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HYPERFINE STRUCTURE PARAMETERS OF THE HEAVY ISOTOPES: CONSISTENT NUCLEAR-QED THEORY

It is presented the new, consistent theoretical nuclear-QED approach to estimating parameters of the hyperfine structure of the heavy isotopes, which is based on the relativistic mean field theory of a nucleus and QED perturbation theory. The hyperfine structure parameters for the heavy isotopes of ^{205}Tl and ^{169}Tm are calculated. The theoretical values of the relative contribution into the hyperfine structure due to the effect of the distribution of the magnetic moment of the nucleus are listed too.

1. Introduction

A development of a new effective nuclear schemes and technologies for sensing different nuclear properties, studying the properties of heavy isotopes is of a great importance in the modern atomic, nuclear physics and technologies [1-3]. Among the most important problems one could mention the studying of nuclei, which are available in the little quantities (for example, the lanthanides isotopes, radioactive nuclei far of the stability boundary), search of the super dense nuclei and its sensing, laser governing by parameters of the proton and other beams and sensing their characteristics etc [1-17]. Such possibilities are provided by the modern laser methods and technologies (see, for example, [1,2]). A high sensibility and resolution ability of laser spectroscopy methods allows investigating the characteristics of nuclei available in the little quantities, heavy isotopes. As an example (see ref. [1-6]) one can mention the CERN technical device for studying the short-lived nuclei which are obtained on the mass-separator in the line with synchrocyclotrone on 600 MeV (ISOLDE apparatus [1]). The shocking results have been obtained in studying of the odd neutron-deficit non-stable isotopes of $^{182-190}$Hg. The intensity of the ion beams of these isotopes with life time 1-60 min was 10^7-10^9 ions/s. Under excitation of fluorescence by dye pulsed laser radiation the second harmonics of radiation was tuning to region of 2537A and the measurement of the hyperfine structure for this line of Hg was carried out during 1-2 min disposing about 10^8 of the mercury isotope atoms. During transition from nucleus ^{186}Hg to nucleus ^{185}Hg it has been discovered the sharp changing of the middle square of the nuclear radius which is interpreted as sharp changing of the nuclear form (increasing of non-soherity and electric quadrupole moment) during decreasing the neutrons number. In refs. [17-25] (see also [4,5]) we have developed new effective theoretical scheme with possibility of advancing corresponding nuclear technology for sensing different spectral parameters, including the hyperfine structure ones, for heavy isotopes and elements available in the little quantities. It is based on the experimental receiving the isotope beams on the CERN ISOLDE type apparatus (see detailed description in refs. [1,3,4]) and the précised theoretical and laser spectroscopy empirical estimating the hyperfine structure parameters, magnetic and electric moments of a nucleus of isotopes. We have carried out sensing and estimating the hyperfine structure parameters, magnetic and electric moments of a nucleus for ^{235}U, ^{201}Hg and rare cosmic isotopes. Theory of the hyperfine structure calculation is based on developed earlier gauge-invariant QED PT formalism with an precise account of the exchange-correlation (inter electron interaction corrections), nuclear and QED effects and nuclear relativistic mean field (RMF) theory. In this paper we consider its application to studying hyperfine structure parameters for some heavy isotopes, in particular, the corresponding data for the ^{205}Tl and ^{169}Tm isotopes are listed.

Let us also remind that the accurate measurements of the hyperfine structure parameters for a whole number of heavy isotopes (e.g. [1,6,16]) not only provide the possibility for testing the quantum electrodynamics (QED) in strong fields, but also sensing the hyperfine structure parameters of spectra for heavy atomic systems, electric charge and magnetic moment distributions inside the nucleus [5-10]. Theoretical calculations fulfilled during the last several years apart from the basis Fermi-Breit relativistic contributions also include the magnetic dipole moment distribution inside the nucleus (Bohr-Weisskopf effect) and radiative QED corrections (e.g. [1-6]). In calculations of the heavy ions the well known multiconfiguration (MC) Dirac-Fock (DF) approach is widely used (e.g.[14-20]).

