ORNL-TM-5174

Inversion of Single-Particle Levels in Nuclear Hartree-Fock and Brueckner-HF Calculations With Broken Symmetry

R. L. Becker
J. P. Svenne

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION • FOR THE U.S. ATOMIC ENERGY COMMISSION

BLANK PAGE

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
Price: Printed Copy $5.45; Microfiche $2.25

ORNL-TM-5174

Contract No. W-7405-eng-26

Physics Division

INVERSION OF SINGLE-PARTICLE LEVELS IN NUCLEAR HARTREE-FOCK AND BRUECKNER-HF CALCULATIONS WITH BROKEN SYMMETRY

R. L. Becker
Oak Ridge National Laboratory
Oak Ridge, Tennessee 37830

and

J. P. Svenne
University of Manitoba
Winnipeg, Manitoba
Canada

DECEMBER 1975

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
ENERGY RESEARCH AND DEVELOPMENT ADMINISTRATION

BLANK PAGE

Inversion of Single-Particle Levels in Nuclear Hartree-Fock and Brueckner-HF Calculations with Broken Symmetry

R. L. Becker
Oak Ridge National Laboratory*
Oak Ridge, Tennessee 37830

and

J. P. Svenne
University of Manitoba†
Winnipeg, Manitoba

Abstract: Energy levels of states connected by a symmetry of the Hamiltonian normally should be degenerate. In self-consistent field theories, when only one of a pair of single-particle levels connected by a symmetry of the full Hamiltonian is occupied, the degeneracy is split and the unoccupied level often lies below the occupied one. We examine inversions of neutron-proton (charge) and time-reversal doublets in odd nuclei, charge doublets in even nuclei with a neutron excess, and spin-orbit doublets in spherical configurations with spin-unsaturated shells. The origin of the level inversion is investigated, and the following explanation offered. Unoccupied single-particle levels, from a calculation in an A-particle system should be interpreted as levels of the (A+1)-particle system. When the symmetry-related level, occupied in the A-particle system, is also calculated in the (A+1)-particle system it is degenerate with or lies lower than

*Research sponsored by the U. S. Atomic Energy Commission under contract with Union Carbide Corporation.

†Work supported in part by the National Research Council of Canada.

the other. That is, when both levels are calculated in the (A+1)-particle system, they are not inverted. It is demonstrated that the usual prescription to occupy the lowest-lying orbitals should be modified to refer to the single-particle energies calculated in the (A+1)- or the (A-1)-particle system. This observation is shown to provide a justification for avoiding an oscillation of occupancy between symmetry-related partners in successive iterations leading to self-consistency.

It is pointed out that two degenerate determinants arise from occupying one or the other partner of an initially degenerate pair of levels and then iterating to self-consistency. The existence of the degenerate determinants indicates the need for introducing correlations, either by mixing the two configurations or by allowing additional symmetry-breaking (resulting in a more highly deformed non-degenerate configuration).

1. Introduction

Symmetry properties have long been recognized as playing a vital role in nuclear self-consistent field (SCF) theories.* Besides making

*We have in mind, along with Hartree-Fock (HF) (see, e.g. the review by Ripka in ref. 7), the newer and less extensively exploited density-dependent Hartree-Fock (DDHF)[1,2], Brueckner-Hartree-Fock (BHF)[3], renormalized Brueckner-Hartree-Fock (RBHF)[4], and Hartree-Fock-Bogoliubov (HFB)[5,6] theories.

it possible to include known facts about the nucleus from the start, these symmetries lead to important simplifications in the calculations and make them more tractable in terms of computer time and storage. If, among the symmetries of the full Hamiltonian, only the self-consistent

symmetries (precisely defined in section 2) are imposed on the SCF Hamiltonian, these introduce no additional approximations into the calculation. However, they do place restrictions[7-9] on the neutron and proton numbers of the nuclei which can be treated and on the kinds of configurations for which the calculations can be done. It can be useful also to make SCF calculations with a simplified full Hamiltonian having a symmetry which the "actual" nucleon-nucleon interaction does not possess,*

*One does not know, of course, the exact effective interaction which should be used in a given SCF theory. But one has learned that the nucleon-nucleon force is very complicated and possesses fewer symmetries than the model forces one would prefer to use for the sake of simplicity.

provided that the symmetry-breaking part of the "actual" interaction is relatively weak. Thus, assuming a symmetry also places restrictions on the two-nucleon interaction.

Two symmetries of the full Hamiltonian assumed in many of the nuclear SCF calculations done up till now are: (i) time-reversal invariance, and (ii) isospin conservation. The latter assumption requires neglecting the isovector part of the Coulomb interaction between nucleons and the small non-charge-independent contributions to the nuclear forces. In order for (i) to be a self-consistent symmetry, the calculations must be restricted to nuclei with even N and even Z; similarly, (ii) requires self-conjugacy, N = Z. Taken together these two symmetries limit consideration to particular configurations of even-even self-conjugate nuclei, here to be called α-particle nuclei[7]. Because of the presence of isovector Coulomb forces in actual nuclei, only the lightest of these nuclei, viz. those with $A \leq 60$, are stable or nearly stable; heavier stable elements strongly prefer a neutron excess.

The set of α-particle nuclei includes all of the stable self-conjugate nuclei which can have closed spherical ℓ-shells, ^{4}He, ^{16}O and ^{40}Ca. In these nuclei the "normal" splitting of the j-subshells, which arises primarily from the two-nucleon spin-orbit interaction[10], is such that the j=ℓ+1/2 level lies below the j=ℓ-1/2 level. From Wong's investigation one may infer that the interaction of a single-particle (s.p.) state j with a filled j'-subshell, which we shall denote by $U_j(j')$, is such that

$$\Delta_\ell(\ell'-1/2) \equiv U_{\ell-1/2}(\ell'-1/2) - U_{\ell+1/2}(\ell'-1/2) > 0, \quad \text{("normal")} \tag{1.1a}$$

$$\Delta_\ell(\ell'+1/2) \equiv U_{\ell-1/2}(\ell'+1/2) - U_{\ell+1/2}(\ell'+1/2) < 0, \quad \text{("abnormal")} \tag{1.1b}$$

and that if the ℓ'-shell is closed there is a partial cancellation between $\Delta_\ell(\ell'\pm1/2)$, with the remainder having the normal sign

$$\Delta_{\ell;\ell'} \equiv \sum_{j'=\ell'\pm1/2} \Delta_\ell(j') > 0. \tag{1.1c}$$

Another subset of the α-particle nuclei includes ^{12}C, ^{28}Si, ^{32}S and ^{56}Ni, which have spherical configurations in which the highest occupied ℓ'-shell is spin-unsaturated, i.e. the "normally lower" j'=ℓ'+1/2 subshell is filled while the j'=ℓ'-1/2 shell is empty. The interactions of the s.p. states j = ℓ ± 1/2 with the spin-unsaturated ℓ'-shell are, by eq. (1.1b), such as to give an "abnormal" contribution to the spin-orbit splitting. A surprising result of some HF[11,12] and RBHF[13,14] calculations (see section 3.1) is that for ℓ = ℓ' (the spin-unsaturated ℓ-shell) the unoccupied j=ℓ-1/2 subshell is found to lie lower than the occupied j=ℓ+1/2 subshell. That is, the uncompensated "abnormal" contribution to

the splitting of states with $j = \ell \pm 1/2$ arising from interactions with the filled $j=\ell+1/2$ subshell outweighs the individually small "normal" contributions from the interactions with the occupied closed ℓ-shells. This poses a problem for the SCF theory, because the occupied levels in the model ground state are supposed to be those with the lowest s.p. energies. This is one example of the level-inversion problem to be considered in this paper.*

*The spherical configurations do not provide very good descriptions of the ground states of these nuclei: ^{12}C, ^{28}Si and ^{32}S are described better as deformed and ^{56}Ni as paired. The possibility of escaping from an inversion or near-degeneracy by taking on correlations is discussed in section 6.

Although most nuclear SCF calculations performed to date are for the α-particle nuclei,** a number have been done for spherical nuclei with a

**We cite a number which employ various interactions and methods of calculation: for the spherical nuclei refs. 15, 12 and 16 (HF), refs. 2, 17 and 18 (DDHF), refs. 19 and 20 (BHF), and refs. 13, 14, 21 and 22 (RBHF); for axially symmetric deformed nuclei refs. 23-25 (HF), ref. 26 (DDHF), and refs. 13 and 27 (BHF and RBHF). As the considerations of the paper do not cover explicitly the HFB method, we have not included any references to HFB calculations.

neutron excess, e.g.[12,16,18,20,21,28]. Moreover, a few have been made for odd nuclei with one "particle" or hole outside closed spherical shells, e.g.[29,14,24,30] and for more strongly deformed odd and odd-odd nuclei, e.g.[30,24]. A frequent result is the intrusion of an unoccupied level below the highest occupied level, i.e. an apparently non-self-consistent inversion of levels. For example, in an odd or odd-odd nucleus an unoccupied state which is similar to the time-reverse of an occupied state lies below the occupied state (see sect. 3.3).

In the case of a breaking of time-reversal invariance a level-inversion can lead to an instability in the iterative process used to achieve self-consistency. Suppose that, as part of the input to one step of the iteration, the "last nucleon" occupies a certain state whereas the time-reversed state is unoccupied, and that in the output of this iteration the time-reversed state is the lower. Then, according to the standard interpretation of SCF theory, in the next iteration the time-reversed state should be taken as occupied, and so on.* This has been

*Note, however, that the particle density of an orbital is the same as that of its time-reverse, so there is no oscillation of density.

done for example in the calculations of odd axially deformed nuclei by Lee and Cusson[24]. They have cited the lower of the energies of the two states as that of the highest lying occupied state (ε_f) and the higher of the two as the energy of the lowest unoccupied state (ε_{f+1}), but their calculations in fact involved the inversion-instability (priv. comm.[24]).

In this paper we examine these level inversion problems in some detail for the HF, BHF, and RBHF theories. We suggest a physically meaningful interpretation[31] which removes the apparent inconsistency between filling the lowest levels and the existence of a level inversion, and which is shown to provide a theoretical justification for avoiding an inversion-instability in successive iterations.

2. Statement of the problem

2.1. SELF-CONSISTENT SYMMETRIES

We shall deal first with the level inversion problem in a formal way that includes all the cases mentioned above. We assume that the full

Hamiltonian of an A-nucleon system is

$$H = \sum_{i=1}^{A} T(i) + \sum_{i,j(i<j)}' v(i,j). \qquad (2.1)$$

A symmetry property of H is expressible as the invariance of H under a transformation. Thus, a symmetry operator for H is defined as a unitary or anti-unitary (in the case of time-reversal) operator which commutes with H. The one-body SCF Hamiltonian, h, for any solution of the SCF problem is a functional of the occupied self-consistent orbitals, ψ_λ, i.e.

$$h = h(\{\psi_\lambda, \lambda \leq A\}).$$

A symmetry operator $\mathcal{S}$ for H which, moreover, is the A-fold product* of

*This requirement excludes symmetries involving permutations of particle labels, which can be reduced only as far as products of two-particle operators.

a s.p. transformation, S, is said to be a self-consistent symmetry for a solution of the SCF problem if S is a symmetry operator for h. A self-consistent symmetry is a propagating symmetry, i.e. one which is preserved in successive iterations. Thus, if a trial set of orbitals yields a s.p. Hamiltonian $h^{(T)}$ which commutes with S, then the self-consistent h obtained at the end of the iteration process will commute with S.

