

Thus, Eq. (A5) is reduced to

$$(V - V_0) \int_0^\infty f(r) u_0^2 dr = B/\alpha = \left(\frac{\hbar^2}{2m}\right)^{1/2} B^{1/2}, \quad (\text{A10})$$

which has the form of Eq. (A1).

For the  $s$ -shell hypernuclei, the use of Eq. (12) as an interpolation formula is based on the following observations: (1) the  $\Lambda$  particle can be approximately regarded as moving in a potential well created by its interaction with the individual nucleons, with the depth of the well determined by the strength of the  $\Lambda$ -nucleon interaction, and (2) the condition expressed by Eq. (A9) is fairly well satisfied. There is a slight complication arising from the fact that the shape of the well depends somewhat on the

depth of the  $\Lambda$ -nucleon potential, but we do not think that this can seriously affect the results obtained by using Eq. (12). In any case, we have taken the extra precaution of always choosing one value of  $U_{0A}$  which yields a value for  $B_\Lambda$  close to that determined experimentally.

There is also another piece of evidence which shows that a two-parameter interpolation formula is quite sufficient for the  $s$ -shell hypernuclei. In Ref. 11, we have used a more careful procedure involving three values of  $U_{0A}$  and a three-parameter interpolation formula. But, this was later found to be unnecessary, since a two-parameter formula would have yielded very nearly the same results as that from a three-parameter formula, if the values of  $U_{0A}$  are chosen properly.

## Nature of Hartree-Fock Calculations in Light Nuclei\*

J. BAR-TOUV

*Department of Nuclear Physics, The Weizmann Institute of Science, Rehovoth, Israel*

AND

C. A. LEVINSON†

*Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania*

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The role of the two-body force, its exchange mixture, and the spin-orbit force in their effect on the Hartree-Fock wavefunctions and spectra is investigated. It is shown that the main features of the Hartree-Fock single-particle field are determined almost completely by the long-range part of the two-body force. The solutions for a long-range model are derived for various systems of different neutron excesses, and the exchange dependence of the energy "gap" between occupied and unoccupied levels is particularly considered. The main effect of the spin-orbit force and the finite range of the two-body force is to mix the orbitals. In the cases where the energy "gap" is large, the mixing is only of the occupied orbitals among themselves. Out of this study it emerges that the most natural representation for the Hartree-Fock single-particle orbitals is that associated with the axially symmetric deformed harmonic oscillator where one takes linear combinations of degenerate orbitals which are time-reversal eigenstates. This prescription results often in nonaxially-symmetric nuclei and is consistent with the results found in exact calculations with realistic forces.

### I. INTRODUCTION

IN recent years the method of self-consistent deformed orbitals has been successfully applied to various nuclear structure problems. In particular, there now exists a number of papers<sup>1-5</sup> dealing with the rotational and vibrational aspects of the low-lying spectra of nuclei in the  $1p$  and  $2s, 1d$  shells. Intershell prob-

lems<sup>6-9</sup> such as the  $O^{16}$  spectrum involving  $1p$  holes and  $2s, 1d$  particles as well as the dipole giant resonances involving the  $1p, 2s, 1d$ , and  $2p, 1f$  shells have also been treated by the method of deformed orbitals.

The success of the above calculations certainly indicate that the underlying Hartree-Fock (HF) approximation has considerable validity in light nuclei. It is the purpose of this paper to discuss the main physical features of these calculations and to investigate the role of the two-body force and its exchange mixture and the spin-orbit force in their effect on the Hartree-Fock wave functions and spectra. Usually these points are obscured

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† On leave from the Weizmann Institute of Science, Rehovoth, Israel.

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since the results are simply presented as the end point of a series of computer calculations. In particular, the appearance of an energy gap in the calculations has been of critical importance in fitting the experimental data and should be understood in its relation to the original two-body Hamiltonian. In light nuclei around  $\text{Ne}^{20}$ , this gap is of the order of 7 MeV as measured by the energy separation of ground and first excited even-parity band heads in  $\text{Ne}^{20}$ . This gap in the Hartree-Fock single-particle spectrum probably persists to some extent in the heavy nuclei and may have quite important consequences there which have not yet been studied. The standard single-particle spectrum as given by the Nilsson model does not include this effect.

It has been found that certain nuclei are axially symmetric and others are not. The symmetry properties of the wave functions will be discussed and will be shown to depend on the exchange mixture of the force and on the constraint of time-reversal invariance.

A key observation of the Copenhagen school is that the Hartree-Fock field is mainly determined by the long-range part of the two-body nuclear force. Following this idea, it is natural to consider an expansion of the two-body force in inverse powers of the range and to study the leading terms separately since they should give the dominant effects in a Hartree-Fock calculation. When this is done, it is easily seen how the energy gap arises as a consequence of the exchange mixture and what is the nature of the Hartree-Fock orbitals. This long-range calculation almost exactly reproduces the results of realistic-range Hartree-Fock calculations done on digital computers. The spin-orbit force is seen to play a small role when the energy gap in the Hartree-Fock spectrum is large and one can understand, in this way, the success of the supermultiplet model in certain cases. A most important parameter governing the structure of the nuclear wave functions is the ratio of the spin-orbit force strength to the magnitude of the energy gap.

The energy gap discussed here arises solely from the long-range part of the force and the particular exchange mixture. This "long-range energy gap" can be approximately predicted for heavy nuclei based on its known value for light nuclei. It appears that this gap is of importance in the structure of heavy nuclei where to a certain extent it opposes the effects of the short-range part of the force and the well-known gap arising therefrom.

## II. THE HARTREE-FOCK APPROXIMATION

There are two applications of Hartree-Fock theory under current investigation. One approach is typified by the work of Kerman and collaborators<sup>10</sup> and Baranger and collaborators.<sup>11</sup> This approach concentrates mainly

on spherical nuclei where the spin and angular part of the orbitals is fixed *a priori* and only the radial dependences are varied to minimize the total energy. The other type of approach with which we are concerned here fixes the radial dependences *a priori* and varies the spin and orbital parts of the wave functions. This method does not address itself to the problems of nuclear matter, but rather is more concerned with questions of nuclear spectra, positions of band heads, moments of inertia, and coupling schemes.

