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Notes on the j-j Coupling Shell Model*

EUGENE FEENBERG

Washington University, St. Louis, Missouri, and Oak Ridge National Laboratory,** Oak Ridge, Tennessee (Received July 29, 1949)

A study of the nuclear shell model based on the hypothesis of strong spin-orbit coupling yields a number of interesting results for even-even and odd-odd nuclei. To secure simple relations all calculations are based on the extreme limiting situation of complete j-j coupling. Maximum symmetry in the space wave function and j-j coupling are generally in sharp conflict. On occasion there is no conflict and then the consequences of the j-j coupling model are found to agree with experiment (notably the spin and magnetic moment of B¹⁰ and the sign of the magnetic moment of K^{40}). The *j*-*j* coupling model yields good results for the magnetic moments of N14 and Ne22, but in both cases the agreement may be illusory because the computed moments are nearly independent of the amount of singlet wave function in the representation of the ground state. Also the model favors I = 5 for the ground state of Na²².

INTRODUCTION

HREE aspects of nuclear structure are particularly relevant for the present discussion:

(a) Spin-orbit coupling. Experimental results on nuclear spins and magnetic moments of light nuclei suggest that parallel orientation of the orbital and spin angular momentum vectors of the individual particles is favored energetically over the antiparallel orientation.¹ The rule may be stated in the form that nuclear multiplets are inverted or regular according as the last orbital shell is less or more than half-filled.² Actually the theoretical basis for the rule is somewhat confused and equivocal because of uncertainty in the form, exchange properties and spin dependence of nuclear forces and the associated relativistic corrections³⁻⁵ as well as in the best choice of nuclear model and the magnitude of configuration interaction.^{6,7}

(b) Odd-even structure of the energy surface. In the successive addition of neutrons (or protons), the odd neutron (or proton) is less tightly bound than the

preceding and following even neutron (or proton).8-10 The simplest interpretation is that two nucleons interact most strongly when both are in essentially equivalent space orbits. With two particles in an orbit, energy is gained from the direct interaction of the particles and from a second-order polarization effect which simulates a direct interaction.¹¹ In the space orbital approximation, two like particles outside of a closed shell or missing from a closed shell are described by singlet wave functions completely symmetrical in the space coordinates of the two particles.

From a more general standpoint, the odd-even structure of the energy surface can be correlated with a pronounced tendency for the ground state space wave function to possess the maximum possible symmetry consistent with the exclusion principle. The actual maximum is associated with Wigner's first approximation¹² in which the space wave functions belong to irreducible representations of the symmetric group. The ground states have then the following spin properties:

Type of nucleus	Spin character
even-even	singlet $(S=0)$
odd-odd	singlet $(S=0)$ or triplet $(S=1)$
even-odd	doublet $(S=\frac{1}{2})$.

⁸ N. Bohr and J. A. Wheeler, Phys. Rev. 56, 426 (1939); particularly Eq. (6).

^{*} Assisted by the Joint Program of the ONR and the AEC. ** Temporary, summer, 1949. ¹ D. R. Inglis, Phys. Rev. 50, 783 (1936); also G. Breit, lectures ¹ D. R. Inglis, Phys. Rev. **50**, 783 (1936); also G. Breit, lectures at Ann Arbor, summer, 1936.
 ² L. Rosenfeld, *Nuclear Forces* (Interscience Publishers, Inc., New York, 1948), p. 317. Denoted by NF in later references.
 ³ S. Dancoff and D. R. Inglis, Phys. Rev. **50**, 784 (1936).
 ⁴ W. Furry, Phys. Rev. **50**, 784 (1936).
 ⁵ G. Breit, Phys. Rev. **51**, 248, 778 (1937).
 ⁶ M. Phillips, Phys. Rev. **57**, 160 (1940); NF, p. 410.
 ⁷ R. Sacks, Phys. Rev. **55**, 825 (1939); NF, p. 411.

