Most negative and most positive expectation values of the spin operator

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Formulas for the most positive and most negative values of the expectation of the spin operator are given and compared with single-particle values. The Nilsson model is used to evaluate these expectations and a scenario is discussed where the value is greater than one.

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The motivation for this work stems from the fact that isoscalar magnetic moments obtained from mirror pairs and $N = Z$ odd-odd nuclei have values that are very close to the single j limit-simplicity in the midst of complexity. We wish to clarify the distinction between the one- and the many-particle aspects of this problem.

For a system of several nucleons we define the expectation value of the spin operator $\vec{\sigma} = 2\vec{S}$:

$$\langle\sigma\rangle = \left\langle \Psi_J^J \sigma_z \Psi_J^J \right\rangle, \tag{1}$$

where Ψ is the many-particle wave function in a state with $M = J$. The magnetic moment of a single nucleon in a state ψ_j^j is called the Schmidt moment. From values of this moment we can infer that for a single nucleon in a state $[L, 1/2]^j$ with $j = L + 1/2$ the value of $\langle\sigma\rangle$ is 1; for a single nucleon with $j = L - 1/2$ the value is $-j/(j+1)$. We next consider a system of many nucleons and use LS wave functions $[L, S]J$. We address the problem of finding the most negative and most positive values of $\langle\sigma\rangle$. We find

$$\langle\sigma\rangle = (1J0J|JJ)2S/(1S0S|SS)\sqrt{(2J+1)(2S+1)} \times W(1SJL;SJ), \tag{2}$$

where W is a Racah coefficient. We have

$$(1J0J|JJ) = -\sqrt{J/(J+1)},$$
$$(1S0S|SS) = -\sqrt{S/(S+1)}, \tag{3}$$

and

$$W = -[S(S+1) + J(J+1) - L(L+1)] \Big/ \sqrt{4S(S+1)(2S+1)J(J+1)(2J+1)}. \tag{4}$$

We find

$$\langle\sigma\rangle = [S(S+1) + J(J+1) - L(L+1)]/(J+1). \tag{5}$$

Let us consider the extremes. For

$$J = L - S, \qquad \langle\sigma\rangle = -2SJ/(J+1). \tag{6}$$

This is the most negative value this quantity can have for a given J. This expression for several nucleons in LS coupling with $J = L - S$ is consistent with the expression for a single nucleon with $j = L - 1/2$ $(-j/(j+1))$, as it must be. The maximum value of $\langle\sigma\rangle$ is obtained by setting $J = L + S$. The value is $2S$. For a single nucleon the value is 1. One can determine $\langle\sigma\rangle$ from mirror pairs:

$$\langle\sigma\rangle = [2\mu(\mathrm{IS}) - J]/(\mu_p + \mu_n - 1/2), \tag{7}$$

where

$$\mu(\mathrm{IS}) = [\mu(T_z) + \mu(-T_z)]/2. \tag{8}$$

In the work of Kramer *et al.* [1], the magnetic moment of ^{21}Mg is measured, which when combined with the moment of ^{21}F yields an isoscalar magnetic moment and an expectation value of the spin operator. These authors refer to the "empirical limits." They use as limits the single-particle Schmidt values $-j/(j+1)$ for $j = L - 1/2$ and 1 for $j = L + 1/2$ and call the results beyond these limits anomalous. By this criterion their own value, $\langle\sigma\rangle = 1.15(2)$, is anomalous. They also refer to anomalies for $A = 9$ found by Matsuta *et al.* [2] and discussed by Utsuno [3]. They obtained a very large value, $\langle\sigma\rangle = 1.44$. A careful reading of the Matsuta *et al.* and Kramer *et al.* papers, however, shows that they do not say that these empirical limits are theoretical limits. Indeed in Ref. [1] the authors report a shell-model calculation with a charge-independent interaction which gives a value of 1.11, close to their measured value. They then go on to include a charge-symmetry-violating interaction which improves the fit. The final result is 1.15. Their shell-model calculation shows that one does not need a violation of charge symmetry to go beyond the empirical limit $\langle\sigma\rangle = 1$.