The most general Hartree-Fock calculations of the latter kind in the *sd* shell reported to date are those of Bar-Touv and Kelson.<sup>4</sup> In this paper, the intrinsic self-consistent structure of the nucleus is derived from the many-body Hamiltonian by solving the self-consistent Hartree-Fock equation:

$$\langle \alpha | h | \beta \rangle = \langle \alpha | K | \beta \rangle + \sum_{\lambda} [\langle \alpha \lambda | V | \beta \lambda \rangle - \langle \alpha \lambda | V | \lambda \beta \rangle], \quad (1)$$

$$h | \lambda \rangle = \epsilon_{\lambda} | \lambda \rangle, \quad (2)$$

where  $|\alpha\rangle$  is a one-particle state, the states  $|\lambda\rangle$  are occupied, and  $h$  is the one-body Hartree-Fock Hamiltonian.  $K$  is the single-body and  $V$  the two-body parts of the Hamiltonian. The most general one-body wave function is made up of orbitals in the *sd* shell and is of the form

$$|\lambda\rangle = \sum_{j,m} a_{j,m}^{\lambda} | j, m \rangle, \quad (3)$$

where the states  $jm$  are the *jj*-coupled single-particle states in the *sd* shell in a fixed harmonic-oscillator potential and only the parameters  $a_{j,m}^{\lambda}$  are varied in the calculation. The Hartree-Fock wave function is simply the determinant of the occupied orbitals:

$$\Psi = \text{Det}(\lambda_1, \lambda_2, \dots, \lambda_A). \quad (4)$$

Clearly the wave function remains invariant if one introduces new orbitals which are linear combinations of the old occupied orbitals. It is sometimes convenient to do this in order to gain insight into the structure of the wave function.

The two-body interaction is of the general form

$$V_{ij} = V_c(r_{ij}) \{ W + MP_{ij}^x + BP_{ij}^{\sigma} - HP_{ij}^{\tau} \}, \quad (5)$$

where  $P^x$ ,  $P^{\sigma}$ ,  $P^{\tau}$  are the space, spin, and isospin exchange operators and  $V_c(r_{ij})$  is a Yukawa or Gaussian potential of definite range and strength.

The one-body interaction is taken to be a standard shell-model type where

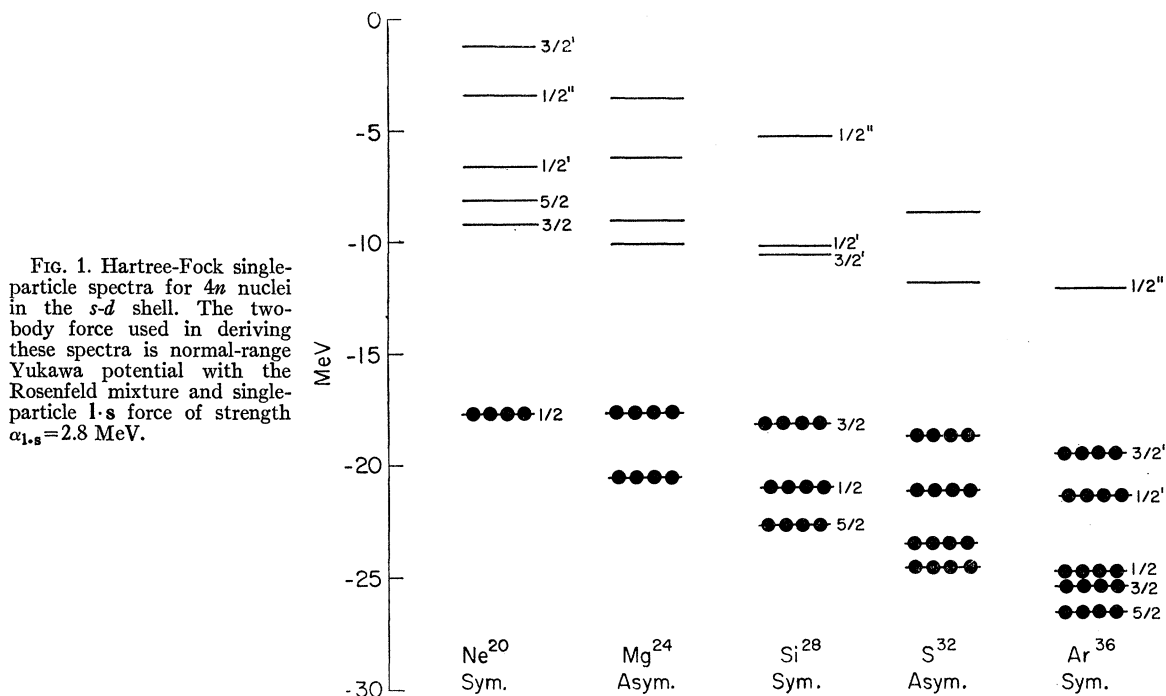
$$K = H_0 + \alpha_{ls} \mathbf{l} \cdot \mathbf{s} + \alpha_l l^2, \quad (6)$$

where  $H_0$  is a harmonic-oscillator Hamiltonian and  $\alpha_{ls}$ ,  $\alpha_l$  are the strength of the spin-orbit and  $l^2$  force.

Further details of the calculation can be found in Ref. (4). In Fig. 1 is shown the single-particle Hartree-Fock spectrum for the  $4n$  nuclei. The parameters  $a_{j,m}^{\lambda}$  are given in Ref. (4).

<sup>10</sup> A. K. Kerman, J. P. Svenne, and F. M. H. Villars, Phys. Rev. 147, 710 (1966).

<sup>11</sup> K. T. R. Davies, S. J. Krieger, and M. Baranger (to be published).



First let us examine the spectra. The dominant qualitative features are:

- (1) There is a constant energy gap of about 8 MeV between the topmost occupied level and the bottommost unoccupied level.
- (2) Qualitatively, the occupied levels are close together and remain at the same energy while the unoccupied levels cluster about a higher energy.

As has been emphasized before, the energy gap manifests itself in the nuclear-energy-level spectra and in the computed moments of inertia through the cranking formula. The Hartree-Fock wave functions are rigorously stable against single-particle excitations and corrections to the approximation can only occur through two-particle excitations. However, with an energy difference of about 16 MeV for two-particle excitations, one sees that the Hartree-Fock wave functions for  $4n$ -type nuclei should be quite stable. (Typical off-diagonal matrix elements being of the order of an MeV or so.) Let us now consider the case where there is no spin-orbit force present. In Fig. 2 is shown the Hartree-Fock spectrum for  $Mg^{24}$ . We see that the occupied levels are essentially degenerate and the unoccupied levels are also approximately degenerate and lie at a considerably higher energy. This phenomenon is quite independent of the exchange mixture. In the limit of infinite-range forces, the degeneracies become exact. So we see already that Hartree-Fock calculations with realistic-range forces give essentially the type of spectrum found in the infinite-range limit. The spin-orbit force does split

these degeneracies further as one can see by comparing Figs. (1) and (2).