¹⁰ See reference 2, Fig. 3.221-1.
¹⁰ K. Way, Phys. Rev. **75**, 1448 (1949).
¹¹ C. F. V. Weizacker, Zeits. f. Physik **96**, 432 (1935).
¹² E. P. Wigner, Phys. Rev. **51**, 106, 947 (1937).

	g factor			
State	Neutron g1	Proton g		
${}^{2}S_{1/2}$	-3.82	5.58		
${}^{2}P_{3/2}$	-1.27	2.53		
${}^{2}P_{1/2}$	1.27	-0.53		
${}^{2}D_{5/2}$	-0.76	1.92		
${}^{2}D_{3/2}$	0.76	0.08		
${}^{2}F_{7/2}$	-0.55	1.65		
${}^{2}F_{5/2}$	0.55	0.35		
${}^{2}G_{9/2}$	-0.42	1.51		
${}^{2}G_{7/2}$	0.42	0.49		
${}^{2}H_{11/2}$	-0.35	1.42		
2Ha/2	0.35	0.58		

TABLE I. Single particle Landé g factors.

There is good evidence from the analysis of binding energies supporting the approximate validity of Wigner's first approximation up to $A \sim 50^{12,13}$ The absence of a noticeable trend with Z or A in the values of allowed (favored)¹⁴ and allowed (unfavored)^{15,16} beta-decay matrix elements suggests a much wider range of validity.

(c) I=0 for even-even nuclei. As yet no exception is known to the rule that even-even nuclei have I=0 in the ground state. However, the existence of two eveneven nuclei with isomeric states (82Pb²⁰⁴ and 32Ge⁷²) and the probable existence of others suggests the advisability of caution in stating and applying the rule. In terms of the explanation offered for b, the rule implies that the state of lowest energy has neither orbital nor spin angular momentum. Studies of exchange force models by variational and perturbation methods yield results conforming to the rule.¹⁷⁻¹⁹

Among recently discussed nuclear shell models, one is based on the hypothesis that (i) strong spin-orbit coupling exists in accordance with the Breit-Inglis rule¹ and (ii) the effective magnitude of the coupling grows with increasing angular momentum in an unspecified, but decisive manner.^{20, 21}

The present note develops certain consequences of the strong spin-orbit coupling model for two particles with respect to the symmetry properties of the space wave function. To secure simple relations, all calculations are based on the extreme limiting situation of complete j-j coupling. It will be shown that j-jcoupling on the one hand and maximum symmetry in the space wave function on the other are generally in sharp conflict. On occasion there is no conflict and then the consequences of the j-j coupling model are found to agree with experiment (notably the spin and magnetic moment of B¹⁰ and the sign of the magnetic moment of

 $_{19}K^{40}$). The j-j coupling model yields good results for the magnetic moments of 7N14 and 11Ne22, but in both cases the agreement may be illusory because the computed moments are nearly independent of the amount of singlet wave function in the representation of the ground state. Also, the model favors I = 5 for the ground state of $_{11}Na^{22}$ rather than the actual I=3.

NOTATION

 $\Theta_{lm}(\theta, \varphi)$ —normalized single particle angular wave function.

$$(2l+1)^{\frac{1}{2}}\psi_{l+\frac{1}{2},p+\frac{1}{2}} = (l+1+p)^{\frac{1}{2}}\Theta_{l,p}\delta(m_{s},\frac{1}{2}) + (l-p)^{\frac{1}{2}}\Theta_{l,p+1}\delta(m_{s},-\frac{1}{2}),$$

