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Brueckner-Hartree-Fock calculations and their density dependence

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Brueckner-Hartree-Fock (BHF) calculations are presented taking into account the Pauli operator in the self-consistent basis rather than in the oscillator basis. The definition of the single particle energies includes an on-shell rearrangement diagram (starting energy rearrangement) stemming from the only partial occupation of the occupied states due to the short range correlations. Further, it includes an off-shell diagram (Pauli rearrangement) term which originates from the density dependence of the Pauli operator. The three additional terms, the correction for the self-consistent Pauli operator, the starting energy, and the Pauli rearrangement terms, contribute significantly to the nucleus. It is shown that the definition of the single particle energies is analogous to that in density dependent Hartree-Fock calculations. One obtains all the effects of a density dependent force within the BHF formalism without making a detour to nuclear matter and thus avoids many of the approximations used in the calculations with density dependent forces. The method is applied here for ^{16}O using the Reid soft core and the Yale potential.

[NUCLEAR STRUCTURE Brueckner-Hartree-Fock calculation in finite nuclei, ^{16}O calculated binding energy, rms radius, charge distribution, electron scattering.]

I. INTRODUCTION

In an attempt to explain some of the properties in finite nuclei starting with a basic nucleon-nucleon force, Brueckner-Hartree-Fock (BHF) calculations[1-7] have been done with some success in the closed shell nuclei. These calculations, however, have been unable to give the correct saturation properties in the nuclei considered. On the other hand, the density dependent forces[8,9] have been rather successful to a much higher degree. These density dependent forces are determined by solving the Bethe-Goldstone (B.G.) equation as a function of the Fermi momentum and thus of the density. This leads to the effective force in the momentum space. In order to be able to use it in finite nuclei one has to transform it to a spatial representation. In doing so one makes several approximations, e.g. Brandow's suggestion, namely of equating the integrands if the matrix elements are equal, averaging over starting energy, momenta and angular momenta, and using the local density approximation. Finally, one fits the nuclear matter data using two parameters. The present paper is an improvement of our previous work,[10,11] where we have tried to explain the behavior of the density dependent forces within the context of the BHF formalism by treating the density dependence in the Pauli operator more carefully. Specifically, we treated the Pauli operator in the self-consistent basis and included off-the-energy-shell diagrams related to the Pauli operator. In the present work we extend the method by taking into account the density matrix dependence of the reaction matrix through the starting energy. This yields an additional rearrangement term (starting energy rearrangement). In first order it is identical with a term contained in the renormalized BHF (RBHF) but derived there in a different way. In contrast to Refs. 10 and 11, where an averaged energy denominator in the BG equation was chosen before the iteration, in this work also the starting energy is treated self-consistently. Preliminary results of this method have been given at a conference in Balatonfüred, Hungary.[12]

II. THEORY

The total energy in the BHF approximation is given by

$$\langle H\rangle=\sum_i \langle i|t|i\rangle+\tfrac{1}{2}\sum_{ik}\langle ik|G(\omega_{ik})|ik\rangle\rho_i\rho_k\,, \qquad (1)$$

where the density matrices ρ are diagonal in the self-consistent single particle states $|i\rangle$, $|k\rangle$, $|l\rangle\ldots$:

$$\rho_i=\begin{cases}1, & i<F;\\ 0, & i>F;\end{cases} \qquad (2)$$

where F stands for the Fermi surface. The self-consistent single particle states can be expanded into oscillator basis states $|a\rangle$, $|b\rangle$, $|c\rangle\ldots$:

$$|i\rangle=\sum_a |a\rangle\langle a|i\rangle\,. \qquad (3)$$

The reaction matrix G in Eq. (1) is defined with the self-consistent Pauli operator Q:

$$G = V + V\frac{Q}{e}G, \tag{4}$$

with

$$e = W - H_s(1) - H_s(2),$$
$$H_s = \sum_i |i\rangle(\epsilon_i - c_i)\langle i| .$$

Here V is the nucleon-nucleon interaction and Q the self-consistent (s.c.) Pauli operator $Q = (1-\rho)(1-\rho)$. The energy denominator e contains the self-consistent single particle Hamiltonian H_s with an arbitrary shift c_i for every state $|i\rangle$. As a first step to calculate G, one calculates the reaction matrix G_O in the oscillator basis, with oscillator Pauli operator Q_O. This was done using the modified versions of the BGOLAP and TGEN codes originally written by M. R. Patterson of Oak Ridge National Laboratory:

$$G_O(W) = V + V\frac{Q_O}{\hat{e}_O}G_O(W), \tag{5}$$

with

$$\hat{e}_O = W - H_O(1) - H_O(2),$$
$$H_O = \sum_a |a\rangle(\epsilon_a - c_{Oa})\langle a| .$$

The intermediate particle spectrum is here defined by the harmonic oscillator Hamiltonian with an individual shift for every level. The self-consistent reaction matrix G is related to the reaction matrix G_O by the identity

$$G(W) = G_O(W) + G_O(W)\left(\frac{Q}{\hat{e}} - \frac{Q_O}{\hat{e}_O}\right)G(W). \tag{6}$$

It is worth noting that in our formalism one requires two different definitions for the intermediate states in Eqs. (4) and (5) to guarantee that the corresponding energy denominators commute with the respective Pauli operators:

$$[Q, \hat{e}] = [Q_O, \hat{e}_O] = 0 . \tag{7}$$

The self-consistent and the oscillator energy denominators $\hat{e}$ and $\hat{e}_O$ are defined apart from individual energy shifts c_i and c_{Oa} for every single particle level. We restrict the number of free parameters to only one by chosing the final energies of the unoccupied single particle states to be the oscillator energies plus a level independent shift:

$$\epsilon_i - c_i = \hbar\omega(N_i + \tfrac{3}{2}) - C ,$$
$$\epsilon_a - c_{Oa} = \hbar\omega(N_a + \tfrac{3}{2}) - C . \tag{8}$$

The correspondence between the self-consistent single particle states $|i\rangle$ and the main oscillator shell N is defined by the largest overlap $|\langle i|Nlj\rangle|$.

