PHYSICAL REVIEW C VOLUME 12, NUMBER 6 DECEMBER 1975

Interpretation of inversions of single-particle levels in self-consistent field theories

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

J. P. Svenne
University of Manitoba,† Winnipeg, Manitoba, R3T 2N2, Canada

(Received 28 July 1975)

An interpretation is offered for the level inversion that usually occurs in self-consistent field calculations when only one of a pair of symmetry-related levels is occupied: the single-particle energy of the level unoccupied in the A-particle system is its energy of removal from the $(A+1)$-particle system. The correction of this energy to convert it to the corresponding energy in system A is simply given. When both symmetry-related levels are calculated in the same system there is no level inversion. The prescription to occupy the lowest levels should be amended to state that the energies should all correspond to removal energies from system A.

[NUCLEAR STRUCTURE Self-consistent field theory (HF, RBHF); broken symmetry. Level inversion explained; oscillation of level occupancies with iteration avoided.]

The various self-consistent field (SCF) theories [1-7] provide a prescription for constructing from the many-body Hamiltonian $H=\sum_{i=1}^{A} t_i + \sum_{i<j}^{A} v_{ij}$ a one-body Hamiltonian $h=h(\{\psi_\lambda, \lambda \leq A\})$ which depends not only on the operators t_i and v_{ij} appearing in H but also on a set of occupied single-particle (s.p.) orbitals $\{\psi_\lambda\}$. The theory is self-consistent in the sense that the orbitals ψ_λ from which h is constructed must themselves be eigenfunctions of h. It is well known that h may have lower symmetry than H, because of the dependence of h on $\{\psi_\lambda\}$. Specifically, if a symmetry operator for H can be expressed as an A-fold product of one-body unitary or antiunitary transformations S, then S is a symmetry operator for h, called a self-consistent symmetry, if and only if S leaves the subspace of occupied orbitals $\{\psi_\lambda, \lambda \leq A\}$ invariant.[8] Such a symmetry is preserved in successive iterations leading to self-consistency.

The symmetry requirements on the subspace impose restrictions on the types of nuclei and particle configurations which can be treated while preserving the symmetry. In order to perform calculations for other nuclei it is necessary to alter the occupied subspace so that it is not invariant under S, and consequently to break the symmetry of h. This almost always leads to an inversion of at least one (inexactly) symmetry-related pair of occupied and unoccupied levels, which appears incompatible with the usual prescription of occupying the A lowest orbitals. We shall give here an example of this problem in its several manifestations, provide an interpretation of such an inversion, and amend the SCF prescription to remove its incompatibility with the inversion. A more detailed discussion will be found in Ref. 6.

We must usually consider SCF solutions with more than one self-consistent symmetry, some of which 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. In this paper all the nondiagonal symmetries with which we shall be concerned lead only to a twofold 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 degenerate partners under S. We may refer to the eigenvalue (d) 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 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, $S_D=\exp[i\pi(j_{z'}-\frac{1}{2})]$ distinguishes between the two sets of partners.

A similar operator can be defined for axially asymmetric fields with ellipsoidal symmetry. 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.

(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 $Q = \frac{1}{2}A - T_3$, is conserved. Each orbital may be chosen to have a definite isospin projection, $\tau = +\frac{1}{2}$ for a neutron and $-\frac{1}{2}$ for a proton. A twofold degeneracy exists between a neutron 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, $N = Z$ ($M_T = 0$).

(iii) Invariance under inversion of intrinsic spins in spherical ($J = 0$) configurations. This is not a symmetry of the "realistic" nucleon-nucleon interactions, since these contain a spin-vector component, namely the two-body spin-orbit interaction $\propto \vec{l}_{12}\cdot(\vec{s}_1 + \vec{s}_2)$, where $\vec{l}_{12}$ is the relative orbital angular momentum. While this contributes most of the spin-orbit splitting in SCF calculations,[9,10] it is not very important for the spin-averaged properties of nuclei. Consequently, it is instructive to consider interactions where such a term is absent. Then inversion of spins is a symmetry of H, and if only "spin-saturated" configurations (i.e., both values of spin occupied) are allowed in SCF calculations, spin inversion is a self-consistent symmetry. Then, in the j-j coupling scheme, both values of j ($l \pm \frac{1}{2}$) for a given l have to be occupied and they are degenerate in energy. This allows calculation only for closed l shells (in practice, only ^{4}He, ^{16}O, and ^{40}Ca).