A necessary and sufficient condition for a symmetry to be self-consistent in HF theory is given in the following lemma[7,8]:

If S is a unitary or anti-unitary s.p. transformation for which $\mathcal{S} \equiv \prod_{i=1}^{A} S(i)$ commutes with H(1,...A), then S commutes with $h(\{\psi_\lambda, \lambda \leq A\})$ if and only if S leaves the subspace of occupied orbitals $\{\psi_\lambda, \lambda \leq A\}$ invariant.

The lemma is a consequence of the fact that the HF Hamiltonian is invariant under any unitary or anti-unitary transformation within the subspace of occupied orbitals. As this property holds also for the BHF and RBHF theories, the lemma can be generalized to apply to these theories. The self-consistent determinantal wave function,

$$\Psi = \det\{\psi_\lambda,\ \lambda \leq A\}$$

is clearly invariant to within a phase under a self-consistent symmetry.

Axial symmetry is always a self-consistent symmetry in the absence of an external magnetic field because

$$[\exp\{i\theta \sum_{i=1}^{A} j_z(i)\},\ H] = 0 \tag{2.2a}$$

and for an axially symmetric field the azimuthal dependence of each orbital wave function can be chosen to correspond to a sharp intrinsic magnetic quantum number, Ω, for which S is diagonal

$$\exp\{i\theta j_z\}\psi_{\alpha\Omega} = \exp\{i\Omega\theta\}\Psi_{\alpha\Omega}, \tag{2.2b}$$

so that the manifold of occupied orbitals is trivially invariant.

When considering a single self-consistent symmetry, S, if it is not already diagonal by choice (as in the case of axial symmetry), one can diagonalize it in the space of occupied orbitals. Its eigenfunctions are invariant to within a phase under S. But we must usually consider SCF solutions with more than one self-consistent symmetry. Often some of the symmetries do not commute among each other. In such cases it will be impossible for the individual orbitals to be eigenfunctions of all the symmetries. It is necessary to choose a basis set of orbitals in

which a commuting set of symmetries are diagonal while the other symmetries are not. If an orbital is transformed into a different orbital by a self-consistent symmetry, then the orbital and its transform are degenerate, for

$$h\psi = \varepsilon\psi \quad \text{and} \quad [S,h] = 0 \tag{2.3}$$

imply

$$h(S\psi) = Sh\psi = \varepsilon(S\psi). \tag{2.4}$$

In this paper all the non-diagonal symmetries with which we shall be concerned lead only to a two-fold degeneracy. For these $S^2\psi \propto \psi$, and S may be referred to as an "interchange" operator. With each such symmetry S, there is another self-consistent symmetry, S_D, with which S does not commute and which distinguishes between each two degenerate partners under S. We may refer to the eigenvalue of S_D, which distinguishes one class of orbitals from that of their partners under S, as the distinction quantum number relative to S. Two partners may be said to have opposite distinctions.

The three cases to be considered here are:

(i) Time-reversal ($\mathcal{T}$) invariance. For axially symmetric fields the time-reversed partner of an orbital has a magnetic quantum number of opposite sign. Thus, if the body-fixed unit vector $\hat{z}'$ is along the axis of symmetry, $S_D = e^{i\pi(j_{z'}-1/2)}$ distinguishes between the two sets of partners. Bar-Touv and Kelson[7] pointed out that the $\mathcal{T}$-adapted orbitals of axially asymmetric fields with ellipsoidal symmetry can be written as superpositions of states $\phi_{\alpha\Omega}$ with Ω-1/2 either even or odd. So here again $d_{\mathcal{T}} = \langle(-1)^{j_{z'}-1/2}\rangle$ distinguishes the partners. If an orbital is occupied then its time-reversed partner also must be occupied

if the subspace of occupied orbitals is to be invariant under time-reversal. Consequently, the nucleon number A must be even. Moreover, if the orbitals do not mix neutron and proton components, then N and Z separately must be even. In the case of axial symmetry the total magnetic quantum number must be zero.

(ii) Charge-independence (invariance under the group of rotations in isospin space, $S(\vec{\theta}) = e^{i\vec{\theta}\cdot\vec{t}}$). This implies that the total isospin, T, as well as the charge $Q = A/2 - T_3$, is conserved. Each orbital may be chosen to have a definite isospin projection, $\tau = +1/2$ for a neutron and $-1/2$ for a proton. A rotation by π about the first or the second axis takes τ into $-\tau$,* leading to a two-fold degeneracy between a neutron

*Because $t_1^2 = (\frac{1}{4})I$, $S \equiv e^{i\pi t_1} = \cos \pi/2 + i2t_1 \sin\pi/2 = i2t_1 = i(t_+ + t_-)$, where $t_\pm$ are the raising and lowering operators.

orbital, with $d_q = (-)^{\tau-1/2} = 1$, and the corresponding proton orbital ($d_q = -1$) with exactly the same space-spin wave function. Consequently, if charge-independence is a self-consistent symmetry, the nucleus must be self-conjugate, N = Z ($M_T = 0$). The same result must hold in an arbitrarily rotated frame, i.e. $M_T' = 0$, and hence we must have T = 0, corresponding to a closed "shell" in isospace.

(iii) Invariance under reflection of intrinsic spins in spherical (J=0) configurations. If rotational invariance, which involves both orbital and intrinsic spin degrees of freedom, is a self-consistent symmetry, the state must have J = 0. A more restrictive symmetry is the one describable in the Russell-Saunders coupling scheme by S = L = 0. This holds in a J=0 configuration if there is invariance also under inversion of intrinsic spins. Invariance of the nucleon-nucleon interaction

under spin reflections requires the absence of the spin-vector component, namely the two-body spin-orbit interaction $\propto \vec{\ell}_{12}\cdot(\vec{s}_1+\vec{s}_2)$ where $\vec{\ell}_{12}$ is the relative orbital angular momentum. While this component is appreciable in the modern "realistic" phenomenological interactions and contributes most of the spin-orbit splitting in SCF calculations, it is not very important for the spin-averaged properties of nuclear states. Consequently, it is instructive to consider model interactions which lack the spin-vector term.

In a Russell-Saunders L=S=J=0 configuration there is only one radial wave function for each ℓ. If we choose to use the j-j coupling scheme, there are in general two radial wave functions, one for each $j(j_{\pm}=\ell\pm 1/2)$. For S = 0 the configuration must have both J-shells filled or both empty because a "spin-unsaturated" configuration, with only one j-subshell filled, does not have a definite intrinsic spin. For example, a $p_{1/2}$ shell has probability 2/3 for S = 1 and 1/2 for S = 0. Moreover, in agreement with the description in Russell-Saunders coupling, the radial wave functions of the two j-subshells must be the same in order that the closed ℓ-shell configuration have S = 0. To continue the example, in a closed p-shell we find

$$\langle (p_{3/2})^4 (p_{1/2})^2 | \vec{S}\cdot\vec{S} | (p_{3/2})^4 (p_{1/2})^2 \rangle = \frac{8}{3}\left[1 - (R_-|R_+)^2\right] \qquad (2.5)$$

where R_- and R_+ are the normalized radial wave functions for the $p_{1/2}$ and $p_{3/2}$ subshells, respectively. If these radial functions are the same, S = 0; otherwise there is a mixture of S values and of L values in the closed ℓ-shell. Thus, the usual terminology, "spin saturated configuration", is strictly applicable to a closed ℓ-shell configuration only in

the absence of a one-body spin-orbit term in the s.p. potential. This is the term which leads to differences in the radial wave functions and the energies of the j-subshells. As a shorthand we may refer to the situation in which the s.p. spin-orbit potential is absent as that of j-degeneracy.

The possible contribution of the tensor interaction $\propto [(\vec{s}_1\cdot\vec{r}_{12})(\vec{s}_2\cdot\vec{r}_{12}) - \frac{1}{3}(\vec{s}_1\cdot\vec{s}_2)]$ to spin-orbit splittings has been of interest for over twenty years. More recently quadratic spin-orbit terms also have been found necessary in realistic interactions. It is important to realize that in HF theory these interactions of even rank (k = 0 and 2) as spin-tensors do not break the self-consistency of j-degeneracy. Only the spin-vector (k=1) component can break the symmetry (Lande and Svenne[10]). On the other hand, once the symmetry is broken, so that the $R_{\pm}$ wave functions are different, then the even-rank components can contribute to the spin-orbit potential.

In Brueckner theory the k=2 components of the bare interaction do contribute to the k=1 component of the reaction matrix. But the effect is rather weak (Landé-Svenne[10]), primarily because there is no contribution in relative s-states. Thus, in BHF and RBHF the spin-orbit splitting in closed ℓ-shell configurations still arises predominantly from the two-body spin-orbit interaction.

In the case of j-degeneracy let us define an interchange operation which transforms the orbitals (j_+,m) and (j_-,m) into each other for $|m| \leq \ell-1/2$. The distinction number for spin-orbit partners is simply $d_j = (-)^{j-\ell-1/2}$. An explicit interchange operator can be constructed as follows: The spin-angle wave functions for the ℓ-shell are the spinor spherical harmonics

$$\mathcal{Y}_{\pm}^{m} \equiv \sum_{\sigma} C\begin{pmatrix} \ell & 1/2 & \ell\pm 1/2 \\ m-\sigma & \sigma & m \end{pmatrix} Y_{\ell}^{m-\sigma} \chi_{1/2}^{\sigma}. \tag{2.6}$$

We make use of a Regge symmetry of the Clebsch-Gordan coefficients relating $C\begin{pmatrix} j_1 & j_2 & j_1+j_2 \\ m\mp j_2 & \pm j_2 & m \end{pmatrix}$ and $C\begin{pmatrix} j_1 & j_2 & j_1-j_2 \\ m\pm j_2 & \mp j_2 & m \end{pmatrix}$ for $|m| \leq j_1-j_2$, which reduces in the spin-orbit case to

$$C\begin{pmatrix} \ell & 1/2 & \ell+1/2 \\ m-\sigma & \sigma & m \end{pmatrix} = (-)^{\sigma-1/2} C\begin{pmatrix} \ell & 1/2 & \ell-1/2 \\ m+\sigma & -\sigma & m \end{pmatrix}. \tag{2.7}$$

One finds that

$$S \equiv (\ell_+ s_- - \ell_- s_+) \left[(\ell+1/2)^2 - j_z^2\right]^{-1/2} \tag{2.8}$$

where $\ell_\pm$ and $s_\pm$ are raising and lowering operators, satisfies

$$S[R_\pm(r)\mathcal{Y}_{\pm}^{m}] = \pm [R_\pm(r)\mathcal{Y}_{\mp}^{m}], \qquad |m| \leq \ell-1/2. \tag{2.9}$$

As remarked above, the radial wave functions of the j-subshells must be the same in order to have j-degeneracy, in which case S is the desired j-interchange operator.*

---

*As defined in eq. (2.8) S annihilates the orbitals with $m = \pm(\ell+1/2)$. In order not to have a singular operator, one can redefine S to act as the identity on the orbitals with $|m| = \ell+1/2$ by adding

$$\delta_{j_z,\ell+1/2} + \delta_{j_z,-\ell-1/2} = \prod_{m=-\ell-1/2}^{\ell-1/2} (j_z-m)/(\ell+1/2-m)$$

$$+ \prod_{m=-\ell+1/2}^{\ell+1/2} (j_z-m)/(-\ell-1/2-m).$$

Clearly, S does not commute with the rotations, though the j-distinction operator does.