We next compare the wave functions for calculations with and without the spin-orbit force. It will be most convenient to display the wave function in a basis where the space part of the orbital is either even or odd under time reversal. In the  $sd$  shell, the wave functions of the orbitals can be taken with real  $a_{jm}^\lambda$ , and the time reversal operation is equivalent to a rotation of  $180^\circ$  about the  $x$  axis or a reflection through a plane perpendicular to the  $x$  axis. In these three cases,  $\Psi_m^j$  simply goes into  $(-1)^{j-m}\Psi_{-m}^j$ . We choose as a representation the six states listed in Table I and their time reversals which correspond here only to a spin flip, and a possible phase change. The notation is such that  $d_2$  means a  $d$  orbital with  $m_L=2$ . The symbol  $\uparrow$  stands for a spin-up Pauli spinor.  $\alpha$  and  $\beta$  are amplitudes for the  $s_0$  and  $d_0$  components in  $\Psi_1$ .

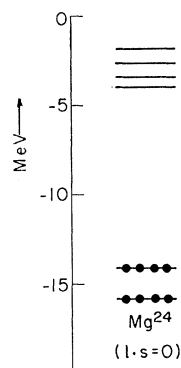


TABLE I. Definitions of the representation used in the present article.

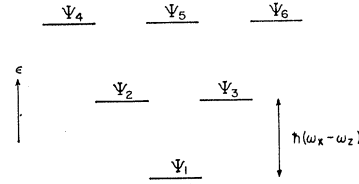
(1)	$(\alpha s_0 + \beta d_0) \uparrow$
(2)	$\left(\frac{d_1 + d_{-1}}{\sqrt{2}}\right) \downarrow$
(3)	$\left(\frac{d_1 - d_{-1}}{\sqrt{2}}\right) \downarrow$
(4)	$\left(\frac{d_2 + d_{-2}}{\sqrt{2}}\right) \uparrow$
(5)	$\left(\frac{d_2 - d_{-2}}{\sqrt{2}}\right) \uparrow$
(6)	$(-\beta s_0 + \alpha d_0) \uparrow$

The wave functions of Ref. 4 corresponding to normal potential range and spin-orbit force are expandable in terms of  $\Psi_1, \dots, \Psi_6$  with  $\alpha=0.44$  and  $\beta=0.90$  and the wave functions of the occupied levels are shown in Table II except for  $\text{Ar}^{36}$  where the wave function of the single unoccupied level is given.

The representation we have chosen is that which gives a solution in the case of a long-range force with no spin-orbit splitting. In the case of a very-long-range force, the  $SU(3)$  representation suggested by Elliot holds. (See the discussion of this point by Flamm *et al.*<sup>12</sup> and the following article by Kugler.<sup>13</sup>) In this case, the orbitals  $\Psi_1 \dots \Psi_6$  are the correct ones with  $\beta=0.82$  and  $\alpha=0.57$ . These are simply the orbitals which occur in the solution of a deformed axially symmetric harmonic oscillator. We note that the values of  $\alpha$  and  $\beta$  in the Bar-Touv-Kelson calculation are not far from this value. For the harmonic oscillator with  $\hbar\omega_z < \hbar\omega_x$  and

TABLE II. Single-particle wave functions of Ref. 4 corresponding to normal potential range and spin-orbit force in the representation defined in Table I.

		$\Psi_1$	$\Psi_2$	$\Psi_3$	$\Psi_4$	$\Psi_5$	$\Psi_6$
$\text{Ne}^{20}$	I	0.97	0.16	0.16	0	0	0
	II	0.45	-0.81	0.24	-0.22	0.08	-0.16
$\text{Mg}^{24}$	I	0.83	0.53	0.08	0.10	0.07	-0.10
	II	0.45	-0.81	0.24	-0.22	0.08	-0.16
	III	0	0	0	0.71	0.71	0
$\text{Si}^{28}$	I	0	0	0	0.71	0.71	0
	II	0.28	-0.12	-0.12	0	0	0.94
	III	0	0.23	-0.23	0.67	-0.67	0
$\text{S}^{32}$	I	-0.07	0.05	0	0.68	0.66	0.31
	II	-0.16	-0.63	0.04	-0.09	0.41	-0.63
	III	-0.16	0.50	-0.25	0.43	-0.19	-0.66
	IV	0.29	0.55	0.13	-0.48	0.57	-0.19
$\text{Ar}^{36}$	I <sup>a</sup>	0.95	-0.2	-0.2	0	0	0.04

<sup>a</sup> I  $\rightarrow$  unoccupied level in  $\text{Ar}^{36}$ .<sup>12</sup> E. Flamm, C. A. Levinson, and S. Meshkov, Phys. Rev. **129**, 297 (1963).<sup>13</sup> M. Kugler, Phys. Rev. **129**, 317 (1963).FIG. 3. Schematic diagram for the single-particle spectrum of an axially symmetric deformed harmonic oscillator in the absence of  $\mathbf{l} \cdot \mathbf{s}$  force.

$\hbar\omega_x = \hbar\omega_y$ , we have the spectrum shown in Fig. 3. If  $\hbar\omega_z < \hbar\omega_x$ , the figure is simply inverted. Bearing this in mind and remembering that the spectrum of an infinite-range force is such that there is a considerable gap between occupied and unoccupied states, we would expect that the effect of the finite range and the spin-orbit force would be simply to mix the occupied levels but not admix much of the unoccupied levels since they are 8 MeV or so away. The results shown in Table II certainly bear out this point of view. In  $\text{Ne}^{20}$ , with only one occupied level, containing four particles ( $\Psi_{1n}, \Psi_{1Tn}, \Psi_{1p}$ , and  $\Psi_{1Tp}$ , where  $T$  stands for time reversal, and  $n$  and  $p$  stand for neutron and proton), we see that  $\Psi_1$  remains fairly pure.

We now look into the  $\text{Mg}^{24}$  case in more detail. The spectra with and without a spin-orbit force but with normal-force range have been referred to earlier and appear in Fig. 1 and Fig. 2. The wave functions for no-spin-orbit force are shown in Table III. We see indeed that the occupied orbits are pure  $\Psi_1$  and  $\Psi_2$  and the unoccupied orbits are linear combinations of  $\Psi_4$  and  $\Psi_6$  or pure  $\Psi_5$  or  $\Psi_3$ . Comparing with the case where the spin-orbit force is turned on, we see that  $\Psi_1$  and  $\Psi_2$  do mix but that the unoccupied levels hardly admix at all because they are too far away in energy. It is the spin-orbit force that mixes the occupied orbitals and, to a lesser extent, the effect of the finite range also mixes orbits. In Fig. 4 we show the effect of finite range on the HF spectra. We see that as the range of the force is varied the spectrum remains quite close to its infinite-range appearance.

