PHYSICAL REVIEW C VOLUME 2, NUMBER 4 OCTOBER 1970

Slater Determinants, Parity Projection, and Hartree-Fock Calculations

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(Received 23 January 1970)

Slater determinants used in a standard Hartree-Fock calculation and built with parity-mixed single-particle orbitals do not have a definite parity; a parity projection after the variation is needed, in general. A different solution is investigated here, in which the projection is performed before the variation. Conditions are studied for the case where the solution is still a Slater determinant. The results of explicit calculations for both methods are compared in the case of a three-nucleon system. A larger binding energy is obtained in the case of projection before variation, and in the corresponding solution (which is not a Slater determinant) considerable parity mixing in single-particle wave functions is allowed.

I. INTRODUCTION

In recent years the Hartree-Fock (HF) approximation has been widely used in nuclear physics. However, among the very many possible solutions of HF equations, only those with some given symmetry have been investigated, as a matter of computational simplification. Most calculations, in fact, have been done for $4n$ nuclei (i.e., with an equal even number of protons and neutrons); only for these nuclei can the largest symmetry be preserved, as the usual symmetry group of the total nuclear Hamiltonian (invariance under three-dimensional rotation-inversion group and under time reversal, in addition to charge independence) is also a symmetry group of the HF Hamiltonian, i.e., it is a consistent symmetry.[1] However, imposing symmetry conditions means that one restricts oneself to those solutions which have the given symmetry; thus, it may happen that the absolute energy minimum is not reached. Moreover, the consistent symmetry group of the HF Hamiltonian need not necessarily be the same group of symmetry of the total Hamiltonian. In particular, in the HF Hamiltonian a parity violation is allowed, in principle, by the presence of tensor forces and of the one-pion exchange potential (OPEP) in a complete realistic nucleon-nucleon interaction. Then, the ground-state energy may be obtained if parity conservation in single-particle (s.p.) wave functions is suppressed.[2] Much theoretical work has been done on the basis of this hypothesis.

However, in the particular case of $4n$ nuclei, it has been shown recently[3] that parity mixing in s.p. orbitals is prevented if the s.p. densities are taken to be invariant under the following consistent symmetries:

(i) time reversal T;

(ii) reflection through a plane, e.g., the x-z plane, $Pe^{-i\pi J_y}$;

(iii) rotation by π about an axis in the plane of reflection symmetry, e.g., the z axis, $e^{i\pi J_z}$,

where P in (ii) is the parity operator.

In actual realistic HF calculations[4, 5] for $4n$ nuclei up to ^{40}Ca, good parity solutions were, indeed, found to be energetically favored. This can be understood also from a physical point of view; in a $4n$ nucleus, contributions from short-range central forces surely dominate with respect to tensor forces and OPEP, and the lowest states have seniority zero.[6, 7]

When the symmetries (i)–(iii) are violated, parity mixing in s.p. orbitals can also be obtained for $4n$ nuclei.[8] In the case of an odd nucleus, symmetry (i) does not hold, and an approximate HF solution presents parity mixing.[9]

In addition, a simple model based on the hypothesis of parity mixing in s.p. orbitals applied to the study of direct reactions[10] seems to be preferable to any other proposed models in the case of two-nucleon transfer reactions[11] such as ^{12}C(^{3}He,p)^{14}N. It must be noted that the spectroscopic factor for this reaction is sensitive to the details of the wave function of the odd-odd ^{14}N nucleus, for which a HF parity-mixed solution exists.[9]

In the case of parity mixing, the Slater determinant (SD) solution of the HF problem is built with s.p. orbitals without definite parity. This means that the state function of the nucleus so obtained does not, in general, possess a definite parity either. This situation is similar to that of other quantum numbers which have to be good quantum numbers of the nucleus, and is a peculiarity of the use of SD's. Let Ω be an operator which commutes with the total Hamiltonian, and ω the relative quantum number associated with the symmetry properties described by Ω. In general, the HF solutions mix several values of ω; the description of a nuclear level thus requires the use of a projection operator $\mathcal{P}_\Omega$ which extracts from the HF wave function the component of a good quantum number ω. This method can be called "projection after variation" (PAV). It does not, in general, give the same results as "projection before variation" (PBV), i.e., a variational calculation based on trial wave functions obtained after projecting the good quantum number ω from the initial SD.

