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Minimization of energy and of energy variance for Slater determinants in nuclei

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Two distinct variational methods for obtaining single determinantal states in light spherical nuclei are studied. The first is the well-known Hartree-Fock method and the second is the minimization of the energy variance method. The equations for determining the self-consistent set of single particle orbits using the new variational procedure are derived. The widths of these states are also evaluated, which provide us with a measure of their departure from the exact eigenstates of the nuclear system. Perturbation theory corrections are also calculated for these determinantal states to estimate the correlation effects. A comparative study of the properties of the Slater determinants using the Hartree-Fock method and the new variational method is also made.

[NUCLEAR STRUCTURE Evaluation of variance for Hartree-Fock states, minimization of energy variance for Slater determinants.]

I. INTRODUCTION

Slater determinant is probably the most widely used approximate wave function for particles in a nucleus. In the last 10 years or so, such a determinant has very often been obtained by the Hartree-Fock (HF) method[1-4] in which one finds the determinant having the lowest energy. It is generally accepted that the HF approximation describes many nuclear properties, including the ground state energy well. In particular, some of the single-particle properties (expectation values of one-body operators in the HF state) show spectacular agreement[4] with experiments. In spite of the agreement one finds with the experiments it is not clear how "good" the HF wave function is. To be more precise, one does not know how well this approximate wave function compares with the "exact" solution of the Hamiltonian in the model space. Often one also does not know how the calculated properties would change with improvement in the wave function. It seems justified therefore not to strive for very good agreement between the HF results and the experimental ones without a proper investigation of corrections to the HF. In view of this, we make a modest beginning here of systematically studying these questions and also investigate a new variational procedure for obtaining Slater determinants. A more detailed discussion of some measures for testing approximate wave functions and the related variational principles is given in Sec. II.

Consider the HF solution for the nuclear system and evaluate its variance[5] $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$. The width σ provides us with a measure of departure of the approximate wave function from the exact solution for the system. Of course, this quantity by itself does not tell us how important the "correlation" effects are for the nuclear properties. One way of learning about these is to improve the wave function by the use of perturbation theory. We have therefore evaluated the correction to the HF wave function and the HF energy in perturbation theory. This is described in Secs. III and IV. The width may also be used as a measure for comparing two approximate wave functions. For example, given the widths of two determinantal states, one can say that the one with the smaller width is closer to the exact solution of the system. In Sec. IV we also discuss how the width of the HF state changes with a change in the size of the vector spaces. We also examine the changes in the ground state energy with this truncation and see how the width is related to the total energy spectrum span of the nuclear system.

Besides studying the HF solution we also examine in Sec. V an alternative variational procedure suggested earlier[6] to obtain determinantal states. In this we minimize the variance σ^2 for the system rather than the energy. It should be clear that the energy of the new determinant Ψ_σ will be higher than that of Ψ_{HF}, but its width will be smaller. If we therefore use the width as a measure of goodness of a wave function, then the state Ψ_σ is an improvement over Ψ_{HF}. Moreover, if we carry out perturbation theory corrections for Ψ_σ and Ψ_{HF}, we expect smaller 2p-h correction for Ψ_σ than for Ψ_{HF}. This is because in the determination of Ψ_σ we are already including some excitations to intermediate 2p-h states. Of course, as far as the energy criterion is concerned the HF solution is superior to the corresponding solution obtained by minimizing σ^2.

The numerical calculations in this paper are carried out for light spherical nuclei within the space of three and four harmonic oscillator shells.

Tabakin interaction has been used. It should be pointed out that the calculations we have carried out are meant for internal comparison of the two variational methods and for illustrating the various points we are making in the paper. It is not our aim to compare the results of our calculations with experimental quantities.

A discussion of the results and some concluding remarks are presented in Sec. VI.

II. MEASURES FOR APPROXIMATE WAVE FUNCTIONS AND CORRESPONDING VARIATIONAL PROCEDURES

We discuss in this section two measures for determining the goodness of an approximate wave function.

First we consider as a measure the width σ of the approximate state, which is defined through the variance σ^2. The variance σ^2 for a state $|\Psi\rangle$ is defined to be

$$\sigma^2(\Psi) = \langle\Psi|H^2|\Psi\rangle - \langle\Psi|H|\Psi\rangle^2 , \tag{2.1}$$

where H is the Hamiltonian of the system. It follows from this definition that if $|\Psi\rangle$ is an exact eigenstate of H then its width σ is zero. Otherwise, $|\Psi\rangle$ will have a nonzero width which will give us a measure of the departure of $|\Psi\rangle$ from an eigenstate of H.