The effective interaction $G(W)$ to calculate the total energy (1) can in principle be calculated solving the Bethe-Goldstone equation [Eq. (4)] if the s.c. Pauli operator and the starting energies are known. This would be very time consuming since the Bethe-Goldstone equation, Eq. (4), would have to be solved in every HF iteration. A more favorable starting point for the calculation of the reaction matrix $G(W)$ is the identity (6). If the s.c. Pauli operator is not too much different from the oscillator Pauli operator Q_O, the iteration of Eq. (6) is converging rapidly:

$$G(W) = G_O(W) + G_O(W)\left(\frac{Q}{\hat{e}} - \frac{Q_O}{\hat{e}_O}\right)G_O(W) + \cdots . \tag{9}$$

The third order term in the above equation was checked numerically and was found to be less than 5% of the second order term, which in turn itself is very small compared to $G_O(W)$. The third and higher order terms are therefore neglected in expansion (9). The expression (9) for the reaction matrix $G(W)$ has two decisive advantages: First, it exhibits separately the dependence on the starting energy W and the Pauli operator Q, two quantities which are responsible for the density dependence of the effective force.[8,9] Secondly, it expresses the effective interaction $G(W)$ by the reaction matrix $G_O(W)$ calculated with the oscillator Pauli operator. The quantities $G_O(W)$ can be tabulated independently of the result of the HF iteration, and have to be calculated only once.

The density dependence is contained in the Pauli operator $Q = (1-\rho)(1-\rho)$, and in the starting energy

$$W_{ik} = \epsilon_i + \epsilon_k , \quad \epsilon_i \approx \langle i|t|i\rangle + \sum_k \langle ik|G|ik\rangle\rho_k . \tag{10}$$

The effective density dependent force is now defined by the expression (9) with the correction term due to the difference between the self-consistent Pauli operator and the oscillator Pauli operator. The Hartree-Fock equations which define the self-consistent single particle states are derived using the variational principle employed for the usual density dependent forces.[8] We should emphasize that we are not trying to justify the use of the variational principle. Instead, we are interested in the comparison of the definition of the s.p. energy given above in the context of the BHF formalism with that of the definition of the s.p. energy coming out of a density dependent Hartree-Fock calculation. We are not using a density dependent force derived by fitting the nuclear matter data, making several approximations on the way. Instead we are taking the realistic nucleon-nucleon forces which fit the phase shift data and looking at their density dependence rather closely in finite nuclei. In order to do that we are using the same variational principle as used with the density dependent forces derived from the nuclear matter. Obviously the validity or the nonvalidity of the variational principle in this context remains the same as for the density dependent forces. Here we want to understand the variational principle, which varies not only the wave functions but also the density dependence of the force, as supplying an essential ingredient of the density dependent forces. This variational principle defines the single particle energies, in the same way as Landau,[13] as the variational of the total energy with respect to the occupation probability of a single particle state.

The variation of the total energy given in Eq. (1), with expression (9), leads[1,10] to

$$
\begin{aligned}
H_i = \frac{\partial\langle H\rangle}{\partial\rho_i} &= \sum_{ab} \langle i|a\rangle H_{ab}\langle b|i\rangle \\
&= \langle i|t|i\rangle + \sum_k \langle ik|G_O(W_{ik})|ik\rangle \rho_k + \sum_k \langle ik|G_O[(1-\rho)(1-\rho)/\hat{e}_{ik} - Q_O/\hat{e}_{Oik}]\, G_O|ik\rangle \rho_k \\
&\quad + \sum_k \langle ik|G_O(W_{ik})|ik\rangle \left[\sum_s \langle ks|\, \frac{\partial G_O}{\partial W_{ks}}\, |ks\rangle \rho_s \right] \rho_k - \sum_{rsk} \langle rs|G_O(W_{rs})|ik\rangle [(1-\rho_k)/e_{rs}] \langle ik|G_O(W_{rs})|rs\rangle \rho_s \rho_r ,
\end{aligned}
\tag{11}
$$

with

$$
\begin{aligned}
\hat{e}_{ik} &= W_{ik} - H_s(1) - H_s(2) \\
\hat{e}_{Oik} &= W_{ik} - H_O(1) - H_O(2) \\
e_{rs} &= W_{rs} - \epsilon_i - \epsilon_k ,
\end{aligned}
$$

where H_s and H_O are defined by Eqs. (4), (5), and (8). Note that ϵ_i in e_{rs} is the hole energy in our case and ϵ_k is the particle energy with the proper shift. The dependence of the effective interaction (9) on the density matrix ρ through the starting energy W and the Pauli operator Q has been varied only in the leading terms depending on W and Q, respectively.

