

## Study of the Neutron-Proton Correlations in the Shell Model\*

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A shell-model treatment is given for the spectra of the nuclei where there are two protons and two neutrons outside a doubly closed shell. The only restriction is that like-nucleons are required to occupy the same angular momentum state. In addition to this general wave function, more restricted wave functions also are investigated, viz., the pairing wave function (as least one pair of like nucleons is coupled to zero angular momentum) which contain no  $n$ - $p$  correlations; the quartetting wave function (two unlike nucleons are first coupled to the maximum angular momentum, then the two pairs are coupled to  $I$ , the nuclear angular momentum) which does contain  $n$ - $p$  correlations; and a superposition of pairing and quartetting wave functions. Results for  $^{44}\text{Ti}$ ,  $^{64}\text{Zn}$ , and  $^{204}\text{Hg}$  are given. The ground states are reproduced quite well by the pairing wave function; it seems, however, to fail for the excited states. The overlap between the general and the quartetting wave function is quite large. Finally, results are also given for the pairing force, which has only a  $T=1$  component.

### I. INTRODUCTION

IT is well known that the low-lying states of the vibrational nuclei can be very well described by the pairing-force theory as long as only one shell is open. If both protons and neutrons are outside of closed shells then one must expect that the  $n$ - $p$  correlations should play as important a role as the correlations between the like nucleons. However, they are not taken into account by the usual pairing force theory.

Briefly, the difficulties encountered by BCS-like treatments are the following. As is well known, the BCS wave function does not have a definite particle number. It has, however, a good angular momentum. Thus, as long as in the considered region of the periodic table the nuclear properties change only slowly with atomic number, the computed characteristics can be expected to be of acceptable accuracy. Similarly, the BCS-like wave functions do not have good isospin when they include  $p$ - $n$  pairing. In contrast to the particle number, the isospin impurity is, however, quite important since the states with higher isospin lie at rather high energy, i.e., of the order of 10 MeV. In addition, the usual pairing Hamiltonian contains only  $T=1$  forces.

An attempt to generalize the BCS method so as to guarantee good isospin was made by Flowers and Vujcic.<sup>1</sup> Working in the LS coupling scheme they showed that this requires the abandonment of pairing in favor of quartetting, i.e., of four-particle correlations. Such a treatment is, however, quite complicated; this is exemplified by the circumstance that the required quasiparticle transformation is nonlinear, as had already been observed earlier by Bloch and Messiah.<sup>2</sup>

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<sup>1</sup> B. Flowers and M. Vujcic, Nucl. Phys. **49**, 586 (1963).

<sup>2</sup> C. Bloch and A. Messiah, Nucl. Phys. **39**, 95 (1962).

Alternatively, one can apply projection methods or variational constraints to BCS-type wave functions to obtain good, or at least improved, isospin, in analogy to the treatments concerning the particle number. Recent papers on this subject are, e.g., by Ginocchio and Weneser,<sup>3</sup> and by Goodwin, Struble, and Goswami<sup>4</sup>; they contain further references.

In this paper, we shall investigate the influence of  $n$ - $p$  correlations in the simplest possible model, viz., a nucleus which has two protons and two neutrons outside of a doubly closed shell. This is the simplest possible system in which both the correlations between like and between unlike nucleons are important. We shall consider the core to be inert, and we will allow the particles to populate all states of the open shell, i.e., we shall use the shell model with configuration interactions. Thus our Hamiltonian consists of an average potential which we take to be of a Woods-Saxon form, and an effective two-body potential. For the latter we take the force as given by Clark and Elliott.<sup>5</sup> It has a Gaussian radial dependence and central as well as tensor force amplitudes. Note that we do not employ the pairing Hamiltonian. In order to keep the problem to a manageable size, we restrict ourselves to the case where two like nucleons occupy the same angular momentum state.

We shall compare the spectra obtained by diagonalization of the Hamiltonian matrix for the following cases:

(I) The general scheme  $G$ : Here the like nucleons are coupled to all possible intermediate angular momenta. This is the most general wave function within our restriction.

(II) The pairing scheme  $P$ : Here at least one pair

<sup>3</sup> J. N. Ginocchio and S. Weneser, Phys. Rev. **170**, 859 (1968).

<sup>4</sup> A. L. Goodman, G. L. Struble, and A. Goswami, Phys. Letters **26B**, 260 (1968).

<sup>5</sup> J. Clark and J. Elliott, Phys. Letters **19**, 294 (1965).

TABLE I. Single-particle potentials for the nuclei considered.

Nucleus	$V_0$ (MeV)	$a$ (fm)	$R$ (fm)	$\alpha$ (MeV)
$^{44}\text{Ti}$	-50	0.65	4.38	20
$^{60}\text{Zn}$	-50	0.65	4.68	20
$^{204}\text{Hg}$	-41 protons -53 neutrons	0.70	7.25	25

of the like nucleons are coupled to zero intermediate angular momentum.

(III) The quartetting scheme  $Q$ : Here each proton-neutron pair is coupled to the maximum possible angular momentum. These two "stretched" pairs are then coupled to  $I$ , the nuclear angular momentum.

(IV) The  $P+R$  scheme: Here the pairing scheme is supplemented with the component of the quartetting scheme which is orthogonal to the pairing wave function.

(V) The primed pairing scheme  $P'$ : This is the pairing scheme computed with the analogue of a pairing Hamiltonian, i.e., the shell-model Hamiltonian is mutilated by putting all  $T=0$  two-body forces equal zero.