It is often convenient, in performing calculations for nuclei where (i), (ii), or (iii) cannot be self-consistent symmetries, to allow a relatively "mild" partial breaking of symmetry. Specifically, we will assume the symmetry S is broken, while the distinction remains a good quantum number. For example, in case (ii), this implies that we can calculate nuclei with $N \neq Z$, but we do not mix neutron and proton orbitals. We will then in general have one or more pairs of orbitals for which the $d = +1$ partner is occupied while $d = -1$ is not (or vice versa). The degeneracy of these two levels is then split and the unoccupied level usually lies lower than the occupied one.

We shall give here just one example of a SCF calculation in which this level inversion can be noted in all three manifestations. Fig. 1 is reproduced from the RBHF calculation by Becker and Patterson[11] of single-hole states in ^{15}O and ^{15}N. This figure shows 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 specific orbitals. Each column of the figure corresponds to a particular valence orbital. The shells in ^{16}O are split in the nuclei with $A = 15$ because the presence of a valence hole with a specific magnetic quantum number m_v implies a nonspherical 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. 1 (its energy does not depend on m_v), in-

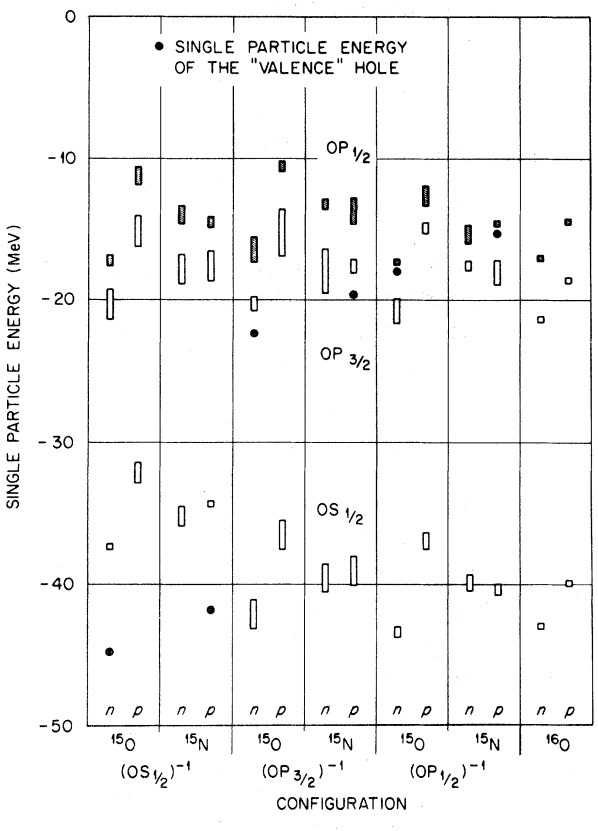

FIG. 1. Renormalized Brueckner single-particle levels in $A = 15$ isobars, from the RBHF calculation of Ref. 11. See text for detailed discussion of this figure. The oscillator range parameter is $b = 1.571$ fm.

variably 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 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; and (iii) that the spin-orbit splitting of the $0p$ levels is reduced by a valence hole in the $0p_{1/2}$ shell. Thus, Fig. 1 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.

The origin of this effect is readily seen to be in the fact that the single-particle energy for the unoccupied state has (at least) one extra matrix element of the interaction which is not present in the energy of the occupied state. This matrix element is negative in each of the cases examined here. We assume that we have a core of A_0 nucleons in which, for every occupied orbital, the orbital with the other value of the distinction quantum number d is also occupied; and one extra nucleon in the $d=+1$ member of the pair of orbitals $\zeta\,(z, d=\pm 1)$. We then find, from the Hartree-Fock equations, that the single-particle energies of these two orbitals are

