Calculation of the weak interactions in dysprosium

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P-odd and P,T-odd transition amplitudes for the two almost degenerate levels of opposite parity with $J = 10$ and $E = 19\,797.96$ cm^{-1} are calculated. Our result for the P-odd amplitude of the interaction with the weak charge of the nucleus is $(70 \pm 40)(-i)$ Hz. The P,T-odd amplitude caused by the electric dipole moment of the electron d_e is $(1.2 \pm 0.5) \times 10^{23}$ Hz/(e cm). We also calculated g factors and hyperfine constants A and B for several levels. These results are in good agreement with experiment. The calculated lifetime of 6 μ sec for the positive parity level is reasonably close to 8 μ sec measured by D. Budker *et al.* [Phys. Rev. Lett. **70**, 3019 (1993)].

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I. INTRODUCTION

In the spectrum of dysprosium there are two almost degenerate metastable levels ($E = 19797.96$ cm^{-1}) of opposite parity but equal angular momentum $J = 10$. As was pointed out in [1,2] this provides an opportunity for a strong manifestation of parity-nonconserving (PNC) weak interactions. These interactions include both time-reversal invariant (T-even) and noninvariant (T-odd) terms. In this paper we shall restrict ourselves to two T-even and two T-odd amplitudes associated with the so-called weak charge Q_W and the anapole moment of the nucleus, the electric dipole moment (EDM) of the electron d_e and the magnetic quadrupole moment of the nucleus M. For a wide discussion of possible manifestations of the weak interactions in atomic physics and the role of atomic measurements for particle physics see Refs. [3,4]. The computational methods are described in a recent review [5].

An experiment on this almost degenerate pair of levels is now under way at the University of California at Berkeley. In the first stage a number of spectroscopic parameters, such as the lifetimes, the hyperfine constants, and the isotope shifts were measured [6–9]. This allows us to check the quality of our wave functions and the reliability of the results for the weak interactions.

II. DESCRIPTION OF THE CALCULATION PROCEDURE

To get correct results for the effects caused by weak interaction both the configuration interaction (CI) and the core polarization must be taken into account. It can be illustrated with an example of two nearly degenerated levels of Dy at $E = 19798$ cm^{-1}. The leading configuration for the even level is $4f^{10}5d6s$ and for the odd one it is $4f^9 5d^2 6s$. So, the one-electron transition between these two levels is a d-f transition and the corresponding weak matrix element is negligibly small. However, the transition amplitude between these two levels is nonzero for two reasons.

(i)There is an admixture of the $4f^9 5d6s6p$ configuration to the even level and the $4f^9 5d6s^2$ configuration to the odd one. Hence, the one-electron s-p transition is possible.

(ii) The d-f matrix element becomes non-zero if one takes into account the core polarization by the residual Coulomb interaction.

The calculations were performed in two steps to take into account both of these effects. In the first step the Hartree-Fock-Dirac (HFD) equations were solved and the configuration interaction within the valence shells was taken into account. For this step we used the program package written at Petersburg State University and kindly given to us by I. I. Tupizin. It includes the HFD program [10] and CI program [11]. In the second step the package developed in Novosibirsk was used [12] to include core excitations.

A. Valence shell calculations

There are four nonrelativistic valence shells in dysprosium, namely the $4f$, $5d$, $6s$, and $6p$ shells. According to the experimental data [13] and theoretical analysis [14], the low-lying levels of Dy belong to the following configurations:

even: $4f^{10}6s^2$, $4f^9 6s^2 6p$, $4f^{10}5d6s$
odd: $4f^9 5d6s^2$, $4f^9 5d^2 6s$, $4f^{10}6s6p$, $4f^{10}5d6p$.

Each of these nonrelativistic configurations includes a set of relativistic configurations corresponding to different occupations of the $(4f_{5/2}, 4f_{7/2})$, $(5d_{3/2}, 5d_{5/2})$, and $(6p_{1/2}, 6p_{3/2})$ subshells. In the CI calculations we were able to include about 30 relativistic configurations for each state. Because of this restriction it was important to optimize the HFD basis set for the valence electrons.

