Removal and Single Particle Energies in Nuclei

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Dedicated to Prof. K. BLEULER *for his Sixtieth Birthday*

The difference between the absolute value of the Hartree—Fock (HF) single particle energy and the removal energy is studied. This total rearrangement is composed out of the orbital (or spatial) and the Brueckner rearrangement. It is shown analytically within the Pauli—Brueckner HF (PBHF) approach that the saturation potential $\langle h \mid \partial V/\partial \varrho \mid h \rangle$ for a density dependent effective force is equal to the Brueckner rearrangement energy of the level $\mid h \rangle$ plus a smaller term. This is in ^{16}O accidentally numerically roughly equal to the orbital rearrangement energy. The numerical calculation in ^{16}O of the rearrangement energies for the proton level yields the maximum value (9 MeV) for the $Os_{1/2}$ state. The Brueckner rearrangement is from a factor two to twenty larger than the orbital rearrangement.

1. Introduction

In the last years the Hartree-Fock (HF) approach yielded more and more reliable results for the ground state properties of nuclei [1–3]. Among other data it produces also the single particle energies. KOOPMANS [4] did demonstrate already in the thirties that their absolute value is identical with the removal energies. This identity was shown only under the following two assumptions:

1. The single particle wave functions are the same in the nucleus with A and with $A-1$ nucleons and

2. the interaction is identical in the initial and the final nucleus.

Both conditions are not fulfilled in a nucleus.

1. The single particle wave functions are the number of nucleons, the HF method yields different single particle functions in the nucleus with A and the nucleus with $A-1$ nucleons. The resulting positive difference between the absolute value of the single particle energy $|\varepsilon_i|$ and the removal energy S_i is named the *orbital or spatial rearrangement energy*.

2. The renormalisation of the realistic force into the Brueckner reaction matrix depends due to the Pauli operator in the Bethe-Goldstone equation on the occupation probabilities of the single particle states. These probabilities are different in the initial and final nucleus. The total rearrangement is not just the sum of both effects due to the strong coupling between them. The orbital rearrangement is restricted to finite nuclei while the second type of rearrangement is also present in nuclear matter. It is called "*Brueckner rearrangement*" and was first studied in nuclear matter by BRUECKNER and GOLDMAN [5] and later by KÖHLER [6, 7]. The orbital rearrangement energy has been calculated by FAESSLER and WOLTER [8] and by MÜTHER et al. [9]. Until now the Brueckner rearrangement has not been calculated in a finite nucleus. BASSICHIS and STRAYER [10] have calculated approximately the Brueckner rearrangement energy in ^{16}O utilizing second order perturbation theory. But they utilized the occupation probabilities of Eq. (18) and not (19). This overestimates [9] the rearrangement effect.

In the last two years HF calculations with density dependent forces [2, 11] and with methods taking this density dependence into account in finite nuclei (without the detour over nuclear matter) gave single particle energies which compare favourably with the experimental removal energies. Naturally one would like to know if the HF single particle energies with density dependent forces include totally or partially the orbital and Brueckner rearrangement effect.

In Chapter 2 we will develop the theory for calculatinig the rearrangement energies. The orbital rearrangement energy is calculated exactly within the framework of the HF approach. The Brueckner rearrangement is calculated by summing the first diagram of Fig. 1 in the Goldstone expansion. In nuclear matter Köhler did show that the second diagram of Fig. 1 contributes 10% of the first diagram while the diagram of Fig. 2 can contribute 20 to 40%. Finally we will show that the HF single particle

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energies calculated with density dependent forces and including the "saturation potential" $(\partial V/\partial \varrho)$ take into account the Brueckner rearrangement in a reasonable approximation but neglect the orbital rearrangement.

In Chapter 3 the numerical results are presented and discussed. In general the Brueckner rearrangement is more than twice as large as the orbital one.

In Chapter 4 the conclusions of this work are summarized.

