$$\Delta\omega \simeq 0.78(\Gamma_\alpha \Gamma_\beta)^{1/2} \quad \text{if } \Gamma_\beta \ll \Gamma_\alpha , \tag{16}$$

$$\Delta\omega \simeq \Gamma_\alpha \qquad \text{if } \Gamma_\alpha \ll \Gamma_\beta . \tag{17}$$

Finally, we shall consider the case which we expect to be most nearly like (3) and (4) in which the upper level has a small comparative population, i.e., $f \ll 1$. Expanding (11) to first-order terms in f, we find that

$$\Delta\omega \simeq \Gamma_\alpha \left(1 - f\Gamma_\alpha \frac{\Gamma_\alpha + \Gamma_\beta}{\Gamma_\alpha^2 + \Gamma_\beta^2} \right), \tag{18}$$

and since $\Gamma_\alpha = \Delta\omega +$ terms of order f, we can replace Γ_α in the coefficient of f in (18) by $\Delta\omega$ and solve for Γ_α to this order; we obtain

$$\Gamma_\alpha \simeq \Delta\omega \left(1 + f\Delta\omega \frac{\Delta\omega + \Gamma_\beta}{(\Delta\omega)^2 + \Gamma_\beta^2} \right), \tag{19}$$

which is an approximate expression for the desired value of Γ_α in terms of the measured Hanle-effect width and the, hopefully, known values of f and Γ_β.

VI. DISCUSSION

The examples we have just discussed for this special semiclassical case for collisional excitation show quite clearly that when cascade or other processes affecting the time dependence of the level of interest are possible, then the relation between the Hanle-effect width and the lifetime is no longer as simple as (4), and that a use of (4) in such a situation can lead to large errors in the lifetime deduced from the measurement. In fact, we have seen an extreme example in which the width gives the lifetime of the cascading level and *not* that of the one being studied.

In the quantum-mechanical treatments of this problem there is generally a step analogous to using (2) and (6), and one will have to look at all of these cases with care. The most complete quantum treatment of similar problems seems to have been given by Macek[8] and possibly one can adapt his very general results to specific situations of interest.

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PHYSICAL REVIEW A VOLUME 3, NUMBER 4 APRIL 1971

Accurate Numerical Hartree-Fock Self-Consistent-Field Wave Functions for Rare-Earth Ions[*]

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Accurate numerical Hartree-Fock (HF) self-consistent-field (SCF) wave functions have been calculated for Pr^{+++}, Ce^{++}, Nd^{+++}, Pr^{++}, Pm^{+++}, Nd^{++}, Sm^{+++}, Pm^{++}, Eu^{+++}, Sm^{++}, Gd^{+++}, Eu^{++}, Tb^{+++}, Gd^{++}, Dy^{+++}, Tb^{++}, Ho^{+++}, Dy^{++}, Er^{+++}, Ho^{++}, Tm^{+++}, and Er^{++} rare-earth ions having an f^N electron configuration in their ground-state manifolds. Calculations, in general, have an accuracy of seven significant digits in the total energy. Values of several Hartree-Fock parameters have also been obtained from these wave functions.

INTRODUCTION

The rare-earth ions are of great importance from the point of view of laser activity and the development of the magneto-optical solid-state devices.[1,2] In order to obtain the electronic energy levels of a rare-earth ion accurately, one must include, apart from the electrostatic interaction, the magnetic interactions such as spin-spin, orbit-orbit, spin-orbit, and spin–other-orbit interactions. Recently work has been in progress[3] on the evaluation of the general expressions of the above-mentioned magnetic interactions in terms of certain interaction parameters for f^N electron configurations. In order to obtain theoretically accurate values of the interaction parameters for a particular atomic system one needs accurate wave functions for the atomic system. This need has led us to the project of evaluating accurate numerical HF SCF wave functions for atomic systems having f^N electron configurations.

In the present work, we have obtained accurate numerical HF SCF wave functions for the triply and doubly ionized rare-earth systems mentioned in the abstract. Use has been made of the double-precision numerical HF SCF wave-function program written by Fischer.[4] The computations were performed on IBM 360/50K computer. All the configurations are established normal f^N configurations except for Gd^{++} $(4f^8)$, for which the normal configuration is actually $4f^7 5d(^9D)$. Also, all the calculations correspond to the ground-state manifold of the systems. Using the present wave functions, we have also obtained the values of the additional Hartree-Fock parameters:

$$a_0(nl) = \lim[P(nl, r)/r^{l+1}] \quad \text{as } r \to 0;$$

$$\sigma_{nl} = Z - (\langle r_H \rangle / \langle r \rangle_{nl}),$$

the screening numbers; $\langle 1/r^3 \rangle_{nl}$; $\langle 1/r \rangle_{nl}$; $\langle r \rangle_{nl}$; $\langle r^2 \rangle_{nl}$; $F^K(4f, 4f)$, the Slater integrals; ζ_{4f}, the spin-orbit parameters[5]; and $M^K(4f, 4f)$, the spin-spin parameters.[6]

Work on the evaluation of accurate numerical HF SCF wave functions and the corresponding Hartree-Fock parameters for actinide ions having a normal f^N electron configuration is in progress and will be published subsequently.