In the case of  $\text{Si}^{28}$ , there is a degeneracy. One solution is mainly  $\Psi_4, \Psi_5, \Psi_6$  and is oblate. This is the one given in Ref. 4. The other solution is mainly  $\Psi_1, \Psi_2, \Psi_3$  and is prolate. (We should like to thank Dr. George Ripka for bringing this to our attention). In  $\text{Ar}^{36}$  where the single unoccupied level is  $\Psi_1$  in the infinite range, no-spin-orbit limit, we see that the unoccupied level remains fairly pure.

TABLE III.  $\text{Mg}^{24}$  single-particle wave function for the case of zero  $\mathbf{l} \cdot \mathbf{s}$  force.

$\text{Mg}^{24}$	$\mathbf{l} \cdot \mathbf{s} = 0$		$\alpha = 0.62$		$\beta = 0.78$		Energy (MeV)
	$\Psi_1$	$\Psi_2$	$\Psi_3$	$\Psi_4$	$\Psi_5$	$\Psi_6$	
I	0.98	0	0	0.16	0	0	-20.00
II	0	1	0	0	0	0	-17.95
III	0	0	1	0	0	0	-5.24
IV	0.11	0	0	-0.68	0	0.72	-4.27
V	0	0	0	0	-1	0	-3.38
VI	-0.12	0	0	0.72	0	+0.68	-2.38

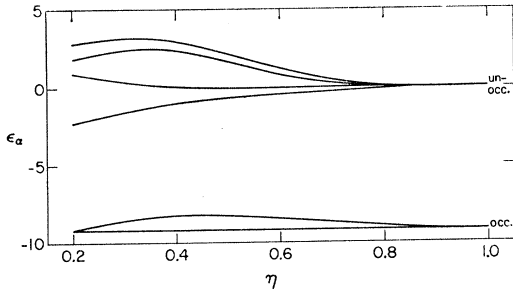


FIG. 4. Range dependence of the self-consistent energies of  $Mg^{24}$ , based on two-body force of Gaussian shape with the Rosenfeld mixture, and zero  $I \cdot s$  force. The range parameter  $\eta$  is defined in Ref. 13.  $\eta$  covers the interval from zero to unity, while the range  $\mu$  changes from zero to infinity. The energies for each  $\eta$  are normalized so that the lowest occupied orbital is of  $-9$  MeV.

We thus see that a study of the actual Hartree-Fock calculations in the  $sd$  shell does indeed indicate that the main underlying zero-order spectrum and representation is that of the infinite-range case. In the next section we will take up the case of the infinite-range limit in detail and discuss the main physical consequences of variations in exchange mixture and the perturbing effects of the spin-orbit and finite-range corrections.

### III. LONG-RANGE LIMIT OF HARTREE-FOCK CALCULATIONS

In this section we are going to discuss the Hartree-Fock calculation as applied to the long-range part of the two-body potential. The expansion of a two-body potential in terms corresponding to decreasing range has been discussed by Kugler.<sup>13</sup> The leading term of zero order is simply a constant. Next comes a term which behaves essentially like  $r_1^2 r_2^2 P_2(\cos\theta_{12})$ , the quadrupole-quadrupole force, which is usually taken as representing the long-range part of the force. The constant part plays the major role in determining the nature of the energy gap, and the quadrupole part determines the structure of the Hartree-Fock orbitals. If one considers a Gaussian potential of the form  $e^{-(r_{12}/\mu)^2}$ , then the expansion we have in mind corresponds to a Taylor series in the inverse range parameter ( $1/\mu$ ):

$$e^{-(r_{12}/\mu)^2} = 1 - (r_{12}/\mu)^2 + \frac{1}{2}(r_{12}/\mu)^4 + \dots \quad (7)$$

For more general potentials, the reader is referred to the paper of Kugler.<sup>13</sup> We now consider the Hartree-Fock problem for an arbitrary exchange mixture but only considering the leading term in the range expansion of the potential, namely a constant potential.

In order to study the single-particle spectra with two-body forces of infinite range in a simple manner, we will discard the single-body part of the Hamiltonian. In doing so, the  $(l, s)$  scheme becomes a good one and each single-particle level is denoted by separate space, spin, and isospin quantum numbers. Denoting the general state by  $|\alpha\rangle = |\alpha_x, \alpha_\sigma, \alpha_\tau\rangle$ , the single-particle Hartree-

Fock energy in a system of  $A$  nucleons is defined by the sum

$$\epsilon_\alpha = \sum_\lambda \{ \langle \alpha_x, \alpha_\sigma, \alpha_\tau; \lambda_x, \lambda_\sigma, \lambda_\tau | V | \alpha_x, \alpha_\sigma, \alpha_\tau; \lambda_x, \lambda_\sigma, \lambda_\tau \rangle - \langle \alpha_x, \alpha_\sigma, \alpha_\tau; \lambda_x, \lambda_\sigma, \lambda_\tau | V | \lambda_x, \lambda_\sigma, \lambda_\tau; \alpha_x, \alpha_\sigma, \alpha_\tau \rangle \}. \quad (8)$$

For two-body infinite range forces ( $V_c(r_{ij})=1$ ) of the general form of Eq. (5), these energies are determined by the sums of two-body wave function overlaps. The contributions of the different wave exchange components may be found by the following simple sums:

$$\begin{aligned} \epsilon_\alpha(W) &= \sum_\lambda [1 - (\alpha_x | \lambda_x)^2 (\alpha_\sigma | \lambda_\sigma)^2 (\alpha_\tau | \lambda_\tau)^2], \\ \epsilon_\alpha(M) &= \sum_\lambda [(\alpha_x | \lambda_x)^2 - (\alpha_\sigma | \lambda_\sigma)^2 (\alpha_\tau | \lambda_\tau)^2], \\ \epsilon_\alpha(B) &= \sum_\lambda [(\alpha_\sigma | \lambda_\sigma)^2 - (\alpha_x | \lambda_x)^2 (\alpha_\tau | \lambda_\tau)^2], \\ \epsilon_\alpha(H) &= - \sum_\lambda [(\alpha_\tau | \lambda_\tau)^2 - (\alpha_\sigma | \lambda_\sigma)^2 (\alpha_x | \lambda_x)^2], \end{aligned} \quad (9)$$

where  $\epsilon_\alpha(W)$  is the  $\epsilon_\alpha$  due to a unit Wigner force and so on. Using Eq. (9) we can easily find the relative spacings of the single-particle levels for any assumed occupied states  $|\lambda\rangle$  and an exchange mixture given by assumed values of  $W, M, B$ , and  $H$ .

$$\epsilon_\alpha = W \epsilon_{\alpha(W)} + M \epsilon_{\alpha(M)} + B \epsilon_{\alpha(B)} + H \epsilon_{\alpha(H)}. \quad (10)$$