The rationale for this choice is the following. As is well known, the basic building block of the wave function of a vibrational nucleus is the pair, i.e., a state of two like nucleons coupled to zero angular momentum. In a similar way the basic building block of a rotational nucleus is the quartet.<sup>6</sup> Insofar as there seems to be competition in any nucleus between the spherical and the deformed shape, it can be expected that these two types of building blocks might compete, the pairing dominating in spherical nuclei and the quartetting dominating in deformed nuclei. Still, the principal admixture to the dominant coupling scheme could very well be the subjugated wave function, i.e., the quartetting scheme in spherical, and the pairing scheme in deformed nuclei.

The paper is organized as follows. The needed definitions and formulas are given in Sec. II. In Sec. III, we give the input parameters, present the level spectra obtained in the different schemes, and discuss the numerical aspects. We also give the wave function and their overlap with the general scheme. The most complete calculations were performed for  $^{44}\text{Ti}$ . Some calculations were also done for  $^{60}\text{Zn}$ ,  $^{64}\text{Zn}$ , and  $^{204}\text{Hg}$ . In Sec. IV, we summarize our study and draw conclusions regarding each scheme.

## II. FORMAL DEVELOPMENT

Consider an even-even nucleus with two protons and two neutrons, or, alternatively, two proton holes and two neutron holes, outside a doubly closed shell. The ground-state angular momentum for this nucleus is zero. The shell-model Hamiltonian for such a problem is

$$H = H_0 + V, \quad (1)$$

<sup>6</sup> M. Danos and V. Gillet, Phys. Rev. **161**, 1034 (1967).

where  $H_0$  is the sum of the single-particle operators,

$$H_0 = \sum_i h_i = \sum_i (T_i + V_i),$$

and  $V$  is the sum of the effective residual two-body potentials,

$$V = \sum_{i < j} V_{ij}.$$

We want the solution to the equation

$$H\Psi = E\Psi,$$

where  $\Psi$  is a four-body wave function

$$\Psi = \Psi(1, 2, 3, 4).$$

As mentioned in the Introduction, we consider the following approximations.

### A. General Scheme $G$

The most general four-body wave function is

$$|\Psi_{M.G.}\rangle = \sum |[(j_1 j_2)^{[J]}(k_1 k_2)^{[J']}]^{[I]}\rangle. \quad (2)$$

Throughout the paper we denote the proton and neutron angular momentum state by  $j$  and  $k$ , respectively; we use the convention of Fano and Racah<sup>7</sup> to indicate angular momentum coupling. In Eq. (2),  $j_1, j_2$  and  $k_1, k_2$  can independently take all values available in the major shell. However, as mentioned in the Introduction, we restrict ourselves to the case  $j_1 = j_2$  and  $k_1 = k_2$ . The configuration in which  $j_1 \neq j_2$  and  $k_1 \neq k_2$  would be less important because of the reduced overlap and, consequently, weaker binding. In any case, the problem would, in general, be unmanageable because of the exceedingly large number of possible configurations. Thus, we take as our most general scheme

$$|\Psi_G\rangle = \sum_{j,k;J \text{ even}} \gamma_{jkJ} |[(j^2)^{[J]}(k^2)^{[J']}]^{[0]}\rangle. \quad (3)$$

The coefficients  $\gamma_{jkJ}$  are obtained by diagonalizing the Hamiltonian. The excited states with spin differing from zero are given by the configurations of the type

$$|\Phi_G\rangle = |[(j^2)^{[J]}(k^2)^{[J']}]^{[I]}\rangle. \quad (4)$$

We shall restrict our attention to the states with even angular momentum  $I$ . We maintain the restriction of like nucleons occupying the same angular momentum state throughout the discussion. The details regarding the computation of the energy matrix are given in Appendix B.

Now we consider the other schemes which involve the superposition of a smaller number of configurations. We will compare them with the general scheme  $G$ .

### B. Pairing Scheme $P$

In the pairing scheme, the ground-state wave function is obtained by coupling each nucleon pair independently to zero angular momentum.

$$|\Psi_P\rangle = \sum \alpha_{jk} |[(j^2)^{[0]}(k^2)^{[0]}]^{[0]}\rangle. \quad (5)$$

<sup>7</sup> U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959).

TABLE II. Single-particle energies for the nuclei considered.

Nucleus	Type of nucleons	The open shell states (energies in MeV)						Ref.
		$2p_{1/2}$	$2p_{3/2}$	$1f_{5/2}$	$1f_{7/2}$			
$^{44}\text{Ti}$	neutrons	0.0	-3.0	-3.0	-7.0			10
	protons	0.0	-1.8	-1.3	-5.3			
$^{60}\text{Zn}$		$2p_{1/2}$	$2p_{3/2}$	$1f_{5/2}$	$1g_{9/2}$			10
	neutrons	-1.0	-4.0	-4.0	0.0			
	protons	-1.0	-2.8	-2.3	0.0			
	neutrons	$3p_{1/2}$	$3p_{3/2}$	$2f_{5/2}$	$2f_{7/2}$	$1h_{9/2}$	$1i_{13/2}$	
$^{204}\text{Hg}$		$3s_{1/2} \times$	$2d_{3/2}$	$2d_{5/2}$	$1g_{7/2}$	$1h_{11/2}$		11
	protons	8.03	8.38	9.70	11.43	9.37		

The excited states with  $I \neq 0$  are given by the superposition of the configurations of the type

$$|\Phi_P\rangle = |[(j^2)^{I1}(k^2)^{01}]^{I1}\rangle + |[(j^2)^{01}(k^2)^{I1}]^{I1}\rangle. \quad (6)$$

Obviously the  $P$  scheme is a subspace of the  $G$  space. Note that we use  $\Psi$  for the wave function and  $\Phi$  for the configuration; the former is a superposition of several  $\Phi$ 's.