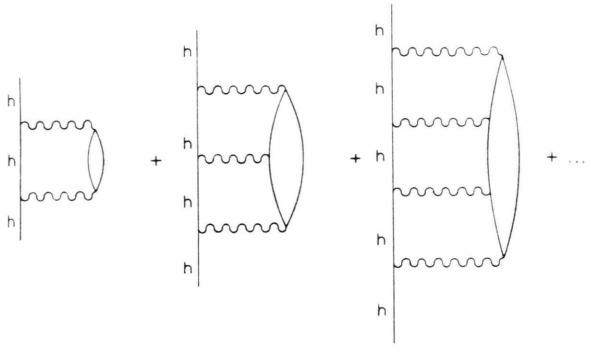

Fig. 1. Series of diagrams for the Brueckner rearrangement energy corresponding to expansion (7) with $^{A-1}e = {}^{A}e$ for the energy denominators.

2. Orbital and Brueckner Rearrangement

The removal or separation energy for the pick up of a nucleon from a nucleus is defined as:

$$S_h = {}^{A}B - {}^{A-1}B^{(h)} = {}^{A-1}E^{(h)} - {}^{A}E\,. \tag{1}$$

Here $^{A}B = -{}^{A}E$ are the total binding and the total energy, respectively. $^{A-1}E^{(h)}$ is the total energy in the $A-1$ nucleon system where the particle in the A system has been removed from the single particle state h. The total energy ^{A}E has to be calculated with the effective interaction ^{A}G and the single particle wave functions $\Phi_i{}^{A}$ in the A nucleon system. Correspondingly $^{A-1}E^{(h)}$ is defined with the effective interaction $^{A-1}G^{(h)}(W)$ (W = starting energy) and the wave functions $\Phi_i{}^{A-1(h)}$. The rearrangement energy R_h is then given by the difference of the absolute value of the HF single particle energy $^{A}\varepsilon_h$ and the separation energy S_h.

$$R_h = |\,\varepsilon_h{}^{A}\,| - S_h\,. \tag{2}$$

In the BHF approach the separation (or removal) energy has the form:

$$\begin{aligned} S_h &= -{}^{A}\varepsilon_h - R_h = {}^{A-1}E^{(h)} - {}^{A}E \\ &= -\langle \Phi_h{}^{A}\,|\,t\,|\,\Phi_h{}^{A}\rangle - \sum_{j=1}^{A}\langle \Phi_h{}^{A}\,\Phi_j{}^{A}\,|\,{}^{A}G\,|\,\Phi_h{}^{A}\,\Phi_j{}^{A}\rangle \\ &\quad - \Big\{\sum_{i=1}^{A}\big(\langle \Phi_i{}^{A}\,|\,t\,|\,\Phi_i{}^{A}\rangle - \langle \Phi_i{}^{A-1(h)}\,|\,t\,|\,\Phi_i{}^{A-1(h)}\rangle\big) \\ &\quad + \tfrac{1}{2}\sum_{\substack{i,j=1\\ i,j\neq h}}^{A}\big(\langle \Phi_i{}^{A}\,\Phi_j{}^{A}\,|\,{}^{A}G\,|\,\Phi_i{}^{A}\,\Phi_j{}^{A}\rangle \\ &\quad - \langle \Phi_i{}^{A-1(h)}\,\Phi_j{}^{A-1(h)} \\ &\quad \cdot {}^{A-1}G^{(h)}\,|\,\Phi_i{}^{A-1(h)}\,\Phi_j{}^{A-1(h)}\rangle\big)\Big\}\,. \end{aligned} \tag{3}$$

The two body matrix elements are here antisymmetrized as in this whole work. The term in the last curly bracket of Eq. (3) is identical with the total rearrangement energy. It is evident that it vanishes if the effective interaction G and the single particle functions Φ_i are the same in the A and the $A-1$ nucleons system. The same interaction but different single particle states yields the *orbital rearrangement* while different interactions ^{A}G and $^{A-1}G^{(h)}$ and the same wave functions give the *Brueckner rearrangement.*

The orbital (or spatial) rearrangement is calculated straightforward by two HF calculations utilizing the same two body matrix elements. The difference in the effective interaction G (which produces for the same single particle wave functions the Brueckner rearrangement) stems from the inaquality of the Pauli operator and the energy denominator in the Bethe-Goldstone equation in the A and the $A-1$ nucleons system.

$${}^{A}G({}^{A}W) = V + V\,({}^{A}Q/{}^{A}e)\;{}^{A}G({}^{A}W)\,. \tag{4}$$

To discuss the Brueckner rearrangement energy we assume that the single particle wave functions are the same.