In order to get some more understanding of the quantity σ, consider the expansion of $|\Psi\rangle$ over the complete set of eigenstates $|\phi_k\rangle$ of our system. We have

$$|\Psi\rangle = \sum \alpha_k |\phi_k\rangle ,$$

where α_k are the coefficients of expansion. A plot of the intensities $|\alpha_k|^2$ versus energy will then provide a picture of the way in which the state $|\Psi\rangle$ is distributed over the exact eigenstates of H. In practice, we seldom know all the α_k's and E_k's, and hence we will not be able to determine the distribution of $|\Psi\rangle$. Let us suppose, however, that we know the energy and the variance of $|\Psi\rangle$. These can be written as

$$\begin{aligned} E &= \langle\Psi|H|\Psi\rangle = \sum_k |\alpha_k|^2 E_k , \\ \sigma^2(\Psi) &\equiv \mu_2 = \sum_k |\alpha_k|^2 E_k^2 - \left(\sum_k |\alpha_k|^2 E_k\right)^2 . \end{aligned} \tag{2.2}$$

We see from these equations that E is the mean energy and σ^2 the second central moment of the distribution—i.e., these are the lowest two moments of the distribution. As we evaluate higher central moments $\mu_p = \langle\Psi|(H-E)^p|\Psi\rangle$ $(p>2)$, we learn more and more about the distribution. It should be clear, therefore, that after the energy the variance is the next simplest quantity that we can evaluate for a state $|\Psi\rangle$. Note that the energy of a state by itself gives no indication at all about the goodness of the wave function, but the width does provide some information. In fact, it gives the spread of $|\Psi\rangle$ over the actual eigenstates of H.

Further, it can be shown by making use of the expansion in Eq. (2.1) that the width can be used to give both a lower and an upper bound to an exact eigen energy of the system. More precisely, we have the relation

$$E - \sigma \leq E_0 \leq E + \sigma ,$$

where E and σ are the energy and the width of the approximate state Ψ, and E_0 is the exact eigen energy closest to E—i.e., $|E-E_0| < |E-E_k|$ for all E_k. Thus, if E is closest to the exact ground state energy then the lowest two moments provide bounds to the exact ground state energy.

Another possible measure which is often used is the overlap of the approximate state $|\Psi\rangle$ with the exact ground state wave function. This is generally very difficult if not impossible to have. Thus this measure is available only in some restricted problems and hence has limited usefulness.

It is worthwhile recalling at this stage that, among variational solutions, the one with the lower energy does not necessarily have a smaller width or a larger overlap with the exact ground state. Furthermore, a smaller width does not imply a larger overlap with the ground state either. Thus the energy, the width, and the overlap provide different criteria for discussing approximate wave functions.

Further, corresponding to each of these criteria one can set up a variational procedure. It should be evident that if we allow for the most general variation in the wave function then each procedure would be equivalent to solving the Schrödinger equation. It is when we put restriction on the variational wave functions that we obtain different variational solutions. For determinantal states, the energy minimization leads to the well-known Hartree-Fock procedure. The minimization of σ^2 for Slater determinants will be discussed in detail in Sec. V and the optimization of the overlap has been considered by Kelson and Shadmon.[9]

III. HARTREE-FOCK APPROXIMATION

There are already many articles[1-4] on the HF approximation and hence we give very few details about the method here.

If Ψ is a Slater determinant describing the states of an A-particle system, then we can write it as

$$|\Psi\rangle = \prod_{i=1}^{A} a_i^\dagger |0\rangle ,$$

where the operator $a_i^\dagger$ creates a fermion in the orbit i, and so on. These $a_i^\dagger$ and the corresponding destruction operators a_i obey the well-known fermion anticommutation rules. In this formalism the Hamiltonian $\mathcal{H}$ of the system has the form shown in Eq. (3.1):

$$\mathcal{H} = \sum_{\mu\nu} \langle \mu | t | \nu \rangle a_\mu^\dagger a_\nu + \frac{1}{4} \sum_{\substack{\mu\nu \\ \mu'\nu'}} \langle \mu\nu | V^A | \mu'\nu' \rangle a_\mu^\dagger a_\nu^\dagger a_{\nu'} a_{\mu'} . \quad (3.1)$$

Here t is the kinetic energy operator $p^2/2m$ and $\langle \mu\nu | V^A | \mu'\nu' \rangle$ is an antisymmetrized matrix element of the two-body interaction. The single-particle states $\mu, \nu, \ldots$ belong to a complete orthonormal set. Before we proceed further we describe the notation used in this work. For details we refer the reader to Ref. 3. The occupied single-particle orbits will be denoted by the Greek letters $\alpha, \beta, \gamma, \lambda, \ldots$, and the unoccupied ones by $i, j, k, l, \ldots$.

In our work the ground state wave function is approximated by a single spherically symmetric Slater determinant having the lowest energy. Such an assumption seems to be reasonable for double-closed shell nuclei like ^{4}He, ^{16}O, ^{40}Ca, etc. Such calculations have been reported earlier in literature[1,3,4]. The assumption of spherical symmetry means that each single-particle orbit is a linear combination of harmonic oscillator (ho) states having the same angular momentum quantum numbers l and j but different radial quantum numbers n. Thus we have

$$|(ljm\tau)_\alpha\rangle = \sum_{n_\alpha} C_{n_\alpha}^\alpha |n_\alpha l_\alpha j_\alpha m_\alpha \tau_\alpha\rangle = \sum_{n_\alpha} C_{n_\alpha}^\alpha |n_\alpha s_\alpha m_\alpha \tau_\alpha\rangle , \quad (3.2)$$

where m stands for the projection of j along the z axis and τ is the third component of the isospin of the nucleon. Also, s_α denotes in a compact way the quantum numbers l_α, j_α. In the HF wave function the expansion coefficients C_n^α are such that they characterize the determinant having the lowest energy.