The procedure is then as follows. The infinite-range solutions are characterized by the states  $|\lambda_x, \lambda_\sigma, \lambda_\tau\rangle$ . Depending on the choice of the functions  $|\lambda_x\rangle$ , one can construct the axially symmetric or the nonaxially symmetric cases. The only characteristic of the wave functions  $|\lambda_x\rangle$  that enters into question is their overlap integrals  $\langle \alpha_x | \lambda_x \rangle$ . Since we are assuming now that the two-body potential is a constant in its spatial dependence, it cannot determine the spatial dependence of the orbitals. The next term in the long-range expansion of the two-body potential, namely the quadrupole force, does determine the spatial dependence to be that going with the deformed harmonic oscillator. So, in our examples, we choose orbitals with this in mind. For example in  $Ne^{20}$  we can consider the solution

$$\Psi_1 \uparrow p, \quad \Psi_1 \downarrow p, \quad \Psi_1 \uparrow n, \quad \Psi_1 \downarrow n.$$

The main point to make for infinite-range forces is simply that all the  $|\lambda_x\rangle$  functions in  $Ne^{20}$  are identical and have unit overlap with each other. In the case of  $Ne^{20}$ , the above solution is the lowest one. Using Eq. (9) we can evaluate the Hartree-Fock energies  $\epsilon_\alpha$ . Simply set  $\langle \alpha_x | \lambda_x \rangle = 0$  for  $\alpha$  unoccupied and  $\langle \alpha_x | \lambda_x \rangle = 1$  for  $\alpha_x = \lambda_x$  the occupied orbit. For example, the energy of the occupied orbit is

$$\epsilon(\Psi_1) = 3W + 3M \quad (11)$$

and the energy of an unoccupied orbit is

$$\epsilon(\Psi_i) = 4M - M + 2B - 2H, \quad i = 2, 3, 4, 5, 6. \quad (12)$$

We thus have a very simple Hartree-Fock spectrum for  $\text{Ne}^{20}$ . The unoccupied orbits are all degenerate. We next consider the most general  $4n$  nucleus consisting of four-fold degenerate levels and each of the four degenerate levels having the same space dependence. The condition that the four degenerate orbitals should have the same space dependence results in determinants with maximum space symmetry. This situation is strongly favored experimentally where the Majorana force is strong and attractive for all exchange mixtures found in shell-model calculations. Another symmetry found in Hartree-Fock calculations is that the wave functions corresponding to degenerate orbitals are time reverses of each other. If we insist that the space part be the same for the degenerate orbitals and that they transform into each other under time reversal, then it follows that the space part of the orbital be even or odd under time reversal. This is indeed found to be the case in actual Hartree-Fock<sup>1-9</sup> calculations carried out with "realistic" forces. If we demand in addition that the orbitals be solutions in a deformed harmonic oscillator (this would result in an HF calculation with a  $P_2$  term), then we get the form chosen for the orbitals  $\Psi_1, \dots, \Psi_6$  in Sec. II. We note that  $m_j$  is not a good quantum number for orbitals  $\Psi_2, \Psi_3, \Psi_4, \Psi_5$  and that nuclei where these orbitals are occupied cannot be axially symmetric. There are exceptions to this, however. For example, if both  $\Psi_2$  and  $\Psi_3$  are occupied then we do not change the determinant if we choose new orbitals

$$d_{1\uparrow} = \frac{\Psi_2 + \Psi_3}{\sqrt{2}}, \quad d_{-1\uparrow} = \frac{\Psi_2 - \Psi_3}{\sqrt{2}},$$

and these new orbitals do yield an axially symmetric contribution to the matter distribution. More generally, the occupied orbitals form a subspace. If this subspace is invariant under the operation of  $J_z$ , then the nucleus in question is axially symmetric. If not, then the nucleus is not axially symmetric. These considerations explain why Bar-Touv and Kelson found some nuclei to be axially symmetric and others to be nonaxially symmetric. The sums in Eq. (9) can easily be carried out, and one finds quite generally that

$$\begin{aligned} \epsilon(\text{occupied}) &= N(W - \frac{1}{4}M + \frac{1}{2}B - \frac{1}{2}H) \\ &\quad + 4M - W - 2B + 2H, \quad (13) \\ \epsilon(\text{unoccupied}) &= N(W - \frac{1}{4}M + \frac{1}{2}B - \frac{1}{2}H), \end{aligned}$$

where  $N$  is the number of particles and  $N = 4n$  where  $n$  is an integer. This extremely simple result shows that the occupied levels are all degenerate and the unoccupied levels are also degenerate. The energy difference between these levels remains constant and is independent of the number of particles  $N$ . In fact the

"gap" is given simply by  $G$  independent of  $N$  where

$$G = -4M + W + 2B - 2H. \quad (14)$$

We thus see that quite generally an infinite-range Hartree-Fock calculation gives a constant gap between degenerate occupied and degenerate unoccupied levels which agrees rather well with the finite-range results.

We next consider nuclei of the form  $(4n+1)$  and consider solutions where the space dependence is the same for groups of 4 orbitals and only the spin-isospin factors vary as spin-up neutron, spin-down neutron, spin-up proton, and spin-down proton. We thus consider systems defined by the diagram in Fig. 5, where  $\lambda$  designates fourfold-occupied levels,  $\alpha$  designates the singly occupied level, and  $\beta$  designates unoccupied levels. Using Eq. (9) we find

$$\begin{aligned} \epsilon(\lambda \uparrow n) &= N\Gamma + (-W - \frac{3}{2}B + 13M/4 + \frac{3}{2}H), \\ \epsilon(\lambda \downarrow n) &= N\Gamma + (-W - \frac{5}{2}B + 17M/4 + \frac{3}{2}H), \\ \epsilon(\lambda \uparrow p) &= N\Gamma + (-W - \frac{3}{2}B + 17M/4 + \frac{5}{2}H), \\ \epsilon(\lambda \downarrow p) &= N\Gamma + (-W - \frac{5}{2}B + 17M/4 + \frac{5}{2}H), \\ \epsilon(\alpha \uparrow n) &= N\Gamma + (-W - \frac{1}{2}B + \frac{1}{4}M + \frac{1}{2}H), \\ \epsilon(\alpha \downarrow n) &= N\Gamma + (-\frac{3}{2}B + \frac{5}{4}M - \frac{1}{2}H), \\ \epsilon(\alpha \uparrow p) &= N\Gamma + (\frac{1}{2}B + \frac{5}{4}M + \frac{3}{2}H), \\ \epsilon(\alpha \downarrow p) &= N\Gamma + (-\frac{1}{2}B + \frac{5}{4}M + \frac{1}{2}H), \\ \epsilon(\beta \uparrow n) &= N\Gamma + (\frac{1}{2}B - \frac{3}{4}M - \frac{1}{2}H), \\ \epsilon(\beta \downarrow n) &= N\Gamma + (-\frac{3}{2}B + \frac{1}{4}M - \frac{1}{2}H), \\ \epsilon(\beta \uparrow p) &= N\Gamma + (\frac{1}{2}B + \frac{1}{4}M + \frac{1}{2}H), \\ \epsilon(\beta \downarrow p) &= N\Gamma + (-\frac{3}{2}B + \frac{1}{4}M + \frac{1}{2}H), \end{aligned} \quad (15)$$

