrelativistic calculations. 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 ions with $Z \leq 40$ an expansion into double series of the PT on the parameters $1/Z$, $\alpha Z$ ($\alpha$ is the fine structure constant) turned out to be quite useful. It permits evaluation of contributions of the different expansion terms: relativistic, QED contributions as the functions of $Z$. Now this topic has been a subject of intensive theoretical and experimental interest. There is a great necessity of developing high precise methods of simultaneous account for the relativistic, radiative and nuclear effects in order to calculate adequately the energy spectra for heavy systems. Speech is about the radiative or QED effects, in particular, the self-energy part of the Lamb shift, vacuum polarization (VP) contribution, correction on the nuclear finite size for superheavy elements and its account for different spectral properties of these systems, including the hyperfine structure parameters and derivatives of the one-electron characteristics on nuclear radius etc ( [1]–[14]). In our paper we present a new, ab initio approach to relativistic calculation of the spectra for superheavy ions with an account of relativistic, nuclear and radiative effects. It is based on the quantum electrodynamical (QED) perturbation theory (PT). The results of relativistic calculation of the eigen values of energy for H atom and superheavy H-like multicharged ion

with account of nuclear and radiative effects are presented. Besides, derivatives of the one-electron characteristics on nuclear radius for atom of hydrogen $^1$H (test calculation), superheavy H-like ion with nuclear charge $Z = 170$, are also listed.

## 2 Quantization of states of the relativistic 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 superheavy atomic systems with account of the relativistic and nuclear effects. The corresponding procedure for quantization of the quasistationary (stationary) states of the relativistic Dirac equation with an account of the cited effects in the advanced total potential is briefly described too. let us consider a superheavy hydrogen-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. 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 [2]):

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

where $E_{n\chi}$ 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. $Z^2$. These units are very comfortable under studying the multicharged ions of isoelectronic sequences of the definite element. The total potential V in Eq. (1) consist of the electric and vacuum-polarization potentials of a nucleus. 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], [4]). As the detailed description of accounting for the main radiative effects, namely self-energy part of the Lamb shift, vacuum polarization (VP) contribution, is presented in ( [2]- [4]), here we are limited by a brief comments. Regarding the vacuum-polarization effect let us note that this effect is usually taken into

account in the first PT theory order by means of the Uehling potential. This potential is usually written as follows ([2],[3]):

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

where $g = \frac{r}{\alpha Z}$. In our theory we use more exact approach, proposed in ( [3]). The Uehling 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 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 Uehling 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]):

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

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-Kutt 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

Energies of the quadruple ($W_q$) and magnetic dipole ($W_\mu$) interactions, which define a hyperfine structure, are calculated as follows (c.f. [13],[14]):

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

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. The electric quadrupole spectroscopic HFS constant $B$ of an atomic state related to the electric field gradient $q$ and to electric quadrupole moment $eQ$ of the nucleus as: $B = eqQ/h$. So, to obtain the corresponding value of $Q$ one must combine the HFS constants data with the electric field gradient obtained in our approach from the QED PT calculation. The details of calculation are presented in ([1]-[4]).

## 4 Results of calculation and conclusion

We have carried out the test calculation of the hyperfine structure parameters (plus derivatives of the energy contribution on nuclear radius) for atom of hydrogen $^1$H and superheavy H-like ion with nuclear charge $Z = 170$. For hydrogen atom there are available sufficiently exact experimental data ( [15]) for hyperfine splitting energies of 1s, 2s levels. For superheavy ion $Z = 170$ there is no experiment and we can analyze only the theoretical results. In Table 1 we present the experimental and theoretical (our calculation) results for hyperfine splitting energies for 1s, 2s levels of hydrogen atom. There is an excellent agreement between the theoretical data and experimental ones.

**Table 1** Experimental and theoretical (our calculation) results for hyperfine splitting energies for 1s, 2s levels of hydrogen atom

| Electron term<br>Quantum numbers of<br>full moment | Experiment<br>$\Delta\nu(F,F')$, MHz<br>$\Delta E(F,F'), 10^{-3}$ cm$^{-1}$ | Our calculations<br>$\Delta\nu(F,F')$, MHz<br>$\Delta E(F,F'), 10^{-3}$ cm$^{-1}$ |
|---|---|---|
| $1s^2S_{1/2}$ (1.0) | 1420.406 | 1419.685 |
| | 47.379 | 47.355 |
| $2s^2S_{1/2}$ (1.0) | 177.557 | 177.480 |
| | 5.923 | 5.920 |

**Table 2** Characteristics of one-electron states for H-like ion with nuclear charge $Z = 170$ (our calculation)

| | $1s_{1/2}$ | $2s_{1/2}$ | $2p_{1/2}$ | $2p_{3/2}$ | $3s_{1/2}$ | $3sp_{1/2}$ | $3p_{3/2}$ |
|---|---|---|---|---|---|---|---|
| A | 4337 | 837 | 3867 | 1.59 | 207 | 322 | 0.615 |
| DA | 1039 | 228 | 941 | 0.0001 | 56.8 | 84.0 | 0.0001 |
| B | 9091 | 1897 | 8067 | 0.007 | 475 | 707 | 0.04 |
| DB | 7245 | 1557 | 6405 | 0.0008 | 394 | 574 | 0.0003 |
| DV | 1255 | 273 | 1108 | 0.0011 | 67.7 | 98.3 | 0.0005 |
| U | 1453 | 282 | 1301 | 1.31 | 69.3 | 109 | 0.62 |
| DU | 2343 | 503 | 2071 | 0.0015 | 127 | 185 | 0.0007 |

In Table 2 we present the results of our calculation for the hyperfine structure parameters (plus derivatives of the energy contribution on nuclear radius) for the superheavy H-like ion with nuclear charge $Z = 170$.

We have used the denotations as follows:

$$A = \frac{10^8 A}{Z^3 g_I}, \quad \text{(eV)};$$

$$DA = \frac{10^{-2}}{Z^4 g_I}\frac{\partial A}{\partial R}, \quad \text{(eV/cm)};$$

$$B = \frac{10^7 BI(2I-1)}{Z^3 Q}, \quad \text{(eV/Barn)};$$

$$DB = \frac{10^{-3} I(2I-1)}{Z^4 Q}\frac{\partial B}{\partial R}, \quad \text{(eV/(Barn cm))};$$

$$U = -\frac{10^4}{Z^4}\langle U(r,R)\rangle, \quad \text{(eV)};$$

$$DU = \frac{10^{-1}}{Z^4}\frac{\partial\langle U(r,R)\rangle}{\partial R}, \quad \text{(eV/cm)};$$

$$DV = \frac{10^{-8}}{Z^3}\frac{\partial\langle V\rangle}{\partial R}, \quad \text{(eV/cm)}.$$

Therefore we have presented a new advanced approach to determination of the eigen values spectra for the superheavy quantum (atomic) systems with an account of relativistic, nuclear (the finite nuclear size effect) and radiative

corrections. This approach is based on the formalism of the gauge-invariant quantum electrodynamical many-body perturbation theory ([1]-[4]). Within its limits, we have elaborated an advanced numerical procedure for quantization of the quasistationary states of the relativistic Dirac equation for superheavy relativistic ions with an account of relativistic, nuclear, radiative corrections. We have also presented the results of calculating the energy eigen values spectra, hyperfine structure parameters, derivatives of the one-electron characteristics on nuclear radius for hydrogen atom and superheavy hydrogen-like ion with account of relativistic, nuclear and radiative effects.

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