The Hartree-Fock equation for the expansion coefficients $\langle a|i\rangle$ and the single particle energies are then given by

$$
\sum_b H_{ab}\langle b|i\rangle = \epsilon_i \langle a|i\rangle . \tag{12}
$$

A look at Eq. (11) reveals that the first two terms correspond to the usual BHF approach with the two self-consistencies for the single particle states and the starting energy W_{ik}, and correspond to the diagram of Fig. 1(a) for the s.p. energy. The inclusion of the third term corrects for the difference between the self-consistent Pauli operator and oscillator Pauli operator and the single particle energy contribution from this term is represented by Figs. 1(c) and 1(d). The last two terms are the rearrangement contributions which originate from the variation of the density dependence in the force (9). The fourth term comes from the variation of the starting energy W. This can be seen by writing the derivative of the reaction matrix G_O with respect to the starting energy W in the following way:

$$
\frac{\partial G_O}{\partial W} = -G_O(W)(Q_O/\hat{e}_O{}^2)G_O(W) . \tag{13}
$$

It corresponds to the diagram in Fig. 1(b). It is an on-the-energy-shell insertion and has been discussed earlier.[1,14,15] The inclusion of this term in the calculation corresponds to the RBHF.[6,15] It can be included in the second term using the partial occupation probabilities for the single particle states $|k\rangle$, defined in the lowest order as

$$
\rho_k \simeq 1 + \sum_s \langle ks|\, \frac{\partial G}{\partial W_{ks}}\, |ks\rangle \rho_s . \tag{14}
$$

We emphasize here that the occupation probability in Eq. (11) is included only to the first order. The second difference between using Eq. (11) without the third and the last term on the right-hand side and doing the conventional RBHF calculation is that Eq. (11) does not take into account the overcounting correction which is used in conventional RBHF[6,15] calculations. These correction terms are not included in order to have an exact correspondence to HF calculations with density dependent forces.[8,9] But as additional information we also give in the tables the binding energy with the overcounting correction.[6,15]

The last term originates[1,10] from the variation of the Pauli operator and corresponds to the off-the-energy-shell diagram of Fig. 1(e). For this reason it is known as the Pauli rearrangement term. This is included in our definition of the single-particle energy. It is also taken into account in Landau's work.[13]

The above comparison shows that our definition of the s.p. energy within the BHF formalism completely overlaps with the defintion of the s.p. energy for the density dependent forces. In this sense our calculation can also be regarded as providing a microscopic description of the density dependent forces.

III. RESULTS

The above described theory is applied to ^{16}O utilizing the Yale[17] and the Reid soft core potential.[18] The Reid soft core potential[18] is defined for relative angular momenta $j \leq 2$. For higher partial waves we take the Yale potential.[17] The details concerning the solution of the reaction matrix in the oscillator basis $G_O(W)$ are given elsewhere.[4,10] The HF equation (12) with the Hamiltonian (11) is solved in an oscillator basis ($\hbar\omega = 13.29$ MeV), including the seven lowest oscillator shells ($2n + l = N \leq 6$). By varying the basis it has been shown that it is large enough for all data discussed here apart from the high momentum transfer electron scattering data ($E_e = 750$ MeV and larger angles).

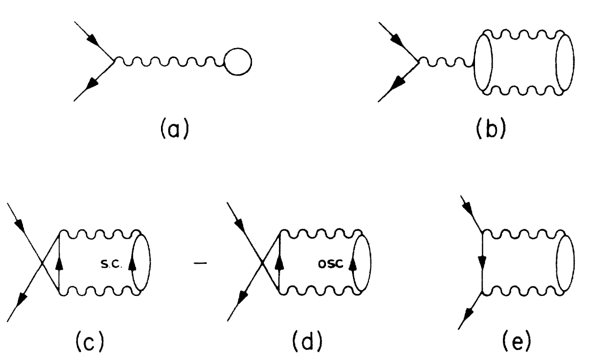

FIG. 1. Diagrams defining the single particle energies in this paper. (a) Corresponds to the usual Brueckner-Hartree-Fock (BHF) approximation. Diagram (b) depicts the starting energy rearrangement term, which is the fourth term on the right-hand side of the Hartree-Fock (HF) Hamiltonian, Eq. (11). It is, in first order, equivalent with the partial occupation probabilities discussed elsewhere (Refs. 1 and 14) and taken into account in the renormalized BHF (RBHF) approach (Refs. 6 and 15). The diagrams (c) and (d) differ by the particle lines which are self-consistent (s.c.) and oscillator (osc) states above the s.c. Fermi surface F and the oscillator Fermi surface F_0, respectively. These two diagrams correct for the difference between the s.c. and the osc Pauli operator Q and Q_0. The contribution e is the Pauli rearrangement term. It originates from the variation of the density (matrix) dependence of the Pauli operator. It corresponds to the last term in Eq. (11) and admixes 1p2h states. It yields automatically an imaginary single particle energy if one describes the intermediate particle states by a continuum (Ref. 13). We describe the intermediate single particle states by a shifted oscillator potential defined in Eqs. (4), (5), and (8). To prevent possible singularities one introduces (Ref. 22) a width Γ into the denominator of this term and takes the real part. The single particle energies, which are most sensitive to this width, are affected by less than 5% if one varies this width between 0 and 5 MeV in our examples.

