Variational Shell-Model Methods for Deformed Orbitals*

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A single-particle representation of deformed orbitals in the s-d shell is obtained by using variational selfconsistent methods. The two-body Rosenfeld potential is taken as the effective interaction. The dependence of the single-particle Hamiltonian on the force parameters, as well as its dependence on the number of nucleons, is investigated. The results are compared with the deformed harmonic-oscillator model, discussed by Mottelson and Nilsson.

INTRODUCTION

HE existence of strongly deformed nuclei has long been established. The use of the spherical j-jcoupling single-particle representation, does not seem proper for these nuclei.2 When the nucleus retains its strong deformation not only for the ground state but for low excited states as well, one expects a singleparticle representation of deformed orbitals to be applicable. The single-particle Hamiltonian, is taken to be spheroidal, with each orbit fourfold degenerate populated by two protons and two neutrons with spins up and down. Nilsson³ chooses the deformed harmonic oscillator, as a Hamiltonian having these properties. This choice has the great advantage of being simple and easily diagonalizable. In fact, neglecting interaction between major shells, one has its eigenvalues and eigenfunctions as a function of the deformation, and the strength of the single-particle l^2 and $l \cdot s$ forces. The particular choice of these parameters, remains to be made for each individual problem. That is generally done by seeking those values for which the expectation value of the total Hamiltonian in the ground state is minimal.4

Since the exact solution of the nuclear many-body problem is impossible, the choice of a proper representation is not merely a matter of mathematical convenience. That is, the quality of the results of approximate calculations and methods, in various nuclear models, depends on the single-particle representation that is being used. This is especially true for models, which essentially assign general nuclear properties, to individual nucleons, e.g., the magnetic moment of oddeven nuclei. It is, therefore, of interest to investigate what representation one would get, assuming spheroidicity (but without restricting oneself to a deformed harmonic oscillator) and using a more general variational principle. The use of these variational methods introduces two main changes: The representation is dependent directly, in a self-consistent way, on the

single- and two-body parts of the total Hamiltonian; the mathematical procedure becomes more complicated, than in the straightforward Nilsson analysis. In this paper we shall deal only with the s-d shell. This shell has the advantage of having enough particles to make the problem nontrivial, yet not too many particles to make it too complicated. Moreover, the nuclei in the first half of the s-d shell display clearly rotational properties, closely related to the deformed shape of the nucleus.

THE VARIATIONAL METHOD

The actual physical Hamiltonian of the nuclear system, is assumed to have the standard second quantized form

$$H = \sum_{\alpha,\beta} \langle \alpha | K | \beta \rangle a_{\alpha}^{+} a_{\beta}$$

$$+ \frac{1}{4} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha \beta | V_{A} | \gamma \delta \rangle a_{\alpha}^{+} a_{\beta}^{+} a_{\delta} a_{\gamma}. \quad (1)$$

The single-body part, K, in the Hamiltonian is a sum of the harmonic-oscillator (h.o.) energy and l² and l·s forces,

$$K = E_{\text{h.o.}} + \alpha_{\mathbf{l} \cdot \mathbf{s}} \mathbf{l} \cdot \mathbf{s} + \alpha_{\mathbf{l}^2} \mathbf{l}^2. \tag{2}$$

The two-body interaction is taken, throughout this paper, to be the Rosenfeld mixture, 5 used by Elliott and Flowers⁶:

$$V = V_{0\overline{3}}(\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2)(0.3 + 0.7 \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2) [(e^{-r/a})/(r/a)] \quad (3)$$

and

$$\langle \alpha\beta | V_A | \gamma\delta \rangle = \langle \alpha\beta | V | \gamma\delta \rangle - \langle \alpha\beta | V | \delta\gamma \rangle$$
.

The sum over states in (1), is a priori restricted to the s-d major shell. Whatever extra shell effects there may be are either neglected, or assumed to be partially included in the single-body force. The harmonicoscillator energy, Eh.o., is therefore an additive constant, while V_0 , α_{l-s} and α_{l^2} are adjustable parameters.

The Hartree-Fock method consists of finding the single-particle determinantal trial wave function ϕ_0 ,

^{*} The research reported in this document has been sponsored *The research reported in this document has been sponsored in part by the Office of Scientific Research, OAR, through the European Office, Aerospace Research, U. S. Air Force.

