Applied computing approach calculations for g-Factor and HFS calculations of Light Ions.

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Abstract. Electron correlation effects on the bound-electron $g$-factor and hyperfine structure in highly charged ions are calculated by a combination of perturbation theory to leading order in $1/Z$, with $Z$ being the atomic number, and a large-scale relativistic configuration interaction method. Our results for lithiumlike ions improve the accuracy of earlier calculations by one or two digits.

1. Introduction

Over the last decades, there has been a growing interest in the $g$-factor of a bound-electron, both theoretically (see e.g. [1, 2, 3]) and experimentally (see e.g. [4, 5, 6]). This interest is rising partly due to the development of experiments on highly charged ions utilizing ion traps. The study of these systems also provides the opportunity to determine fundamental constants such as the mass of the electron [7, 8]. Experiments on ions of high $Z$ are of great interest from theoretical and experimental point of view and are to be performed in the nearest future. Currently, high-precision experiments of the $g$-factor of Li-like Ca are being performed. Furthermore, the precision theory of the $g$-factor of heavy B-like and H-like ions including higher-order QED and nuclear corrections is anticipated to yield, in combination with planned experiments, an independent determination of the fine-structure constant $\alpha$ [9].

In all applications involving many-electron systems, the effect of the interelectronic interaction has to be taken into account to high accuracy. First-order contributions in $1/Z$ were calculated by perturbation theory. Higher-order contributions were evaluated by means of the configuration interaction Dirac-Fock-Sturmian method in Ref. [10, 11].

Hyperfine splitting (HFS) in highly charged ions gives a sensitive tool for testing quantum electrodynamic (QED) effects in strongest electric and magnetic fields. High-precision measurements of the ground-state hyperfine splitting were executed for a number of H-like ions, including $^{209}$Bi, $^{165}$Ho, $^{185}$Re, $^{207}$Pb, $^{203}$Tl and $^{205}$Tl in Ref. [12]. This experimental progress has motivated an effort for accurate calculations. The theoretical uncertainty of the hyperfine splitting is dominated by the nuclear effects, especially by the Bohr-Weisskopf effect caused by the inhomogeneous nuclear magnetization distribution [13]. Recent theoretical research has proved that if a specific difference between the HFS for H- and Li-like ions (or H- and B-like ions...
ions) of the same isotope is applied, the Bohr-Weisskopf effect can be largely cancelled and a higher accuracy for testing strong-field QED can be reached than with studies on the binding energy.

2. Interelectronic-interaction correction

Let us start by writing the interelectronic-interaction correction $\Delta g_{\text{int}}$:

$$
\Delta g_{\text{int}} = 2 \left[ \frac{(\alpha Z)^2}{Z} B(\alpha Z) + \frac{(\alpha Z)^2}{Z^2} C(\alpha Z) + \frac{(\alpha Z)^2}{Z^3} D(\alpha Z) + \ldots \right],
$$

(1)

Here, $B(\alpha Z)$, $C(\alpha Z)$, and $D(\alpha Z)$ are the functions that define the interelectronic-interaction correction terms of first, second, and third orders in $1/Z$, respectively. The derivation of the interelectronic-interaction correction in first order in the expansion parameter $1/Z$ was considered in detail in Ref. [?, ?]. In our calculation we divide this contribution into two parts, namely, the part which may be also derived from standard quantum mechanical perturbation theory,

$$
\Delta E_{\text{int}} = \sum_{m_e} \left[ \sum_P (-1)^P \sum_n \frac{\langle P_v P_c | I(\Delta_{P_v}) | n c \rangle \langle n | \delta V | v \rangle}{\varepsilon_v - \varepsilon_n} ight. \\
+ \sum_P (-1)^P \sum_n \frac{\langle v | \delta V | n c \rangle \langle I(\Delta_{P_v}) | P_v P_c \rangle}{\varepsilon_v - \varepsilon_n} \\
+ \sum_P (-1)^P \sum_n \frac{\langle P_v P_c | I(\Delta_{P_v}) | v n \rangle \langle n | \delta V | c \rangle}{\varepsilon_v - \varepsilon_n} \\
+ \sum_P (-1)^P \sum_n \frac{\langle c | \delta V | n \rangle \langle v n | I(\Delta_{P_v}) | P_v P_c \rangle}{\varepsilon_v - \varepsilon_n} \right],
$$

(2)

and a QED part involving derivatives with respect to the frequency of the exchanged photon:

$$
- \sum_{m_e} \left[ \langle v c | I'(\Delta_{vc}) | v c \rangle (\langle v | \delta V | v \rangle - \langle c | \delta V | c \rangle) \right] .
$$