The HF Hamiltonian (11) has been solved including different terms. The self-consistent solution of the first two terms with self-consistent starting energies corresponds to the Brueckner-Hartree-Fock (BHF) approach.[3-5] The first, second, and fourth term correspond to the renormalized BHF (RBHF) Hamiltonian.[6,15] Again one has to satisfy both the HF and the starting energy self-consistency. As mentioned earlier, there are two differences between our RBHF and other RBHF calculations.[6,15] First, the occupation probabilities are included in our calculations only in first order. Secondly, we do not include the overcounting corrections, which reduces the potential energy by 3%. Hence our results are more bound by approximately 1 MeV/particle than for other calculations. But for additional information we also give the binding energies corrected for overcounting in Tables I and II. However, one should have in mind that especially for the DBHF method the correction is not adequate since there the starting energy rearrangement and the Pauli rearrangement are strongly coupled,[16] while the correction for the total binding energy is only suitable for the starting energy rearrangement. The first four terms of the Hamiltonian (11) include in addition the self-consistent Pauli operator (RBHF + s.c. Q) instead of the oscillator Pauli operator. If one also includes the Pauli rearrangement which is the last term in Eq. (11), we name the method the density dependent Brueckner-Hartree-Fock (DBHF) method.

The only free parameter in these calculations is the energy shift C of the intermediate particle spectrum for the unoccupied states defined in Eqs. (4), (5), and (8). For both interactions, the Yale[17] and the Reid soft core potential,[18] we choose the shift C so that the energy of the $1s_{1/2}$ state of the first unoccupied oscillator shell agrees with the self-consistent BHF single particle energy of the $1s_{1/2}$ level. This choice corresponds to $C = 41.5$ MeV and $C = 42$ MeV, respectively. To see the influence of this shift we also give results for $C = 46.5\ \text{MeV} = \frac{7}{2}\hbar\omega$ for the Yale and $C = 38$ MeV for the Reid soft core potential.

All different approaches have been initially calculated with the matching self-consistent starting energies. But it turned out that the choice of the starting energies in the correction term for the self-consistent Pauli operator [third term of Eq. (11)] and for the Pauli rearrangement [last term of Eq. (11)] is not too sensitive. We therefore

TABLE I. Single particle energies ϵ in MeV, occupation probabilities P (14), binding energy per nucleon (BE/A) and rms charge radius $\langle r_c^2 \rangle^{1/2}$ for ^{16}O resulting from various self-consistent calculations with the Yale (Ref. 17) potential. The basis includes the seven lowest oscillator shells ($2n + l = N \leq 6$; $\hbar\omega = 13.29$ MeV). The results for Brueckner-Hartree-Fock [BHF ≅ first two terms of Eq. (11)], for BHF with the self-consistent Pauli operator [BHF + s.c. Q = first three terms of Eq. (11)], for BHF with s.c. Pauli operator plus Pauli rearrangement term [BHF + s.c. Q + P.r. ≅ first three terms and last term of Eq. (11)], for the renormalized BHF with the s.c. Pauli operator [RBHF + s.c. Q ≅ first four terms of Eq. (11)] and for the density dependent BHF [DBHF ≅ all terms in Eq. (11)] are given for the intermediate particle spectrum with the shifts $C = (2 + \frac{3}{2})\hbar\omega \approx 46.5$ MeV and $C = 41.5$ MeV (shift to the self-consistent position of the $1s_{1/2}$ level). The binding energies are corrected for the center of mass motion (B.E. = B.E.$_{\text{uncorr}} + \frac{3}{4}\hbar\omega$). The single particle energies are not corrected for the center of mass motion (Davies and Becker Ref. 6). The binding energy with the overcounting correction of the renormalized Brueckner-Hartree-Fock (RBHF) is also included [(BE/A)$_c$]. The rms radius is corrected for the finite size of the proton and for c.m. motion ($\langle r_c^2 \rangle = \langle r_p^2 \rangle + 0.65\ \text{fm}^2 - \frac{3}{2}\hbar/m\omega A$). The experimental separation energies should not be directly compared with the HF energies (Refs. 19 and 20).

				$2n_1 + l_1 \leq 6$						
		$C = 46.5$ MeV				s.c. Particle spectrum $C = 41.5$ MeV				
^{16}O		BHF	BHF + s.c. Q	BHF + s.c. Q + P.r.	DBHF	BHF	BHF + s.c. Q	RBHF + s.c. Q	DBHF	Expt.
$0s_{1/2}$	ϵ	−48.56	−47.91	−44.31	−35.10	−46.03	−42.74	−34.34	−29.28	−40 ± 8
	P	1.0	1.0	1.0	0.87	1.0	1.0	0.79	0.89	
$0p_{3/2}$	ϵ	−25.99	−25.64	−24.47	−17.89	−23.53	−22.27	−15.81	−14.81	−18.4
	P	1.0	1.0	1.0	0.81	1.0	1.0	0.77	0.83	
$0p_{1/2}$	ϵ	−21.58	−21.30	−19.42	−13.58	−19.49	−18.38	−13.03	−11.25	−12.1
	P	1.0	1.0	1.0	0.83	1.0	1.0	0.80	0.85	
$0s_{1/2}$	ϵ	−51.77	−50.98	−47.32	−38.64	−49.04	−45.71	−37.67	−32.52	
	P	1.0	1.0	1.0	0.83	1.0	1.0	0.75	0.84	
$0p_{3/2}$	ϵ	−28.83	−28.40	−27.15	−20.74	−26.26	−24.92	−18.51	−17.40	−21.9
	P	1.0	1.0	1.0	0.79	1.0	1.0	0.76	0.81	
$0p_{1/2}$	ϵ	−24.70	−24.36	−22.43	−16.71	−22.49	−21.36	−15.99	−14.14	−15.7
	P	1.0	1.0	1.0	0.82	1.0	1.0	0.77	0.83	
BE/A (MeV)		6.59	6.56	7.26	9.14	5.71	5.36	8.32	7.98	7.98
(BE/A)$_c$ (MeV)		6.59	6.56	7.26	6.96	5.71	5.36	6.99	5.16	
$\langle r_c^2 \rangle^{1/2}$ (fm)		2.37	2.39	2.44	2.55	2.41	2.48	2.55	2.69	2.7 ± 0.1