$$(2l+1)^{\frac{1}{2}} \psi_{l-\frac{1}{2}, p+\frac{1}{2}} = (l-p)^{\frac{1}{2}} \Theta_{l, p} \delta(m_{s}, \frac{1}{2}) \\ - (l+1+p)^{\frac{1}{2}} \Theta_{l, p+1} \delta(m_{s}, -\frac{1}{2}), \\ {}^{3}S_{1}(1, 2) = \delta(m_{s1}, \frac{1}{2}) \delta(m_{s2}, \frac{1}{2}), \\ {}^{3}S_{0}(1, 2) = 2^{-\frac{1}{2}} \left[\delta(m_{s1}, \frac{1}{2}) \delta(m_{s2}, -\frac{1}{2}) \\ + \delta(m_{s2}, \frac{1}{2}) \delta(m_{s1}, -\frac{1}{2}) \right], \\ {}^{3}S_{-1}(1, 2) = \delta(m_{s1}, -\frac{1}{2}) \delta(m_{s2}, -\frac{1}{2}), \\ {}^{1}S_{0}(1, 2) = 2^{-\frac{1}{2}} \left[\delta(m_{s1}, \frac{1}{2}) \delta(m_{s2}, -\frac{1}{2}) \\ - \delta(m_{s2}, \frac{1}{2}) \delta(m_{s1}, -\frac{1}{2}), \right], \\ (p+\frac{1}{2}, q+\frac{1}{2})_{\pm}^{i} = 2^{-\frac{1}{2}} \left[\psi_{j, p+\frac{1}{2}}(1) \psi_{j, q+\frac{1}{2}}(2) \right]$$

$$\pm \psi_{j, p+\frac{1}{2}}(2)\psi_{j, q+\frac{1}{2}}(1)],$$

$$(p, q)_{\pm} = 2^{-\frac{1}{2}} \left[\Theta_{l, p}(1) \Theta_{l, q}(2) \pm \Theta_{l, p}(2) \Theta_{l, q}(1) \right].$$

The last two definitions fail for p = q. Obvious modifications are then required to maintain the normalization of the symmetrical combination.

TWO LIKE PARTICLES IN EOUIVALENT ORBITS

The wave function

$$(l+1)^{\frac{1}{2}}\Psi_{0}(1,2) = \sum_{0}^{l} (-1)^{p} (p+\frac{1}{2}, -p-\frac{1}{2})^{l+\frac{1}{2}}$$
(1)

describes two like particles in $j = l + \frac{1}{2}$ orbits combined to produce an antisymmetrical state with zero angular momentum. The problem set here is the determination of the statistical weight of the singlet component in Ψ_0 . A straightforward calculation yields

$$\begin{split} & 2l+1)(l+1)^{\frac{1}{2}}\Psi_{0}(1,2) \\ &= {}^{3}S_{1}\sum_{0}^{l}(-1)^{p}\{(l+1+p)(l-p)\}^{\frac{1}{2}}(p,-p-1) \\ &+ {}^{3}S_{-1}\sum_{0}^{l}(-1)^{p}\{(l+1+p)(l-p)\}^{\frac{1}{2}}(p+1,-p)_{-} \\ &+ {}^{3}S_{0}2^{\frac{1}{2}}\sum_{1}^{l}(-1)^{p}p(p,-p)_{-} \\ &+ (l+1) {}^{1}S_{0}\bigg[(0,0)_{+}+2^{\frac{1}{2}}\sum_{1}^{l}(-1)^{p}(p,-p)_{+}\bigg]. \end{split}$$

¹³ W. Barkas, Phys. Rev. 55, 691 (1939).

 ¹⁴ E. P. Wigner, Phys. Rev. 56, 519 (1939); A. M. Feingold and
 E. P. Wigner, unpublished notes (1949).
 ¹⁵ N. Feather and H. O. W. Richardson, Proc. Phys. Soc. 61, 452

^{(1948).}

<sup>(948).
&</sup>lt;sup>16</sup> E. Feenberg and K. C. Hammack, Phys. Rev. **75**, 1877 (1949).
¹⁷ W. Heisenberg, Zeits. f. Physik **96**, 473 (1935).
¹⁸ E. Feenberg and M. Phillips, Phys. Rev. **51**, 597 (1937).
¹⁹ Tyrrell, Carroll, and Margenau, Phys. Rev. **55**, 790 (1939).
²⁰ M. G. Mayer, Phys. Rev. **75**, 1969 (1949).
²¹ Haxel, Jensen, and Suess, Phys. Rev. **75**, 1766 (1949).

