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**DEFORMED BRUECKNER-HARTREE-FOCK CALCULATIONS
FOR LIGHT NUCLEI**

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ABSTRACT

For the first time the Brueckner-Hartree-Fock (BHF) method is applied to nuclei whose intrinsic structure is nonspherical. One aim is to investigate whether the energy dependent reaction matrix calculated from a "realistic" nucleon-nucleon interaction leads to deformations similar to, or rather different from, those obtained from energy independent interactions in Hartree-Fock (HF) calculations. Reaction matrix elements were calculated as a function of "starting energy" for the Hamada-Johnston interaction, using a Pauli operator appropriate to ^{16}O and a shifted oscillator spectrum for virtual excited states. Binding energies, single-particle energies, radii, and shape deformations of the intrinsic state in unrenormalized as well as renormalized BHF are discussed and compared with previous HF studies. Results are presented for ^{12}C , ^{16}O , and ^{20}Ne .

INTRODUCTION

The connection between the nuclear many-body problem and the prediction of properties of finite nuclei has been studied with increased intensity in the last few years (ref. 1). Advances in computational technology have made it possible to drop the "closed-shell-core" assumption which was common to most nuclear structure calculations (ref. 2). Thus it has become feasible to attempt to understand nuclear phenomena in terms of a microscopic theory without the additional uncertainties which result when an inert core is assumed. (The inert core effects are usually manifested through the need for effective charges in calculating electromagnetic properties and the need for effective interactions in obtaining matrix elements of the nuclear Hamiltonian.)

A natural starting point for many microscopic studies of nuclear systems has been the Hartree-Fock (HF) method (ref. 3), which has contributed significantly to our understanding of the properties of nuclei (ref. 4). The use of the HF method has been limited somewhat by the type of interactions available for use in calculations, but it is certainly the most convenient method available presently for investigating nuclear many-body systems. For the most part HF studies have been restricted to the use of (1) phenomenological effective interactions (ref. 5) or (2) various types of effective interactions based directly or indirectly on nuclear matter calculations (ref. 6). Microscopic studies of both spherical and deformed nuclei have been made using such effective interactions. Ultimately, however, one would like to begin with a "realistic" nucleon-nucleon interaction and, with as few approximations as possible, calculate nuclear properties based on a many-body theory. The Brueckner-Goldstone (BG) theory provides a starting point for such calculations.

Following the pioneering work of Brueckner (ref. 7) and Goldstone (ref. 8), there came a large number of papers clarifying the theory and extending it beyond applications to nuclear matter (ref. 9). In recent years, the usefulness of the nuclear-matter calculations in studying properties of finite nuclei was demonstrated by Kuo and Brown (ref. 10), and the development of Brueckner theory for closed-shell nuclei was advanced considerably by the work of Kohler and McCarthy (ref. 11) and by Becker, MacKellar and Morris (ref. 12).

There do remain uncertainties in the many-body theory, because of a lack of understanding of the two-body force and some questions regarding the importance of higher order Brueckner-Goldstone diagrams (ref. 13) and three-body clusters (ref. 14). However, if one hopes to understand the structure of nuclei in terms of a true microscopic picture, a Brueckner-Hartree-Fock (BHF) type of calculation appears to be the most reasonable approach presently available.

The application of the BHF method to the investigation of properties of finite nuclei has thus far been limited to spherical, closed-shell nuclei. Among the most significant of the calculations made to date have been those of the Oak Ridge groups (refs. 15 and 16). Self-consistent BHF studies by Davies et al. demonstrated the ease and reliability with which such calculations could be made, although they found the nuclei to be too small and underbound. Several authors suggested that occupation probabilities may play an important role in BHF treatments of finite nuclei (ref. 17). The inclusion of occupation probabilities in finite-nucleus Brueckner calculations by Becker made a substantial difference

in the single particle energies, and it was found that the depletion factors for normally occupied single-particle orbits were of the order of 15 percent (ref. 17). Subsequent calculations by Davies and McCarthy show that good results for the binding energy can be obtained when such higher-order diagrams are included; however, the nuclei are still too small.

