PACS 31.30.Gs

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HYPERFINE STRUCTURE PARAMETERS FOR COMPLEX ATOMS WITHIN RELATIVISTIC MANY-BODY PERTURBATION THEORY

Abstract. The calculational results for the hyperfine structure (HFS) parameters for the Mn atom (levels of the configuration $3d^6 4s$) and the results of advanced calculating the HFS constants and nuclear quadrupole moment for the radium isotope $^{223}_{88}Ra$ are obtained on the basis of computing 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 relativistic Hartree-Fock Dirac-Fock and many-body perturbation theory methods calculations is explained by using the different schemes of taking into account the inter-electron correlations as well as nuclear and radiative ones.

1. Introduction

The study of the parameters of the hyperfine structure (HFS) and the characteristics associated with it is of great importance for modeling the properties of nuclei, the search for superdense nuclei, and a number of other problems in nuclear physics. Nuclear size effects in the energy structure of the states of the electron shell of a heavy atom are essentially used in physical research and for technological purposes. The scheme for measuring isotopic shifts of atomic levels based on the method of laser photoionization has become classical, in particular, for Hg isotopes (A = 193-201), this method has been used to measure the root-mean-square radii of the charge distribution in the nucleus and the total moments. Such information can, in principle, be used to simulate intranuclear forces.

In connection with the foregoing, interest has sharply increased in the corresponding theoretical calculations of the HFS characteristics of the spectra of heavy atoms and ions with allowance for relativistic, correlation, and nuclear effects and, of course, in testing new effects predicted on the basis of quantum electrodynamics (QED). It is known that QED corrections (vacuum polarization, self-energy contribution) to the energies of transitions with the participation of K and L-electrons, as well as the effects of the finiteness of the nucleus at large nuclear charges Z> 60, are on the order of the binding energy of valence electrons. Taking them into account is fundamental for determining the energetically allowed channels of decay of states with vacancies and predicting the complete kinetics of decay.

The multi-configuration relativistic Hartree-Fock (RHF), Dirac-Fock (DF), multi-configuration DF (MCDF) approaches (see, for example, refs. [1-33]) are the most reliable versions of calculation for multi-electron systems with a large nuclear charge.

In this paper we present the calculational results for the HFS structure parameters for the Mn atom (levels of the configuration $3d^6 4s$) and the results of advanced calculating the HFS constants and nuclear quadrupole moment for the radium isotope $^{223}_{88}Ra$, using the optimized method of the relativistic many-body perturbation theory with the Dirac-Kohn-Sham zeroth approximation and a correct and effective taking into account the exchange-correlation, relativistic, nuclear and radiative corrections [9-30]. Analysis of the data shows that an account of the cited cor-

rections 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. [19-30]). 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. [20]). 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 [21,22].

A procedure of taking into account the radiative QED corrections is in details given in the refs. [19,20].

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:

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

$$= -\frac{2\alpha}{3\pi r}C(g), \qquad (5)$$

where $g=r/(\alpha Z)$. In our calculation we use more exact approach [20]. The Uehling potential, determined as a quadrature (5), 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 the methods [19-24]. The radiative shift and the relativistic part of energy in an atomic system are, in principle, defined by one and the same physical field. 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.[19-24,30-35]. 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:

$$(RA)_{-2} = \int_0^\infty dr r^2 F(r)G(r)U(1/r^2, R),$$

$$(RA)_{-3} = \int_0^\infty dr r^2 [F^2(r) + G^2(r)U(1/r^2, R) \cdot \quad (8)$$

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. The key elements of the numerical approach to computing the corresponding matrix elements are presented in [31-44]. All calculations are performed on the basis of the numeral code Superatom-ISAN (version 93).

3. Results and Conclusions

In this subsection we go on the presentation of the experimental data and the results of the calculation of the HFS parameters for the Mn element. Let us remind that Mn has one stable isotope with a mass number of 55, a nuclear spin of 5/2, a magnetic dipole moment of 3.46871668 $\mu_я$ and an electric quadrupole moment of Q = 0.33 (1) barn. Basic electronic configuration: $3d^5 4s^2$ ($^6S_{5/2}$). Given the complexity of the spectrum, theoretical study of the HFS should be based on a full multi-electron calculation. An useful review and detailed analysis of the studies of the HFS of the Mn atom was given, for example, in [6].

In table 1 we present the available experimental (A_{exp}, B_{exp}) and theoretical (our calculation) values of the energy levels and the HFS parameters for the Mn levels of the configuration $3d^6 4s$. Earlier [37] we have presented the analogous data for the levels of configuration $3d^5 4s^2$,3d64s. The reasonable agreement between theoretical and measured data can be reached by way of using the optimized wave functions basises and complete, correct accounting for the exchange-correlation corrections.

Table 1. Experimental (A_{exp}, E_{exp}) and theoretical values of the energies of the levels (cm^{-1}) and HFS constants (MHz) (see text) for the levels of the configuration $3d^6 4s$.