### C. Quartetting Scheme $Q$

In order to study the neutron-proton correlations we introduce a scheme where the nucleons in each of the two neutron-proton pairs are coupled to the maximum possible angular momentum. In the ground state the two pairs are then coupled to zero angular momentum, in general to angular momentum  $I$ :

$$|\Psi_Q\rangle = \sum_{j,k;K=j+k} \alpha \beta_{jk} |[(jk)^{K1}(jk)^{K1}]^{I1}\rangle. \quad (7)$$

$\alpha$  is the antisymmetrization operator necessary to ensure the antisymmetry between two identical nucleons. In principle,  $K$  can take all values from  $|j-k|$  to  $|j+k|$ . However, a study of the two-body matrix

elements shows that the most important contribution should be expected to come from the configurations with  $K=j+k$ . In fact, the binding energy in this case is comparable to the binding energy of the state with  $K=0$  for the case where  $j=k$ . If  $j \neq k$ , the state with  $K=j+k$  has the largest binding energy. This is illustrated in Appendix A, where the two-body matrix elements are given for some  $j$  and  $k$ .

The quartetting scheme thus is the analog of the  $P$  scheme in the case of identical particles, where the configuration  $(j^2)^{01}$  has the largest binding compared with  $(j^2)^{J1}$ ,  $J \neq 0$ .

Now we shall expand Eq. (7) in terms of the set of states defined by the general scheme

$$|[(jk)^{K1}(jk)^{K1}]^{I1}\rangle = \frac{1}{\chi} \sum_{J \text{ even}} \begin{bmatrix} j & k & K \\ j & k & K \\ J & J' & I \end{bmatrix} |[(j^2)^{J1}(k^2)^{J'1}]^{I1}\rangle. \quad (8)$$

The summation in Eq. (8) is restricted to even  $J$  because of the antisymmetry between like nucleons. The recoupling coefficients are defined in terms of the

TABLE III. The two-body force parameters (in MeV).

Nucleus	Central				Tensor		Ref.
	$A^{13}$	$A^{31}$	$A^{11}$	$A^{33}$	$B^{13}$	$B^{33}$	
$^{44}\text{Ti}$	-41.5	-38.0	97.3	14.8	-95.1	12.1	5
$^{60}\text{Zn}$	-37.3	-41.3	100	15	0	0	5
$^{64}\text{Zn}$	-40	-20	-26	+6	0	0	11 (CAL)
$^{204}\text{Hg}$	-40	-24	-24	+25	0	0	11 (COP)

TABLE IV. Comparison with the results of Ref. 12 and the present results for the  $^{44}\text{Ti}$  ground state. Column a: results of Ref. 12 where only the  $f_{7/2}$  shell was considered. Columns b and c: our results where all the shells were considered using the force mixtures given by Refs. 5 and 11, respectively; however, only the numbers of the  $f_{7/2}$  shell are quoted.  $Q$  correlations are obtained by squaring the sum of the amplitudes of the primed columns, which are respectively 96, 61, and 82%.  $P$  correlations are obtained by squaring the  $J=0$  amplitude in the unprimed columns and are 58, 85, and 75%, respectively.

$J$	Amplitudes of the states			$Q$ correlation amplitudes		
	a	b	c	a'	b'	c'
0	0.7608	0.9243	0.866	0.5166	0.6327	0.5952
2	0.6090	0.1855	0.408	0.4355	0.1325	0.2923
4	0.2093	0.1144	0.145	0.0304	0.0166	0.0215
6	0.0812	0.1434	0.095	0.0004	0.0008	0.0005

9- $j$  coefficients<sup>8</sup> by

$$\begin{bmatrix} j_1 & k_1 & I_1 \\ j_2 & k_2 & I_2 \\ J_1 & J_2 & I \end{bmatrix} = \hat{I}_1 \hat{I}_2 \hat{J}_1 \hat{J}_2 \begin{bmatrix} j_1 & k_1 & I_1 \\ j_2 & k_2 & I_2 \\ J_1 & J_2 & I \end{bmatrix}, \quad (9)$$

where

$$\hat{I} = (2I+1)^{1/2}. \quad (10)$$

The normalization constant  $\chi$  is given by  $\langle \Phi_Q | \Phi_Q \rangle = 1$ , which leads to

$$\chi^2 = \sum_{J=0, \text{ even}}^{J_{\max}} \begin{bmatrix} j & k & K \\ j & k & K \\ J & J & I \end{bmatrix}^2. \quad (11)$$

#### D. $P+R$ Scheme

In order to investigate the competition between the pairing and the quartetting scheme, discussed in the Introduction, we consider a wave function which is a superposition of pure pairing and pure quartetting. However, the  $Q$  scheme is not orthogonal to the  $P$  scheme. Hence we employ the Schmidt orthogonalization procedure to obtain that part of  $Q$  which is orthogonal to  $P$ ,

$$|\Phi_R\rangle = \frac{|\Phi_Q\rangle - \langle \Phi_Q | \Phi_P \rangle |\Phi_P\rangle}{(1 - |\langle \Phi_P | \Phi_Q \rangle|^2)^{1/2}}. \quad (12)$$

Substituting  $|\Phi_Q\rangle$  as expressed in terms of the set defined in (3), we get

$$|\Phi_R\rangle = \frac{1}{N} \sum_{J', J=2}^{J_{\max}} \begin{bmatrix} j & k & K \\ j & k & K \\ J & J' & I \end{bmatrix} |[(j^2)^{[J]}(k^2)^{[J']}]^{[I]}\rangle, \quad (13)$$

where  $N$  is given by

$$N^2 = \sum_{J', J=2}^{J_{\max}} \begin{bmatrix} j & k & K \\ j & k & K \\ J & J' & I \end{bmatrix}^2. \quad (14)$$

<sup>8</sup> R. Caswell and L. Maximon, National Bureau of Standards Technical Note 409, 1966 (unpublished).