The results discussed above indicate that the nuclear many-body problem is now sufficiently well understood to make it reasonable to examine the degree to which one can use it to predict nuclear properties while, at the same time, attempting to refine and extend our present knowledge of the problem. Since the majority of nuclei are not of the spherical, closed-shell type, it is of interest to determine whether the energy dependent reaction matrix obtained from BHF calculations leads to deformations, gaps, etc, which are similar to those resulting from standard HF calculations with effective interactions. The light deformed nuclei provide a good starting point for such a study, since the number of particles involved is small enough to keep the problem tractable and the simple HF approximation is understood well enough to provide guidelines for what is recognized to be a rather complicated problem. Although there are some conceptual difficulties associated with obtaining physical states from deformed intrinsic systems when BHF is used, there is still much to be gained from a study of properties of the intrinsic system. For instance, it would be interesting to see how deformations, single particle energies, and energy gaps are affected when one does BHF and renormalized

BHf rather than the simpler HF calculation using an energy independent interaction. One aim of this paper is to discuss and compare such calculations.

THEORY

The deformed intrinsic HF state of a many-body system is nondegenerate in the body-fixed frame, and therefore Goldstone's linked cluster perturbation expansion is valid (ref. 18). If one makes the usual association of terms in the perturbation series with Brueckner-Goldstone diagrams, then the only departure from the more familiar spherical situation is that propagation lines are now associated with deformed single particle states. It follows that summations and cancellations of particular diagrams are identical for finite spherical and deformed systems. As usual, summation of terms corresponding to a series of ladder diagrams is accomplished by solving the integral equation

$$t_{12}(E_s) = v_{12} - v_{12} \frac{Q}{h_{12} - E_s} t_{12}(E_s) \quad (1)$$

Here $t_{12}(E_s)$ is Brueckner's reaction matrix, v_{12} is a nucleon-nucleon interaction with short range repulsion, E_s is the "starting energy," Q is the Pauli operator, and $h_{12} = h_1 + h_2$. The single-particle Hamiltonians include single-particle (SP) potentials which are defined to cancel certain classes of diagrams; these potentials are deformed for the case of interest here.

Because of the hard core in v_{12} , it is convenient to define a correlated two-particle wavefunction, ψ_{12} , by means of the equation

$$t_{12}(E_s)\phi_{12} = v_{12}\psi_{12} \quad (2)$$

from which one can obtain the integral form of the Bethe-Goldstone equation:

$$\psi_{12} = \phi_{12} - v_{12} \frac{Q}{h_{12} - E_s} \psi_{12} \quad (3)$$

The solution of this equation is very difficult, so the usual procedure is to define a "reference" t-matrix

$$t_{12}^R(E_s) = v_{12} - v_{12} \frac{Q^R}{h_{12}^R - E_s} t_{12}^R(E_s) \quad (4)$$

to be solved for as a first approximation to the nuclear t-matrix; one also obtains the reference Bethe-Goldstone equation:

$$\psi_{12}^R(E_s) = \phi_{12} - v_{12} \frac{Q^R}{h_{12}^R - E_s} \psi_{12}^R(E_s) \quad (5)$$

The nuclear t-matrix may then be obtained through use of the relation

$$t_{12}(E_s) = t_{12}^R(E_s) - t_{12}^R(E_s) \left[\frac{Q^R}{h_{12}^R - E_s} - \frac{Q}{h_{12} - E_s} \right] t_{12}(E_s) \quad (6)$$

Now, it is clear that the solution of equation (5) will also be complicated if h_{12} contains deformed single-particle potentials. This is immediately obvious if we try to transform to relative and center-of-mass coordinates which is necessary since v_{12} is nearly always given in that representation. On the other hand, if we solved equation (5) with a spherical reference operators, h_{12}^R , and Q^R and then iterated equation (6), the problem would be greatly simplified. (This is essentially what we have in mind.)