In the case of the total angular momentum, the PBV method has already been extensively and successfully used[12] and also compared with the corresponding PAV method.[13]

In this work we shall investigate the advantages of the PBV method connected with the parity projection from a SD built with s.p. orbitals without definite parity.

In Sec. II the two methods (PBV and PAV) are discussed for the case of using initial SD as a trial wave function. Section III is devoted to some conditions which are necessary for the solution of the PBV method to still be a SD. The general formalism of parity PBV is developed in Sec. IV and applied to the case of a three-nucleon system in Sec. V, where comparison with PAV and the standard HF approximation is also done. The conclusions are drawn in Sec. VI.

II. PROJECTION BEFORE AND AFTER VARIATION

Let V be an m-dimensional vector space formed by the complex linear combinations of a set $\{\varphi_\alpha\}$ of m linearly independent s.p. wave functions; then

$$\psi_i = \sum_{\alpha=1}^{m} X_\alpha^i \varphi_\alpha \tag{1}$$

is an element of V. According to Navon and Bose,[14] let K_N be the space formed by all the SD's of order N which can be constructed, each starting from N linearly independent s.p. wave functions ψ_i. It is clear that K_N is not a vector space, because a linear combination of two SD's is not, in general, a SD: if and only if the two SD's differ by at most one s.p. wave function, is such a linear combination still a SD. Then any elementary continuous variation in the space K_N can be expressed as the sum of two SD's differing from each other by only one orbital; and the variational principle restricted to the space K_N leads to the well-known Brillouin condition and to the HF equations. The topological structure of K_N is thus responsible for the nuclear s.p. properties, which are so well reproduced in the HF approximation.

In order to reach a correlated ground-state function it would be preferable, from a strict theoretical point of view, to use the method of superposition of configurations.[15] In this case the variational procedure is applied to a trial antisymmetric wave function which may be expanded in SD's built up from a complete s.p. basis set. Even in the simplified version of a multiconfiguration HF theory,[16] such a program is obviously very difficult to perform with a realistic Hamiltonian.

In any case, at the end of the calculation one always meets the other difficulty: that the single SD of the HF approximation and the superposition of SD's do not have, in general, the required definite quantum numbers, and a PAV is needed.

An approach, whose difficulty is intermediate between standard HF and multiconfiguration theory, is the method of PBV. Let us denote by K_P the space of all state functions obtained by applying the projection $\mathcal{P}_\Omega$ to all the elements of K_N. Of course, K_P is also not a vector space. Furthermore, let us suppose that K_C is the set of all state functions which belong both to K_P and to K_N:

$$K_C = K_N \cap K_P .$$

The solution of the variational method in the PBV theory, which must be found in K_P, will not necessarily be in K_C. It is still an antisymmetric state function (as in the multiconfiguration method) and, moreover, has the required symmetry, i.e., ω is a good quantum number.

In order to see the power of the PBV method, let us consider the case of a HF solution in K_C: the HF method is then equivalent to that of PAV, as ω is already a good quantum number for the final solution. When performing the method of PBV, the same solution (in K_C) or one with lower energy (in that part of K_P complementary to K_C) must be found.

On the other hand, if the HF solution is not in K_C, then in order to obtain the good quantum number ω a projection must be performed, and a final-state function belonging to K_P is obtained. (If, e.g., Ω is the parity operator, it has been shown[17] that a gain in the binding energy is also possible by this projection.) However, the same result (but, in general, a better result) is achieved by a PBV which allows us to explore the whole K_P space.

Thus, in any case, PBV is preferable to PAV.

