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Note

A Simple Strategy for Finding the Low-Lying Solutions of the Restricted Nuclear Hartree–Fock Equations

INTRODUCTION

The Raleigh–Ritz (RR) method provides a simple means of approximating the lower lying eigenstates of a bounded (or semi-bounded) operator. Obviously, how good the approximation is depends strongly on the choice of Ritz basis vectors. Recently, in the case of strongly interacting systems described by a many body effective Hamiltonian operator, it has been suggested that an optimized choice of these basis vectors can be generated from variational methods such as, for example, the Hartree–Fock (HF) method [1–6]. The idea is simply to use the lowest lying solutions obtained from the variational method as the Ritz basis vectors. Such a prescription clearly does not impose any a priori structure on the basis vectors. Using variational methods to ascertain the structure of the Ritz vectors is physically appealing. To some extent the choice of the basis vectors is then intimately connected to the dynamics of the system since, in both the basis generation and the RR step, the same interaction is used. Furthermore, in the case of the HF equations, the dimensionality of the basis generation is determined by the number of single particle states and not by the dimensionality of the many-body space. If not too many basis states are required, good approximate nuclear structure calculations in very large model spaces are certainly feasible. The difficulty, of course, is to construct an operationally efficient strategy for generating these basis states. In the present work, we concentrate on the specific problem of finding the lowest lying solutions of the non-linear restricted HF equations. The present method can be extended quite easily to other more general variational methods such as the Hartree–Fock–Boguliubov method.

The general strategy that evolves, we believe, is applicable to a wider class of nuclear structure problems. At finite temperatures, the aforementioned method which is designed to approximate the low-lying eigenspectrum, provides an excellent means of approximating the results for heated nuclei in the canonical ensemble [7]. Fluctuations in the number of particles are not introduced as in the case of most finite temperature mean field calculations. Using constrained variational methods with angular momentum constraints to generate the basis states, provides a convenient means of approximating the spectrum of states with a particular angular momentum [8, 9]. In this manner symmetry restoration of the basis states by projection after variation can be circumvented in a simple manner.

There are, however, certain severe computational problems involved in the pre-

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sent strategy. Clearly, we require something more than an efficient means of solving the HF equations. If no further restrictions are placed on the structure of the basis states, other than that they are solutions of a particular variational method, it is important to devise a strategy in which the lowest lying solutions are found only once and not repeatedly. In order to avoid finding the same solution of the HF equations more than once, we have made use of penalty functions involving the overlap with previously obtained solutions of the HF equations. The inclusion of these penalty functions initially results in a set of equations which no longer may be cast into the form of a non-linear eigenvalue problem. Hence many of the methods developed for finding the HF groundstate solution cannot be applied to this more general problem. Furthermore, the use of penalty functions guarantees that the solutions found are distinct but does not necessarily yield the lowest lying solutions of the HF equations.

In the case of the restricted HF equations there are two useful methods of solving the equations. If one is interested in obtaining the lowest lying solution, it is generally accepted that a good strategy is to construct the single particle HF Hamiltonian and to diagonalize it repeatedly in the model space. Choosing the single particle states with the lowest lying single particle energies as the occupied single particle states in the next iteration step usually ultimately yields the HF ground state or a very small subset of the low-lying solutions. The reason for this is simply that the total HF energy, the quantity to be minimized, is to a large extent just the sum of the occupied single particle state energies.

However, if one is interested in generating a set of the lower lying solutions of the HF equations, the diagonalization strategy is inadequate. In this case it is advantageous to solve the restricted HF equations via Newton–Raphson methods [4, 10] or in larger systems via modified Crank–Nicolson schemes [11, 12]. Here one chooses the occupation of the single particle orbitals initially and iterates only within the space of these occupied orbitals. It is not possible to rearrange the occupation of the single particle orbitals according to the single particle energies as in the diagonalization procedure, because the complete set of single particle orbitals and energies is not known. Because no rearrangement takes place, it is possible to generate many more solutions of the HF equations simply by choosing different sets of initially occupied orbitals. However, there is no a priori guarantee that a set of occupied single particle orbitals will lead to either a new or even a low lying solution of the HF equations.