The calculation of the reaction matrix provides the necessary ingredients for a Brueckner-Hartree-Fock calculation. The set of self-consistent equations to be solved are

$$h|\lambda\rangle = e_\lambda|\lambda\rangle \quad (7)$$

where

$$\langle\lambda|h|\mu\rangle = \langle\lambda|K|\mu\rangle + \langle\lambda|U|\mu\rangle \quad (8)$$

and the specific form of $\langle\lambda|U|\mu\rangle$ depends on whether λ and μ refer to hole-hole, hole-particle, or particle-particle states (ref. 12). The dependence of U on the occupied SP states results in a double self-consistency requirement: the SP states, λ , are eigenstates of $(K + U)$ and U itself depends on the energies of the filled SP states. It therefore appears that, in order to do BHF correctly, we must recalculate the reaction matrix after each iteration in a self-consistency procedure. Fortunately this can be avoided by the technique introduced by McCarthy and Davies (ref. 16), in which t is expressed as a power series:

$$t_{12}(E_s) = \sum_{n=1}^N A_n E_s^n \quad (9)$$

If the reaction matrix is calculated for several starting energies, the coefficients A_n may be obtained by a suitable fitting procedure. Once the reaction matrix is obtained as a function of starting energy, it would be possible after each iteration in the BHF problem to use equation (6) to make the Pauli corrections. In practice one would probably get sufficiently accurate results if these corrections were only made for the last two or three steps in the iterative procedure.

The usual method of solving equations (7) is to introduce a finite set of basis vectors which span several major shells. The equations then become:

$$\sum_b \left\{ \langle a|K|b \rangle + \langle a|U|b \rangle \right\} C_b^\lambda = e_\lambda C_a^\lambda \quad (10)$$

where the coefficients C_k^λ express the deformed orbitals in terms of a spherical oscillator representation, i.e.

$$|\lambda \rangle = \sum_k C_k^\lambda |k \rangle \quad (11)$$

The method of Davies, Baranger, Tarbutton and Kuo (ref.) may be used to calculate the matrix elements of U in the oscillator representation:

$$\begin{aligned} \langle a|U|b \rangle = & \frac{1}{2} \sum_{a'cd} \sum_{\xi} \sum_{\lambda}^{\text{occ.}} \rho_{aa'}^{\xi} \rho_{dc}^{\lambda} \langle a'c|t_{12}^A(\epsilon_{\lambda\xi})|bd \rangle \\ & + \frac{1}{2} \sum_{b'cd} \sum_{\eta} \sum_{\lambda}^{\text{occ.}} \rho_{bb'}^{\eta} \rho_{dc}^{\lambda} \langle ac|t_{12}^A(\epsilon_{\lambda\eta})|b'd \rangle \end{aligned} \quad (12)$$

where

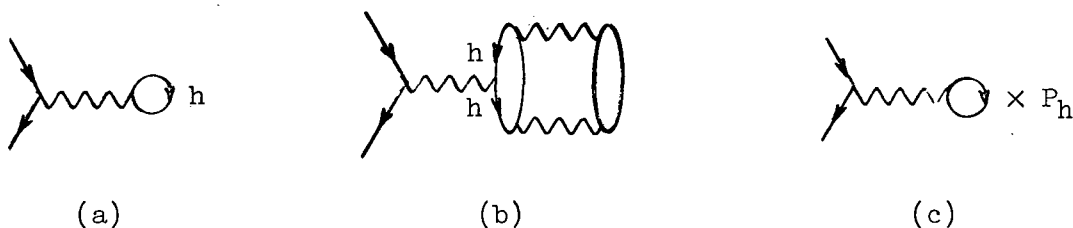
$$\rho_{ab} \equiv C_a^{\lambda*} C_b^{\lambda}$$

Although this expression is obtained using an approximation involving the starting energies, it has been pointed out by Davies et al. that one is primarily interested in occupied states and related properties, so that particle-hole and particle-particle matrix elements (which are given only by eq. (12)) will be less important since the effects on the occupied states only enter in second order (ref. 16). Furthermore, it has been shown by Davies and Baranger (ref. 16) that the exact expression gives essentially the same results for light nuclei.