1 A. Bohr, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 26, No. 14 (1952).

2 I. Unna, thesis, 1962 (unpublished).

3 S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 29, No. 16 (1955).

4 T. D. Newton, Can. J. Phys. 38, 700 (1960).

L. Rosenfeld, Nuclear Forces (North-Holland Publishing Company, Amsterdam, 1948), p. 233.
 J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) A229, 536 (1955).

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minimizing the expectation value $\langle \phi_0 | H | \phi_0 \rangle$,

$$\delta \langle \phi_0 | H | \phi_0 \rangle = 0$$
.

The self-consistent equivalent is that the occupied single-particle states $\{\lambda\}$, are eigenfunctions of the Hartree-Fock Hamiltonian, which, in turn, depends on the states $\{\lambda\}$ through

$$\langle \alpha | h | \beta \rangle = \langle \alpha | K | \beta \rangle + \sum_{\lambda=1}^{A} \langle \alpha \lambda | V_A | \beta \lambda \rangle.$$
 (4)

The general solution of the self-consistency problem is quite difficult. In the approach used here all the preliminary assumptions are incorporated beforehand into the mathematical procedure. Axial symmetry is introduced, by taking for the trial states, eigenfunctions of j_z . In the s-d shell each such state is a (normalized) linear combination of the form

$$|\lambda; k\rangle = \sum_{i} C_{\lambda k}^{i} |jk\rangle,$$
 (5)

where the sum goes over the $d^{5/2}$, $d^{3/2}$, and $s^{1/2}$ states. The coefficients $C_{\lambda k^j}$ are the parameters over which the variation will be performed. The fourfold degeneracy is built into the process by using a determinantal wave function, where, along with each single-particle k state, one includes also the states obtained from it by interchanging protons and neutrons, and by reflecting across the x-y body fixed reference plane. That is, a proton and a neutron are taken in the state (5) and in the state $|\lambda; -k\rangle$, where

$$|\lambda; -k\rangle = \sum_{j} (-1)^{j-k} C_{\lambda k}{}^{j} |j-k\rangle.$$
 (5a)

The fourfold degeneracy of h, therefore, comes as a result of taking the sum in Eq. (4) over configurations of 4n nucleons in the s-d shell. h is diagonal in m and in τ_z , but is not diagonal in j. We compute it in the $\langle jm|$ representation. Equation (4) becomes explicitly

 $\langle jm\tau_z|h|j'm\tau_z\rangle = \langle jm\tau_z|K|j'm\tau_z\rangle$

$$+\sum_{\lambda=1}^{A} \langle jm\tau_z; \lambda | V_A | j'm\tau_z; \lambda \rangle, \quad (6)$$

where the state λ is given by (5), and characterized by $\tau_{z\lambda}$. Since we have the matrix elements of the two-body interaction in the $\langle j_1 j_2 JT |$ representation, we transform (6), using coupling and decoupling relations, where $M=m+m_{\lambda}$ and $T_z=\tau_z+\tau_{z\lambda}$. We get

 $\langle jm | h | j'm \rangle = \langle jm | K | j'm \rangle$

$$+\sum_{\lambda=1}^{A}\sum_{j''j'''}A(|T_z|;m,jj'j''j''';m_{\lambda}) \times C_{\lambda m_{\lambda}}{}^{j''}C_{\lambda m_{\lambda}}{}^{j'''}, \quad (7)$$

where the coefficients $A(|T_z|; m; jj'j''j'''; m_{\lambda})$ are

given by

$$A(|T_{z}|; m; jj'j''j'''; m_{\lambda})$$

$$= \frac{1}{2} \sum_{J} \begin{bmatrix} j & j'' & J \\ m & m_{\lambda} & M \end{bmatrix} \begin{bmatrix} j' & j''' & J \\ m & m_{\lambda} & M \end{bmatrix}$$

$$\times \{\langle jj''JT = 1 | V_{A}| j'j'''JT = 1 \rangle$$

$$+ \langle jj''JT = |T_{z}| | V_{A}| j'j'''JT = |T_{z}| \rangle \}. \quad (8)$$

In the sum over occupied states, we perform separately the sum over each quartet of states with the same $|m_{\lambda}|$. Thus,

$$\langle jm | h | j'm \rangle = \langle jm | K | j'm \rangle + \sum_{|m_{\lambda}|} \sum_{j''j'''} B_{|m_{\lambda}|}(m, jj'j''j''') \times C_{|m_{\lambda}|}^{j''} C_{|m_{\lambda}|}^{j'''}, \quad (9)$$

where

$$B_{|m_{\lambda}|}(m; jj'j''j''') = \sum_{|m_{\lambda}| |T_{z}|} A(|T_{z}|; m, jj'j''j'''; m_{\lambda}). \quad (10)$$

