

Calculation of hyperfine structure constants for ytterbium

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Abstract. We calculate energies and hyperfine structure constants A and B for low-lying levels of ^{173}Yb . The latter is treated as a two-electron atom. To account for valence–valence correlations the configuration interaction method is used. Valence–core correlations are accounted for within the many-body perturbation theory which is used to construct effective two-electron operators in the valence space.

1. Introduction

Two years ago a method for calculation of the low-lying energy levels of many-electron atoms was proposed [1]. Calculations for Tl [1], Ca, Sr, Ba and Yb [2] and Ba [3] confirmed its effectiveness. Later, this method was generalized for other observables, such as hyperfine structure (HFS) constants [4] and polarizabilities [5]. Within this method valence–valence correlations are treated non-perturbatively, while core–valence and core–core correlations are treated within the many-body perturbation theory (MBPT).

Here we report calculations for the HFS constants of the low-lying levels of Yb. Our interest in this atom is caused in part by an extremely large parity nonconserving (PNC) amplitude for the $^1S_0(6s^2) \rightarrow ^3D_1(5d6s)$ transition. It was first suggested by DeMille [6] and later confirmed in [7, 8], that this amplitude is approximately 100 times larger than the PNC amplitude for the $6s \rightarrow 7s$ transition in Cs and 10 times larger than that for the $6p \rightarrow 7p$ transition in Tl. This makes Yb a very promising candidate for the future PNC experiment. Therefore, accurate atomic calculations for Yb are needed. Moreover, it is important to have a reliable estimate of the accuracy of such calculations. The PNC amplitude is very sensitive to the behaviour of the wavefunction in the vicinity of the nucleus. Of course, the same applies to HFS constants. That makes HFS calculations very important for the future analysis of the theoretical accuracy for the PNC amplitude.

We also have a more general interest in Yb as an atom with a relatively shallow 4f core shell. For such an atom it is not obvious at all, that core–valence correlations can be treated by means of the MBPT. In our earlier paper [2] we have shown that the method works for the low-lying energy levels and here we extend our analysis to the HFS constants. We also show here, that with some caution it is possible to calculate the HFS constants of the levels, which lie above the core excitation threshold.

In the next section of this paper we define effective operators for the valence electrons and briefly describe how MBPT can be used to calculate these operators (for more details see [1, 4]). In section 3 we give some details of the calculations followed by the discussion of the results in section 4.

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2. Effective operators for valence electrons

At present there are several methods of calculation for many-electron atoms. For atoms with one electron above a closed core a conventional MBPT is quite effective (see, for example, [9]). For atoms with several valence electrons the multi-configurational Hartree–Fock (MCHF) method is often used [10]. Lately the coupled-cluster method has become very popular [11–13]. All these methods were used to calculate HFS constants of different atoms (see, for example, [14–19]).

The most complicated problem in precise atomic calculations is associated with the necessity to treat valence–valence, core–valence, and core–core correlations. The former are usually too strong to be treated perturbatively, while other types of correlations cannot be effectively treated within non-perturbative techniques, such as MCHF or configuration interaction (CI) method.

Therefore, it is natural to try to combine MBPT with one of the non-perturbative methods. In [1] it was suggested to use MBPT in order to construct an effective Hamiltonian for valence electrons. After that, the Schrödinger equation for valence electrons is solved within the CI approach. That allows us to find the low-lying energy levels. In order to calculate other atomic observables, one needs to construct corresponding effective operators for valence electrons [4]. The latter effectively account for the core–valence and core–core correlations, which are of particular importance for such singular operators as HFS ones.

Suppose, that we are interested in atomic levels with energies $E_i - E_0 < \varepsilon$, where E_0 is the ground state energy. In the first approximation we can assume that inner electrons with the Hartree–Fock energies $|\varepsilon_n| \gg \varepsilon$ form the core, which is described by the wavefunction

$$\Psi_{\text{core}} = (N_c!)^{-1/2} \det(\phi_1, \phi_2, \dots, \phi_{N_c}), \quad (1)$$

$$h_{\text{DF}}\phi_n = \varepsilon_n\phi_n, \quad (2)$$

where h_{DF} is the Dirac–Fock operator, and N_c is the number of core electrons. Note, that this operator can include the field of some valence electrons as well. For example, it is natural to consider Yb as a two-electron atom with the core $[1s^2, \dots, 4f^{14}]$, and operator h_{DF} can be calculated for configuration $1s^2, \dots, 4f^{14}6s^2$ (so-called, V^N -approximation, N is the number of electrons in the atom).