where  $\Gamma = W + \frac{1}{2}B - \frac{1}{4}M - \frac{1}{2}H$  and  $N$  is the number of particles.  $\Gamma$  vanishes for a saturating force and in any case the term  $N\Gamma$  is common to all the energies and thus plays no role in considering relative spacings. Hence relative spacings are independent of the number of particles involved and depend only on the "occupation structure" of the nucleus (i.e., whether it is a  $4n$  type, a  $4n+1$  type, etc.).

For comparison, we write the  $4n$ -nucleus energies:

$$\begin{aligned} \epsilon(\lambda) &= N\Gamma + (-W - 2B + 4M + 2H), \quad (16) \\ \epsilon(p) &= N\Gamma. \end{aligned}$$

Comparing the  $4n$  energies with the  $4n+1$  energies, we see that the states  $\lambda$  on the average are unaffected. The singly occupied state  $\alpha$  is unshifted from its position in the  $4n$  nucleus if we consider saturating forces. This is because the relative shift in  $\alpha$  is proportional to  $\Gamma$

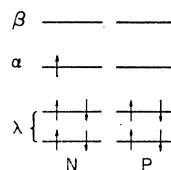


FIG. 5. Schematic diagram for  $4n+1$  spectrum.  $\lambda$  are the fully occupied states,  $\alpha$  are occupied with the extra nucleon, and  $\beta$  are the unoccupied levels.

which vanishes for saturating forces. The unoccupied levels in the  $4n+1$  system do shift a bit. In the  $4n+1$  nuclei, we find that with realistic exchange mixtures the unoccupied  $\alpha$  state lies lower than the occupied one. No matter what one chooses for the occupied  $\alpha$  state it will invariably lie above the unoccupied  $\alpha$  states. Perhaps it is more physical to consider an ensemble of occupied  $\alpha$  states where each one of the four possible states is occupied with equal probability  $\theta$ . We take  $\theta$  to be  $\frac{1}{4}$  for a  $4n+1$  nucleus,  $\theta=\frac{1}{2}$  for a  $4n+2$  nucleus,  $\theta=\frac{3}{4}$  for  $4n+3$ , and  $\theta=1$  for  $4n+4$ . Consider  $p$  states  $\lambda$  and one state  $\alpha$  with occupation probability  $\theta$  and unoccupied levels  $\beta$  as shown in Fig. 6. The energies are then given by

$$\begin{aligned}\epsilon(\lambda) &= 4(p+\theta)\Gamma + (-W+2M-2B+H), \\ \epsilon(\alpha) &= 4(p+\theta)\Gamma + \theta(-W+2M-2B+H), \\ \epsilon(\beta) &= 4(p+\theta)\Gamma.\end{aligned}\quad (17)$$

We thus find the extremely simple result that as a level becomes occupied it sinks from its unoccupied position to a fully occupied position in a linear manner. The other levels remain relatively unshifted. (Even absolutely unshifted for  $\Gamma=0$  saturating mixtures.) If a level is occupied to an amount  $\theta$ , then it is shifted below the degenerate unoccupied states by an amount  $\theta G$  where  $G$  is the gap in the spectra of  $4n$ -type nuclei.

We now go on to discuss nuclei of the form  $4n+2q$  corresponding to nuclei of the  $4n$  type with  $q$  doubly occupied neutron levels. This is shown schematically in Fig. 7. The energies are independent of spin, so we only record spin up. The results are

$$\begin{aligned}\epsilon(\lambda \uparrow n) &= N\Gamma + [-W-2B+(4-\frac{1}{2}q)M+(2-q)H], \\ \epsilon(\lambda \uparrow p) &= N\Gamma + [-W-2B+(4+\frac{1}{2}q)M+(2+q)H], \\ \epsilon(\alpha \uparrow n) &= N\Gamma + [-W-2B+(2-\frac{1}{2}q)M+(1-q)H], \\ \epsilon(\alpha \uparrow p) &= N\Gamma + [(2+\frac{1}{2}q)M+(1+q)H], \\ \epsilon(\gamma \uparrow n) &= N\Gamma + [-\frac{1}{2}qM-qH], \\ \epsilon(\gamma \uparrow) &= N\Gamma + [\frac{1}{2}qM+qH].\end{aligned}\quad (18)$$

These results can be written in a more transparent fashion if we introduce the expression

$$\beta = -(M+2H).\quad (19)$$

This is the same term introduced by Lane<sup>14</sup> and denoted by  $V_1/A$  in order to discuss the isobaric dependence of the interaction of a nucleon with a nucleus. (See also Sherr *et al.*<sup>15</sup> and further references therein.) In terms of

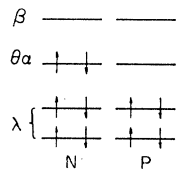
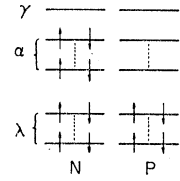


FIG. 6. Schematic diagram for the case where each one of the four possible  $\alpha$  states is occupied with equal probability  $\theta$ .

<sup>14</sup> T. A. Lane, Nucl. Phys. **35**, 676 (1962).

<sup>15</sup> R. Sherr *et al.*, Phys. Rev. **139**, B1272 (1965).

FIG. 7.  $4n+2q$  nucleus.  $\lambda$  fully occupied,  $\alpha$  half occupied, and  $\gamma$  unoccupied levels.