TABLE II. Single particle energies ϵ in MeV, occupation probabilities P (14), binding energy per particle (BE/A) and rms charge radius $\langle r_c^2 \rangle^{1/2}$ for ^{16}O resulting from various self-consistent calculations with the Reid (Ref. 18) soft core potential. The details are described in Table I. The intermediate particle shifts are $C = 42$ MeV and $C = 38$ MeV (shift to the self-consistent position of the $1s_{1/2}$ level).

		s.c. Spectrum $C = 42$ MeV				$C = 38$ MeV				
^{16}O		BHF	RBHF	RBHF + s.c. Q	DBHF	BHF	RBHF	RBHF + s.c. Q	DBHF	Expt.
$\pi 0s_{1/2}$	ϵ	−50.76	−38.93	−37.93	−32.94	−48.96	−36.77	−35.91	−31.74	−40 ± 8
	P	1.00	0.82	0.83	0.86	1.00	0.80	0.81	0.85	
$\pi 0p_{3/2}$	ϵ	−25.72	−18.17	−17.87	−16.44	−24.05	−16.60	−16.36	−15.31	−18.4
	P	1.00	0.79	0.80	0.81	1.00	0.80	0.80	0.82	
$\pi 0p_{1/2}$	ϵ	−21.00	−14.93	−14.62	−12.60	−19.51	−13.69	−13.45	−11.75	−12.1
	P	1.00	0.80	0.80	0.81	1.00	0.80	0.81	0.83	
$\nu 0s_{1/2}$	ϵ	−54.22	−41.75	−40.72	−35.46	−52.39	−39.49	−38.62	−34.31	
	P	1.00	0.81	0.82	0.86	1.00	0.79	0.80	0.84	
$\nu 0p_{3/2}$	ϵ	−28.77	−20.56	−20.24	−18.62	−27.06	−18.91	−18.66	−17.51	−21.9
	P	1.00	0.79	0.80	0.81	1.00	0.80	0.80	0.82	
$\nu 0p_{1/2}$	ϵ	−24.31	−17.56	−17.25	−15.06	−22.78	−16.25	−16.02	−14.24	−15.7
	P	1.00	0.80	0.80	0.81	1.00	0.80	0.81	0.83	
BE/A (MeV)		6.36	8.40	8.11	8.34	5.77	7.63	7.40	7.56	7.98
(BE/A)$_c$ (MeV)		6.36	7.32	7.08	5.71	5.77	6.60	6.41	5.23	
$\langle r_c^2 \rangle^{1/2}$ (fm)		2.33	2.44	2.48	2.57	2.358	2.487	2.52	2.60	2.7 ± 0.1

used afterwards for these two terms the starting energies of the RBHF approach. In addition, we kept in these two small terms the excited particle spectrum constant at the *sd* shell in order to reduce the computational work. These are not serious approximations, since there are two small correction terms and any reasonable approximation should be a good one. This is not apparent at first since the denominator in the Pauli rearrangement term may even change sign. We went back to check this numerically by introducing an imaginary term in the denominator of the Pauli rearrangement term to avoid any singularities, taking finally the real part of the calculation. In the extreme case where the denominator was made minimum we found the effect on the single particle energies (where the effect is largest) to be less than 5% compared with the more exact calculation. This justifies our approximations used in these two terms.

The effect of the different terms in the HF Hamiltonian (11), which are depicted in Fig. 1, can be seen from the results displayed in Tables I and II and in Figs. II to VI.

It is well known[6,15] that the RBHF approach reduces the absolute value of the single particle energies drastically. Tables I and II show reductions between 12 and 8 MeV for $0s_{1/2}$ single particle energies. The binding energy per particle is increased by about 2 MeV. The overcounting correction[6,15] reduces this to half of the value.

Next we show the effect of the two new terms included in our calculation. First we look at the effect of using the self-consistent Pauli operator rather than the oscillator Pauli operator. Its effect is small as expected. The single particle energy becomes more repulsive; the reduction in the extreme case is up to 1 MeV or 4 MeV depending on the order in which the terms are included. The binding energy per A (BE/A) is reduced up to a maximum of 0.35 MeV. However, it does reduce the density at the center of the nucleus and this increases the rms radius.

The Pauli rearrangement term is more important. It reduces the single particle energy in the $0s$ state up to 5 MeV. It does reduce the density of the nucleus at the center up to 25%, and this in-