Let us say that many-electron wavefunction Ψ belongs to the valence subspace if core electrons are in the state (1). We will denote the projector operator on this subspace by P . Then, operator $Q = 1 - P$ will project on the subspace for which at least one of the core electrons is excited to one of the states ϕ_n with $n > N_c$.

One can show [1], that the Schrödinger equation

$$H\Psi = E\Psi \quad (3)$$

is equivalent to the following equation in the P -subspace for the function $\Phi = P\Psi$:

$$(PHP + \Sigma(E))\Phi = E\Phi, \quad (4)$$

$$\Sigma(E) = PV'R_Q(E)V'P, \quad (5)$$

where V' is the operator of the residual Coulomb interaction and $R_Q(E)$ is the Green function in Q -subspace:

$$V' = H - H_0, \quad (6)$$

$$R_Q(E) = Q \frac{1}{E - QHQ} Q. \quad (7)$$

Operator H_0 is defined in terms of one-electron operator (2):

$$H_0 = \sum_{i=1}^N h_{\text{DF}}(\vec{r}_i) - W. \quad (8)$$

The constant W on the right-hand side of this equation is introduced to compensate the double counting of the two-electron interaction in the sum. It can be fixed, for example, by the requirement:

$$\langle \Psi_{\text{core}} | H_0 | \Psi_{\text{core}} \rangle = \langle \Psi_{\text{core}} | H | \Psi_{\text{core}} \rangle, \quad (9)$$

which implies, that

$$W = W_0 \equiv \sum_{i=1}^{N_c} \varepsilon_i - \langle \Psi_{\text{core}} | H | \Psi_{\text{core}} \rangle. \quad (10)$$

It is also possible to use W as a free parameter to match the energy spectrum. This subject is discussed in more detail elsewhere [20].

Equations (3)–(7) yield:

$$\Psi = (P + R_Q(E)V'P)\Phi. \quad (11)$$

The orthonormality condition $\langle \Psi_i | \Psi_k \rangle = \delta_{i,k}$ is approximately equivalent to the following condition for Φ :

$$\langle \Phi_i | 1 - \partial_E \Sigma(\bar{E}) | \Phi_k \rangle \approx \delta_{i,k}, \quad (12)$$

where $\bar{E} \approx (E_i + E_k)/2$. Note, that only the last of equations (4)–(12) is approximate.

The operator in the left-hand side of equation (4) plays the role of an effective Hamiltonian H_{eff} . Equations (4)–(7) allow us to construct it with the help of the conventional diagrammatic technique [1, 2], which is based on the following representation of the Green function:

$$R_Q(E) = R_Q^0(E) + R_Q^0(E)V'R_Q(E), \quad (13)$$

$$R_Q^0(E) = Q \frac{1}{E - QH_0Q} Q. \quad (14)$$

In particular, if we restrict ourselves to the second-order MBPT, we have to replace $R_Q(E)$ in the right-hand side of (5) by $R_Q^0(E)$.

Suppose now, that we know the solutions of equation (4) and we want to use them to calculate an observable a , which is associated with the one-electron operator A :

$$a = \langle \Psi | A | \Psi \rangle. \quad (15)$$

Let us define effective operator A_{eff} so, that

$$a = \langle \Phi | A_{\text{eff}} | \Phi \rangle. \quad (16)$$

The following approximation for A_{eff} was suggested in [4]

$$A_{\text{eff}} \approx P A P + P V' R_Q^0(E) A_{\text{rpa}} P + P A_{\text{rpa}} R_Q^0(E) V' P, \quad (17)$$

where A_{rpa} corresponds to the well known random-phase approximation (RPA).

Note, that only the first-order MBPT corrections are completely included in (17). Some second-order corrections, the, so-called, structural radiation, as well as many higher-order corrections, are omitted. Nevertheless, this approximation accounts for several of the most important MBPT corrections to all orders. The diagrammatic representation of equation (17) can be found in [4].