III. PARITY PROJECTION AND SLATER DETERMINANTS

A system of N Fermi particles can be described, as usual, by the following SD:

$$\Phi = (N!)^{-1/2} \det\{\psi_i\} , \tag{2}$$

where ψ_i is of the form of Eq. (1), and $i = 1, \ldots, N$. Φ is thus an element of K_N. It is easy to recognize that Φ can always be expanded as

$$\Phi = \sum_{k=1}^{M} C_k \Phi_k, \quad M = \binom{m}{N} , \tag{3}$$

where

$$\Phi_k = (N!)^{-1/2} \det\{\varphi_\alpha\} \tag{4}$$

represents the kth SD of order N built with a subset of N functions φ_α from among all M possible SD's of this kind. The expansion coefficients C_k are known if the $N \times m$ matrix A (whose matrix elements are $A_{i\alpha} = X^i_\alpha$) is known. In fact, C_k is the determinant of order N derived from this matrix:

$$C_k = \det\{X^i_{\alpha_k}\}, \tag{5}$$

where the set of indices $\{\alpha_k\}$ is the same which appears in the construction of the corresponding Φ_k.

Conversely, given a (complex) matrix A with m columns ($\alpha = 1, \ldots, m$) and N rows ($i = 1, \ldots, N$), with elements $A_{i\alpha} = X^i_\alpha$ such that

$$\sum_{\alpha=1}^{m} X^{i*}_\alpha X^j_\alpha = \delta_{ij}, \quad i, j = 1, \ldots, N \tag{6}$$

and given a set of m linearly independent s.p. wave functions $\{\varphi_\alpha\}$ ($\alpha = 1, \ldots, m$), one can construct all possible C_k's and Φ_k's according to Eqs. (4) and (5). Then one finds that

$$\sum_{k=1}^{M} C_k \Phi_k = \Phi', \tag{7}$$

where Φ' is a SD and belongs to K_N. In addition, the numbers X^i_α assume the meaning of expansion coefficients for the s.p. wave function, as in Eq. (1).

It may happen, of course, that some C_k in Eq. (7) vanishes, since two rows (columns) can be made proportional to each other. This case is frequent if there are many elements equal to zero in the original matrix A. In any case, Eq. (7) always holds.

Then, from Eqs. (3) and (7) we may state the following theorem: A superposition of SD's, $\sum_k C_k \Phi_k$, is still a SD if and only if:

(i) There is an $N \times m$ matrix A [whose elements are subject to the condition (6)] such that the C_k's are given by Eq. (5).

(ii) There is a set of m linearly independent s.p. wave functions $\{\varphi_\alpha\}$ such that the Φ_k's are given by Eq. (4).

(iii) $k = 1, \ldots, M$, as in Eq. (3).

Condition (i) is always satisfied if $m = N + 1$, according to Theorem III of Foldy,[18] where general (laborious) criteria are also devised to insure that a completely antisymmetric function of N variables be a SD.

Now, let us consider the parity operation. If the functions of the set $\{\varphi_\alpha\}$ are not all of the same parity, Φ has no definite parity. A state function with good parity can be obtained as

$$\Psi_\pm = \mathcal{P}_\pm \Phi, \tag{8}$$

where the parity projection operator is:

$$\mathcal{P}_\pm = \tfrac{1}{2}(1 \pm P). \tag{9}$$

It is clear that the following expansion is possible:

$$\Psi = \sum_k{}' C_k \Phi_k, \tag{10}$$

where the symbol $\sum'$ means that the sum is only over all SD's Φ_k with the same parity as Ψ. (Here and in the following we shall omit the labels ± when confusion is impossible.)

The operation indicated by Eq. (8) is thus equivalent to dropping some (in general nonvanishing) terms in the expansion (3). By the above theorem, therefore, Ψ is, in general, an element of K_P, but not of K_N.

When dealing with PBV and PAV methods, it is important to know whether or not the final solution belongs to K_C, i.e., whether or not it fulfills the conditions of the above theorem. Here, we are only able to suggest a direct inspection of the set $\{\varphi_\alpha\}$, with which the Φ_k's in Eq. (10) are built, and of the matrix A which generates the corresponding C_k's.

A particular case is that of a matrix A with so many vanishing elements that all C_k's of the "wrong" parity are zero; then, $\Psi \equiv \Phi$. This is the case for the HF solutions of Refs. 4, 5, and of our Sec. V.

IV. PARITY PROJECTION BEFORE VARIATION

In this section we give the general formalism necessary for the case of parity projection before doing the variational calculation. Similar approaches have already been proposed by Zeh[19] and Ebenhöh[20] without considering any computational details. A direct application of these methods seems, indeed, very laborious.