2.2. SYMMETRY BREAKING

In calculations for which a transformation S cannot be a self-consistent symmetry (either because of the choice of nucleus, nuclear configuration, or nuclear interaction), an unrestricted SCF calculation would contain no reference to the transformation S. There would be more degrees of freedom in the s.p. orbitals than for the case in which S is a self-consistent symmetry. Sometimes the SCF theory for such "unsymmetrical" cases is approximated by artificially imposing the symmetry through the use of a symmetry-restricted SCF procedure.

Consider, for example, a nucleus with $A = A_o+1$ where $A_o = 2N_o = 4n$. One can start the iterations with a trial configuration specified in terms of orbitals with the symmetries of the nucleus A_o, e.g. the self-consistent orbitals or, less accurately, those of an oscillator shell model (spherical or deformed, depending on the nucleus). To impose the symmetry artificially one can put half of the "last" nucleon in each of the two lowest, previously unoccupied, degenerate orbitals.* Because the addition of a nucleon violates both time-reversal invariance and charge-independence, the situation is actually a little more complicated than described: if nucleus A_o is axially symmetric, one would put one-fourth nucleon in each of the four degenerate states $(\pm\Omega, \pm\tau)$. If this "averaging over configurations" is done at each iteration, there is an exact four-fold degeneracy among the final self-consistent "valence"

*This is a very simple case of a symmetry-restricted SCF theory for open shell systems employing fractional occupancies for the open shells, which was initiated by Hartree and improved by Roothaan[32], whose method has been extended to the general case of several open shells[33]. This approach has been applied to nuclei in a few papers, e.g. Davies, et al.[15,17].

orbitals. One finally constructs four determinants each containing a different one of the valence orbitals. Another example of imposing a symmetry is that of an isoscalar-restricted HF Hamiltonian for nuclei with a general neutron excess[34]. Because no inversion occurs, we are not concerned in this paper with symmetry-restricted SCF theories. We may note that the existence of several degenerate determinants (not orbitals) indicates a failure to take into account deformations or other kinds of correlation which would appear if the degenerate configurations were allowed to mix.

A relatively mild loss of symmetry occurs when a symmetry group is only partially broken, a subgroup remaining as a self-consistent symmetry. More generally, consider the case in which the symmetry S is broken but the distinction symmetry, S_D, is still a self-consistent symmetry, so one does not have to allow mixing of orbitals of opposite distinctions. That is, in the case of ellipsoidal symmetry without time-reversal invariance one still does not mix states with opposite values of $(-)^{\Omega-1/2}$; with the breaking of charge independence by $N \neq Z$ and/or isovector Coulomb interactions one can still employ orbitals of definite isospin projection (n or p); and in spherical configurations one still requires invariance under combined rotations in space and spin space and does not mix $j = \ell + 1/2$ and $j = \ell - 1/2$. However, since the manifold of occupied s.p. states is no longer invariant under the interchange transformation S, the partner of an occupied orbital is not necessarily occupied.

Moreover, the partner under S of a self-consistent orbital is not self-consistent in general, though it usually will be similar to a self-consistent orbital. For example, consider again the case of a nucleus

$A = 4n+1$ in which the initial trial determinant is constructed of self-consistent orbitals of the self-conjugate nucleus A-1. The "last" nucleon goes into a "valence" state of definite $d_{\mathcal{J}} = (-)^{\Omega-1/2}$ and $d_q = (-)^{\tau-1/2}$. Its partner under time reversal has the opposite sign of $d_{\mathcal{J}}$ and is not occupied. Its partner under n-p interchange has the opposite sign of d_q and is not occupied. These zeroth-iteration partner states are self-consistent orbitals in the field of nucleus A-1 (= 4n), but in succeeding iterations the partners of the valence orbital fail to be eigenfunctions of the s.p. Hamiltonian of nucleus A.

It is in these situations with partial symmetry breaking that the problem of level inversion occurs. When one of the pair of "formerly" degenerate levels is occupied, the other (unoccupied one) usually comes lower in energy[11-14,24]. We discuss in the next section some representative HF and RBHF calculations which give a level inversion.

3. Samples of calculated level inversions

3.1. j-INVERSION IN SPIN-UNSATURATED SPHERICAL CONFIGURATIONS OF N=Z NUCLEI

In BHF and RBHF calculations[13,14] of ^{12}C, ^{28}Si, and ^{32}S with the Hamada-Johnston interaction[35] and in Rouben and Saunier's HF calculation[12] of ^{56}Ni with the Saunier-Pearson[36] effective interaction SP2 the s.p. energy of the unoccupied neutron $(\ell-1/2)$-subshell is lower than that of the occupied $(\ell+1/2)$-subshell (see table 1), and similarly for the corresponding proton states. Spin-orbit forces have been included, so the breaking of j-degeneracy arises both from the spin-unsaturation and from the spin-and-orbit-dependent interactions.

3.2. n-p INVERSION IN NUCLEI WITH A NEUTRON EXCESS; CASE OF A SPIN-UNSATURATED SPHERICAL CONFIGURATION

Figure 1 shows the results of a HF calculation[37] for ^{48}Ca (and of ^{40}Ca for comparison) in which the Coulomb interaction has been left out. The two-term separable nuclear interaction of Tabakin, as modified by Clement and Baranger[38], was used. One sees that each proton level lies lower than the corresponding neutron level. In particular, the unoccupied proton $f_{7/2}$ level is below the occupied neutron $f_{7/2}$ level. Unlike a breaking of time-reversal invariance, an n-p level inversion does not give rise to an apparent inconsistency with the prescription to occupy the lowest levels: because of the conservation of N and Z it is consistent to fill the lowest neutron and proton levels separately. However, the inclusion of the Coulomb force in the calculation raises the proton levels about even with the neutron levels and obviates the problem.

3.3. INVERSIONS OR REDUCED NORMAL SPLITTINGS IN ODD NUCLEI WITH ONE PARTICLE OR HOLE RELATIVE TO A SPHERICAL CORE

Very little work on odd nuclei has appeared in the literature, and in the few published results[30,29,24] little or nothing was said about how the breaking of time-reversal invariance was actually handled. But generally the unoccupied partner lies lower, and the usual prescription to occupy the A lowest-lying s.p. states leads to an oscillation of occupancy from iteration to iteration (see sect. 1).

A renormalized Brueckner calculation of single-hole states in ^{15}O and ^{15}N calculated with the Hamada-Johnston interaction and pure oscillator s.p. wave functions was reported in ref. 29. We have reproduced, as fig. 2a here, fig. 1 of ref. 29 and have accompanied it by a similar figure[39] for ^{16}O plus one particle, fig. 2b. These figures show in the

right-hand column the RBHF energies of s.p. states normally occupied in ^{16}O. The other columns show the corresponding energies in the nuclei in which a single neutron or a single proton has been removed from (fig. 2a) or added to (fig. 2b) specific orbitals. Each column of the figure corresponds to a particular valence orbital. The shells in ^{16}O are split in the nuclei with A = 15 or 17 because the presence of a valence "particle" or hole with a specific magnetic quantum number, m_v, implies a non-spherical term in the s.p. potential and an m-dependence in the s.p. energies. The individual s.p. energies are not shown; instead the broadened shells are indicated by rectangles, the length of the rectangle representing the spread.

One notes three things here: (i) that each (unoccupied) hole level, represented by a circle in fig. 2a (its energy does not depend on m_v), invariably lies below the filled states of the same shell with $m \neq m_v$. For example in ^{15}N with a proton missing from the $0p_{1/2}$ shell (see the third to last column), the s.p. energy of the hole (circle) is more negative than the s.p. energy of the other (occupied) proton $0p_{1/2}$ state (shaded square); (ii) that when the hole is a neutron the occupied proton states are raised relative to the neutron ones, and vice versa; similarly, when the "particle" is a neutron the proton states are lowered relative to the neutron ones, and vice versa; and (iii) that the spin-orbit splitting of the 0p levels is reduced by a valence hole in the $0p_{1/2}$ shell or a "particle" in the $0d_{5/2}$ shell. Thus, fig. 2 illustrates the tendency toward level inversion manifested in all three cases of partial symmetry breaking discussed in this paper, namely the breaking of time-reversal invariance when N or Z is odd, of charge independence when $N \neq Z$, and of intrinsic-spin independence when an ℓ-shell is not spin-saturated.

4. Origin of the effect

The HF equation can be derived from the variational principle[40]

$$\delta[\langle\Psi|H|\Psi\rangle - \eta\langle\Psi|\Psi\rangle] = 0 \tag{4.1}$$

where H is the full Hamiltonian (2.1) and Ψ is a Slater determinant of s.p. wave functions ψ_λ. The variational principle is satisfied when the ψ_λ are eigenstates of the HF s.p. Hamiltonian h, given by

$$h \equiv T + U \tag{4.2}$$

where the HF s.p. potential U is defined in an arbitrary basis $\{|a\rangle,|b\rangle,\ldots\}$ in terms of the self-consistent occupied s.p. states λ by

$$\langle a|U_{HF}|b\rangle = \sum_{\lambda}^{occ} \langle a\lambda|v|b\lambda\rangle_A. \tag{4.3}$$

The matrix elements of the interaction are antisymmetrized, as indicated by the subscript A. The BHF equations are quite similar except that the two-body matrix elements of the interaction v are replaced by those of the two-body Brueckner reaction matrix (see e.g. ref. 19)

$$G(E_s) = v + v \frac{Q}{E_s - h_{12}^R} G(E_s). \tag{4.4}$$

Here the "Pauli operator", Q, is a projection operator which excludes normally occupied s.p. states from appearing in the intermediate pair states, h_{12}^R is an unperturbed (reference) pair Hamiltonian

$$h_{12}^R = h^R(1) + h^R(2) \tag{4.5}$$

where h^R is the reference s.p. Hamiltonian for normally empty s.p. states, and E_s is the energy available to the pair ("starting energy"). The BHF potential energy of a normally occupied s.p. state λ is

$$\langle\lambda|U_{BHF}|\lambda\rangle = \sum_{\lambda'}^{occ} \langle\lambda\lambda'|G(\varepsilon_\lambda+\varepsilon'_\lambda)|\lambda\lambda'\rangle. \tag{4.3a}$$

The RBHF equations[4,22)]* differ from the BHF equations only in that the

*The RBHF approximation referred to here is closely related to the lowest self-consistent truncation of the generalized-time-ordered version of the Brueckner-Goldstone expansion discussed by Brandow[41)]. A somewhat different RBHF approximation results from the lowest truncation of the extended-generalized-time-ordered series[42)]. The remarks of the present paper hold also for this second RBHF approximation.

reaction matrix element is multiplied by the "true" occupation probability of the normally occupied state with which an interaction is taking place, P_λ. That is,

$$\langle a|U_{RBHF}|b\rangle = \sum_{\lambda}^{occ} \langle a\lambda|G(E_s)|b\lambda\rangle\, P_\lambda. \tag{4.3b}$$

The fractional occupation probabilities can be calculated, in the RBHF approximation, by a finite set of algebraic equations involving only the normally occupied states[4)]. The coefficients in these equations can be expressed either in terms of Bethe-Goldstone defect functions[4)] or, more conveniently for rapid numerical calculations, in terms of the energy derivative of the reaction matrix[41,43)].

We now consider the inversion problem by relating the nucleus A, for which there is an inversion, to that nucleus, A_o, nearest to it in the periodic table for which there is no symmetry breaking. For the latter nucleus the occupied states, labeled by λ, will be called core states.