Since we are concerned with light nuclei the center-of-mass motion cannot be neglected, and its effect on the HF wave function, its energy, and width have to be properly taken care of. The operator for the center-of-mass energy is $\vec{P}^2/2mA$, where $\vec{P}$ is the total momentum. If we subtract $\vec{P}^2/2mA$ from the total nuclear Hamiltonian we get the intrinsic Hamiltonian H,

$$H = \mathcal{H} - \vec{P}^2/2mA . \quad (3.3)$$

All the calculations described in this paper have been carried out with the intrinsic Hamiltonian H of Eq. (3.3). This method for including the center-of-mass motion (c.m.m) correction was used by Kerman, Svenne, and Villars.[1]

Having obtained the HF wave function we can improve upon it by including 2p-2h corrections to it in perturbation theory. It should be pointed out that by definition the Hamiltonian H does not connect the HF state with 1p-1h state. We can also evaluate the second-order correction $E(2)$ in energy. The expression for the total energy E is given by

$$E = E_{\rm HF} + E(2) ,$$

where

$$E(2) = -\frac{1}{4} \sum_{\alpha\beta kl} \frac{\langle \alpha\beta | H | kl \rangle \langle kl | H | \alpha\beta \rangle}{\epsilon_k + \epsilon_l - \epsilon_\alpha - \epsilon_\beta} . \quad (3.4)$$

Here ϵ_i refer to the HF single-particle energies.

The wave function corrected to first order may be written as

$$\Psi_{\rm HF}^{(1)} = \alpha \left[\Psi_{\rm HF} + \sum_i C_i \Psi_i \right] . \quad (3.5)$$

Here α^2 is the intensity of the HF state, and C_i^2 is the intensity evaluated in second-order perturbation theory of the 2p-2h state Ψ_i. The normalization condition is given by $\alpha^2[1 + \sum_i C_i^2] = 1$.

IV. WIDTHS OF HF WAVE FUNCTIONS

A. A method for evaluating widths

Now we describe in detail a method[5] for evaluating the variance defined in Eq. (2.1). To evaluate it we make an intermediate state expansion in the complete set of particle-hole (p-h) states built on the wave function Ψ. The Eq. (2.1) leads to

$$\sigma^2(\Psi) = |\langle \Psi | H | \Psi_{0\rm ph} \rangle|^2 + \sum_{\rm 1ph} |\langle \Psi | H | \Psi_{1\rm ph} \rangle|^2 + \sum_{\rm 2ph} |\langle \Psi | H | \Psi_{2\rm ph} \rangle|^2 - |\langle \Psi | H | \Psi \rangle|^2 . \quad (4.1)$$

Note that the series on the right-hand side in Eq. (4.1) terminates at two particle-hole states since H, being a two-body operator, will not connect states higher than 2 p-h states to the ground state. Now, since $|\Psi_{0\rm ph}\rangle \equiv |\Psi\rangle$, the first and last terms in Eq. (4.1) are identical. Thus we get

$$\sigma^2(\Psi) = \sum_{\rm 1ph} |\langle \Psi | H | \Psi_{1\rm ph} \rangle|^2 + \sum_{\rm 2ph} |\langle \Psi | H | \Psi_{2\rm ph} \rangle|^2 . \quad (4.2)$$

From Eq. (4.2) we see that the width of the wave function $|\Psi\rangle$ arises from the one particle-hole and

two particle-hole excitations only.

Since the Hamiltonian H cannot connect the HF states with the 1p-h states, we obtain for the width of the HF state

$$\sigma^2(\Psi_{\mathrm{HF}}) = \sum_{2\mathrm{ph}} |\langle \Psi_{\mathrm{HF}} | H | \Psi_{2\mathrm{ph}} \rangle|^2 . \tag{4.3}$$

We see therefore that the width of the HF ground state arises purely from the 2p-h excitations.

We now give explicit expressions for the variance. In the formalism of second quantization we can write

$$\begin{aligned} |\Psi_{1\mathrm{ph}}\rangle &= a_k^\dagger a_\alpha |\Psi\rangle , \\ |\Psi_{2\mathrm{ph}}\rangle &= a_k^\dagger a_l^\dagger a_\alpha a_\beta |\Psi\rangle . \end{aligned} \tag{4.4}$$

With these the Eqs. (4.2) and (4.3), respectively, reduce to Eqs. (4.5) and (4.6):

$$\sigma^2(\Psi) = \sum_{\alpha k} \langle \alpha | \tilde{\epsilon} | k \rangle \langle k | \tilde{\epsilon} | \alpha \rangle + \frac{1}{4} \sum_{\alpha\beta kl} \langle \alpha\beta | V^A | kl \rangle \langle kl | V^A | \alpha\beta \rangle \tag{4.5}$$

and

$$\sigma^2(\Psi_{\mathrm{HF}}) = \frac{1}{4} \sum_{\alpha\beta kl} \langle \alpha\beta | V^A | kl \rangle \langle kl | V^A | \alpha\beta \rangle . \tag{4.6}$$