The singlet term is found to occur with the statistical weight

$$(l+1)/(2l+1)$$
.

Similarly, one finds

$$l^{\frac{1}{2}}\Phi_{0}(1,2) = \sum_{0}^{l-1} (-1)^{p} (p + \frac{1}{2}, -p - \frac{1}{2})_{-}^{l-\frac{1}{2}}, \quad (3)$$

the antisymmetric wave function with zero angular momentum constructed from pairs of orbits with $j=l-\frac{1}{2}$. Proceeding as before, the singlet term is found to occur with the statistical weight l/(2l+1). The single formula (2j+1)/2(2l+1) includes both cases.

As illustrations, consider the application to ${}_{38}\text{Sr}^{88}$ and ${}_{40}\text{Zr}^{92}$ assuming I=0 for the ground states of both nuclei as required by c. In Wigner's first approximation, the space part of the wave functions belong to irreducible representations of the symmetric group denoted by the partition symbol $4 \cdots 42 \cdots 2$. In the language of the shell model, assuming L-S coupling, two holes in the proton 3p shell or two particles in the neutron 4d shell generate ${}^{1}S_{0}$ ground states, completely symmetrical in the space coordinates of the two particles. With complete j-j coupling on the other hand, the statistical weight of the ${}^{1}S_{0}$ component is 0.33 $(l=1, j=\frac{1}{2})$ and 0.60 (l=2, j=5/2).

The only certain conclusion warranted by the preceding argument is that the hypothesis of strong spinorbit coupling as postulated by Mayer requires an extreme degree of departure from the maximum possible symmetry, consistent with the exclusion principle, in the space wave function. However, continuing on less certain ground, several plausible lines of argument may be cited against the possibility of such large admixture of triplet components as occur in the preceding examples. The simple and qualitatively satisfying explanation discussed under b of the greater binding energy of the even particle now fails. The ground states of even-even nuclei are now linear combinations of ${}^{1}S_{0}$ and ${}^{3}P_{0}$ components with approximately equal statistical weights. Also the theoretical basis for the separation of allowed beta-transitions into distinct favored and unfavored groups is lost.

One can, however, find in property c an argument for a tendency toward j-j coupling. The two particle wave functions with maximum spin are

$$\Psi_{2l} = (l + \frac{1}{2}, l - \frac{1}{2})_{-}^{l+1},$$

$$\Psi_{2l-2} = (l - \frac{1}{2}, l - \frac{3}{2})_{-}^{l-\frac{1}{2}}, \quad l > 0.$$
(4)

The statistical weight of the singlet component is $(2l+1)^{-1}$ for the first and $(4l-1)(2l+1)^{-2}$ for the second. In view of these results it is a reasonable supposition that the statistical weight of the singlet component for states in the antisymmetric j^2 function space attains a maximum at I=0. If now strong forces tending

TABLE II. Spins and magnetic moments of odd-odd nuclei.

Nucleus	Experimental* Mag- netic Spin moment		Compute mc <i>j-j</i> coupling	ed magnetic oment Singlet component removed	Statistical weight of the triplet component in <i>j-j</i> coupling	Pre- dicted spin in <i>j-j</i> coupling	
3Li6	1	0.82	0.63	0.785	0.444	3	
5B10	3	1.80	1.88	1.88	1.000	3	
7N14	1	0.40	0.37	0.34	0.778	1	
$_{11}Na^{22}$	3	1.75	1.73	1.86	0.640	5	
19K40	4	-1.29	-1.70	1.16	0.74		

*S. Millman and B. Kusch, Phys. Rev. 60, 91 (1941); J. Zacharias, Phys. Rev. 61, 270 (1942); Gordy, Ring, and Burg, Phys. Rev. 74, 1191 (1948); and L. David, Phys. Rev. 74, 1193 (1948).

to favor energetically states of maximum symmetry in the space wave function (i.e., Majorana forces) coexist with strong spin-orbit forces, the opposing tendencies should favor zero spin for the ground state.