Each s.p. level of nucleus A_o, whether occupied or not, is two-fold degenerate with respect to the distinction quantum number $d = \pm 1$. In considering nucleus A we shall be concerned with the s.p. states corresponding to those in A_o of a particular two-fold degenerate level, $\zeta = (z,d)$. The main effect producing the splitting of this level in nucleus A is the change in potential energy resulting from the changed occupancy. This effect appears in first order perturbation theory, as well as in higher orders. The change in the s.p. wave functions, on the other hand, does not affect the energy splitting in first order, but does contribute in second and higher orders. The first-order effect is expected to dominate.*

*If it does not, there is a great deal of "core polarization" in A and the relevance of the self-consistent symmetry in A_o to the nucleus A is rather tenuous.

Consequently, we shall give a discussion of the splitting based on employing the orbitals of nucleus A_o. Some comments on the effects of distortion of the orbitals are given in sect. 5.

4.1. ODD NUCLEI, $A = A_o \pm 1$

If partial occupancy occurs only for one degenerate pair, one can choose the unperturbed core states to be the filled states either of nucleus A+1 or of A-1. Consider first the description in terms of a core A_o = A-1 and a valence "particle". Let us assume that only the d=+ member of the pair of states $\zeta = (z,d=\pm)$ is occupied. The s.p. energies are

$$\varepsilon_\zeta = \langle\zeta|T|\zeta\rangle + \langle\zeta|U|\zeta\rangle. \tag{4.6}$$

If the wave functions are those of the nucleus A_o, the kinetic energy is independent of the distinction number, d, i.e. $\langle\zeta|T|\zeta\rangle = \langle z|T|z\rangle$.

However, the potential energy reflects the occupancy of $(z,+)$. In the HF theory

$$\langle\zeta|U|\zeta\rangle = \sum_{\lambda}^{\text{core}} \langle\zeta,\lambda|v|\zeta,\lambda\rangle_A + \langle\zeta,z+|v|\zeta,z+\rangle_A. \tag{4.7}$$

The first term is independent of d, since the degeneracy in the orbitals λ is summed over, so we can write

$$\varepsilon_\zeta = \varepsilon_z^{(o)} + \langle\zeta,z+|v|\zeta,z+\rangle_A \tag{4.8a}$$

with

$$\varepsilon_z^{(o)} = \langle z|T|z\rangle + \sum_{\lambda}^{\text{core}} \langle\zeta,\lambda|v|\zeta,\lambda\rangle_A. \tag{4.8b}$$

Now look at the s.p. energies of the two states ζ:

$$\varepsilon_{z+} = \varepsilon_z^{(o)} + \langle z+,z+|v|z+,z+\rangle_A = \varepsilon_z^{(o)} \tag{4.9a}$$

$$\varepsilon_{z-} = \varepsilon_z^{(o)} + \langle z-,z+|v|z-,z+\rangle_A \equiv \varepsilon_z^{(o)} + v_{-+}. \tag{4.9b}$$

In the first equation the matrix element $\langle z+,z+|v|z+,z+\rangle_A$ is identically zero since it is antisymmetrized. However, in the second equation the matrix element, which we have called v_{-+} for simplicity, is non-zero.

Thus, the degeneracy of the completely empty level z in nucleus A_o is broken when the level is half filled in nucleus A_o+1 because the energy of the unoccupied sublevel contains a mutual interaction energy with the occupied state, while the occupied state does not have a corresponding interaction with itself. That is, a test particle in the "unoccupied" state (z,-) experiences one more interaction than does the nucleon in the occupied state (z,+).

Consider next the description in terms of a core $A_o = A+1$ and a "valence hole". In this case also, as in the "particle" description we have the result

$$\varepsilon_{z-} - \varepsilon_{z+} = v_{-+}. \tag{4.10}$$

An inversion,

$$\varepsilon_{z-}(\text{unoccupied}) < \varepsilon_{z+}(\text{occupied}) \tag{4.11}$$

occurs if $v_{-+} < 0$. In the cases we have examined v_{-+} is always negative. For example, table 2 gives values of v_{-+} in the 0p and 1s-0d shells of the spherical harmonic oscillator basis for four effective interactions. These interactions were constructed in quite different ways and, taken together, pretty well sample the range of possibilities allowable for a successful shell model effective interaction in these two major shells. Because the addition or removal of a nucleon breaks both time-reversal invariance and charge-independence, there are two sets of matrix elements to be considered, those involving states differing in the distinction number d_τ and those differing in d_q.

From table 2 one sees in the case of the Tabakin interaction that if the $0d_{5/2}$ neutron state with m = 3/2 is occupied, then the $0d_{5/2}$ neutron state with m = -3/2 lies lower, if unoccupied, by about 0.6 MeV, and the $0d_{5/2}$, m = 3/2 proton state, if unoccupied, lies lower by about 1.9 MeV in the absence of Coulomb interactions. In the case of the Saunier-Pearson interaction cited in table 2, one sees that if the $0p_{3/2}$ proton state with m = 3/2 is emptied, then its s.p. energy is about 2.9 MeV below the occupied $0p_{3/2}$ proton state with m = -3/2 and about 3.4 MeV

below the occupied $0p_{3/2}$, m = 3/2 neutron state (in the absence of Coulomb interactions). Similar results for one 0s or 0p hole in the ^{16}O core have been shown in fig. 2a, which was calculated from the Hamada-Johnston interaction, the appropriate reaction matrix elements (G_{-+}) of which, times the "true" occupation probability P_{z+}, are given in table 2 also.

It is fairly easy to understand that v_{-+} should be negative in the time-reversal case, since it is precisely these matrix elements coupled to J = 0 that are the pairing interaction, which is known to be strongly attractive. Likewise, the neutron-proton force is known to be largely attractive, but it is not clear why all n-p matrix elements cited in table 2 should turn out to be attractive.

These considerations apply also to deformed odd nuclei. For axially symmetric configurations one replaces m by Ω, the magnetic quantum number in a body-fixed coordinate system. In tri-axial ellipsoidal configurations the distinction number $d_{\tilde{z}} = \langle (-)^{j_z, -1/2} \rangle$ is still appropriate for labeling the time-reversed partners (see sect. 2).

4.2. SPIN-UNSATURATED SPHERICAL NUCLEI

The spin-orbit case has to be discussed separately because it involves a sum over the magnetic quantum number, m. We consider first the nuclei for which a $j=\ell+1/2$ subshell is filled both by neutrons and protons and the $j=\ell-1/2$ subshell is completely empty (see sects. 1 and 3.1). If we neglect the Coulomb interaction and the difference in radial wave functions of the j-subshells, it will suffice to generalize the previous notation only to the extent of writing $\zeta = (z,j,m,\tau)$, where we prefer to use j in place of the distinction number $d_j = 2(j-\ell) = (-)^{j-\ell-1/2}$. Then eqs. (4.6) and (4.7), generalized to the RBHF theory, are replaced by

$$\varepsilon_{zjm\tau} = \langle z|T|z\rangle + \sum_{\lambda}^{\text{core}} \langle zjm\tau,\lambda|G|zjm\tau,\lambda\rangle_A \, P_\lambda$$

$$+ \sum_{\tau'=-1/2}^{1/2} \sum_{m'=-(\ell+1/2)}^{\ell+1/2} \langle zjm\tau, z(\ell+1/2)m'\tau'|G|zjm\tau, z(\ell+1/2)m'\tau'\rangle_A \, P_{z,\ell+1/2}$$

$$\equiv \varepsilon_{zj}^{(o)} + U_{zj}(z,\ell+1/2) \tag{4.12a}$$

in which $\varepsilon_{zj}^{(o)}$ consists of the first two terms of eq. (4.12a) and is independent of m and τ after summing over the closed-core shells λ. The sums in the last term can be evaluated to give

$$U_{zj}(z,\ell+1/2) = \frac{1}{2(2j+1)} \sum_{TJ} (2T+1)(2J+1)[1+\delta_{j,\ell+1/2}]$$

$$\times \langle zj, z(\ell+1/2|^{J,T}G|zj, z(\ell+1/2)\rangle_A \, P_{z,\ell+1/2} \tag{4.12b}$$

which also is independent of m and τ.* The potential energy of interaction

*Here the (J,T)-coupled matrix elements are with respect to normalized antisymmetrical pair states. An element $\langle n_1\ell_1 j_1, n_2\ell_2 j_2|^{J,T}G|n_3\ell_3 j_3, n_4\ell_4 j_4\rangle$ contains a factor $\left[1 + \delta^{n_1\ell_1 j_1}_{n_2\ell_2 j_2}\right]^{-1/2} \left[1 + \delta^{n_3\ell_3 j_3}_{n_4\ell_4 j_4}\right]^{-1/2}$. In eq. (4.12b) this factor is canceled by the explicit factor $[1 + \delta_{j,\ell+1/2}]$.

with the spin-saturated core levels λ depends on j, giving a splitting of normal sign

$$\Delta_z^{\text{core}} \equiv \varepsilon_{z,\ell-1/2}^{(o)} - \varepsilon_{z,\ell+1/2}^{(o)} > 0 \tag{4.13}$$

as in eq. (1c). If there is no effective two-body spin-orbit force, the

first-order splitting from interactions with the core, Δ_z^{core}, vanishes[10]. But with realistic forces, RBHF calculations[4,21,22] give the large splittings that are seen experimentally in the regions near ^{4}He, ^{16}O, and ^{40}Ca and that are assumed in the Mayer-Jensen shell model. By adding the "abnormal" contribution to the splitting from the interaction with the $(z,\ell+1/2)$ subshell (see eq. (1b))

$$\Delta_z^{unsat} \equiv U_{z,\ell-1/2}\ (z,\ell+1/2) - U_{z,\ell+1/2}\ (z,\ell+1/2) < 0 \tag{4.14}$$

one obtains

$$\Delta\varepsilon_z \equiv \varepsilon_{z,\ell-1/2} - \varepsilon_{z,\ell+1/2} = \Delta_z^{core} + \Delta_z^{unsat}. \tag{4.15}$$

There is an inversion of the spin-orbit partners, to first order, if

$$\Delta_z^{core} < |\Delta_z^{unsat}|. \tag{4.16}$$

In table 3 the matrix elements $U_{zj}(z,\ell+1/2)$ in the 0p and 0d shells are given. One sees that Δ_z^{unsat} is negative and of five to ten MeV in magnitude. This is sufficient to overcome the normal "core" splitting and give a spin-orbit inversion in calculations for the spherical configurations of ^{12}C, ^{28}Si, ^{32}S and ^{56}Ni, as we have seen in table 1.