After obtaining the matrix elements of U as defined in equation (12), the solution of equation (10) essentially reduces to the standard HF problem. The binding energy is given by the same expression in both HF and BHF:

$$E_1 = \frac{1}{2} \sum_{\lambda}^{\text{occ.}} \left[\langle \lambda | K | \lambda \rangle + e_{\lambda} \right]$$

The renormalized BHF (RBHF) takes into account the depletion of normally occupied single-particle states resulting from two-nucleon correlations (ref. 17). The main difference between RBHF and the BHF approximation is that RBHF includes, along with the BHF contribution to the SP potential (fig. 1(a)), the contribution of figure 1(b)



which, in the unrenormalized Brueckner theory, is regarded as one of two third-order rearrangement potentials. Brandow urged that such potentials be included in the definition of the self-consistent field, where it would renormalize the BHF term, rather than be calculated only as a rearrangement correction (ref. 19). In the RBHF approximation the SP potential is that of figure 1(c), which includes the contribution of figures 1(a) and (b), and the particle occupation probabilities are set equal to zero. A complete renormalization of the entire perturbation series has been obtained by Brandow and is discussed in detail elsewhere (ref. 13).

DISCUSSION

Reaction matrix elements were calculated as a function of "starting energy" for the Hamada-Johnston interaction using a Pauli operator appropriate to ^{16}O and a shifted oscillator spectrum for the virtual excited states. Detailed descriptions of the method used to solve the reference Bethe-Goldstone equations may be found in reference 12. The t-matrix so obtained is essentially the spherical reference t-matrix with which the deformed calculations are begun, i.e., the oscillator representation of the t-matrix elements as they appear in equation (12). At the beginning of each iteration in the solution of the self-consistency problem the starting energies from the previous iteration are used; however, the Pauli corrections are not made. The "on shell" prescription is used for the particle-particle matrix elements in the deformed BHF calculations, although an approximate "off-shell" prescription was used in the original spherical calculations (ref. 12). The choice of the shift parameter, C, used in the calculations has been discussed in reference 12.

Properties of the intrinsic states of ^{12}C , ^{16}O , and ^{20}Ne have been calculated for oscillator lengths of 1.57 fm and 1.77 fm, using BHF and renormalized BHF. The variational problem was solved subject to the condition that the deformed intrinsic states possess axial symmetry and four-fold degeneracy. Expectation values of operators are calculated with the uncorrelated wavefunctions. The results have not been corrected for Coulomb and center-of-mass effects; such corrections should almost cancel each other for the nuclei studied here.

The HF calculations with which our results are compared are those of Zofka and Ripka (ZR) in which the effective interaction of Negele was used (ref. 20). This interaction is a density dependent one which was found to yield good binding energies, sizes, single-particle energies and electron scattering cross sections for certain spherical nuclei. Much of the improvement in binding energy and radius, however, is due to adjustment of the strength and range of the interaction to obtain the desired saturation properties of nuclear matter or selected finite nuclei. It should be noted that the calculations of ZR generally overestimate the nuclear sizes (and therefore quadrupole moments, etc.) but it is nevertheless felt that their results are the most relevant with which to compare at the present time. ZR refers to the values quoted here as calculation II. For this set of calculations, perturbation theory was used to correct for the fixed starting energy and Coulomb interaction. Whenever possible, the ZR values appropriate to neutrons are quoted, since we do not treat the Coulomb interaction in the calculations reported here.

Our results for ^{12}C are presented in table I. As expected from experience with spherical, close-shell nuclei, the RBHF calculation yields better values than the BHF for both oscillator lengths. An oblate shape for the nucleus is predicted, in agreement with the usual HF studies. Note that the radius predicted by the ZR calculation is considerably larger than experiment, and that their intrinsic quadrupole moment is 30 percent larger than the largest RBHF result. This is not surprising since the radius given by RBHF is only 2.37 fm, as compared to 2.59 fm given by ZR. We also observe that deformation increases when occupation

probabilities are included, and that the level ordering is unchanged. In all cases, the nucleus is underbound, although ZR's results are 20 percent larger than the RBHF results. The intrinsic properties of ^{12}C do not seem to be very sensitive to the oscillator length. Proton separation energies are given in the column labelled experiment. Results are given for neutrons in the (BHF, RBHF) calculations, but the Coulomb effects should only increase the results by about 2 MeV.

It has been known for some time that ordinary HF calculations do not provide good results for separation energies, and we observe that the ZR calculation differs by 20 percent from experiment for the most tightly bound state, although the p states are well represented. This is somewhat better than previous HF predictions of SP energies, however, since one usually finds that at least one of the predicted SP energies differs significantly (~50 percent) from experiment. Unrenormalized BHF is known to suffer from large rearrangement corrections and is also not expected to agree very well with experiment; this too is observed. The RBHF results are clearly the best of the three calculations.