3. Hyperfine structure calculations

We use basis representation for diagrams for effective Hamiltonian and effective HFS operators. That implies that all sums over intermediate states run over some finite set of one-electron states. The latter should effectively account for both the discrete and continuous part of the spectrum of the Dirac–Fock operator (2).

In this calculation basis set included 167 four-component orbitals: 1—23s, 2—22p, 3—22d, 4—15f, 5—15g and 6—13h. Core orbitals as well as valence orbitals 6s, 7s, 6p, 7p, and 5d, 6d were obtained by solving Dirac–Fock equations for appropriate configurations, while higher virtual orbitals were formed, as described in [1, 4, 21, 22]. After that operator (2) was diagonalized in order to have a quasi-Dirac–Fock basis set.

This basis set was used to solve the RPA equations for HFS operators and to calculate diagrams for effective Hamiltonian and effective HFS operators. After that, the solution of equation (4) was found in the CI approximation. On this stage it was possible to truncate our basis set to 7—15s, 6—15p, 5—14d, 5—10f and 5—7g orbitals. We made complete CI on this shorter basis set.

We calculated the effective Hamiltonian H_{eff} in the second order of MBPT. That means, that zero order approximation (14) for the Green function was used in (5). The choice of the constant W suggested by equation (10) resulted in some underestimation of the binding energy for levels of the configuration 5d6s and for the $^1P_1^o$ level of the configuration 6s6p. For these levels $W = W_0 + 0.4$ au was used. Our final results for the ground state are given in table 1 and for several low-lying levels in table 2.

In the next stage we used corresponding wavefunctions to calculate HFS constants. These calculations are similar to those of the papers [4] and [5]. Results are given in tables 3 and 4. In the analysis of theoretical accuracy, which is done in the next section, it is very important to know the scale of different contributions to the final answer. Therefore, in tables 3 and 4 we give results of the Dirac–Fock calculation, of the conventional two-electron CI and of the two-electron CI with an effective Hamiltonian. Final values include effective operator corrections (17) and normalization correction (12). The latter usually decreases the answer by 1–2%.

4. Discussion

We have pointed out above, that the effective Hamiltonian can be safely used only for the energy levels below the core excitation threshold. For Yb this threshold lies at $23\,189\text{ cm}^{-1}$ above the ground state and many of the levels from table 2 lie higher. Nevertheless, theoretical spectrum is quite good up to the level $^1P_1^o(6s7p)$, which appears 1634 cm^{-1} below its experimental

Table 1. Two-electron energies E_{val} of the Yb ground state in different approximations (au). MBPT corrections were calculated with $W = W_0$ (see equation (10)).

| DF ^a | MBPT ^b | CI ^c | CI+MBPT ^d | Experiment ^e |
|-----------------|-------------------|-----------------|----------------------|-------------------------|
| 0.606 810 | 0.654 308 | 0.632 398 | 0.677 601 | 0.677 584 |

^a Single-configuration approximation.

^b Single-configuration approximation with MBPT correlation.

^c Conventional CI method for two outer electrons.

^d CI+MBPT method: two-electron CI with an effective Hamiltonian formed within a second order of MBPT.

^e This is the sum of the first two ionization potentials of Yb [23].

Table 2. The low-lying levels of Yb in V^N approximation. E_{val} is the two-electron energy and Δ is the interval from the ground state. The multiplet splittings are given in parentheses. Levels marked with † were calculated with $W = W_0 + 0.4$ au and the levels marked with ‡ were calculated with $W = W_0 + 0.1$ au.

