UDC 539.184

O. Yu. Khetselius, T. A. Florko, A. V. Smirnov, Yu. Ya. Bunyakova

Odessa State Environmental University, 15, Lvovskaya str., Odessa, Ukraine
Odessa National Politechnical University, 1, Shevchenko av., Odessa, Ukraine
e-mail: nuckhet@mail.ru

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

It is presented the consistent theoretical nuclear-QED approach to estimating parameters of the hyperfine structure and electric quadrupole moment of the mercury isotope 201Hg. 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 Dirac-Fock (single configuration approximation) as well as their generalized versions with the limited accounting the exchange-correlation effects do not give a sufficiently high accuracy.

1. Introduction

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 atomic method with possibility of advancing corresponding nuclear technology for sensing different parameters, including the hyperfine structure ones, for heavy isotopes and elements available in the little quantities. It is based on experimental receiving the isotope beams on the CERN ISOLDE type apparatus (see detailed description in [1,3,4]) and the précised theoretical and laser spectroscopy empirical estimating the hyperfine structure parameters, nuclear magnetic and electric moments of isotopes. We carried out

sensing and estimating the hyperfine structure (HFS) parameters, magnetic and electric moments of a nucleus for [235]U, and others. The HFS calculation theory is based on developed earlier gauge-invariant QED PT formalism with an precise account for exchange-correlation (inter electron interaction corrections), nuclear and QED effects and nuclear relativistic mean field (RMF) theory. New theory has been called as the nuclear-QED PT [26]. Here we present the results of advanced studying the hyperfine structure parameters and electric quadrupole moment a nucleus for the mercury isotopes, namely [201]Hg.

Following, [24,25], 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 multi-configuration (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-nlj} 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]):

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

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

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

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

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 ($=3,57\ 10^{20}Z^2$m^{-2}; $=6,174\ 10^{30}Z^3$m^{-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 advanced data (the Superatom package [4,5] is used) on the HFS parameters and quadrupole electric moment for the ^{201}Hg.

In Table 1 there are listed the experimental and calculated values of the nuclear electric quadrupole moment Q (mb) for ^{201}Hg (from [5,6,23,26]. The calculations were performed on the basis of the non-correlated DF, in the many approximation of DF (MCDF), taking into account the Breit and QED corrections, as well as on the basis of our method (the RMF model for the charge distribution in a nucleus).

Table 1

The values of the nuclear electric quadrupole moment Q (mb) for mercury

Q (мб)	Method	Reference	Год
383,1	At-Nucl	Our work	2013
380,5	Atomic	Glushkov et al	2006
387 (6)	Atomic	Pyykko et al	2005
347	Nuclear	Fornal et al	2001
(43)	Atomic	Ulm et al	1988
385	Muonic	Gunther et al	1983
(40)	Muonic	Hahn et al	1979
485	Muonic	Hahn et al	1979
(68)	Solid	Edelstein-	1975
386	Atomic	Pound	1960
(49)	Atomic	McDermott	1959
267	Atomic	etal	1957
(37)	Solid	Murakawa	1954
390	Atomic	Blaise-	1935
(20)		Chantrel	
455		Dehmelt et al	
(40)		Schuler-	
420		Schmidt	
500			
(50)			
600			
500			

As can be seen, the value of the moment of Q, obtained by us, in the best agreement with the data obtained by a group of Ulm. Comparison of the results of calculations in the framework of our method and the DF (the single-and many-approximation based on the Breit and QED corrections) shows that our values of the constants A are in better agreement with experiment than the DF.

In Table 2 there are listed the experimental and calculated values of the hyperfine constants (in MHz) for the $^3P_1$ state of the neutral mercury atom [5,6,23,26]. 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.

Table 2

Experimental and Calculations meaning of the nuclear electric quadrupole moment Q (mb) for ^{201}Hg and the HFS constants (MHz) for the $^3P_1$ state of the neutral atom of mercury ^{201}Hg

Method	Q (mb)	A (MHz)	B (MHz)
DF	478,13	-4368,266	---
MCDF (Breit+QED)	386,626	-5470,810	---
RMBT	380, 518	-5460, 324	-286,512
This work: EXC	-92,980	-1161,242	-58,478
This work: Breit-QED	-2,582	-20,384	-1,002
This work Total.	380, 518	-5458,420	-283,313
Experiment	Table 1	-5454,569 (0,003)	-280,107 (0,005)

Note: EXC- exchange-correlation contribution;

Analysis shows that 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.

References

1. Letokhov V.S., Non-linear selective photoprocesses in atoms and molecules.-Moscow: Nauka, 1987.-380P.
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.-400P.
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., Chernyakova 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., Hol-

brow 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, N6.-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.032502-1-8.

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.-210P.

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. Techn.-2006.-N3.-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.-N2.-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.-N3.-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., Hyper fine structure of radium// Photoelectronics.-2005.-N14.-P.83-85.

25. Khetselius O.Yu., Hyperfine structure parameters of the heavy isotopes: Consistent nuclear-QED theory // Photoelectronics.-2013.-N22.-P.146-152.

26. Khetselius O.Yu., Quantum structure of electroweak interaction in heavy finite ermi-systems.-Odessa: Astroprint, 2011.

27. 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.

28. 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.

29. 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.

30. Sobel'man I.I. Introduction to theory of atomic spectra.-Moscow: Nauka.-1977.

31. Radtsig A.A.,Smirnov B.M., Parameters of atoms and ions. – Moscow,1986.

UDC 539.184

O. Yu. Khetselius, T. A. Florko, A. V. Smirnov, Yu. Ya. Bunyakova

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

Abstract.

It is presented the consistent theoretical nuclear-QED approach to estimating parameters of the hyperfine structure and electric quadrupole moment of the mercury isotope [201]Hg. 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 Dirac-Fock (single configuration approximation) as well as their generalized versions with the limited accounting the exchange-correlation effects do not give a sufficiently high accuracy.

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

УДК 539.184

О. Ю. Хецелиус, Т. А. Флорко, А. В. Смирнов, Ю. Я. Бунякова

ПАРАМЕТРЫ СВЕРХТОНКОЙ СТРУКТУРЫ IЗОТОПОВ Hg В РАМКАХ ПОСЛЕДОВАТЕЛЬНОЙ ЯДЕРНО-КЭД ТЕОРИИ

Резюме.

Рассмотрен последовательный теоретический ядерно-КЭД подход к оценке параметров сверхтонкой структуры и электрического квадрупольного момента ядра изотопа [201]Hg. Анализ данных показывает, что учет межэлектронных корреляционных эффектов имеет критически важное значение при расчете параметров сверхтонкой структуры и, следовательно, применение к задаче традиционных методов типа метода Дирака-Фока (в одно- конфигурации приближении), а также его обобщенных версий с ограниченным учетом обменного корреляционных эффектов не дает возможности достичь достаточно высокой точности описания искомых свойств.

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

УДК 539.184

О. Ю. Хецелиус, Т. О. Флорко, А. В. Смірнов, Ю. Я. Бунякова

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

Резюме.

Розглянуто послідовний теоретичний ядерно-КЕД підхід до оцінки параметрів надтонкої структури та електричного квадрупольного моменту ядра ізотопу ^{201}Hg. Аналіз даних показує, що урахування між електронних кореляційних ефектів має вирішальне значення при розрахунку параметрів надтонкої структури і, отже, застосування до задачі традиційних методів типу методу Дірака-Фока (в одно-конфігураційному наближенні), а також його узагальнених версій з обмеженим урахуванням обмінно-кореляційних ефектів не дає можливості досягнути достатньо високої точності опису шуканих властивостей. .

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