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THE HYPERFINE STRUCTURE OF HEAVY ELEMENTS ATOMS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

The hyperfine structure and electric quadrupole moment of the mercury isotope are estimated within the relativistic many-body perturbation theory formalism with a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections. Analysis of the data shows that an account of the interelectron correlation effects is crucial in the calculation of the hyperfine structure parameters. The fundamental reason of physically reasonable agreement between theory and experiment is connected with the correct taking into account the inter-electron correlation effects, nuclear (due to the finite size of a nucleus), relativistic and radiative corrections. The key difference between the results of the RHF, RMPT methods calculations is explained by using the different schemes of taking into account the inter-electron correlations.

1. Introduction

The research on the hyperfine structure characteristics of the heavy neutral and highly ionized atoms is of a great fundamental importance in many fields of atomic physics (spectroscopy, spectral lines theory), astrophysics, plasma physics, laser physics and so on (see, for example, refs. [1-37]). The experiments on the definition of hyperfine splitting also enable to refine the deduction of nuclear magnetic moments of different isotopes and to check an accuracy of the various calculational models employed for the theoretical description of the nuclear effects. The multi-configuration relativistic Hartree-Fock (RHF) and Dirac-Fock (DF) approaches (see, for example, refs. [1,2]) are the most reliable versions 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 refs. [1-4] and references there).

In the present paper we present the calculational results for the hyperfine structure and electric quadrupole moment of the isotope $^{223}_{88}Ra$, estimated within the relativistic many-body perturbation theory formalism with a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections [3,4,10-20]. Analysis of the data shows that an account of the interelectron correlation effects is crucial in the calculation of the hyperfine structure parameters.

2. Relativistic method to computing hyperfine structure parameters of atoms and ions

Let us describe the key moments of the approach (more details can be found in refs. [3,4,10-20]). The electron wave functions (the PT zeroth basis) are found from solution of the relativistic Dirac equation with potential, which includes ab initio mean-field potential, electric, polarization potentials of a nucleus. The charge distribution in the Li-like ion is modelled within the Gauss model. The nuclear model used for the Cs isotope is the independent particle model with the Woods-Saxon and spin-orbit potentials (see refa. [3,4]). Let us consider in details more simple case of the Li-like ion. We set the charge distribution in the Li-like ion nucleus $\rho(r)$ by the Gaussian function:

$$\rho(r|R) = \left(4\gamma^{3/2}/\sqrt{\pi}\right)\exp\left(-\gamma r^2\right) \qquad (1)$$

where $\gamma=4/\pi R^2$ and R is the effective nucleus radius. The Coulomb potential for the spherically symmetric density $\rho(r)$ is:

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

Consider the DF type equations. Formally they fall into one-electron Dirac equations for the orbitals with the potential $V(r|R)$ which includes the electrical and the polarization potentials of the nucleus; the components of the Hartree potential (in the Coulomb units):

$$V(r|i) = \frac{1}{Z}\int d\vec{r}'\rho(r|i)/|\vec{r}-\vec{r}'| \qquad (4)$$

Here $\rho(r|i)$ is the distribution of the electron density in the state $|\, i >$, V_{ex} is the exchange inter-electron interaction. The main exchange and correlation effects will be taken into account in the first two orders of the PT by the total inter-electron interaction [3,4].

A procedure of taking into account the radiative QED corrections is in details given in the refs. [4,44]. Regarding the vacuum polarization effect let us note that this effect is usually taken into consideration in the first PT theory order by means of the Uehling-Serber potential. This potential is usually written as follows:

$$U(r) = -\frac{2\alpha}{3\pi r}\int_1^\infty dt \exp\left(-2rt/\alpha Z\right)\left(1+1/2t^2\right)\frac{\sqrt{t^2-1}}{t^2} \equiv -\frac{2\alpha}{3\pi r}C(g), \qquad (5)$$

where $g=r/(\alpha Z)$. In our calculation we use more exact approach [3]. The Uehling potential, determined as a quadrature (6), 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 – 1%.

A method for calculation of the self-energy part of the Lamb shift is based on an idea by Ivanov-Ivanova et al [38-41], which generalizes the known hydrogen-like method by Mohr and radiation model potential method by Flambaum-Ginges (look details in Refs. [4,44,45]). The radiative shift and the relativistic part of energy in an atomic system are, in principle, defined by one and the same physical field [38]. One could suppose that there exists some universal function that connects the self-energy correction and the relativistic energy. Its form and properties are in details analyzed in Refs.[4,45]. Unlike usual purely electronic atoms, the Lamb shift self-energy part in the case of a pionic atom is not significant and much inferior to the main vacuum-polarization effect.