It appeared that the HFD orbitals significantly differ for the configurations with 9 and 10 $4f$ electrons. To construct the most appropriate basis set we examined the relative energies of the levels of different configurations. Our main basis set was obtained in the following way. The complete system of HFD equations was solved for the $4f^{10}6s5d$ configuration to find the core orbitals, as well as the $4f$ and $6s$ orbitals. Then, the $6p$ orbitals were obtained for the $4f^9 6s5d6p$ configuration with the $4f, 6s$, and the core orbitals frozen. At the next stage, the $5d$ orbitals were calculated for the $4f^9 6s5d^2$ configuration with all orbitals except $5d$ frozen. The $6d$ orbitals were obtained in the double charged ion of the $4f^9 6d$ configuration. For this basis set the relative positions of the different configurations were in reasonable agreement with [13,14]. Nevertheless, it appeared necessary to improve the $5d$ orbital for the $4f^{10}5d6s$ configuration by adding the excited $6d$ orbitals. No other excitations from the valence shells were included. We also checked our results with a different basis set which was obtained starting from the $4f^{10}6s^2$ configuration. It turned out that the g factors and the hyperfine structure constants are relatively stable while weak interaction results were much more sensitive to choice of the basis set (see below).

All five levels of the ground state multiplet ($J = 8,\ldots,4$) were calculated with 25 relativistic configurations corresponding to $4f^{10}6s^2$, $4f^{10}6p^2$, $4f^{10}5d^2$ nonrelativistic configurations. We also made calculations for the ground state alone with the addition of the $4f^9 5d6s6p$ configuration. After that we calculated four even levels with $J = 9, 10, 11$ of the $4f^{10}5d6s$ configuration. In this calculation the contributions of the $4f^{10}6s6d$, $4f^{10}6p^2$, $4f^9 5d^2 6p$, and $4f^9 5d6s6p$ configurations were included. Finally, four odd levels with $J = 9, 10$ for the $4f^{10}6s6p$ and $4f^9 5d^2 6s$ configurations were calculated with the addition of the $4f^{10}5d6p$, $4f^9 5d6p^2$, $4f^9 5d6s^2$, and $4f^9 6s6p^2$ configurations.

The resultant wave functions of the levels were used to form the single-particle density matrices and the single-particle transition matrices. The former were used to calculate the g factors, the magnetic dipole, and the electric quadrupole hyperfine constants A and B. The latter were used to calculate the $E1$ transition amplitudes and matrix elements of the weak interactions.

B. Core excitations

A technique to take into account the core polarization effect was developed in [12]. It uses a self-consistent numerical solution of the time-dependent relativistic Hartree-Fock equations (TDHF) in external fields which corresponds to inclusion of the random-phase-approximation exchange chain of diagrams in all orders of perturbation theory in the residual Coulomb interaction.

To adapt this technique to the case of dysprosium some assumptions have to be made. First of all we need a spherically symmetric potential which must be the same for the Hartree-Fock orbitals and for TDHF equations. As in [12] we made our calculations for dysprosium in the V^{N-1} approximation. Namely, we considered the $6s^2 4f_{5/2}^6 4f_{7/2}^3$ configuration of external electrons, so that the potential had the form

$$V(r) = V_c(r) + 3V_0(r)\ , \tag{1}$$

for all atomic core and excited states except the $4f_{7/2}$ state. In (1) $V_c(r)$ is the Hartree-Fock potential of the closed subshells including $6s$ and $4f_{5/2}$ and $V_0(r)$ is the spherically symmetrical part of the direct Coulomb field created by a $4f_{7/2}$ electron. For the $4f_{7/2}$ state the self-interaction must be subtracted "by hand" so that the potential for the $4f_{7/2}$ state has the form

$$V(r) = V_c(r) + 2V_0(r).$$

We consider the $6s$ state in the TDHF calculations as a core state to take into account all possible $6s$-ns excitations including excitations to the continuous spectrum. To avoid double counting the $6s$-$6p$ transition should be excluded at this stage, since it has been taken into account in CI calculations when the configurations with both $6s$ and $6p$ states are included. There is no such problem for the $4f$ state because the corresponding contributions are negligibly small.