These remarks leave the issue unsettled, but may help to direct attention to an important problem.

TWO UNLIKE PARTICLES

The spins and magnetic moments of odd-odd nuclei offer further opportunities for testing the hypothesis of strong spin-orbit coupling. A table of Landé g factors facilitates the calculations (see Table I).

The formula

$$\mu/\mu_0 = \frac{1}{2}I \left[g_1 + g_2 + (g_1 - g_2) \frac{(j_1 - j_2)(j_1 + j_2 + 1)}{I(I+1)} \right], \quad (5)$$

valid for pure j-j coupling, yields the magnetic moments listed in column 4 of Table II.

The excellent agreement of j-j coupling moments with the experimental values may be illusory. First of all, the values listed in the last column of Table II represent the ground state spins expected if strong forces tending to produce j-j coupling are associated with strong forces tending to favor energetically states of maximum symmetry in the space wave function. The discrepancies at Li⁶ and Na²² suggest that spin-orbit coupling plays a secondary role in determining the ground state angular momenta of these nuclei. Secondly, the complete omission of the singlet components in the j-j coupling wave functions (excluding K⁴⁰) does not change the moments appreciably (except in Li⁶ where the omission of the singlet component results in a notable improvement).

In the shell model description of K^{40} , the $(3d)^{-1}(4f)^1$ configuration generates four L-S coupling type states with I=4; ${}^{3}H_{4}$, ${}^{3}G_{4}$, ${}^{3}F_{4}$, and ${}^{1}G_{4}$ all with positive magnetic moments.²² The alternative simple possibility of j-j coupling yields one state with I=4 from each of the configurations ${}^{2}D_{3/2} {}^{2}F_{5/2}$, ${}^{2}D_{5/2} {}^{2}F_{7/2}$, and ${}^{2}D_{3/2} {}^{2}F_{7/2}$. Only the last named possesses a negative

²² D. R. Inglis,"Phys. Rev. 60, 837 (1941); NF, p. 416.

magnetic moment. Thus the negative magnetic moment of K^{40} may be cited as supporting the j-j coupling shell model. Considering, however, the absence of symmetry effects (because of the non-equivalence of the 3d and 4forbits), it is not unlikely that the appearance of extreme j-j coupling may be produced by a relatively weak coupling of the spin and orbital motion. Within the limits of the ground state configuration, the most general wave function is a linear combination of the four above-mentioned L-S coupling states. The expectation value of the magnetic moment operator then contains cross terms connecting the several pure L-S type components. These cross terms create the possibility of a negative magnetic moment.

Recent studies of energy distribution in the 38Sr⁹⁰ and 39Y90 beta-transitions23,24 provide unambiguous evidence for the assignment I=2 to the ground state of 39Y90. A direct measurement of the spin and magnetic moment of this nucleus would yield information on the coupling scheme in a $(3p)^{-1}(4d)^1$ configuration. The various simple ways of constructing states with I=2and the associated magnetic moments are tabulated below:

State	$^{1}D_{2}$	${}^{3}P_{2}$	$^{3}D_{2}$	${}^{3}F_{2}$	$P_{3/2}D_{5/2}$	$P_{3/2}D_{3/2}$	$P_{1/2}D_{3/2}$	$P_{1/2}D_{5/2}$
μ/μ_0	0.33	0.38	0.57	0.30	-0.97	3.29	0.88	-1.60

The wave functions listed in the Appendix may be used to compute quadrupole moments. It is uncertain whether such calculations can yield significant results because of the sensitivity of quadrupole matrix elements to the admixture of small components in the wave function from excited configurations. Whereas magnetic moments depend quadratically on the amplitudes of the admixture, quadrupole moments are linear functions when these amplitudes are small. Consequently, a simple wave function may produce a significant result for the magnetic moment while failing completely on the quadrupole moment (i.e., the ${}^{2}P_{3/2}$ wave function derived from $(2p)^3$ for Li⁷).²⁵