$\beta$ , the isobaric shift parameter  $G$  the gap parameter, and  $\Gamma$  the parameter which vanishes for saturating forces, we can rewrite the energies as

$$\begin{aligned}\epsilon(\lambda \uparrow n) &= N\Gamma + \frac{1}{2}q\beta - G, \\ \epsilon(\lambda \uparrow p) &= N\Gamma - \frac{1}{2}q\beta - G, \\ \epsilon(\alpha \uparrow n) &= N\Gamma + \frac{1}{2}q\beta + (-W-2B+2M+H), \\ \epsilon(\alpha \uparrow p) &= N\Gamma - \frac{1}{2}q\beta + (2M+H), \\ \epsilon(\gamma \uparrow n) &= N\Gamma + \frac{1}{2}q\beta, \\ \epsilon(\gamma \uparrow p) &= N\Gamma - \frac{1}{2}q\beta,\end{aligned}\quad (20)$$

where  $q$ , the number of double occupied neutron levels, is equal to  $T_z$  of the nucleus. It is clear from the above equations that neutrons and protons shift relative to each other by an amount  $q\beta$ . The completely unoccupied levels  $\gamma$  still are a distance  $G$  above the completely occupied levels  $\alpha$  just as in the  $4n$ -type nuclei. The doubly occupied levels  $\alpha$  lie somewhere in the gap region. For forces which are predominantly Majorana, the  $\alpha$  states lie midway in the gap region between the completely occupied and the completely unoccupied levels. It is clear that  $\beta$  measures the part of the symmetry energy in nuclei which comes from the potential energy. In addition, there is a part coming from the kinetic energy.<sup>16</sup>

For completeness we record the case of neutrons alone which may be useful in considering the very heavy nuclei. They may be described schematically by Fig. 8. For such nuclei, only two exchange mixtures enter corresponding to the  $T$  equals 1 forces. They are singlet-even ( ${}^1E$ ) and triplet-odd ( ${}^3O$ ) where

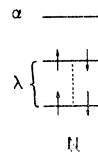
$$\begin{aligned}{}^1E &= \frac{1}{4}(W-B+M-H), & {}^3E &= \frac{1}{4}(W+B+M+H), \\ {}^3O &= \frac{1}{4}(W+B-M-H), & {}^1O &= \frac{1}{4}(W-B-M+H).\end{aligned}\quad (21)$$

The energies are given by

$$\begin{aligned}\epsilon(\lambda) &= N[{}^1E+3{}^3O]+2{}^1E-6{}^3O, \\ \epsilon(\alpha) &= N[{}^1E+3{}^3O].\end{aligned}$$

We thus see that an energy gap appears between occupied and unoccupied levels of magnitude  $(6{}^3O-2{}^1E)$ , which is independent of the number of particles.

FIG. 8. Schematic diagram for even-number neutron excess.  $\lambda$  doubly occupied,  $\alpha$  unoccupied levels.



<sup>16</sup> Reference 14, p. 679 ff.

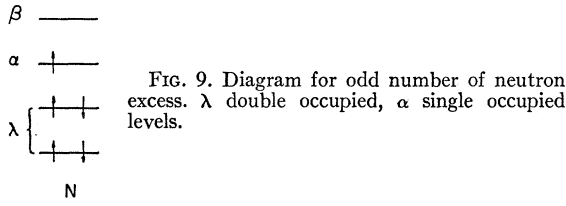


FIG. 9. Diagram for odd number of neutron excess.  $\lambda$  double occupied,  $\alpha$  single occupied levels.

Next consider pure neutron configurations with an odd number of neutrons. This is shown schematically in Fig. 9. The energies are given by

$$\begin{aligned}
 \epsilon(\lambda \uparrow) &= N(^1E + 3^3O) + ^1E - 5^3O, \\
 \epsilon(\lambda \downarrow) &= N(^1E + 3^3O) + 3^1E - 7^3O, \\
 \epsilon(\alpha \uparrow) &= N(^1E + 3^3O) + ^1E - ^3O, \\
 \epsilon(\alpha \downarrow) &= N(^1E + 3^3O) + 3^1E - 3^3O, \\
 \epsilon(\beta \uparrow) &= N(^1E + 3^3O) + ^3O - ^1E, \\
 \epsilon(\beta \downarrow) &= N(^1E + 3^3O) - ^3O + ^1E.
 \end{aligned} \quad (22)$$

It is probably more physical to consider an ensemble where there are  $p$  doubly occupied levels  $\lambda_i$  and the odd particle has probability  $\theta$  to be in the  $\alpha$  spin-down state. The state  $\gamma$  is unoccupied. This is shown schematically in Fig. 10. The Hartree-Fock energies for this case are

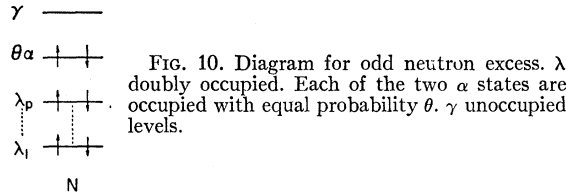


FIG. 10. Diagram for odd neutron excess.  $\lambda$  doubly occupied. Each of the two  $\alpha$  states are occupied with equal probability  $\theta$ .  $\gamma$  unoccupied levels.

then

$$\begin{aligned}
 \epsilon(\lambda) &= 2(p + \theta)(^1E + 3^3O) + (2^1E - 6^3O), \\
 \epsilon(\alpha) &= 2(p + \theta)(^1E + 3^3O) + \theta(2^1E - 6^3O), \\
 \epsilon(\gamma) &= 2(p + \theta)(^1E + 3^3O).
 \end{aligned} \quad (23)$$

The gap parameter for the pure neutron case is thus

$$G_n = -2^1E + 6^3O = W + 2B - 2M - H. \quad (24)$$

We thus see that in the pure neutron case all fully occupied levels are degenerate and are separated from the fully unoccupied levels by an energy  $G_n$ , while the singly occupied level (corresponding to  $\theta = \frac{1}{2}$ ) lies half-way between.

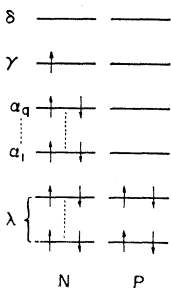


FIG. 11. Schematic diagram for odd mass nucleus with variable neutron excess.  $\lambda$  fully occupied,  $\alpha$  doubly occupied,  $\gamma$  single occupied, and  $\delta$  unoccupied states.