The energies of electric quadruple and magnetic dipole interactions are defined by a standard way with the hyperfine structure constants, usually expressed through the standard radial integrals:

$$A=\{[(4,32587)10^{-4}Z^2\chi g_I]/(4\chi^2-1)\}(RA)_{-2},$$

$$B=\{7.2878\ 10^{-7}\ Z^3Q/[(4\chi^2-1)I(I-1)\}\ (RA)_{-3}, \qquad (7)$$

Here g_I is the Lande factor, Q is a quadruple momentum of nucleus (in Barn); $(RA)_{-2}$, $(RA)_{-3}$ are the radial integrals usually defined as follows:

$$(RA)_{-2} = \int_\infty drr\ F(r)G(r)U(1/r\ , R)$$

$$(RA)_{-3} = \int_\infty drr \qquad . \qquad (8)$$

The radial parts F and G of the Dirac function two components for electron, which moves in the potential $V(r,R)+U(r,R)$, are determined by solution of the Dirac equations. To define the hyperfine interaction potentials $U(1/r^n,R)$, we use the method by Ivanov et al [11]. The key elements of the optimized relativistic energy approach to computing oscillator strengths are presented in [39,41,42,46-53]. Let us remind that an initial general energy formalism combined with an empirical model potential method has been developed by Ivanov-Ivanova et al [11], further more general ab initio gauge-invariant relativistic approach has been presented in [42], where the calibration of the single model potential parameter b has been performed on the basis of the special *ab initio* procedure within relativistic energy approach (see also [4,45]). All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results and Conclusions

In this subsection we present experimental data and the results of the calculation of the HFS constants and the nuclear quadrupole moment for the radium isotope. In Table 1 we list the experimental and calculational data on the magnetic dipole constant HFS A (MHz) for the $^{223}_{88}Ra$ 7s7p $^1P_1$, $^3P_1$, $^3P_2$ states. The data are obtained on the basis of calculations in the framework of the standard uncorrelated DF method, MKDF method with taking into account for the Breit and standard QED corrections, the relativistic configuration interaction method with taking into account for the correlation corrections within the random phase approximation (RCI-RPA) [6], as well as our results (Gaussian model for charge distribution in the core) [2,3,6,7].

It is important to note that the key quantitative factor in the agreement of the theory with experiment is associated with a correct allowance for interelectronic correlations, an amendment to the finite size of the nucleus, and Breit and QED radiation effects [3,4].

Table 1

The experimental and calculational data on the magnetic dipole constant HFS A (MHz) for the $^{223}_{88}Ra$ 7s7p $^1P_1$, $^3P_1$, $^3P_2$ states (see text)

Method/ State	$^1P_1$	$^3P_1$	$^3P_2$
DF	-226.59	803.97	567.22
MCDF (Breit+QED)	-330.3	1251.9	737.1
RCI-RPA	-242.4	-	-
Our data	-339.1	1209	704.5
Exp.	-344.5 (0.9)	1201.1 (0.6)	699.6 (3.3)

The analysis shows that the contribution due to the electron – electron correlations to the values of the HFS constants is ~ 100–500 MHz for various states. This circumstance explains the low degree of consistency in accuracy of the data provided, obtained in the framework of different versions of the DF method. The key difference between the results of the calculation in the framework of our approach and the MCDF is due to different methods of taking into account the electron-electron correlations. The contributions of higher-order QED TV corrections and corrections for the finite core size can reach 1–2 tens of MHz, and it seems obviously important to consider them more correctly. In addition, it is necessary to take direct account of nuclear polarization contributions, which can be done within the framework of solving the corresponding nuclear problem, for example, using the shell model with Woods-Saxon and spin-orbit potentials. Such an approach is outlined in Refs [3,4].

In Table 2 we present the measured values of the nuclear quadrupole moment Q (in barns) for the isotope, obtained experimentally by the ISOLDE Collaboration group (CERN) based on various methods (see [6]). In addition, this table presents the calculated values of the nuclear quadrupole moment Q (in barns) for the isotope, obtained on the basis of calculations in the framework of the methods of MKDF (including Breit and QED corrections), relativistic many-particle TV (RMBPT) and our data (taken from works [2,3,6,7] and references in them).