Our variational problem lies in the minimization of the following expectation value:

$$E_\pm = \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Phi|H|\Phi\rangle \pm \langle\Phi|HP|\Phi\rangle}{1 \pm \langle\Phi|P|\Phi\rangle}. \tag{11}$$

TABLE I. The ground-state energy E (in MeV) for ^{3}He and ^{3}H, as computed in the HF approximation and in the PBV method.

b (fm)	$E(^3\text{He})$ HF	$E(^3\text{He})$ PBV	$E(^3\text{H})$ HF	$E(^3\text{H})$ PBV
1.4	0.88		−0.16	
1.5	0.80		−0.22	
1.6	0.61	−0.89	−0.36	−1.91

Let us first consider how to calculate $\langle\Phi|P|\Phi\rangle$. $P\Phi$ is also a SD, which we denote by $\bar{\Phi}$:

$$\bar{\Phi} = (N!)^{-1/2}\det\{\bar{\psi}_i\}, \tag{12}$$

where, to be consistent, we have defined $\bar{\psi}_i = P\psi_i$. Since $\langle\Phi|\bar{\Phi}\rangle$ is the overlap of two SD's, it is known[21] that it equals the determinant of the overlap matrix O defined by its matrix elements

$$O_{ij} = \langle\psi_i|\bar{\psi}_j\rangle. \tag{13}$$

Thus,

$$\langle\Phi|\bar{\Phi}\rangle = \det O. \tag{14}$$

As the Hamiltonian H consists of a one-body and a two-body part,

$$H = \sum_{i=1}^{N} T_i + \tfrac{1}{2}\sum_{i\neq j=1}^{N} V_{ij}, \tag{15}$$

it turns out that

$$\langle\Phi|H|\bar{\Phi}\rangle = \sum_{i,j=1}^{N}(-)^{i+j}\langle\psi_i|T|\bar{\psi}_j\rangle\langle\Phi_i|\bar{\Phi}_j\rangle + \sum_{i<r}\sum_{j<s}(-)^{i+j+r+s}\langle\psi_i\psi_r|V|\bar{\psi}_j\bar{\psi}_s\rangle\langle\Phi_{ir}|\bar{\Phi}_{js}\rangle, \tag{16}$$

where

$$\Phi_i = [(N-1)!]^{-1/2}\det\{\psi_1, \ldots, \psi_{i-1}, \psi_{i+1}, \ldots, \psi_N\}, \tag{17}$$

$$\Phi_{ir} = [(N-2)!]^{-1/2}\det\{\psi_1, \ldots, \psi_{i-1}, \psi_{i+1}, \ldots, \psi_{r-1}, \psi_{r+1}, \ldots, \psi_N\}, \tag{18}$$

and $\langle\psi_i\psi_r|V|\bar{\psi}_j\bar{\psi}_s\rangle$ is the antisymmetrized matrix element.

Expanding the orbitals ψ_i as in Eq. (1) (using, e.g., a set of harmonic-oscillator wave functions), one has

$$\begin{aligned} E_\pm = \Big\{ &\sum_{ij}\sum_{\lambda\mu}[\delta_{ij} \pm (-)^{i+j}\pi_\mu\langle\Phi_i|\bar{\Phi}_j\rangle]\langle\varphi_\lambda|T|\varphi_\mu\rangle X_\lambda^{i*}X_\mu^j + \sum_{\substack{i<r\\ j<s}}\sum_{\lambda\mu\nu\rho}[\delta_{ij}\delta_{rs} \pm (-)^{i+j+r+s}\pi_\mu\pi_\rho\langle\Phi_{ir}|\bar{\Phi}_{js}\rangle] \\ &\times\langle\varphi_\lambda\varphi_\nu|V|\varphi_\mu\varphi_\rho\rangle X_\lambda^{i*}X_\nu^{r*}X_\mu^jX_\rho^s\Big\}\Big\{1 \pm N^{-1}\sum_{ij}(-)^{i+j}\sum_\lambda X_\lambda^{i*}X_\lambda^j\pi_\lambda\langle\Phi_i|\bar{\Phi}_j\rangle\Big\}^{-1}, \end{aligned} \tag{19}$$

where $P\varphi_\lambda = \pi_\lambda\varphi_\lambda$.

