Application of Self-Consistent Field Methods to Rotational Motion in *sd* Shell Nuclei*

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A self-consistent field calculation of the single-particle orbitals in the *sd* shell is presented. The calculation is based on a standard shell-model Hamiltonian employing a single-particle spin-orbit force and two-body Yukawa interaction with a Rosenfeld exchange mixture. Using these orbitals the low-lying rotational spectra of the *sd* shell nuclei are computed. The variational formula of Skyrme and the cranking model yield moments of inertia which compare well with the experimental data. The rotation-particle coupling interaction is diagonalized and good fits to the nuclear rotational spectra are obtained.

I. INTRODUCTION

THE program of this paper is to use shell-model concepts and methods to compute nuclear collective properties. In particular, the collective properties of the spectra of nuclei in the first half of the *sd* shell are treated here. A discussion of how one can apply the shell-model Hamiltonian for the computation of moments of inertia[1] (to be referred to as I) and self-consistent wave functions and intrinsic spectra[2] (to be referred to as II) has been given elsewhere. In this paper these methods are brought to bear on observed nuclear spectra. In the case of odd-even nuclei the even-even core is first treated and its moment of inertia and wave function calculated. Next, the extra core particle is added and its polarizing effect on the core is computed and the rotation particle coupling (RPC) interaction is diagonalized. This yields the spectra of the various observed bands. The shell-model interaction used in this paper is that given by Elliott and Flowers.[3] The strength of the two-body force is varied along with the position of the single-particle levels. The effects of changes in the exchange mixture or the range of the two-body interaction are not studied.

That this method works for the nuclei studied is hardly surprising. There has been ample experimental and theoretical[4,5] evidence that nuclei in the first half of the *sd* shell are essentially "collective." It is, however, particularly gratifying that one can easily carry out the calculations from a rather fundamental viewpoint. The given Hamiltonian is not chopped into various phenomenological pieces but bears some resemblance to what one hopes the ultimate shell-model force will look like.

The methods used here will probably have to be modified in treating the heavy rotational region where the pairing interaction modifies the form of the wave function. However, no overriding objection to the general approach seems present.

Some initial steps have[6] been taken in the direction of applying shell-model methods to the calculation of a vibrational potential and thus computing the vibrational parameters.

It is felt that too little attention has been given in the past to the interesting possibility of using shell-model Hamiltonians in calculations of self-consistent orbitals, moments of inertia and collective properties in general. The main technical advantage in this direction is that one can often avoid the real weakness of the shell model, namely the evaluation of matrix elements between states of many particles where J is a good quantum number. In spite of the many sophisticated theories of angular momenta and their couplings the program of direct calculation of nuclear properties in the shell-model scheme with configuration interaction for many-particle systems cannot, at present, be carried out. It may even be argued that a representation with good J obscures the real physical aspect of the wave function. Certainly, in the case of a deformed rotating nucleus or a vibrating one, this is true. It is therefore natural to consider the shell-model approach applied directly to various collective wave functions.

II. THE MODEL

The existence of a ground-state rotational band in even-even nuclei, and a series of rotational bands in neighboring odd-even nuclei, leads very naturally, as first pointed out by Bohr and Mottelson,[7] to the description of these nuclei in terms of a rotational collective model. The even-even nucleus is described as a

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[1] C. A. Levinson, Phys. Rev. **132**, 2184 (1963).
[2] I. Kelson, Phys. Rev. **132**, 2189 (1963).
[3] J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) **A229**, 536 (1955).
[4] A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **30**, No. 1 (1955).
[5] H. E. Gove and A. E. Litherland, Phys. Rev. **113**, 1078 (1957).
[6] E. Flamm, C. A. Levinson, and S. Meshkov, Phys. Rev. **129**, 297 (1963).
[7] A. Bohr and B. R. Mottelson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **27**, No. 16 (1953).

simple rotator. Since, quantum mechanically, a spherical object cannot give rise to a rotational spectrum, one assigns to the nucleus a deformed shape. From the point of view of a single-particle approximation of the nuclear states, that would mean that the single-particle orbits of the nucleons do not have j, angular momentum, as a good quantum number. However, if we retain a spheroidal shape k, the z component of angular momentum in the body-fixed system, would characterize these states. The odd-even nucleus fits very simply into the picture. The even-even core is still a simple rotator with a moment of inertia $\mathcal{J}$, while the extra nucleon can be in a set of single-particle levels, all of which are eigenfunctions of a spheroidal Hamiltonian n.

The Hamiltonian of the system is thus given by[8]

$$H=A\mathbf{R}^2+h, \tag{1}$$

where $A=\hbar^2/2\mathcal{J}$ and $\mathbf{R}$ is the angular momentum of the even-even core. Since $\mathbf{R}^2$ is not a constant of motion, (1) is better re-expressed in terms of the total angular momentum $\mathbf{I}=\mathbf{R}+\mathbf{j}$

$$H=A(\mathbf{I}-\mathbf{j})^2+h=A(\mathbf{I}^2+\mathbf{j}^2)+h-2A\mathbf{I}\cdot\mathbf{j}. \tag{2}$$

This Hamiltonian may be diagonalized very easily, by making use of the symmetric top eigenfunctions $D_{MK}{}^I$, and the known single-particle eigenfunctions χ_K of h. Incorporating the properties of invariance under rotation and reflection, the following set of functions is obtained

$$\phi_{MK}{}^{I,\tau}=\frac{(2I+1)^{1/2}}{4\pi}\{D_{MK}{}^I(\theta_i)\chi_K{}^\tau(\mathbf{r}') +(-1)^{I-j}D_{M-K}{}^I(\theta_i)\chi_{-K}{}^\tau(\mathbf{r}')\}, \tag{3}$$

θ_i represent the collective-angle variables of the nucleus, whereas $\mathbf{r}'$ are the body-fixed coordinates of the extra nucleon. This separation is indeed appropriate for (2), the eigenfunctions of which are linear combinations of the form

$$\Psi_M{}^I=\sum_{K,\tau}\alpha_K{}^{I,\tau}\phi_{MK}{}^{I,\tau}. \tag{4}$$

The only term in (2) which is not diagonal in K is the scalar product $-2A\mathbf{I}\cdot\mathbf{j}$ (the RPC term). It has nondiagonal elements between states $\phi_{MK}{}^{I,\tau}$ with $\Delta k=1$, and diagonal elements, possibly, only for $K=\frac{1}{2}$. These diagonal matrix elements cause the so-called decoupling of the $K=\frac{1}{2}$ rotational band from the total rotational motion of the nucleus. When the eigenstates of h are given by

$$\chi_K=\sum_i C_K{}^i\phi_K{}^i, \tag{5}$$

this decoupling effect is quantitatively reflected in the decoupling factor

$$a=\sum_j(-1)^{j-1/2}(j+\tfrac{1}{2})(C_{1/2}{}^j)^2, \tag{6}$$

and the diagonal elements are

$$\langle\phi_{M1/2}{}^{I,\tau}|H|\phi_{M1/2}{}^{I,\tau}\rangle =A[I(I+1)+(-1)^{I-1/2}a(I+\tfrac{1}{2})]. \tag{7}$$