The equations of the previous paragraph are easily generalized to nuclei with a neutron excess. With neglect of Coulomb interactions and differences in s.p. wave functions of the j-subshells, we have for a configuration like that of the ground state of ^{48}Ca or ^{90}Zr with only one spin-unsaturated neutron shell, in the RBHF theory

$$\epsilon_{zjm\tau} = \langle z|T|z\rangle + \sum_{\lambda}^{\text{core}} \langle zjm\tau,\lambda|v|zjm\tau,\lambda\rangle_A \, P_\lambda$$

$$+ \sum_{m'=-(\ell+1/2)}^{\ell+1/2} \langle zjm\tau,z(\ell+1/2)m'1/2|v|zjm\tau,z(\ell+1/2)m'1/2\rangle_A \, P_{z,\ell+1/2}$$

$$\equiv \epsilon^{(o)}_{zj} + U_{zj\tau}(z,\ell+1/2,1/2) \tag{4.17a}$$

where

$$U_{zj\tau}(z,\ell+1/2,1/2) = \frac{1}{2(2j+1)} \sum_{T,J} [\delta_{\tau,-1/2} + 2\delta_{\tau,1/2}\,\delta_{T,1}](2J+1)$$

$$\cdot [1 + \delta_{j,\ell+1/2}] \langle zj,z(\ell+1/2)|^{J,T}G|zj,z(\ell+1/2)\rangle_A \, P_{z,\ell+1/2}. \tag{4.17b}$$

Values of $U_{zj\tau}(z,\ell+1/2,1/2)$ in the 0p and 0d shells are given in table 3. Neutron-proton splittings as well as spin-orbit splittings are tabulated. The "abnormal" spin-orbit splitting from interactions with the unsaturated shell is reduced by roughly one half because of the absence of protons in that shell. Thus, calculations for ^{48}Ca do not exhibit inversions of the 0p, 0d, or 0f spin-orbit doublets, although the normal splittings are smaller in magnitude[10,12,37] than in ^{40}Ca.

Equation (4.17) can be generalized to more complicated configurations by including a term U for each spin-unsaturated shell. The s.p. levels in ^{60}Ni, which has three spin-unsaturated ℓ-shells (the neutron and proton 0f shell and the neutron 1p shell), should show a particularly great tendency toward spin-orbit inversion. However, because other levels are nearby, configuration mixing should be important, and the HF determinant is probably not a very good model ground state. Configuration mixing is minimized for ground states of nuclei in which N and Z are

"magic numbers". Beyond ^{56}Ni only $^{208}_{82}Pb_{126}$ qualifies. But for such a heavy nucleus there are many more spin-saturated core levels; their "normal" contributions to the spin-orbit splitting may overcome the "abnormal" contributions from the $i_{13/2}$ neutron shell and the $h_{11/2}$ proton shell.* Thus, spin-orbit inversions appear to be limited to fairly light spherical nuclei.

*See, however, the inversion of the $h_{9/2}$-$h_{11/2}$ doublet produced by the interaction[36] SP2 in the calculation of Rouben and Saunier[12], table 4, second last column.

5. Interpretation

One way of overcoming the inversion problem would be to allow breaking of the distinction symmetry, S_D, as well as the interchange symmetry, S. However, in all of the three cases discussed here this complete symmetry breaking considerably increases the labor of the calculation.** When time-reversal invariance is broken, the proposal would imply breaking also axial or ellipsoidal symmetry by allowing components with even values of Ω-1/2 to mix with odd ones in the expansion of the self-consistent orbitals. The mixing coefficients would then not only double in number because of the additional mixing, but also would be complex because of the breaking of time-reversal invariance, a four-fold increase in difficulty. If charge-independence is partially broken, the "complete breaking" proposal implies giving up charge conservation by

**In some cases, however, breaking S_D may be preferable to other methods of achieving a sufficiently accurate description of the nuclear state (see sect. 6).

mixing neutron and proton components in the self-consistent orbitals, thereby producing solutions in which Z and N are not good quantum numbers. One is no longer dealing with a particular nuclide unless states of good T_3 are projected from the self-consistent determinant. For spherical nuclei with spin-unsaturated shells, complete symmetry breaking would imply mixing components with $j = \ell + 1/2$ and $\ell - 1/2$ for $|m| \leq \ell - 1/2$. This would destroy rotational invariance, which could be restored only by projecting states of $J = 0$. Since the deformed ℓ-shell could polarize the core, it probably would be preferable to allow all shells to deform, as in a conventional deformed SCF calculation.

Instead we consider retention of the distinction symmetry in the s.p. wave functions, and justify the intrusion of unoccupied levels below occupied ones in the spectrum of the SCF Hamiltonian. The fact is, the SCF equations per se have nothing to say about the interpretation of unoccupied levels. The equations demand merely that matrix elements of h between occupied and unoccupied levels be zero (Brillouin's theorem in the case of HF theory). The occupied states are the only ones entering into the definition of the SCF Hamiltonian and, hence, are the only ones involved in the self-consistency process. However, if the SCF equations are solved approximately by matrix diagonalization in a finite dimensional basis, some of the unoccupied orbitals are obtained as a bonus.

The question of which s.p. states should be filled in the SCF determinantal approximation to the ground state has a definite answer in HF theory, namely those A s.p. states which give the determinant having the lowest energy,

$$E = \langle\Psi|H|\Psi\rangle = \frac{1}{2}\sum_{\lambda}^{occ}\left[\langle\lambda|T|\lambda\rangle + \varepsilon_\lambda\right]$$

$$\varepsilon_\lambda = \langle\lambda|T+U|\lambda\rangle \tag{5.1}$$

$$\langle\lambda|U|\lambda\rangle = \sum_{\lambda'}^{occ}\langle\lambda\lambda'|v|\lambda\lambda'\rangle_A .$$

Suppose one has achieved self-consistency with a particular set of occupied orbitals (C_1) and wishes to investigate a slightly different configuration (C_2). One can start the iterations for C_2 with eigenfunctions of the s.p. Hamiltonian $h(C_1)$; at least one of the orbitals occupied in this approximation to C_2 is unoccupied in C_1. After iterating to self-consistency the orbitals occupied in C_2, which are eigenfunctions of $h(C_2)$, will differ slightly from those of $h(C_1)$. The differences between corresponding eigenfunctions of $h(C_1)$ and $h(C_2)$ are referred to as resulting from <u>orbital rearrangement</u>. The s.p. energies are changed also; the differences are called orbital-rearrangement energies. To the extent that the orbital rearrangement is negligible, the difference between the HF energy of $\Psi_1 \equiv \Psi(C_1)$ and of a configuration C_2 with only one "particle" and one "hole" relative to C_1 can be calculated easily. If we restrict the label λ to refer only to the "core states", those occupied both in Ψ_1 and Ψ_2, then $C_1 = (\{\lambda\},h)$ and $C_2 = (\{\lambda\},p)$. The HF energies of Ψ_1 and Ψ_2 are

$$E_1 = \sum_{\lambda}\langle\lambda|T|\lambda\rangle + \langle h|T|h\rangle + \frac{1}{2}\sum_{\lambda\lambda'}\langle\lambda\lambda'|v|\lambda\lambda'\rangle_A + \sum_{\lambda}\langle\lambda h|v|\lambda h\rangle_A \tag{5.2a}$$

and

$$E_2 = \sum_{\lambda}\langle\lambda|T|\lambda\rangle + \langle p|T|p\rangle + \frac{1}{2}\sum_{\lambda\lambda'}\langle\lambda\lambda'|v|\lambda\lambda'\rangle_A + \sum_{\lambda}\langle\lambda p|v|\lambda p\rangle_A \tag{5.2b}$$

so that

$$E_2 - E_1 = \langle p|T|p\rangle + \sum_{\lambda} \langle \lambda p|v|\lambda p\rangle_A - \epsilon_h$$
$$= \epsilon_p - \epsilon_h - \langle hp|v|hp\rangle_A \tag{5.3}$$

where the s.p. energy ϵ_p is that of state p as an unoccupied state in the SCF of state Ψ_1.

In the application to the inversion problem p = (z,-) and h = (z,+) (see sect. 4). Then by eq. (4.10c)

$$E_2 - E_1 = \epsilon_{z-} - \epsilon_{z+} - v_{-+} = 0. \tag{5.4}$$

Thus, these two configurations, which differ only in containing one or the other member ($d = \pm 1$) of a pair of valence orbitals almost connected by a (slightly broken) interchange symmetry, are degenerate.

The usual prescription, to fill those s.p. states having the lowest s.p. energies, follows from eq. (5.3) with the neglect of the particle-hole interaction term. But for the level-inversion problem it is this neglect which gives rise to the difficulty. The significance of the interaction term in eq. (5.3) can be understood in a different way as follows. First notice that, with neglect of orbital rearrangement corrections, the ϵ_p given by eq. (4.9b) is also the s.p. energy of state p in that configuration of nucleus A+1 in which p is a valence particle, because $\langle pp|v|pp\rangle_A = 0$. Next, notice that the s.p. energy of the state h in this same configuration ($\{\lambda\}$,h,p) of nucleus A+1 is

$$\epsilon_h^{(A+1)} = \epsilon_h + \langle hp|v|hp\rangle_A. \tag{5.5}$$

Thus,

$$E_2 - E_1 = \varepsilon_p^{(A+1)} - \varepsilon_h^{(A+1)}. \tag{5.6}$$

Consequently, the usual prescription for occupation of s.p. states should be modified slightly to refer to the s.p. energies in the configuration of the adjacent nucleus, A+1, in which both states p and h are occupied. This modification removes the inconsistency that in comparing s.p. energies in nucleus A, ε_p involves A interactions with other particles whereas ε_h involves only A-1 interactions (no self-energy). For the inversion problem

$$\varepsilon_{z+}^{(A+1)} = \varepsilon_z^{core} + v_{-+} = \varepsilon_{z-}^{(A+1)} \tag{5.7}$$

so that $E_2 - E_1 = 0$ as in eq. (5.4). In nucleus A+1 with both (z,-) and (z,+) occupied, the interchange transformation S is a self-consistent symmetry. This is the reason for the degeneracy in eq. (5.7). An alternative analysis can be carried out with reference to the nucleus A-1 with a hole in s.p. state h, again yielding for the inversion problem $E_2 - E_1 = 0$.

Similar considerations hold in the RBHF approximation, but not in the ordinary BHF approximation. The difference is related to the fact that in BHF theory the s.p. energies differ from the corresponding separation energies by large "Brueckner rearrangement energies" associated with the non-static nature of the effective interaction (the starting-energy dependence of the reaction matrix). The renormalization with occupation probabilities restores the connection between separation and s.p. energies, i.e. in RBHF theory there is an analogue[39] of Koopmans' theorem in HF theory. Now E_1 and E_2 can be written in terms of the

binding energy $E^{(A-1)}$ of the nucleus A-1, which provides the common core for configurations C_1 and C_2 of nucleus A, and the separation energies $\mathcal{E}_p$ and $\mathcal{E}_h$:

$$E_1 = E^{(A-1)} + \mathcal{E}_h \quad , \quad E_2 = E^{(A-1)} + \mathcal{E}_p \tag{5.8}$$

so that

$$E_2 - E_1 = \mathcal{E}_p - \mathcal{E}_h. \tag{5.9}$$

Then by the analogue of Koopmans' theorem in RBHF theory

$$E_2 - E_1 = \varepsilon_p^{(A-1)} - \varepsilon_h^{(A-1)} \tag{5.10}$$

just as in the HF approximation. For the inversion problem

(p = z-, h = z+)

$$\varepsilon_{z\pm}^{(A-1)} = \varepsilon_z^{core}. \tag{5.11}$$

so that E_1 and E_2 are degenerate.

The inversion-instability in the case of the breaking of time-reversal invariance in odd or odd-odd nuclei is avoided easily. The preceding discussion shows that there are two degenerate determinants. One can put the valence particle in a state of distinction d = + and leave it there from iteration to iteration even though the unoccupied partner with d = - has a lower s.p. energy in the nucleus A (but not, as we have seen, in nucleus A+1). The particle-hole excitation based on the d = + solution, obtained by "exciting" the d = + partner to the d = - level, does not lie lower in energy than the original configuration, but is degenerate with it, as shown by eq. (5.4). Each is an equally good HF ground state.