We would say that their results are not anomalous if the theoretical limits are used. For $J = 5/2$ an LS wave function component with $L = 0$, $S = 5/2$, would yield an upper limit of 5—much larger than the Schmidt limit of 1. For $L = 1$, $S = 3/2$, we get 3. It would be correct to say that these configurations are not the major components of the complete nuclear wave function, so it is still surprising that values greater than 1 are obtained. For $A = 9$, $J = 3/2$, there are several LS configurations with $\langle\sigma\rangle > 1$. For example, there is $[311]L = 0T = 3/2$, $S = 3/2$, for which $\langle\sigma\rangle = 3$, and $[221]L = 1T = 3/2$, $S = 3/2$, for which $\langle\sigma\rangle = 11/5$ [4]. Note that the supermultiplet quantum numbers at the left in these two examples are not needed to evaluate $\langle\sigma\rangle$; only L and S are needed. However, they are included to show that these

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TABLE I. Experimental values of the spin operator obtained from mirror pairs.

Mirror pairs	J	Odd proton	Odd neutron	Sum	$\langle\sigma\rangle$
^{9}Li-^{9}C	3/2	3.439	−1.394	2.048	1.434
^{21}F-^{21}Ne	5/2	3.93	−0.983	2.947	1.176
^{21}Ne-^{21}Na	3/2	2.386	−0.662	1.724	0.589
^{23}Na-^{23}Mg	3/2	2.218	−0.536	1.681	0.479
^{25}Mg-^{25}Al	5/2	3.646	−0.855	2.790	0.766

states obey the Pauli principle. Useful references are studies by Wigner [4] and Bohr and Mottelson [5].

The Nilsson one-body interaction [6] consists of a spin-orbit term, an L^2 term (to make up for the deficiency of the oscillator radial shape), and, most important, a deformed potential $V(r) = 1/2m\omega^2 r^2[1 - 4/3\delta P_2(\cos(\vartheta)]$. As the deformation parameter δ approaches zero we go toward the weak-deformation limit. For very large δ we come to the asymptotic limit where the angle spin part of the wave function decouples to the form $Y_{L,\Lambda}$, $\chi_{1/2,\Sigma}$. For finite δ the spin-orbit interaction prevents Λ and Σ from being good quantum numbers. One gets a sum over various Λ and Σ with the constraint that $\Lambda + \Sigma = K$. The formula for the laboratory magnetic moment in the rotational model using the notation of Bohr and Mottelson [7] is

$$\mu = g_R J + (g_K - g_R)K^2/(J+1) \times [1 + \delta_{K,1/2}(2I+1)(-1)^{J+1}b], \quad (9)$$

where

$$(g_K - g_{R)})b = \langle K(g_L - g_R)L_+\bar{K}\rangle + \langle K(g_S - g_R)S_+\bar{K}\rangle \quad (10)$$

and $|\bar{K}\rangle$ is the time reverse of the state $|K\rangle$. Since g_R is Z/A, for mirror pairs the summed g_R is 1. Hence, if K is not equal to 1/2, we obtain

$$2\mu(\text{IS}) = J + (Kg_K - K)K/(J+1), \quad (11)$$

where $Kg_K = \langle g_L L_z + g_S S_z\rangle$ is evaluated in the intrinsic state. Here g_L is also 1 and $g_S = 2(\mu_p + \mu_n) = 1.760$. Keeping in mind that $A = 9$ and $A = 21$, let us consider intrinsic states in the weak-deformation limit, $p_{3/2,K=3/2}$ and $d_{5.2,K=5/2}$, respectively. We find that

$$Kg_K - K = (\mu_p + \mu_n + L - K), \quad (12)$$

$$2\mu(\text{IS}) = J + (\mu_p + \mu_n + L - K)K/(J+1), \quad (13)$$

TABLE II. Isoscalar Schmidt moments.

	2μ(IS)	$\langle\sigma\rangle$
$s_{1/2}$	0.880	1.000
$p_{3/2}$	1.880	1.000
$d_{5/2}$	2.880	1.000
$p_{1/2}$	0.373	−1/3
$d_{3/2}$	1.272	−3/5

where $Kg_K = \langle g_L L_z + g_S S_z\rangle$ is evaluated in the intrinsic state. When we combine this with the expression at the beginning, we obtain

$$j = L + 1/2 \qquad 2\mu(\text{IS, Schmidt}) = L + \mu_p + \mu_n, \quad (14)$$

where $[\mu(\text{Nilsson}) - \mu(\text{Schmidt})]/\mu(\text{Schmidt}) = -8.1\%$ for $A = 9$, and -3.8% for $A = 21$. Although the percent changes are rather small, the deviations of $\langle\sigma\rangle$ from unity (the Schmidt value) are large. In more detail,

$$A = 9 : J = 3/2, \quad 2\mu(\text{IS}) = 1.728, \quad \langle\sigma\rangle = 0.600,$$
$$A = 21 : J = 5/2, \quad 2\mu(\text{IS}) = 2.771, \quad \langle\sigma\rangle = 0.713.$$

Note that for the above states $\langle\sigma\rangle$ is equal to 1 in the intrinsic frame but considerably less than 1 in the laboratory frame.