2. Theoretical approach to calculating hyperfine structure parameters

Let us describe the key moments of the theoretical scheme. Full details of the whole method of calculating the hyperfine structure constants can be found in [4,5,17-24]. The wave electron functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential, electric, polarization potentials of nucleus. All correlation corrections of the second and high orders of PT (electrons screening, particle-hole interaction etc.) are accounted for [17]. The concrete nuclear model is used as described below. A quantitative estimate of the nuclear moments demands realistic proton single-particle wave functions which one could obtain by employing the RMF model of a nucleus. Though we have no guaranty that these wave-functions yield a close approximation to nature, the success of the RMF approach supports our choice (e.g.[26]). These wave functions do not suffer from known deficiencies of other approaches, e.g., the wrong asymptotics of wave functions obtained in a harmonic oscillator potential. The RMF model has historically been designed as a renormalizable meson-field theory for nuclear matter and finite nuclei. The realization of nonlinear self-interactions of the scalar meson led to a quantitative description of nuclear ground states. As a self-consistent mean-field model (for a comprehensive review see Ref. [25]), its ansatz is a Lagrangian or Hamiltonian that incorporates the effective, in-medium nucleon-nucleon interaction. Recently self-consistent models have undergone a reinterpretation which explains their quantitative success in view of the facts that nucleons are composite objects and that the mesons employed in RMF have only a loose correspondence to the physical meson spectrum [25-28]. RMF models are effective field theories for nuclei below an energy scale of 1GeV, separating the long- and intermediate-range nuclear physics from short-distance physics, involving, i.e., short-range correlations, nucleon form factors, vacuum polarization etc, which is absorbed into the various terms and coupling constants. As it is indicated in refs.[27] the strong attractive scalar (*S:* -400 MeV) and repulsive vector (*V:* +350 MeV) fields provide both the binding mechanism (*S* + *V:* -50 MeV) and the strong spin-orbit force (*S* – *V:* -750 MeV) of both right sign and magnitude. In our calculation we have used so called NL3 (c.f.[25]), which is among the most successful parametrizations available.

The scheme of accounting for the finite size effect is in details described in ref. [17]. Here we only note that if the point-like nucleus possesses by some central potential *W(R)* then transition to potential of the finite nucleus is realized by substitution *W(r)* on

$$W(r|R) = W(r)\int_0^r dr\, r^2 \rho(r|R) + \int_r^\infty dr\, r^2 W(r)\rho(r|R) \ .$$

In our case the Coulomb potential for spherically symmetric density $\rho(r|R)$ is:

$$V_{nucl}(r|R) = -((1/r)\int_0^r dr' r'^2 \rho(r'|R) + \int_r^\infty dr' r' \rho(r'|R)$$

Further the standard Dirac-Fock -like equations for a multi-electron system {core-*nl*j} are solved. Formally they fall into one-electron Dirac equations for the orbitals *nlj* with potential: $V(r)=2V(r|SCF)+V(r|nlj)+V_{ex}+V(r|R)$. It includes the electrical and polarization potentials of a nucleus with a finite size. The part V_{ex} accounts for exchange inter-electron interaction. The exchange effects are accounted for in the first two PT orders by the total inter-electron interaction [17]. The core electron density is defined by iteration algorithm within QED procedure [4]. The radiative QED (the self-energy part of the Lamb shift and the vacuum polarization contribution) are accounted for within the QED formalism [4,25]. The hyperfine structure constants are defined by the radial integrals of the known type (e.g. [29,17]):

$$A=\{[(4,32587)10^{-4}Z^2cg_I]/(4c^2-1)\}$$

$$\int_0^\infty drr^2F(r)G(r)U(1/r^2,R)$$

$$B=\{7.2878\ 10^{-7}\ Z^3Q/[(4c^2-1)I(I-1)\}$$

$$\int_0^\infty drr^2[F^2(r)+G^2(r)U(1/r^2,R)$$

Here I is a spin of nucleus, g_I is the Lande factor, Q is a quadruple momentum of nucleus; radial integrals are calculated in the Coulomb units (=$3.57\times10^{20}Z^2$m^{-2}; =6.174 10^{30} Z^3m^{-3}). Radial parts F and G of two components of the Dirac function for electron, which moves in the potential are defined by solution of the Dirac equations (PT zeroth order). The other details can be found in refs. [17-25].

3. Estimating the hyperfine structure parameters and conclusions

Earlier we have studied the hyperfine structure of spectra for the elements Be, C, Al, U, which have above cited rare, cosmic isotopes. Here we present the results of studying (the Superatom package [4,5] is used) the hyperfine structure parameters for the heavy isotopes of ^{205}Tl and ^{169}Tm. In table 1 we present the values of the hyperfine splitting Dn(*F*, *F'*) (in MHz) for ^{169}Tm ($^2F_{7/2}$) (nuclear spin 1/2) with available theoretical (MCDF) and experimental or compilation data [30].

