Dynamical basis generation method with an application to the four-nucleon problem

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A variational method inspired by the Hartree-Fock approximation but not restricted to a single Slater determinant trial space is investigated. The physical motivation is that a method should attempt to find a subspace of collective states which are most strongly coupled to the ground state. This method attempts to do this by providing a systematic technique to generate basis states from the collective Hartree-Fock type of state. In the resulting basis space a residual diagonalization is easily performed. Results of a test with the four-nucleon problem with realistic effective nuclear Hamiltonians are shown.

I. INTRODUCTION

In nuclear structure studies one is often only interested in the low-lying bound states. Consequently, if one does not need the corresponding complete set of eigenstates, the large diagonalizations which occur in a shell-model calculation may be avoided. This is the motivation for shape mixing calculations in deformed nuclei, where one mixes solutions of the Hartree-Fock (HF) equations, which frequently possess different deformations or shapes. Configuration mixing calculations have also been performed with configurations constructed from one-particle—one-hole (1p-1h) excitations of the ground state.

From a theoretical standpoint there is clear motivation to base an approach on the variational principle, as the many-body Schrödinger equation arises from it when no restrictions are placed on the trial wave functions (TWF's). Approximations are then introduced simply by restricting the class of admissible TWF. In the HF case the TFW is a single Slater determinant. Improvements of the HF case can then be obtained by enlarging the class of TWF to include more configurations, and one obtains the multiconfiguration HF approach (MCHF).[1] Here, however, one often confronts the problem of not knowing *a priori* which configurations should be included. Progress in this respect has been achieved by Miller *et al.*,[2–5] who have proposed a systematic approach for generating a set of basis states via variational methods. These states can then be used in configuration mixing calculations, providing a good description of the lowest-lying states of a many-body system. The essential idea of Miller *et al.* is that of generating a set of basis states which are all solutions to the HF variational equations.[2–5] Quite interesting results are obtained, but one still faces the technical difficulty of solving the HF problem not only once, but as many times as the number of basis states desired.

The purpose of the present work is to employ a method developed by Bozzolo *et al.*[6] and already applied to a soluble model. This method is based on the variational principle, as is the one of Miller *et al.*, and it constitutes a more efficient way of generating the basis states that precede a configuration mixing calculation.

The paper is organized as follows: Section II presents a summary of the formalism so that the present work is self-contained, while Sec. III deals with some practical considerations. Section IV presents our results and conclusions.

II. FORMALISM

According to Thouless,[7] the unperturbed ground state of a N-fermion system ($|\Phi_0\rangle$) and the corresponding Hartree-Fock state ($|\mathrm{HF}\rangle$) are related by means of a unitary transformation $\exp(iF)$

$$|\mathrm{HF}\rangle = \exp(iF)\,|\Phi_0\rangle\ , \tag{1}$$

where F is a one-body operator to be determined by the variational principle applied to the many-body Hamiltonian H,

$$\delta\langle \mathrm{HF}\,|\,H\,|\,\mathrm{HF}\rangle = 0\ . \tag{2}$$

We can truncate the expansion of $\exp(iF)$ to obtain the Kth order of approximation to the HF ground state energy,[8]

$$E(K) = \sum_{n=0}^{K} \frac{1}{n!}\left[\sum_i t_{ii}^{(n)} + \tfrac{1}{4}\sum_{ij}\left(V_{ijij}^{(n)} - V_{ijji}^{(n)}\right)\right]\ , \tag{3}$$

where the quantities $t^{(n)}$ and $V^{(n)}$ are obtained from the kinetic energy and two body potential, respectively. They can be easily determined if we make use of the commutation relationship between H and F:

$$t_{ij}^{(n+1)} = i\sum_{\alpha\beta}\left[f_{\alpha\beta}\left(t_{i\alpha}^{(n)}\delta_{\beta j} - t_{\beta j}^{(n)}\delta_{i\alpha}\right) + f_{\alpha\beta}^{*}\left(t_{i\beta}^{(n)}\delta_{\alpha j} - t_{\alpha j}^{(n)}\delta_{\beta i}\right)\right], \tag{4}$$