### III. NUMERICAL RESULTS

In this section, we shall discuss the results of the numerical calculations. The theory applies to two protons and two neutrons outside a doubly closed shell, or two proton holes and two neutron holes. Hence, we could consider  $^{20}\text{Ne}$ ,  $^{36}\text{Ar}$ ,  $^{44}\text{Ti}$ ,  $^{60}\text{Zn}$ ,  $^{204}\text{Hg}$ , and  $^{212}\text{Po}$ . However,  $^{36}\text{Ar}$  and  $^{20}\text{Ne}$  are  $2s-1d$  shell nuclei; and hence there are too few configurations available to make the problem interesting.  $^{212}\text{Po}$  has not been computed because the size of the matrix is too large. We also do some calculations for  $^{64}\text{Zn}$  in which the  $p_{3/2}$  neutron shell is filled. We discuss the energy spectra and the wave functions.

#### A. Input Numbers

There are essentially three types of input numbers: the diagonal energies, the parameters concerning the two-body matrix elements, and the parameters which determine the radial wave functions of the single-particle shell-model states.

##### 1. Parameters or Single-Particle States

To obtain the radial wave functions, one solves the Schrödinger equation with the potential<sup>9</sup>

$$V(r) = V_c(r) - \alpha(\hbar/2M_n c)^2 (\mathbf{1} \cdot \mathbf{s}) (1/r) (dV_c/dr), \quad (15)$$

where

$$V_c(r) = V_0 / \{1 + \exp[(r-R)/a]\}. \quad (16)$$

Thus, the necessary parameters are the well depth  $V_0$ , the diffuseness parameter  $a$ , the nuclear radius  $R$ , and the spin-orbit interaction parameter  $\alpha$ . For each nucleus they are chosen to reproduce roughly the single-particle energies. The values used are given in Table I.

##### 2. Single-Particle Energies $\epsilon_j^0$ and $\epsilon_k^0$

The single-particle energies are taken from the work of Kisslinger and Sorensen.<sup>10</sup> They are given in Table II for each nucleus.

<sup>9</sup> R. Caswell, National Bureau of Standards Technical Note 410, 1966 (unpublished).

<sup>10</sup> L. Kisslinger and R. Sorensen, Rev. Mod. Phys. **35**, 853 (1963).

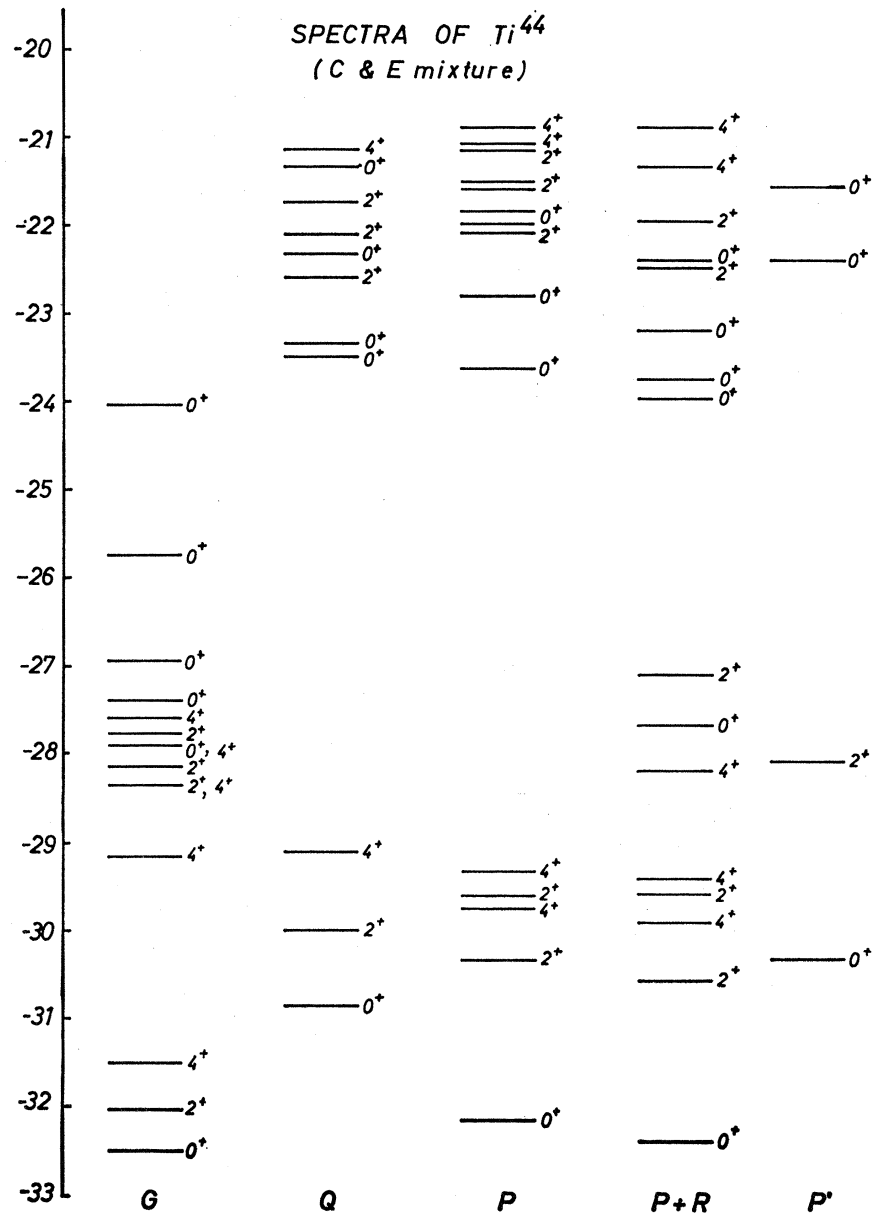


FIG. 1. Energy levels of  $^{44}Ti$  as computed by the different schemes discussed in Sec. II, using two-body force mixture given by Clark and Elliott (Ref. 5).