Table 1. **The hyperfine splitting Dn(F, F') (in MHz) of levels for ^{169}Tm ($^2F_{7/2}$)**

Isotope; Spin of nucleus	Term	Quantum numbers total moment *F*, *F'*	Δν(*F*, *F'*), MHz [30]	Theory, MCDF	Theory, Present Wok
^{169}Tm ($^2F_{7/2}$) 1/2	4 $^2F_{7/2}$	(4, 3)	1496.55	1484.8	1496.12

Table 2 lists the experimental (A^{Exp}) and theoretical values of the constant A (in GHz) for the valence states ^{205}Tl, in particular, the theoretical value obtained by calculation within the method of single DF (A^{DF}), the method including single- and double- excited states (A^{SD}), DF method, taking into account the configuration interaction (A^{DF+C}), multiconfiguration DF method (A^{MCDF}), relativistic cluster-coupled method, taking into account the finite size of the nucleus (A^{RCC-FS}), a modified Hartree-Fock (A^{gHF}), the time-dependent relativistic Hartree-Fock theory (A^{TDRHF}), the same method, but taking into account the correlations and the finite size of the nucleus ($A^{TDRHF+C}$) and the nuclear-QED theory (A^{N-QED}) (from [14 -18]). Analysis of the data shows that an account of the interelectron correlation effects is crucial in the calculation of the hyperfine structure parameters and therefore the conventional methods such as the method of DF (of single approximation) as well as the method with the limited accounting the exchange-correlation effects do not give a sufficiently high accuracy. Significantly better data in terms of accuracy and consistency to the experiment results are obtained on the basis of the calculation in the framework of the relativistic cluster-coupled method, taking into account the finite size of the nucleus (A^{RCC-FS}), the time-dependent relativistic theory with accounting the correlations and the finite size of the nucleus ($A^{TDRHF+C}$) and nuclear-QED theory. Naturally, a precise agreement between theory and experiment can be reached by means accounting for not only the relativistic and exchange-correlation effects, but the radiative QED corrections, the nuclear effects of Bohr-Weisskopf, Breit-Rosenthal-Crawford-Schawlow etc too.

Table 2. **Experimental (A^{Exp}) and theoretical values of the constant A (in GHz) for the valence states of ^{205}Tl (see text)**

Method/State	$6p_{1/2}$	$6p_{3/2}$	$7s_{1/2}$
A^{DF}	17.68	1.304	7.78
A^{DF+C}	20.86	0.256	12.67
A^{RCC+FS}	21.43 21.30	0.317 0.339	12.92 12.76
A^{SD-DF}	18.73	1.381	-
A^{MCDF}	20.32	1.485	-
A^{gHF}	20.89	0.895	-
A^{RMBPT}	21.663	0.248	12.666
A^{TDRHF} $A^{TDRHF+C}$	24.06 21.30	-1.885 0.600	13.06 12.56
A^{N-QED}	21.3098	0.2535	12.2713
A^{exp}	21.3108	0.2650	12.2972

In Table 3 we list the theoretical value of the relative contribution (the value of $D/l_{c,m}$) into the hyperfine structure due to the effect of the distribution of the magnetic moment of the nucleus. There are presented data, estimated by the different methods, namely, the single-configuration Dirac-Fock (DF) method, the relativistic cluster-coupled method, taking into account the finite size of the nucleus (ARCC-FS) and nuclear-QED theory (see [14-18]). The cited parameter has a simple physical meaning. The shift in the hyperfine structure constant for two different isotopes (nuclear $g=m/I$ factor) is usually estimated as: A_1g_2/A_2g_1-1=D.

On the other hand, the variation of the charge distribution in a nucleus core, as known from the theory of the isotope shift, leads to the known correction: $l_{c,m}=k_c<d<(r_c)^2>$, where the k_c factor takes into account the higher moments of the distribution of the charge. For ^{205}Tl there are known the experimental data on the parameters D and $l_{c,m}$, derived from the values of the magnetic moments ^{203}m =1.622258m_N и ^{205}m =1.638315m_N [16]. The analysis shows that the contribution to the «perturbation» of the hypefine structure for the thallium has roughly equal to the effects of Bohr-Weisskopf and Breit-Rosenthal-Crawford-Schawlow.