$$\begin{aligned} &R_h(\text{Brueckner}) \\ &= \tfrac{1}{2}\sum_{\substack{i,j=1\\ i,j\neq h}}\langle i\,j\,|\,{}^{A}G({}^{A}W) - {}^{A-1}G^{(h)}({}^{A-1}W)\,|\,i\,j\rangle\,. \end{aligned} \tag{5}$$

To simplify the calculation of expression (5) one expresses ^{A-1}G by ^{A}G. The exact equation [12]

$${}^{A}G - {}^{A-1}G = -{}^{A}G\left[\frac{{}^{A-1}Q}{{}^{A-1}e} - \frac{{}^{A}Q}{{}^{A}e}\right]{}^{A-1}G \tag{6}$$

can be iterated:

$${}^{A}G - {}^{A-1}G = -\{{}^{A}G\;p^{(h)}\;{}^{A}G + {}^{A}G\;p^{(h)}\;{}^{A}G\;p^{(h)}\;{}^{A}G\ldots\}$$

with:
$$p^{(h)} \equiv \frac{{}^{A-1}Q}{{}^{A-1}e} - \frac{{}^{A}Q}{{}^{A}e}\,. \tag{7}$$

In the approximation ${}^{A}e = {}^{A-1}e$ one is only summing the diagrams in Figure 1. The energy denominator ${}^{A-1}e$ can also be expanded into quantities of the A nucleons system:

$$ {}^{A-1}\varepsilon_i^{(h)} \approx {}^{A}\varepsilon_i - \langle i\,h \,|\, {}^{A}G \,|\, i\,h \rangle \,. \tag{8} $$

The lowest terms which originate from such an expansion correspond to the diagrams in Figure 2. KÖHLER [7] did show in nuclear matter that the third order diagrams in Figs. 1 and 2 yield up to 10% and 40% respectively of the leading second order diagram from Figure 1. We took into account the first term of the right hand side of Eq. (7) which corresponds to the second order diagram of Figure 1.

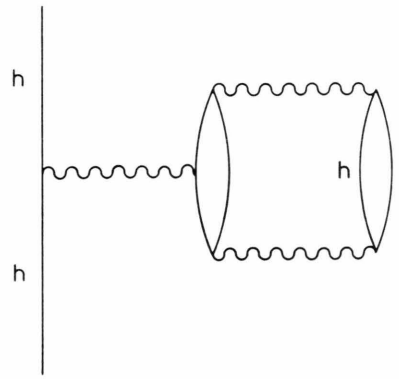

Fig. 2. Lowest order diagrams of the expansion (7) for the Brueckner rearrangement energy arising from the difference of the energy denominators ${}^{A}e$ and ${}^{A-1}e$.

$$ R_h(\text{Brueckner}) = -\sum_{\substack{i,j<F \\ i,j\neq h}} \sum_{m>F} |\langle i\,j \,|\, {}^{A}G({}^{A}W) \,|\, h\,m \rangle|^2 ({}^{A}\varepsilon_i + {}^{A}\varepsilon_j - {}^{A}\varepsilon_h - {}^{A}\varepsilon_m)^{-1} \tag{9} $$

$|h\rangle$ = selfconsistent hole state,
$|i\rangle, |j\rangle, |m\rangle$ = selfconsistent single particle states in A nucleons system.

The above expression is normally positive since the average value for the energy denominator is negative.

The total rearrangement energy (2) can now be calculated by performing two HF calculations to get the removal energy according to:

$$ S_h = {}^{A-1}E^{(h)}_{\text{BHF}} - {}^{A}E_{\text{BHF}} \,. $$

The two body elements in the $A-1$ system are given by:

$$ {}^{A-1}G \approx {}^{A}G + {}^{A}G \,\frac{{}^{A-1}Q^{(h)} - {}^{A}Q}{{}^{A}e}\, {}^{A}G \tag{10} $$

with $\quad {}^{A}e \equiv {}^{A}W - H_0 \,.$

Although Eqs. (3) and (9) establish clearly that the absolute value of the HF single particle energy is different from the experimental removal energy, recent [2, 11, 13] HF calculations yield single particle energies which agree very nicely with the separation energies S_h. These calculations are all utilizing density dependent effective forces [2, 11] or take the density dependence in some other way into account [13]. It seems therefore that the density dependence is modifying the single particle energies so that the rearrangement effect is at least taken partially into account.