III. DISCUSSION OF THE MODEL

The principal assumptions on which the simple rotational model is based, are the existence of a collective rotational Hamiltonian of the core, and the validity of the single-particle deformed orbit picture for the odd nucleon: To what extent these assumptions are related to each other, as well as their basic connection with a more fundamental physical picture—is not answered by the model. Fitting the experimental data thus becomes a matter of adjusting the parameters that appear in the problem. The value of A, as well as the form of h and its eigenvalues and eigenfunctions, have to be determined phenomenologically.

In previous work[9] with this model, h was taken to have the form of a deformed harmonic oscillator and the value of A was either taken from the data or computed with a cranking formula including the effects of pairing. In principle, of course, h should represent the average field in which the nucleons move. This field can be computed using the Hartree-Fock method.[10] In the full Hartree-Fock approach the orbitals are completely arbitrary and are varied over all possible radial and angular dependences. In our "Hartree-Fock" calculation, we take a standard shell-model radial dependence and vary only over linear combinations of spins and angular dependences in a given major shell. These calculations are described in detail in paper II. The calculation of the moment of inertia parameter A is carried out by the variational method of Skyrme which is discussed in detail in paper I or with the Inglis cranking formula.[11] Thus, all of the information needed to compute nuclear structure in the rotational regions is computed directly from a given shell-model Hamiltonian and is given a self-consistent basis.

In the case of even-even nuclei the collective motion presents a single low-lying rotational band and some high excited bands. In this work only the low-lying band in even-even nuclei is discussed so that only a moment of inertia is computed. The details of moment of inertia calculations are given in the next sections.

The spectra of the odd-even nuclei presents a much more stringent test for the model. In these nuclei one must carry out an RPC matrix diagonalization. This

[8] S. A. Moszkowski, *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1957), Vol. 39, p. 411.

[9] K. H. Bhatt, Nucl. Phys. **39**, 375 (1962).

[10] A good summary of the subject is given by F. Villars, in *Rendiconti della Scuola Internazionale di Fisica* "Enrico Fermi," *XXIII Corso: Fisica Nucleara* (Academic Press Inc., New York and London, 1963).

[11] D. R. Inglis, Phys. Rev. **96**, 1059 (1954).

involves the single-particle energy spacings as well as the details of the self-consistent wave functions. Also, in odd-even nuclei several bands occur simultaneously among the low-lying states and the details of their mixing must be correctly understood.

In addition a new effect occurs—that of particle core polarization. It is clear that the even-even core single-particle structure does not remain unchanged while the external nucleon is allowed to go from orbit to orbit. This polarization (details are given in paper II) has two important effects.

(1) When a particle changes orbit, its effect on the underlying even-even core changes. This causes a small change in each of the particle wave functions in the core and a consequent change in the total energy of the core which is sometimes quite important. This change in energy of the system is referred to as a polarization effect and serves to renormalize the single-particle energies of a particle outside a core.

(2) If the surface tension of the core is low enough, then the polarizing effect of the outside particle is enough to change the moment of inertia of the core. This effect is actually seen in the spectra of Al^{25} and Al^{27}.

It is a great advantage of the self-consistent methods used in this paper that polarization effects can be computed in detail and with sufficient accuracy to check against the observed data.

IV. REGION OF APPLICABILITY

The nuclei that are suitable for treatment by these methods are odd-even nuclei, where the numbers of protons and neutrons differ by one. The charge symmetry as well as the averaging procedure in paper II demand that mirror nuclei should be treated in pairs. In coming to determine the region of applicability, the following points should be considered:

(1) The even-even core has to have a ground-state rotational band, as well as an intrinsic single-particle structure, which is deformed and stable against vibrations (in particular γ vibrations).

(2) The odd-particle states should be well separated from the occupied states of the core, so that no single- or double-particle excitations will compete energetically. In this context it may be stressed that the variational methods for obtaining single-particle level schemes tend to increase the gap between occupied and unoccupied states. This will be discussed in detail in later sections.

These criteria limit our calculations to the first half of the *s-d* shell. Around mass number[12] 28 (Si^{29}) the sign of the deformation changes, and is experimentally not quite clear. Around mass number 32, condition (2) is severely violated. Single- and double-particle excitations, as from the $\frac{1}{2}'$—to the $\frac{3}{2}'$ orbit are very likely to occur and play an important role.

Four pairs of mirror nuclei are thus left for detailed treatment:

$$Ne^{21}\text{–}Na^{21};\quad Na^{23}\text{–}Mg^{23};\quad Mg^{25}\text{–}Al^{25};\quad Al^{27}\text{–}Si^{27}.$$

V. DETAILS OF THE CALCULATION

The basic two-body interaction is taken to be the Rosenfeld[13] mixture, having the form

$$V=V_0V_{TS}\frac{e^{-r/a}}{r/a}, \tag{8}$$

where $a=1.37\times10^{-13}$ cm, and V_{TS} has the following eigenvalues

$$V_{00}=1.8\quad V_{01}=-1.0\quad V_{10}=-0.6\quad V_{11}=0.333\cdots. \tag{9}$$

V_0 was chosen to be 42.5 MeV, and is actually one of the parameters in the problem. The single-body part was taken throughout to be a pure $\mathbf{l}\cdot\mathbf{s}$ force, with a $d^{5/2}$–$d^{3/2}$ splitting of 6.2 MeV. All the calculations were done with oscillator functions of range 1.65×10^{-13} cm.

The choice of V_0 and $\alpha_{\mathbf{l}\cdot\mathbf{s}}$ is interdependent. Increasing V_0, has through the self-consistent calculations, an effect similar to that of increasing the spin-orbit force. But once those parameters are chosen our detailed model yields unambiguously the rotational spectra. The Rosenfeld mixture, though, may not be very satisfactory, since it probably tends to overemphasize the singlet-triplet part of the force. Another debatable point, is whether the single-particle part of the force should be taken to be the same for the whole range of nuclei in question. The calculations of nuclear spectra in this paper indicate that the experimental data is consistent with little or no change in the strength of the single-particle spin-orbit force.