Table 3. **Experimental and theoretical values for the $D/l_{c,m}$ (10^{-4}/fm^2) for the valence states of the ^{205}Tl: single-configuration Dirac-Fock (DF), relativistic cluster-coupled method with accounting the finite size effect (A^{RCC-FS}) and nuclear-QED theory (A^{N-QED})**

Method/State	$6p_{1/2}$	$6p_{3/2}$	$7s_{1/2}$
$(\Delta/\lambda_{c,m})^{DF}$	-2.26	-	-7.95
$(\Delta/\lambda_{c,m})^{RCC+FS}$	-2.48	43.0	-7.62
$(\Delta/\lambda_{c,m})^{N-QED}$	-2.4735	42.68	-7.54
Experiment Δ $\lambda_{c,m}$	-2.4762 -1.04 0.42	42.79 16.26 0.38	-7.56 -3.4(18) 0.45(24)

References

1. Letokhov V. S., Non-linear selective photoprocesses in atoms and molecules.-Moscow: Nauka, 1987.- 380 P.
2. Klaft I., Borneis S., Engel T., Fricke B., Grieser R., Huber G., Kuhl T., Marx D., Neumann R., Schroder S., Seelig P., Volker L. Precision laser spectroscopy of ground state hyperfine splitting of H-like $^{209}Bi^{82+}$ // Phys.Rev.Lett.-1994.-Vol. 73.-P. 2425-2427.
3. Glushkov A.V., Relativistic and correlation effects in spectra of atomic systems.-Odessa: Astroprint, 2006.-400 P.
4. Glushkov A.V., Khetselius O.Yu., Ambrosov S.V., Loboda A.V., Gurnitskaya E.P., QED calculation of heavy ions with account for the correlation, radiative and nuclear effects // Recent Adv. in Theor. Phys. and Chem. Systems (Springer). - 2006.-Vol. 15.-P. 285-300.
5. Glushkov A. V., Khetselius O. Yu., Ambrosov S. V., Loboda A. V., Chernyako-

va Yu.G., Svinarenko A. A., QED calculation of the superheavy elements ions: energy levels, radiative corrections and hfs for different nuclear models// Nucl. Phys.A.: Nucl.and Hadr. Phys. –2004.-Vol.734.-P. 21-28.
6. Freeman A. J., Frankel R. H., Hyperfine interactions.-N-Y.: Plenum, 1987.-340P.
7. Nagasawa T., Haga A., Nakano M., Hyperfine splitting of hydrogenlike atoms based on relativistic mean field theory // Phys.Rev.C.-2004.-Vol.69.-P. 034322:1–10.
8. Tomaselli M, Kuhl T., Nortershauser W., Borneis S., Dax A., Marx D, Wang H, Fritzsche S., Hyperfine splitting of hydrogenlike thallium // Phys. Rev.A-2002.-Vol. 65.-P. 022502.
9. Tomaselli M., Kuhl T., Seelig P., Holbrow C. and Kankeleit E., Hyperfine splittings of hydrogenlike ions and the dynamic-correlation model for one-hole nuclei // Phys.Rev.C.-1998.-Vol.58, N3.-P. 1524-1534.
10. Tomaselli M., Schneider S. M., Kankeleit E., Kuhl T., Ground state magnetization of ^{209}Bi in a dynamic-correlation model // Phys.Rev.C.-1995.-Vol. 51, N 6.-P. 2989-2997.
11. Benczer-Koller N., The role of magnetic moments in the determination of nuclear wave functions of short-lived excited states // J.Phys.CS.-2005.-Vol. 20.-P. 51-58.
12. Bieron J., Pyykko P., Degree of accuracy in determining the nuclear electric quadrupole moment of radium // Phys. Rev. A.- 2005.-Vol. 71.-P. 032502.
13. Derevianko A., Porsev S. G., Dressing lines and vertices in calculations of matrix elements with the coupled-cluster method and determination of Cs atomic properties // Phys.Rev. A.-2005.-Vol.71.-P. 032509.
14. Safronova M. S., Johnson W. R., Safronova U. I., Excitation energies, hyperfine constants, E1,E2,M1 transition rates and lifetimes of $6s^2nl$ states in TlI and PbII // Phys.Rev.A.-2005.-Vol. 71.-P. 052506.
15. Martensson A. M., Gouch D. S., Hanaford P., Relativistic coupled-cluster approach to hyperfine structure of Tl atom // Phys. Rev.A.1993 -.Vol. 49.-P. 3351-3360.
16. Martensson A. M., Magnetic moment distributions in Tl nuclei // Phys. Rev. Lett.-1995.-Vol. 74.-P. 2184-2188.
17. Khetselius O. Yu., Hyperfine structure of atomic spectra.-Odessa: Astropritn, 2008.-210 P.
18. Khetselius O. Yu., Relativistic perturbation theory calculation of the hyperfine structure parameters for some heavy-element isotopes // Int. Journ. of Quantum Chemistry.-2009.-Vol. 109.- N14.-P. 3330-3335
19. Khetselius O. Yu., Gurnitskaya E. P., Sensing the electric and magnetic moments of a nucleus in the N-like ion of Bi // Sensor Electr. and Microsyst. Tech.- 2006.-N 3.-P. 35-39.
20. Khetselius O. Yu., Gurnitskaya E. P., Sensing the hyperfine structure and nuclear quadrupole moment for radium // Sensor Electr. and Microsyst. Techn.-2006.-N 2.-P. 25-29.
21. Glushkov A. V., Khetselius O. Yu., Gurnitskaya E. P., Florko T. A., Sensing of nuclei available in little quantities by means of laser spectroscopy of hyperfine structure for isotopes: new theoretical scheme (U ,Hg) // Sensor Electr. and Microsyst. Techn.- 2007.-N 3.-P. 21-26.
22. Khetselius O. Yu., On possibility of sensing nuclei of the rare isotopes by means of laser spectroscopy of hyperfine structure // Sensor Electr. and Microsyst. Techn.-2007.-N4.-P. 11-16.
23. Khetselius O. Yu., Hyperfine structure of energy levels for isotopes ^{73}Ge, ^{75}As, ^{201}Hg // Photoelectronics.-2007.-N16.-P. 129-132.
24. Khetselius O. Yu., Hyperfine structure of radium // Photoelectronics.-2005.-