The self-consistent condition implies that the states λ are eigenstates of h, that is, for each $|m_{\lambda}|$,

$$\sum_{j} C_{|m_{\lambda}|}{}^{j}h|j|m_{\lambda}|\rangle = E_{\lambda} \sum_{j} C_{|m_{\lambda}|}{}^{j}|j|m_{\lambda}|\rangle.$$
 (11)

The variational problem is solved, using an iterative method on Eqs. (9) and (11). An initial set of the parameters of the occupied orbits is chosen, $C_{\lfloor m \lambda \rfloor}{}^{j(0)}$. This choice automatically fulfills condition (5a). At each step, the next iterated set, $C_{\lfloor m \lambda \rfloor}{}^{j(n+1)}$, is obtained in the following way. The set $C_{\lfloor m \lambda \rfloor}{}^{j(n)}$ defines the single-body Hamiltonian $h^{(n+1)}$, through

$$\langle jm | h^{(n+1)} | j'm \rangle$$

$$= \langle jm | K | j'm \rangle + \sum_{|m_{\lambda}|} \sum_{j''j'''} B_{|m_{\lambda}|}(m,j,j'j''j''')$$

$$\times C_{|m_{\lambda}|} j'''^{(n)} C_{|m_{\lambda}|} j'''^{(n)} \qquad (9a)$$

which, when diagonalized, yields

$$\sum_{j} C_{|m_{\lambda}|}^{j(n+1)} h^{(n+1)} |j| m_{\lambda}| \rangle$$

$$= E_{\lambda}^{(n+1)} \sum_{j} C_{|m_{\lambda}|}^{j(n+1)} |j| m_{\lambda}| \rangle. \quad (11a)$$

The convergence of the method is, in general, a consequence of the properties of the $B_{|m\lambda|}$ coefficients, and quite independent of the parameters $C_{|m\lambda|}i^{(0)}$, initially chosen. However, as more and more orbits are being filled, the behavior of the energy surface $\langle \Phi_0 | H | \Phi_0 \rangle$, as a function of the $C_{|m\lambda|}i$ becomes more complicated. A detailed investigation of that expectation value, then reveals the exact nature of the point of equilibrium. As

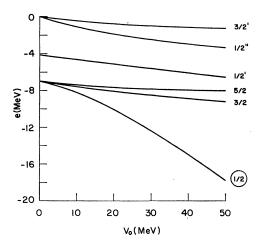


Fig. 1. Single-particle self-consistent energies, for Ne²⁰, as a function of the strength of the two-body interaction, V_0 . $e_{3/2} = 0$, $e_{1/2} = -4.2$ MeV, $e_{5/2} = -7.0$ MeV.

a result, we obtain the energies and eigenfunctions of nonoccupied single-particle levels as well.

The separation of the sum in Eq. (4) to different quartets of orbits, offers a great advantage. We can solve the self-consistent problem, with any particular set of coefficients $B_{|m_{\lambda}|}$, multiplied through by a constant θ_{λ} . As θ_{λ} goes from zero to unity, the change will mathematically reflect the transformation of the single-body Hamiltonian, as the $|m_{\lambda}|$ orbit is being gradually filled. Physically, this enables us to treat configurations not containing exactly 4n nucleons. It is true that this process involves an averaging effect over protons and neutrons. We should, therefore, only treat nuclei with equal numbers of protons and neutrons, or pairs of mirror nuclei simultaneously.

RESULTS

Table I' gives the eigenvalues and wave functions of the single-body Hamiltonians for different values of filling-numbers θ of the various orbits, for fixed V_0 , $\alpha_{1\text{-s}}$ and α_{1} . The left column gives the k of the states; the italicized number is the self-energy in MeV, followed by its eigenfunction, given by the coefficients $C_K{}^i$, starting with $C_K{}^{i\max}$.