$$\begin{aligned} V_{ijkl}^{(n+1)} = i\sum_{\alpha\beta}\big[&f_{\alpha\beta}\left(V_{ij\alpha l}\delta_{\beta k} + V_{ijk\alpha}^{(n)}\delta_{\beta l} - V_{i\beta kl}^{(n)}\delta_{\alpha j} - V_{\beta jkl}^{(n)}\delta_{\alpha i}\right) \\ &+ f_{\alpha\beta}^{*}\left(V_{ij\beta l}^{(n)}\delta_{\alpha k} + V_{ijk\beta}^{(n)}\delta_{\alpha l}\right. \\ &\left. - V_{i\alpha kl}^{(n)}\delta_{\beta j} - V_{\alpha jkl}^{(n)}\delta_{\beta i}\right)\big]\ , \end{aligned} \tag{5}$$

$$V^{(0)}_{ijkl}=V_{ijkl};\quad t^{(0)}_{ij}=t_{ij};\quad \alpha\notin\Phi_0,\quad \beta\in\Phi_0\ . \tag{6}$$

The parameters $f_{\alpha\beta}$ are the matrix elements of the operator F and are determined by minimizing, for successive values of K, the approximate ground state energy $E(K)$.

Off hand we do not know how many solutions for the parameters f will be obtained, but we do know that these solutions should approximate solutions of Eq. (2). That is, each set of parameters should approximate a local minimum or maximum of the Hartree-Fock energy surface. Since our interest is to generate an efficient basis for the low-lying spectra, the approximate solutions corresponding to local minima of the HF energy surface would be a natural choice. Here we demonstrate how to generate such a basis in a convenient fashion.

Suppose now that at order K, we obtain M different sets of parameters f. We can then determine a nonorthonormal, undercomplete basis given by the states generated with the M different solutions so obtained:

$$|\Psi^{(j)}_K\rangle=\exp(iF_j)\,|\Phi_0\rangle\quad j=1,\ldots,M\ . \tag{7}$$

We then diagonalize in this undercomplete basis. This yields the following generalized eigenvalue problem:

$$\sum_{j=1}^{M} H^{(K)}_{ij}d^{(K)}_j=E^{(K)}\sum_{j=1}^{M}\sigma^{(K)}_{ij}d^{(K)}_j\quad i=1,\ldots,M\ , \tag{8}$$

where

$$H^{(K)}_{ij}=\langle\psi^{(i)}_K\,|\,H\,|\,\psi^{(j)}_K\rangle \tag{9}$$

and

$$\sigma^{(K)}_{ij}=\langle\psi^{(i)}_K\,|\,\psi^{(j)}_K\rangle\ . \tag{10}$$

The lowest eigenvalue of Eq. (8) will be our new approximation, at order K for the ground state energy.

III. PRACTICAL CONSIDERATIONS

A. Evaluation of matrix elements in the dynamical basis

The evaluation of the matrix elements of H in the dynamical basis (9) is the most time-consuming aspect of the calculation. It is useful to derive a recursive algorithm which would enable us to go from a given order or approximation K to the next one in a more efficient way.

By expanding the unitary operator $\exp(iF)$ implicit in (9), we obtain

$$H^{(K)}_{ij}=\sum_{\lambda\mu\sigma\tau}H_{\lambda\mu\sigma\tau}\sum_{\substack{n=0\\ n+m\le K}}^{K}\sum_{m=0}^{K}\frac{(-1)^{n_i n+m}}{n!m!}X^{(i,j)}_{n,m} \tag{11}$$

with

$$X^{(i,j)}_{n,m}=\langle\Phi_0\,|\,F^n_i a^\dagger_\lambda a^\dagger_\mu a_\tau a_\sigma F^m_j\,|\,\Phi_0\rangle\ . \tag{12}$$

The underlying philosophy of this approach is that the coefficients f are suitable expansion parameters. Hence, in obtaining all ingredients for our calculations we consistently retain all contributions to the same fixed order in f. This leads to the restricted sums in (11). By inspection of Eq. (11) we are able to obtain a recursive relationship between $H^{(K-1)}_{ij}$ and $H^{(K)}_{ij}$, namely,

$$H^{(K)}_{ij}=H^{(K-1)}_{ij}+\frac{i^K}{K!}\sum_{\lambda\mu\sigma\tau}H_{\lambda\mu\sigma\tau}\sum_{r=0}^{K}\begin{bmatrix}K\\ r\end{bmatrix}(-1)^r X^{(i,j)}_{r,K-r}\ . \tag{13}$$

