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SELF-CONSISTENT PAULI CORRECTIONS IN BRUECKNER-HARTREE-FOCK CALCULATIONS

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ABSTRACT

A scheme is introduced which makes it feasible to make completely self-consistent Brueckner-Hartree-Fock (BHF) and renormalized BHF calculations for spherical, closed-shell and axially-symmetric deformed nuclei. The usual requirement or orbital (HF) self-consistency has been imposed, as well as self-consistency in the starting energies and occupation probabilities. Previously only approximate forms have been used for the Pauli operator. This approximation is removed here and a method for making the necessary Pauli corrections to the reaction matrix during the approach to self-consistency is presented. A discussion of the symmetries which reduce the problem to one of manageable proportions is included.

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SUMMARY

The Brueckner-Hartree-Fock method is extended to include self-consistency in the reaction matrix as well as the usual self-consistencies. Corrections to the G-matrix are made using an approximate iterative procedure rather than the exact matrix inversion. Consideration of only spherical and axially symmetric deformed nuclei makes it possible to reduce the computational problem to one of manageable proportions by making use of the symmetries of the nuclear wave functions.

INTRODUCTION

Nuclear many-body theory has now progressed to the point where it becomes possible to make a quantitative connection between the (realistic) nucleon-nucleon interaction and properties of finite nuclei. These theoretical developments (referred to generally as Brueckner theories) are excellently summarized in several recent review articles (refs. 1 to 3). Applications of the theory to spherical (closed-shell) nuclei have been numerous (refs. 4 and 5), and recently the theory and its application have been extended to deformed nuclei (ref. 6). Significantly, all of these Brueckner-type calculations have yielded saturation at radii which are too small.

On the other hand, ordinary Hartree-Fock (HF) calculations but with density-dependent or velocity-dependent effective interactions have been very successful in predicting binding energies and shapes of finite nuclei (refs. 7 and 8). Despite the considerable degree of phenomenology inherent in such investigations, it is apparent that their underlying assumptions are good approximations to the realities of the nuclear medium, and that there is much to be learned from them. In particular, those who employ the more complicated Brueckner theories must wonder whether some neglected aspect of these theories could provide the equivalent of density or velocity dependence.

So far, Brueckner-type calculations have been carried out in a largely but not completely self-consistent manner. The usual requirement of "orbital" or Hartree-Fock self-consistency has been imposed, as well as self-consistency in the starting energies and (in renormalized BHF calculations) in the occupation probabilities; but only approximate forms have been used for the Pauli operator, which forbids scattering into intermediate states which are normally occupied. Since the correct form for the Pauli operator is not determined until the calculation has been completed, all current methods have the drawback that their output is inconsistent with their input. While this drawback is recognized and deplored, the enormous computational difficulties involved have so far prevented any attempts to treat the Pauli operator exactly. It is certainly conceivable, however, that current approximations make the resulting effective interaction (reaction matrix) less sensitive to details of the nuclear environment than would otherwise be the case, and that the success of the phenomenological calculations lies in their simulation of this sensitivity by means of density or velocity dependence.

If complete Pauli corrections are sought, it will be necessary to make corrections to the reaction matrix during the approach to self-consistency. A method for doing this in the general case of a deformed nucleus will be presented here, together with a discussion of those symmetries which reduce the problem to one of manageable proportions.

METHOD

All modern theories of nuclear matter and finite nuclei make use, in one form or another, of the reaction matrix $G(\omega)$ which satisfies

$$G(\omega) = V + V \frac{Q}{\omega - h} G(\omega) \qquad (1)$$

This equation describes the scattering of two nucleons which are moving in some average field, with V representing the interaction between them and ω the "starting energy." The unperturbed motion of the nucleons (i.e., in the absence of V) is described by the two-body Hamiltonian h, which is usually taken to be a sum of one-body Hamiltonians

$$h = h_1 + h_2$$

$$h_i = T_i + U_i$$

in which T represents the kinetic energy operator and U the average field felt by the nucleon.

The reaction matrix is used in place of V in many-body theories, the argument being that in this way multiple scattering between a given pair of nucleons is treated exactly. For this reason it is important to exclude, from the description of the multiple scattering, any effects which have already been included in the description of the unperturbed nuclear state. This is accomplished by means of the projection operator Q, which prohibits either of the nucleons from scattering into any of the single-particle orbitals which make up the unperturbed ground state. Because this restriction is similar to that arising from the indistinguishability of the nucleons, the operator Q is often called the Pauli operator.