RESULTS AND DISCUSSION

The tables of all the numerical HF SCF wave functions and the various Hartree-Fock parameters are much too long to be presented here. Therefore, they are given in a supplementary technical report.[7] It contains two tables, the first of which lists the radial wave functions given to six digits after the decimal point. We also give there the maximum error for each wave function, and this effectively tells[7] us the number of significant figures to which a particular wave function is self-consistent. The orbital wave functions are assumed to be self-consistent to at least four significant digits. However, the inner wave functions are much more self-consistent than the outer ones; for example, all the $1s$ wave functions are self-consistent to at least six significant figures. Occasionally, there are nodes in the tail of the inner wave functions beyond those required by the orthogonality conditions. However, within the accuracy of the present calculations, such oscillations were confined to $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ functions only. The magnitudes of such oscillations of $P(nl, r)$ in the tail region (called "wobblings") were always less than 0.000146. Thus, the orbital wave functions are without tail oscillations to three decimal places.

The second table of the above-mentioned technical report[7] gives the total energy (E), the one-electron energy parameters ($\epsilon_{nl,nl}$), and the additional Hartree-Fock parameters mentioned earlier for all the systems.

In the present paper, Table I gives the values of the Hartree-Fock parameters for $\text{Pr}^{+++}(4f^2)$, ^3H and $\text{Nd}^{+++}(4f^3)$, ^4I, and Table II presents the total energy (E in a.u.) and the virial-theorem[8] ratio for all the systems.

The convergence tolerance in $\epsilon_{nl,nl}$ iterations were specified to be $2(Z - \sigma_{nl})^2 \times 10^{-7}$, where σ_{nl} is the screening number of the shell and Z is the atomic number. Since σ_{nl} increases as we go to the outer shells, the convergence tolerance in the corresponding $\epsilon_{nl,nl}$ iterations decreases. However, it is to be noted that $|\epsilon_{nl,nl}|$ also decreases as we go to the outer shells, $|\epsilon_{1s,1s}|$ being the largest. The $\epsilon_{1s,1s}$ values are self-consistent to almost seven significant digits. Furthermore, the accuracy of the total energy E largely depends on the accuracy to which $\epsilon_{1s,1s}$ can be determined. As can be seen from the Table II, the virial theorem is satisfied to at least six significant digits, and in most cases to seven significant digits. Convergence tolerance in the normalization iterations was specified to be $4 \times 10^{(n-9)}$ where n is the principal quantum number.

As has been pointed out earlier, the computer program used is a double-precision (sixteen significant digits) program. Thus the accumulative round-off errors, affecting the last significant figure in the results of the present calculations, which would have occurred in a single-precision (eight significant digits) computer representation, have been avoided.

The program used puts special emphasis on the accuracy of the inner-electron distribution. Therefore, the Hartree-Fock parameters which depend more on the outer-electron distribution are expected to have lesser numerical accuracy, especially for complex atomic systems.

Since the self-consistent-field procedure is an iterative procedure, one requires initial estimates of the wave functions. In the program used, as the calculation proceeds, the convergence criterion is relaxed. Thus, with poor estimates the program may stop with results less self-consistent than those obtained with good estimates. The pro-

TABLE I. Hartree-Fock parameters for Pr^{+++} ($4f^2$), ^3H and Nd^{+++} ($4f^3$), ^4I [one-electron energy parameters $\epsilon_{nl,\,nl}$ in rydbergs; $a_0(nl)$, σ_{nl}, $\langle 1/r^3\rangle_{nl}$, $\langle 1/r\rangle_{nl}$, $\langle r\rangle_{nl}$, $\langle r^2\rangle_{nl}$, total energy E, and Slater integrals $F^K(4f,\ 4f)$ in atomic units; and spin-orbit parameter ζ_{4f} and spin-spin parameters $M^K(4f,\ 4f)$ in cm^{-1}].