To obtain a set of the lowest lying solutions of the HF equations in a reasonably efficient manner, the following strategy was devised. For a given set of occupied orbitals, a few iterations are performed via the HF diagonalization procedure in order to rearrange the occupation of the orbitals in the trial state according to their single particle energies. At this point subsequent iterations are performed via the Newton–Raphson procedure. To avoid obtaining the same solution more than once, penalty functions that involve the overlaps between the trial state and previously obtained solutions of the HF equations are introduced. These functions involve multipliers, which are then reduced to zero to obtain the next solution.

In the next section the details of the strategy are presented. The numerical results obtained are given in Section 3.

2. Applications of the Method

We begin by considering the two methods of solution of the Hartree–Fock equations. The full many-body Hamiltonian may be written in second quantized form as

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | \hat{H}_0 | \beta \rangle a_\alpha^+ a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{V} | \gamma\delta \rangle a_\alpha^+ a_\beta^+ a_\delta a_\gamma, \tag{1}$$

where the $a_\alpha^+(\alpha_\beta)$ are the single particle creation (annihilation) operators and $\hat{H}_0$, $\hat{V}$ denote the single particle energy and two-body residual effective interaction operators, respectively. In the restricted Hartree–Fock approximation the many-body state $|\Phi\rangle$ is required to be a single Slater determinant of A single particle orbitals $|\alpha\rangle$, each of which is expanded in terms of the orthonormal basis $|j\rangle$, $j = 1, 2, ..., N$,

$$|\alpha\rangle = \sum_{j=1}^{N} d_j^\alpha |j\rangle, \tag{2}$$

where the expansion coefficients fulfill the orthonormality requirement

$$\sum_j d_j^{\alpha *} d_j^\beta = \delta_{\alpha\beta}, \qquad \alpha, \beta = 1, 2, ..., A. \tag{3}$$

The expectation value of the Hamiltonian may then be expressed as

$$\begin{aligned} \langle \Phi | \hat{H} | \Phi \rangle = & \sum_{\alpha ij} d_i^{\alpha *} e_i \delta_{ij} d_j^\alpha \\ & + \tfrac{1}{2} \sum_{\alpha\beta ijkl} d_i^{\alpha *} d_j^{\beta *} \langle ij | \hat{V} | \tilde{kl} \rangle d_l^\beta d_k^\alpha, \end{aligned} \tag{4}$$

where the $\langle ij | \hat{V} | \tilde{kl} \rangle$ are the fully antisymmetrized matrix elements of the two-body interaction and e_i are the eigenvalues of the single particle Hamiltonian $\hat{H}_0$. Minimizing this expectation value with respect to the expansion coefficients subject to the constraint above yields the HF single particle eigenvalue problem

$$\sum_j h_{ij}^{\mathrm{HF}} d_j^\alpha = \varepsilon_\alpha d_i^\alpha, \tag{5a}$$

where

$$h_{ij}^{\mathrm{HF}} = e_i \delta_{ij} + \sum_{\beta kl} d_k^{\beta *} \langle ik | \hat{V} | \tilde{jl} \rangle d_l^\beta. \tag{5.b}$$

For an initial choice of the expansion coefficients, diagonalization of the HF Hamiltonian matrix, h^{HF}, yields the new set of N eigenvalues and N eigenvectors. We then choose the eigenvectors corresponding to the lowest A eigenvalues to be the new expansion coefficients of the occupied orbitals in the next iteration step. This procedure repeatedly tends to generate a very small subset of the low-lying solutions which almost always includes the Hartree–Fock ground state. It is, however, very difficult to adapt this procedure to produce a larger set of basis states efficiently or to prevent the same solution being obtained more than once.

The second method of solution proceeds by minimizing the HF energy directly, subject to penalty constraints to obtain a new distinct solution; that is, one such that

$$\langle \Phi | \Psi \rangle \neq 1,$$

where Ψ is any previous solution, we introduce the positive definite penalty function

$$\frac{\beta}{1 - |\langle \Phi | \Psi \rangle|^2},$$

which tends to infinity if the trial state approaches Ψ.