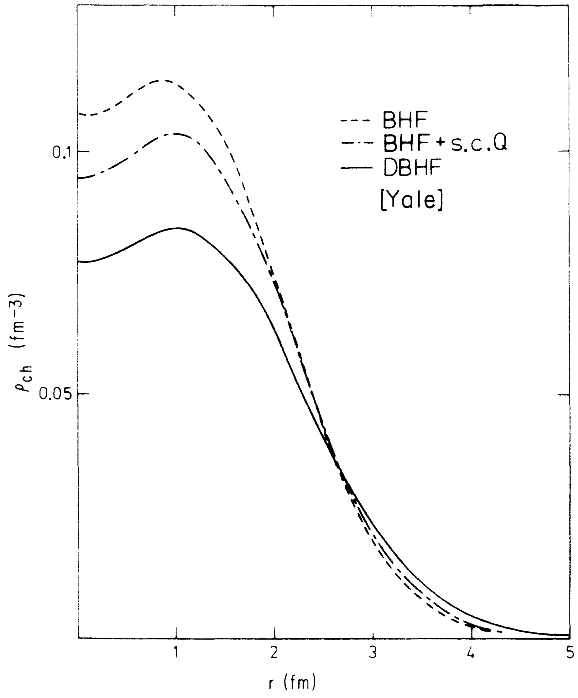

FIG. 2. Charge distribution for ^{16}O with the Yale (Ref. 17) potential. The particle spectrum is shifted by $C = 41.5$ MeV, so that the lowest unoccupied s state ($1s_{1/2}$) agrees with the self-consistent result of the BHF calculation. The dotted lines are for BHF, the dashed-dotted lines for BHF plus s.c. Q, and the solid lines for density dependent Brueckner-Hartree-Fock (DBHF), which includes all terms of the Hamiltonian, Eq. (11). The distribution takes into account the finite size of the proton and the c.m. correction (Ref. 8).

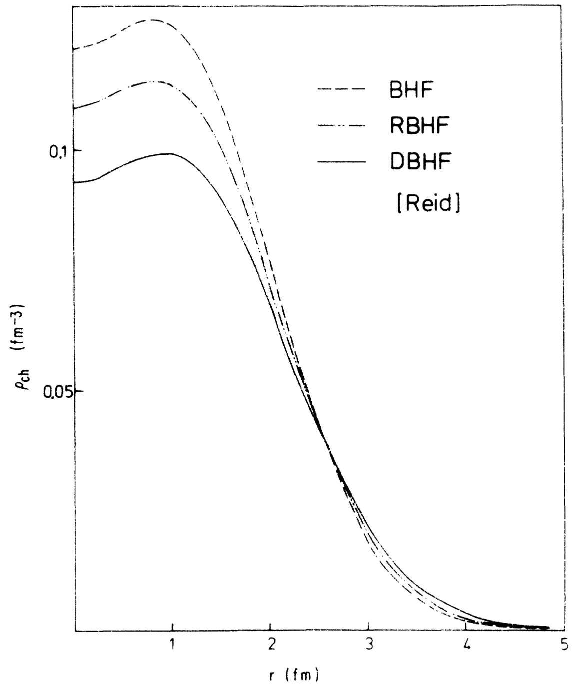

FIG. 3. Charge distribution for ^{16}O using the Reid soft core (Ref. 18) potential in the Brueckner-Hartree-Fock (BHF, dotted line), the renormalized BHF [RBHF ≅ first, second, and fourth term of Eq. (11), dashed-dotted line] and the density dependent BHF (DBHF, solid line) approaches. The shift of the particle spectrum is $C = 42$ MeV. The distribution is corrected for the finite size of the proton and the center of mass motion (Ref. 8).

creases the rms radius while keeping the BE/A practically the same (BE/A changes at most by 0.45 MeV). Hence this term does help the saturation of the nucleus more significantly. Both terms taken together do help quite a bit to saturate the nucleus at the correct density, namely, the BE/A changes only by 0.06 MeV while the radius increases from 2.44 to 2.57 fm for the Reid soft core potential (see Table II). Hence it is obvious that these two terms, although unimportant for the BE/A, are quite important for the s.p. energies and rms radius and also for the density distribution of the nucleus.

In order to test our density distribution we calculated the electron scattering cross section.[19]

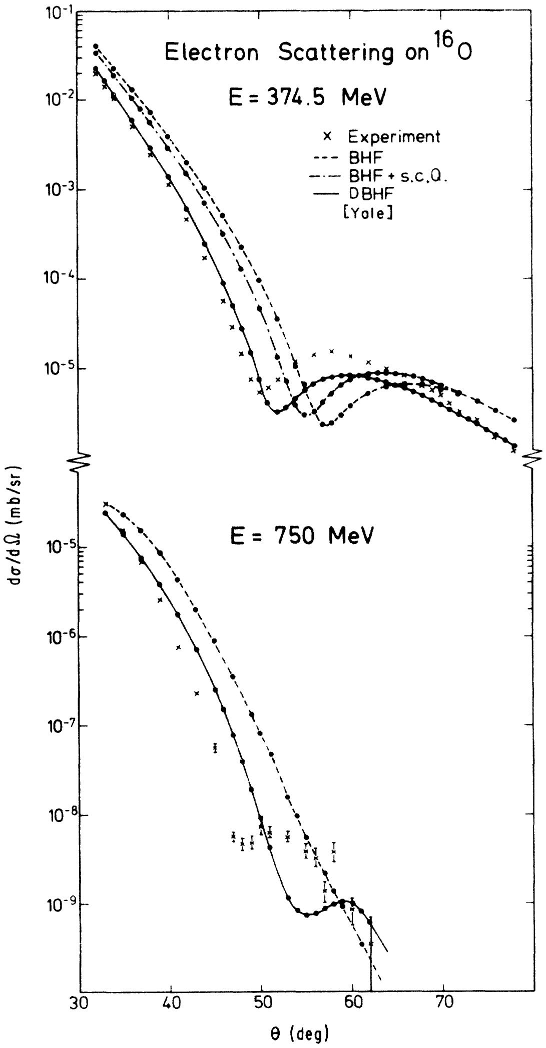

FIG. 4. Elastic electron scattering from the charge distribution calculated with the Yale potential shown in Fig. 2 for ^{16}O at 374.5 MeV (top part of figure) and at 750 MeV (bottom part). The different approaches are described in Fig. 2. The crosses represent the experimental data (Ref. 18).