We now consider $K = 1/2$ bands. Since g_l and g_R are both 1, the first term in Eq. (9) vanishes and we have

$$(g_K - g_R)b = \langle K|(g_S - g_R)S_+\bar{K}\rangle. \quad (15)$$

We now list in Table I experimental results for $\langle\sigma\rangle$. The Schmidt results are given in Table II. All the values are rounded to up to three digits beyond the decimal point.

In the single-j model for the configurations $(d_{5/2})^n$, the values are as follows:

$$J = 3/2, \quad 2\mu(\text{IS}) = 3/5[\mu(\text{IS, Schmidt})] = 1.728,$$
$$\langle\sigma\rangle = 0.6, \quad J = 5/2, \quad 2\mu(\text{IS}) = 2.880, \quad \langle\sigma\rangle = 1.0.$$

In the weak-deformation limit of the Nilsson model, one obtains

$$J = 3/2, \quad \psi_{j,K} = d_{5/2,3/2}, \quad 2\mu(\text{IS}) = 1.637, \quad \langle\sigma\rangle = 0.360,$$
$$J = 5/2, \quad \psi_{j,K} = d_{5/2,5/2}, \quad 2\mu(\text{IS}) = 2.771, \quad \langle\sigma\rangle = 0.713.$$

Note that the single-j and weak-deformation Nilsson values are not the same. The first two mirror pairs in Table I have isospin $T = 3/2$ and the others have $T = 1/2$. The $T = 1/2$ values of $\langle\sigma\rangle$ are within the single-particle limits but this is not the case for $T = 3/2$. More complete intrinsic wave functions for the cases where $J = K$ were obtained by Ripka and Zamick [8]. They give results for odd proton and odd neutron nuclei from which we can easily infer the isoscalar results. The notation in Table III is such that $C(j)$ is the probability amplitude that the odd particle is in the jj coupling state n, L, j.

In Tables IV and V we give a selected list of 2μ(IS) and $\langle\sigma\rangle$. In Table V things are rearranged to show the evolution of the expectation of the spin operator from the weak-deformation limit to the asymptotic limit.

In the Nilsson model, two identical particles in the same spatial state have opposite spins so only the odd particle contributes to $\langle\sigma\rangle$ and the value is less than or equal to 1. To obtain values of $\langle\sigma\rangle$ greater than 1, components in which the particles are not in the lowest intrinsic states must be introduced. As an example in the weak-deformation limit we form the intrinsic state where a particle is promoted from $p_{3/2,3/2}$ to $p_{1/2,-1/2}$. Thus, the unpaired states are $p_{3/2,1/2}$, $p_{3/2,3/2}$, and $p_{1/2,-1/2}$. One obtains

$$2\mu(\text{IS}) = I + K/(I+1)[\Sigma(\langle L_z\rangle + 1.760\langle S_z\rangle) - K]. \quad (16)$$

TABLE III. Ripka-Zamick expressions modified to yield isoscalar magnetic moments.

	2μ(IS)
p shell	
$J = K = 1/2$	0.3733
$J = K = 3/2$	1.7320
s-d shell	
$J = K = 1/2$	$0.1780C^2(5/2) - 0.1746C^2(3/2) + 0.3804C^2(1/2) - 0.5C(5/2)C(3/2) + 0.5$
$J = K = 3/2$	$0.1368[C^2(5/2) - C^2(3/2)] - 0.3645C(5/2)C(3/2) + 1.5$
$J = K = 5/2$	2.7720

This is a $K = 3/2$ band and for $J = 3/2$ we find that $\langle L_z \rangle = 2/3$, $\langle S_z \rangle = 5/6$, $2\mu(\text{IS}) = 1.88$, and $\langle \sigma \rangle = 1$. This does not get us what we want. However, if we go to the asymptotic limit, the unpaired states are $Y_{1,0}\uparrow$, $Y_{1,1}\uparrow$, and $Y_{1,-1}\uparrow$. In this limit we find that $\langle L_z \rangle = 0$, $\langle S_z \rangle = 3/2$, $2\mu(\text{IS}) = 2.164$, and $\langle \sigma \rangle = 1.8$. This works.