This penalty function is included in the minimization; that is

$$\frac{d}{dd_m^{\gamma *}} \left\{ \langle \Phi | | H \Phi \rangle - \sum_{\alpha\gamma} \varepsilon_{\alpha\gamma} \left(\sum_j d_j^{\alpha *} d_j^{\gamma} - \delta_{\alpha\gamma} \right) + \frac{\beta}{1 - |\langle \Phi | \Psi \rangle|^2} \right\} = 0. \tag{6}$$

The penalty multiplier must ultimately be reduced to zero, re-solving the above equations at each stage. For a given choice of the penalty multiplier after a converged solution of Eq. (6) is obtained, the new penalty multiplier is taken to be the product of the old multiplier and the overlap squared; that is $\beta = \beta' |\langle \Phi | \Psi \rangle|^2$. When β is less than 10^{-3}, it is set equal to 0. Any number of penalty functions may be used with separate multipliers, thus allowing us to produce a set of distinct solutions.

This minimization problem may be solved using a Newton–Raphson method. Since the states $|\Phi\rangle$ and $|\Psi\rangle$ are Slater determinants, their overlap is easily seen to be

$$\langle \Phi | \Psi \rangle = \det A, \tag{7}$$

where A is the matrix of the overlap of the single particle orbitals

$$A_{\alpha\lambda} = \sum_{j=1}^{N} d_j^{\alpha *} c_j^{\lambda}, \qquad \alpha, \lambda = 1, 2, ..., A, \tag{8}$$

where the c_j^{λ} denote the expansion coefficients of the single particle orbitals $|\lambda\rangle$ of the Slater determinant $|\Psi\rangle$

$$|\lambda\rangle = \sum_{j=1}^{N} c_j^{\lambda} |j\rangle, \qquad \lambda = 1, ..., A. \tag{9}$$

Expanding the determinant in terms of the minors $M(A)_{\alpha\lambda}$,

$$\det A = \sum_{\lambda} (-)^{\lambda+\alpha} A_{\alpha\lambda} M(A)_{\alpha\lambda} \tag{10}$$

yields the explicit system of equations for d_j^{α},

$$F_i^{\alpha}(d, \varepsilon) = 0 \tag{11a}$$

$$\sum_{j=1}^{N} d_j^{\alpha *} d_j^{\gamma} = \delta_{\alpha\gamma}, \tag{11b}$$

where

$$F_i^{\alpha}(d, \varepsilon) = \sum_{j} h_{ij} d_j^{\alpha} - \sum_{\gamma} \varepsilon_{\alpha\gamma} d_i^{\gamma} + \frac{2\beta \sum_{\lambda} c_i^{\lambda} (-)^{\lambda+\alpha} M(A)_{\alpha\lambda} (\det A)}{(1-(\det A)^2)^2} \tag{11c}$$

and h_{ij} is given in Eq. (5b). Here one clearly sees that equations to be solved cannot be brought into the form of a non-linear eigenvalue problem.

The derivatives necessary for the Newton–Raphson method are then

$$\begin{aligned}\frac{\partial F_i^{\alpha}}{\partial d_j^{\gamma}} &= h_{ij}\,\delta_{\alpha\gamma} + \sum_{kl} [\langle ij|\,\hat{V}\,|\tilde{k}l\rangle + \langle il|\,\hat{V}\,|\tilde{k}j\rangle]\, d_k^{\alpha}\, d_l^{\gamma} - \varepsilon_{\alpha\gamma}\,\delta_{ij} \\ &+ \frac{2\beta(\sum_{\lambda} c_i^{\lambda} (-)^{\lambda+\alpha} M(A)_{\alpha\lambda})(\sum_{\rho} c_j^{\rho} (-)^{\rho+\gamma} M(A)_{\gamma\rho})}{(1-(\det A)^2)^2} \left[1 + \frac{4(\det A)^2}{1-(\det A)^2}\right] \\ &+ \frac{2\beta(\sum_{\lambda\rho} c_i^{\lambda} c_i^{\rho} (-)^{\lambda+\alpha+\rho+\gamma} M(A)_{\alpha\gamma,\lambda\rho}) \det A}{(1-(\det A)^2)^2},\end{aligned} \tag{12a}$$