EFFECT OF CHANGING Vo

The deformation of the nucleus is caused by the interaction between particles, which tend, for semi-filled shells, to prefer deformed over spherical orbitals. It is interesting to see how the single-particle spectra changes with the strength of the two-body interaction. That is shown in Fig. 1 for Ne²⁰ ($\theta_{1/2}=1$) and in Fig. 2 for Mg²⁴($\theta_{1/2}=\theta_{3/2}=1$). The resemblance to the Nilsson curve (which is a function of η) is striking especially for

Table I. Single-particle self-consistent Hamiltonians for $V_0 = 50$ MeV, $e_{3/2} = 0$, $e_{1/2} = -4.2$ MeV, $e_{5/2} = -5.0$ MeV. (The italicized numbers are the self energies in MeV.)^a

	$\theta_{1/2}=1$	$\theta_{1/2} = 1 \\ \theta_{3/2} = \frac{1}{2}$	$\theta_{1/2} = 1 \\ \theta_{3/2} = 1$	$\theta_{1/2} = 1 \theta_{3/2} = 1 \theta_{5/2} = \frac{1}{2}$	$\theta_{1/2} = 1 \\ \theta_{3/2} = 1 \\ \theta_{5/2} = 1$
$K=\frac{1}{2}$	-16.7977 0.7106 - 0.3911 0.5848	$\begin{array}{r} -17.9103 \\ 0.7043 \\ -0.3557 \\ 0.6143 \end{array}$	$\begin{array}{r} -19.0182 \\ 0.7118 \\ -0.3072 \\ 0.6316 \end{array}$	-19.2201 0.7644 - 0.3102 0.5652	-21.1816 -0.5025 0.2894 0.8147
$K = \frac{3}{2}$	- 7.2580 0.9925 - 0.1224	$\begin{array}{r} -10.0787 \\ 0.9772 \\ -0.2121 \end{array}$	-13.1306 0.9628 -0.2700	-14.0767 0.9787 -0.2051	-17.4118 0.6302 0.7764
$K = \frac{3}{2}$	- 5.7057 1.0000	- <i>6.7812</i> 1.0000	- 7.7585 1.0000	-10.8785 1.0000	-20.9543 1.0000
$K = \frac{1}{2}'$	- 6.2566 0.6835 0.1866 - 0.7057	- 8.5308 0.6915 0.5395 - 0.4803	-11.6878 0.6158 0.7054 -0.3508	$\begin{array}{r} -12.5096 \\ 0.5786 \\ 0.7167 \\ -0.3893 \end{array}$	- 8.8411 0.8517 0.3278 0.4087
$K = \frac{1}{2}$	7 - 3.1975 0.1668 0.9012 0.4000	- 5.0192 - 0.1606 0.7631 0.6260	- 5.9875 - 0.3379 0.6387 0.6913	- 7.7605 - 0.2842 0.6246 0.7274	- 4.7548 0.1488 - 0.8973 0.4112
$K = \frac{3}{2}'$	- 1.0034 0.1224 0.9925	$\begin{array}{r} -\ 2.3641 \\ 0.2121 \\ 0.9772 \end{array}$	- 3.5626 0.2700 0.9628	- 7.1271 0.2051 0.9787	- 8.9939 - 0.7764 0.6302

^a Around mass number 27, where the $d_{\delta/2}$ ^{5/2} level is being filled, there is an abrupt change from positive to negative deformation. This is in agreement both with other calculations and, most probably, with experimental data. (See Ref. 7.)

the second case. This resemblance also occurs when the corresponding wave functions are compared. The variation of $x(=C_{1/2}^{5/2})$ and $y(=C_{1/2}^{3/2})$ as a function of η , and as a function of V_0 , is illustrated in Fig. 3.

THE DEPENDENCE ON $\alpha_{l.s}$ AND α_{l^2}

The dependence of the single-particle Hamiltonian on the single-particle part K, is summarized in Tables II and III; where, for Ne²⁰ and Mg²⁴ respectively, the

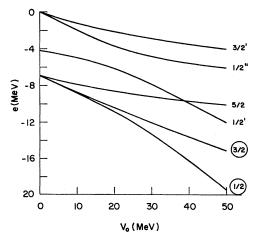


Fig. 2. Single-particle self-consistent energies, for Mg²⁴, as a function of the strength of the two-body interaction, V_0 . $e_{3/2}=0$, $e_{1/2}=-4.2$ MeV, $e_{5/2}=-7.0$ MeV.