In the case of spin-unsaturated spherical shells let the neutron or proton subshell $(z,\ell+1/2,\tau)$ be filled and the neutron and proton subshells with $j = \ell-1/2$ be empty. Consider the energy of state $(z,\ell+1/2,m,\tau)$ in the configuration of nucleus A+1 in which there is a valence particle in state $(z,\ell-1/2,m',\tau)$. The extra interaction in $\varepsilon^{A+1}_{z,\ell+1/2,m,\tau}$ not contained in $\varepsilon^{A}_{z,\ell+1/2,\tau}$, namely

$$v^{\tau}_{m+,m'-} \equiv \langle z,\ell+1/2,m,\tau;\ z,\ell-1/2,m',\tau|v|z,\ell+1/2,m,\tau;\ z,\ell-1/2,m',\tau\rangle_A \qquad (5.12)$$

can give enough extra binding to make

$$\varepsilon^{A+1}_{z,\ell+1/2,m,\tau} < \varepsilon^{A+1}_{z,\ell-1/2,m',\tau} = \varepsilon^{A}_{z,\ell-1/2,\tau}. \qquad (5.13)$$

The dependence of these energies on m and m' is rather weak, so it is useful to average over m' in (5.12), obtaining an energy $\overline{v^{\tau}_{+-}}$ which is independent of m. This average interaction is expressible in terms of the s.p. potential of eq. (4.17b) (with $j_{\pm} \equiv \ell\pm1/2$) as

$$\overline{v^{\tau}_{+-}} = \frac{1}{(2j_-+1)}\, U_{zj_+\tau}(zj_-\tau) = \frac{1}{(2j_++1)}\, U_{zj_-\tau}(zj_+\tau) = \overline{v^{\tau}_{-+}} \qquad (5.14)$$

Here the second equality, which arises formally from eq. (4.17b) and a symmetry of the two-body matrix elements, states the fact that $(2j_++1)U_{zj_+\tau}(zj_-\tau)$ and $(2j_-+1)U_{zj_-\tau}(zj_+\tau)$ both represent the mutual interaction energy of the neutrons (or protons) in shell j_+ with those in j_-. If both neutrons and protons occupy the shell j_+, then we might average also over τ', obtaining

$$\overline{\overline{v_{+-}}} = \frac{1}{2(2j_-+1)}\left[U_{zj_+\tau}(z,j_-,\tau) + U_{aj_+\tau}(z,j_-,-\tau)\right] = \frac{1}{2(2j_++1)}\left[U_{zj_-\tau}(z,j_+,\tau)\right. \tag{5.15}$$

$$\left. + U_{zj_-\tau}(z,j_+,-\tau)\right] \equiv \frac{1}{2(2j_++1)}\, U_{zj_-}(zj_+) = \overline{\overline{v_{-+}}}.$$

In table 1 the row labeled $\varepsilon^{A+1}_{\ell+1/2}$ contains renormalized-Brueckner-approximation values of the s.p. energy of the shell $(n^\ell j_+)$ in the nucleus with A+1 nucleons when one nucleon is in the otherwise empty subshell $(n^\ell j_-)$. These energies were obtained with Brueckner self-consistency, i.e. the starting energies of the reaction matrix elements were self-consistent. The last row in table 1 gives the estimate of $\varepsilon^{A+1}_{\ell+1/2}$ obtained from eq. (5.15) and table 3. For ^{28}Si and ^{32}S the estimate of $\overline{\overline{v_{+-}}}$ is somewhat too large in magnitude because the oscillator range parameter b is too small. One sees that $\varepsilon^{A+1}_{\ell+1/2}$ is fairly well approximated and that

$$\Delta^{A+1}_\ell \equiv \varepsilon^{A+1}_{\ell-1/2} - \varepsilon^{A+1}_{\ell+1/2} \approx \Delta_\ell - \overline{\overline{v_{+-}}} \tag{5.16}$$

is of normal sign (> 0), so that the spin-orbit doublet is not inverted when properly treated. We expect this feature would be retained in calculations of higher dimensionality.

6. Inversions as signals of needed correlations

It was demonstrated in sect. 5 that two degenerate determinants arise from occupying one or the other partner of a degenerate pair of s.p. levels of nucleus A_o = A-1 and then iterating to self-consistency in the nucleus A. Although we have shown the inversion of s.p. levels to be unphysical, the existence of the degenerate determinants indicates

that the SCF description of the nuclear state in terms of either determinant alone will not be very accurate. The degeneracy indicates the need for a supplementary calculation in which the two determinants (actually four if both time-reversal and isospin invariance are broken simultaneously) are allowed to mix, thereby giving a state of lower energy with some correlations between the nucleons. A more accurate version of this would be a two (or four) dimensional mixed-configuration HF calculation, in which one diagonalizes H after each HF iteration.

An alternative way of lifting the degeneracy is to allow the distinction symmetry, S_D, to be broken,* leading to a more deformed self-

*See the beginning of sect. 5.

consistent field. Thus, deformations in the ground states of nuclei with spherical configurations having an inversion or near degeneracy of an occupied and an unoccupied level may be thought of as arising as a means of escaping the degeneracy. From the standpoint of the spherical basis, the projection of a state of good angular momentum from a non-spherical determinant contains configuration mixing and hence "correlations". The mixing leads to a state of lower symmetry. The deformed intrinsic s.p. levels have a greater energy gap at the Fermi surface. The appearance of an inversion or even a significant reduction of the normal spin-orbit splitting at the Fermi surface in spherical calculations provides a signal that a deformed solution of lower energy may exist. This is the case for ^{12}C, ^{28}Si and ^{32}S in table 1. Similarly an axially symmetric solution with an inversion or near degeneracy can deform to a lower-lying axially asymmetric solution with a large gap at the Fermi surface.

The authors gratefully acknowledge interesting discussions with Ron Cusson, Edith Halbert, and Paul (H. C.) Lee.

References

1) K. A. Brueckner and D. T. Goldman, Phys. Rev. 116 (1959) 424

2) J. W. Negele, Phys. Rev. C1 (1970) 1260

3) K. A. Brueckner, J. L. Gammel and H. Weitzner, Phys. Rev. 110 (1958) 431; R. J. Eden and V. J. Emery, Proc. Roy. Soc. (London) A248 (1958) 266

4) R. L. Becker, Phys. Rev. Letters 24 (1970) 400; Phys. Letters 32B (1970) 263; in The nuclear many-body problem, eds. F. Calogero and C. Ciofi Degli Atti, vol. 2 (Editrice Compositori, Bologna, 1974) paper III-10

5) N. N. Bogoliubov, Uspekhi Fiz. Nauk 67 (1959) 549 [Soviet Phys.-Uspekhi 67 (1959) 236]; Y. Nambu, Phys. Rev. 117 (1960) 648

6) M. Baranger, Phys. Rev. 122 (1961) 992; J. G. Valatin, Phys. Rev. 122 (1961) 1012

7) J. Bar-Touv and I. Kelson, Phys. Rev. 138 (1965) B1035; G. Ripka, in Fundamentals in nuclear theory, eds. A. deShalit and C. Villi (Intern. Atomic Energy Agency, Vienna, 1967) p. 623

8) M. Bouten and P. Van Leuven, Physica 34 (1967) 461

9) P. U. Sauer, Nuovo Cimento 57 (1968) 62; A. L. Goodman, G. L. Struble, J. Bar-Touv and A. Goswami, Phys. Rev. C2 (1970) 380

10) C. W. Wong, Nucl. Phys. A108 (1968) 481; A. Lande and J. P. Svenne, Nucl. Phys. A124 (1969) 241

11) M. K. Pal and A. P. Stamp, Phys. Rev. 158 (1967) 924; A. P. Stamp, Nucl. Phys. A105 (1967) 627

12) R. M. Tarbutton and K. T. R. Davies, Nucl. Phys. A120 (1968) 1; B. Rouben and G. Saunier, Phys. Rev. C5 (1972) 1223

13) R. L. Becker, R. C. Braley, W. F. Ford and M. R. Patterson, Oak Ridge National Laboratory Report, ORNL-TM-3951 (1972).

14) R. L. Becker and M. R. Patterson, to be published

15) A. K. Kerman, J. P. Svenne and F. M. H. Villars, Phys. Rev. 147 (1966) 710; K. T. R. Davies, S. J. Krieger and M. Baranger, Nucl. Phys. 84 (1966) 545; D. Vautherin and M. Veneroni, Phys. Letters 25B (1967) 175

16) J. Shao, W. H. Bassichis and E. L. Lomon, Phys. Rev. C6 (1972) 758

17) S. J. Krieger, M. Baranger and K. T. R. Davies, Phys. Letters 22 (1966) 607

18) J. Nemeth and D. Vautherin, Phys. Letters 32B (1970) 561; D. Vautherin and D. M. Brink, Phys. Rev. C5 (1972) 626; X. B. Campi and D. W. L. Sprung, Nucl. Phys. A194 (1972) 401; J. W. Ehlers and S. A. Moszkowski, Phys. Rev. C6 (1972) 217; G. Fai and J. Nemeth, Nucl. Phys. A208 (1973) 463

19) R. L. Becker, A. D. MacKellar and B. M. Morris, Phys. Rev. 174 (1968) 1264; J. M. Irvine, Nucl. Phys. A120 (1968) 576

20) K. T. R. Davies, M. Baranger, R. M. Tarbutton and T. T. S. Kuo, Phys. Rev. 177 (1969) 1519

21) K. T. R. Davies and R. J. McCarthy, Phys. Rev. C4 (1971) 81

22) R. L. Becker, K. T. R. Davies and M. R. Patterson, Phys. Rev. C9 (1974) 1221

23) W. H. Bassichis, A. K. Kerman and J. P. Svenne, Phys. Rev. 160 (1967) 746; S. S. M. Wong, J. LeTourneaux, N. Quang-hoc and G. Saunier, Nucl. Phys. A137 (1969) 318; W. F. Ford and R. C. Braley, Nucl. Phys. A134 (1969) 265; W. F. Ford, R. C. Braley and J. Bar-Touv, Phys. Rev. C4 (1971) 2099

24) H. C. Lee and R. Y. Cusson, Ann. Phys. (N.Y.) 72 (1972) 353; private communication from H. C. Lee and from R. Y. Cusson

25) E. Boeker, Nucl. Phys. A91 (1967) 27; Y. Abgrall, G. Baron, E. Caurier and G. Monsegno, Nucl. Phys. A131 (1969) 609; S. J. Krieger, Phys. Rev. C1 (1970) 76

26) J. Zofka and G. Ripka, Nucl. Phys. A168 (1971) 65

27) W. F. Ford, R. C. Braley, R. L. Becker and M. R. Patterson, in The nuclear many-body problem, eds. F. Calogero and C. Ciofi Degli Atti, vol. 2 (Editrice Compositori, Bologna, 1974) paper III-11

28) D. Vautherin and M. Veneroni, Phys. Letters 29B (1969) 203; W. H. Bassichis and A. K. Kerman, Phys. Rev. C2 (1970) 1768; D. R. Tuerpe, W. H. Bassichis and A. K. Kerman, Nucl. Phys. A142 (1970) 49

29) R. L. Becker and M. R. Patterson, Nucl. Phys. A178 (1971) 88

30) M. R. Gunye, Nucl. Phys. 118 (1968) 174; ibid. A120 (1968) 691; ibid. A128 (1969) 457; Phys. Letters 37B (1971) 125

31) J. P. Svenne and R. L. Becker, Bull. Am. Phys. Soc. 17 (1972) 910; R. L. Becker and J. P. Svenne, to be published in Phys. Rev. C, Dec. 1975

32) C. C. J. Roothaan, Rev. Mod. Phys. 32 (1960) 179

33) S. Huzinaga, Phys. Rev. 120 (1960) 866; F. W. Birss and S. Fraga, J. Chem. Phys. 38 (1963) 2552

34) D. M. Brink and J. P. Svenne, Nucl. Phys. A154 (1970) 449

35) T. Hamada and I. D. Johnston, Nucl. Phys. 34 (1962) 383

36) G. Saunier and J. M. Pearson, Phys. Rev. C1 (1970) 1353

37) A. Lande and J. P. Svenne, Nucl. Phys. A164 (1971) 49

38) F. Tabakin, Ann. Phys. (N.Y.) 30 (1964) 51; D. M. Clement and E. U. Baranger, Nucl. Phys. A108 (1968) 27

39) R. L. Becker and M. R. Patterson, unpublished

40) V. Fock, Z. Physik 61 (1930) 126; J. C. Slater, Phys. Rev. 35 (1930) 210; F. Villars, Proc. Int. School of Physics "Enrico Fermi", Course XXIII, ed. V. F. Weisskopf (Academic Press, New York, 1963) p. 1

41) B. H. Brandow, Phys. Rev. 152 (1966) 863

42) R. W. Jones, F. Mohling and R. L. Becker, Nucl. Phys. A220 (1972) 45

43) R. J. McCarthy and K. T. R. Davies, Phys. Rev. C1 (1970) 1644

Figure Captions

Fig. 1. Single-particle levels in ^{40}Ca and ^{48}Ca, from the Hartree-Fock calculation of ref. 37. The Tabakin[38] interaction was used, with no Coulomb interaction and an oscillator radius parameter b = 1.732 fm.