The results are shown in Figs. 4 and 5, for the density distributions plotted in Figs. 2 and 3. The agreement with the electron scattering data at 379.5 MeV with the effect of the two additional terms (s.c. Pauli operator and Pauli rearrangement terms) is rather good. The agreement at 750 MeV is also improved. However, our basis should be enlarged to expect any better agreement with the electron scattering data at this energy.

We have listed the experimental numbers for the s.p. energy, BE, and rms radius in Tables I and II. One should be careful in comparing the single particle energies of the theoretical calculation with

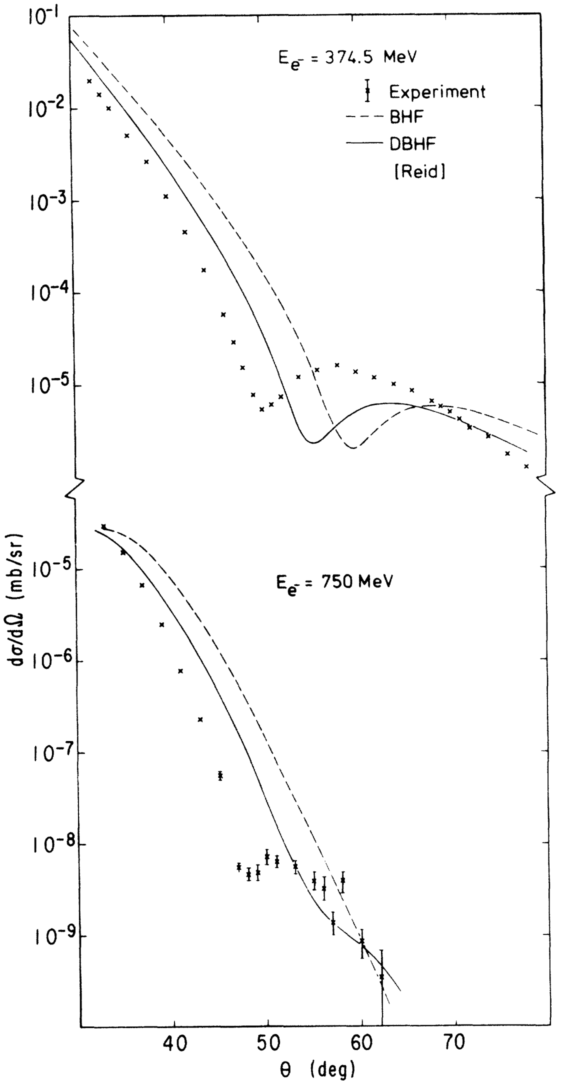

FIG. 5. Elastic electron scattering cross section at 374.5 and 750 MeV for the charge distribution of ^{16}O calculated with the Reid soft core potential (Ref. 18) shown in Fig. 3. The two curves are for the BHF (dotted line) and for the DBHF [all terms of Eq. (11), solid line]. The shift of the intermediate particle spectrum is $C = 42$ MeV.

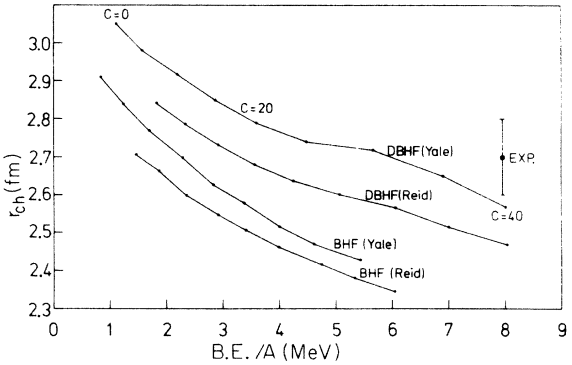

FIG. 6. Binding energies per particle versus rms radius with varying shifts for Yale (Ref. 17) and Reid (Ref. 18) soft core potentials. The point with the error bar indicates the experimental value.

those of the experimental ones. While it is true that the introduction of the rearrangement terms introduced here does bring physically the s.p. energies calculated here closer to the experimental ones,[16] there is still not a one-to-one corresponence since the final hole state in a pickup reaction is mixed with 1p2h and 2p3h states.[20,21] Comparing the single particle energies for the 0s and 0p state in Ref. 10, Table I (second to last row corresponding to the BHF + s.c. Q + P.r. approach) with the results of DBHF in Table I of this work ($C = 46.5$ MeV) one finds the following changes: The inclusion of the starting energy rearrangement and the self-consistent starting energy W lowers the absolute value for the 0s single particle energy and increases these numbers for the 0p states. This can be explained with the starting energy dependence of G matrix elements. While the self-consistent absolute values of W for the 0s nucleons are larger than the averaged values in Ref. 10, this leads to a reduction of the matrix elements and therefore also of the single particle energies. The opposite is true for the 0p states.

The elastic electron scattering cross sections do not agree so well as for phenomenological density dependent forces.[8] This may be caused by one of the three facts:

(i) Negele[8] fits two free parameters to nuclear matter data while this is a parameter free calculation. The electron scattering data are mainly determined by the half-density radius and the slope of the density distribution at this point. Negele fits the half-density radius, then the slope comes out alright in his case. One naturally expects the partly fitted results to be better.