Evidently the Pauli operator, and hence the reaction matrix, cannot be determined unless the occupied single-particle orbitals are known.

But in all the theories, the single-particle orbitals are eigenstates of a Hamiltonian which depends in some way on the reaction matrix. Thus yet another type of self-consistency is required, which has been avoided in calculations so far by the use instead of an approximate reaction matrix $G_o(\omega)$ obtained with an approximate Pauli operator Q_o. (It should be re-emphasized that this approximation is only a computational expedient, since in principle the correct Q could be obtained by solving for the reaction matrix and the nuclear orbitals simultaneously.)

Actually the approximation goes farther than that, because the two-body Hamiltonian h also depends on the single-particle orbitals. Usually it is replaced by a "reference" Hamiltonian, h_o, and the corresponding $G_o(\omega)$ is termed the "reference" reaction matrix.

In any event, $G(\omega)$ and $G_o(\omega)$ satisfy a relation (ref. 1) of the form

$$G(\omega) = G_o(\omega) + G_o(\omega)\left[\frac{Q_o}{\omega - h_o} - \frac{Q}{\omega - h}\right]G(\omega) \tag{2}$$

derived by eliminating the two-body interaction V. This equation has been used in some instances to obtain corrections to the reference reaction matrix, but not in a fully self-consistent way. It is possible to achieve complete self-consistency, but the corrections must be made more than once as the calculation unfolds.

Since the determination of nuclear structure is basically a nonlinear problem, all methods of solution which do not approximate the nonlinearity must proceed iteratively. Thus at any stage, say the n^{th}, there is a single-particle Hamiltonian $H^{(n)}$, whose eigenfunctions may be labeled $\phi_\lambda^{(n)}$. In the iterative process these eigenfunctions are used to form the next Hamiltonian $H^{(n+1)}$, and the calculation continues until the eigenfunctions and eigenvalues do not change from iteration to iteration. The various methods in current use (HF, BHF, RBHF) differ from one another in practice only in the way in which the new Hamiltonian is generated from the previous eigenfunctions.

To date all such calculations have employed a fixed reaction matrix determined in some approximate manner at the outset (ref. 9). But a slight modification of (2) provides a means of correcting the reaction matrix at each iteration. For, once the eigenfunctions $\phi_\lambda^{(n)}$ have been found, the Pauli operator $Q^{(n)}$ corresponding to them may be constructed, and the corrected reaction matrix $G^{(n)}$ obtained by solving

$$G^{(n)} = G_o^{(n)} + G_o^{(n)}\left[\frac{Q^{(n)}}{\omega - h^{(n)}} - \frac{Q_o^{(n)}}{\omega - h_o^{(n)}}\right]G^{(n)} \tag{3}$$

$$G^{(n)} = G^{(n-1)} + G^{(n-1)}\left[\frac{Q^{(n)}}{\omega - h^{(n)}} - \frac{Q^{(n-1)}}{\omega - h^{(n-1)}}\right]G^{(n)} \tag{4}$$

and used to form the new Hamiltonian $H^{(n+1)}$ as before. When convergence is near, it is legitimate to replace $G^{(n)}$ by $G^{(n-1)}$ on the right-hand side of (4) and then the reaction matrix changes at each iteration by the (matrix) amount

$$\Delta G = X_1 - X_0 \tag{5}$$

$$X_1(\omega) = G(\omega)\,\frac{Q^{\mathrm{NEW}}}{\omega - h^{\mathrm{NEW}}}\,G(\omega) \tag{5a}$$

$$X_0(\omega) = G(\omega)\,\frac{Q^{\mathrm{OLD}}}{\omega - h^{\mathrm{OLD}}}\,G(\omega) \tag{5b}$$

SYMMETRY CONSIDERATIONS

All current nuclear structure calculations require that the reaction matrix be expressed in terms of a suitable single-particle basis. Generally the basis functions are spherical, i.e., they may be specified by the quantum numbers $\{n, \ell, j, m, \tau\}$, ℓ representing the orbital angular momentum, j the total angular momentum, m the z-component of total angular momentum, and τ the z-component of isospin, with n standing for any other quantum numbers needed to distinguish the state (usually the radial quantum number). In the coordinate representation, a particular basis function labeled by the index "a" will be denoted by

$$\phi_a(\underset{\sim}{x}) \equiv \left\langle \underset{\sim}{x} \middle| a \right\rangle \equiv \left\langle \underset{\sim}{x} \middle| n_a \ell_a j_a m_a \tau_a \right\rangle \tag{6}$$

$\underset{\sim}{x}$ of course standing for the space and spin coordinates of the nucleon.

