Calculation of lifetimes of low-lying odd-parity levels of Sm

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Ab initio calculations of $E1$ transition amplitudes from low-lying odd-parity levels ^9G_J ($J=0-4$) and ^9F_J ($J=1,2$) levels to the even-parity states ^7F_J ($J=0-5$), ^9H_J ($J=1-5$), and ^9D_J ($J=2,3$) were performed using the configuration-interaction method. Using the results obtained for these $E1$ amplitudes, the oscillator strengths and probabilities of the corresponding transitions were calculated. The estimates of the lifetimes of the odd-parity states are also presented. [S1050-2947(97)06410-X]

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I. INTRODUCTION

In recent years the existence of parity nonconservation in heavy atoms has become well established [1,2]. Effects due to parity nonconservation can be substantially enhanced in rare-earth atoms since these are heavy and have close energy levels of opposite parity. Both circumstances are known to lead to an enhancement of parity-nonconserving effects. Samarium has a very dense spectrum of levels [3]. For this reason it is not difficult to find pairs of levels of opposite parity separated by a small energy interval that are convenient for a parity-nonconservation search [4–8].

It is clear that theoretical predictions of the magnitude of the effect are very important in choosing a particular system for an experiment. Among the parameters of importance for parity violation experiments are the $E1$ amplitudes of transitions between opposite-parity levels. Unfortunately, because of the complexity of the samarium spectrum, the semiempirical calculations of $E1$ amplitudes carried out so far [9–11] agree poorly with experimental data [12–18].

In this work we perform *ab initio* calculations of $E1$ transition amplitudes from low-lying odd-parity levels ^9G_J (total angular moment $J=0-4$) and ^9F_J ($J=1,2$) levels to the states ^7F_J ($J=0-5$), ^9H_J ($J=1-5$), and ^9D_J ($J=2,3$) using the configuration-interaction (CI) method. Using the results obtained for these $E1$ amplitudes, we calculate the oscillator strengths and probabilities of the corresponding transitions. The estimates of the lifetimes of the odd-parity states are also presented.

II. METHOD OF CALCULATION

Samarium has nuclear charge $Z=62$. There are several isotopes of Sm with mass numbers $A=144-154$ and among them there are two odd neutron number isotopes ($A=147$ and 149) with nuclear spin $I=7/2$. The principal configuration of the ground-state term (^7F_J) is $4f^6 6s^2$. The other levels considered in this work are even-parity levels ^9H_J and ^9D_J ($4f^6 5d6s$) and the lowest odd-parity levels ^9G_J and ^9F_J ($4f^6 6s6p$) (see Fig. 1).

For the calculation we used the widely known CI method. Alternatively, we can use the multiconfiguration Hartree-Fock method (see the corresponding GRASP code described elsewhere [19]).

In the first stage of the calculation we constructed one-electron wave functions using a Hartree-Fock-Dirac (HFD) code written by Brattsev, Deineka, and Tupitsyn [20] with subsequent modification by Tupitsyn (in particular, the finite nuclear size was accounted for). One-electron wave functions were constructed in the following way. The HFD equations were solved self-consistently for $1s^2,\ldots,4f^6$, $6s^2$ electrons. The orbitals obtained were frozen and the $5d$ orbital was found from the HFD equation for the configuration $4f^6 6s5d$. Further, the $6p$ shell was added. The electron from the $5d$ shell was moved to the $6p$ shell, all orbitals were frozen again, and the $6p$ orbital was found from the HFD equation for the configuration $4f^6 6s6p$. In this way, HFD orbitals $1s,\ldots,6s$, $5d$, and $6p$ were obtained. The virtual orbitals nl and $n'l'$ (where $n=7,8$, $l=s,p$, and $n'=6$, $l'=d$) were constructed from $n-1$ l and $n'-1$ l' orbitals, correspondingly, by multiplication of the latter by r and subsequent orthogonalization with all other orbitals. In this way $6d$, $7s$, and $7p$ orbitals were constructed from the HFD $5d$, $6s$, and $6p$ orbitals, correspondingly. After that $8s$ and $8p$ orbitals were constructed from $7s$ and $7p$ orbitals in an analogous fashion. This method of construction of virtual orbitals has been applied previously to calculations in Bi and Yb [21,22]. (A detailed description of this approach is given in [21].) In this way, the basis set consisting of HFD and virtual orbitals was formed.