The core polarization effect was taken into account for the PNC, EDM, and magnetic hyperfine interactions where the renormalization of higher wave contributions (e.g., d-f) is very large.

Note that the potential (1) is not the same as for the CI calculations. So we used the core polarization calculations to obtain correction factors for single-electron matrix elements rather than obtaining their absolute values.

III. RESULTS AND DISCUSSION

The first problem which has to be solved is a reliable identification of the energy levels. For the dysprosium atom where the spectrum is so dense, it is not easy. In Table I the results of the valence shell calculations are given for the energies, g factors, and hyperfine constants of the ground multiplet and the low-lying levels of both parities and $J = 9, 10, 11$. It is seen from this table that the differences between the calculated and measured level energies are large in comparison with the characteristic level spacings. On the other hand, the g factors are reproduced much better and can be used to distinguish between the levels with equal J and parity. It is probably

TABLE I. Energies, g factors, and hyperfine constants A, B for ground multiplet and several low-lying excited states with $J = 9, 10, 11$.

N	leading config.	J^p	Term	Energy (cm^{-1}) Expt. [a]	Calc.	g factor Expt. [a]	Calc.	A (MHz) Expt. [b]	Calc.	B (MHz) Expt. [b]	Calc.
I	$4f^{10}6s^2$	8^+	^5I	0	0	1.24159	1.242	163	170	1153	1366
II	$4f^{10}6s^2$	7^+	^5I	4134	4159	1.17346	1.175	178	186	1066	1277
III	$4f^{10}6s^2$	6^+	^5I	7051	7206	1.07155	1.072	196	206	1015	1198
IV	$4f^{10}6s^2$	5^+	^5I	9212	9501	0.911	0.907	227	241	944	1136
V	$4f^{10}6s^2$	4^+	^5I	10925	11285	0.618	0.614	288	305	1015	1188
VI	$4f^{10}5d6s$	9^+	$^3[8]$	17515	18895	1.316	1.319		237		706
VII	$4f^{10}5d6s$	10^+	$^3[9]$	18463	19614	1.282	1.290		220		1188
VIII	$4f^{10}5d6s$	11^+	$^3[10]$	19349	20421	1.27	1.268		204		1910
IX	$4f^{10}5d6s$	10^+	$^3[10]$	19798	21269	1.21	1.209	159	152	1865	1819
X	$4f^{10}6s6p$	9^-	$(8,1)^0$	15972	13936	1.29	1.305		241		−296
XI	$4f^{10}6s6p$	10^-	$(8,2)^0$	17513	15307	1.30	1.294		225		2434
XII	$4f^{10}6s6p$	9^-	$(8,2)^0$	17727	15605	1.25	1.248		186		2061
XIII	$4f^95d^26s$	10^-	$^9K^o$	19798	26249	1.367	1.373	218	206	2060	2228

[a]Reference [13].
[b]References [7,15–17].

not surprising since the main contribution to the angular momentum **J** and thus to the g factor values comes from the f-shell electrons. This shell appears to be rather firm and is weakly affected by the interaction of the nonrelativistic configurations (of course, the configuration mixing of the relativistic configurations is important). Another reason why the results for the g factors are good is that in this case the radial integrals are trivial.

There is quite a different situation for the hyperfine constants. Here the contributions of electrons with small angular momenta are enhanced because these electrons penetrate closer to the nucleus. The radial integrals here are not trivial and depend on both upper and lower components of the relativistic radial functions in the vicinity of the nucleus. Nevertheless, as seen in Table I our results for the hyperfine constants A and B are in good agreement with the experimental values obtained in [15–17,7]. For the A constant the discrepancy is less than 10%, while for the B constant it is larger, but still lies within 20%. The lower accuracy for the quadrupole constant can be explained by the neglect of the core polarization which is more important in this case [18].