Here the matrix element $\langle \alpha | \tilde{\epsilon} | k \rangle$ of the single-particle Hamiltonian is given by

$$\langle \alpha | \tilde{\epsilon} | k \rangle = \langle \alpha | t | k \rangle + \sum_{\lambda=1}^{A} \langle \alpha\lambda | V^A | k\lambda \rangle . \tag{4.7}$$

B. Numerical results

We have carried out radial Hartree-Fock and width calculations for the double-closed shell nuclei ^{4}He, ^{16}O, and ^{40}Ca. The calculations were done in the space of the first four oscillator major shells. The single-particle orbits were expanded in the spherical oscillator basis states as described in Eq. (3.2). The correction due to the center-of-mass motion was included. The correction arising from Coulomb repulsion was, however, not considered. Thus the binding energies presented here refer to the nuclear energies only.

It should be pointed out that five distinct types of uncoupled matrix elements of V^A enter into the calculation of width. These are $\langle pp | V^A | pp \rangle$, $\langle pn | V^A | pn \rangle$, $\langle p\bar{p} | V^A | p\bar{p} \rangle$, $\langle p\bar{n} | V^A | p\bar{n} \rangle$, and $\langle p\bar{n} | V^A | \bar{p}n \rangle$. Here p stands for a proton in a certain state and $\bar{p}$ a proton in the time reversed state. Similarly for n and $\bar{n}$. Note that of these five types only the first four enter in the ordinary Hartree-Fock calculation.

We have done calculations using the Tabakin[7,8] matrix elements. We show in Table I the results of our calculation.

The HF energies for the Tabakin interaction are, as is well-known,[1] low compared with the experimental binding energies. Further, the second-order correction in energy $E(2)$ is approximately 20% of E_{HF} for ^{4}He and ^{16}O, which is not negligible. This was first noted by Kerman *et al.*[1] The widths σ are large for the HF solutions of all the nuclei shown. In ^{16}O the HF determinant has a spread of about 24 MeV about the HF energy. This large spread implies that the ground state wave function of ^{16}O (and of other nuclei discussed) cannot be described by a single HF determinant. In fact, the HF intensity shown in column 6 of the table gives us a measure of the importance of the HF state in the wave function corrected to first order [see Eq. (3.5)].

We see from the values of α^2 [see Eq. (3.5)] given in Table I that except for ^{4}He there is a sizable admixture of the 2p-h states in the other nuclei. In column 5, the rms radius r calculated using the HF determinant is shown. We have also studied the effect of the c.m.m term on the HF energy E_{HF} as well as the width σ_{HF}. We find that the HF energy for the Hamiltonian H [see Eq. (3.3)] is lower by about 11 MeV compared to that for the Hamiltonian $\mathcal{H}$. The width σ_{HF} is also smaller by about 2 MeV when the c.m.m term is included. This trend for both E_{HF} and σ_{HF} follows from the positive definite nature of the c.m.m term. Finally, recalling the discussion in Sec. II about the bounds on the exact energy, we see that the interaction used here may give an additional binding of about 3 MeV per particle in ^{4}He, 1.5 MeV per particle in ^{16}O, and 0.5 MeV per particle in ^{40}Ca.

TABLE I. Some properties of the HF ground states of spherical nuclei. Calculation in four oscillator major shells with c.m. correction. Interaction: Tabakin (b = 1.81 fm for ^{4}He and ^{16}O, b = 2.03 fm for ^{40}Ca).

Nucleus	E_{HF} (MeV)	$E(2)$ (MeV)	E(Total) (MeV)	r(HF) (fm)	α^2(HF)	Width (MeV)
^{4}He	−10.25	−1.93	−12.18	1.83	0.97	12.32
^{16}O	−44.29	−9.14	−53.43	2.42	0.86	24.29
^{40}Ca	−125.16	−15.67	−140.83	3.44	0.55	21.34

It should be emphasized again that the HF calculations of energy, rms radius, and the perturbation corrections to E_{HF} and Ψ_{HF} are meant basically for making comparisons with the results of the new variational method (see Sec. V). These quantities have been calculated earlier and in much larger spaces as well. Of course the evaluation of σ_{HF} has not been done before even in these primitive spaces.

C. Effect of enlarging the space

The spectroscopic space one deals with in nuclear physics is a finite vector space. Moreover, one also tries to simulate the effect of the real interaction in the Hilbert space by an effective interaction in the truncated space. Several interesting problems arise from this process of reducing the infinite Hilbert space. Here we ask ourselves the question how the widths are affected by truncating or equivalently by enlarging the given finite space. If a wave function calculated in a given space is transported into another larger space and allowed to spread there, one can then study the effect of the enlargement of space on the width of the wave function. We show in Table II the results of one such calculation. To start with, we made a spherical HF calculation for ^{16}O in three oscillator major shells. Then we opened the $0f$-$1p$ major shell and allowed the three-shell wave function to spread. As can be seen from Table II, this spread is greater than both the three major shell and four major shell HF widths. These calculations do not include c.m. correction. This result shows that a proper self-consistent solution in four shells (column 3) is a definite improvement over a three-shell HF solution considered in the space of four shells. The difference arises from the mixing of the $0p$ and $1p$ oscillator orbits.