In the next step, the CI was included. In this stage all electrons were divided into two groups: the core electrons

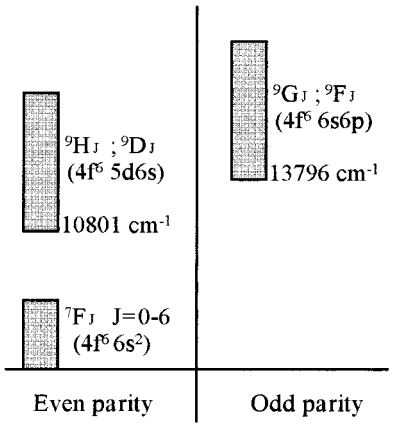

FIG. 1. Scheme of the low-lying odd-parity and even-parity levels.

TABLE I. Energies and g factors of the low-lying levels in Sm (one-configuration approximation and including the CI). The multiplet splittings are indicated in parentheses.

Level	E (cm^{-1}) One-configuration calculation	E (cm^{-1}) CI calculation	E (cm^{-1}) Expt. [3]	g factor One-configuration calculation	g factor CI calculation	g factor Expt. [3]
$^7F_0$	0	0	0			
$^7F_1$	285	285	293	1.498 99	1.498 98	1.498 39
$^7F_2$	811	810	812	1.498 59	1.498 59	1.497 79
$^7F_3$	1524	1523	1490	1.498 23	1.498 22	1.497 07
$^7F_4$	2377	2376	2273	1.497 60	1.497 60	1.496 25
$^7F_5$	3332	3331	3125	1.496 93	1.496 92	1.495 32
$^7F_6$	4361	4361	4021	1.496 15	1.496 14	1.494 17
$^9H_1$	7650	12 737	10 801	−0.977	−0.979	−0.98
$^9H_2$	7877 (227)	12 693 (226)	11 045 (224)	0.676	0.673	0.67
$^9H_3$	8215 (565)	13 300 (563)	11 406 (605)	1.089	1.086	1.08
$^9H_4$	8658 (1008)	13 744 (1007)	11 877 (1076)	1.254	1.251	1.25
$^9H_5$	9200 (1550)	14 288 (1551)	12 445 (1644)	1.336	1.334	1.33
$^9D_2$	9343	14 589	12 313	2.602	2.605	2.56
$^9D_3$	9676	14 970	12 847	2.048	2.053	2.05
$^9G_0$	7236	11 339	13 796			
$^9G_1$	7437 (201)	11 533 (194)	13 999 (203)	1.501	1.501	1.50
$^9G_2$	7820 (584)	11 906 (567)	14 380 (584)	1.502	1.502	1.50
$^9G_3$	8363 (1127)	12 442 (1103)	14 916 (1120)	1.501	1.501	1.49
$^9F_1$	8393	12 674	14 864	3.225	3.164	3.10
$^9F_2$	8500	12 551	15 040	2.505	2.542	2.365
$^9G_4$	9047 (1811)	13 120 (1781)	15 579 (1783)	1.500	1.500	1.500

TABLE II. Reduced matrix elements $|\langle {}^7F_J \| r \| {}^9L'_J \rangle|/a_0$ ($L' \equiv G,F$), a_0 is Bohr's radius. Upper numbers, $4f^6(6s6p+5d6p) \rightarrow 4f^6(6s^2+6p^2)$; medium numbers, $4f^6(6s6p+5d6p) \rightarrow 4f^6 6s^2$; lower numbers, $4f^6 6s6p \rightarrow 4f^6 6s^2$.

$F \backslash L'$	$^9G_0$	$^9G_1$	$^9G_2$	$^9G_3$	$^9G_4$	$^9F_1$	$^9F_2$
		0.168				0.270	
$^7F_0$		0.233				0.355	
		0.131				0.197	
	0.095	0.004	0.277			0.302	0.182
$^7F_1$	0.135	0.007	0.381			0.398	0.244
	0.082	0.011	0.211			0.243	0.149
		0.091	0.009	0.360		0.151	0.225
$^7F_2$		0.131	0.015	0.494		0.197	0.303
		0.083	0.025	0.268		0.133	0.198
			0.068	0.008	0.417		0.116
$^7F_3$			0.100	0.016	0.572		0.155
			0.065	0.030	0.306		0.113
				0.044	0.005		
$^7F_4$				0.068	0.013		
				0.045	0.030		
					0.025		
$^7F_5$					0.040		
					0.026		