Shell	$\epsilon_{nl,\,nl}$	$a_0(nl)$	σ_{nl}	$\langle 1/r^3\rangle_{nl}$	$\langle 1/r\rangle_{nl}$	$\langle r\rangle_{nl}$	$\langle r^2\rangle_{nl}$
			$\mathrm{Pr}^{+++}(4f^2)$, ^3H, $Z=59$				
1*s*	−2951.401	898.0646	0.705		58.463	0.025731	0.000885
2*s*	−470.5045	293.7728	4.44		13.539	0.109963	0.014195
2*p*	−444.7063	4743.134	5.57	6883.65	13.527	0.093574	0.010632
3*s*	−106.3783	133.6664	11.8		5.0599	0.286055	0.093306
3*p*	−95.04221	2263.074	13.8	1368.72	4.9828	0.276295	0.088302
3*d*	−74.18748	7414.512	16.6	228.040	4.8559	0.247558	0.071994
4*s*	−24.23053	63.32501	22.1		2.1267	0.650578	0.476315
4*p*	−19.78075	1050.583	24.7	287.295	2.0309	0.670253	0.509328
4*d*	−11.84682	3405.426	29.9	39.5681	1.8187	0.721786	0.602084
5*s*	−5.252789	25.50012	34.9		0.83189	1.55703	2.70880
5*p*	−3.835885	395.6205	37.8	40.5803	0.74858	1.71827	3.31555
4*f*	−3.290174	1806.551	39.5	5.52706	1.3674	0.924501	1.06324
$E=-8919.8340$							
$F^0(4f,\ 4f)=0.9953251$		$F^2(4f,\ 4f)=0.4789446$		$F^4(4f,\ 4f)=0.3016848$		$F^6(4f,\ 4f)=0.2174157$	
$\zeta_{4f}=923.445$		$M^0(4f,\ 4f)=2.261$		$M^2(4f,\ 4f)=1.267$		$M^4(4f,\ 4f)=0.8601$	
			$\mathrm{Nd}^{+++}(4f^3)$, ^4I, $Z=60$				
1*s*	−3056.725	921.1211	0.707		59.463	0.025298	0.000856
2*s*	−489.1280	301.6617	4.45		13.786	0.108006	0.013692
2*p*	−462.8005	4957.528	5.58	7264.30	13.775	0.091872	0.010247
3*s*	−110.9591	137.6670	11.8		5.1665	0.280314	0.089594
3*p*	−99.33840	2374.264	13.8	1454.53	5.0904	0.270509	0.084638
3*d*	−77.96073	7957.056	16.6	243.423	4.9661	0.241930	0.068726
4*s*	−25.14896	65.39307	22.3		2.1760	0.636408	0.455857
4*p*	−20.56030	1105.765	24.9	307.198	2.0800	0.654910	0.486368
4*d*	−12.36796	3676.566	30.1	42.6604	1.8679	0.703067	0.571421
5*s*	−5.361445	26.18252	35.5		0.84700	1.52901	2.61304
5*p*	−3.904695	413.0939	38.4	42.7058	0.76168	1.68819	3.20202
4*f*	−3.481826	2058.581	39.7	6.18549	1.4234	0.886259	0.975660
$E=-9282.5251$							
$F^0(4f,\ 4f)=1.037941$		$F^2(4f,\ 4f)=0.5006535$		$F^4(4f,\ 4f)=0.3156171$		$F^6(4f,\ 4f)=0.2275324$	
$\zeta_{4f}=1070.85$		$M^0(4f,\ 4f)=2.553$		$M^2(4f,\ 4f)=1.433$		$M^4(4f,\ 4f)=0.9731$	

gram accepts the initial estimates of the wave functions either as input data or as screened hydrogenlike functions. In the latter case, estimates of the screening numbers are required as input data. In the present calculations, we first used the screened hydrogenlike wave functions as the initial estimates. Values for the screening numbers were obtained[9] using the Hartree-Fock-Slater (HFS) wave functions of Herman and Skillman.[10] In order to further improve the results, the wave functions thus obtained were used as initial estimates and the calculations were repeated. However, it was found that the improvement was not significant enough so as to encourage one to recycle again. This indicates that HFS values of the screening numbers are fairly reliable.