| Level | Theory | | Experiment ^a Δ (cm ⁻¹) |
|--|-----------------------|------------------------------|---|
| | E_{val} (au) | Δ (cm ⁻¹) | |
| Even states | | | |
| ³ D ₁ (5d6s)† | -0.566 086 | 24 441 | 24 489 |
| ³ D ₂ (5d6s)† | -0.564 919 | 24 697 (256) | 24 752 (263) |
| ³ D ₃ (5d6s)† | -0.562 415 | 25 247 (550) | 25 271 (519) |
| ¹ D ₂ (5d6s)† | -0.551 500 | 27 642 | 27 678 |
| ³ S ₁ (6s7s) | -0.529 514 | 32 501 | 32 695 |
| ¹ S ₀ (6s7s) | -0.521 725 | 34 210 | 34 351 |
| ³ D ₁ (6d6s) | -0.496 053 | 39 845 | 39 809 |
| ³ D ₂ (6d6s) | -0.495 902 | 39 877 (33) | 39 838 (29) |
| ³ D ₃ (6d6s) | -0.495 384 | 39 991 (114) | 39 966 (128) |
| ¹ D ₂ (6d6s) | -0.494 733 | 40 135 | 40 062 |
| Odd states | | | |
| ³ P ₀ ^o (6s6p)‡ | -0.598 858 | 17 282 | 17 288 |
| ³ P ₁ ^o (6s6p)‡ | -0.595 599 | 17 997 (715) | 17 992 (704) |
| ³ P ₂ ^o (6s6p)‡ | -0.587 613 | 19 750 (1753) | 19 710 (1718) |
| ¹ P ₁ ^o (6s6p)† | -0.563 354 | 25 074 | 25 068 |
| ³ P ₀ ^o (6s7p) | -0.504 463 | 38 000 | 38 091 |
| ³ P ₁ ^o (6s7p) | -0.504 096 | 38 080 (80) | 38 174 (83) |
| ³ P ₂ ^o (6s7p) | -0.502 388 | 38 455 (375) | 38 552 (378) |
| ¹ P ₁ ^o (6s7p) | -0.500 224 | 38 930 | 40 564 |

^a [23].

Table 3. Magnetic dipole (A) and electric quadrupole (B) hyperfine structure constants of low-lying even-parity levels for ¹⁷³Yb. The electric quadrupole moment is taken to be 2.80 b.

| | ³ D ₁ (5d6s) | ³ D ₂ (5d6s) | ³ D ₃ (5d6s) | ¹ D ₂ (5d6s) | ³ S ₁ (6s7s) | ³ D ₁ (6s6d) | ³ D ₂ (6s6d) | ³ D ₃ (6s6d) | ¹ D ₂ (6s6d) |
|-------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|---------------------------------------|
| A (MHz) | | | | | | | | | |
| DF | 447 | -200 | -348 | -18 | -1225 | 490 | -206 | -337 | 28 |
| CI | 443 | -288 | -348 | 62 | -1489 | 633 | -468 | -437 | 238 |
| H_{eff} | 588 | -398 | -469 | 105 | -1910 | 830 | -677 | -567 | 380 |
| Total | 596 | -351 | -420 | 131 | -1938 | 838 | -683 | -569 | 392 |
| Experiment ^a | 563(1) | -362(2) | -430(1) | 100(18) | -1879(10) | 818.7(4) | -732.5(4) | -559.9(5) | 438.5(4) |
| B (MHz) | | | | | | | | | |
| DF | 151 | 206 | 353 | 379 | 0 | 32 | 45 | 76 | 81 |
| CI | 156 | 229 | 368 | 676 | 0.3 | 38 | 55 | 92 | 115 |
| H_{eff} | 219 | 314 | 492 | 693 | 0.2 | 38 | 62 | 92 | 115 |
| Total | 290 | 440 | 728 | 1086 | 0.2 | 58 | 96 | 150 | 184 |
| Experiment ^a | 335(1) | 482(22) | 909(29) | 1115(89) | < -3(18) | 59.3(2) | 52.5(2) | 139.6(3) | 142.2(2) |

^a HFS constants for configuration 5d6s were measured in [24], for ³S₁-state in [25], and for configuration 6s6d in [26].

position. This huge discrepancy can be attributed to interaction with the $J = 1$ level at 38 422 cm⁻¹, which is supposed to belong to the configuration 4f¹³5d²6s [23]. This level can also interact with ³P₁^o(6s7p), which makes calculations for this level less reliable. For

Table 4. Magnetic dipole (A) and electric quadrupole (B) hyperfine structure constants of low-lying odd-parity levels for ^{173}Yb .