TABLE III. Reduced matrix elements $|\langle {}^9L_J \| r \| {}^9L'_J \rangle|/a_0$ ($L \equiv H,D$; $L' \equiv G,F$). Upper numbers, transition $4f^6(6s6p+5d6p) \rightarrow 4f^6(5d6s+6d6s)$; medium numbers, transition $4f^6(6s6p+5d6p) \rightarrow 4f^6 5d6s$; lower numbers, transition $4f^6 6s6p \rightarrow 4f^6 5d6s$.

$L \backslash L'$	$^9G_0$	$^9G_1$	$^9G_2$	$^9G_3$	$^9G_4$	$^9F_1$	$^9F_2$
	1.931	2.041	0.874			0.038	0.042
$^9H_1$	2.394	2.530	1.084			0.052	0.054
	2.953	3.121	1.340			0.084	0.062
		2.646	2.529	1.016		0.055	0.123
$^9H_2$		3.285	3.136	1.260		0.080	0.161
		4.063	3.878	1.565		0.129	0.185
			3.357	2.806	0.993		0.163
$^9H_3$			4.174	3.481	1.236		0.213
			5.181	4.313	1.543		0.243
				4.053	2.918		
$^9H_4$				5.047	3.626		
				6.284	4.501		
					4.735		
$^9H_5$					5.906		
					7.370		
		0.224	0.369	0.166		1.887	2.664
$^9D_2$		0.269	0.466	0.187		2.230	3.143
		0.354	0.625	0.278		2.818	3.887
			0.220	0.507	0.197		2.475
$^9D_3$			0.250	0.657	0.221		2.867
			0.390	0.896	0.381		3.449

and the valence electrons. We define the core as $[1s^2,\ldots,5s^2,5p^6]$, leaving eight electrons in the valence field. Several additional configurations were added to the principal configurations of all three terms. For the ground-state term (^7F_J), as well as for the low-lying odd-parity levels (see below), the configurations obtained by (i) one- and two-electron excitations of $6s$ and $6p$ electrons to $5d$, $6p$, $7s$, and $7p$ shells; (ii) one-electron excitations of $6s$ and $6p$ electrons to $6d$, $8s$, and $8p$ shells; and (iii) excitation of the f electron to $5d$ and $6p$ shells were taken into account. Thus the following configurations were included for the ^7F_J term:

$$4f^6(6s^2+6s5d+6s7s+6s6d+6s8s+5d^2+6p^2+7s^2$$

$$+7p^2+6p7p+5d7s)+4f^5(6s^2 6p+6s5d6p).$$

It proved to be very important to take into account the configuration $4f^6 6p^2$. The admixture of the latter to the principal configuration $4f^6 6s^2$ is found to be at the level of 7% in probability. This is important from the point of view of the location of energy levels of the ground-state term with respect to those of the other terms. Comparing columns 2 and 3 in Table I, we see that the ^7F_J term proved to be 4000 cm^{-1} deeper in energy when the CI was included than in the single-configuration case. Mostly this was due to the admixture of the $4f^6 6p^2$ configuration. In addition, there is a strong one-electron transition ($6p \rightarrow 6s$) from the $4f^6 6p^2$ configuration to the principal configuration $4f^6 6s6p$ of odd-parity levels. This admixture has a significant contribution to the magnitudes of the $^9G(^9D) \rightarrow {}^7F$ $E1$ amplitudes (see Table II).

In contrast, accounting for the f-shell excitations (e.g., including configurations $4f^5 6s^2 6p$ and $4f^5 6s5d6p$) hardly influences the results at all. In fact, it confirms the conclusion arrived at in [11] that due to the weak electrostatic interaction between the deep-lying $4f$ electrons and external $6s$ and $6p$ electrons, the open $4f^6$ shell may be treated as the core, the quantum state of which does not change during a transition.