The minimum of $E_\pm$ can be found, in principle, by solving simultaneously the set of coupled nonlinear equations

$$\frac{\partial E_\pm}{\partial X_\alpha^i} = 0, \quad i = 1, \ldots, N; \quad \alpha = 1, \ldots, m, \tag{20}$$

under the condition (6) for the unknown complex coefficients X_α^i. However, such a solution is very complicated from a computational point of view, so it seems to be easier to make use of a computer code which minimizes directly the expression (19) as a function of X_α^i's, as has already been done in the case of angular momentum projection.[12]

V. NUMERICAL COMPUTATIONS

As an illustration of the preceding considerations we have performed numerical computations both with the HF approximation and with the PBV method. The choice of the particular nuclear system is very limited if one has to look for the minimum of expression (19), as the number of free parameters probably cannot exceed 30. Therefore, in order to have a reasonably large s.p. space and to study an odd nucleus, we have restricted our investigations to a three-body system (^{3}He and ^{3}H), for which the ground-state good quantum numbers are (total spin) $J = \frac{1}{2}$, (isospin) $T = \frac{1}{2}$, and positive parity. Of course, other refined approaches are more suitable for the description of such a system.[22] However, this example is already sufficient to illustrate our preceding considerations.

Our s.p. wave functions are

$$\psi_i \equiv \psi_{jm\tau}(\vec{r}_i) = \sum_{nl} X_{nl}^i\varphi_{nljm\tau}(\vec{r}_i), \tag{21}$$

where the principal quantum number n can take the values 0, 1, 2; the orbital angular momentum $l = 0, 1$; the total s.p. spin j is kept fixed at the value $\frac{1}{2}$; and $\tau = \frac{1}{2}$ $(-\frac{1}{2})$ specifies protons (neutrons). Owing to the Pauli principle, the third component of the spin j is $m = \pm\frac{1}{2}$ for identical nucleons. Moreover, we have chosen $m = \frac{1}{2}$ $(= J)$ for the unpaired nucleon (proton for ^{3}H and neutron for ^{3}He).

We are then left with 18 complex coefficients X_α^i, which can be reduced to 30 independent real parameters if we choose X_{00}^i to be real and utilize the normalization condition (6).

In the total Hamiltonian of ^{3}He, the Coulomb energy has been taken into account. In addition, the intrinsic Hamiltonian of the nucleus has been used, i.e., we have subtracted the c.m. kinetic energy according to Gunye.[23] The nuclear two-body interaction has been simulated by the effective force derived by Elliott *et al.*[24] Since matrix elements in the harmonic-oscillator basis of this force are tabulated for discrete values of the oscillator size parameter $b = (\hbar/m\omega)^{1/2}$, we have chosen $b = 1.4$, 1.5, and 1.6 fm as reasonable values in the HF approximation. When dealing with the PBV method, b is fixed at the value for which the corresponding HF energy has been found to be lowest.

TABLE II. Expansion coefficients X_{nl} as obtained in the PBV method for ^{3}He. For comparison, the X_{nl} obtained in the HF approximation are given in parentheses, when different from zero. i is the imaginary unit.

m	τ	X_{00}	X_{01}	X_{10}	X_{11}	X_{20}	X_{21}	HF energy (MeV)
$\frac{1}{2}$	$\frac{1}{2}$	0.938 (0.997)	0.339i	−0.044 (−0.064)	−0.050i	0.027 (0.040)	0.016i	−6.66
$-\frac{1}{2}$	$\frac{1}{2}$	0.889 (0.995)	0.449i	−0.051 (−0.081)	−0.056i	0.038 (0.059)	0.019i	−6.13
$\frac{1}{2}$	$-\frac{1}{2}$	0.957 (0.999)	0.280i	−0.033 (−0.035)	−0.055i	0.016 (0.020)	0.016i	−7.99

Our computer codes for the HF approximation are based on the usual iterated diagonalization of the HF Hamiltonian. In the case of the PBV method we have used the subroutine OPTNOV in the library of the 1108 Univac computer at the Centro di Calcolo of the University of Pavia. This subroutine finds the extremum of a given function without calculating its derivatives.