$$\epsilon_{z+} = \epsilon_z^{(0)} \tag{1a}$$

and

$$\epsilon_{z-} = \epsilon_z^{(0)} + v_{-+}\,. \tag{1b}$$

Here $\epsilon_z^{(0)}$ is the contribution to the s.p. energy due to the fully occupied core orbitals and v_{-+} is the antisymmetrized two-body matrix element[12]

$$v_{-+} = \langle z-, z+ \,|\, v \,|\, z-, z+ \rangle_A\,. \tag{2}$$

The corresponding matrix element v_{++} is missing from Eq. (1a) since it is zero because of the antisymmetrization. Thus these two levels are nondegenerate, and ϵ_{z-} (unoccupied) $< \epsilon_{z+}$ (occupied), since $v_{-+} < 0$ in all the cases we have examined; see Table I.

The spin-orbit case is complicated by two factors: the $(2j+1)$-fold degeneracy of each spherical orbital, and the explicit two-body spin-orbit interaction in most "realistic" nucleon-nucleon potentials. We take the distinction quantum number $d=\pm 1$ to identify the two spin-orbit partners $j = l \pm \frac{1}{2}$ for a given l. But each of these states has a further $(2j+1)$-fold degeneracy which always holds in the case of spherical nuclei. As a result, v_{-+} is not just a single matrix element as in (4) but a sum over the magnetic quantum numbers. We define for this case

$$U_d(d') = \sum_{m'} \langle zdm, zd'm' \,|\, v \,|\, zdm, zd'm' \rangle_A\,. \tag{3}$$

After the sum on m' is carried out this is independent of m, but $U_+(+)$ is nonzero, since the sum will contain terms with $m' \neq m$ which do not have to be zero. Thus, with this definition of $U_d(d')$ Eqs. (1a) and (1b) have to be replaced by

$$\epsilon_{zd} = \epsilon_{zd}^{(0)} + U_d(+)\,. \tag{1c}$$

This leads to a spin-orbit splitting resulting from interactions with the spin-unsaturated shell (only $d=+$ occupied),

$$\Delta_z^{\text{unsat}} = U_-(+) - U_+(+), \tag{4}$$

which has been shown by Wong[9] to be always negative. If there were no two-body spin-orbit force this would be the only contribution to the spin-orbit splitting, and there would be a level-inversion independent of the strength of the interaction. However, if a spin-orbit component is present in the two-body interaction, the "core" contribution $\epsilon_z^{(0)}$ to the single-particle energy will depend on the distinction of the level and there will be a positive contribution to the spin-orbit splitting,

$$\Delta_z^{\text{core}} = \epsilon_{z-}^{(0)} - \epsilon_{z+}^{(0)}\,. \tag{5}$$

In this case there is a competition between the negative Δ_z^{unsat} and the positive Δ_z^{core} which may or may not result in a level inversion, depending on the strength of the interaction. In any case, the presence of Δ_z^{unsat} will always reduce the spin-orbit splitting for spin-unsaturated shells. See Table II for some typical results.

For a number of applications, mixing of states differing in their distinction quantum number is best avoided. We must then find a physically consistent interpretation for the unoccupied single-particle levels lying below occupied ones. Interpretation of the single-particle energies must rest in Koopmans' theorem[11,13]; that is, they should be related to separation energies. The single-particle energy ϵ_α of an unoccupied level of an A-particle system is (neglecting center of mass, orbital rearrangement, and s.p.-strength splitting effects[5]) the separation energy for removing a particle from state α in the $(A+1)$-particle system,