The reaction matrix is a two-body operator, and so its matrix elements will be of the form $\langle ab|G(\omega)|cd\rangle$. Because only antisymmetrized matrix elements are ever needed,

$$\langle ab|G(\omega)|cd\rangle = -\langle ab|G(\omega)|dc\rangle = -\langle ba|G(\omega)|cd\rangle \tag{7}$$

and it suffices to consider pairs $A = \{ab\}$ and $B = \{cd\}$ such that $a < b$ and $c < d$. In most calculations the reaction matrix is real, and it is always Hermitian (for fixed ω), so that

$$\langle A|G(\omega)|B\rangle = \langle B|G(\omega)|A\rangle \tag{8}$$

Thus only matrix elements with $A \leq B$ need to be calculated. The net result of all these simplifications is to reduce the number of matrix elements required by essentially a factor of 8.

Further reductions can only come about from symmetry effects, such as invariance with respect to spatial and isospin rotations and time-reversal invariance. Unfortunately, although V always possesses such symmetries, $G(\omega)$ may not because of its dependence on the nuclear orbitals through h and Q. For instance, although all stationary states of nuclei are also states of sharp angular momentum, the so-called intrinsic state of a permanently deformed nucleus - for which the basic structure calculations are performed in one version of the current theory - is characterized by having a rather broad spread of angular momenta forming a basis for the rotational "band."

In like manner, the isospin and time-reversal symmetries possessed by stationary nuclear states are generally not found in the intrinsic state. The exception occurs for doubly-even nuclei with $N = Z$, whose orbitals may be filled in such a way as to preserve the symmetries. Furthermore, these nuclei are quite often axially symmetric, so that the z-component of total angular momentum is conserved. The enormous reduction in calculation time which results from all this makes such nuclei extremely desirable for theoretical studies.

Accordingly, it is convenient to divide the pair states $A = \{ab\}$ into groups with the same parity ($\pi_A = \pi_a + \pi_b$), the same z-component of angular momentum ($M_A = m_a + m_b$), and the same total isospin ($T_A = 0$ or 1, $\tau_A = \tau_a + \tau_b$). In this way the reaction matrix is made block diagonal, each block being characterized by the appropriate conserved quantum numbers.

When isospin is conserved a further simplification results, since the $T_A = 1$ matrix elements are independent of τ_A (a consequence of the Wigner-Eckart theorem). Thus only two of the four submatrices need to be computed.

A similar result occurs when time-reversal invariance holds, but for different reasons. To begin with, the pair states of the basis may always be arranged so that for each state $|A\rangle$ there is a time-reversed counterpart $|\bar{A}\rangle$, the two satisfying

$$|\bar{A}\rangle = \mathcal{T}|A\rangle, \qquad |A\rangle = \mathcal{T}|\bar{A}\rangle \tag{9}$$

where $\mathcal{T}$ is the time-reversal operator. The matrix element of an arbitrary operator Ω between $|\bar{A}\rangle$ and $|\bar{B}\rangle$ may then be written (ref. 10)

$$\langle\bar{A}|\Omega|\bar{B}\rangle = \langle\mathcal{T}A|\Omega|\mathcal{T}B\rangle \tag{10a}$$

$$= \langle\mathcal{T}A|\Omega\,\mathcal{T}B\rangle \tag{10b}$$

$$= \langle A|\mathcal{T}^{-1}\Omega\,\mathcal{T}B\rangle^* \tag{10c}$$

$$\langle\bar{A}|\Omega|\bar{B}\rangle = \langle A|\mathcal{J}^{-1}\Omega\mathcal{J}|B\rangle^* = \langle A|\bar{\Omega}|B\rangle^* \tag{10d}$$

where $\bar{\Omega}$ is the time-reversed form of Ω. (The step from (10b) to (10c) follows from the antiunitary nature of the time-reversal operator.) When the operator Ω is time-reversal invariant,

$$\langle A|\bar{\Omega}|B\rangle^* = \langle A|\Omega|B\rangle^* \tag{11}$$

and when the phases have been chosen so that the matrix element is real,

$$\langle\bar{A}|\Omega|\bar{B}\rangle = \langle A|\Omega|B\rangle \tag{12}$$

Note that $\Omega = \bar{\Omega}$ only for nuclei whose intrinsic state is time reversal invariant.