We have a number of symmetries which further simplify the calculations:

$$(-1)^K[X^{(j,i)}_{r,K-r}]^*=X^{(i,j)}_{r,K-r}\ , \tag{14}$$

$$[X^{(j,i)}_{m,n}]^*=X^{(i,j)}_{n,m}\ , \tag{15}$$

$$X^{(i,j)}_{mn}=(-1)^{n+m}X^{(i,j)}_{nm}\ . \tag{16}$$

The next stage is to evaluate the quantities $X^{(i,j)}_{nm}$ which are Φ_0 expectation values of disordered strings of creation and destruction operators. We address this problem in a simple way by means of the following result:[9]

$$\langle\Phi_0\,|\,a^\dagger_{x_1}a^\dagger_{x_2}\cdots a^\dagger_{x_N}a_{y_N}\cdots a_{y_2}a_{y_1}\,|\,\Phi_0\rangle = D\begin{Bmatrix}y_1\cdots y_N\\ x_1\cdots x_N\end{Bmatrix}_{\phi_0}, \tag{17}$$

where

$$D\begin{Bmatrix}y_1\cdots y_N\\ x_1\cdots X_n\end{Bmatrix}_{\phi_0}$$

is an $N\times N$ determinant with elements $\delta_{x_i y_i}$ and where all states $x,\ y\in\phi_0$. Using the properties of determinants, it is then quite easy to evaluate quantities like (17).

B. The choice of $|\Phi_0\rangle$

As a final practical consideration, we note that it is important to have an easy initial test since it yields a linear set of equations which may be rapidly solved before proceeding with the full problem. Furthermore, we will suggest how to use the $K=2$ case to improve $|\Phi_0\rangle$ if the initial choice of $|\Phi_0\rangle$ is found to be unsuitable.

In the $K=2$ case, the minimization problem is reduced to that of solving a linear set of equations,

$$\sum_{\tau}\epsilon_{\sigma\tau}f_{\tau\mu}-\sum_{\nu}\epsilon_{\nu\mu}f_{\sigma\nu}-\sum_{\tau\nu}\{f_{\tau\nu}V_{\sigma\nu\tau\mu}+f^*_{\tau\nu}V_{\sigma\tau\mu\nu}\}=i\epsilon_{\sigma\mu}\qquad \begin{matrix}\sigma,\tau\in\phi_0\\ \mu,\nu\notin\phi_0\end{matrix} \tag{18}$$

for N fermions, with

$$\epsilon_{\alpha\beta}=t_{\alpha\beta}+\sum_{\mu=1}^{N}V_{\alpha\mu\beta\mu}\ . \tag{19}$$

Equations (18) and (19) were originally proposed by Mann and Gross.[9]

The advantage in studying this case is not only its extreme simplicity from the numerical point of view, but

also it provides us with a criterion to establish the suitability of our reference state. If after solving (18) we obtain values for the parameters f small enough to warrant a second order approximation, then $|\Phi_0\rangle$ can be considered a good choice for a more extensive calculation. In other words, $|\Phi_0\rangle$ appears to be a reasonable initial approximation to $|\mathrm{HF}\rangle$.

For a higher order of approximation ($K>2$), the problem becomes nonlinear and it is convenient to then use the recursive method of Eq. (13) done with a computer. However, we quote in the Appendix the expressions for $K=3$ for the approximate energy, in order to provide at least one critical test for the application for the recursive method.

For those situations in which the solution of Eqs. (18) and (19) show that $|\phi_0\rangle$ is not a suitable reference state, we use a recently developed method which gives a definite prescription for the construction of a good starting Slater determinant. This is called the modified second order approximation (MSOA). This involves choosing an arbitrary one-parameter unitary transformation in which

$$c_\alpha^\dagger = \sum_\beta d_{\alpha\beta}(\theta) a_\beta^\dagger , \tag{20}$$

where the $d_{\alpha\beta}(\theta)$ are the conventional matrices of the rotation group[10] and where θ is chosen to minimize $\langle\phi_0(\theta)|H|\phi_0(\theta)\rangle$. We found that this scheme is adequate for choosing the reference state ϕ_0 so that out "perturbative" approach is efficient. Of course, many linear transformations which mix single particle (s.p.) levels in the vicinity of the Fermi level will probably suffice in order to determine an adequate $|\phi_0\rangle$, the detailed form being a matter of convenience.

IV. RESULTS AND CONCLUSIONS

As an application of the method outlined in this work, we studied the ^{4}He nucleus, focusing our attention on the total binding energy E. We made use of the realistic effective Hamiltonian described in Ref. 8, which is based on the Reid soft core potential[11] and evaluated in a harmonic oscillator basis. We compare our results with those obtained from a spherical HF calculation (SHF) in the full two space ($0s$-$0p$ and $1s$-$0d$ shells). We also quote the results of an exact diagonalization in the two space. Our calculations were done in a particular subspace of the full two space, in which we retain only the s orbitals. The exact problem is then a 70×70 diagonalization.