For the low-lying odd-parity levels of the ^9G_J term ($J=0-4$) and the ^9F_J ($J=1,2$) levels the following configurations were considered:

$$4f^6(6s6p+5d6p+7s6p+6d6p+8s6p+6s7p+6s8p$$

$$+7s7p+5d7p)+4f^5(6s6p^2+6s^2 5d+6s5d^2).$$

In this case one can note a rather large (of the order of 4%) admixture of the $4f^6 5d6p$ configuration. Taking into account that there is one-electron transition $4f^6 5d6p \rightarrow 4f^6 5d6s$, the essential contribution to the $^9G \rightarrow {}^9H(^9D)$ $E1$ transition amplitudes caused by this admixture appears reasonable (see Table III).

For the levels of another even multiplet ^9H_J ($J=1-5$) and levels ^9D_J ($J=2,3$) the following configurations were taken into account: one-electron excitations of $6s$ and $5d$

electrons to $5d$, $6d$, and $7s$ shells; excitations of $6s$ and $5d$ electrons to the $6p$ shell; and excitation of the f electron to $6s$ and $6p$ shells:

$$4f^6(5d6s+6d6s+5d7s+5d6d+5d^2+6s7s+6p^2)$$
$$+4f^5(6s^26p+6s5d6p).$$

Here we accounted for a smaller number of configurations than in the two previous cases for the following reasons. (i) Each added nonrelativistic configuration originates a large number of determinants. For instance, we were obliged to omit the configuration $4f^55d^26p$ that gives about 45 000 determinants. (ii) The amplitudes $^9G\rightarrow{}^9H$ that give significant contributions to lifetimes of low-lying odd-parity levels are rather large (~ 1 a.u.). For this reason the account for excitations to high-lying shells (such as $8s$ and $8p$) is of less importance for them than, e.g., for amplitudes $^9G\rightarrow{}^7F$.

For the $^9G\rightarrow{}^9H$ transitions, it was important to account for the configuration $4f^66d6s$. It gives 2% admixture to the main configuration $4f^65d6s$. In addition, there is a rather strong one-electron $E1$ transition from $6d$ to $6p$. The contribution to the $^9G\rightarrow{}^9H$ $E1$ transition amplitudes due to the $4f^66d6s$ configuration is approximately 20% (see Table III).

In Tables II and III we illustrate the importance of admixed configurations mentioned above (namely, $4f^66p^2$ to $4f^66s^2$ for the ^7F term, $4f^66d6s$ to $4f^65d6s$ for the ^9H term, and $4f^65d6p$ to $4f^66s6p$ for the ^9G term) for calculations of $E1$ amplitudes $^9L_J\rightarrow{}^7F_J$ ($L=G,F$) and $^9L_J\rightarrow{}^9L'_J$ ($L'=H,D$). The results obtained for reduced matrix elements $|\langle{}^7F_J\|r\|{}^9L'_J\rangle|$, defined according to

$$\langle J'M'|d_q|JM\rangle=(-1)^{J'-M'}\begin{pmatrix} J' & 1 & J \\ -M' & q & M\end{pmatrix}\langle J'\|d\|J\rangle,$$

are presented in Table II. The results for the following three cases are reflected: (i) The one-configuration approximation, e.g., $4f^66s6p\rightarrow 4f^66s^2$ (lower numbers in each entry); (ii) $4f^6(6s6p+5d6p)\rightarrow 4f^66s^2$ (middle numbers); and (iii) $4f^6(6s6p+5d6p)\rightarrow 4f^6(6s^2+6p^2)$ (upper numbers).

Analyzing results of Table II, we see that each added configuration changes the reduced matrix elements at least at a 25% level. But for the majority of transitions the corresponding contributions to $E1$ amplitudes from $4f^65d6p$ and $4f^66p^2$ configurations have opposite sign and partially cancel each other. A curious observation is that the transitions $^9G_J\rightarrow{}^7F_{J'}$, for which $J+J'$ is an even number, are exceptions from this rule. For them the two contributions mentioned add. Since the corresponding matrix elements are small ($\leqslant 0.03$ a.u.), all of them change by several factors.

In an analogous fashion, the reduced matrix elements $|\langle{}^9L_J\|r\|{}^9L'_J\rangle|$ ($L=G,F$; $L'=H,D$) are given in Table III for the following cases: (i) The one-configuration approximation, e.g., $4f^66s6p\rightarrow 4f^65d6s$ (lower numbers in each entry); (ii) $4f^6(6s6p+5d6p)\rightarrow 4f^65d6s$ (middle numbers); and (iii) $4f^6(6s6p+5d6p)\rightarrow 4f^6(5d6s+6d6s)$ (upper numbers). For these transitions (in contrast with the previous case) contributions from both configurations added have the same sign, leading to a reduction of the corresponding $E1$ amplitudes at least at a 50% level.