The first SCF calculations on rare-earth ions were done by Ridley[11] for Pr^{+++} and Tm^{+++}. However, these calculations did not include the "exchange" which is known to produce significant changes in the wave functions. Later, Freeman and Watson[12] obtained approximate analytic HF SCF wave functions for Ce^{+++} ($4f$), ^2F; Pr^{+++} ($4f^2$), ^3H; Nd^{+++} ($4f^3$), ^4I; Sm^{+++} ($4f^5$), ^6H; Eu^{++} ($4f^7$), ^8S; Gd^{+++} ($4f^7$), ^8S; Dy^{+++} ($4f^9$), ^6H; Er^{+++} ($4f^{11}$), ^4I; and Yb^{+++} ($4f^{13}$), ^2F. Accuracy of their wave functions was quite limited in the inner regions owing to the small size of the *s* and *p* basis sets used. They only reported the $4f$ orbitals which are in terms of four basis functions. Sovers[13] obtained numerical tabulations of the $4f$ wave functions from the corresponding analytic expansions of Freeman and Watson.[12] Synek and Corsiglia[14] performed analytic calculations for $\mathrm{Pr}^{+++}(4f^2)$, ^3H, and $\mathrm{Nd}^{+++}(4f^3)$, ^4S, ^4D, ^4F, ^4G, and ^4I with minimum basis sets for *s* and *p* wave functions, with five basis functions for *d* wave functions, and with six basis functions for *f* wave functions. Recently, Synek and co-workers[15] have carried out more accurate analytic HF SCF wave function calculations for $\mathrm{Pr}^{+++}(4f^2)$, ^3H, and $\mathrm{Nd}^{+++}(4f^3)$, ^4I, describing the *s*, *p*, *d*, and *f* sym-

TABLE II. Total energy E (a.u.) and virial theorem for various rare-earth systems.

Z	System	Term	E	Virial Theorem
58	$\mathrm{Ce}^{++}\,(4f^2)$	^3H	-8566.4243	-2.0000002
59	$\mathrm{Pr}^{+++}(4f^2)$	^3H	-8919.8340^{a}	-2.0000009^{a}
59	$\mathrm{Pr}^{++}(4f^3)$	^4I	-8920.6931	-2.0000006
60	$\mathrm{Nd}^{+++}(4f^3)$	^4I	-9282.5251^{b}	-1.9999999^{b}
60	$\mathrm{Nd}^{++}\,(4f^4)$	^5I	-9283.3752	-2.0000003
61	$\mathrm{Pm}^{+++}(4f^4)$	^5I	-9653.7230	-1.99999917
61	$\mathrm{Pm}^{++}(4f^5)$	^6H	-9654.5840	-1.9999991
62	$\mathrm{Sm}^{+++}(4f^5)$	^6H	-10033.518	-1.9999996
62	$\mathrm{Sm}^{++}(4f^6)$	^7F	-10034.440	-2.0000002
63	$\mathrm{Eu}^{+++}(4f^6)$	^7F	-10422.032	-2.0000008
63	$\mathrm{Eu}^{++}(4f^7)$	^8S	-10423.022	-1.9999995
64	$\mathrm{Gd}^{+++}(4f^7)$	^8S	-10819.364	-1.9999995
64	$\mathrm{Gd}^{++}(4f^8)$	^7F	-10820.092	-1.9999999
65	$\mathrm{Tb}^{+++}(4f^8)$	^7F	-11225.235	-2.0000008
65	$\mathrm{Tb}^{++}\,(4f^9)$	^6H	-11226.035	-1.9999995
66	$\mathrm{Dy}^{+++}(4f^9)$	^6H	-11640.063	-2.0000001
66	$\mathrm{Dy}^{++}(4f^{10})$	^5I	-11640.914	-2.0000000
67	$\mathrm{Ho}^{+++}(4f^{10})$	^5I	-12063.899	-1.9999995
67	$\mathrm{Ho}^{++}(4f^{11})$	^4I	-12064.757	-1.9999987
68	$\mathrm{Er}^{+++}(4f^{11})$	^4I	-12496.782	-2.0000004
68	$\mathrm{Er}^{++}(4f^{12})$	^3H	-12497.614	-2.0000021
69	$\mathrm{Tm}^{+++}(4f^{12})$	^3H	-12938.732	-1.9999996

[a] Synek and Timmons (Ref. 15) in their analytic HF SCF wave functions obtained $E = -8919.8142$ and virial theorem ratio $= -2.0000037$.

[b] Synek and Grossgut (Ref. 15) in their analytic HF SCF wave functions obtained $E = -9282.5000$ and virial theorem ratio $= -1.9999999$.

metries with ten, eight, five, and six basis functions, respectively. For the states considered, this work provided significant improvement over the previous work of Synek and Corsiglia,[14] especially for the s and p wave functions.