We also show in columns 5 and 6 the width for the pure oscillator determinant $(0s)^4(0p)^{12}$ in the space of $N=3$ and $N=4$ oscillator shells. Again we see that the HF solutions are better in the sense of widths than the pure oscillator states.

Another feature we observe is that the widths become larger and larger as we enlarge the space. This would mean that as we carry out calculations in increasingly larger spaces the HF solution gets worse; in other words, there is an increasingly greater departure from the model eigenstate. We can understand this increase in width with increase in the size of the space as simply arising from a large number of states the HF state can mix with. It should be remembered, however, that although the HF state may have a sizable matrix element with a distant state, the mixing of this state (in the HF state) will be small because of the energy denominator which enters in the expression for the mixing amplitudes.

In view of this we have evaluated the ratio of the width with the spectrum span that the model nucleus has in the space. The spectrum span was determined by assuming the nuclear states (in a finite space) to have a Gaussian distribution[10] in energy. The parameters[10] which define the Gaussian density are the centroid energy and width. These were evaluated[10] and the ground state E_g determined by using Ratcliff's[10] procedure. The spectrum span was then taken to be $2(E_c - E_g)$. Although this method is probably not as accurate as some of the other methods suggested in Ref. 10, it provides a reasonable estimate of the spectrum span.

This ratio is shown in column 9 of Table II. We find that it is very small and more or less constant, implying thereby that in each case the HF state can mix appreciably with only those states which lie within this small fraction of the spectrum span.

Although in our examples the widths of the states increase with an increase in the size of the vector space, it might be interesting to consider interactions where the widths "saturate" as the space is enlarged. Note that since the width is a sum of squares of matrix elements, such a constraint on the interaction is nonperturbative and also more severe than demanding convergence in perturbation theory.

V. MINIMIZATION OF ENERGY VARIANCE

A. An alternative to Hartree-Fock method

We gave in Sec. III a brief description of the Hartree-Fock approximation to the ground state of

TABLE II. Effect of enlargement of space on width (σ). Nucleus is ^{16}O, N is the number of oscillator major shells in which σ was calculated.

Interaction	$\sigma(\Psi^N_{HF})$ (MeV)		$\sigma(\Psi^{N=3}_{HF}$ in four-major-shell space) (MeV)	$\sigma(\Psi^N_{\text{pure ho}})$ (MeV)		Spectrum span S		Ratio σ/S	
	$N=3$	$N=4$		$N=3$	$N=4$	$N=3$	$N=4$	$N=3$	$N=4$
Tabakin (b =1.81 fm)	18.29	26.49	29.99	19.41	30.73	461.44	672.034	0.0396	0.0394

a nucleus. However, the large widths seen in the HF determinants (see Sec. IV) imply that though the HF determinants are the best in the energy sense, they do not seem to be so in the width sense. Naturally, one would like to know whether a single Slater determinant designed to give minimum energy variance rather than minimum energy would provide a better description of the ground state of a nucleus.

Consider a Slater determinant $|\Psi\rangle$ for a nucleus consisting of A nucleons. Then with the energy variance $\sigma^2(\Psi)$ defined as in Eq. (2.1) we require that for a first-order variation in $|\Psi\rangle$ the variance σ^2 is stationary with the constraint that $|\Psi\rangle$ is normalized, i.e.,

$$\delta\sigma^2(\Psi) = 0 ,$$

where δ denotes the variation. Then from Eq. (2.1) we have

$$\delta(\langle\Psi|H^2|\Psi\rangle - |\langle\Psi|H|\Psi\rangle|^2) = 0 . \tag{5.1}$$

Since $|\Psi\rangle$ and its conjugate $\langle\Psi|$ can be varied independently, we choose to vary $\langle\Psi|$. Now for a first-order change in $\langle\Psi|$ we must have

$$\delta\langle\Psi| = \eta\langle\Psi_{1\text{ph}}| ,$$

where η is an infinitesimal and $\langle\Psi_{1\text{ph}}|$ is a one particle-hole state. With this the Eq. (5.1) becomes

$$\langle\delta\Psi|H^2|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\delta\Psi|H|\Psi\rangle = 0 ,$$

i.e.,

$$\langle\Psi_{1\text{ph}}|H^2|\Psi\rangle - 2\langle\Psi|H|\Psi\rangle\langle\Psi_{1\text{ph}}|H|\Psi\rangle = 0 . \tag{5.2}$$

In order to evaluate the first term in Eq. (5.2) we carry out an intermediate state expansion where we choose for the intermediate states the complete set of particle-hole (p-h) states $\{\Psi'_{n\text{ph}}\}$ ($n = 0, 1, 2, \ldots$) built on the state $|\Psi\rangle$. Note that the p-h states with $n \geq 3$ do not contribute to the first term in Eq. (5.2) because H is a two-body operator. Since $|\Psi'_{0\text{ph}}\rangle \equiv |\Psi\rangle$, Eq. (5.2) simplifies to

$$\sum_{\Psi'_{1\text{ph}}} \langle\Psi_{1\text{ph}}|H|\Psi'_{1\text{ph}}\rangle\langle\Psi'_{1\text{ph}}|H|\Psi\rangle + \sum_{\Psi'_{2\text{ph}}} \langle\Psi_{1\text{ph}}|H|\Psi'_{2\text{ph}}\rangle\langle\Psi'_{2\text{ph}}|H|\Psi\rangle - \langle\Psi|H|\Psi\rangle\langle\Psi_{1\text{ph}}|H|\Psi\rangle = 0 . \tag{5.3}$$