3. Parameters Concerning Two-Body Matrix Elements

In the case of  $^{44}Ti$  and  $^{60}Zn$  these parameters are taken from the analysis of Clark and Elliott<sup>5</sup> in which the authors deduce an effective potential from shell-model calculations. They computed 48 shell-model matrix elements with a two-body potential of the form

$$V_{ij} = \exp(-r^2/a^2) \times \left\{ \sum_{T,S} A^{TS} P^{TS} + \sum_T (B^{T3} P^{T3}) S_{ij} + \sum_T (C^{T3} P^{T3}) L \cdot S \right\}, \tag{17a}$$

where  $P^{2T+1} 2S+1$  are projection operators; the *A*'s, *B*'s,

and *C*'s are constants, and

$$a = 1.8 \text{ fm},$$

$$S_{ij} = 3r^{-2} (\delta_i \cdot r) (\delta_j \cdot r) - (\delta_i \cdot \delta_j),$$

$$S = \frac{1}{2} (\delta_i + \delta_j), \quad L = r \times p. \tag{17b}$$

Then they compared the matrix elements with those deduced from known experimental spectra. The mixture constants *A*, *B*, and *C* were determined by a least-squares fit. In the present work, we have slightly varied the values of these amplitudes—within the given error limits—so as to obtain roughly a vibrational level spacing for the lowest levels.

We also use the mixture as given in Ref. 11. There

<sup>11</sup> V. Gillet, A. Green, and E. Sanderson, Nucl. Phys. 88, 321 (1966).

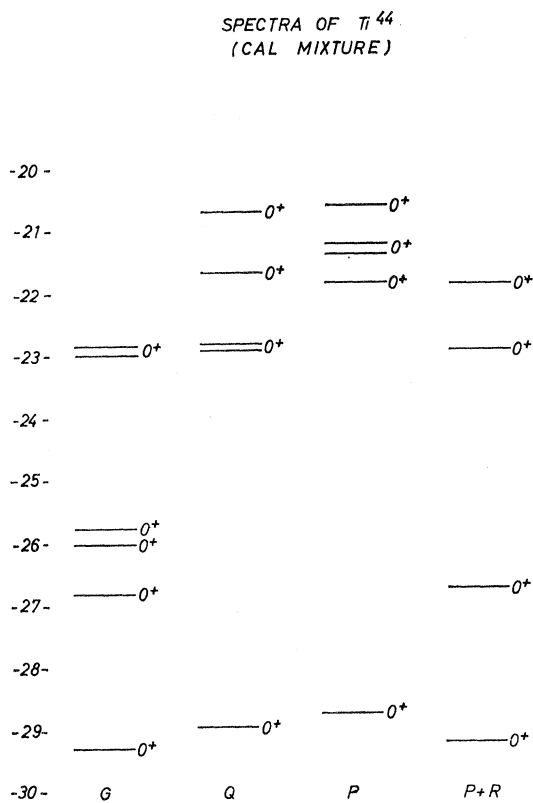


FIG. 2.  $0^+$  levels of  $^{44}Ti$  computed with the CAL mixture (Ref. 11).

the parameters were chosen to give good results for particle-hole calculations of  $^{12}C$ ,  $^{16}O$ , and  $^{208}Pb$ , referred to as COP mixture and of  $^{40}Ca$  which is referred to as CAL mixture. The former is used for  $^{204}Hg$  and the latter for  $^{64}Zn$ . The chosen parameters are given in Table III for each nucleus.

## B. Discussion of Results

### 1. Nucleus $^{44}Ti$

The Woods-Saxon potential parameters, the single-particle energies and the two-body force parameters are chosen as shown in the Tables I, II, and III, respectively. The justification for the parameters comes from the fact that the binding energy of  $^{44}Ti$  with respect to  $^{40}Ca$  is 32.5 MeV, the level spacing between the lowest  $0^+$  and  $2^+$  state is 0.5 MeV and the single-particle energy for the  $f_{7/2}$  shell is 8 MeV. These numbers agree well with the values inferred from the experimental spectra of the neighboring nuclei.

While adjusting the two-body parameters to obtain the level spacing of the lowest levels for the general case, we found that the inclusion of tensor forces reduces the level spacing, and the whole spectrum is shifted upwards by about 2 MeV. Increasing the  $T=0$  amplitudes also reduces the level spacing between

the  $0^+$  and  $2^+$  levels and lifts the spectrum. Thus, both the effects are repulsive in this case. However, the general features remain unchanged.

The obtained level scheme is shown in Fig. 1. Only the states with  $I=0, 2$ , and 4 were computed. Perhaps the most surprising feature of the  $G$  scheme is the quasirotational character of the spectrum. It has a large energy gap, viz., 3-4 MeV, and a 0-2-4 sequence. The level spacings are more those of a vibrational nucleus while the absence of a  $0^+$  and a  $2^+$  state around the energy of the  $4^+$  level, i.e., of the other members of the two-phonon excitation, is incompatible with a vibrational spectrum. On the other hand, a good rotator should also have a  $K=2$  band. There is no trace of it in the computed spectrum. For a definite interpretation, information on the static and transition  $E2$  moments would be required. Also, the  $6^+$  and  $8^+$  spectra would be useful. Anyway, this is not the central aim of the present paper.

