MENU 2007
11th International Conference
on Meson-Nucleon Physics and
the Structure of the Nucleon
September10-14, 2007
IKP, Forschungzentrum Jülich, Germany

# NUCLEAR ELECTRIC QUADRUPOLE MOMENTS AND HYPERFINE STRUCTURE PARAMETERS FOR HEAVY ISOTOPES

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**Abstract**

Consistent calculation of the nuclear electric quadrupole moments and hyperfine structure parameters for heavy elements is carried out within the gauge-invariant QED perturbation theory with using the optimized one-quasiparticle representation with account of relativistic, correlation, nuclear, QED effects. The charge distribution in a nucleus is modelled within the Gauss model. Nuclear electric quadrupole moments Q, the hyperfine structure constants for a number valent states of $^{201}$Hg, $^{223}$Ra are defined.

## 1 Introduction

In last years a studying the spectra of heavy elements isotopes is of a great interest for further development as atomic and as nuclear theories (c.f.[1-8]). Well known multi-configuration Dirac-Fock (MCDF) approach is the most reliable version of calculation for atomic systems, but , as a rule, detailed description of the method for studying role of the nucleus finite size effect (NFSE) is lacking. As alternative approach one can consider the PT on parameters *1/Z*, $\alpha Z$ ($\alpha$ is a fine structure constant). It permits evaluations of the relative contributions of different expansion energy terms: nonrelativistic, relativistic ones, as the functions of Z. But, the serious problems are connected with correct definition of the QED corrections: the Lamb shift (LS), the LS self-energy (SE) part, vacuum polarization (VP), the nuclear finite size correction etc. Here we present the results of calculation of the nuclear electric quadrupole moments and hyperfine structure parameters for

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heavy elements (Hg, Ra) within the gauge-invariant QED perturbation theory with using the optimized one-quasiparticle representation and correct account of relativistic, correlation, nuclear, QED effects [9-14].

# 2 QED perturbation theory approach with account of the nuclear corrections

The wave functions zeroth basis is found from the Dirac equation solution with potential, which includes the core ab initio potential, electric, polarization potentials of nucleus (the gaussian form for charge distribution in the nucleus is used). We set the charge distribution in the nucleus by the Gaussian function:

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

Here $\gamma = 4/\pi R^2$; $R$ is an effective nucleus radius, defined as: $R = 1.60 \times 10^{-13} z^{1/3}$ $(cm)$.

The Coulomb potential for spherically symmetric density $\rho\left(r|R\right)$ is:

$$V_{nucl}\left(r|R\right) = -\left((1/r\right)\int\limits_0^r dr' r'^2 \rho\left(r'\middle|R\right) + \int\limits_r^\infty dr' r' \rho\left(r'\middle|R\right)$$

One can write the DF-like equations for a N-electron system. Formally they fall into one-electron Dirac equations for the corresponding orbitals with potential: which includes the electrical and polarization potentials of the nucleus. The correlation corrections are taken into account within the Green functions method (with the use of the Feynman diagram technique). There have taken into account all correlation corrections of the second order and dominated classes of the higher orders diagrams (electrons screening, particle-hole interaction, mass operator iterations) [9-14]. The part $V_{ex}$accounts for exchange inter-electron interaction. The main exchange effect will be taken into account . The rest of the exchange-correlation effects are accounted for in the first two PT orders by the total inter-electron interaction [12]. The core electron density is defined by iteration algorithm within gauge invariant QED procedure [10]. The magnetic inter-electron interaction is accounted in the lowest (on $\alpha^2$ parameter), the LS polarization part - in the Uehling-Serber approximation, self-energy part of the LS is accounted effectively within the Ivanov-Ivanova non-perturbative procedure [15].

Table 1: Presented values of nuclear electric quadrupole moment $Q$(mb) of $^{201}$Hg [3]

| $Q$(mb) |
| --- |
| 380 387 (6) 347 (43,0) 385 (40) 485 (68) 386 (49) 267 (37) 390 (20) 455 (40) 420 500 (50) 6 |

# 3 Hyperfine structure constants and nuclear quadrupole moment for $^{201}$Hg isotope.

We carried out the calculation of the hyperfine structure constants and nuclear quadrupole moment for $^{201}$Hg isotope. Mercury has one stable isotope $^{201}$Hg ($I = 3/2$)with relative abundance 13,2% . The isotope $^{199}$Hg with relative abundance 16,9% has two excited states at 158 and 208 keV. Values of the quadrupole moments for several radioactive isotopes with masses from 185 to 203 were reported by Ulm et al. (c.f.[3]). A comprehensive compilation of the quadrupole moments for the isotopes in the mass range 185-206 was included in the tables of Raghavan. Most of these data are based on the primary $Q(^{201}\mathrm{Hg})$ value, combined with measured isotopic ratios. A number of available experimental values of the quadrupole moment $Q(^{201}\mathrm{Hg})$ are quoted in table 1. The "muonic 3d" value of 386(49)mb was used in a recent "year-2001" summary of nuclear quadrupole moments [3]. In table 2 we present our calculated values of the nuclear electric quadrupole moment $Q$(mb) of $^{201}$Hg and magnetic dipole hyperfine structure constants A (MHz) of the $^3P_1$ state of neutral mercury, compared with the uncorrelated DF, MCDF (with account Breit and QED corrections) [3]. Our final result fits between the latest values obtained by the group of Ulm. Regarding an error bar, preliminary analysis gives an estimate $\Delta Q$ ~7mb.