(3)

where, $v$ and $c$ are the valence and core electron states, $m_e$ is the angular momentum projection of the core electron, $\delta = \varepsilon_v - \varepsilon_c$, $\delta V(\tilde{x}) = e \tilde{\alpha} \cdot \tilde{A}_c(\tilde{x})$ is the interaction operator of the external magnetic field, $I(\omega) = \epsilon^2 \alpha^\rho \alpha^\sigma D_{\rho\sigma}(\omega)$, $D_{\rho\sigma}(\omega, \tilde{x} - \tilde{y})$ is the interaction operator which can be derived from the exchange of a virtual photon between two electrons. The photon propagator is denoted by

$$
D_{\rho\sigma}(\omega, \tilde{x} - \tilde{y}) = g_{\rho\sigma} \frac{\exp(i|\omega|\|\tilde{x} - \tilde{y}\|)}{4\pi|\tilde{x} - \tilde{y}|}.
$$

(4)

The related contribution to the $g$-factor is denoted as $\Delta g_{\text{int}} = \Delta E_{\text{int}} / \mu_0 H m_v$, where $\mu_0 = |e|/2m$ is the Bohr magneton and $m_v$ is the angular momentum projection of the valence electron.

Eq. (2) contains sums over intermediate states excluding the valence $2s$ reference state. We use a relativistic Sturmian basis set of single-electron wave functions (see the next section for more details) to perform the summation numerically. In order to saturate these sums, we take into account all virtual orbitals with $s$ and $d$ symmetries with principal quantum numbers up to 50.
3. Higher-order corrections by means of the configuration interaction method

Higher-order contributions of the electron-electron interaction in powers of $1/Z$ may be evaluated perturbatively or by some all-order procedure. We use here a configuration interaction method to evaluate second- and higher-order terms. The schema of our calculation is following: firstly we perform the calculation of occupied one-electron wave functions by Dirac Fock (DF) method, next calculation is calculation DF-Sturm equations, that means that we add to our DF basis virtual DS orbitals, than we calculate DS orbitals for the negative Dirac spectrum so as to double the one-electron basis. Finally we apply the Restricted Active Space. Dirac-Sturm (DS) equations are solved for the each value of the relativistic quantum number $\kappa$. This set of functions yields a basis of one-electron functions that we use for the calculations.

To implement the configuration interaction (CI) methods and the many-particle perturbation theory (PT), it is necessary to first build a basis of single-electron functions. The natural choice for such functions is the populated orbitals of the DF or MCDF method. The set of these functions must then be supplemented with additional vacant (virtual) orbitals. Virtual orbitals can, for example, be obtained as the eigenfunctions of an DF operator.

In Breit approximation, the system can be described by the Hamiltonian

$$H = \sum_i h_D(i) + \sum_{i,j} V(i,j),$$

where $h_D$ is a one-electron Dirac Hamiltonian

$$h_D = c(\alpha \cdot \rho) + (\beta - 1)c^2 + V(r),$$

and $V(i,j)$ is a two-electron interaction Coulomb-Breit operator

$$V(i,j)\alpha \left[ \frac{1}{r_{ij}} - \frac{\alpha_i \cdot \alpha_j}{r_{ij}^2} - \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{2r_{ij}^3} \right]$$

$$\hat{H} = \sum_i \hat{h}_i + \sum_{i<j} \hat{v}_{ij}.$$  

In the central-field approximation, the single-electron Dirac-Fock orbital is a four-component Dirac spinor

$$\Psi_{n\kappa\mu}(r) = \frac{1}{r} \left( \begin{array}{c} P_{n\kappa}(r) \\ iQ_{n\kappa}(r) \\ \chi_{\kappa,\mu}(\theta, \vartheta) \\ -\chi_{-\kappa,\mu}(\theta, \vartheta) \end{array} \right),$$

where $\kappa = (-1)^{j+1/2-1}(j+1/2)$ is the relativistic quantum number, $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are radial functions and $\chi_{\kappa\mu}$ is the spherical Pauli spinor

$$\chi_{\kappa\mu}(\vec{r}, \sigma) = \sum_m \sum_{m_s} C_{lm,1/2m_s}^{\mu} Y_{lm}(\vec{r}) \cdot \eta_{m_s}(\sigma).$$

The Sturm orbitals are localised in the region where the weight function is slice to constant and approximately coincide with the occupied HF or DF states. Such orbitals are excluded from consideration and, in their place, the HF or DF orbitals are included in the basis. The relativistic Sturm operator, like the DF operator, has a negative Dirac spectrum. However, unlike the DF operator, the negative spectrum of the Sturm operator is discrete, and the corresponding orbitals decay exponentially with increasing $r$. Thus, in the non-relativistic case, the single-electron basis is constructed as following: the basic functions of the occupied states were chosen as numerical solutions of the HF equations and for virtual states the eigenfunctions of the Sturm operator.
were used. In the relativistic case, the basis doubles due to the addition of the Sturm orbitals corresponding to the negative Dirac spectrum. The combined relativistic basis of the DF orbitals and the Sturm functions will be called the Dirac-Sturm (DS) basis. Let’s consider the Fock operator $h^F$ and generalized eigenvalue problem on a Sturmian:

$$h^S \phi_j = \lambda_j W(r) \phi_j, \quad h^S = h^F - \varepsilon_0$$

(11)

$$h^S = h^F - \varepsilon_0$$

(12)

Here $W(r)$ is a weight function that asymptotically approach zero and $\varepsilon_0$ is usually the one-electron energy of one of the valence states.