For each of the pairs of nuclei in question only the lowest possible band for each k was included in the calculation. Higher K bands, if existing, are well separated and are weakly coupled to the lowest ones. Thus, for nuclei with mass number 21, 23 three rotational bands

$$k=\tfrac{1}{2}'\quad k=\tfrac{3}{2}\quad k=\tfrac{5}{2}$$

and their mixing by the RPC were computed. For mass number 25, 27 only two bands were considered

$$k=\tfrac{1}{2}'\quad k=\tfrac{5}{2},$$

because in Mg^{24} the $k=\frac{3}{2}$ orbit is completely filled. In the latter case the two orbits are not mixed by the RPC force, and the problem splits into two parts: the structure of each band, and their relative position.

[12] H. E. Gove, *Proceedings of the International Conference on Nuclear Structure, Kingston, 1960*, edited by D. A. Bromley and E. W. Vogt (University of Toronto Press, Toronto, 1960), p. 438.

[13] L. Rosenfeld, *Nuclear Forces* (North-Holland Publishing Company, Amsterdam, 1948), p. 233.

TABLE I. Moment of inertia parameter A, in MeV, calculated by the cranking formula, using Nilsson and self-consistent single-particle wave functions, for Ne^{20} and Mg^{24}. μ is the coefficient of the l^2 single-particle force.

	Nilsson				Self-consistent			
	$\mu=0$ $\eta=2$	$\mu=0$ $\eta=4$	$\mu=0.167$ $\eta=2$	$\mu=0.167$ $\eta=4$	$\mu=0$ $V_0=40$ MeV	$\mu=0$ $V_0=50$ MeV	$\mu=0.167$ $V_0=40$ MeV	$\mu=0.167$ $V_0=50$ MeV
Ne^{20}	0.052	0.120	0.048	0.116	0.208	0.272	0.205	0.270
Mg^{24}	0.068	0.109	0.074	0.114	0.178	0.154	0.189	0.163

VI. MOMENTS OF INERTIA

An alternative method to the Skyrme formula for computing the moment of inertia is the Inglis cranking formula[11] given by

$$\mathcal{I}=2\sum_{\sigma,\mu}\frac{|(\sigma|J_x|\mu)|^2}{E_\sigma-E_\mu}\quad\begin{matrix}\sigma\equiv\text{"unoccupied" level}\\ \mu\equiv\text{"occupied" level.}\end{matrix}\qquad(10)$$

The energies in the denominator are the eigenvalues of the Hartree-Fock Hamiltonian. The difference $(E_\sigma-E_\mu)$ is not[10] the energy required to lift a particle from the state μ to the state σ. If we call this latter energy $\delta E_\mu{}^\sigma$ then the two are related by the formula:

$$\delta E_\mu{}^\sigma=(E_\sigma-E_\mu)-(\sigma\mu|V|\sigma\mu)+(\sigma\mu|V|\mu\sigma),\qquad(11)$$

where V is the two-body part of the original Hamiltonian. If Φ_0 is the ground-state determinant and $\Phi_\mu{}^\sigma$ is the determinant obtained by promoting a particle in the μ orbital to the σ orbital, then we have

$$\delta E_\mu{}^\sigma=(\Phi_\mu{}^\sigma|H|\Phi_\mu{}^\sigma)-(\Phi_0|H|\Phi_0).\qquad(12)$$

In an odd-even nucleus where the effects of polarization are important the determinant $\Phi_\mu{}^\sigma$ is computed variationally from $\delta(\Phi_\mu{}^\sigma|H|\Phi_\mu{}^\sigma)=0$. The resulting value of $\delta E_\mu{}^\sigma$ is then somewhat different from the result where $\Phi_\mu{}^\sigma$ is taken to be made up out of the orbitals based on the usual single-particle Hamiltonian (see paper II for details about polarization calculations). $\delta E_\mu{}^\sigma$ is the relevant energy spectrum for computing spectra of odd-even nuclei while $E_\sigma-E_\mu$ is required in the cranking formula.

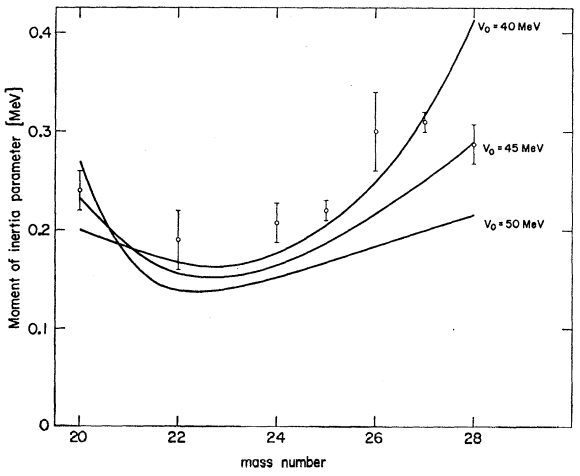

FIG. 1. The moment of inertia parameter for the ground-state bands, obtained by using the cranking formula for different V_0. The continuous curve corresponds to gradually varying $\theta_{3/2}$, $\theta_{5/2}$ from zero to unity between masses 20–24 and 24–28, respectively. The experimental moments of inertia parameters are shown for comparison for mass numbers 21 and 23. See Figs. 7, 8 where the full RPC diagonalization is carried out.

Moments of inertia computed with the cranking model are shown in Fig. 1 where results for various choices of the two-body force strength V_0 are shown. In each case the moment of inertia of the ground-state band is calculated and also, for comparison, are shown the experimentally observed moment of inertia parameters. The agreement between theory and experiment is indeed gratifying.

The rate of change of computed moment of inertia with respect to a change in V_0 depends on the surface tension of the nucleus. As one moves from Ne^{20} toward Si^{28} the figure shows that the moment of inertia parameter changes more and more with a fixed 10-MeV change in V_0. This indicates that the heavier nuclei in this group have a smaller surface tension and one would not be surprised to find vibrational degrees of freedom becoming more important as the surface tension goes down.

In Table I is shown a comparison between the cranking formula moment of inertia parameters computed with self-consistent orbitals and then with the Nilsson Mottelson[14] wave functions and energy spacings.

The great difference between the Nilsson-Mottelson results and the self-consistent calculation is due to the quite different energy denominators in the two calculations. In Fig. 2 is shown a comparison of Nilsson-Mottelson single-particle spectra with the self-consistent results. In a true self-consistent calculation, the single-particle level spectrum depends strongly on the nature of the occupied levels. This is not the case for the deformed harmonic oscillator model of Nilsson and Mottleson, where the values of $E_\sigma-E_\mu$ which are required for the cranking model formula [Eq. (10)] are quite different from those computed self-consistently. The wave functions, on the other hand, do not differ greatly and hence the numerator in Eq. (10) is approximately the same for both cases.