It is useful to examine the contributions of different shells to the A and B constants. The levels IX and XIII from Table I are of main interest to us. For these two almost degenerate levels of different parity we obtained the following:
Level IX:

$$A = 152 \times (0.88 + 0.05 + 0.07 + 0)\ \text{MHz}, \quad (2a)$$

$$B = 1819 \times (0.71 + 0.29 + 0 + 0)\ \text{MHz}. \quad (2b)$$

Level XIII:

$$A = 206 \times (0.54 + 0.05 + 0.37 - 0.04)\ \text{MHz}, \quad (2c)$$

$$B = 2228 \times (1.42 - 0.42 + 0 + 0)\ \text{MHz}. \quad (2d)$$

In these equations the numbers in parentheses are the relative contributions of the f, d, s, and p shells correspondingly. It is seen that the first three contributions are significant, while that of the p shell is almost negligible (note that for these states the discrepancy in A, B between the theory and the experiment is about 6%). It means that the comparison with the experimental hyperfine constants cannot serve as a test for the contribution of the p orbitals to the electronic wave function. This contribution is especially important for the calculations of P-odd weak interactions, where s-p is the only nonzero amplitude (other amplitudes can contribute due to the polarization effects only).

In Table II the results for the $E1$ transition amplitudes are given. The calculations were performed in the length (L) and velocity (V) gauges. For the L gauge the results appeared to be much more stable in comparison to the V gauge. Indeed, the amplitude for the latter depends explicitly on the transition frequency, which is poorly reproduced in our calculations. But even for the L gauge there are large cancellations between different contributions. They are caused in part by approximate selection rules mainly associated with the coupling of f electrons and in part by the configuration interaction. The latter appears to be very important for the d-f transitions from the XIII state. The admixtures of the s-p and p-d amplitudes dominate here. For example, the leading contributions to the reduced matrix element for the XIII–IX transition correspond to the $f_{5/2}$-$d_{3/2}$, $f_{5/2}$-$d_{5/2}$, $s_{1/2}$-$p_{1/2}$, $s_{1/2}$-$p_{3/2}$, and $p_{3/2}$-$d_{5/2}$ terms,

$$R = 0.11 \times (-2.26 - 0.10 + 2.63 + 0.41 + 0.41 - 0.10)\ . \quad (3)$$

The sum in parentheses is equal to unity, while the sum of the absolute values is almost six times larger. Of course, it reduces the accuracy of our results for small amplitudes like this.

The amplitude under consideration was measured in [7] and appeared to be an order of magnitude smaller

TABLE II. $E1$ transition amplitudes. Numbers are given in atomic units for the reduced matrix elements in the length and velocity gauges.

	VI[a]		VII		VIII[b]		IX	
	L	V	L	V	L	V	L	V
X	7.2	4.8	−7.0	−4.9			− 3.8	−4.6
XI	3.6	1.8	−7.1	−4.2	11.0	7.6	− 0.3	−0.2
XII	−3.0	−0.6	2.8	0.8			−10.0	−7.2
XIII	0.0	0.0	0.1	−0.2	0.0	0.3	0.1	−0.3

[a]Levels are labeled as in Table I

[b]$E1$ transitions to the states X and XII are forbidden ($\Delta J = 2$).

than the calculated one. Unfortunately, there is no direct experimental information on large dipole amplitudes from Table II. However, in the same paper [7] the lifetime measurements were made for the IX and XIII levels. For the first of them the lifetime is determined by two relatively strong transitions to the X and XII states. Using the amplitudes in the L gauge we obtained a lifetime of 6 μsec which has to be compared with 8 μsec measured in [7]. As seen from Table II, there are no strong transitions for the state XIII. It agrees with the fact that its lifetime is more than an order of magnitude larger.

Finally, we calculated the matrix elements of the weak interaction operators for the two pairs of close-lying states of different parity:

Levels VI, XI: $\Delta J = 1$, (d-p type transition);

Levels IX, XIII: $\Delta J = 0$, (f-d type transition).