One immediate consequence of (12) is that no negative-M submatrices need be computed, since each will be equal to the corresponding positive-M submatrix. For $M = 0$ the situation is more involved, and it is convenient to further subdivide this set so that one group of states is mapped into the other by time reversal. There are many ways of doing this; one simple method is to place pair states with $m_a < m_b$ in the group [A], and those with $m_a > m_b$ in the group $[\bar{A}]$. By the foregoing argument matrix elements of the type $\langle\bar{A}|\Omega|\bar{A}'\rangle$ need not be computed, and when the pair states are from different groups,

$$\langle A|\Omega|\bar{A}'\rangle = \langle\bar{A}|\Omega|A'\rangle \tag{13a}$$

$$= \langle A'|\Omega|\bar{A}\rangle \tag{13b}$$

(Eq. (13a) follows from (12), and (13b) from (8).) By symmetry, then, it is only necessary to compute

$$\langle A|\Omega|A'\rangle, \qquad A \leq A', \text{ and} \tag{14a}$$

$$\langle A|\Omega|\bar{A}'\rangle, \qquad A \leq A' \tag{14b}$$

when $M = 0$.

DETAILS OF THE CALCULATION

Both terms in (5) are similar in form, so that what must be calculated are matrix elements of the general type

$$\left\langle ab\left|G(\omega)\,\frac{Q}{\omega - h}\,G(\omega)\right|cd\right\rangle \equiv \langle ab|Y(\omega)|cd\rangle \tag{15}$$

Now in all current versions of nuclear many-body theory, the eigenfunctions ϕ_λ may be used to construct (in a manner to be specified shortly) orbital pair states $|\lambda\mu\rangle$ which diagonalize both Q and h. Hence the needed matrix elements may be obtained from

$$\sum_{\lambda\mu}{}' \frac{\langle ab|G(\omega)|\lambda\mu\rangle\langle\lambda\mu|G(\omega)|cd\rangle}{\omega - \varepsilon_{\lambda\mu}} \tag{16}$$

where $\sum'$ indicates the legacy of Q, namely that only the unoccupied orbitals are to be included in the summation.

This expression may be simplified in several ways. First, because of the antisymmetric nature of the matrix elements, the summation may be restricted to those orbital pairs $\Lambda = \{\lambda\mu\}$ with $\lambda < \mu$ and the result then multiplied by 2. Second, if the orbital pairs are labeled by the same general quantum numbers that label the basis pairs, the summation will be further restricted to those pairs with the same quantum numbers as {ab} and {cd}. Equation (15) may thus be written

$$Y(\omega)_A^B = 2 \sum_{\Lambda}{}'' \frac{G(\omega)_A^\Lambda G(\omega)_B^\Lambda}{\omega - \varepsilon_\Lambda} \tag{17}$$

where $\sum''$ indicates the further restrictions and an obvious shorthand for the matrix elements has been introduced.

The economy of expression displayed in (17) is achieved only through the use of mixed-representation matrix elements of $G(\omega)$. These are related to the basis-representation matrix elements by

$$G(\omega)_A^\Lambda = 2 \sum_B G(\omega)_A^B \rho_B^\Lambda \tag{18}$$

where ρ_B^Λ is the projection of $|\Lambda\rangle$ onto the basis pair-state $|B\rangle$:

$$|\Lambda\rangle = \sum_B \rho_B^\Lambda |B\rangle \tag{19a}$$

$$\rho_B^\Lambda = \langle B|\Lambda\rangle \tag{19b}$$

(The factor of 2 appears as before because of the use of ordered pairs.) Although calculation of the mixed-representation matrix elements is a rather lengthy intermediate step which must be performed for both terms in (5), overall time is greatly reduced owing to the appearance of a single, rather than a double, pair-state summation in (17).