III. RESULTS AND DISCUSSION

The energy spectrum and g factors obtained for the low-lying levels in the single-configuration approximation and including the configuration interaction are presented in Table I. In Table I results are presented only for five low-lying ^9H levels and for five low-lying ^9G levels. Other levels of these multiplets were not calculated for the following reason. During the calculations we needed to find eigenvalues and eigenvectors of energy matrices of size up to 90 000 constructed in the space of determinants. Of course, these matrices are too large to be solved efficiently using standard methods of direct diagonalization. In addition, they are usually sparse (that is, they have many zero elements). A rapidly convergent method that allows one to find a few lower eigenvalues and eigenvectors of such matrices was developed by Davidson in [23]. A detailed description of this method can be found elsewhere [24]. Using Davidson's procedure significantly modified and adopted for our purposes by Kozlov and Mitrushchenkov, we could reliably calculate several low-lying levels for each term.

Comparing calculated level energies with the experimental ones (see Table I), we see that the multiplet splitting of the ground term ^7F is reproduced with accuracy better than 8%. Of course, such a coincidence between experimental and calculated energies is not as good as, e.g., in comparison with Ref. [25], where the energies of the ground-state ^7F term were reproduced with an accuracy of 0.1%. The authors of [25] assumed that the ratios of the Slater integrals F_4/F_2 and F_6/F_2 (see [26]) were those of a $4f$ hydrogenic eigenfunction. With this assumption it was possible to express the elements of the energy matrix in terms of the radial integral F_2 and spin-orbit coupling constant ξ, which were found semiempirically. It is important to note that the 0.1% agreement was achieved without accounting for spin-spin, spin-other-orbit, and configuration interactions. Comparing columns 2 and 3 of Table I, we see that taking into account the configuration interaction did not change the multiplet splitting of the ground-state term. It agrees well with the results of Ref. [25].

The multiplet splitting of the other even-parity term ^9H_J is also reproduced at the 8% level, while the multiplet splitting of the odd-parity multiplet ^9G_J is reproduced even more accurately (better than 5%). Even-parity levels $^9D_2$ and $^9D_3$ as well as odd-parity levels $^9F_1$ and $^9F_2$ were not reproduced as well. It is not surprising because, in accordance with [3], the main configuration $4f^65d6s$ contributes to $^9D_2$ and $^9D_3$ at the 85% level (in probability) and, correspondingly, admixture of other configurations is rather large. Hence some configurations that are not important for $E1$ amplitudes (but are important for energies of levels) might be neglected by us. A similar explanation holds for $^9F_1$ and $^9F_2$ odd-parity levels, for which the main configuration $4f^66s6p$ contributes even less ($\leqslant 57\%$).

As it was noted in [25], the attempt to use $4f$ hydrogenic eigenfunction for calculations of Slater integrals for the high-lying levels (other than levels of the ground-state term) did not allow the precision to be anywhere near that of the ground-state term. Thus, taking into account that our main motivation here is to calculate $E1$ amplitudes, the accuracy achieved in this approach for level energies for all three mul-

TABLE IV. Reduced matrix elements $|\langle {}^7F_J \| r \| {}^9L'_J \rangle|/a_0$ and $|\langle {}^9L_J \| r \| {}^9L'_J \rangle|/a_0$ ($L \equiv H,D$; $L' \equiv G,F$) (including the configuration interaction).

$L \backslash L'$	$^9G_0$	$^9G_1$	$^9G_2$	$^9G_3$	$^9G_4$	$^9F_1$	$^9F_2$
$^7F_0$		0.221				0.361	
$^7F_1$	0.143	0.027	0.345			0.451	0.230
$^7F_2$		0.146	0.055	0.432		0.251	0.304
$^7F_3$			0.117	0.068	0.484		0.175
$^7F_4$				0.083	0.068		
$^7F_5$					0.051		
$^9H_1$	1.948	2.063	0.885			0.026	0.053
$^9H_2$		2.666	2.555	1.030		0.040	0.158
$^9H_3$			3.375	2.839	1.011		0.210
$^9H_4$				4.077	2.961		
$^9H_5$					4.772		
$^9D_2$		0.204	0.364	0.171		1.787	2.642
$^9D_3$			0.160	0.470	0.189		2.746

tiplets can be considered adequate.