By expressing $|\Psi_{1\text{ph}}\rangle$, $|\Psi'_{1\text{ph}}\rangle$, and $|\Psi'_{2\text{ph}}\rangle$ in the second quantized notation as in Eq. (4.4) and making extensive use of Wick's theorem, we finally obtain the following equation:

$$\sum_l \langle k|\tilde{\epsilon}|l\rangle\langle l|\tilde{\epsilon}|\alpha\rangle - \sum_\beta \langle k|\tilde{\epsilon}|\beta\rangle\langle\beta|\tilde{\epsilon}|\alpha\rangle + \sum_{\beta l} \langle l|\tilde{\epsilon}|\beta\rangle\langle\beta k|V^A|l\alpha\rangle + \sum_{\beta l} \langle\beta|\tilde{\epsilon}|l\rangle\langle kl|V^A|\alpha\beta\rangle + \frac{1}{2}\sum_{\beta l m} \langle\beta k|V^A|lm\rangle\langle lm|V^A|\beta\alpha\rangle - \frac{1}{2}\sum_{\beta\gamma m} \langle km|V^A|\beta\gamma\rangle\langle\beta\gamma|V^A|\alpha m\rangle = 0 . \tag{5.4}$$

Here $\langle i|\tilde{\epsilon}|j\rangle$ is a matrix element of the one-body Hamiltonian defined below:

$$\langle i|\tilde{\epsilon}|j\rangle = \langle i|t|j\rangle + \sum_{\lambda \text{ occupied}} \langle i\lambda|V^A|j\lambda\rangle .$$

Also, it should be recalled that Greek letters α, β, γ, λ, etc., refer to occupied single-particle states, and k, l, m, etc., to the unoccupied single-particle states.

Next we define a single-particle operator

$$\hat{\sigma}^2 = \sum_{\alpha k} \Big\{ \sum_l \langle k|\tilde{\epsilon}|l\rangle\langle l|\tilde{\epsilon}|\alpha\rangle - \sum_\beta \langle k|\tilde{\epsilon}|\beta\rangle\langle\beta|\tilde{\epsilon}|\alpha\rangle + \sum_{\beta l} \langle l|\tilde{\epsilon}|\beta\rangle\langle\beta k|V^A|l\alpha\rangle + \sum_{\beta l} \langle\beta|\tilde{\epsilon}|l\rangle\langle kl|V^A|\alpha\beta\rangle + \frac{1}{2}\sum_{\beta l m} \langle\beta k|V^A|lm\rangle\langle lm|V^A|\beta\alpha\rangle - \frac{1}{2}\sum_{\beta\gamma m} \langle km|V^A|\beta\gamma\rangle\langle\beta\gamma|V^A|\alpha m\rangle \Big\} a_k^\dagger a_\alpha , \tag{5.5}$$

where k and α are arbitrary. Then Eq. (5.4), which we obtained by minimizing $\sigma^2(\Psi)$, implies that the operator $\hat{\sigma}^2$ does not connect the occupied and the unoccupied single-particle spaces. This property allows us to diagonalize the $\hat{\sigma}^2$ matrix in the space of occupied single-particle levels only. As in the Hartree-Fock method, the matrix elements of $\hat{\sigma}^2$ are functionals of occupied orbits. So one starts with a trial set of occupied orbits, sets up the $\hat{\sigma}^2$ matrix, and diagonalizes it to obtain a new set of orbits. This initiates the next cycle of the iterative procedure which goes on till the input and the output wave functions are the same. At this point one claims that the wave function so obtained is self-consistent; with this wave function one then computes the energy variance using the expression in Eq. (4.5).

B. Numerical results

We have carried out the energy variance minimization calculations for the double-closed shell nuclei ^{4}He, ^{16}O, and ^{40}Ca. We have assumed that the Slater determinants are spherically symmetric. The calculations were done in the space of the first four oscillator major shells using the Tabakin[7,8] matrix elements. We now give the matrix elements of the one-body operator $\hat{\sigma}^2$ of Eq. (5.5) in the basis of harmonic oscillator orbitals $|nlj\rangle$ using the notation of Sec. III.