It is important that all four levels are metastable. For the first pair of levels the transition frequency is 1.17 cm^{-1}, while the hyperfine structures of the IX and XIII levels overlap and the transition frequencies lie in the microwave region. Since $\Delta J = 1$ for a transition between the VI and XI levels, the matrix element between them is not zero only for the nuclear spin-dependent interactions H_M and H_A. However, one can expect larger matrix elements for this transition because of the d-p type of the transition and the fact that for both levels VI and XI the f shell is in the same $^5I_8$ state [13].

A derivation of the effective atomic operators for the weak interactions can be found, e.g., in [3]. First of all, it is the interaction of the electron EDM d_e with the electric field of the atom (atomic units are used throughout the paper if the opposite is not stated explicitly):

$$H_d = 2d_e \begin{pmatrix} 0 & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} [-\boldsymbol{\nabla}\phi(\mathbf{r})] \ , \tag{4}$$

where $\phi(\mathbf{r})$ is the atomic potential and σ_i are the Pauli matrices. Another source of P,T violation is the interaction of the nuclear magnetic quadrupole moment M with the atomic magnetic field. This interaction depends on the nuclear spin $\mathbf{I}$ and thus plays the role of a P,T-odd correction to the hyperfine structure,

$$H_M = -\frac{M}{4I(2I-1)} T_{i,k} \frac{3}{2r^5} \gamma_0\gamma_j r_l (\epsilon_{j,l,i} r_k + \epsilon_{j,l,k} r_i) \ , \tag{5}$$

$$T_{i,k} = I_i I_k + I_k I_i - \frac{2}{3} I(I+1)\delta_{i,k} \ , \tag{6}$$

where γ_j are the Dirac matrices and $\epsilon_{j,l,i}$ is the antisymmetric tensor.

One can also consider the P-odd interactions of electrons with the weak charge Q_W and the anapole moment of the nucleus:

$$H_Q = \frac{G\alpha}{2\sqrt{2}} Q_W \gamma_5 n(\mathbf{r}) \ , \tag{7}$$

$$H_A = \frac{G\alpha}{\sqrt{2}} k_A \mathbf{I}\gamma_0\boldsymbol{\gamma} n(\mathbf{r}) \ , \tag{8}$$

where G is the Fermi constant, α is the fine structure constant, $n(\mathbf{r})$ is the nuclear density normalized to unity, and k_A is the anapole moment constant of the nucleus. For the weak charge of the nucleus we used the value

$$Q_W = -N + Z(1 - 4\sin^2\theta) \approx -N + 0.08Z \ , \tag{9}$$

where N and Z are the numbers of neutrons and protons in the nucleus and θ is the Weinberg angle. In this equation we assumed that $\sin^2\theta = 0.23$. Our results for the interactions (4), (5), (7), (8) are given in Table III, where the electronic parts W_i of the matrix elements are listed. The connection with the matrix elements between states with the total angular momentum F and its projection M is the following:

TABLE III. Parameters W_i for the P,T-odd and P-odd interactions caused by the electron EDM, the magnetic quadrupole moment of the nucleus, the weak charge of the nucleus and the anapole moment of the nucleus. Definitions are given in the text.

Transition	W_d [Hz/(e cm)]	W_M [Hz/(e cm^2)]	W_Q (Hz)	W_A (Hz)
XI-VI		-1.23×10^{32}		−13
XIII-IX	1.0×10^{23}	0.23×10^{32}	−34	−8.5

TABLE IV. Radial integrals in atomic units for H_d and H_Q operators with and without the core polarization.

	H_d		H_Q	
	Valence	Total	Valence	Total
$6s_{1/2}$-$6p_{1/2}$	-3.69	-3.15	59.0	65.6
$6p_{3/2}$-$5d_{3/2}$	-0.20	-0.32	0.0	-7.1
$5d_{5/2}$-$4f_{5/2}$	-0.14	-0.17	0.0	-0.55

$$\langle FMJI|H_d|FMJI\rangle = W_d d_e, \tag{10a}$$

$$\langle FMJ'I|H_M|FMJI\rangle = (-1)^{(F+J+I+1)}\left(\frac{(I+1)(2I+3)}{6}\right)^{1/2}\begin{Bmatrix} J' & I & F \\ I & J & 2 \end{Bmatrix} W_M M, \tag{10b}$$

$$\langle FMJI|H_Q|FMJI\rangle = W_Q, \tag{10c}$$

$$\langle FMJ'I|H_A|FMJI\rangle = (-1)^{(F+J+I+1)}\left[I(I+1)(2I+1)\right]^{1/2}\begin{Bmatrix} J' & I & F \\ I & J & 1 \end{Bmatrix} W_A k_A. \tag{10d}$$