[14] S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **29**, No. 16 (1955).

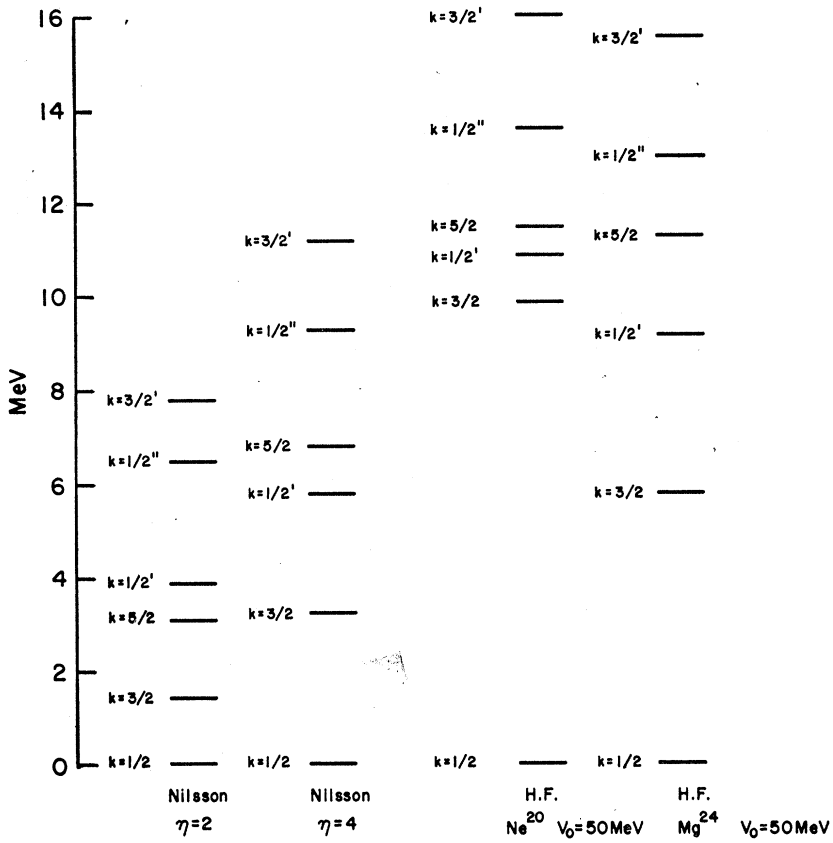

FIG. 2. A comparison between the deformed harmonic oscillator spectrum of Nilsson and Mottelson (for $\eta=2$ and $\eta=4$), and the self-consistent single-particle spectrum (for Ne^{20} and Mg^{24}). The two sets of single-particle spectra go to the same spherical spectrum for $\eta=0$ or $V_0=0$.

VII. RESULTS

The single-particle spectra resulting from the self-consistent calculations are shown for even-even nuclei in Fig. 3 and for odd-even nuclei in Fig. 4. In these calculations the force parameters were those discussed in Sec. V. The orbitals were labeled by the k quantum number and a "filling parameter" θ_k is introduced for each orbital. θ_k gives the fraction of filling of each orbital and is discussed in detail in paper II. In the odd-even spectra the effect of polarization is included and levels occupied by the even-even core are not shown. The odd-even spectrum in Fig. 4 was used in the RPC diagonalization. However, for a cranking-model calculation one must use the "unpolarized" spectrum in Fig. 3. The "unpolarized" odd-even spectrum is not given explicitly but can be read off by interpolation from Fig. 3.

Tables II and III give the corresponding single-particle wave functions.

A. Ne^{20} Moment of Inertia

The procedure for computing the moment of inertia with the Skyrme formula is given in detail in paper I. Summarizing briefly: The "intrinsic" Hamiltonian H is introduced where

$$H \equiv H - AJ^2 \text{J} . \qquad (13)$$

J^2 is the total angular-momentum operator and H is the shell-model Hamiltonian. A best determinantal wave function is found variationally for various par-

TABLE II. Single-particle self-consistent energies and wave functions for even-mass nuclei. The italicized numbers are the self-energies in MeV, followed by the components of the eigenfunctions, in the $|jm\rangle$ representation, starting with $C_K^{j\max}$. $V_0=42.5$ MeV.

	$\theta_{1/2}=1$	$\theta_{1/2}=1$ $\theta_{3/2}=\frac{1}{2}$	$\theta_{1/2}=1$ $\theta_{3/2}=1$	$\theta_{1/2}=1$ $\theta_{3/2}=1$ $\theta_{5/2}=\frac{1}{2}$
$k=\frac{1}{2}$	*0*	*0*	*0*	*0*
	0.829	0.819	0.816	0.870
	−0.397	−0.360	−0.294	−0.297
	0.394	0.448	0.498	0.393
$k=\frac{3}{2}$	*7.142*	*5.805*	*3.799*	*3.005*
	0.995	0.987	0.974	0.991
	−0.098	0.163	−0.226	−0.134
$k=\frac{5}{2}$	*8.587*	*9.392*	*8.690*	*6.167*
	1.000	1.000	1.000	1.000
$k=\frac{1}{2}'$	*9.435*	*9.653*	*8.412*	*7.285*
	0.528	0.569	0.518	0.455
	0.321	0.614	0.755	0.790
	−0.787	−0.546	−0.403	−0.411
$k=\frac{1}{2}''$	*12.161*	*11.882*	*11.290*	*10.300*
	0.186	−0.079	−0.257	−0.186
	0.860	0.702	0.586	0.536
	0.475	0.708	0.768	0.823
$k=\frac{3}{2}'$	*13.888*	*13.547*	*13.186*	*10.745*
	0.098	0.163	0.226	0.134
	0.995	0.987	0.974	0.991