$$ \varepsilon_i = \langle i \,|\, t \,|\, i \rangle + \sum_{k<F} \langle i\,k \,|\, V \,|\, i\,k \rangle + \tfrac{1}{2} \sum_{l,k<F} \langle l\,k \,|\, \frac{\partial V}{\partial \varrho_i} \,|\, l\,k \rangle \,. \tag{11} $$

If ε_i is in this case approximately $-S_i$ then the last term of (11) should correspond to the rearrangement energy. If we are utilizing a selfconsistent Pauli operator

$$ \langle a\,b \,|\, Q_{\text{HF}} \,|\, c\,d \rangle = (\delta_{ac} - \varrho_{ac})\,(\delta_{bd} - \varrho_{bd}) $$
$$ |a\rangle, |b\rangle, |c\rangle, |d\rangle = \text{oscillator basis states} \tag{12} $$

as in the Pauli-Brueckner-Hartree-Fock (PBHF) approach [13] we are getting also a density dependent force. This yields the so called [13] Pauli rearrangement potential, which corresponds to the last term in Equation (11).

$$ \begin{aligned} \langle h \,|\, U \,|\, h \rangle &= \tfrac{1}{2} \sum_{k,l<F} \langle l\,k \,|\, \frac{\partial\, {}^{A}G}{\partial \varrho_h} \,|\, l\,k \rangle \\ &= \tfrac{1}{2} \sum_{\substack{k,l<F \\ mn}} \langle l\,k \,|\, {}^{A}G \,|\, m\,n \rangle \\ &\cdot \frac{\partial}{\partial \varrho_h} \{(1-\varrho_m)\,(1-\varrho_n)\}\, \frac{1}{e^A}\, \langle m\,n \,|\, {}^{A}G \,|\, l\,k \rangle \\ &= -\sum_{\substack{k,l<F \\ m>F}} |\langle k\,l \,|\, {}^{A}G \,|\, h\,m \rangle|^2 \,(\varepsilon_k + \varepsilon_l - \varepsilon_h - \varepsilon_m)^{-1} \,. \end{aligned} \tag{13} $$

Here we utilized the fact that the effective matrix elements ${}^{A}G$ calculated with the selfconsistent Pauli operator (12) can be written:

$$ \tilde{G} = G + G\left(\frac{Q_{\text{HF}}}{{}^{A}e} - \frac{Q}{{}^{A}e}\right) G + \ldots \tag{14} $$

Q = oscillator Pauli operator.

A comparison of the last term in Eq. (13) with the Brueckner rearrangement energy (9) shows that the Pauli rearrangement (13) (which corresponds for density dependent effective forces to the saturation potential $\partial V/\partial \varrho$) is up to

$$\delta_h = -\sum_{\substack{l<F \\ m>F}} |\langle h\, l \,|\, {}^A G \,|\, h\, m\rangle|^2 \,(\varepsilon_l - \varepsilon_m)^{-1} \quad (15)$$

identical with the Brueckner rearrangement energy. Since δ_h is always positive one expects that the saturation potential is larger than the Brueckner rearrangement. In many cases one finds (see Chapter 3) that δ_h is of the order of the orbital rearrangement energy and the saturation potential agrees accidentally with the total rearrangement energy.

3. Numerical Procedure and Results

The HF solutions have been calculated utilizing the program of TRIPATHI, FAESSLER and MACKELLAR [13] which considers the density dependence of the effective force G in the finite nucleus. This dependence stems from the Pauli operator. It is handled without the usual detour [2] over nuclear matter. The total energy can be written [13]:

$$\langle H\rangle = E = \mathrm{tr}(t\,\varrho) + \tfrac{1}{2}\,\mathrm{tr}(G\,\varrho\,\varrho) + \tfrac{1}{2}\,\mathrm{tr}\left(G\left\{\frac{(1-\varrho)\,(1-\varrho)}{e} - \frac{Q}{e}\right\}\varrho\,\varrho\right). \quad (16)$$