Table 2.

The values of the electric quadrupole moment Q (in barns) for isotope of $^{223}_{88}Ra$

Method	Q (barn)
MCDF (Breit+QED)	1.21 (0.03)
RMBPT	1.28
QED theory	1.22
Our data	1.213
Pykko, Recommend.	1.221 (old) 1.210 (new)
ISOLDE Collaboration fs RaII	1.254 (0.003) {0.066]
Wendt et al, fs RaI	1.19 (0,12)
ISOLDE Collaboration fs RaI	1.190 (0,007) {0,126}
ISOLDE Collaboration B(E2)	1.2

Our final data lie between the latest experimental values of the Wendt group (ISOLDE Collaboration), but have less error definitions.

The fundamental reason of physically reasonable agreement between theory and experiment is connected with the correct taking into account the inter-electron correlation effects, nuclear (due to the finite size of a nucleus), relativistic and radiative corrections.

The key difference between the results of the RHF, RMPT methods calculations is explained by using the different schemes of taking into account the inter-electron correlations. The contribution of the PT high order effects and nuclear contribution may reach the units and even dozens of MHz and should be correctly taken into account. So, it is necessary to take into account more correctly the spatial distribution of the magnetic moment inside a nucleus (the Bohr-Weisskopf effect), the nuclear-polarization corrections etc too. These topics require the separated accurate treatment.

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THE HYPERFINE STRUCTURE OF HEAVY ELEMENTS ATOMS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

Summary

The hyperfine structure and electric quadrupole moment of the isotope $^{223}_{8}R$ are estimated within the relativistic many-body perturbation theory formalism with a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections. Analysis of the data shows that an account of the interelectron correlation effects is crucial in the calculation of the hyperfine structure parameters. The fundamental reason of physically reasonable agreement between theory and experiment is connected with the correct taking into account the inter-electron correlation effects, nuclear (due to the finite size of a nucleus), relativistic and radiative corrections. The key difference between the results of the RHF, RMPT methods calculations is explained by using the different schemes of taking into account the inter-electron correlations.

Keywords: Hyperfine structure –Heavy atoms – Relativistic perturbation theory – Correlation, nuclear, radiative corrections

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СВЕРХТОНКАЯ СТРУКТУРА ТЯЖЕЛЫХ АТОМОВ В РАМКАХ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме

Параметры сверхтонкой структуры и электрический квадрупольный момент изотопа радона рассчитаны на основе релятивистской многочастичной теории возмущений с эффективным аккуратным учетом обменно-корреляционных, релятивистских, ядерных и радиационных поправок. Анализ данных показывает, что учет эффектов межэлектронной корреляции имеет критическое значение при вычислении параметров сверхтонкой структуры. Физически разумное согласие теории и прецизионного эксперимента может быть обеспечено благодаря полному последовательному учету межэлектронных корреляционных эффектов, ядерных, релятивистских и радиационных поправок. Ключевое различие между результатами расчетов в приближениях Дирака-Фока, различных версиях формализма теории возмущений в основном связано с использованием различных схем учета межэлектронных корреляций.

Ключевые слова: Сверхтонкая структура - тяжелый атом - релятивистская теория возмущений - корреляционные, ядерные, радиационные поправки

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НАДТОНКА СТРУКТУРА ВАЖКИХ АТОМІВ В РАМКАХ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ

Резюме

Параметри надтонкої структури і електричний квадрупольний момент ізотопу радону розраховані на основі релятивістської багаточастинкової теорії збурень з ефективним акуратним урахуванням обмінно-кореляційних, релятивістських, ядерних і радіаційних поправок. Аналіз даних показує, що урахування ефектів міжелектронної кореляції має критичне значення при обчисленні параметрів надтонкої структури. Фізично розумне узгодження теорії і прецизійного експерименту може бути забезпечено завдяки повному послідовному обліку міжелектронних кореляційних ефектів, ядерних, релятивістських та радіаційних поправок. Ключова відмінність між результатами розрахунків в наближеннях Дірака-Фока, різних версіях формалізму теорії збурень в основному пов’язано з використанням різних схем обліку міжелектронних кореляцій.

Ключові слова: Надтонка структура – важкий атом - релятивістська теорія збурень – кореляційні, ядерні, радіаційні поправки