Comparing experimental and calculated g values (see Table I), we see that, excluding $^9F_1$, $^9F_2$, and $^9D_2$ levels, they coincide up to the third decimal place. The generally good agreement between experimental and calculated g values seems natural for two reasons. (i) The g values can be calculated in a simple manner. (For instance, one does not need to calculate radial integrals.) (ii) The configuration interaction weakly influences g values. In fact, g values obtained in the one-configuration approximation hardly differ from the final values at all (compare columns 5 and 6 in Table I). For g values of the ground-state term we display six decimal places for the sake of a convenient comparison. As for the discrepancy between experimental and calculated g values for $^9F_1$, $^9F_2$, and $^9D_2$ levels, the reason is the same as for discrepancies of energies: Some important configurations were not taken into account for these levels.

The calculated reduced $E1$ matrix elements of the $^9L_J \rightarrow {}^9L'_J$ ($L=G,F$; $L'=H,D$) and $^9L_J \rightarrow {}^7F_J$ transitions are presented in Tables II–IV. Note that in the calculations of $E1$ amplitudes both the length gauge and velocity gauge can be used. During these calculations only the former was used. This is because the expression for a matrix element of the $E1$ transition written in the velocity gauge includes the difference of energies between levels under consideration. Thus, if an energy interval is calculated incorrectly, the corresponding matrix element also will be incorrect. As seen from Table I, the intervals between the ground-state term (^7F) and the two other terms (^9H and ^9G), as well as those between ^9H and ^9G terms themselves, were not reproduced well. For instance, the ^9G term was calculated to be lower in energy than the ^9H term. For this reason, it was meaningless to use the velocity gauge.

The values presented in Tables II–IV are easily understood starting from LS coupling. $E1$ transitions $^9G_J \rightarrow {}^9H_J$ and $^9F_J \rightarrow {}^9D_J$ are allowed in LS coupling since the total spin S does not change and $|\Delta L|=1$ (L is the total orbital angular momentum). Therefore, the corresponding $E1$ amplitudes are of the order of 1 a.u., as expected. As for the $^9G_J \rightarrow {}^7F_J$, $^9G_J \rightarrow {}^9D_J$, $^9F_J \rightarrow {}^7F_J$, and $^9F_J \rightarrow {}^9H_J$ transitions, they should be suppressed in LS coupling because one of the selection rules ($|\Delta L| \leqslant 1$ or $\Delta S=0$) is not fulfilled for them. Although the samarium spectrum generally cannot be satisfactorily described in LS coupling (as illustrated by the poor agreement of oscillator strengths calculated in [11,12] with the experimental data [12,14]), the selection rules for L and S ($|\Delta L|=1$, $\Delta S=0$) work rather well for the terms considered here.

From the analysis of the results given in Tables II–IV, it is seen that the magnitudes of $E1$ amplitudes are strongly influenced by the configuration interaction. The amplitudes calculated including the CI differ by 30–60 % compared to those obtained in the one-configuration approximation. The differences are even more significant for small amplitudes (by small ones we mean the amplitudes of the order of 10^{-2} a.u.). For the transitions $^9G_J \rightarrow {}^9H_J$ this is mostly caused by the admixture of $4f^6 5d 6p$ to $4f^6 6s 6p$ for the ^9G term and by the admixture of $4f^6 6d 6s$ to $4f^6 5d 6s$ for the ^9H term. To some extent, this explains why the results obtained by semiempirical methods (which do not take into account the configuration interaction) agree poorly with experimental data.

Let us now discuss the accuracy of the results presented in Table IV. Unfortunately, the accuracy is not high, especially for the small amplitudes. In practice, in the calculations of the reduced matrix elements we tried to account for configurations that give contributions as small as 10^{-3} a.u. However, as we saw, the configurations obtained by excitation of $5s$ and $5p$ electrons also gave contributions to the corresponding $E1$ amplitudes of the order of 10^{-3} a.u.

Unfortunately, it is extremely difficult in the framework of the CI method to take into account the core polarization as well as electron excitations for high-lying levels. This is because each new additional nonrelativistic configuration (which originates several relativistic ones) strongly increases the number of determinants one needs to take into account in the construction of the energy matrix.