In the present work we have presented accurate numerical HF SCF wave functions for the triply and doubly ionized rare earths listed in the abstract in their ground states. The important results, which have been presented in Tables I and II, can be used for comparison with the calculations of Synek and co-workers[15] for Pr^{+++} and Nd^{+++}. It can be seen that we have lower energy values *and* a better virial-theorem ratio for Pr^{+++}. It may be pointed out that a lower total energy *only* does not imply greater variational accuracy since systematic errors can be introduced in a numerical computation. Regarding the tail wobbling of the $P(nl, r)$ functions for Pr^{+++} and Nd^{+++}, it may be noted here that as compared to the wave functions of Synek and co-workers,[15] the presently obtained functions have smoother tails.

The "tail procedure" used by Fischer[4] has been described by her in an earlier paper.[16] However, in connection with the wobbling, it is important to mention here that Handy, Marron, and Silverstone[17] have recently claimed that the choice of the slope of the wave function at the outermost point in Fischer's tail procedure[16] neglects exchange. This does not seem to be correct. In the notation of Fischer,[16] when a boundary condition is applied at r_{N+1}, a value of y_{N+1} is guessed by assuming $y_{N+1} = cy_N$. One could set $y_{N+1} = 0$ (which is actually done later by Fischer[16]) and then back substitute for y_N, $y_{N-1}, \ldots$, etc. The wrong value of y_{N+1} introduces an error in the boundary condition, but as shown by Fischer and Usmani,[18] the effect of this error decreases as one moves away from the boundary. It may also be remarked here that Synek and co-workers[15] did not impose the cusp-condition restriction[15] on the choice of their basis functions. This implies that the wave functions obtained by these workers cannot be regarded to be quite accurate near the nucleus. On the contrary, in the numerical Hartree-Fock calculation, a series expansion is assumed near the origin which automatically satisfies the cusp condition. As a result, more emphasis has been placed on the inner-electron distribution in the present calculations.

In conclusion, we hope that the present results of the Hartree-Fock calculations on the rare-earth ions will further facilitate the research in the applied solid-state physics concerning these ions.

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Energy Shift Due to Nuclear Polarization in a High Orbital State of Muonic Atom[*]

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The effect of the electromagnetic polarization of the nucleus is considered on the energy levels of the high orbital states in a muonic atom. A simplified calculation is carried out to estimate the approximate dependence of the shifts of the energy levels on the atomic number Z for the orbital states $3s$, $3p$, and $3d$. To do this, a formulation is proposed in which the energy shift is regarded as the amount of energy which flows into the system when the approximated second-order electromagnetic interaction between muon and nucleus is adiabatically switched on. The many-body property of the nucleus is formally expressed as the correction term to the photon self-energy part which represents the dielectricity of nuclear matter. Then the formal parallel holds between the present treatment of nuclear polarization and that of vacuum polarization in field theory. The applicability of the theory is restricted to the high orbital state, in which the bound-state wave function is less sensitive to the nuclear polarization effect, and its energy fluctuation is much less than the energy attributed to the muonic state.

I. INTRODUCTION

Because in some respects the muon can be considered as a heavy electron, the measurements of x rays from muonic atoms have provided much useful information in the study of nuclear structure.[1-3] However, among several corrections necessary to make the information precise, the largest uncertainty has been in the theoretical estimates of the nuclear polarization effect, as pointed out by Ravenhall.[2] Nuclear polarization by electrons was first considered by Breit *et al.*[4] as a possible cause of even-odd straggling, and also by Reiner and Wilets,[5] who found that the effect was too small as far as the monopole, dipole, and quadrupole interactions were concerned. In a muonic atom, Fitch and Rainwater[6] pointed out this effect as a possible correction to muonic energy levels. For shifts of the 1s level, some theoretical estimates had been made by Cooper and Henley,[7] Lakin and Kohn,[8] and Nuding.[9] The predicted values were considerably high, while later calculations based on the collective excitations of the nucleus gave smaller values. The giant resonance was taken into account by Pieper and Greiner,[10] and the effect of a valence proton was considered by Scheck.[11]

By much effort and improvement of experimental technique, accurate measurements have been achieved with better statistics and higher precision. In particular, the Chicago group[12] has been able to assess the discrepancy between their experimental energy value and the calculated one, which is tentatively interpreted as the shift due to nuclear polarization effects in Pb^{206}. The shift for the $1s$ level extrapolated from Cole's result[13] is compatible with the measured value. In his calculations, the giant dipole resonance and the quasielastic peaks in electron inelastic scattering are considered as in nuclear excitation spectra. The result is consistent with Chen's recent calculations[14] which refer specifically to Pb^{208}.

The purpose of the present paper is to estimate the energy shift in higher orbital states. It is