⁷ H. E. Gove, Proceedings of the International Conference on Nuclear Structure, Kingston, edited by D. A. Bromley and E. W. Vogt (University of Toronto Press, Toronto, Canada 1960), p. 438.

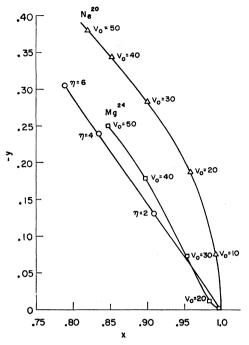


Fig. 3. The variation of the equilibrium point for Ne20 and M_8^{24} , as a function of V_0 , compared to the Nilsson model. $e_{3/2} = 0$, $e_{1/2} = -4.2$ MeV, $e_{5/2} = -7.0$ MeV.

 $d^{5/2}$ -state position is being changed relative to the $s^{1/2}$ and $d^{3/2}$ states.8

POLARIZATION EFFECTS

The single-particle Hamiltonian for a particular nucleus generates, as we have seen, not only the occupied, but the nonoccupied orbitals as well. For eveneven nuclei, with equal numbers of protons and neutrons, the determinantal stationary ground state is relatively stable. The single-particle self-consistent representation may then serve as a proper basis for a perturbation treatment of low-excited nuclear levels. In odd-even nuclei, an extra nucleon is added to the stable core treated before. The properties of the lowlying levels of such a nucleus would depend, to a great degree, on a set of intrinsic nuclear states, where, in each one, the odd nucleon occupies a different orbital.9 This is, in particular, true for varieties of the collective rotational model.¹⁰ The first attempt might be to use, for the odd nucleon, the nonoccupied orbitals obtained in the variational calculation for the even-even core. However, following the ideas of the present analysis, such a choice clearly neglects the two-body interactions of the nucleons in the core with the odd nucleon. Moreover, this effect depends quantitatively on which level the latter occupies. Each configuration of the odd nucleus,

¹⁰ K. H. Bhatt, Nucl. Phys. 39, 375 (1962).

Table II. Single-particle self-consistent Hamiltonians for Ne 20 ; $V_0 = 50$ MeV, $e_{3/2} = 0$, $e_{1/2} = -4.2$ MeV.

	$e_{5/2} = -5.5$	$e_{5/2} = -6.0$	$e_{5/2} = -6.5$	$e_{5/2} = -7.0$
$K = \frac{1}{2}$	-17.0157	-17.2291	<i> 17.4417</i>	- 17.6565
	0.7439	0.7724	0.7973	0.8193
	-0.3928	- 0.3911	-0.3868	-0.3805
	0.5406	0.5003	0.4633	0.4290
$K = \frac{3}{2}$	<i>- 7.7414</i>	- 8 <i>.2304</i>	<i>- 8.7252</i>	<i>- 9.2254</i>
	0.9940	0.9950	0.9961	0.9968
	-0.1097	-0.0985	-0.0886	-0.0800
$K = \frac{5}{2}$	— 6.2792	- <i>6.8571</i>	— 7.4364	— 8.0155
-	1.0000	1.0000	1.0000	1.0000
$K = \frac{1}{2}'$	-6.3477	- 6.4298	- 6.5035	- 6.5685
-	0.6480	0.6145	0.5825	0.5520
	0.2264	0.2616	0.2929	0.3211
	-0.7272	- 0.7443	- 0.7581	-0.7695
		-11-2-0	******	******
$K = \frac{1}{2}''$	- 3.2435	- 3.2934	- 3.3473	<i>- 3.4052</i>
	0.1633	0.1602	0.1575	0.1550
	0.8912	0.8823	0.8744	0.8672
	0.4230	0.4424	0.4590	0.4731
			3.1070	3.1701
$K = \frac{3}{2}'$	- 1.0753	- 1.1495	- 1.2236	-1.2968
4	0.1097	0.0985	0.0886	0.0800
	0.9940	0.9950	0.9961	0.9968
	0.5510	0.7700	0.2201	0,2200

is therefore treated separately, to form a stationary determinantal state. This is done with the help of the filling parameters θ . For mass number A=21 nuclei (Ne21 and Na21), the following configurations are

TABLE III. Single-particle self-consistent Hamiltonians for Mg^{24} ; $V_0 = 50$ MeV, $e_{3/2} = 0$, $e_{1/2} = -4.2$ MeV.