Taking a look at the approximation schemes one sees first of all that the usual pairing Hamiltonian, i.e., the  $P'$  scheme, which has no  $T=0$  force, is in extremely poor agreement with the general scheme. The  $Q$  scheme describes the level spacing of the first three levels fairly well; however, the whole spectrum is shifted upwards by 2 MeV. Also, the gap is larger by about 2 MeV. The spectrum thus shows very strong "collective" features. If one considers the first three levels as an essential feature for the "collective" character, the  $Q$  scheme gives good results. The  $P$  scheme does well in keeping the ground state low enough but the "collective" features are poorly reproduced. The gap is as bad as that of the  $Q$  scheme.

Going to the  $P+R$  scheme does not improve the low-energy part of the spectrum very much. There evidently is still insufficient off-diagonal interaction between the two lowest  $2^+$  and the two lowest  $4^+$  states. Also, the higher part of the spectrum is still very badly reproduced.

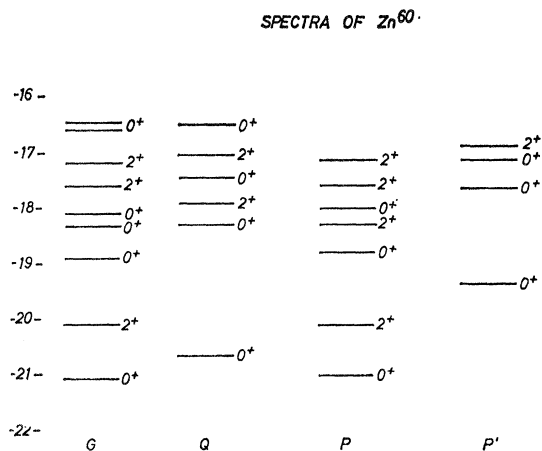


FIG. 3. Energy levels of  $^{60}Zn$ . Modified Clark and Elliott forces were employed.

We now go over to the discussion of the wave functions. In Table IV, we list the amplitudes of the dominant configuration, viz.,  $(f_{7/2})^4$ , as obtained in the  $G$  scheme, i.e., the coefficients  $\gamma_{7/2, 7/2, J}$  of Eq. (3). For purposes of comparison we also list the amplitudes of Ref. 12 in which only  $f_{7/2}$  orbitals were considered.

Now we ask how much quartetting and pairing correlations are present in the general wave function  $G$ . Referring to Eqs. (3), (5), and (8), we have

$$|\langle \psi_G | \psi_Q \rangle|^2 = \left| \frac{1}{\chi} \sum_{J \text{ even}} \begin{bmatrix} j & k & K \\ j & k & K \\ J & J & 0 \end{bmatrix} \gamma_{jkJ} \right|^2, \quad (18)$$

$$|\langle \psi_G | \psi_P \rangle|^2 = |\gamma_{j_0}|^2. \quad (19)$$

It turns out that both the overlaps are large and of comparable magnitude for this nucleus. The terms of the sum of the right-hand side of (18) are listed in the primed columns of Table IV.

In order to see whether a relatively more attractive  $T=0$  force favors the  $Q$  scheme, the calculations for the  $I=0$  spectrum were repeated with CAL mixture.<sup>11</sup> Figure 2 shows the results and the  $Q$  scheme gives indeed a better description of the ground state than the  $P$  scheme. However, again the gap is too large in both these schemes. The  $P+R$  scheme begins to fill in the gap, as it did with the CE mixture. With the CAL forces the  $Q$  correlations were found to be 82%, whereas the  $P$  correlations were 77%. Table IV shows the general wave function and the  $Q$  correlations (only the  $f_{7/2}$  shell is given) for this nucleus.

## 2. Nucleus $^{60}\text{Zn}$

Only the  $0^+$  and  $2^+$  spectra for this case have been computed. To obtain a level spacing of roughly 1 MeV, we had to discard the tensor force completely. Here an increment of the  $T=0$  amplitudes also reduces the level spacing. As seen from Table III, we have taken in

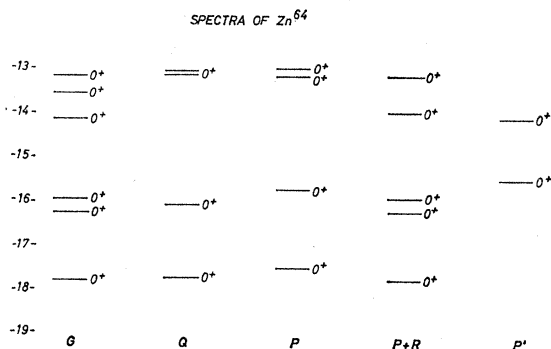


FIG. 4.  $0^+$  levels of  $^{64}\text{Zn}$  computed with the CAL mixture (Ref. 11).

<sup>12</sup> J. McCullen, B. Bayman, and L. Zamick, Phys. Rev. **134**, B15 (1964).

