Quasi-Deuterons in Light Nuclei

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Abstract. The role of pairing correlations for nucleon pairs with isospin $T = 1$ and $T = 0$ is investigated for ground-states of nuclei in the mass region $12 \leq A \leq 42$. For that purpose the two-nucleon densities resulting from nuclear shell-model calculations in one and two major shells are analyzed. Various tools are applied in this analysis including the sensitivity of correlation effects on components of the $NN$ interaction. Significant effects on the resulting energies are observed due to the formation of $T = 0$ pairs. The formation of quasi-deuterons is maximal for symmetric nuclei with $N = Z$. The formation of $T = 0$ pairs is less sensitive to the density of single-particle states close to the Fermi energy than the $T = 1$ pairing. Therefore the correlations in $T = 0$ pairs are relevant also for excitations across shell-closures. This robustness also explains why $T = 0$ pairing does not lead to such a clear evidence in comparing energies of neighbored nuclei as the “odd-even mass staggering” due to the formation of $T = 1$ pairing.

Keywords: Isoscalar pairing, Shell-model, Correlations, Two-body density

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1. Introduction

The occurrence of pairing correlations between nucleons of the same isospin is a well established feature in the study of ground state properties of nuclei. The pairing term is an important ingredient of the nuclear mass formula to describe the odd-even mass staggering in the binding energies of nuclei\cite{1}. Therefore it has been an obvious extension of mean-field or Hartree-Fock calculations of nuclei to account for the formation of proton-proton ($pp$) and neutron-neutron ($nn$) pairs by performing Hartree-Fock Bogoliubov (HFB) calculations for nuclei all over the nuclear mass table (For example see Refs.\cite{2, 3, 4, 5} and references cited there).

While the importance of $pp$ and neutron-neutron $nn$ pairing correlations is established, no clear evidence has empirically been observed for corresponding $pn$
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At first sight this is rather astonishing since the proton-neutron interaction is more attractive than the interaction between like nucleons and leads to the only bound states of two nucleons in the deuteron channel $^3S^1D_1$. Therefore one should expect stronger two-nucleon correlations in the form of $pn$ pairing than $pp$ or $nn$ pairing also in nuclei.

Indeed, this expectation is supported by the study of pairing correlations in isospin symmetric infinite nuclear matter. BCS calculations for infinite nuclear matter predict values for the pairing gap of $pp$ or $nn$ pairing in the $^1S_0$ channel of the order of 1 to 2 MeV, which is in reasonable agreement with empirical data for $nn$ and $pp$ pairing in finite nuclei. Corresponding calculations for $pn$ pairing in the $^3S^1D_1$ channel yield much larger values for the pairing gap, which are of the order of 10 MeV. Therefore one may expect that it should also be seen in finite nuclei, in particular in light nuclei with equal number of protons and neutrons.

Efforts have been made to determine the $pn$ pairing in nuclei by solving the corresponding HFB equations or to extract corresponding correlations from wavefunction of shell-model calculations in one major shell or performing variational calculations in large model spaces, which account for superpositions of various symmetry-projected HFB states. Neither these theoretical studies nor the analysis of empirical data, as discussed above, provide any clear evidence for strong $pn$ pairing effects occurring in infinite nuclear matter.

It has been argued that the strong spin-orbit field in light nuclei may spoil the isoscalar spin 1 $pn$ pairing correlations. Bertsch and Zuo demonstrated that a spin triplet pairing condensate may occur in large nuclei, where the spin-orbit term tends to become smaller. Their study is based on a Woods-Saxon description for the mean field of the nucleons and a phenomenological contact interaction to generate the pairing correlations.

More recent studies tried to investigate the modifications $T=1$ as well as $T=0$ pairing-correlations in a transition from nuclear matter to finite nuclei. These studies are based on realistic models for the $NN$ interaction and support the reduction of $T=0$ pairing due to the spin-orbit term as discussed by Bertsch and Zuo for open shell nuclei with $N=Z$ like $^{28}$Si. The studies in Ref predict rather strong effects of $T=0$ pairing for the closed-shell nuclei $^{16}$O and $^{40}$Ca.

In the present study we extend a systematic study of $T=0$ and $T=1$ pairing correlations by analyzing the results of configuration-mixing shell-model calculations for the ground-state of light nuclei. Special attention has been paid to the contributions to the energy resulting from the $pp$ and $nn$ interaction, which are compared to the contributions of the $pn$ interaction in pairs of nucleons with $T=0$ and $T=1$. Two-nucleon densities are investigated and analyzed in terms of a partial wave decomposition.

Results of calculations for $sd$-shell nuclei, assuming an inert core of $^{16}$O and accounting for all configurations of valence nucleons in the $1s0d$ shell are presented in section 2. In section 3 we discuss corresponding results for nuclei around $^{16}$O and $^{40}$Ca considering configurations of nucleons in two major shells ($1p$ and $1s0d$ for nuclei
with mass number $A$ around 16 and 1s0d and 1p0f for $A$ around 40). The conclusions from the present study are summarized in the final section 4.