	$e_{5/2} = -5.5$	$e_{5/2} = -6.0$	$e_{5/2} = -6.5$	$e_{5/2} = -7.0$
$K = \frac{1}{2}$	-19.1640 0.7509 -0.2992 0.5887	-19.2952 0.7865 -0.2871 0.5467	$ \begin{array}{r} -19.4137 \\ 0.8188 \\ -0.2711 \\ 0.5060 \end{array} $	-19.5201 0.8483 -0.2514 0.4660
$K = \frac{3}{2}$	-13.6024 0.9662 -0.2578	-14.0864 0.9692 -0.2464	-14.5847 0.9718 -0.2358	$ \begin{array}{r} -15.0995 \\ 0.9741 \\ -0.2259 \end{array} $
$K = \frac{5}{2}$	- 8.3453 1.0000	- 8.9437 1.0000	- <i>9.5502</i> 1.0000	-10.1629 1.0000
$K = \frac{1}{2}'$	$\begin{array}{r} -11.8051 \\ 0.5822 \\ 0.7206 \\ -0.3765 \end{array}$	-11.9036 0.5461 0.7366 -0.3989	$\begin{array}{r} -11.9839 \\ 0.5077 \\ 0.7531 \\ -0.4184 \end{array}$	$\begin{array}{r} -12.0455 \\ 0.4670 \\ 0.7697 \\ -0.4352 \end{array}$
$K = \frac{1}{2}$ "	$\begin{array}{r} - \ 6.0321 \\ - \ 0.3115 \\ 0.6254 \\ 0.7154 \end{array}$	- 6.0799 - 0.2882 0.6123 0.7362	- 6.1328 - 0.2675 0.5995 0.7553	- 6.1918 - 0.2492 0.5868 0.7704
$K = \frac{3}{2}'$	- 3.6794 0.2578 0.9662	- 3.8041 0.2464 0.9692	- 3.9338 0.2358 0.9718	- 4.0667 0.2259 0.9741

a As the $s^{1/2}$ states goes below the $d^{5/2}$ states, the equilibrium point becomes more and more spherical. This change is very abrupt for Ne²⁰, and more gradual for Mg²⁴. This is shown in Fig. 4, where the expectation value of Q_0 (the intrinsic quadrupole moment) is plotted against $e(s^{1/2})$ for Ne²⁰ and Mg²⁴. The $d^{3/2}$ and $d^{5/2}$ levels are held fixed at 0 and -5.0 MeV, respectively. It should be noted that the experimental value of $\langle Q_0 \rangle$ contains a considerable contribution from the O¹⁶ core (see Ref. 8).

⁸ S. A. Moszkowski, Handbuch der Physik (Springer-Verlag,

Berlin, 1957), Vol. 39, p. 411.

9 A. Bohr and B. Mottelson, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. 27, No. 16 (1953).

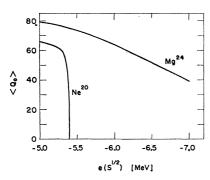


Fig. 4. The expectation value of Q_0 (in arbitrary units of 3.1114 mb) for Ne²⁰ and Mg²⁴, as a function of $e(s^{12})$ $V_0 = 50$ MeV, $e(d^{3/2}) = 0$, $e(d^{5/2}) = -5.0$ MeV.

treated:

$$\begin{array}{ll} \{\theta_{1/2} \! = \! 1 & \theta_{3/2} \! = \! \frac{1}{4} \} \; (K \! = \! \frac{3}{2} \; \text{intrinsic state}) \, , \\ \{\theta_{1/2} \! = \! 1 & \theta_{5/2} \! = \! \frac{1}{4} \} \; (K \! = \! \frac{5}{2} \; \text{intrinsic state}) \, , \\ \{\theta_{1/2} \! = \! 1 & \theta_{1/2}' \! = \! \frac{1}{4} \} \; (K \! = \! \frac{1}{2}' \; \text{intrinsic state}) \, . \end{array}$$