## SPECTRA OF $\text{Hg}^{204}$

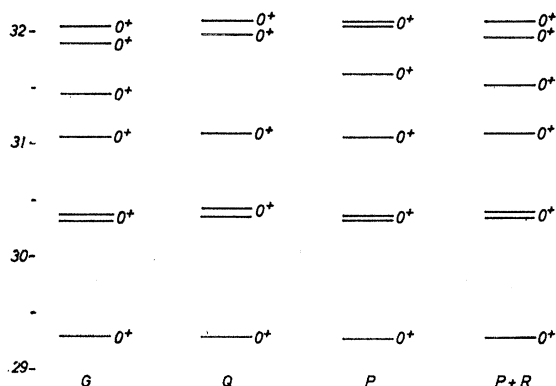


FIG. 5.  $0^+$  levels of  $^{204}\text{Hg}$  computed with the COP mixture (Ref. 11).

this case the  $T=0$  amplitudes to be smaller as compared with  $T=1$ . Naturally, this leads to a bad fit for the  $Q$  scheme since the success of the  $Q$  scheme depends on the large  $n-p$  matrix elements for the case  $j+k=K$  and decreasing the  $T=0$  amplitudes will favor the  $P$  scheme. From Fig. 3 one sees that the  $P$  scheme does very well compared to the  $G$  scheme. It is not even necessary to consider the  $P+R$  scheme. The  $P'$  scheme does poorly compared with the general scheme also in this case.

The important amplitudes in the  $G$  scheme are

$$[(p_{3/2}^2)^{[0]}(p_{1/2}^2)^{[0]}]^{[0]} = 0.36,$$

$$[(p_{3/2}^2)^{[0]}(p_{3/2}^2)^{[0]}] = 0.76.$$

Thus the  $p_{3/2}$  shell plays the major role here.

## 3. Nucleus $^{64}\text{Zn}$

Only the  $0^+$  spectrum was computed for this nucleus. The single-particle energies as well as the single-particle parameters are taken to be the same as given for  $^{60}\text{Zn}$ . However, the  $p_{3/2}$  neutron shell is now closed. The important amplitudes, therefore, are different and the configurations  $[(p_{3/2}^2)^{[J]}(f_{5/2}^2)^{[J]}]^{[0]}$ , where  $J=0$  and  $2$ , carry 93% of the total strength of the ground state.

The CAL mixture is used which has a relatively strong attractive even-triplet amplitude. The  $Q$  correlations in the ground state of the general wave function are 91%, and the  $P$  correlations are 77%. Figure 4 shows that the  $Q$  scheme gives somewhat better results than the  $P$  scheme. The  $P+R$  scheme does very well and the  $P'$  scheme gives only two levels within the chosen energy range.

## 4. Nucleus $^{204}\text{Hg}$

The general wave function for the lowest ground state shows that almost 97% of the strength is distributed amongst configurations involving the  $s_{1/2}$  pro-

TABLE V. The matrix elements  $\langle (f_{7/2}^2); JT | V | (f_{7/2}^2); JT \rangle$  for  $^{44}\text{Ti}$ .

$J$	Central		Tensor	
	$T=0$	$T=1$	$T=0$	$T=1$
0	0	-1.860	0	-0.620
1	1.834	0	-0.947	0
2	0	-0.506	0	+0.001
3	0.262	0	-1.001	0
4	0	-0.171	0	-0.001
5	-0.450	0	0.665	0
6	0	-0.036	0	-0.112
7	-2.3	0	-0.170	0

ton state or the  $p_{1/2}$  neutron state. This is associated with the fact that the hole energies for these two states are the lowest.

Now one sees from Eq. (8), where  $|\Psi_Q\rangle$  is expressed in terms of the complete set, i.e., the  $G$  scheme, that if one of the angular momenta is  $\frac{1}{2}$  then the summation over  $J$  is reduced to only one term, viz.,  $J=0$  and hence  $|\Psi_Q\rangle$  in this case equals  $|\Psi_p\rangle$ . This is the reason why the  $0^+$  spectra in Fig. 5 show similar behavior for all the cases we have considered. Therefore, further calculations involving  $I=2^+$  and  $4^+$  were not carried out.

#### IV. CONCLUSIONS

Perhaps the most paradoxical aspect of the obtained results is the high content of both the  $Q$  and  $P$  correlations in the  $G$  wave function, and the rather small improvement achieved in  $^{44}\text{Ti}$  when going from the  $P$  to the  $P+R$  scheme. The first aspect results simply from the nonorthogonality of the  $P$  and  $Q$  wave functions. The second aspect is associated with the fact that basically  $P$  and  $Q$  are quite different coupling schemes: that part of, say,  $Q$ , which is orthogonal to  $P$ , i.e., an  $R$  state, requires more than a two-body recoupling to interact with a  $P$  state. The  $G$  states supply an assortment of states which can serve as inter-

TABLE VI.  $\langle g_{7/2}^2 i_{13/2}; JT | V | g_{7/2}^2 i_{13/2}; JT \rangle$  as a function of  $J$  for  $^{204}\text{Hg}$ .

$J$	$T=0$	$T=1$
3	-1.397	0.712
4	-0.390	0.336
5	-0.525	0.233
6	-0.406	0.115
7	-0.349	0.159
8	-0.433	-0.039
9	-0.266	0.122
10	-0.913	-0.404

mediates between the  $P$  and the  $R$  states thus greatly enhancing the coupling between these two major components. This effect has been observed by Raynal and Gillet<sup>13</sup> who investigated the mixing of pairing and stretch wave functions. As the number of valence nucleons increases, more and more particles must be recoupled and the off-diagonal matrix elements very soon become negligibly small. Consequently, the states there degenerate into either a pure stretch or a pure pairing configuration. The admixture of more general states thus becomes even more important as the number of valence nucleons increases.

Returning now to the present calculation we see that clearly a Hamiltonian which does not consider the  $T=0$  forces is quite inadequate. However, the pairing scheme does very well when employing a force with a  $T=0$  admixture. The importance of the quartetting scheme

TABLE VII.  $\langle i_{13/2}^2; J1 | V | i_{13/2}^2; J1 \rangle$  as a function of  $J$  for  $^{204}\text{Hg}$ .