N14.-P.83-85.

25. Khetselius O.Yu., Quantum structure of electroweak interaction in heavy finite ermi-systems.-Odessa: Astroprint, 2011.
26. Serot B. D., Advances in Nuclear Physics Vol. 16: The Relativistic Nuclear Many Body Problem / Serot B. D., Walecka J. D.-Plenum Press, New York, 1986.
27. Burvenich T. J., Evers J., Keitel C. H., Dynamic nuclear Stark shift in superintense laser fields // Phys.Rev.C.-2006.-Vol.74.-P. 044601-1-044601-10.
28. Dikmen E., Novoselsky A., Vallieres M., Shell model calculation of low-lying states of ^{110}Sb // J.Phys.G.: Nucl. Part. Phys.- 2007.-Vol. 34.-P. 529-535.
29. Sobel'man I. I. Introduction to theory of atomic spectra.-Moscow: Nauka.- 1977.
30. Radtsig A. A.,Smirnov B. M., Parameters of atoms and ions. – Moscow, 1986.

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Abstract

It is presented the new, consistent theoretical nuclear-QED approach to estimating parameters of the hyperfine structure of the heavy isotopes, which is based on the relativistic mean field theory of a nucleus and QED perturbation theory. The hyperfine structure parameters for the heavy isotopes of ^{205}Tl and ^{169}Tm are calculated. The theoretical values of the relative contribution into the hyperfine structure due to the effect of the distribution of the magnetic moment of the nucleus are listed too.

Key words: hyperfine structure, heavy isotopes, nuclear-QED approach

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ПАРАМЕТРЫ СВЕРХТОНКОЙ СТРУКТУРЫ ТЯЖЕЛЫХ ИЗОТОПОВ В РАМКАХ ПОСЛЕДОВАТЕЛЬНОЙ ЯДЕРНО-КЭД ТЕОРИИ

Резюме

Представлен новый, последовательный теоретический ядерно-КЭД подход к оценке параметров сверхтонкой структуры тяжелых изотопов, основанный на релятивистской теории среднего поля ядра и КЭД теории возмущений. Рассчитаны параметры сверхтонкой структуры спектров тяжелых изотопов ^{205}Tl и ^{169}Tm. Также приведены оценки теоретических значений относительного вклада в значения параметров сверхтонкой структуры вследствие эффекта распределения магнитного момента в ядре.

Ключевые слова: сверхтонкая структура, тяжелые изотопы, ядерно-КЭД теория

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ПАРАМЕТРИ НАДТОНКОЇ СТРУКТУРИ ВАЖКИХ ІЗОТОПІВ В РАМКАХ ПОСЛІДОВНОЇ ЯДЕРНО-КЕД ТЕОРІЇ

Резюме

Розвинуто новий послідовний теоретичний ядерно-КЕД підхід до оцінки параметрів надтонкої структури важких ізотопів, який базується на релятивістській теорії середнього поля ядра і КЕД теорії збурень. Розраховані параметри надтонкої структури спектрів важких ізотопів ^{205}Tl і ^{69}Tm. Також наведені оцінки теоретичних значень відносного внеску до параметрів надтонкої структури завдяки ефекту розподілу магнітного моменту в ядрі.

Ключові слова: надтонка структура, важкі ізотопи, ядерно-КЕД теорія