If the weight function $W(r)$ tends to a constant value as $r \to 0$, then the asymptotic behaviour of the Sturm functions near zero coincides with the asymptotic behavior of the DF orbitals, since in this case $Z^* = Z$. The eigenfunctions with $\lambda_j < 0$ correspond to the negative spectrum. In other words, Sturmian orbitals with the same $\kappa$ have approximately the same radius.

To build a basis for the Slater determinants we use the concept of limited active space. Herein, the set of all Slater determinants which is included in the expansion of the multiconfiguration wave function, is obtained by generating all determinants from a given list of non-relativistic atomic configurations. The list of all non-relativistic configurations is constructed by considering single, double, triple, and quadruple excitations from one or more reference configurations. Reference configurations include those whose atomic terms and wave functions are to be determined. When generating a list of configurations herein, we used the concept of Restricted Active Space (RAS). According to this model, the entire space of single-electron radial wave functions is divided into four subspaces: inactive occupied cores (frozen core), occupied cores (closed shells), active inhabited (valence orbitals) and vacant inhabited (unfilled, highly-excited orbitals). In the DFS method, the DS orbitals belong to this space. Applying this method allows us to generate a list of all non-relativistic configurations that are included in the calculation using the CI method. In the next stage, a list of all relativistic configurations corresponding to a given set of non-relativistic configurations of the atom is constructed. Then, a list of Slater determinants $\det_\alpha \{ \phi_i(x_j) \}$, corresponding to a given set of relativistic configurations is generated.

4. Results

The interelectronic interaction correction of first order in $1/Z$ (see Table) is calculated by means of perturbation theory, and it includes the frequency-dependence of the exchanged virtual photon, as well as the derivative term. Second and higher-order terms are extracted from the CI calculation. The uncertainty of these terms is estimated by analyzing the dependence of results on the configuration set used. The uncertainty of the Dirac value is given by the error bar of the fine-structure constant, while the uncertainty of the finite nuclear size correction is determined by the error bar of the nuclear radius. See the text for further details.

The coefficients of the $Z\alpha$ expansion of the finite interelectronic interaction contribution were obtained by performing accurate numerical calculations and fitting their results to the known expansion form. To perform the calculation and to increase the accuracy of the calculation a large Sturmian basis set with the following maximal principal quantum numbers for a given symmetry: $25s, 20p, 20d, 15f, 15g, 14h, and 13k$ was used.
Table 1. Contributions to the $g$-factor of Li-like ions of selected elements.

| $g$-factor contribution   | $^{28}\text{Si}^{11+}$      | $^{40}\text{Ca}^{17+}$      | $^{129}\text{Xe}^{51+}$      |
|---------------------------|-----------------------------|-------------------------------|-------------------------------|
| Dirac value               | 1.998254750677(1)           | -1.996426010901(3)            | -1.97275020536(2)            |
| Finite nuclear size       | 0.00000000002580            | 0.0000000123764               | -0.0000031791498             |
| Interelectronic interaction | -0.0003215918(3)           | -0.00046115642(1)             | -0.0013072791(6)             |
| $1/Z$ with $\omega$-dependence | 0.00000069(1)              | 0.00000069(1)                 | 0.00000069(2)                |
| $1/Z^2$ and higher orders | -0.0003147(1)               | -0.0004543(1)                 | -0.0013004(2)                |
| total                     | -0.0003147(1)               | -0.0004543(1)                 | -0.0013004(2)                |

| $g$-factor contribution   | $^{208}\text{Pb}^{79+}$    | $^{209}\text{Bi}^{80+}$      | $^{238}\text{U}^{89+}$       |
|---------------------------|-----------------------------|-------------------------------|-------------------------------|
| Dirac value               | -1.9320029038(1)            | -1.93006881925(6)             | -1.91072262359(7)            |
| Finite nuclear size       | -0.0007568743480            | -0.0008434443120              | -0.0002322518350             |
| Interelectronic interaction | -0.00212903(1)             | -0.00219231(1)                | -0.00252792(1)               |
| $1/Z$                     | -0.00212903(1)              | -0.00219231(1)                | -0.00252792(1)               |
| $1/Z^2$ and higher orders | 0.00000773(7)               | 0.00000779(7)                 | 0.00000859(8)                |
| total                     | -0.00212130(7)              | -0.00218452(7)                | -0.00251933(8)               |

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6. References

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