For mass number A = 25 (Mg²⁵ and Al²⁵):

$$\begin{array}{ll} \{\theta_{1/2} \! = \! 1 & \theta_{3/2} \! = \! 1 & \theta_{5/2} \! = \! \frac{1}{4} \} \ (k \! = \! \frac{5}{2} \ \text{intrinsic state}) \, , \\ \{\theta_{1/2} \! = \! 1 & \theta_{3/2} \! = \! 1 & \theta_{1/2} \! : \! = \! \frac{1}{4} \} \ (k \! = \! \frac{5}{2} \ \text{intrinsic state}) \, . \end{array}$$

Higher k states are well separated from these groups (see Figs. 1 and 2), and are insignificant in the treatment of low-lying levels. In the calculations of the $k=\frac{1}{2}$ ' states, an orthogonality condition between equal k states is incorporated into the iterative process.

The first result of these calculations is a change in the total energy of the even-even system. This change may be absorbed in the energies of the nonoccupied single-particle levels of the core, resulting in a renormalization of their values. The correction added is simply given by

$$\Delta \epsilon_{k} = \langle \Phi_{k}(2N+1) | H(2N+1) | \Phi_{k}(2N+1) \rangle - \langle \Phi_{0}(2N) | H(2N) | \Phi_{0}(2N) \rangle - \langle k | h | k \rangle, \quad (12)$$

where $\Phi_k(2N+1)$ and H(2N+1) refer to the odd-even system; $\Phi_0(2N)$, H(2N) and h, to the even-even system.

Figure 5 shows the renormalization effect on the physically important k levels. This effect, as is well

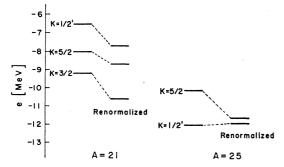
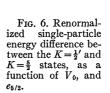
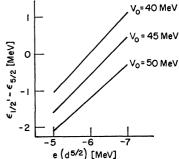


Fig. 5. Renormalization of single-particle excited energy levels, due to polarization, for A=21 and A=25. $V_0=50$ MeV, $e_{3/2}=0$, $e_{1/2}=-4.2$ MeV, $e_{5/2}=-7.0$ MeV.

seen, is most important for the difference of the $k=\frac{1}{2}'$ and $K=\frac{5}{2}$ states in A=25. In this case, the experimental situation is also very clear. It is interesting to see the dependence of the renormalized difference of energies $\epsilon_{1/2}'-\epsilon_{5/2}$, on the initial force parameters. This is illustrated in Fig. 6. One can see that the difference indeed becomes positive, for acceptable values of V_0 and $e(d^{5/2})$. The $e(s^{1/2})$ value is kept constant at -4.2 MeV.

The rearrangement of the intrinsic structure of the core, may be regarded as a polarization effect of the odd nucleon, and changes of collective properties might occur. For the $k=\frac{5}{2}$ configuration, the odd nucleon has to be in a pure $j=\frac{5}{2}$ state, namely $d_{5/2}^{5/2}$. Its interaction





energy with the core nucleons is given by

$$V_{d_{5/2}}^{5/2}, \text{ core} = \sum_{\lambda} \langle \lambda; d_{5/2}^{5/2} | V | \lambda; d_{5/2}^{5/2} \rangle$$

$$= \sum_{\lambda} \sum_{j,j'} \langle j m_{\lambda}; d_{5/2}^{5/2} | V | j' m_{\lambda}; d_{5/2}^{5/2} \rangle$$

$$\times C_{\lambda m_{\lambda}}^{j} C_{\lambda m_{\lambda}}^{j'}. \quad (13)$$

This is clearly equivalent to adding an extra singleparticle operator to the self-consistency problem of the bare core, the matrix elements of this operator being simply

$$\langle jm | 0_p | j'm \rangle = \langle jm; d_{5/2}^{5/2} | V | j'm; d_{5/2}^{5/2} \rangle.$$
 (14)

At this point, we can easily see the connection with the Nilsson representation, which is obtained by diagonalizing a one-body operator. In Nilsson terms, the polarization effect would mean the following: Two configurations of an odd number of nucleons, although differing in the occupied level of a single nucleon, are best treated as being generated by different values of the deformation η . If we regard the moment of inertia as macroscopically related to the deformation of the nucleus, that would explain the occurrence of different moments of inertia for different k bands.

ACKNOWLEDGMENT

The author wishes to thank Professor C. A. Levinson for constant help and encouragement in the course of this work.