$$\epsilon_\alpha^{(A+1)} = E_\alpha(A+1) - E(A), \tag{6a}$$

where $E_\alpha(A+1)$ is the total energy in the $(A+1)$-

TABLE I. 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 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 nlj	Label z $\lvert m\rvert$	Tabakin [a] $b=1.732$	SP [b] $b=1.752$	Shell model [c] $12<A<28$	HJ [d] $b=1.571$
Time reversal $(-)^{m-1/2}$	$0p_{2/3}$	$\frac{1}{2}$ or $\frac{3}{2}$	−1.86	−2.86	−1.09	−2.09
	$0p_{1/2}$	$\frac{1}{2}$	−0.10	−1.04	−0.28	−0.43
	$0d_{5/2}$	$\frac{1}{2}$	−0.73	−0.78	−0.55	−1.27
	$0d_{5/2}$	$\frac{3}{2}$	−0.56	−0.81	−0.44	−1.00
	$0d_{5/2}$	$\frac{5}{2}$	−0.83	−0.76	−0.62	−1.44
	$1s_{1/2}$	$\frac{1}{2}$	−2.15	−1.55	−1.14	−2.49
	$0d_{3/2}$	$\frac{1}{2}$ or $\frac{3}{2}$	0.20	0.03	−0.14	−0.65
n-p interchange $(-)^{\tau-1/2}$	$0p_{3/2}$	$\frac{1}{2}$	−2.81	−2.48	−1.77	−3.76
	$0p_{3/2}$	$\frac{3}{2}$	−3.89	−3.35	−2.12	−4.79
	$0p_{1/2}$	$\frac{1}{2}$	−0.34	−1.53	−1.27	−2.61
	$0d_{5/2}$	$\frac{1}{2}$	−1.65	−1.34	−1.24	−3.22
	$0d_{3/2}$	$\frac{3}{2}$	−1.95	−1.59	−1.33	−3.47
	$0d_{5/2}$	$\frac{5}{2}$	−2.84	−2.54	−1.75	−5.17
	$1s_{1/2}$	$\frac{1}{2}$	−2.67	−2.88	−1.84	−5.20
	$0d_{3/2}$	$\frac{1}{2}$	−0.30	−0.98	−1.06	−2.92
	$0d_{3/2}$	$\frac{3}{2}$	−1.23	−1.63	−1.30	−4.05

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

[b] SP denotes G. Saunier and J. M. Pearson, Phys. Rev. C 1, 1353 (1970).

[c] J. M. Irvine, *Nuclear Structure Theory* (Pergamon, Oxford, 1972), pp. 249–251.

[d] HJ denotes reaction matrix elements of Ref. 11 of the interaction of T. Hamada and I. D. Johnston, Nucl. Phys. 34, 382 (1962), multiplied by the "true" occupation probabilities (Ref. 5).

TABLE II. Inversion of spin-orbit doublets in spin-unsaturated shells of spherical configurations of light $N=Z$ nuclei. Single-neutron energies are given in 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 $\epsilon^{A+1}_{l+1/2}$ is the s.p. energy in the nucleus with $A+1$ nucleons.

	RBHF [a] $D=2$	RBHF [b] $D=1$			HF [c] $D=4$
	^{12}C	^{12}C	^{28}Si	^{32}S	^{56}Ni
b	1.571	1.571	1.885	1.885	1.997
l	1	1	2	2	3
$\epsilon_{l+1/2}$	−13.2	−12.9	−12.0	−14.3	−12.5
$\epsilon_{l-1/2}$	−13.6	−14.5	−13.4	−15.1	−15.2
Δ_l	−0.4	−1.6	−1.4	−0.8	−2.7
$\epsilon^{A+1}_{l+1/2}$		−16.2		−15.3	
$\Delta_l^{\rm unsat}$		−8.8	−11.4	−11.4	
$\Delta_l^{\rm core}=\Delta_l-\Delta_l^{\rm unsat}$		7.2	10.0	10.6	

[a] R. L. Becker, R. C. Braley, W. F. Ford, and M. R. Patterson, Oak Ridge National Laboratory Report No. ORNL-TM-3951, 1972 (unpublished).

[b] R. L. Becker and M. R. Patterson (unpublished).

[c] B. Rouben and A. Saunier, Phys. Rev. C 5, 1223 (1972).

particle system with the extra particle occupying orbital α, and $E(A)$ is the total energy of the A-particle ground state. On the other hand, for occupied orbitals ϵ_α is the removal energy from system A,

$$\epsilon_\alpha^{(A)} = E(A) - E_{\alpha^{-1}}(A-1), \tag{6b}$$

where $E_{\alpha^{-1}}(A-1)$ is the total energy of the $(A-1)$-particle system with a hole in state α.