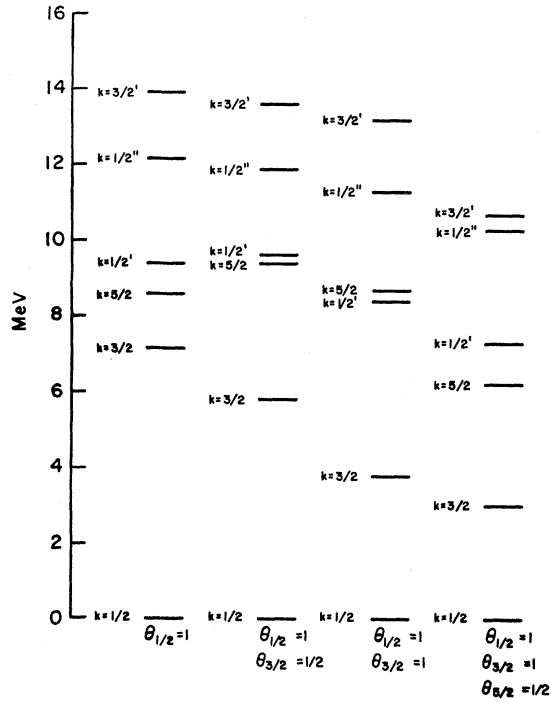

FIG. 3. Self-consistent single-particle spectra for even-mass nuclei. The parameters employed are $V_0=42.5$ MeV, $\alpha_{l,s}=2.48$ MeV ($d_{5/2}-d_{3/2}$ splitting equals 6.2 MeV). It is interesting to note the relative gap between occupied and unoccupied orbits. In particular the contraction of the $k=\frac{1}{2}-k=\frac{3}{2}$ gap as the $k=\frac{3}{2}$ is being filled and the corresponding effect for the $k=\frac{3}{2}-k=\frac{5}{2}$ gap should be noticed.

ticular values of A, the moment of inertia parameter. If $|\Phi_A\rangle$ designates the variational determinant corresponding to H, then, in order to find the best value of A, one must minimize the expression

$$I_A{}^2\equiv\langle\Phi_A|\,(H-\langle\Phi_A|H|\Phi_A\rangle)^2|\Phi_A\rangle \qquad (14)$$

as a function of A. Since the orbitals in $|\Phi_A\rangle$ have been determined self-consistently, H has vanishing matrix elements to single-particle excitations. Hence, the expression for I_A reduces to

$$I_A{}^2=\sum_{\mu\nu;\,\sigma\tau}|\langle\mu\nu|\,V_A|\sigma\tau\rangle|^2, \qquad (15)$$

where $\mu\nu$ are "occupied" levels and $\sigma\tau$ are unoccupied levels. V_A is the antisymmetrized two-body part of H. As A is varied in the neighborhood of the minimum of $I_A{}^2$ both V_A and the orbitals change. The strongest dependence of A occurs for matrix elements in the above sum for which the matrix element of H can cancel against that of AJ^2. Matrix elements such that $\langle\mu\nu|J^2|\sigma\tau\rangle$ is identically zero have a very slow dependence on A and contribute only a "background."

In the case of Ne^{20} the most important matrix elements are those between the states:

$$(\tfrac{1}{2}\,\tfrac{1}{2})\rightarrow(\tfrac{3}{2}\,\tfrac{1}{2}') \quad (\tfrac{1}{2}\,\tfrac{1}{2})\rightarrow(\tfrac{3}{2}\,\tfrac{3}{2})$$
$$(\tfrac{1}{2}\,\tfrac{1}{2})\rightarrow(\tfrac{3}{2}\,\tfrac{1}{2}'') \quad (\tfrac{1}{2}\,\tfrac{1}{2})\rightarrow(\tfrac{1}{2}'\,\tfrac{1}{2}').$$

TABLE III. Single-particle self-consistent energies and wave functions for odd-mass nuclei, including polarization effects (same format as Table II).

Mass number:	21	23	25	27
$k=\frac{3}{2}$	*0*	*0*		
	0.991	0.981		
	−0.134	−0.194		
$k=\frac{5}{2}$	*2.817*	*3.382*	*0*	*0*
	1.000	1.000	1.000	1.000
$k=\frac{1}{2}'$	*3.515*	*3.074*	*0.748*	*1.299*
	0.615	0.530	0.513	0.444
	0.427	0.680	0.748	0.835
	−0.663	−0.507	−0.421	−0.324
$k=\frac{1}{2}''$	*5.943*	*7.879*	*3.600*	*4.311*
	0.099	−0.120	−0.235	−0.176
	0.792	0.652	0.594	0.436
	0.602	0.748	0.769	0.882
$k=\frac{3}{2}'$	*7.580*	*8.419*	*5.725*	*4.740*
	0.134	0.194	0.201	0.094
	0.991	0.981	0.979	0.996

Cancellation between the matrix elements of H and J^2 occurs in the neighborhood of $A=0.2$. Plots of $I_A{}^2$ versus A are given in Fig. 5. In heavier nuclei the cancellations are not as good and the background terms are larger, thus making for a less pronounced minimum. This may indicate that our choice for the form of the orbitals is a poorer approximation for the heavier nuclei.

The dependence of $A_{\min}$ on V_0 is simply through a proportionality relation. Thus, for

$e_{3/2}=0$, $e_{1/2}=-4.2$ MeV, $e_{5/2}=-7.0$ MeV, (no l^2 force).

$$V_0=50\text{ MeV}\quad A_{\min}=0.23\text{ MeV}$$
$$V_0=40\text{ MeV}\quad A_{\min}=0.184\text{ MeV}.$$

For $e_{3/2}=0$, $e_{1/2}=-4.2$ MeV, $e_{5/2}=-6.0$ MeV,

$$V_0=50\text{ MeV}\quad A_{\min}=0.205\text{ MeV}$$
$$V_0=40\text{ MeV}\quad A_{\min}=0.164\text{ MeV},$$

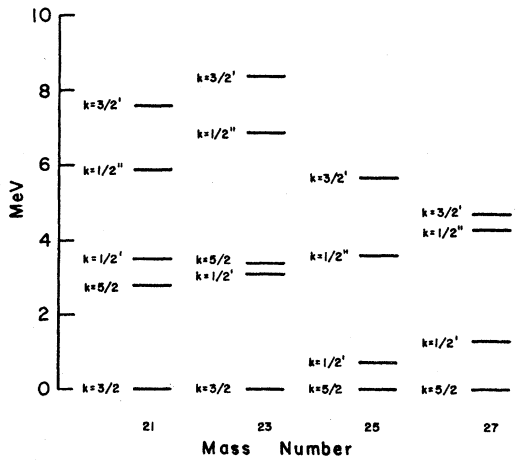

FIG. 4. Self-consistent single-particle spectra for odd-mass nuclei where polarization corrections of nonoccupied states are included. The parameters employed are $V_0=42.5$ MeV, $\alpha_{l,s}=2.48$ MeV.

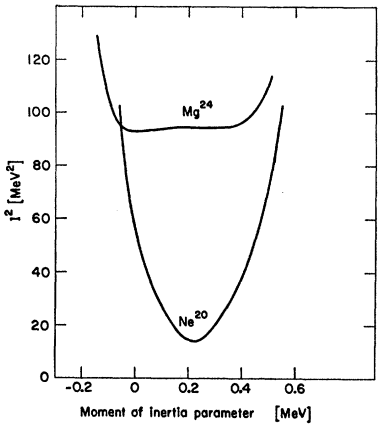

FIG. 5. I^2 versus moment of inertia parameter for Ne^{20} and Mg^{24}.

where e_j is the single-particle energy due to the spin-orbit force.