$$\partial F_i^{\alpha} / \partial \varepsilon_{\beta\gamma} = -d_i^{\gamma}\,\delta_{\alpha\beta}, \tag{12b}$$

and

$$\frac{\partial}{\partial d_i^{\gamma}} \left[\sum_{j} d_j^{\alpha *} d_j^{\beta} - \delta_{\alpha\beta}\right] = d_i^{\beta}\,\delta_{\alpha\gamma} + d_i^{\alpha *}\,\delta_{\beta\gamma}, \tag{12c}$$

where we have used the expansion of the minors of A in terms of the second minors $M(A)_{\alpha\alpha',\lambda\lambda'}$,

$$M(A)_{\alpha\lambda} = \sum_{\lambda'} (-)^{\lambda'+\alpha'} A_{\alpha'\lambda'} M(A)_{\alpha\alpha',\lambda\lambda'}. \tag{13}$$

This method is efficient for generating many different solutions since the occupation of the single particle orbitals is to a certain extent fixed by the choice of the initial expansion coefficients. As a result, the solutions are found over a wide range of energies, and there is no way to ensure that a low lying solution will be found for a given choice of the start coefficients. In larger systems, where storage limitations

may make it necessary to eliminate the inversion problem inherent in the Newton–Raphson method, it may be advantageous to use the imaginary time step method [12] to solve Eq. (11a) and (11b).

We propose a method that is a combination of both methods above. Starting from a set of coefficients, we first perform a few diagonalization iterations to rearrange the single particle orbitals such that those corresponding to the lowest single particle energies are occupied. The resulting coefficients are then used as initial values for a Newton–Raphson type minimization with any necessary penalty functions, which allows us to generate a distinct set of low-lying solutions.

Solutions may be generated in specific symmetry classes, for example, axial or time reversal symmetry, by generating start coefficients with a definite symmetry. Both the Hartree–Fock and Newton–Raphson procedures preserve the symmetries of the coefficients [13, 4], provided that the solutions used in the penalty functions have the same symmetry as that of the start coefficients. Hence it is generally worthwhile to look for solutions with a definite symmetry before attempting to find solutions that do not possess any symmetry.

3. Numerical Results

In the present work we have attempted to find the lowest lying axially symmetric HF states with isospin $T=0$ in ^{20}Ne. The ^{20}Ne nucleus has been taken to consist of an inert ^{16}O core plus four active valence particles in the 2s–1d shell. In the 2s–1d shell we used an effective Hamiltonian with the Vary–Yang interaction [14], including additional third-order corrections to the G matrix to provide a more complete accounting of the core polarization effects [15] and the following single particle energies:

$$e_{d_{5/2}} = -5.00 \text{ MeV}$$

$$e_{d_{3/2}} = 0.08 \text{ MeV}$$

$$e_{s_{1/2}} = -4.13 \text{ MeV}.$$

To solve the HF equations, the HF orbitals were expanded in a truncated harmonic oscillator basis with expansion coefficients $\{d_\nu^i\}$. Isospin symmetry was respected, yielding a twofold degeneracy in the HF orbitals and guaranteeing solutions of the HF equations with $T=0$.

It should be noted that if one is only interested in the HF ground state for a deformed nucleus, choosing the appropriate Nilsson single-particle orbitals backexpanded in a harmonic oscillator basis for the occupied orbitals is an ideal choice, yielding a converged solution of the HF equations in a few iterations. Choosing simple low-lying 1p–1h excitations in either the Nilsson basis or, with respect to the HF ground state as the initial guess for the occupied orbitals, does not, however, in general lead to low-lying solutions of HF equations. In fact, previous calculua-

tions in ^{20}Ne with a slightly different interaction seem to indicate that the important low-lying basis states have a large component of 4p–4h configurations with respect to the HF ground state [1]. Furthermore, earlier shape mixing calculations [16] have pointed out that a simple nonself-consistent basis containing the HF ground state, plus low-lying one-particle one-hole excitations with respect to the HF ground state is not sufficient to approximate the low-lying $T=0$ spectrum in ^{20}Ne.