All of the predictions are within 10 percent of the measured values. An analogue of Koopmans' Theorem for separation energies in RBHF has recently been established (ref. 21). Thus we may associate the energy of the first unoccupied orbit in ^{12}C with the separation energy of the last neutron in ^{13}C . Experimentally, the number is found to be 4.95 MeV (ref. 23). The RBHF prediction is about 4.5 MeV, in very good agreement with the measured result.

Table II contains the results for ^{16}O . Since these results are for spherical ^{16}O and this case has been discussed extensively in other studies, we do not feel it necessary to go into detail here. Efforts to obtain the deformed excited state in ^{16}O have thus far been unsuccessful. This state has been found, in standard HF studies, to be a 4p-4h state lying some 20 to 25 MeV above the ground state. The 4p-4h states which we have been able to study so far have been very unstable.

Of the even Z-even N nuclei in the s-d shell, ^{20}Ne has proved most amenable to description by means of standard HF theory. The various properties of this nucleus which are primarily long range in character may be obtained with good accuracy from a prolate intrinsic state with a rather large hexadecapole moment. Those properties primarily short-range in character, particularly the binding energy, are of course poorly given in standard HF theory.

Our BHF and RBHF results for ^{20}Ne are presented in table III. All the calculations yield prolate intrinsic states with the same level ordering, and as for the preceding cases, the RBHF predictions are somewhat more satisfactory than the BHF. The rms radius of ^{20}Ne has not been measured, but can be inferred from measurements on neighboring nuclei to be about 2.8 cm. Again we find the BHF and RBHF radius values too small, and the ZR value somewhat too large, and all the calculations underbind the nucleus.

In spite of these deficiencies, which are found in BHF and RBHF calculations for spherical nuclei as well, it is gratifying to note that the successful features of the standard HF theory seem also to be present in the Brueckner version. As evidence of this, we may observe the similarity

of values for the "long-range observables" $\langle R^2 \rangle^{1/2}$, Q_2 , and Q_4 , which are listed in table III for both HF and RBHF calculations with $b = 1.77$ fm. If this similarity persists for other values of the oscillator parameter, one would be justified in claiming that renormalized Brueckner-Hartree-Fock calculations give a fundamental description of ^{20}Ne with a consistent degree of accuracy for all its observables. Hopefully this would give even greater emphasis to investigation of the chief drawback of RBHF theory, namely its persistent prediction of nuclei which are too small and too loosely bound.

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TABLE I. - RESULTS FOR ^{12}C (P_λ IS THE OCCUPATION PROBABILITY FOR STATE λ)

b, fm	1.57		1.77		1.67	
Calculation	BHF	RBHF	BHF	RRHF	ZR ^a	Expt ^b
-E/A, MeV	4.6	5.6	4.5	5.2	6.4	7.7
$\langle R^2 \rangle^{1/2}$, fm	2.17	2.30	2.25	2.37	2.59	2.40 ± 0.03
Δ , MeV	12.7	11.2	11.9	10.4	9.8	
$\langle Q_2 \rangle$, fm ² ----	-25.4	-29.6	-26.6	-30.7	-40.9	
$\langle Q_4 \rangle$, fm ⁴	17.7	23.4	19.1	26.7		
$(m_\lambda^\pi, P_\lambda)$	(1/2 ⁺ , 1.0) -46.2	(1/2 ⁺ , 0.81) -35.4	(1/2 ⁺ , 1.0) -43.9	(1/2 ⁺ , 0.84) -34.5	(+) -28	35.5 ± 1.0
e_λ ,	(3/2 ⁻ , 1.0) -23.2	(3/2 ⁻ , 0.82) -16.5	(3/2 ⁻ , 1.0) -21.8	(3/2 ⁻ , 0.84) -15.9	(-) -15	15.0 ± 0.5
MeV	(1/2 ⁻ , 1.0) -21.8	(1/2 ⁻ , 0.83) -15.5	(1/2 ⁻ , 1.0) -20.4	(1/2 ⁻ , 0.85) -14.9	(-) -15	15.0 ± 0.5
C, MeV	48.64	46.84	40.76	38.76		

^aThe orbital energies in the ZR column refer to proton separation energies.