We assert that in deciding which orbitals should be occupied, one should compare energies all of which correspond to removal energies from the same system, either system A or $A+1$. If we do the SCF calculation for A we should calculate $\epsilon_{z,+}$ in the configuration in which $(z,+)$ is occupied and $(z,-)$ is empty, and $\epsilon_{z,-}$ in the configuration in which $(z,-)$ is occupied and $(z,+)$ is empty. These energies are both equal to $\epsilon_z^{(0)}$ [or, in the spin-orbit case with a symmetry-breaking spin-orbit two-body force, to $\epsilon_{z,+}^{(0)} + U_+(+) = \epsilon_{z,+}$ and $\epsilon_{z,-}^{(0)} + U_-(+) - v_{-m,+m}$]. Alternatively, except in the spin-orbit case, we could do the SCF calculation for the configuration of $A+1$ in which both $(z,+)$ and $(z,-)$ are occupied, for which S is a self-consistent symmetry. Then

$$\epsilon_{z,d}^{(A+1)} = \epsilon_z^{(0)} + \sum_{d'=\pm} v_{dd'} . \tag{7a}$$

Thus

$$\epsilon_{z,+}^{(A+1)} = \epsilon_{z,+} + v_{+-}, \tag{7b}$$

where $\epsilon_{z,+}$, given by Eq. (1a) or (1c), is the single-particle energy calculated in the A-particle system, but for the level $(z,-)$ Eqs. (7a) and (1b) or (1c) give exactly the same result. From Eq. (7a), when both levels are calculated in the $(A+1)$-particle system, there is no longer any level inversion, but they are degenerate, since $v_{+-} = v_{-+}$. This is the same result we obtained for the calculations in the A-particle system. Our interpretation, then, is that it is not inconsistent with occupying the lowest single-particle levels, that one unoccupied level intrudes below occupied ones, since this intruder is actually a level of the $(A+1)$-particle system. The prescription must simply be amended to state that the levels should all refer to the same system A or $A+1$.

We have seen that for system A there are two degenerate solutions of the SCF problem with $(z,+)$ or $(z,-)$ occupied, each equally good. The oscillation of occupancies of states $(z,\pm)$ often observed in performing SCF calculations of this type is a consequence of the iteration procedure being unable to select between these two solutions. The procedure should be modified to hold the occupancy of $(z,+)$ fixed. However, the existence of the two degenerate solutions should be a signal that correlations could be important. They could be included either by configuration mixing, or by further symmetry breaking.

---

*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.

[1]G. Ripka, in *Fundamentals in Nuclear Theory*, edited by A. de-Shalit and C. Villi (International Atomic Energy Agency, Vienna, 1967), p. 623.

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

[3]J. W. Negele, Phys. Rev. C 1, 1260 (1970).

[4]K. A. Brueckner, J. L. Gammel, and A. Weitzner, Phys. Rev. 110, 431 (1958).

[5]R. L. Becker, in *The Nuclear Many-Body Problem*, edited by F. Calogero and C. Ciofi Degli Atti (Editrice Compositori, Bologna, 1974), Vol. 2, Paper III-10.

[6]R. L. Becker and J. P. Svenne, Oak Ridge National Laboratory Report No. ORNL-TM-5174, 1975 (unpublished).

[7]We refer here not only to the Hartree-Fock (HF) theory (Ref. 1), but also to the density-dependent HF (DDHF) (Refs. 2 and 3), Brueckner-Hartree-Fock (BHF) (Ref. 4), and renormalized BHF (RBHF) (Ref. 5) theories. See Ref. 6 for a more complete list of references.

[8]J. Bar-Touv and I. Kelson, Phys. Rev. 138, B1035 (1965); M. Bouten and P. Van Leuven, Physica (The Hague) 34, 461 (1967).

[9]C. W. Wong, Nucl. Phys. A108, 481 (1968).

[10]A. Lande and J. P. Svenne, Nucl. Phys. A124, 241 (1969).

[11]R. L. Becker and M. R. Patterson, Nucl. Phys. A178, 88 (1971).

[12]In the BHF theory, replace v by the reaction operator G in Eq. (2); in the RBHF, also multiply the matrix element by the occupation probability P_{z^+}.

[13]At least as far as the HF and RBHF theories are concerned. For BHF, Koopmans' theorem does not apply because of the Brueckner rearrangement energy (Ref. 2).