The last term is the correction for the difference between the selfconsistent Pauli operator (12) expressed by the selfconsistent density matrices ϱ in the oscillator representation and between the oscillator Pauli operator Q. The effective matrix elements are solutions of Bethe-Goldstone equation in an oscillator space up to $12\,\hbar\,\omega$ with the oscillator Pauli operator Q employing the Yale potential and adding the elements of the Coulomb repulsion between the protons. The procedure for solving the Bethe-Goldstone equation is the same as the one of BECKER et al. [14]. The variation of the total energy (16) with respect to the density matrix ϱ yields the HF matrix.

$$h_{ab} = \langle a\,|\,t\,|\,b\rangle + (G\,\varrho)_{ab} + \left(G\,\frac{(1-\varrho)\,(1-\varrho) - Q}{e}\,G\,\varrho\right)_{ab} - \left(G\,\frac{1-\varrho}{e}\,G\,\varrho\,\varrho\right)_{ab}. \quad (17)$$

The two first terms on the right hand side represent the Brueckner-Hartree-Fock (BHF) matrix. The third term gives the correction for the difference between the selfconsistent and the oscillator Pauli operator (Pauli-Brueckner HF = PBHF). The last term of Eq. (17) is the Pauli rearrangement term (PBHF with rearrangement).

In order to calculate the rearrangement energy (2) and (3) one has to perform also a HF calculation in the $A-1$ nucleons system where the A-th particle is missing in the selfconsistent state $|\,h\rangle$. If the A nucleons system is a doubly closed shell nucleus (here ^{16}O) then the $A-1$ system may be deformed. To limit the numerical efforts for a basis $\leqq 12\,\hbar\,\omega$ to a manageable amount we have to restrict the wave functions to spherical symmetry. This symmetry is violated if one occupies out of $n = 2j+1$ degenerate levels $n-1$ and leaves one unoccupied. To conserve the spherical symmetry we utilize the following occupation probabilities (density matrix in the selfconsistent basis):

$$\varrho_k = \begin{cases} 1 & \text{for} \quad k<F;\ k \neq h_1, \ldots, h_n, \\ 1-1/n & \text{for} \quad k = h_1, \ldots, h_n, \\ 0 & \text{for} \quad k>F. \end{cases} \quad (18)$$

Here $|\,h_1\rangle$ is the single particle state out of which the nucleons has been picked up and $|\,h_2\rangle, \ldots, |\,h_n\rangle$ are the states which are degenerate with $|\,h_1\rangle$ due to the rotational symmetry. The correct occupation probabilities would be:

$$\tilde{\varrho}_k = \begin{cases} 1 & \text{for} \quad k<F,\ k \neq h_1, \\ 0 & \text{else}. \end{cases} \quad (19)$$

The expectation value of a one body scalar operator like the kinetic energy does not depend on the choice of the occupation probabilities (18) or (19). But the expectation value of a two body scalar operator (like the interaction) is different for the choice (18) and (19), since it is not a scalar in the space of particle "1" and "2" independently. We are calculating here the difference of such an expectation value between the two alternatives (18) and (19).

$$\langle \Psi(\varrho)\,|\,G\,|\,\Psi(\varrho)\rangle = \sum_{\substack{k,l<F \\ \neq h}} \langle i\,j\,|\,G\,|\,i\,j\rangle + 2\left(1-\frac{1}{n}\right)\sum_{\substack{i<F;\neq h \\ j=h}} \langle i\,j\,|\,G\,|\,i\,j\rangle + \left(1-\frac{1}{n}\right)\left(1-\frac{1}{n}\right)\sum_{i,\,j=h} \langle i\,j\,|\,G\,|\,i\,j\rangle\,. \quad (20)$$