In Table I the energy minimum is given for the different cases. A considerable gain in the binding energy is evident for the PBV method. There are probably two reasons for the large discrepancy with experiment ($E = -7.73$ MeV for ^{3}He and -8.49 MeV for ^{3}H) in both cases. First, neither method is the most appropriate for studying a three-nucleon system, as the trial wave functions, though dependent on many parameters, are not very flexible. Second, the nuclear interaction used, though realistic, seems to underbind light nuclei appreciably.[25]

However, as can be seen from Tables II and III, it is remarkable that in the HF approximation all "wrong" parity components vanish, so that our HF solution is in K_C, as in other calculations,[4, 5] and is coincident with the PAV result. In contrast, considerable parity mixing in s.p. wave functions is allowed in the PBV method, and the final solution (in K_P) is not a SD. This result has been obtained in spite of the fact that our force is known to underestimate $^3S_1$ matrix elements and, therefore, spin-orbit splitting and all other nuclear properties depending on the noncentral part of the interaction.[25]

Another interesting fact can be seen from Tables II and III. All "wrong" parity components are characterized by a pure imaginary coefficient, although our PBV solution is not invariant under time reversal.

Finally, in order to have an indication about the parity doublet,[26] i.e., about the difference $E_- - E_+$, we have found, by minimization of E_- in Eq. (19), that $E_- = 5.5$ MeV for ^{3}H and $E_- = 6.1$ MeV for ^{3}He. Also, a considerable amount of parity mixing in s.p. orbitals is present in the state function describing this excited level of negative parity.

VI. CONCLUSIONS

The use of SD's in a standard HF calculation has been shown to be very limited, as the appropriate symmetry properties of the nuclear ground state are not taken into account. Therefore, we have again proposed the projection of the desired good quantum numbers from the trial SD before performing the variational calculation, instead of doing a projection after variation. The former procedure, indeed, gives better results in general (see Sec. II).

In particular, we have considered the problem of parity projection when single-particle wave functions with undefined parity are used. Such parity mixing is shown to be possible in the frame of a PBV method and in the case of an odd nucleus (^{3}He

TABLE III. Results for ^{3}H. The notation is the same as in Table II.

m	τ	X_{00}	X_{01}	X_{10}	X_{11}	X_{20}	X_{21}	HF energy (MeV)
$\frac{1}{2}$	$\frac{1}{2}$	0.961 (0.999)	0.269i	−0.026 (−0.028)	−0.047i	0.015 (0.020)	0.013i	−8.25
$-\frac{1}{2}$	$-\frac{1}{2}$	0.886 (0.996)	0.459i	−0.033 (−0.063)	−0.046i	0.035 (0.056)	0.017i	−7.25
$\frac{1}{2}$	$-\frac{1}{2}$	0.939 (0.998)	0.338i	−0.028 (−0.046)	−0.042i	0.026 (0.038)	0.014i	−7.79

and ^{3}H). A final solution which is a superposition of SD's, has, in fact, been found to give a larger binding energy than in the case of HF approximation. This seems to agree with the present trend of describing nuclei by a mixture of configurations.

In our investigation we were limited in the choice of the nuclear system by the number of free parameters. It would be desirable to perform similar calculations for the case of systems composed of a larger number of nucleons.

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PHYSICAL REVIEW C VOLUME 2, NUMBER 4 OCTOBER 1970

Nuclear Lifetime of the Ne^{19} 275-keV Level

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(Received 21 May 1970)

The mean life of the 275-keV second excited state of Ne^{19} was measured to be 61.4 ± 3.0 psec. The He^3(Ne^{20}, α)Ne^{19} reaction and the gas-target recoil-distance technique were used. The 275-keV state decays by $E1$ emission to the ground state. The strength of this $E1$ transition is equal within errors to that of the mirror transition in F^{19}. This result is discussed.

I. INTRODUCTION

A well-known consequence of charge symmetry is that corresponding $E1$ transitions in conjugate nuclei (whether $\Delta T = 0$ or ± 1) have equal strengths.[1] The rule for $\Delta T = 0$ transitions follows from the vanishing of the isoscalar $E1$ matrix element. We can most easily test this rule by comparing corre-