$J$	$T=1$
0	-0.299
2	+0.026
4	+0.040
6	+0.046
8	+0.061
10	+0.078
12	+0.089

depends upon the following two factors: (1) The shells that play the major role in the nucleus have high angular momentum. (2) The attraction of the  $T=0$  amplitudes is much stronger than that of the  $T=1$  amplitudes.

It is interesting to note that the fact that the two-body matrix elements show the maximum binding for the maximum angular momentum has a purely geometric origin, but whether the  $Q$  scheme is important or not, depends partly on the chosen force parameters.

In  $^{44}\text{Ti}$ , the important shell is  $f_{7/2}$  and hence the first criterion is satisfied but not the second. To verify our observation the calculations were repeated with the CAL mixture which satisfies the second criterion. Then the  $Q$  correlations in the general wave function were 82%, and the  $P$  correlations 75%.

In  $^{60}\text{Zn}$ , the important shell is  $p_{3/2}$  and hence neither of the criteria is satisfied; the results, therefore, show that the  $Q$  scheme is not satisfactory. In  $^{64}\text{Zn}$ , the  $f_{5/2}$  neutron state becomes important since the  $p_{3/2}$  neutron state is closed. Hence, both criteria are satisfied and the  $Q$  scheme reproduces the first four levels very well.

In  $^{204}\text{Hg}$ , the important shells are  $s_{1/2}$  and  $p_{1/2}$  and

<sup>13</sup> V. Gillet and J. Raynal, Nucl. Phys. **A122**, 193 (1968).



hence the pairing scheme does very well.

Going to the  $P+R$  scheme, we usually get a better agreement for one or two higher levels; it does especially well in  $^{64}\text{Zn}$ .

In conclusion, it seems that the  $Q$  configurations play quite an important role and that it is essential to consider the proton-neutron correlation also in spherical nuclei.

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#### APPENDIX A

The matrix elements of  $^{44}\text{Ti}$  for the configuration  $[f_{7/2}^2]^{[J]}$  vary with  $J$  as shown in Table V. The two-body force parameters are discussed in Sec. III. Thus

we see that the only two important matrix elements are the ones with  $J=0$  and  $J=J_{\text{max}}=7$  which supports the assumption  $j+k=K$ ; also, the  $[f_{7/2}^2]^{[7]}$   $T=0$  matrix element is the largest.

In order to show that the overlap is not small even in the case when neutron and proton orbitals are different, the matrix elements for  $^{204}\text{Hg}$  are given in Tables VI and VII.  $g_{7/2}$  is a proton state and  $i_{13/2}$  is a neutron state for this nucleus.

Thus Tables VI and VII show the following features noted in Secs. I and II:

(1) Neutron-proton matrix elements—when they occupy different orbitals—are not any smaller than the similar matrix elements of like nucleons (Tables VI and VII).

(2) The state with  $J=j+k$  has the largest binding energy.

(3) In most cases the  $T=0$  matrix elements are larger than the  $T=1$  matrix elements.

#### APPENDIX B

The  $0^+$  energy matrix in the general case was computed as follows:

$$\begin{aligned} \langle \Phi_G | H | \Phi_G \rangle &= \sum_{J, J'} \langle [ (j^2)^{[J]} (k^2)^{[J']} ]^{[0]} | H | [ (j'^2)^{[J']} (k'^2)^{[J']} ]^{[0]} \rangle \\ &= (2\epsilon_j^0 + 2\epsilon_k^0) \delta_{jj'} \delta_{kk'} + \sum_{J, J'} \langle [ (j^2)^{[J]} (k^2)^{[J']} ]^{[0]} | V | [ (j'^2)^{[J']} (k'^2)^{[J']} ]^{[0]} \rangle. \end{aligned}$$

Now,  $V = V_{nn} + V_{pp} + 4V_{np}$ . For example, the second term will be

$$\begin{aligned} \langle (j^2)^{[J]} | V_{pp} | (j'^2)^{[J']} \rangle \delta_{kk'} \delta_{JJ'} + \langle (k^2)^{[J]} | V_{nn} | (k'^2)^{[J']} \rangle \delta_{jj'} \delta_{JJ'} \\ + 4 \sum \begin{bmatrix} j & j & J \\ k & k & J \\ L & L & 0 \end{bmatrix} \begin{bmatrix} j' & j' & J' \\ k' & k' & J' \\ L' & L' & 0 \end{bmatrix} \langle [ (jk)^{[L]} (j'k)^{[L']} ]^{[0]} | V_{np} | [ (j'k')^{[L']} (jk)^{[L]} ]^{[0]} \rangle, \end{aligned}$$

where the third term has a recoupled form of the original and reduces to

$$4 \sum \begin{bmatrix} j & j & J \\ k & k & J \\ L & L & 0 \end{bmatrix} \begin{bmatrix} j' & j' & J' \\ k' & k' & J' \\ L' & L' & 0 \end{bmatrix} \langle (jk)^{[L]} | V | (j'k')^{[L']} \rangle \delta_{LL'} \delta_{jj'} \delta_{kk'}.$$

Thus, in this case the neutron-proton pair is coupled to all possible intermediate angular momenta. The generalization of this to the case of the pairing and the quartetting scheme is trivial. Note that by similarity the latter also has all possible intermediate angular momenta in the  $V_{np}$  matrix elements. These formulas can be easily extended to the cases of  $I=2^+$  and  $4^+$ . The details are given in Ref. 14. The two-body matrix elements were computed with the method described in Ref. 15.

<sup>14</sup> J. Shah, thesis, University of Maryland, 1967 (unpublished).

<sup>15</sup> J. Shah, University of Maryland Technical Report No. 658, 1967 (unpublished).