$$
\begin{aligned}
&\langle s_\alpha n_\alpha | \hat{\sigma}^2 | s_\alpha n'_\alpha \rangle \\
&= \sum_{s_l n_l n'_l} \langle s_\alpha n_\alpha | \tilde{\epsilon} | s_l n_l \rangle \langle s_l n'_l | \tilde{\epsilon} | s_\alpha n'_\alpha \rangle \hat{\delta}_{\alpha l} C^{l*}_{n'_l} C^{l}_{n_l} - \sum_{s_\beta n_\beta n'_\beta} \langle s_\alpha n_\alpha | \tilde{\epsilon} | s_\beta n_\beta \rangle \langle s_\beta n'_\beta | \tilde{\epsilon} | s_\alpha n'_\alpha \rangle \hat{\delta}_{\alpha\beta} C^{\beta*}_{n'_\beta} C^{\beta}_{n_\beta} \\
&+ \frac{1}{2(2j_\alpha+1)} \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_l n_l n'_l}} \Big[\langle s_l n_l | \tilde{\epsilon} | s_\beta n_\beta \rangle \hat{\delta}_{l\beta} \sum_{JT} (2T+1)(2J+1) \langle\langle (s_\beta n'_\beta, s_\alpha n_\alpha) | V^A | (s_l n'_l, s_\alpha n'_\alpha) \rangle\rangle_{JT} C^{l*}_{n_l} C^{\beta*}_{n'_\beta} C^{l}_{n'_l} C^{\beta}_{n_\beta} \\
&\qquad + \langle s_\beta n_\beta | \tilde{\epsilon} | s_l n_l \rangle \hat{\delta}_{l\beta} \sum_{JT} (2T+1)(2J+1) \langle\langle (s_l n'_l, s_\alpha n_\alpha) | V^A | (s_\beta n'_\beta, s_\alpha n'_\alpha) \rangle\rangle_{JT} C^{\beta*}_{n_\beta} C^{l*}_{n_l} C^{\beta}_{n'_\beta} C^{l}_{n_l} \Big] \\
&+ \frac{1}{2(2j_\alpha+1)} \left(\frac{1}{2}\right) \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_l n_l n'_l \\ s_m n_m n'_m}} \sum_{JT} (2T+1)(2J+1) \langle\langle (s_\beta n_\beta, s_\alpha n_\alpha) | V^A | (s_l n_l, s_m n_m) \rangle\rangle_{JT} \langle\langle (s_l n'_l, s_m n'_m) | V^A | (s_\beta n'_\beta, s_\alpha n'_\alpha) \rangle\rangle_{JT} \\
&\qquad \times C^{\beta*}_{n_\beta} C^{l*}_{n'_l} C^{m*}_{n'_m} C^{\beta}_{n'_\beta} C^{l}_{n_l} C^{m}_{n_m} \\
&- \frac{1}{2(2j_\alpha+1)} \frac{1}{2} \sum_{\substack{s_\beta n_\beta n'_\beta \\ s_\gamma n_\gamma n'_\gamma \\ s_m n_m n'_m}} \sum_{JT} (2T+1)(2J+1) \langle\langle (s_\alpha n_\alpha, s_m n_m) | V^A | (s_\beta n_\beta, s_\gamma n_\gamma) \rangle\rangle_{JT} \langle\langle (s_\beta n'_\beta, s_\gamma n'_\gamma) | V^A | (s_\alpha n'_\alpha, s_m n'_m) \rangle\rangle_{JT} \\
&\qquad \times C^{\beta*}_{n'_\beta} C^{\gamma*}_{n'_\gamma} C^{m*}_{n_m} C^{\beta}_{n_\beta} C^{\gamma}_{n_\gamma} C^{m}_{n'_m} .
\end{aligned} \tag{5.6}
$$

Here the $C^{\beta}_{n_\beta}$, etc., are the expansion coefficients, the δ function $\hat{\delta}_{\alpha k} = \delta_{l_\alpha l_k} \delta_{j_\alpha j_k}$, and so on.

The high degree of nonlinearity of the equations in Eq. (5.6) is evident. Whereas the Hartree-Fock method gives rise to a set of simultaneous cubic equations, the present method yields a set of simultaneous equations of the seventh degree. Consequently the numerical solution of Eq. (5.6) becomes harder and poses some convergency problems. Another source of complication is the existence of multiple minima. We have not studied all the solutions corresponding to different local minima, but they may provide some interesting information about high lying states having $J=0$ and $T=0$. For comparison with the HF results we have always chosen the solution having the lowest energy.

We show in Table III the results of calculations made with Tabakin matrix elements. In this table we show the same quantities as were shown in Table I, for the HF solution. We see that the energies obtained by the two different variational procedures are nearly equal in all the nuclei studied. This shows that a variance minimum solution exists in the neighborhood of the HF solution. The maximum difference of about 2.3 MeV in the energies obtained by the two procedures is found in the case of ^{16}O. Further, the minimum variance obtained is at best only a few percent smaller than the variance of the HF solution. This means that the wave function obtained by minimization of σ^2 is not really very different from the HF one. In other words the HF solution nearly minimizes the width in the ground state domain.

We have also calculated using the minimum variance wave function, second-order perturbation corrections to the energy arising from 1p-h and 2p-h excitations. The total correction in energy is denoted by $E(2)$ in Table III. It should be emphasized that unlike the HF solution the state Ψ_σ gives nonzero contribution from 1p-h intermediate states.

TABLE III. Some properties of the Ψ_σ solution for spherical nuclei. Calculation in four oscillator major shells with c.m. correction. Interaction: Tabakin ($b=1.81$ fm for ^{4}He and ^{16}O, $b=2.03$ fm for ^{40}Ca).