B. Projection Results for Ne^{20}

For the case of Ne^{20} it is interesting to evaluate the amplitudes a_J of each J state, and the corresponding expectation values of the Hamiltonian, i.e.,

$$a_J=\langle\phi_0|P^J|\phi_0\rangle, \tag{16}$$

$$E_J=\langle\phi_0|HP^J|\phi_0\rangle, \tag{17}$$

where P^J is the projection operator for angular momentum J.

This is done by operating on

$$\phi_0=\sum_{J=0}^{J\max} a_J\Psi_0{}^J \tag{18}$$

repeatedly with J_+, thus

$$J_+{}^n\phi_0\equiv\phi_n=\sum_{J=n}^{J\max} a_J\pi_n{}^J\Psi_n{}^J, \tag{19}$$

where

$$\pi_n{}^J=\prod_{m=0}^{n-1}[(J-m)(J+m+1)]^{1/2}. \tag{20}$$

Equation (19) gives rise to two triangular sets of linear equations,

$$\langle\phi_n|\phi_n\rangle=\sum_{J=n}^{J\max}(\pi_n{}^J)^2a_J{}^2 \tag{21}$$

and

$$\langle\phi_n|H|\phi_n\rangle=\sum_{J=n}^{J\max}(\pi_n{}^J)^2a_J{}^2E_J. \tag{22}$$

The results of solving these equations are summarized in Table IV and the energy levels obtained are also compared to the experimental values in Fig. 6. In addition, Fig. 6 displays the Ne^{20} spectrum based on the Skyrme-formula moment of inertia and the cranking-formula moment of inertia using the same $V_0=42.5$ MeV.

TABLE IV. Projected energies and amplitudes for all the J states of the Ne^{20} ground-state band. The absolute energy values E correspond to adjusting the single-particle $d^{3/2}$ state to zero energy.

	E_J [MeV]	(E_J-E_0) [MeV]	$a_J{}^2$
$J=0$	−44.77	0	0.125
$J=2$	−43.19	1.58	0.436
$J=4$	−39.92	4.85	0.329
$J=6$	−36.56	8.21	0.094
$J=8$	−32.42	12.35	0.016

It should be noted, that if the projected energy levels are exactly those of a rotator, the following relation holds true

$$\langle\phi_0|H|\phi_0\rangle=E_0+A\langle J_+\phi_0|J_+\phi_0\rangle. \tag{23}$$

C. Mass Numbers 21 and 23

We consider here odd-even nuclei where the odd group contains 11 nucleons. The odd particle is in a $k=\frac{3}{2}$ orbit and the ground states indeed are $I=\frac{3}{2}^+$. The nuclei in this group of isospin $\frac{1}{2}$ are divided into two groups. Mass number 21—the pair of mirror nuclei Ne^{21}–Na^{21}, and mass number 23—the pair of mirror nuclei Na^{23}–Mg^{23}.

The rotational nature and structure of these nuclei is not quite clear. First, spin assignments are quite difficult. Second, the identification of rotational bands is somewhat doubtful. Third, some states do not belong to any possible rotational band. This suggests that aside from a blurred rotational pattern, one should include other possible low-energy states, such as core excitations.

From the point of view of the present calculations, the addition of two particles in going from mass number 21 to mass number 23 results in a change in the single-particle spectrum and wave functions. This in turn changes the magnitude of the RPC matrix elements and thus changes the calculated spectrum.

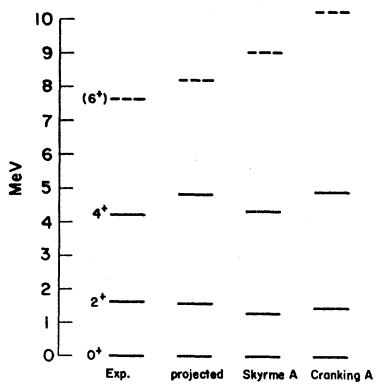

FIG. 6. A comparison between the experimental ground-state rotational band of Ne^{20}, and the calculations using the projection method, the Skyrme method and the cranking formula. The same $V_0=42.5$ MeV is used in all three methods.

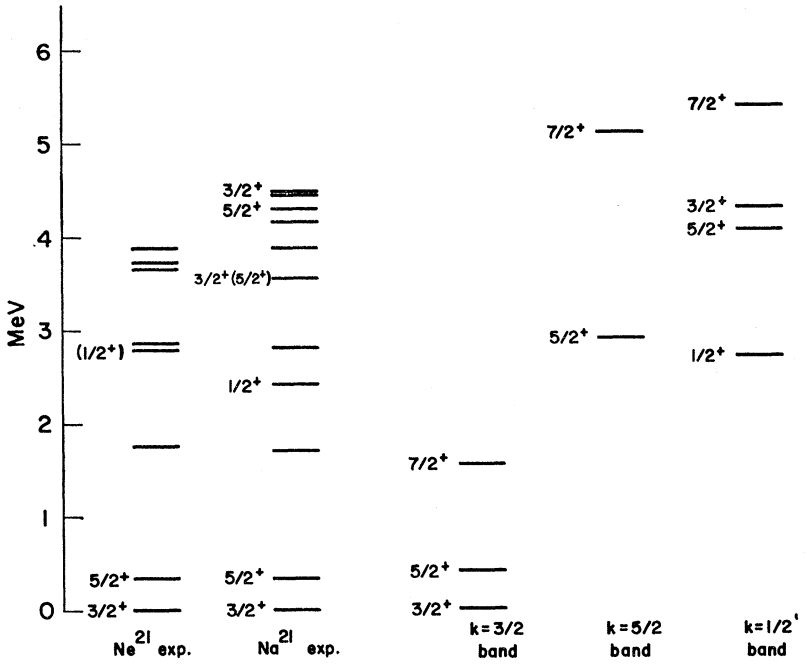

FIG. 7. The three lowest calculated rotational bands for mass number 21, compared to experiment. A, the moment of inertia parameter is taken here to be 0.23 MeV. See Fig. 1 for cranking values of A versus V_0.

The final wave functions resulting from the RPC diagonalization are given in Table V. In this calculation only the orbits $k=\frac{3}{2}, \frac{1}{2}, \frac{5}{2}$ were included. The remaining orbits were neglected since they were much higher in energy. It would be inconsistent to include them while excluding core excitations. The final calculated energies are shown in Figs. 7 and 8.