Fig. 2. Renormalized Brueckner single-particle levels in (a) A=15 and (b) A=17 isobars, from the RBHF calculation of ref. 29. The calculation used the Hamada-Johnston[35] interaction. See text for detailed discussion of these figures. The oscillator range parameter is b = 1.571 fm.

Table 1

Inversion of spin-orbit doublets in spin-unsaturated shells of spherical configurations of light N=Z nuclei as calculated in refs. 12-14. Single-neutron energies are given in MeV. (For ^{56}Ni the proton energies cited by Rouben and Saunier (RS)[12] have been converted by assuming a Coulomb displacement energy of 9.6 MeV.) The dimensionality D is the number of radial oscillator wave functions from which each SCF orbital was constructed. The oscillator range parameter $b = (\hbar/M\omega)^{1/2}$ is in fm. The energy $\varepsilon^{A+1}_{\ell+1/2}$ is the s.p. energy in the nucleus with A+1 nucleons (see sect. 5).

	RBHF				HF
	D = 2	D = 1			D = 4
	^{12}C	^{12}C	^{28}Si	^{32}S	^{56}Ni
reference	13	13	14	14	12(RS)
b	1.571	1.571	1.885	1.885	1.997
ℓ	1	1	2	2	3
$\varepsilon_{\ell+1/2}$	-13.2	-12.9	-12.0	-14.3	-12.5
$\varepsilon_{\ell-1/2}$	-13.6	-14.5	-13.4	-15.1	-15.2
Δ_ℓ	- 0.4	- 1.6	- 1.4	- 0.8	- 2.7
$\varepsilon^{A+1}_{\ell+1/2}$		-16.2		-15.3	
				b = 1.571	
Δ^{unsat}_ℓ (see table 3)		- 8.8	-11.4	-11.4	
$\Delta^{core}_\ell = \Delta_\ell - \Delta^{unsat}_\ell$		7.2	10.0	10.6	
$\overline{\overline{v_{+-}}}$, eq. (5.16)		- 3.0	- 2.5	- 2.5	
$\Delta^{A+1}_\ell = \Delta_\ell - \overline{\overline{v_{+-}}}$		1.4	1.1	1.7	
$\varepsilon_{\ell+1/2} + \overline{\overline{v_{+-}}}$		-15.9	-14.5	-16.8	

Table 2

Some examples of the matrix elements v_{-+} (in MeV) responsible for (m,-m) and (n,p) inversions in spherical shell model configurations of odd-A nuclei, associated with breaking time-reversal invariance and with partial breaking of charge independence. The first three interactions given here are taken, respectively, from F. Tabakin[38], G. Saunier and J. M. Pearson[36], and pp. 249-251 of J. M. Irvine, Nuclear Structure Theory (Pergamon Press, Oxford, 1972). The latter are obtained from phenomenological shell model calculations and consequently may not be very suitable for HF calculations. However, they are included here for comparison. The fourth effective interaction involves reaction matrix elements[29,39] of the Hamada-Johnston interaction[35] multiplied by the "true" occupation probability, P_{z+}, of the occupied partner state as prescribed in the RBHF approximation[4]. The range parameter $b = (\hbar/M\omega)^{1/2}$ of the spherical oscillator basis with respect to which the matrix elements are calculated is given in fm. The matrix elements depend strongly on b. The value 1.571 is more appropriate for the 0p states in nuclei with $12 \leq A \leq 16$ and 1.74 is more appropriate for states of the s-d shell in nuclei with $16 \leq A \leq 28$.

Interchange transformation and distinction number, d.	State $n\ell j$	label $\lvert m \rvert$	v_{-+} Tabakin b: 1.732	v_{-+} SP 1.752	v_{-+} Shell model 12<A<28	$G_{-+}P_{+}$ HJ 1.571
Time reversal $(-)^{m-1/2}$	0p3/2	1/2 or 3/2	-1.86	-2.86	-1.09	-2.09
	0p1/2	1/2	-0.10	-1.04	-0.28	-0.43
	0d5/2	1/2	-0.73	-0.78	-0.55	-1.27
	"	3/2	-0.56	-0.81	-0.44	-1.00
	"	5/2	-0.83	-0.76	-0.62	-1.44
	1s1/2	1/2	-2.15	-1.55	-1.14	-2.49
	0d3/2	1/2 or 3/2	0.20	0.03	-0.14	-0.65
n-p interchange $(-)^{\tau-1/2}$	0p3/2	1/2	-2.81	-2.48	-1.77	-3.76
	"	3/2	-3.89	-3.35	-2.12	-4.79
	0p1/2	1/2	-0.34	-1.53	-1.27	-2.61
	0d5/2	1/2	-1.65	-1.34	-1.24	-3.22
	"	3/2	-1.95	-1.59	-1.33	-3.47
	"	5/2	-2.84	-2.54	-1.75	-5.17
	1s1/2	1/2	-2.67	-2.88	-1.84	-5.20
	0d3/2	1/2	-0.30	-0.98	-1.06	-2.92
	"	3/2	-1.23	-1.63	-1.30	-4.05

Table 3

Contribution from interactions with the occupied $j=\ell+1/2$ subshell of a spin-unsaturated ℓ-shell (in MeV) to:

(1) $U_{zj\tau}(z,\ell+1/2,1/2)$, eq. (4.17b), or $U_{zj}(z,\ell+1/2)$, eq. (4.12b), a part of the single-particle potential energy of state $zj\tau$;

(2) $\Delta^{p-n}_{zj} = U_{z,j,-1/2}(z,\ell+1/2,1/2) - U_{z,j,1/2}(z,\ell+1/2,1/2)$, showing proton-neutron inversion produced by an excess neutron subshell;

(3) $\Delta^{n \text{ or } p}_{z} = U_{z,\ell-1/2,\tau}(z,\ell+1/2,1/2) - U_{z,\ell+1/2,\tau}(z,\ell+1/2,1/2)$, showing spin-orbit inversion produced by an excess neutron subshell;

(4) $\Delta_z = \sum_{\tau'=\pm 1/2} \left[U_{z,\ell-1/2,\tau}(z,\ell+1/2,\tau') - U_{z,\ell+1/2,\tau}(z,\ell+1/2,\tau')\right] = \Delta^n_z+\Delta^p_z$, showing spin-orbit inversion produced by a $j=\ell+1/2$ subshell containing both neutrons and protons. These spin-orbit splittings are denoted by Δ^{unsat} in the text; they are partially compensated by Δ^{core} (see table 1 and fig. 1). The four interactions used are the same as those of table 2.

Nucleus	Potential or Splitting	Interaction: Tabakin 1.732	SP 1.752	Shell Model 12<A<28	HJ 1.571
^{8}He	$U_{0p3/2n}(0p3/2n)$	- 4.03	- 6.21	- 2.38	- 3.47
	$U_{0p3/2p}(0p3/2n)$	- 9.72	- 9.84	- 5.83	-11.77
	$\Delta^{p-n}_{0p3/2}$	- 5.69	- 3.63	- 3.45	- 8.30
	$U_{0p1/2n}(0p3/2n)$	- 6.12	- 8.64	- 6.73	- 6.90
	$U_{0p1/2p}(0p3/2n)$	-12.19	-13.90	-13.77	-17.09
	$\Delta^{p-n}_{0p1/2}$	- 6.07	- 5.26	- 7.04	-10.19
	Δ^{n}_{0p}	- 2.09	- 2.43	- 4.35	- 3.43
	Δ^{p}_{0p}	- 2.47	- 4.06	- 7.94	- 5.32

Table 3 (Continued)

Nucleus	Potential or Splitting	Interaction: Tabakin 1.732	SP 1.752	Shell model 12<A<28	HJ 1.571
^{12}C	$U_{0p3/2}(0p3/2)$	-13.76	-16.05	- 8.22	-15.24
	$U_{0p1/2}(0p3/2)$	-18.32	-22.54	-20.50	-23.99
	Δ_{0p}	- 4.56	- 6.49	-12.28	- 8.75
^{22}O	$U_{0d5/2n}(0d5/2n)$	- 2.59	- 3.24	- 1.84	- 4.84
	$U_{0d5/2p}(0d5/2n)$	- 7.63	- 6.79	- 5.45	-14.40
	$\Delta^{p-n}_{0d5/2}$	- 5.04	- 3.55	- 3.61	- 9.56
	$U_{0d3/2n}(0d5/2n)$	- 5.68	- 7.42	- 6.63	- 8.17
	$U_{0d3/2p}(0d5/2n)$	-10.40	-11.63	-13.03	-22.50
	$\Delta^{p-n}_{0d3/2}$	- 4.72	- 4.21	- 6.40	-14.33
	Δ^{n}_{0d}	- 3.09	- 4.18	- 4.79	- 3.33
	Δ^{p}_{0d}	- 2.77	- 4.84	- 7.58	- 8.10
^{28}Si or	$U_{0d5/2}(0d5/2)$	-10.21	-10.03	- 7.29	-19.24
^{32}S	$U_{0d3/2}(0d5/2)$	-16.07	-19.04	-19.67	-30.67
	Δ_{0d}	- 5.86	- 9.01	-12.38	-11.43