There are many studies of isoscalar magnetic moments. In the work of Mavromatis *et al.* [9] it is noted that only with a tensor interaction can one get corrections to the isoscalar moments of closed major shells plus or minus one nucleon. The systematics of isoscalar moments is discussed in the works of Talmi [10], Zamick [11], Brown [12], Brown and Wildenthal [13], Arima [14], Towner [15], and Talmi [16]. Closely related to mirror pairs are studies of odd-odd $N = Z$ nuclei. It was noted by Yeager *et al.* [17] that both experimental results and large-scale shell-model calculations were close to the single-j results. To understand, these corrections to the Schmidt value in first-order perturbation theory were performed by Zamick *et al.* [18]. They found that isoscalar corrections were much smaller than isovector ones for ^{57}Cu and ^{57}Ni mirror pairs. The calculations went in the direction of reducing $\langle \sigma \rangle$. For problems other than this one, the supermultiplet quantum numbers of Wigner [4] are required if one works in the LS coupling basis.

In summary, it was shown that the range over which $\langle \sigma \rangle$ can vary is considerably wider than that given by the single-particle model. We use the Nilsson model to study this problem and we note some simplicities for the isoscalar mode. The rotational g factor g_R gets replaced by 1 and the expression for a $K = 1/2$ band is simplified. We show that in this model we can get a value of σ greater than 1 only by allowing more than one nucleon to be unpaired. In our example, we have three unpaired particles.

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TABLE IV. Nilsson isoscalar results.

Intrinsic state	2μ(IS)	$\langle \sigma \rangle$
	Weak deformation limit $J = j$	
$p_{3/2,3/2}$	1.728	0.600
$p_{3/2,1/2}$	1.728	0.600
$p_{1/2,1/2}$	0.3733	$-1/3$
$d_{5/2,5/2}$	2.771	0.729
$d_{5/2,3/2}$	2.598	0.257
$d_{5/2,1/2}$	2.706	0.543
$d_{3/2,3/2}$	1.363	−0.360
$d_{3/2,1/2}$	1.363	−0.360
$s_{1/2,1/2}$	0.880	1.000
	Asymptotic $J = 3/2$	
$Y_{1,1}\uparrow$	1.728	0.600
$Y_{1,1}\downarrow$	1.424	-0.200
$Y_{1,0}\uparrow$	1.880	1.000
	Asymptotic $J = 1/2$	
$Y_{1,1}\downarrow$	0.373	$-1/3$
$Y_{1,0}\uparrow$	0.880	1.0
	Asymptotic $J = 5/2$	
$Y_{2,2}\uparrow$	2.771	0.729
$Y_{2,2}\downarrow$	2.446	−0.143
$Y_{2,1}\uparrow$	2.609	0.286
$Y_{2,0}\uparrow$	2.880	1.000
	Asymptotic $J = 3/2$	
$Y_{2,2}\downarrow$	1.272	−0.600
$Y_{2,1}\uparrow$	1.728	0.600
$Y_{2,1}\downarrow$	1.424	−0.200
$Y_{2,0}\uparrow$	1.728	0.600
	Asymptotic $J = 1/2$	
$Y_{0,0}\uparrow$	0.880	1.000
$Y_{2,1}\downarrow$	$-1/3$	−0.439

TABLE V. Expectation values of the spin operator for $J = K$.

Weak deformation limit	$\langle \sigma \rangle$	Asymptotic limit	$\langle \sigma \rangle$
$p_{3/2,1/2}$	0.6	$Y_{1,0}\uparrow$	1.0
$p_{3/2,3/2}$	0.6	$Y_{1,1}\uparrow$	0.6
$p_{1/2,1/2}$	$-1/3$	$Y_{1,1}\downarrow$	−0.2
$d_{5/2,1/2}$	0.543	$Y_{2,0}\uparrow$	1.000
$d_{5/2,3/2}$	0.360	$Y_{2,1}\uparrow$	0.286
$d_{5/2,5/2}$	0.729	$Y_{2,2}\uparrow$	0.729
$d_{3/2,1/2}$	−0.360	$Y_{2,0}\uparrow$	0.600
$d_{3/2,3/2}$	−0.360	$Y_{2,2}\downarrow$	−0.600
$s_{1/2}$	1.000	$Y_{2,1}\downarrow$	−0.439

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