Note: [a] standard value of Raghavan [3]; [b]combines the $^{199}$Hg (I=5/2) value with the 201/199 ratio;

[c] direct muonic measurement on $^{201}$Hg; [d] solid $HgCl_2$ plus $^{199}$Hg nuclear primary value;

# 4 Hyperfine structure constants and nuclear quadrupole moment for $^{223}$Ra isotope

Further we present the experimental data and our theoretical results (QEDPT with the gauss model of charge distribution in a nucleus) calculating the energies and constants of the hyperfine structure, nuclear moments $Q$ for atom of radium $^{223}_{88}Ra$. It has the external valent shell 7s$^2$ and can be treated as

Table 2: Calculated values of the nuclear electric quadrupole moment $Q$(mb) of $^{201}$Hg and magnetic dipole hyperfine structure constants $A$ (MHz) of the $^3$P$_1$ state of $^{201}$Hg, compared with the uncorrelated DF, MCDF (with account Breit and QED corrections) [3].

| Method | $Q$ (mb) | $A$ (MHz) | $B$ (MHz) |
|---|---|---|---|
| Uncorelated DF | 478,13 | -4368,266 | — |
| MCDF (Breit+QED) | 386,626 | -5470,810 | — |
| This work | 380, 518 | -5464, 324 | -286,512 |
| Experiment | See table 1 | -5454,569 (0,003) | -280,107 (0,005) |

Table 3: Experimental and theoretical data on magnetic dipole constant of the hyperfine structure A (in MHz) for the states: 7s7p $^1$P$_1$, $^3$P$_1$ and $^3$P$_2$of radium (calculation by different methods: DF, MCDF with accounting for the Breit and QED corrections, relativistic method of configuration interaction with accounting for correlation corrections within random phase approximation (RCI-RPA) and QED perturbation theory method) [4].

| Method/State | $^1$P$_1$ | $^3$P$_1$ | $^3$P$_2$ |
|---|---|---|---|
| DF | -226,59 | 803,97 | 567,22 |
| MCDF (Brait+KED) | -330,3 | 1251,9 | 737,1 |
| RCI-RPA | -242,4 | - | - |
| QEDPT | -339,1 | 1209 | 704,5 |
| Experiment | -344,5(0,9) | 1201,1(0,6) | 699,6(3,3) |

the two-quasiparticle system. In table 10 we present the experimental and theoretical data on magnetic dipole constant of the hyperfine structure A (in MHz) for the states: 7s7p $^1$P$_1$, $^3$P$_1$ and $^3$P$_2$of radium $^{223}_{88}Ra$. In table 3 we present also the results of calculation by other methods, namely: standard uncorrelated Dirac-Fock (DF) method, multiconfiguration DF method (MCDF) with accounting for the Breit and QED corrections, relativistic method of configuration interaction with accounting for correlation corrections within random phase approximation (RCI-RPA) [4].

In table 4 we present the values of electric quadrupole moment Q (in barn) for isotope of $^{223}$Ra [3], which are experimentally obtained by the ISOLDE Collaboration (CERN) within different methodics and theoretically on the basis of calculations by MCDF (with account of the QED and Breit corrections), relativistic multi-body perturbation theory (RMBPT) and our QED perturbation theory (QEDPT).

The key factor of agreement between theory and experiment is connected with a correct accounting for interelectron correlation effects, corrections

Table 4: Values of electric quadrupole moment Q (in barn) for isotope of $^{223}$Ra

| Method | Q (barn) |
|---|---|
| MCDF (Breit plus 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) | 1,2 |
| QEDPT | 1,22 (0,03) |

due to the finite size of nucleus, the Breit and radiative QED corrections. The key difference between calculation results by MCDF, RMBT, QEDPT methods is connected with different schemes of accounting for interelectron correlations. The well-known MCDF [1-4] method is not gauge-invariant one and an accounting of multi-electron correlations is not fully fulfilled. ¿From the other side, contributions of the high orders QED PT corrections, nuclear contributions may reach dozens of MHz and must be correctly accounted for. It is necessary also to take into account more correctly the spatial distribution of magnetic moment inside a nucleus (the Bohr-Weisskopf effect), the nuclear-polarization corrections that can be done within solving the corresponding nuclear task, for example with using the shell model with Woods-Saxon and spin-orbit potentials [12-14].

# Acknowledgments

The author is very much thankful to Prof.Dr.Hartmut Machner and also Prof.Dr. S. Krewald , Mrs. S. Schadmand for invitation to make contributions on The Eleventh International Conference on Meson-Nucleon Physics and the Structure of the Nucleon-MENU2007 (Juelich, Germany) and support . Author acknowledges the support of the Abdus Salam ICTP Centre (Trieste, Italy), University of Dresden (Germany).

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