D. Mass Numbers 25 and 27

Here we are concerned with odd-even nuclei, where the odd group contains 13 nucleons. The odd particle is in a $k=\frac{5}{2}$ orbit, and the ground states indeed are $I=\frac{5}{2}+$. Here, too, nuclei of isospin $\frac{1}{2}$ are divided into two groups. Mass number 25 nuclei: Mg^{25} and Al^{25}, and mass number 27 nuclei: Al^{27} and Si^{27}.

All the nuclei in this group, display similar properties indicating rotational nature, and similar deformation. The spectra of each pair of mirror nuclei, shows greater similarity than in the previous case (Sec. C). Although the spin assignments of some levels is not quite clear, rotational bands have been positively identified.[15]

The excited low-lying orbits are the $k=\frac{5}{2}$ and $k=\frac{1}{2}'$ levels. Other levels are quite separated from these, and in addition the RPC coupling to them is small. This is a lucky circumstance. $k=\frac{1}{2}'$ and $k=\frac{5}{2}$ bands do not intermix through the RPC. We thus may treat the two low-lying $k=\frac{5}{2}$ and $k=\frac{1}{2}$ bands practically independently.

The k equals $\frac{5}{2}$ band calculation, then, is simply a question of the moment of inertia of the band while the k equals $\frac{1}{2}'$ problem involves a calculation of the energy of the band head, the moment of inertia of the band and the decoupling factor for the band.

In the case of these nuclei the variational method

TABLE V. Results of RPC diagonalization for mass numbers 21 and 23. $E_K{}^{I,\tau}$ is the energy in MeV above the ground-state $E_{3/2}{}^{3/2}$. The wave functions are given in terms of the mixing coefficient $\alpha_k{}^\tau$ for each I submatrix.

		Mass number 21				Mass number 23			
I^π	K^τ	$E_K{}^{I,\tau}$ (in MeV)	$\alpha_{1/2'}$	$\alpha_{3/2}$	$\alpha_{5/2}$	$E_K{}^{I,\tau}$ (in MeV)	$\alpha_{1/2'}$	$\alpha_{3/2}$	$\alpha_{5/2}$
$\frac{1}{2}+$	$\frac{1}{2}'$	2.57	1.000			2.49	1.000		
$\frac{3}{2}+$	$\frac{1}{2}'$	4.21	0.988	−0.156		3.22	0.992	−0.129	
$\frac{3}{2}+$	$\frac{3}{2}$	0	0.156	0.988		0	0.129	0.992	
$\frac{5}{2}+$	$\frac{1}{2}'$	4.04	0.901	−0.381	0.205	4.19	0.939	−0.317	0.134
$\frac{5}{2}+$	$\frac{3}{2}$	0.39	0.240	0.835	0.495	0.45	0.226	0.862	0.453
$\frac{5}{2}+$	$\frac{5}{2}$	2.77	−0.361	−0.397	0.844	2.84	−0.259	−0.396	0.881
$\frac{7}{2}+$	$\frac{1}{2}'$	5.36	0.887	0.405	0.223	4.53	0.902	−0.419	0.101
$\frac{7}{2}+$	$\frac{3}{2}$	1.57	0.234	0.809	0.539	1.69	0.296	0.777	0.556
$\frac{7}{2}+$	$\frac{5}{2}$	5.11	−0.398	−0.426	0.660	5.00	−0.314	−0.470	0.825

[15] A. E. Litherland, H. McManus, E. B. Paul, D. A. Bromley, and H. E. Gove, Can. J. Phys. **36**, 378 (1958).

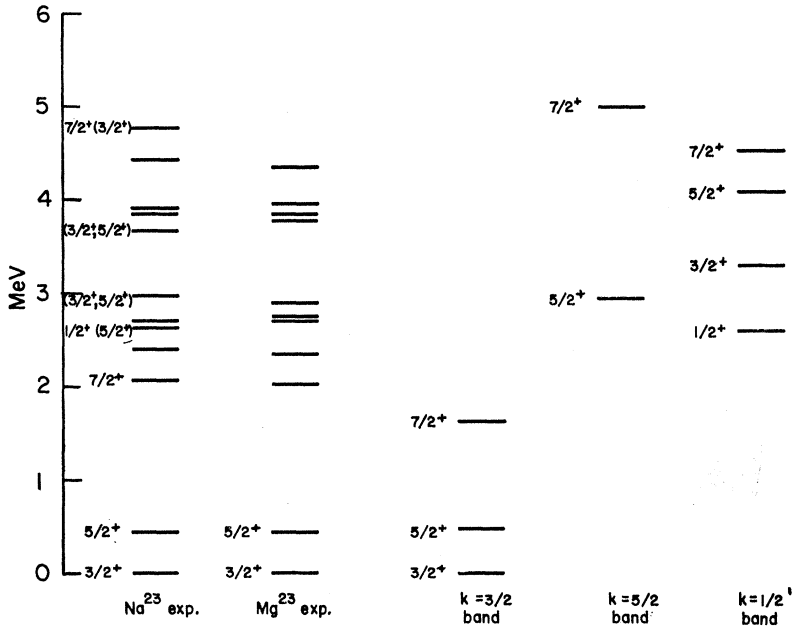

FIG. 8. The three lowest calculated rotational bands for mass number 23, compared to experiment. A, the moment of inertia parameter is taken here to be 0.19 MeV. The main difference between Fig. 8 and Fig. 7 is the change of the structure of the $k=\frac{1}{2}'$ band. See Fig. 1 for cranking values of A versus V_0.

of Skyrme for the moment of inertia is not sufficiently accurate. As seen in Fig. 5, the minimum in the $I^2(A)$ curve for Mg^{24} is very broad and only defines A to within plus or minus 0.15 MeV. This broadness is due to the fact that the matrix elements $\langle\mu\nu|\mathbf{J}^2|\sigma\tau\rangle A$ cancel those of $\langle\mu\nu|H|\sigma\tau\rangle$ at different values of A. We interpret this qualitatively as being due to a decrease in the surface tension since a rather broad group of intrinsic states are all about equally good.

This interpretation is further supported by the results using the cranking model. As discussed in the section Moments of Inertia, the stronger dependence of the moment of inertia parameter on V_0 as one goes to heavier nuclei indicates a decrease in surface tension.