APPENDIX

Li⁶:
$${}^{2}P_{3/2}(\text{neutron}){}^{2}P_{3/2}(\text{proton}), j_{1} = j_{2} = 3/2, I = 1.$$

 $(45)^{1/2}\psi_{1,1} = 3[3^{1/2}(3/2, -1/2)_{+}{}^{3/2} - 2^{1/2}(1/2, 1/2)_{+}{}^{3/2}]$
 $= {}^{3}S_{1}\{3(1, -1)_{+} - 2^{3/2}(0, 0)_{+}\} + {}^{3}S_{0}(0, 1)_{+}$
 $- 2^{1/2} {}^{3}S_{-1}(1, 1)_{+} + 5 {}^{1}S_{0}(1, 0)_{-}.$

B¹⁰:
$${}^{2}P_{3/2} \binom{\text{neutron}}{\text{hole}} {}^{2}P_{3/2} \binom{\text{proton}}{\text{hole}},$$

 $j_{1} = j_{2} = 3/2, I = 3.$
 $\psi_{3,3}(3/2, 3/2)_{+} = {}^{3}S_{1}(1, 1)_{+}.$
N¹⁴: ${}^{2}P_{1/2} \binom{\text{neutron}}{\text{hole}} {}^{2}P_{1/2} \binom{\text{proton}}{\text{hole}},$
 $j_{1} = j_{2} = 1/2, I = 1.$

$$\begin{aligned} 3\psi_{1,1} &= 3(1/2, 1/2)_+ \\ &= {}^3S_1(0, 0)_+ - 2^{1/2} \, {}^3S_0(0, 1)_+ + 2 \, {}^3S_{-1}(1, 1)_+ \\ &- 2^{1/2} \, {}^1S_0(0, 1)_- \end{aligned}$$

Na²²: ${}^{2}D_{5/2}$ (neutron) ${}^{2}D_{5/2}$ (proton),

$$j_1 = j_2 = 5/2, I = 3.$$

$$15\psi_{3,3} = 5[5^{1/2}(5/2, 1/2)_+ - 2(3/2, 3/2)_+]$$

$$= {}^3S_1[(75)^{1/2}(2, 0)_+ - 8(1, 1)_+] + {}^3S_0(2, 1)_+$$

$$- 2 {}^3S_{-1}(2, 2)_+ + 9 {}^1S_0(2, 1)_-$$

K⁴⁰:
$${}^{2}D_{3/2} \left(\stackrel{\text{proton}}{\text{hole}} \right) {}^{2}F_{7/2} (\text{neutron}),$$

 $j_1 = 3/2, j_2 = 7/2, I = 4.$

$$(350)^{1/2}\psi_{4,4} = (35)^{1/2} [3^{1/2}\psi_{3/2} \ _{3/2}(1)\psi_{7/2} \ _{5/2}(2) - 7^{1/2}\psi_{3/2} \ _{1/2}(1)\psi_{7/2} \ _{7/2}(2)]$$

$$= {}^{3}S_{1}[(18)^{1/2}\Theta_{21}(1)\Theta_{32}(2) - (98)^{1/2}\Theta_{20}(1)\Theta_{33}(2)] + {}^{3}S_{0}[(96)^{\frac{1}{3}}\Theta_{21}(1)\Theta_{33}(2) - 6\Theta_{22}(1)\Theta_{32}(2)] - (12)^{1/2} {}^{3}S_{-1}\Theta_{22}(1)\Theta_{33}(2) - {}^{1}S_{0}[(54)^{1/2}\Theta_{21}(1)\Theta_{33}(2) - 6\Theta_{22}(1)\Theta_{32}(2)]$$

 ²³ Braden, Slack, and Shull, Phys. Rev. **75**, 1964 (1949).
 ²⁴ E. N. Jensen and L. J. Laslett, Phys. Rev. **75**, 1949 (1949).
 ²⁵ P. Kusch, Phys. Rev. **76**, 138 (1949).