As a last example, we consider an odd-mass-number nucleus with a variable neutron excess as shown schematically in Fig. 11. The energies are given by

$$\begin{aligned}
 \epsilon(\lambda \uparrow n) &= N\Gamma + [-W - \frac{3}{2}B + 13M/4 + \frac{3}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\lambda \downarrow n) &= N\Gamma + [-W - \frac{5}{2}B + 17M/4 + \frac{3}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\lambda \uparrow p) &= N\Gamma + [-W - \frac{3}{2}B + 17M/4 + \frac{5}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\lambda \downarrow p) &= N\Gamma + [-W - \frac{5}{2}B + 17M/4 + \frac{5}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\alpha \uparrow n) &= N\Gamma + [-W - \frac{3}{2}B + \frac{5}{4}M + \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\alpha \downarrow n) &= N\Gamma + [-W - \frac{5}{2}B + \frac{5}{4}M + \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\alpha \uparrow p) &= N\Gamma + [\frac{1}{2}B + \frac{5}{4}M + \frac{3}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\alpha \downarrow p) &= N\Gamma + [-\frac{1}{2}B + \frac{5}{4}M - \frac{3}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\gamma \uparrow n) &= N\Gamma + [-W - \frac{1}{2}B + \frac{1}{4}M + \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\gamma \downarrow n) &= N\Gamma + [-\frac{3}{2}B + \frac{5}{4}M - \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\gamma \uparrow p) &= N\Gamma + [\frac{1}{2}B + \frac{5}{4}M + \frac{3}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\gamma \downarrow p) &= N\Gamma + [-\frac{1}{2}B + \frac{5}{4}M + \frac{1}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\delta \uparrow n) &= N\Gamma + [\frac{1}{2}B - \frac{3}{4}M - \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\delta \downarrow n) &= N\Gamma + [-\frac{3}{2}B + \frac{1}{4}M - \frac{1}{2}H] + \frac{1}{2}q\beta, \\
 \epsilon(\delta \uparrow p) &= N\Gamma + [\frac{1}{2}B + \frac{1}{4}M + \frac{1}{2}H] - \frac{1}{2}q\beta, \\
 \epsilon(\delta \downarrow p) &= N\Gamma + [-\frac{3}{2}B + \frac{1}{4}M + \frac{1}{2}H] - \frac{1}{2}q\beta.
 \end{aligned} \quad (25)$$

#### IV. RESULTS WITH "BEST" FORCE PARAMETERS

In this section we will present some typical infinite range aspects. For this purpose we need some "typical" values of  $M$ ,  $B$ ,  $H$ , and  $W$ . In another paper<sup>17</sup> a detailed study of binding energies is carried out and the whole question of exchange mixtures is gone into in quite a bit of detail. The various exchange mixtures used in the past are shown to belong to a family, all of which obey the same conditions. As a function of mass number, the parameters  $M$ ,  $B$ ,  $H$ , and  $W$  go more or less like  $(1/A)$ . If we normalize at mass number 20 then a "typical" set of force parameters is given in Table IV.

As we go to different mass numbers the relative magnitudes remain constant but the absolute values decrease with increasing mass number, so our results for the HF spectra should hold relatively for all mass numbers. It should be pointed out that the main features of the HF spectra remain about the same when

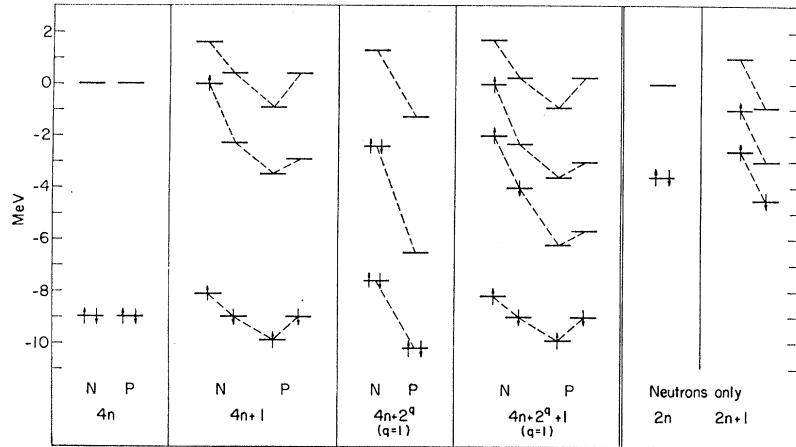
TABLE IV. Exchange parameters for the "best" force and the corresponding values for  $G$ ,  $\beta$ , and  $\Gamma$  defined in the text.

Parameter	MeV	Parameter	MeV
$W$	-0.35	$G$	8.85
$B$	-0.60	$\beta$	2.60
$M$	-2.60	$G_n$	3.65
$H$	0.00	$\Gamma$	0

<sup>17</sup> W. H. Bassichis, C. A. Levinson, and G. Ripka (to be published).



FIG. 12. Single-particle relative spacings in various neutron excess nuclei for long-range two-body force with the exchange mixture given in Table IV.



comparison is made between the various exchange mixtures given in the past. That is to say,  $G$  remains fairly constant from one exchange mixture to the next.  $\Gamma$  and  $G_n$  do show variation, however. It is interesting that  $G_n$ , the pure neutron gap, is about  $\frac{1}{2}G$ , the  $4n$ -nucleus gap.

The spectra for the "typical" force are shown in Fig. 12. The general trends are clear. The gap between occupied and unoccupied levels is modified as discussed earlier by the presence of partially filled levels. In Fig. 12 the singly occupied level is not averaged over by introducing the parameter  $\theta$ , and we see the phenomena of unoccupied neutron levels lying below occupied ones as discussed earlier. In the cases where there are  $q$  doubly occupied neutron levels, only the  $q$  equals one or zero case is shown since the other cases can be derived from these by merely shifting all neutron levels by an amount  $\frac{1}{2}q\beta$  and all proton levels by an amount  $-\frac{1}{2}q\beta$ .

## V. CONCLUSIONS

It has been shown in considerable detail that the results of Hartree-Fock calculations which involve only orbital and spin degrees of freedom are determined almost completely by the long-range part of the two-body force. The solutions for a long-range model were then exhibited, and the dependence of the energy gap on the exchange dependence was shown. A very simple picture emerged. Completely occupied states are degenerate and sink lowest in energy. Then, as a state becomes more and more occupied, it also sinks proportionally. The energy "gap" between occupied and

unoccupied levels is a very important aspect of the Hartree-Fock approximation. The larger the gap, the better the approximation. The main effects of the spin-orbit force and the finite range of the two-body potential are to mix the occupied orbitals. This mixing leaves the Hartree-Fock determinant invariant. For typical cases in the  $sd$  shell, the energy gap is so large that unoccupied states do not mix appreciably with the occupied states. When a neutron excess occurs, the partially occupied levels lie about midway between occupied and unoccupied levels. Thus the "gap" is cut in two, and the spin-orbit force is able to mix levels more easily. This qualitatively explains why series of nuclei like the oxygen isotopes or the calcium isotopes seem to display spectra consistent with the  $jj$  model.

From this study it emerges that the most natural representation for the one-body orbitals in these Hartree-Fock calculations is that associated with the axially symmetric deformed harmonic oscillator where one takes linear combinations of the degenerate orbitals which are eigenstates of time reversal. This prescription will result often in nonaxially symmetric nuclei and is consistent with the result found in exact calculations with realistic forces.

## ACKNOWLEDGMENTS

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