On the other hand, convergence of our procedure is rather rapid. Namely, accounting for one-electron excitations to $7s$ and $7p$ shells (and to the $6d$ shell for the ^9H_J term) contributes to the $E1$ amplitudes at a level of 10^{-2} a.u., while accounting for configurations obtained by one-electron excita-

TABLE V. Oscillator strengths (-10^4 f) for $E1$ transitions from odd-parity to even-parity levels. (The configuration interaction is taken into account.) Upper numbers, present calculations; lower numbers, experimental results [12,14].

even \ odd	$^9G_0$	$^9G_1$	$^9G_2$	$^9G_3$	$^9G_4$	$^9F_1$	$^9F_2$
		6.9				19.6	
$^7F_0$		70[a]				500[a]	
		12.5				28.2	
$^7F_1$	8.4	0.10	10.2			30.0	4.7
			21.6			31.7	13.3
$^7F_2$		2.8	0.25	11.4		9.0	8.0
		5.7	0.77	29.8			20.2
$^7F_3$			1.1	0.27	11.1		2.5
			2.9	1.2	33.6		6.0
$^7F_4$				0.38	0.21		
$^7F_5$					0.11		
$^9H_1$	345.2	137.8	17.0			0.03	0.07
$^9H_2$		212.6	13.2	17.8		0.06	0.61
$^9H_3$			205.8	122.7	14.4		0.97
$^9H_4$				219.1	109.5		
$^9H_5$					240.8		
$^9D_2$		0.71	1.7	0.33		82.5	115.6
$^9D_3$			0.24	2.0	0.33		100.4

[a]Calculation in Ref. [9].

tions to $8s$ and $8p$ shells contributes to these $E1$ amplitudes at a level of 10^{-3} a.u. In spite of this, for the small amplitudes ($\leqslant 0.1$ a.u.) we can comment only about the qualitative agreement with the experimental data (see Table V and the discussion below). The situation for the large $E1$ amplitudes ~ 1 a.u., especially for transitions $^9G_J \rightarrow {}^9H_J$, is more predictable. Comparing the results of Tables III (upper numbers) and IV, we see that the corresponding matrix elements changed only by several percent. We can estimate the accuracy of the matrix elements mentioned on the level 10–15 %.

Using the results obtained for reduced matrix elements, it is easy to calculate oscillator strengths of the corresponding transitions [27]. In relativistic units $c=\hbar=1$ (c is the speed of light)

$$f(\gamma J \rightarrow \gamma' J') = -\frac{2m}{3}\frac{\omega}{2J+1}|\langle \gamma J \| r \| \gamma' J' \rangle|^2, \qquad (1)$$

where γ, γ' are sets of quantum numbers defining the initial and final states, m is the electron mass, and $\omega = (E_{\gamma J} - E_{\gamma' J'})$. Note that we use the experimental values of the energies.

The calculated oscillator strengths together with the available experimental data are given in Table V. The experimental values for relative oscillator strengths were taken from [12]. Then using the calibration coefficient given in [14] they were converted to absolute oscillator strengths $f(^9L_J \rightarrow {}^7F_J)$ $(L=G,F)$ and after that recalculated in a trivial way to oscillator strengths $f(^7F_J \rightarrow {}^9L_J)$. (To the best of our knowledge, there are no experimental oscillator strengths data for other transitions.)

A comparison of the calculated oscillator strengths with the experimental ones shows reasonable agreement within a factor of 1.5–3. (The good coincidence between the calculated and the experimental oscillator strength for the $^9F_1 \rightarrow {}^7F_1$ transition, as well as the discrepancy 4.5 times for that of the $^9G_3 \rightarrow {}^7F_3$ transition, can be treated as rather accidental.) The main reason for such a difference, as already mentioned, is the possibility to account for an admixture of only a few of the most important configurations in the calculation.