The HF Slater determinant $\Psi(\varrho)$ is here calculated with the occupation ϱ. The symbol "h" indicates here all n degenerate single particle states $h_1, \ldots, h_n$. If one introduces the two average values

$$\langle h_2\,h_3\,|\,\bar{G}_1\,|\,h_2\,h_3\rangle = \frac{1}{n(n-1)}\sum_{i,\,j=h} \langle i\,j\,|\,G\,|\,i\,j\rangle\,, \qquad \langle h_2\,h_3\,|\,\bar{G}_2\,|\,h_2\,h_3\rangle = \frac{1}{(n-1)\,(n-2)}\sum_{\substack{i,\,j=h \\ \neq h_1}} \langle i\,j\,|\,G\,|\,i\,j\rangle\,, \quad (21)$$

one is able to write:

$$\langle \Psi(\varrho) \,|\, G \,|\, \Psi(\varrho) \rangle = \sum_{i<F;\, \neq h} \langle i\,j \,|\, G \,|\, i\,j \rangle + 2\,\frac{n-1}{n}\, n \sum_{i<F;\, \neq h} \langle i\,h_2 \,|\, G \,|\, i\,h_2 \rangle$$
$$+ (n-1)\,(n-2)\ \langle h_2\,h_3 \,|\, \bar{G}_1 \,|\, h_2\,h_3 \rangle + \frac{n-1}{n}\ \langle h_2\,h_3 \,|\, \bar{G}_1 \,|\, h_2\,h_3 \rangle\,. \quad (22)$$

The last two terms of Eq. (22) have been separated out of the last term of Equation (20). The expectation value with the exact density matrix $\tilde{\varrho}$ of Eq. (19) may be written in a similar way utilizing the second of the Equations (21).

$$\langle \Psi(\tilde{\varrho}) \,|\, G \,|\, \Psi(\tilde{\varrho}) \rangle = \sum_{i,j<F;\, \neq h} \langle i\,j \,|\, G \,|\, i\,j \rangle + 2\,(n-1) \sum_{i<F;\, \neq h} \langle i\,h_2 \,|\, G \,|\, i\,h_2 \rangle$$
$$+ (n-1)\,(n-2)\ \langle h_2\,h_3 \,|\, \bar{G}_2 \,|\, h_2\,h_3 \rangle\,. \quad (23)$$

Apart of the different way of averaging in the last term of Eq. (23) this expression is identical with the first three terms on the right hand side of the expectation value (22) with the smeared out occupation probabilities. One verifies immediately that by averaging the position of the picked uk nucleon $|\,h_1\rangle$ over the whole shell h the two average values (21) are identical. Furthermore one sees that the third terms on the right and side of Eqs. (22) and (23) disappears for te important $n=2$ $(j=1/2)$. One finds therefore from (22) and (3) with the help of Eq. (21) the equation

$$\langle \Psi(\tilde{\varrho}) \,|\, G \,|\, \Psi(\tilde{\varrho}) \rangle = \langle \Psi(\varrho) \,|\, G \,|\, \Psi(\varrho) \rangle - \frac{1}{n^2} \sum_{i,j=h} \langle i\,j \,|\, G \,|\, i\,j \rangle\,, \quad (24)$$

which is exact for $n=2$ and for $n>2$ correct in the spirit of the occupation probabilities of Equation (18). In the numerical procedure we use the probabilities (18) and correct later on for the error by utilizing Equation (24).

The above described calculations have been performed for ^{16}O for proton hole states in the $Os_{1/2}$, $Op_{3/2}$, and $Op_{1/2}$ shell. An average starting energy of $W=-78$ MeV has been chosen. The intermediate oscillator energy spectrum has been shifted downward by $C=56.5$ MeV. If one considers the sd shell levels as the most important intermediate levels this implies an average energy denominator $\bar{e}=\Delta=-58$ MeV with $h\,\omega=13.3$ MeV for the oscillator basis.

For calculating the Brueckner rearrangement energy (9) we utilized the same average energy denominator. In reality the absolute value might be smaller in this case, so that we are perhaps underestimating the Brueckner rearragement energy. The calculated value might be considered as a lower limit.

In Table 1 and 2 the results for the proton single particle states in ^{16}O are listed for the basis $\leqq 8\,\hbar\,\omega$ and the larger basis $\leqq 12\,\hbar\,\omega$. The results show that the basis up to $8\,\hbar\,\omega$ is not large enough for the quantitative values, although they show the same qualitative relations between the different rearrangement energies as the results in the large ($\leqq 12\,\hbar\,\omega$) basis. The effect of the center of mass correction on the rearrangement energy has been discussed in detail by MÜTHER et al. [9]. Since it is not included here the results disaggree slightly with Table II of Reference [13].