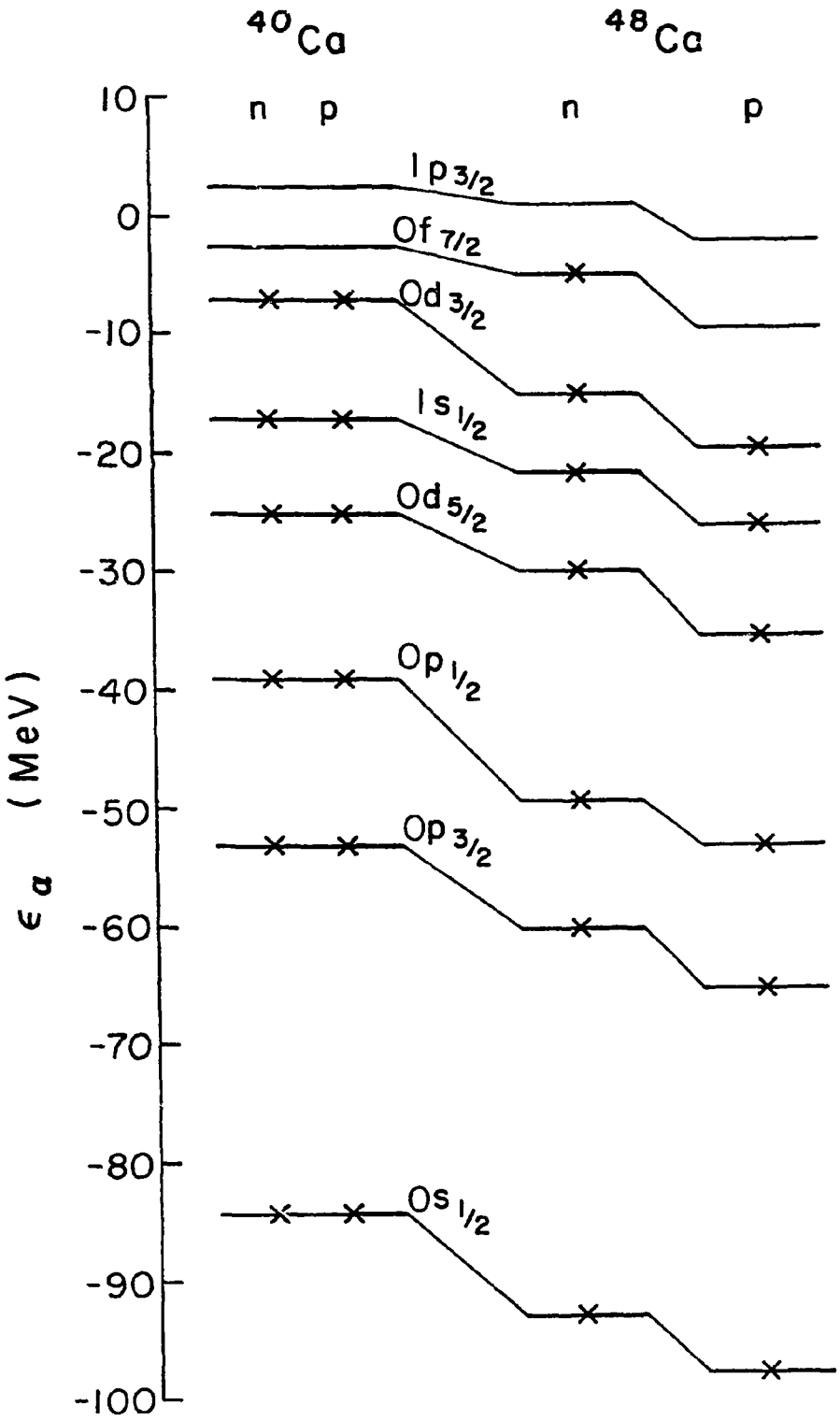
40Ca
48Ca
n
p
n
p
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
εα (MeV)
1p3/2
0f7/2
0d3/2
1s1/2
0d5/2
0p1/2
0p3/2
0s1/2

Fig. 1

BLANK PAGE

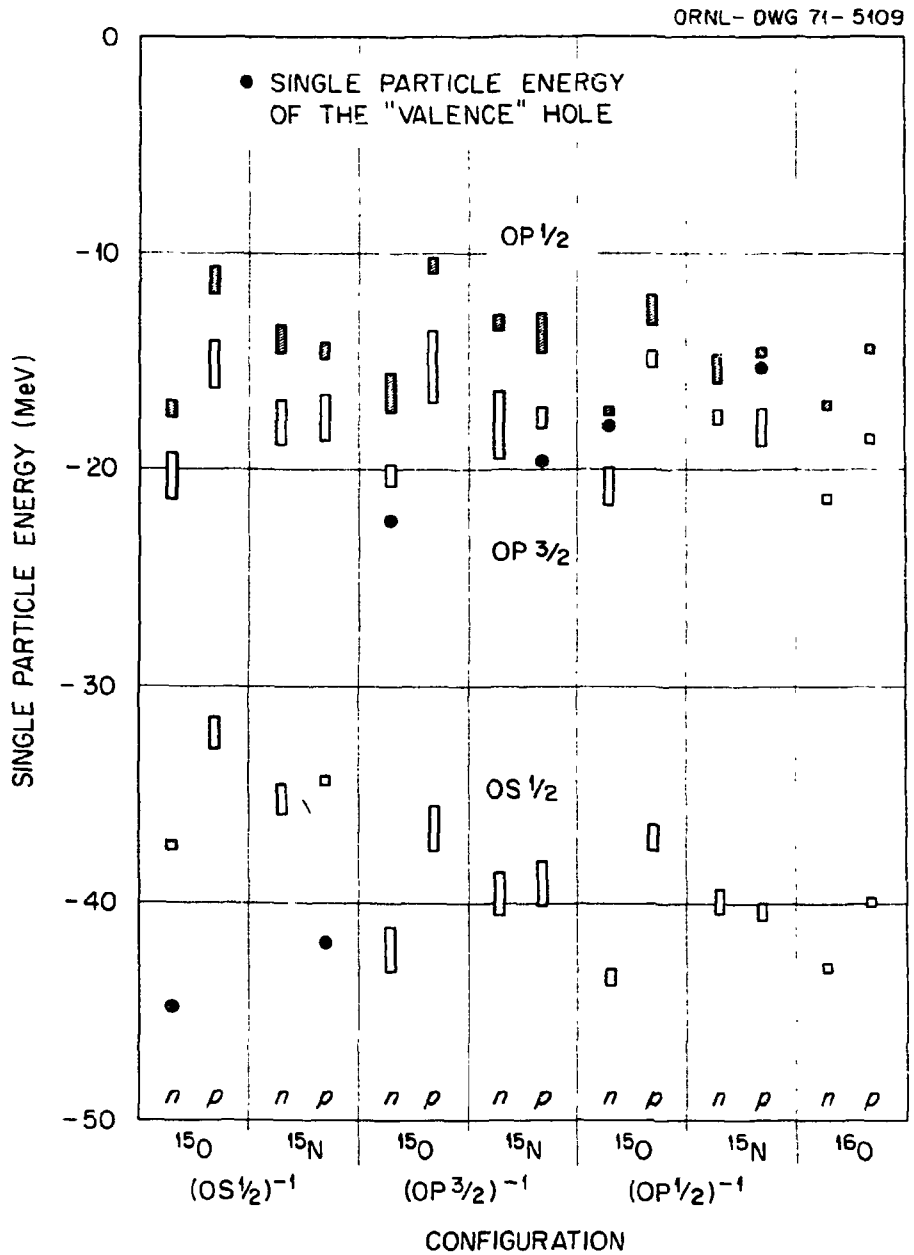
ORNL- DWG 71- 5109
SINGLE PARTICLE ENERGY OF THE "VALENCE" HOLE
SINGLE PARTICLE ENERGY (MeV)
0
-10
-20
-30
-40
-50
OP 1/2
OP 3/2
OS 1/2
n p n p n p n p n p n p n p
15O 15N 15O 15N 15O 15N 16O
(OS1/2)-1 (OP3/2)-1 (OP1/2)-1
CONFIGURATION

Fig. 2a

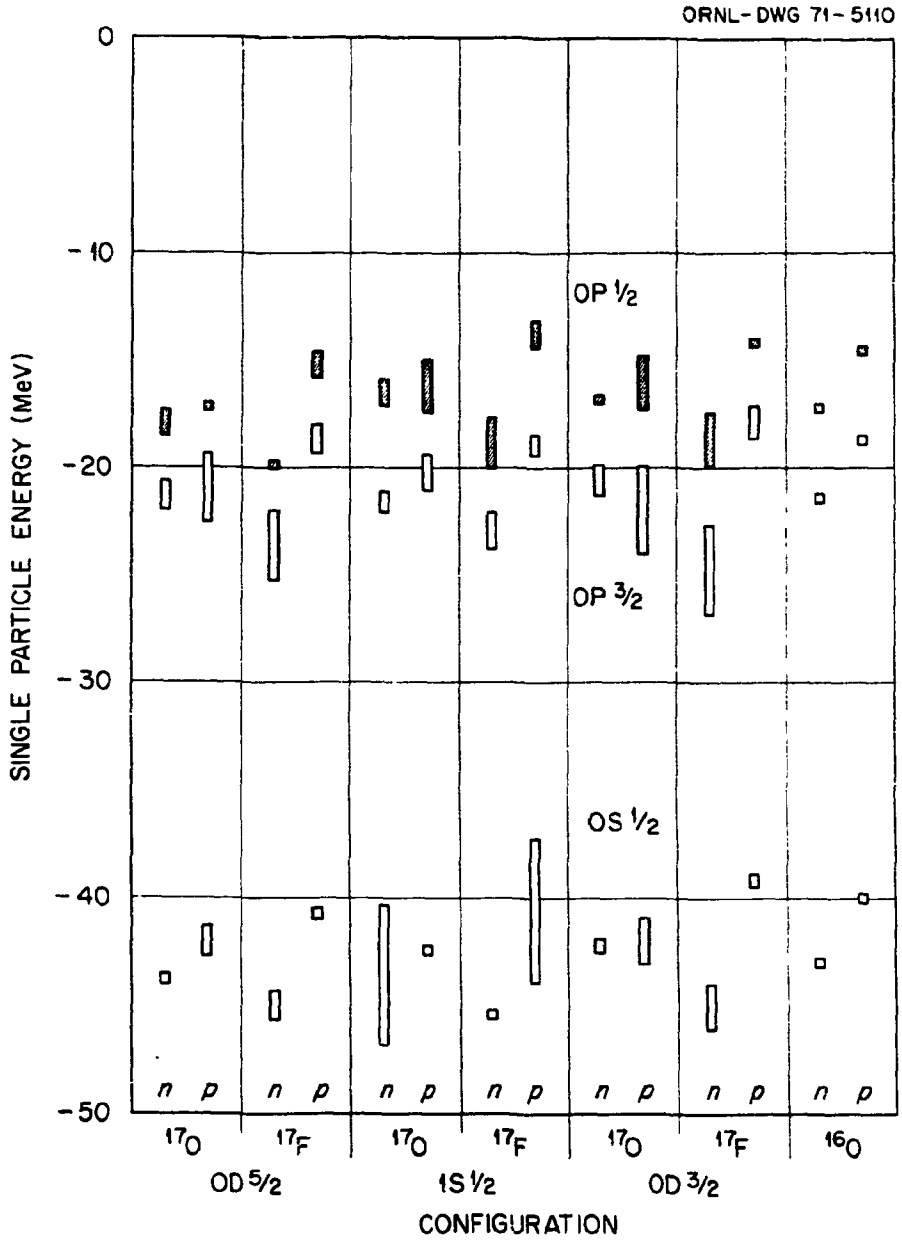
ORNL-DWG 71-5110
0
-10
-20
-30
-40
-50
SINGLE PARTICLE ENERGY (MeV)
0P 1/2
0P 3/2
0S 1/2
n p n p n p n p n p n p n p
17O 17F 17O 17F 17O 17F 16O
0D 5/2
1S 1/2
0D 3/2
CONFIGURATION

Fig. 2b