To proceed further it is necessary to introduce an explicit notation for the isospin. Let $\chi_T(12)$ denote singlet ($T = 0$) and triplet ($T = 1$) isospin functions for two nucleons labeled 1 and 2. A pair state $|ab\rangle$ with a definite isospin is then of the form

$$\langle \underset{\sim}{x}_1 \underset{\sim}{x}_2 | ab \rangle = \frac{1}{\sqrt{2}} \left\{ \langle \underset{\sim}{x}_1 | a \rangle \langle \underset{\sim}{x}_2 | b \rangle + (-1)^T \langle \underset{\sim}{x}_1 | b \rangle \langle \underset{\sim}{x}_2 | a \rangle \right\} \chi_T(12) \tag{20a}$$

$$= \langle \underset{\sim}{x}_1 \underset{\sim}{x}_2 | abT \rangle \chi_T(12) \tag{20b}$$

or symbolically

$$|abT\rangle = \frac{1}{\sqrt{2}} \{ |a\rangle |b\rangle + (-1)^T |b\rangle |a\rangle \} \tag{20c}$$

A similar decomposition of the orbital pair state $|\lambda\mu\rangle$ can be made, leading to the expression

$$\rho^{\lambda\mu T}_{abT} = C^\lambda_a C^\mu_b + (-1)^T C^\lambda_b C^\mu_a \tag{21}$$

where C^λ_a is the projection of $|\lambda\rangle$ onto the basis state $|a\rangle$:

$$|\lambda\rangle = \sum_a C^\lambda_a |a\rangle \tag{22a}$$

$$C^\lambda_a = \langle a | \lambda \rangle \tag{22b}$$

In this notation two-body matrix elements are written

$$\langle abT | G(\omega) | cdT \rangle = \langle ab | G_T(\omega) | cd \rangle = G_T(\omega)^{cd}_{ab} \tag{23}$$

and have the exchange character $(-1)^T$. (It should be noted that the projection of the time-reversed orbit $|\bar{\lambda}\rangle$ onto the time-reversed basis state $|\bar{a}\rangle$ is also equal to C^λ_a, provided this coefficient is real.)

The only remaining problem, aside from the technical questions of efficient sequencing and indexing, is the energy-dependence or ω-dependence of the reaction matrix. It is clear from its definition that $G(\omega)$ is a meromorphic function with poles at the eigenvalues $\varepsilon_{\lambda\mu}$, but in practice these poles, which form the intermediate-state spectrum, are expected to be relatively far removed from the range of ω-values needed for boundstate investigations. Such an assumption must be verified in each instance, of course, but when true it permits an accurate approximation of the form $G(\omega) \cong G_N(\omega)$ with

$$G_N(\omega) = \sum_{n=0}^{N} G_n P_n(\omega) \tag{24}$$

where $P_n(\omega)$ is a polynomial of order n. Equation (24) is inconvenient for Pauli corrections when the basis space is very large, and so it is rearranged to read

$$G_N(\omega) = \sum_{\nu=0}^{N} G_N(\omega_\nu)\mathcal{P}_\nu(\omega) \tag{25}$$

where each $\mathcal{P}_\nu(\omega)$ is a Lagrange-interpolation polynomial of order N characterized by

$$\mathcal{P}_\nu(\omega_\mu) = \delta_{\mu\nu} \tag{26}$$

With this formulation the Pauli corrections may be performed directly on the matrix coefficients $G_N(\omega_\nu)$. The roots ω_ν are quite arbitrary, but round-off error is minimized if they are confined to the ω-range of interest and spread rather uniformly throughout it. The coefficients $G_N(\omega_\nu)$ may be obtained directly from $G(\omega)$, if desired, or a least-squares procedure used to obtain (24) which is then evaluated at the various values ω_ν.

CONCLUDING REMARKS

The problem of making Pauli and spectral corrections to the reaction matrix for spherical and axially-symmetric deformed nuclei has been discussed. This additional self-consistency in BHF and RBHF calculations is usually avoided due to the complexity of the numerical computations. A significant reduction in complexity of the problem results when an iterative method is used to obtain the new G-matrix (instead of matrix inversion), and the symmetries of the intrinsic state are used to reduce the number of matrix elements which must be computed. The completely self-consistent RBHF problem is then reduced to one of manageable proportions.

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