(ii) The derivation of the phenomenological density dependent forces in nuclear matter uses approximations which may change partly the character of the force.

(iii) In Ref. 8 the HF calculations are performed in r and not in a finite configuration space. This may improve their results for high momentum transfer compared to the cross sections given here.

Figure 6 shows the binding energies per particle plotted versus the rms radius for the Yale[17] and the Reid soft core[18] potential for different intermediate particle shifts C. The Yale force seems to be doing better than the Reid soft core potential in the sense that it passes closer to the experimental point. The numerical calculations yield 1.7 MeV additional binding per particle per $\Delta C = 10$ MeV shift for the Yale potential and 1.2 MeV per $\Delta C = 10$ MeV shift for the Reid soft core potential.

IV. CONCLUSIONS

The BHF calculations presented here for the Yale and the Reid soft core potential take into account the Pauli operator in the self-consistent basis. In addition a related rearrangement term is also included. Both these terms are found to give improved saturation properties for both potentials employed. The treatment of the Pauli operator in the self-consistent basis, as we have shown, does include the density dependent effects automatically. The results of our calculations show all the features known from the phenomenological density dependent forces. It reduces the separation energies, increases the rms radius and the binding energy. The charge distribution is lowered in the center of the nucleus and is greatly improved as shown by the electron scattering data. It therefore seems that for the density dependent forces the detour over nuclear matter can be avoided.

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[1] D. J. Thouless, Phys. Rev. 112, 906 (1958); K. A. Brueckner and D. T. Goldman, *ibid.* 117, 207 (1960); K. A. Brueckner, H. W. Meldner, and J. D. Perez, Phys. Rev. C 7, 537 (1973).

[2] M. Baranger, *Nuclear Structure and Nuclear Reactions*, in *Proceedings of the International School of Physics, "Enrico Fermi," Varenna, 1967, Course XL*, edited by M. Jean and R. A. Ricci (Academic, New York, 1969), p. 511.

[3] K. T. R. Davies, M. Baranger, R. M. Tarbutton, and

T. T. S. Kuo, Phys. Rev. 177, 1519 (1969); K. T. R. Davies and M. Baranger, Phys. Rev. C 1, 1640 (1970).

[4] R. L. Becker, A. D. MacKellar, and B. M. Morris, Phys. Rev. 174, 1264 (1968).

[5] B. R. Barrett, R. G. L. Hewitt, and R. J. McCarthy, Phys. Rev. C 2, 1199 (1970); 3, 1137 (1971).

[6] K. T. R. Davies and R. L. Becker, Nucl. Phys. A176, 1 (1971); K. T. R. Davies and R. J. McCarthy, Phys. Rev. C 4, 81 (1971); R. J. McCarthy and K. T. R. Davies, *ibid.* 1, 1644 (1970); K. T. R. Davies, R. J. McCarthy, and P. U. Sauer, *ibid.* 6, 1461 (1972).

[7] A. Kallio and B. D. Day, Nucl. Phys. A124, 177 (1970); R. K. Tripathi and P. Goldhammer, Phys. Rev. C 6, 101 (1972).

[8] J. W. Negele, Phys. Rev. C 1, 1260 (1970); D. W. L. Sprung and P. K. Banerjee, Nucl. Phys. A168, 273 (1971).

[9] J. Nemeth and G. Ripka, Nucl. Phys. A194, 329 (1972).

[10] R. K. Tripathi, A. Faessler, and A. D. MacKellar, Phys. Rev. C 8, 129 (1973).

[11] A. Faessler, A. D. MacKellar, and R. K. Tripathi, Nucl. Phys. A215, 525 (1973).

[12] A. Faessler, R. K. Tripathi, and H. Müther, in Proceedings of the Symposium on Correlations in Nuclei, Balatonfüred, Hungary, 1973, edited by J. Nemeth (to be published).

[13] L. D. Landau, Sov. Phys.—JETP 3, 920 (1956); 5, 101 (1957); 8, 70 (1959).

[14] B. Brandow, in *Lectures in Theoretical Physics*, edited by K. T. Mahanthappa and W. E. Brittin (Gordon and Breach, New York, 1969), Vol. XIB; Rev. Mod. Phys. 39, 771 (1967); Phys. Rev. 152, 863 (1966).

[15] R. L. Becker, Phys. Rev. Lett. 24C, 400 (1970); Phys. Lett. 32B, 263 (1970); R. L. Becker, K. T. R. Davies, and M. R. Patterson, Phys. Rev. C 9, 1221 (1974).

[16] H. Müther, A. Faessler, and K. Goeke, Nucl. Phys. A215, 213 (1973).

[17] K. E. Lassila, M. H. Hull, H. M. Ruppel, P. A. McDonald, and G. Breit, Phys. Rev. 126, 881 (1962).

[18] R. V. Reid, Ann. Phys. (N.Y.) 50, 411 (1968).

[19] I. Sick and J. S. McCarthy, Nucl. Phys. A150, 631 (1970).

[20] U. Wille and R. Lipperheide, Nucl. Phys. A189, 113 (1972); W. Fritsch, R. Lipperheide, and U. Wille, *ibid.* 198, 515 (1972).

[21] A. Faessler, S. Kusuno, and G. L. Strobel, Nucl. Phys. A203, 513 (1973).

[22] K. A. Brueckner, J. L. Gammel, and J. T. Kubis, Phys. Rev. 118, 1438 (1960); H. S. Köhler, *ibid.* 137, B1145 (1965).