To test the proposed strategy for finding the lowest lying solutions of the HF equations we have therefore randomly constructed 15 different sets of expansion coefficients for the occupied orbitals in ^{20}Ne, each of which possesses axial as well as time-reversal symmetry. These sets of expansion coefficients were used as the initial guesses in all the numerical calculations.

In Table I we present the results in which no penalty functions have been used. Repeated diagonalizations of the HF Hamiltonian, starting with the aforementioned sets of expansion coefficients, in the majority of cases yields the lowest lying solution or the HF ground state. Three other low lying solutions are also found, again in every instance more than once. If no diagonalization of the HF Hamiltonian is performed and the solutions are obtained via the Newton–Raphson method without penalty functions, the majority of the solutions have variational energies that do not lie very low. In fact, one does not even obtain the ground state solution. We do not always find a solution for each set of expansion coefficients as we have limited the number of iterations in the Newton–Raphson method to 200. As the number of mutual diagonalizations of the HF Hamiltonian is increased, the solutions found tend towards the same subset of multiple low-lying solutions obtained via the diagonalization procedure. When the Newton–Raphson method

TABLE I

The Variational Energies of the Solutions of the HF Equations in MeV Obtained from a Set of 15 Randomly Constructed Initial Choices of the Expansion Coefficients of the Occupied Orbitals, which Have Both Time Reversal as well as Axial Symmetry

0	1	2	3	HF
	−38.964(3)	−38.964(7)	−38.964(6)	−38.964(7)
−30.609(2)	−30.609(2)	−30.609(3)	−30.609(2)	−30.609(2)
−30.111		−30.111	−30.111(2)	−30.111(2)
−29.564(1)	−29.564(2)			
			−27.891(3)	−27.891(4)
−27.552(2)	−27.552(3)	−27.552(1)		
− 2.489(5)				
− 2.064(2)				

Note. No penalty functions have been used. The first columns give the solutions obtained when 0–3 diagonalizations of the HF Hamiltonian have been performed. The numbers in parentheses refer to the number of times the solution has been obtained. In the last column the solutions are obtained via the HF diagonalization procedure.

TABLE II

The Variational Energies of the Solutions of the HF Equations in MeV Obtained from the Same Set of 15 Start and Number of Diagonalizations of the HF Hamiltonian Coefficients Used in Table I

0	1	2	3
−38.964	−38.964	−38.964	−38.964
−30.609	−30.609	−30.609	−30.601
	−29.564	−29.564	−29.564
	−27.891	−27.891	−27.891
−27.552	−27.552	−27.552	−27.552
− 2.496			
− 2.064			− 2.064

Note. Penalty functions have been used to eliminate repeated solutions.

has been preceded by three diagonalizations of the HF Hamiltonian, essentially the same subset of multiple solutions is obtained as in the diagonalization procedure.

In Table II the results in which penalty functions have been used to eliminate finding the same solution more than once are given. If at least one diagonalization has been performed before the Newton–Raphson method is applied, we have been able to obtain five of the six lowest lying solutions of the HF equations. In most cases we do not find more than about five solutions. In part this is due to the fact that after some of the solutions have been found, it is increasingly more difficult to find a set of start coefficients that is linearly independent to the previously obtained HF solutions. We suspect that this is why we have not found the HF solution with the variational energy of −30.111. Lastly, because the penalty multipliers must eventually be reduced to zero, solutions of Eq. (6) must be found for decreasing values of β. Again, we have limited the maximum number of iterations in Newton–Raphson for each value of β to 200. In some cases converged solutions were not always obtainable for this number of allowed iterations.

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