Along with a decrease in surface tension we would expect a higher degree of polarization by the extra core particle. This would then imply that the different bands in a given nucleus would have different moments of inertia depending on the polarizing effect of the extra core particle. For example, the K equals $\frac{5}{2}$ orbital is a pure $d_{5/2}{}^{5/2}$ orbital and has a negative quadrupole moment. Hence, one would expect it to decrease the deformation of the underlying Mg^{24} core which has a positive quadrupole moment and hence the moment of inertia of the system would decrease (an increase in A). On the other hand, the K equals $\frac{1}{2}$ orbital has a positive quadrupole moment and one would expect a decrease in A. This expectation is consistent with the experimental data, and is predicted quantitatively by the cranking formula. The results of applying the cranking formula to the $k=\frac{1}{2}'$, $\frac{5}{2}$ and bands decoupling to $k=\frac{1}{2}'$ bands are shown in Figs. 9 and 10 where experimental results are shown for comparison.

TABLE VI. Calculated versus experimental nuclear magnetic moments in nuclear magnetons. g_R is taken to be equal to z/A, and the approximate value of $\partial\mu_{\text{cal}}/\partial g_R$ is tabulated.

Nucleus	Spin	μ_{exp}	μ_{cal}	$\frac{\partial\mu_{\text{cal}}}{\partial g_R}$
Ne^{21}	$\frac{3}{2}+$	-0.66	-0.62	~ 0.6
Na^{21}	$\frac{3}{2}+$		$+2.09$	~ 0.6
Na^{23}	$\frac{3}{2}+$	$+2.22$	$+2.29$	~ 0.6
Mg^{23}	$\frac{3}{2}+$		-0.52	~ 0.6
Mg^{25}	$\frac{5}{2}+$	-0.85	-1.01	~ 0.85
Al^{25}	$\frac{5}{2}+$		$+3.70$	~ 0.85
Al^{27}	$\frac{5}{2}+$	$+3.64$	$+3.71$	~ 0.85
Si^{27}	$\frac{5}{2}+$		-1.01	~ 0.85

E. Nuclear Magnetic Moments

Another property of the odd-even nuclei, which is sensitive to the single-particle structure, is their mag-

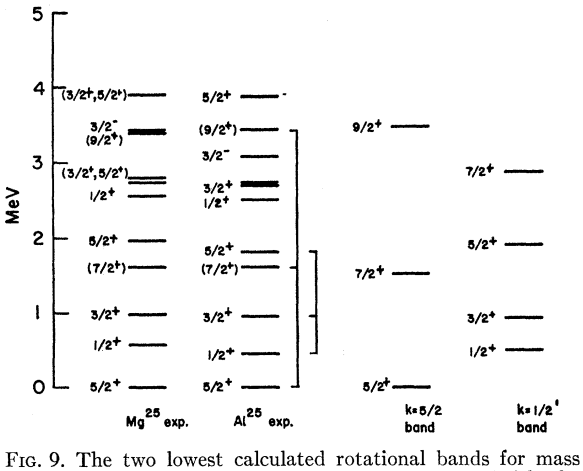

FIG. 9. The two lowest calculated rotational bands for mass number 25, compared to experiment. In accordance with the cranking formula A, the moment of inertia parameter is 0.22 MeV for the $k=\frac{5}{2}$ band and 0.17 MeV for the $k=\frac{1}{2}'$ band. The decoupling factor of the $k=\frac{1}{2}'$ band is $a=-0.15$.

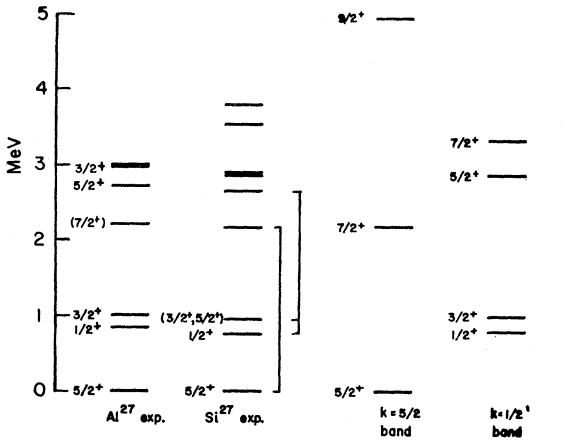

FIG. 10. The two lowest calculated rotational bands for mass number 27, compared to experiment. In accordance with the cranking formula A, the moment of inertia parameter, is 0.31 MeV for the $k=\frac{5}{2}$ band and 0.22 MeV for the $k=\frac{1}{2}'$ band. The decoupling factor of the $k=\frac{1}{2}'$ band is $a=-0.70$.

netic moments. The magnetic moment is

$$\mu=1/(I+1)\langle \mathfrak{y}\cdot \mathbf{I}\rangle, \tag{24}$$

where the operator $\mathfrak{y}$ is given by

$$\mathfrak{y}=g_l\mathbf{l}+g_S\mathbf{S}+g_R\mathbf{R}. \tag{25}$$

The value of g_R was taken to be z/A, in accordance with irrotational flow model. However, since possible deviations might occur from that value, the magnitude of $\partial\mu/\partial g_R$ was calculated. Table VI gives calculated magnetic moments compared to experimental values. The nuclei with ground-state spins $\frac{1}{2}$ and $\frac{3}{2}$ display the greatest sensitivity to the orbital structure, and therefore to the self-consistent single-particle field.

VIII. CONCLUSIONS

The main conclusion is that in the first half of the *sd* shell, the model of a rotating particle core system is essentially correct and that the parameters in this model can be quantitatively understood in terms of a standard shell-model Hamiltonian. The self-consistent calculations for the single-particle orbitals and spectra, although resembling those of the Nilsson model, differ from them in a very important respect. In the self-consistent calculations, a single-particle level is depressed as its occupation number increases. This is clearly due to the strong mutual attractions between particles in the same orbits, both the neutrons and the protons. In the Nilsson-Mottelson model, this effect is almost completely neglected and the levels shift only slightly due to the small changes in the equilibrium deformation of the nucleus. The level depressions found in the self-consistent calculations are a reflection of the pairing properties of the two-body interaction both in the T equals one and T equal zero isospin states. The consequent effect on the cranking formula is to increase the important energy denominators and thus bring the prediction of the model into agreement with experiment. The fact that the Skyrme formula and the cranking-model formula agree is gratifying since the accuracy of the Skyrme formula is expected to be quite good because it is based on a variational principle (see paper I).

As long as pairing effects leading to a breakdown in the validity of single-determinant wave functions do not become dominant, it is conceivable that the methods presented here will be sufficient for understanding certain collective aspects of the low excited states of nuclei. Certainly the second half of the *sd* shell presents an interesting challenge where vibrational degrees of freedom probably become important. Outside of a few regions of pure jj coupling, the pf shell seems to present a fruitful region for application of the methods described in this paper.

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