From calculated $E1$ amplitudes, it is possible to estimate the lifetimes of the odd-parity ^9G_J and ^9F_J levels since we have calculated amplitudes of the main decay channels of these states. Note that it is important to include $^9G_J \rightarrow {}^7F_J$ $E1$ amplitudes in spite of the fact that the latter are at least several times smaller than the $^9G_J \rightarrow {}^9H_J$ ones. This is because the transition rate is

$$W(\gamma J \rightarrow \gamma' J') = \frac{4\alpha}{3}\frac{\omega^3}{2J+1}|\langle \gamma J \| r \| \gamma' J' \rangle|^2 \qquad (2)$$

TABLE VI. Probabilities W (10^3 sec^{-1}) for $E1$ transitions from odd-parity levels to even-parity levels. The configuration interaction is taken into account.

even \ odd	$^9G_0$	$^9G_1$	$^9G_2$	$^9G_3$	$^9G_4$	$^9F_1$	$^9F_2$
$^7F_0$		90.4				288.7	
$^7F_1$	101.9	1.3	134.7			424.6	68.7
$^7F_2$		33.0	3.1	151.4		117.9	107.7
$^7F_3$			11.9	3.2	147.4		30.8
$^7F_4$				4.0	2.5		
$^7F_5$					1.1		
$^9H_1$	206.4	93.9	14.5			0.03	0.1
$^9H_2$		123.7	98.1	17.8		0.06	0.6
$^9H_3$			121.3	100.7	16.7		0.9
$^9H_4$				134.8	100.0		
$^9H_5$					157.6		
$^9D_2$		0.1	0.5	0.1		35.8	57.3
$^9D_3$			0.04	0.6	0.2		32.2

(where $\alpha = 1/137$ is the fine-structure constant) and the small magnitudes of the $^9G_J \rightarrow {}^7F_J$ $E1$ amplitudes are compensated for by the large magnitude of ω^3 since the energy interval between the ^9G_J and ^7F_J terms is approximately four times greater than that between the ^9G_J and ^9H_J terms.

From the experimental point of view it is often important to know the transitions probabilities from a given state. Substituting the results obtained for reduced matrix elements (see Table IV) in Eq. (2), it is easy to calculate the corresponding probabilities. The results for ^9G_J ($J=0-4$) and ^9F_J ($J=1,2$) levels are presented in Table VI.

The lifetime τ of a level is the inverse of the total transition rate. After simple calculations we obtain

$$\tau(^9G_0) = 3.2\times 10^{-6} \text{ sec},$$

$$\tau(^9G_1) = 2.9\times 10^{-6} \text{ sec},$$

$$\tau(^9G_2) = 2.6\times 10^{-6} \text{ sec},$$

$$\tau(^9G_3) = 2.4\times 10^{-6} \text{ sec},$$

$$\tau(^9G_4) = 2.4\times 10^{-6} \text{ sec},$$

$$\tau(^9F_1) = 1.2\times 10^{-6} \text{ sec},$$

$$\tau(^9F_2) = 3.4\times 10^{-6} \text{ sec}.$$

The accuracy of the calculated lifetimes is determined by the accuracy of the corresponding reduced matrix elements discussed above. The lifetimes of the $^9G_3$ and $^9G_4$ levels are slightly overestimated because we did not account for the transitions $^9G_3 \rightarrow {}^9D_4$ and $^9G_4 \rightarrow {}^9D_J$ ($J=4,5$). But, as seen from Table IV, the amplitudes $^9G_J \rightarrow {}^9D_J$ are approximately one order of magnitude smaller than $^9G_J \rightarrow {}^9H_J$. For this reason their contributions to the corresponding lifetimes are small. The result $\tau(^9G_1) = 2.9\times 10^{-6}$ sec is in good agreement with the estimate (2 μsec) made by Budker and DeMille [8].

IV. CONCLUSION

Calculations of $E1$ transition amplitudes from the low-lying odd-parity levels to the levels of two low-lying even-parity terms in samarium were carried out in the framework of the configuration-interaction method. The following conclusions can be drawn from these calculations.

(a) It is necessary to take into account the configuration interaction because it substantially affects the $E1$ amplitudes. The configuration-interaction method gives much better agreement between calculated and experimental oscillator strengths for Sm than semiempirical methods, but further improvement of the calculations is still desirable. Unfortunately, it is hardly possible to achieve an improvement within the frame of the configuration-interaction method, so some other approaches should be developed.

(b) Configurations obtained by f-shell excitations, as well as the core excitations, can be neglected in the first approximation.

(c) The selection rules $\Delta S = 0$ and $|\Delta L| = 1$ work rather well for the given terms.

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