As discussed in Sec. III B, we begin by using the $K=2$ case to test the acceptability of $|\Phi_0\rangle$. The reference state $|\phi_0\rangle$ chosen initially for our calculation consists of fully occupied orbitals. Table I shows the labeling adopted for the s.p. states. Within this subspace of the full two-space, Eq. (18) yields the following results for the parameters f:

$$f_{31}=f_{42}=f_{75}=f_{86}=-0.45i ; \tag{21}$$

all others are 0.

When these coefficients are substituted into Eqs. (3)—(5), we obtain the result that $E(K=2)=-30.896$ MeV. However, the result is immediately suspect, since the f coefficients deviate substantially from zero and we have not accounted for renormalization of the TWF in our application of the variational method. This problem has been studied extensively[8] and as mentioned in Sec. III B one way to overcome this difficulty is to use the MSOA approach. Here we simply mix states with the same projection of spin and isospin but with different principal quantum numbers, as follows:

$$\begin{aligned} |1'\rangle &= \cos\theta\,|1\rangle + \sin\theta\,|3\rangle , \\ |3'\rangle &= -\sin\theta\,|1\rangle + \cos\theta\,|3\rangle . \end{aligned} \tag{22}$$

The symmetry seen in the second order results [Eq. (21)] is conserved by this unitary transformation. The angle θ is determined by minimizing the transformed reference state expectation value of H, yielding $\bar\theta=0.242$. The corresponding results for the parameters f and the new approximate ground state energy are

$$f_{31}(\bar\theta)=f_{42}(\bar\theta)=f_{75}(\bar\theta)=f_{86}(\bar\theta)=-0.59.10^{-6}i ; \tag{23}$$

all others $=0$, and

$$E_{\mathrm{MSOA}}(\bar\theta)=-27.486 \text{ MeV} . \tag{24}$$

Thus we have faced the difficulty discussed in Sec. III B and have overcome it with the simple implementation of the MSOA method. In this particular simple example the MSOA and spherical Hartree-Fock are equivalent but, in general, the MSOA is more limited than spherical Hartree-Fock.[8]

For higher orders of approximation ($K>2$), we face the numerical problem of a 32-parameter minimization. This number of variables does not depend on the order of approximation k, but does depend on the model space we have chosen.

A first attempt to solve the $K>2$ problem within a small model space could indicate simplifications which can be made when going to larger spaces. From the MSOA results [see Eqs. (23) and (24)], we see that we can restrict ourselves to the search of only one variable, which is the imaginary part of, say, f_{31}. When proceeding to higher orders of approximation the problem becomes nonlinear and therefore the energy surface may possess several maxima and minima.

TABLE I. Sequence numbers assigned to single particle orbitals in a harmonic oscillator basis. The principal quantum number is n, the magnetic projection is m_j, and the isospin projection is m_t.

	n	m_j	m_t
1	0	$-\frac{1}{2}$	$-\frac{1}{2}$
2	0	$\frac{1}{2}$	$-\frac{1}{2}$
3	1	$-\frac{1}{2}$	$-\frac{1}{2}$
4	1	$\frac{1}{2}$	$-\frac{1}{2}$
5	0	$-\frac{1}{2}$	$\frac{1}{2}$
6	0	$\frac{1}{2}$	$\frac{1}{2}$
7	1	$-\frac{1}{2}$	$\frac{1}{2}$
8	1	$\frac{1}{2}$	$\frac{1}{2}$

TABLE II. Ground state energies of the four-nucleon system in the $0s$-$0p$—$1s$-$0d$ space within various approximations. The first entry is for a single Slater determinant of harmonic oscillator wave functions ($h\omega=22$ MeV). The SHF results involve radial mixing of s orbitals only as do the MSOA results. The main results of this paper are the $K=2$ (third order) and $K=3$ results with residual 2×2 and 3×3 diagonalizations, respectively.