Level	Term	E_{exp}	E_{th}
$3d^6 4s$	$a^4F_{9/2}$	34938.7	34882
$3d^6 4s$	$a^4F_{7/2}$	35041.4	34977
$3d^6 4s$	$a^4F_{5/2}$	35115.0	35042
$3d^6 4s$	$a^4D_{7/2}$	-	23208
$3d^6 4s$	$a^4D_{5/2}$	-	23473
Level	Term	A_{exp}	A_{th}
$3d^6 4s$	$a^4F_{9/2}$	649(7)	646
		643(4)	646
$3d^6 4s$	$a^4F_{7/2}$	588(5)	580
		576(12)	580
$3d^6 4s$	$a^4F_{5/2}$	437(3)	436
		440(5)	436
$3d^6 4s$	$a^4D_{7/2}$	171(15)	170
$3d^6 4s$	$a^4D_{5/2}$	-	136
Level	Term	B_{exp}	B_{th}
$3d^6 4s$	$a^4F_{9/2}$	200	198
$3d^6 4s$	$a^4F_{7/2}$	150	149
$3d^6 4s$	$a^4F_{5/2}$	-	21

Further we present experimental data and the results of advanced calculating the HFS constants and nuclear quadrupole moment for the radium isotope $^{223}_{88}Ra$. The mercury atom has an external valet configuration $7s^2$ and is considered by us as a two-quasiparticle system.

Table 2 shows the experimental and calculated data on the HTS magnetic dipole constant A (MHz) for the7s7p $^1P_1$, $^3P_1$, $^3P_2$ states of the atom $^{223}_{88}Ra$. The data of calculations within the framework of the standard uncorrelated DF method, MCDF taking into account the Breit and standard QED corrections, the relativistic method of configuration interaction taking into account the correlation corrections in the framework of the random phase approximation (RCI-RPA) [6], as well as our QED approach (Gaussian model for charge distribution in the nucleus) [8,33,35].

Table 2. The experimental and calculated data on the HTS magnetic dipole constant A (MHz) for the7s7p $^1P_1$, $^3P_1$, $^3P_2$ states of the atom $^{223}_{88}Ra$ (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	-	-
RMBPT	-339.1	1209	704.5
This work	-340.4	1207.4	703.9
Experiment	-344.5 (0.9)	1201.1 (0.6)	699.6 (3.3)

In Table 3 we present the measured values of the nuclear quadrupole moment Q (in barns) for the isotope obtained experimentally by the ISOLDE Collaboration (CERN) group based on various techniques (see [6]). In addition, this table presents the calculated values, obtained on the basis of calculations within the framework of the MCDF method (taking into account the Breit and QED corrections), relativistic many-particle PT (RMBPT) and our approach (Refs. [1-6]).

Table 3. The values of electric quadrupole moment Q (mb) for isotope of $^{223}_{88}Ra$

Method	*Q* (mb)
MCDF (Breit+QED)	1.21 (0.03)
ISOLDE Collaboration fs RaII	1.254 (0.003) [0.066]
Wendt et al, fs RaI	1.19 (0.12)
RMBPT	1.28
ISOLDE Collaboration fs RaI	1.190 (0.007) [0.126]
ISOLDE Collaboration B(E2)	1.20
This work	1.225 (0.005)

It is important to note that the key quantitative factor of the agreement between theory and experiment is associated with correct accounting for electron-electron correlations, correction for the finite size of the nucleus, taking into account Breit and QED radiation effects. Analysis shows that the contribution due to electron-electron correlations to the HFS constants is ~ 100-500 MHz for various states. This circumstance explains the low degree of consistency in the accuracy of the data presented, obtained within the framework of various versions of the DF method. The contributions of higher-order corrections to the QED TV and corrections for the finite size of the nucleus can reach 1–2 tens of MHz, and it seems important to take them into account more correctly. In addition, it is necessary to take into account the nuclear polarization contributions directly, 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 [34, 35]. The key difference between the results of calculations within the different theoretical schemes is associated with different methods of accounting for electron-electron correlations.

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PACS 31.30.Gs

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Summary. The calculational results for the hyperfine structure (HFS) parameters for the Mn atom (levels of the configuration $3d^6 4s$) and the results of advanced calculating the HFS constants and nuclear quadrupole moment for the radium isotope ${}^{223}_{88}Ra$ are obtained on the basis of computing 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 relativistic Hartree-Fock Dirac-Fock and many-body perturbation theory methods calculations is explained by using the different schemes of taking into account the interelectron correlations as well as nuclear and radiative ones.

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

PACS 31.30.Gs

Макушкина М.П., Антошкина О.А., Хецелиус О.Ю.

ПАРАМЕТРЫ СВЕРХТОНКОЙ СТРУКТУРЫ СЛОЖНЫХ АТОМОВ В РАМКАХ РЕЛЯТИВИСТСКОЙ МНОГОЧАСТИЧНОЙ ТЕОРИИ ВОЗМУЩЕНИЙ

Резюме. Представлены результаты расчетов параметров сверхтонкой структуры (СТС) атома Mn (уровни конфигурации $3d^6 4s$) и результаты уточненного вычисления а констант СТС и квадрупольного момента ядра для изотопа радия ${}^{223}_{88}Ra$ 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, а также учета ядерных и радиационных поправок.

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

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ПАРАМЕТРИ НАДТОНКОЇ СТРУКТУРИ СКЛАДНИХ АТОМІВ В РАМКАХ РЕЛЯТИВІСТСЬКОЇ БАГАТОЧАСТИНКОВОЇ ТЕОРІЇ ЗБУРЕНЬ

Резюме. Представлені результати розрахунків параметрів надтонкої структури (НТС) атома Mn (рівні конфігурації $3d^6 4s$) і результати уточненого обчислення a констант НТС і квадрупольного моменту ядра для ізотопу радію $^{223}_{88}Ra$ 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, а також врахування ядерних і радіаційних поправок.

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