^bProton separation energies from ref. 22.

TABLE II. - RESULTS FOR $^{16}_0$

b, fm	1.57		1.77		1.67	
Calculation	BHF	RBHF	BHF	RBHF	ZR ^a	Expt ^b
-E/A, MeV	6.2	7.3	6.2	7.0	7.5	7.98
$\langle R^2 \rangle^{1/2}$, fm	2.16	2.27	2.25	2.33	2.72	2.67 \pm 0.03
Δ , MeV	18.0	16.9	17.2	15.8	17.0	
$\langle Q_2 \rangle$, fm ²	0.0	0.0	0.0	0.0	0.0	
$\langle Q_4 \rangle$, fm ⁴	0.0	0.0	0.0	0.0	0.0	
$(m_\lambda^\pi, P_\lambda)$	(1/2 ⁺ , 1.0) -56.7	(1/2 ⁺ , 0.79) -43.9	(1/2 ⁺ , 1.0) -54.9	(1/2 ⁺ , 0.83) -43.6	(+) -33	43 \pm 5
e_λ	(3/2 ⁻ , 1.0) -30.0	(3/2 ⁻ , 0.80) -21.3	(3/2 ⁻ , 1.0) -28.3	(3/2 ⁻ , 0.82) -20.9	(-) -17	21.8
MeV	(1/2 ⁻ , 1.0) -30.0	(1/2 ⁻ , 0.80) -21.3	(1/2 ⁻ , 1.0) -28.3	(1/2 ⁻ , 0.82) -20.9	(-) -17	21.8
	(1/2 ⁻ , 1.0) -23.5	(1/2 ⁻ , 0.80) -17.0	(1/2 ⁻ , 1.0) -22.6	(1/2 ⁻ , 0.82) -16.8	(-) -17	15.7
C, MeV	50.46	48.64	42.62	40.64		

^aThe orbital energies in the ZR column refer to proton separation energies.

^bProton separation energies from ref. 22.

TABLE III. - RESULTS FOR ^{20}Ne

b, fm	1.57		1.77		1.83	
Calculation	BHF	RBHF	BHF	RBHF	ZR ^a	Expt ^b
-E/A, MeV	5.8	7.1	6.1	6.9	7.1	8.2
$\langle R^2 \rangle^{1/2}$, fm	2.36	2.47	2.46	2.56	3.05	(2.55) ^b
Δ , MeV	7.6	7.4	7.9	7.5	6.9	
$\langle Q_2 \rangle$, fm ²	56.9	63.6	62.1	70.4	97.9	(69.8) ^b
$\langle Q_4 \rangle$, fm ⁴	130.7	150.7	167.7	202.9		(214) ^b
$(m_\lambda^\pi, P_\lambda)$	(1/2 ⁺ , 1.0) -61.5	(1/2 ⁺ , 0.79) -47.7	(1/2 ⁺ , 1.0) -59.9	(1/2 ⁺ , 0.83) -47.3	(+) -34	
e_λ	(1/2 ⁻ , 1.0) -38.2	(1/2 ⁻ , 0.79) -28.3	(1/2 ⁻ , 1.0) -36.5	(1/2 ⁻ , 0.81) -27.8	(-) -23	
MeV	(3/2 ⁻ , 1.0) -32.1	(3/2 ⁻ , 0.80) -22.8	(3/2 ⁻ , 1.0) -30.3	(3/2 ⁻ , 0.82) -22.3	(-) -17	
	(1/2 ⁻ , 1.0) -27.1	(1/2 ⁻ , 0.79) -19.4	(1/2 ⁻ , 1.0) -25.9	(1/2 ⁻ , 0.81) -19.1	(-) -17	
	(1/2 ⁺ , 1.0) -18.6	(1/2 ⁺ , 0.81) -12.0	(1/2 ⁺ , 1.0) -18.4	(1/2 ⁺ , 0.82) -12.6	(+) -10	
C, MeV	50.46	48.63	42.62	40.64		

^aProton separation energies as referred to in table I.

^bThese values are obtained from a standard HF calculation with $b = 1.77$ fm.