$\langle\phi_0 \mid H \mid \phi_0\rangle$	−21.866 MeV
SHF (spherical Hartree-Fock, two space)	−27.486 MeV
$\langle\phi_0(\bar{\theta}) \mid H \mid \phi_0(\bar{\theta})\rangle$ (MSOA, second order)	−27.486 MeV
Third order (2×2 diagonalization)	−27.590 MeV
Fourth order (3×3 diagonalization)	−27.667 MeV
Exact diagonalization	−27.669 MeV

At this stage of our applications we found it practical merely to retain those sets of coefficients for which all numbers were smaller (in absolute value) than some critical value. Of course, in applications with larger model spaces we would be motivated to evaluate the expectation value of H for each set and eliminate those sets corresponding to maxima in the energy surface. With this criterion in mind, we proceed to the third and fourth order of approximation, using the reference state determined by the MSOA approach. Two basis states were selected from the third order approximation (with $|f|<0.1$) and three from the fourth order approximation. This results in a 2×2 and a 3×3 diagonalization in the third and fourth order approximations, respectively.

Table II shows a summary of the results for the ground state energy. From this table we obtain a clear hierarchy of approximations to the ground state energy and ground state wave function. We start with the expectation value of H in a harmonic oscillator basis but encounter a major improvement in the SHF approximation due to the dominant role of radial mixing. The restricted application of the MSOA yields a wave function which coincides with SHF. From this stage there is a very rapid progression to the exact results with the method of dynamical basis generation proposed here. The $K=3$ approximation with two solutions retained for a residual 2×2 diagonalization produces a result already within 79 keV of the exact result. One further recursion to the $K=4$ approximation and a 3×3 diagonalization yields a ground state within 2 keV of the exact 70×70 diagonalization. These results demonstrate that this method of dynamical basis generation does appear to capture the essential physical phenomena of the ground state wave function with minimal effort. We are especially pleased to note that the mixing of only three states produced by this method yields a result within 2 keV of the exact result.

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APPENDIX

We can rewrite Eq. (3) as

$$E(K)=\tfrac{1}{2}\sum_{n=0}^{K}\frac{T^{(n)}}{n!}\ , \tag{A1}$$

where

$$T^{(n)}=\sum_{ij\in\phi_0}V_{ijij}^{(n)}+2\sum_{i\in\phi_0}t_{ii}^{(n)}\ . \tag{A2}$$

For $K=3$ we have for the $T^{(n)}$,

$$T^{(1)}=2i\sum_{\substack{AB\\ \alpha}}(f_{\alpha A}-f_{\alpha A}^{*})H_{AB\alpha B}\ , \tag{A3}$$

$$T^{(2)}=2\sum_{\substack{AB\\ \alpha\beta}}(f_{\alpha B}f_{\beta A}^{*}H_{A\alpha\beta B}+f_{\alpha A}f_{\beta A}^{*}H_{\alpha B\beta}-f_{\alpha B}f_{\beta A}H_{AB\beta\alpha})-2\sum_{\substack{ABC\\ \alpha}}f_{\alpha c}f_{\alpha A}^{*}H_{ABCB}+\text{H.c.}\ , \tag{A4}$$

and

$$\begin{aligned}T^{(3)}=&-4i\sum_{\substack{AB\\ \alpha\gamma}}\epsilon_{B\alpha}f_{\gamma B}f_{\gamma A}^{*}f_{\alpha A}-2i\sum_{\substack{AM\\ \alpha\gamma}}\epsilon_{A\alpha}f_{\alpha B}^{*}f_{\gamma B}f_{\gamma A}-4i\sum_{\substack{AB\\ \alpha\alpha'\gamma}}H_{A\alpha\alpha'\gamma}f_{\alpha\beta}^{*}(f_{\alpha' A}F_{\gamma B}^{*}-f_{\gamma A}^{*}f_{\alpha'\beta})\\ &-2i\sum_{\substack{ABC\\ \alpha\gamma}}H_{ABC\gamma}f_{\alpha c}^{*}(f_{\gamma A}^{*}f_{\alpha B}-f_{\alpha A}^{*}f_{\gamma B}+f_{\gamma A}f_{\alpha B}^{*})-2i\sum_{\substack{AB\\ \alpha\gamma}}\delta_{\gamma B}f_{\gamma A}f_{\alpha B}^{*}f_{\alpha A}\\ &-2i\sum_{\substack{ABC\\ \alpha\gamma}}{}'H_{CB\alpha A}f_{\alpha B}^{*}(f_{\gamma C}f_{\gamma A}^{*}+f_{\gamma C}^{*}f_{\gamma A})+\text{H.c.}\end{aligned} \tag{A5}$$

In all cases, A, B, $C\in\phi_0$ and α, α', $\gamma\notin\phi_0$.

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