Nucleus	$E(\sigma)$ (MeV)	$E(2)$ (MeV)	E(total) (MeV)	$r(\sigma)$ (fm)	$\alpha^2(\sigma)$	Width (MeV)
^{4}He	−9.65	−2.96	−12.61	1.75	0.97	11.72
^{16}O	−41.98	−10.66	−52.64	2.30	0.87	23.08
^{40}Ca	−125.07	−15.87	−140.94	3.43	0.55	21.29

It is seen that the second-order perturbation corrections $E(2)$ obtained for the two solutions do not differ very much. However, the 2p-h intermediate state contribution to $E(2)$ calculated for the minimum variance wave function is found to be less than that obtained for the HF wave function. The reason for this is as follows: in minimizing energy variance we are minimizing the sum of one particle-hole and two particle-hole contributions to the ground state wave function, as is clear from Eq. (4.2). Thus the minimum variance wave function already contains some two particle-hole contributions in contrast to the HF wave function which, does not and cannot contain such a contribution. We find that in the case of ^{16}O this difference in the 2p-h second-order correction is about 1.7 MeV. Thus the present method provides us with a determinantal wave function that has less 2p-h second-order perturbation correction than the HF determinant. Let us next consider the intensity of the state Ψ_σ in the wave function $\Psi_\sigma^{(1)}$ (corrected to first order in perturbation theory). If we compare the numbers in column 6 of Tables I and III, we find that in almost every case the intensity of Ψ_σ in $\Psi_\sigma^{(1)}$ is almost the same as the intensity of Ψ_{HF} in $\Psi_{HF}^{(1)}$.

We show in column 5 in Table III the r.m.s. radius r obtained by using Ψ_σ. It is seen that the minimum variance method gives a nuclear radius smaller than the HF method. This is due to the fact that the HF single-particle orbits have less mixing compared to the single-particle orbits obtained from the minimum variance method.

VI. SUMMARY AND CONCLUDING REMARKS

In this paper we have studied two different variational methods for obtaining Slater determinant states in light spherical nuclei. These are the Hartree-Fock and the minimization of energy variance methods. The results indicate that at least for the cases studied both the variational methods give rise to determinants which are very similar. The difference in energy and the width between the two variational solutions is in all the cases studied only a few ($\lesssim 5$) percent. It is tempting therefore to conclude that in the ground state domain of spherical nuclei the HF determinant is just about the best determinant one can have. Our calculations therefore provide a different and more detailed justification of the use of HF method to generate Slater determinants. It should be remembered that while minimizing σ^2 we obtained several solutions corresponding to different local minima. One of these (Ψ_σ) is close in energy to the HF solution, but the others, which lie at various excitation energies and sometimes have width smaller than that for Ψ_σ, may provide approximations to some excited states. This aspect needs to be studied more.

One can also study the two variational methods for nonspherical nuclei. The determinants in these cases would not be eigenstates of angular momentum and hence one would have to carry out the angular momentum projection. It is possible that for such nuclei the projected ground state obtained from Ψ_σ may have a lower energy than the one obtained from Ψ_{HF}. The alternative variational method may therefore have more interesting consequences (in the ground state region) for deformed nuclei than for the spherical ones.

Furthermore, in both the methods the determinants have large widths so that neither approach leads to wave functions which are close to the exact ground state of the system. This does not mean that the approximate states cannot give reasonably accurately the expectation values of some operators. As mentioned earlier, the width by itself does not give us an idea about how important the admixtures with other states are in correcting the energy or some other quantity. Our calculations show that the correlation effects, discussed in perturbation theory, are fairly important and contribute about 20% to the uncorrelated energy. Hence these corrections ought not to be neglected.

It seems therefore that in order to improve the wave function it is necessary to explicitly include 2p-2h states. It does not seem possible to incorporate the correlations in a single determinant by the use of a different variational principle. The inclusion of the 2p-2h states can be carried out in a nonperturbative way by evaluating the lowest three moments of H for the Hartree-Fock state. These moments of H can be evaluated directly from the Hamiltonian matrix elements, without making an intermediate state expansion, by using the spectral distribution method.[10] This will be discussed separately.

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[1]N. Ullah and R. K. Nesbet, Nucl. Phys. 39, 239 (1962); Phys. Rev. 134, B308 (1964); A. K. Kerman, J. P. Svenne, and F. M. H. Villars, Phys. Rev. 147, 710 (1966).
[2]G. Ripka, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt (Plenum, New York, 1968), Vol. I, Chap. 3.
[3]R. M. Tarbutton and K. T. R. Davies, Nucl. Phys. A120, 1 (1968).
[4]J. W. Negele, Phys. Rev. C 1, 1260 (1970).
[5]J. C. Parikh and J. P. Svenne, Phys. Rev. C 6, 34 (1972).
[6]K. H. Bhatt and J. C. Parikh, Phys. Lett. 44B, 338 (1973).
[7]F. Tabakin, Ann. Phys. (N.Y.) 30, 51 (1964).
[8]D. M. Clement and E. U. Baranger, Nucl. Phys. A108, 27 (1968).
[9]I. Kelson and G. Shadmon, Ann. Phys. (N.Y.) 63, 497 (1971).
[10]J. B. French and K. F. Ratcliff, Phys. Rev. C 3, 94 (1971); K. F. Ratcliff, *ibid.* 3, 117 (1971).