| | $^3P_1^o$ (6s6p) | $^3P_2^o$ (6s6p) | $^1P_1^o$ (6s6p) | $^3P_1^o$ (6s7p) | $^3P_2^o$ (6s7p) |
|------------------|--|---------------------|--|-----------------------|----------------------|
| | A (MHz) | | | | |
| DF | -664 | -527 | -25 | -667 | -507 |
| CI | -765 | -556 | 98 | -1044 | -666 |
| H_{eff} | -1075 | -741 | 187 | -1468 | -862 |
| Total | -1094 | -745 | 191 | -1488 | -871 |
| Experiment | -1094.0(7) ^a -1094.2(6) ^d | -738 ^b | 60(5) ^b 58(3) ^e | -1144(1) ^c | -854(2) ^c |
| | B (MHz) | | | | |
| DF | -454 | 715 | 811 | -90 | 150 |
| CI | -533 | 860 | 428 | -80 | 163 |
| H_{eff} | -633 | 1013 | 642 | -82 | 192 |
| Total | -822 | 1335 | 848 | -111 | 264 |
| Experiment | -826.5(1) ^a -827.2(5) ^d | 1312 ^b | 604(7) ^b 588(2) ^e | 12(4) ^c | 267(25) ^c |

^a [26].^b [28].^c [24].^d [27].^e [29].

other levels from table 2 there are no close levels with the same J and the same parity, which correspond to the excitations from the 4f-shell.

The perturber levels, discussed above, correspond to the poles of the Green function $R_Q(E)$ and, thus, to the poles of the operator $\Sigma(E)$. As long as we use an approximate Green function (14) instead of the exact one, the poles of $\Sigma(E)$ are shifted from the physical poles. In order to use an effective Hamiltonian, we have to keep far enough from the poles of the exact Green function and from the poles of the approximate Green function. As we go further up above the core excitation threshold, both sets of poles become denser. For this reason, it is hardly possible to use the effective operator technique there.

Let us now proceed to the calculations of HFS constants presented in tables 3 and 4. In these tables the first two rows correspond to the non-perturbative part of the calculation, while the two lower rows include MPBT corrections associated with the effective Hamiltonian and the effective HFS operators. One can see, that the average MBPT contribution is about 30% for magnetic constant A and about 40% for the electric quadrupole constant B . Thus, theoretical accuracy for the constant A is normally higher. Indeed, we have neglected higher-order corrections to the effective Hamiltonian and to the effective HFS operators, that can only be justified if MBPT corrections are small.

For six levels ($^3D_2(5d6s)$, $^3D_3(5d6s)$, $^3S_1(6s7s)$, $^3D_1(6s6d)$, $^3D_3(6s6d)$, and $^3P_2^o(6s7p)$) MBPT corrections to the constant A are less than 25%. For all these levels the difference between the theory and experiment is within 3%. For the constant B the smallest MBPT corrections (about 35%) correspond to levels $^3D_1(6s6d)$ and $^3P_1^o(6s6p)$, where we have agreement with the experiment within 2%. Constant B for $^3S_1(6s7s)$ -state differs from zero only because of the configuration interaction.

On the other hand, when MBPT corrections are 40% or more, the accuracy of the theory becomes uncertain. The most striking discrepancy with the experiment takes place for levels $^1D_2(5d6s)$, $^3D_2(6s6d)$ and $^1P_1^o(6s6p)$. For all of them MBPT corrections appear to be 40–50%.

The only exception of this rule is the level $^3P_1^0(6s7p)$, where MBPT corrections for both constants are about 30%, but even the sign of the constant B differs from the experiment. As we pointed out above, this level can interact with the perturber level $4f^{13}5d^26s(J = 1)$, which is located at $38\,422\text{ cm}^{-1}$. Constant B for this level is relatively small and even small admixture of the perturber can result in the change of its sign, while the larger constant A should be less affected by such a mixing.

5. Conclusion

In this paper we have checked the applicability of the CI+MBPT method for Yb. The first core excitation here lies only $23\,189\text{ cm}^{-1}$ above the ground state, which seems to restrict us to only few lowest levels. Actually, the method works quite well up to $38\,930\text{ cm}^{-1}$, where the first significantly perturbed level arises.

When the method is used for calculations of HFS constants, the accuracy of calculations depends on the scale of the MBPT corrections. When the total MBPT correction contributes less than 25% to the value of the constant, the accuracy appears to be better than 3%. In contrast, when MBPT corrections account for more than 40% of the theoretical value, the accuracy becomes uncertain. In this case one can use the MBPT correction only as a rough estimate of the theoretical error. We expect, that similar relation holds for other one-electron operators as well.

For the studied levels of Yb the average MBPT correction is approximately 30% for the constant A and 40% for the constant B . Therefore, precision calculations of the constant A are possible for the majority of levels, while precision calculations of the constant B are possible only as exception.

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