The orbital rearrangement energy is practically independent of the fact if one looks to the results of the Brueckner HF (BHF) or to the Pauli-Brueckner HF (PBHF) approach without Pauli rearrangement, although the total binding and the separation energies are quite different in the two methods. The Brueckner rearrangement energy is considerably larger. The total rearrangement has its maximum value for the $Os_{1/2}$ state with almost 9 MeV. It has not to be the sum of the orbital and the Brueckner rearrangement energy due to the coupling between both.

Finally the saturation potential or Pauli rearrangement (13) is given. It should be identical with the Brueckner rearrangement (9) up to the positive term (15). Therefore it is larger than the Brueckner rearrangement and within 1 MeV as large as the

Table 1. Proton Rearrangement Energies in ^{16}O for the Basis $\leqq 8\,\hbar\omega$.

Rearrangement energies of the proton levels for ^{16}O in the oscillator basis $\leqq 8\,\hbar\omega$. The force is the Yale potential [18] and the basis is calculated with the oscillator energy $\hbar\omega = 13.3$ MeV. The starting energy has been chosen as the weighted average of the occupied single particle energies of former calculations [14] as $W = -78$ MeV. The intermediate single particle energies have been shifted by $c = 56.5$ MeV downward. This yields an average energy denominator $e \equiv \Delta = -58$ MeV if one takes the sd shell as the most important intermediate states for ^{16}O. The total binding energy in the BHF approach is $B_{BHF} = 117.48$ MeV while the Pauli BHF (PBHF) yields $B_{PBHF} = 104.81$ MeV. The table shows in its upper part the single particle energies in the A nucleons system (^{16}O) in the BHF and the PBHF (without Pauli rearrangement) approach. The second and the third part give the orbital rearrangement for these two approaches calculated with the reaction matrix ^{A}G of the A nucleons system. The fourth part utilizes the single particle wave functions of ^{16}O of the PBHF method to calculate with the effective interactions ^{A}G and ^{A-1}G the Brueckner rearrangement energy. The fifth part gives the total rearrangement for the PBHF approach. The last part shows the Pauli rearrangement energy [14] which corresponds to the saturation potential $\partial V/\partial\varrho$ for density dependent effective forces. The symbols $^{A}\varepsilon_h$, $^{A-1}\varepsilon_h$, B, S_h, R_h indicate the single particle energies for the state $|\,h\,\rangle$ in the A and the $A-1$ nucleons system, the total binding energy, the removal energy (1), (3), and the rearrangement energy (2).

holes		$s_{1/2}$	$p_{3/2}$	$p_{1/2}$
$-{}^{A}\varepsilon_h$(BHF)	[MeV]	61.90	26.14	19.97
$-{}^{A}\varepsilon_h$(PBHF)	[MeV]	56.21	24.72	19.03
Orbital Rearrangement; BHF				
^{A-1}B	[MeV]	57.98	91.62	97.62
S_h	[MeV]	59.50	25.86	19.86
R_h	[MeV]	2.40	0.28	0.11
$-{}^{A-1}\varepsilon_h$	[MeV]	56.70	25.54	19.73
Orbital Rearrangement; PBHF				
^{A-1}B	[MeV]	50.90	80.41	85.90
S_h	[MeV]	53.91	24.40	18.91
R_h	[MeV]	2.30	0.32	0.12
$-{}^{A-1}\varepsilon_h$	[MeV]	51.10	24.06	18.77
Brueckner Rearrangement; PBHF				
^{A-1}B	[MeV]	51.94	81.02	87.68
S_h	[MeV]	52.87	23.79	17.13
R_h	[MeV]	3.34	0.93	1.90
$-{}^{A-1}\varepsilon_h$	[MeV]	58.03	24.85	19.32
Total Rearrangement: PBHF				
^{A-1}B	[MeV]	55.47	81.98	87.78
S_h	[MeV]	49.34	22.83	1703
R_h	[MeV]	6.87	1.89	2.00
$-{}^{A-1}\varepsilon_h$	[MeV]	55.29	24.36	19.07
Pauli Rearrangement; PBHF with Rearrangement				
$-{}^{A}\varepsilon_h$	[MeV]	51.05	23.66	16.85
R_h	[MeV]	5.16	1.06	2.18

Table 2. Proton Rearrangement Energies in ^{16}O for the Basis $\leqq 12\,\hbar\omega$.