For the scalar interactions H_d and H_Q the core polarization was taken into account in the way discussed in the previous section. The radial integrals for these operators calculated with and without the core polarization are presented in Table IV. They have the following form:

$$I_d = -\int_0^\infty g_i g_k \frac{d\phi}{dr}\, dr\ , \tag{11}$$

$$I_Q = 4\pi \int_0^\infty (f_i g_k - g_i f_k) n\, dr\ , \tag{12}$$

where f_i and g_i are the large and small components of the Dirac radial wave function.

It is interesting to analyze relative contributions to the W_i parameters. We shall do it again using an example of the XII–IX transition. For the W_d parameter the two main contributions come from the f-d and p-s terms: 56% and 43%, respectively. The core polarization affects these terms in the opposite way (see Table IV) and the final result is only 2% larger than the valence contribution. For the W_Q parameter there is only one valence contribution from the p-s transition. The core polarization induces the f-d and d-p terms. It reduces the amplitude by 15%.

So, even for the contact P-odd interaction H_Q, the valence contribution dominates over that of the core. We expect that the same is true for the interactions with the anapole moment and the magnetic quadrupole moment of the nucleus. The first of these interactions is also contact, and one might expect larger core contributions than for the second one. However, the W_a parameter appears to be large in comparison with W_Q. Indeed, according to Eqs. (7)–(9) it is supposed to be approximately Z times smaller than W_Q ($Q_W \approx -N \sim Z$). But, as it follows from Table III, the ratio is only about four. It is caused by the fact that the s-p amplitude is much larger in the vector channel then in the scalar one. For this reason, it is likely that the core polarization is not more important here than for the weak charge.

In Ref. [2] an estimate was made for the EDM of dysprosium in the metastable state VI caused by the magnetic quadrupole moment of the nucleus,

$$d_{atom} = 2.7 \times 10^{-3}\frac{m_p c}{\hbar} M. \tag{13}$$

This dipole moment arises from the admixture of the state XI by the interaction H_M (10),

$$d_{atom} = 2\frac{\langle F,M,J,I|D|F,M,J',I\rangle\langle F,M,J',I|H_M|F,M,J,I\rangle}{\Delta E}$$
$$= 7.864 \times 10^{-3}\frac{M\langle J||D||J'\rangle W_M}{\Delta E} = 1.1 \times 10^{-2}\frac{m_p c}{\hbar} M, \tag{14}$$

where we used L-gauge value for the $E1$ amplitude (in V form the result is two times smaller).

We would like to note in conclusion that the weak interaction results are very sensitive to the choice of a basis set. The results presented above were obtained using the main basis set described in Sec. II. We made a check using a different basis set which was obtained starting from the $4f^{10}6s^2$ configuration. The energy levels, g factors, and hyperfine structure constants are relatively stable with respect to the basis set while the weak interactions results change significantly. For example, we obtained a value of about 100 Hz for the W_Q parameter for the XIII - IX transition in comparison with 34 Hz presented in Table III. For other W_i parameters the results with the new basis set were also about two times larger than those presented in Table III. Stability of the g factors and hyperfine constants does not allow us to choose between the different basis sets. The energy levels are more sensitive, but the agreement with experiment data is not very good for both basis sets, especially for the levels of interest—IX and XIII (see Table I). There is also poor agreement between the L and V forms of the $E1$ transition amplitudes for both basis sets (see Table II). More configurations should probably be taken into account to achieve a better stability of the weak interactions results. This problem deserves further consideration.

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