Rearrangement energies of the proton levels for ^{16}O in the oscillator basis $\leqq 12\,\hbar\omega$. The further details are the same as in Table 1. The binding energies of ^{16}O are: $B_{BHF} = 122.5$ MeV and B_{PBHF} (without Pauli rearrangement) $= 102.33$ MeV.

holes		$s_{1/2}$	$p_{3/2}$	$p_{1/2}$
$-{}^{A}\varepsilon_h$(BHF)	[MeV]	64.67	27.40	20.28
$-{}^{A}\varepsilon_h$(PBHF)	[MeV]	55.43	24.80	18.65
Orbital Rearrangement; BHF				
^{A-1}B	[MeV]	60.58	95.46	102.34
S_h	[MeV]	61.87	26.99	20.11
R_h	[MeV]	2.80	0.41	0.17
$-{}^{A-1}\varepsilon_h$	[MeV]	58.65	26.55	19.93
Orbital Rearrangement; PBHF				
^{A-1}B	[MeV]	49.44	77.94	83.86
S_h	[MeV]	52.89	24.39	18.47
R_h	[MeV]	2.54	0.41	0.18
$-{}^{A-1}\varepsilon_h$	[MeV]	50.14	23.93	18.28
Brueckner Rearrangement; PBHF				
^{A-1}B	[MeV]	51.86	79.05	87.06
S_h	[MeV]	50.47	23.28	15.27
R_h	[MeV]	4.96	1.52	3.38
$-{}^{A-1}\varepsilon_h$	[MeV]	57.88	25.01	19.20
Total Rearrangement: PBHF				
^{A-1}B	[MeV]	55.79	80.52	86.96
S_h	[MeV]	46.54	21.81	15.37
R_h	[MeV]	8.89	2.99	3.28
$-{}^{A-1}\varepsilon_h$	[MeV]	55.50	24.48	18.83
Pauli Rearrangement; PBHF with Rearrangement				
$-{}^{A}\varepsilon_h$	[MeV]	48.02	23.07	14.72
R_h	[MeV]	7.41	1.73	3.93

total rearrangement energy. This is probably the secret of the good agreement which one reaches with density dependent forces. BECKER, PATTERSON [15] and KÖHLER, LIN [16] have recently shown that the asbolute value of the single particle energies and the separation energies are approximately equal (Koopmans theorem) for the renormalized Brueckner-Hartree-Fock (RBHF) approach and for phenomenological density dependent forces, respectively, if one neglects the orbital rearrangement. For the numerical calculations both are utilizinig the occupation probabilities (18) instead of (19). This yields to unreliable numerical results [9] [see also Eq. (24)].

4. Conclusion

The relation between the Hartree-Fock (HF) single particle energy ε_h and the removal energy S_h is very important since the first one can easily be calculated while the second can be measured directly [17]. The absolute values of the two energies are unequal due to the change of the selfconsistent potential and therefore the single particle wave functions *(orbital rearrangement)* and due to the alteration of the Brueckner matrix *(Brueckner rearrangement)* going from the A to the $A-1$ nucleons system.

The agreement which one gets for the separation energies and the single particle energies utilizing density dependent effective interactions $V(\varrho; r_{12})$ is justified. We show here that the single particle expectation value of the saturation potential $\langle h \mid \partial V/\partial \varrho \mid h \rangle$ is equal to the Brueckner rearrangement energy R_h (Brueckner) plus a smaller additional term which is numerically (accidentally) approximately equal to the orbital rearrangement energy. The above proof is performed with an expression for the effective force selfconsistently derived in the finite nucleus [13].

The numerical calculations yield that the Brueckner rearrangement in ^{16}O is by a factor two larger than the orbital rearrangement for the $Os_{1/2}$ proton state and up to almost a factor twenty for the $p_{1/2}$ level. The orbital rearrangement decreases drastically goinig from the $Os_{1/2}$ state to the levels near the Fermi surface. Although the Bueckner rearrangement decreases too, it shows a much weaker variation. But the value of the Brueckner rearrangement energy for the low lying hole states might be increased by taking a more realistic energy denominator in Equation (9). the largest value of the total rearrangement is almost 9 MeV for the $Os_{1/2}$ proton level in ^{16}O.

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