2. Nuclei in the sd-shell

Most of the nuclear structure calculations discussed in this manuscript have been performed using a realistic model for the $NN$ interaction, which is based on the One-Boson-Exchange Potential (OBEP) A defined in Ref.\[26\]. This interaction has been chosen as we also want to study the dependence of $NN$ correlations on various parameters of a relativistic meson-exchange model. As we will demonstrate below, most of the results discussed are not very sensitive to the $NN$ interaction used.

The OBEP A interaction has been determined by fitting the $NN$ phase shifts and the data of the deuteron using the Thompson equation. In order to derive matrix elements of a two-nucleon interaction to be used in a shell-model calculation we assume oscillator wave function (using an oscillator length $b = 1.76$ fm, which is appropriate for nuclei around $^{16}$O and solve the corresponding Bethe-Goldstone equation for a starting energy of -10 MeV. The single-particle energies have been determined from the corresponding Hartree-Fock definition for $^{16}$O, which yields -1.13 MeV, -0.26 MeV, and 3.96 MeV for the 0$d_{5/2}$, the 1$s_{1/2}$, and the 0$d_{3/2}$ shell, respectively. The shell-model calculation have been performed using a Fortran code, which has been inspired and checked by comparison with the package “KShell”, developed by N. Shimizu et al.\[27\].

Results for the energy per valence nucleon and various contributions to this energy for the ground-states of Ne, Mg and Si isotopes are displayed in Fig.1. Before we discuss some details for these results we would like to draw the attention to Fig.2 which shows the corresponding results, which have been obtained using quite a different Hamiltonian, the single-particle energies and the effective interaction USD defined by Brown et al.\[28\]. This Hamiltonian has been fitted to describe nuclear data all over the sd-shell with a shell-model diagonalization.

Although the origin of the two interaction models leading to the results displayed in Figs.1 and 2 is rather different the main features of the various contributions to the energy for the ground states show rather similar features. Only the results for the total energy exhibit some differences. The fact that the binding energies obtained from the Brown-Wildenthal interaction are consistently larger than the corresponding values derived from the OBEP A interaction model is mainly due to the fact that the single-particle energies entering the USD calculations (-3.95 MeV, -3.16 MeV, 1.65 MeV) are more attractive as compared to the values (-1.13 MeV, -0.26 MeV, 3.96 MeV) used for the OBEP A calculations.

Another difference in the calculated energies per valence nucleon is the feature that the Brown-Wildenthal interaction yields a minimal energy for each chain of isotopes displayed in Fig.2 whereas the OBEP A interaction model leads to energies per nucleon, which tend to decrease with increasing neutron number. This difference is related to the fact that fit of the Brown-Wildenthal interaction includes a dependence of the two-body
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**Figure 1.** (Color online) Contributions to the energy per valence nucleon $A$ of Ne (left panel), Mg (middle panel), and Si isotopes (right panel) as a function of neutron number $N$ as derived from shell-model calculations for the $sd$ shell using the $G$-matrix evaluated for the One-Boson-Exchange potential $A$ as described in the text. Results are presented for the total energy ($E_{\text{tot}}$ black dots connected by solid line), the contributions resulting from the $pn$ interaction in pairs with isospin $T = 0$ ($pn, T = 0$, red triangles connected by dashed line) and the contributions obtained from $pn$ pairs with $T = 1$ (green squares connected by dashed line), $pp$ pairs (magenta stars connected by dotted line) and $nn$ pairs (blue diamonds connected by a yellow line).

interaction, which weakens the interaction by a factor

$$
\left(\frac{\tilde{A}}{18}\right)^{(-0.3)}.
$$

where $\tilde{A}$ stands for the total number of nucleons for the nucleus considered. It would be possible to account for a mass dependence of the OBEP $A$ interaction model by considering e.g. a mass dependence of the oscillator functions or reducing the starting energy in the solution of the Bethe-Goldstone equation. Note, however, that it is not the focus of the present investigation to provide an optimal model for the residual interaction. Instead we are interested to discuss features of the correlated many-body states which are general and do not depend on details of the interaction.

Such a feature is the “odd-even mass staggering”, in the energy per nucleon for the various chains of isotopes displayed in Figs. 1 and 2. This means that nuclei with even number of neutrons tend to have a larger binding energy than those with odd neutron
Figure 2. (Color online) Contributions to the energy per nucleon for the ground-states of Ne, Mg and Si isotopes evaluated for the USD interaction of Brown et al.\cite{28}. Further details see Fig.1. Note that for the total energy per valence nucleon a shift of 2 MeV has been added to allow the use of the same energy scale in the figure.

Number $N$ can be traced back to corresponding energy contribution of neutron-neutron pairs, which are represented in those figures by blue triangles connected by yellow lines. This feature is typically interpreted as a signal for the formation of pairs of protons or neutrons, which is suppressed by a blocking effect for an odd number of protons or neutrons.

This pairing effect is a consequence of the attraction of a pair of nucleons with total isospin $T = 1$ in the $^1S_0$ partial wave. Therefore it should be visible by analyzing the two-nucleon density inspecting the contribution, which is due to a pair of nucleons in the $^1S_0$ partial wave for the relative coordinates. Assuming oscillator functions, as we have done in calculating the interaction OBEP A described above, one can easily calculate this contribution using the Talmi-Moshinsky\cite{29} transformation and determine the matrix elements for the two-nucleon projection operator

$$\langle \alpha \beta, JT | \hat{P}^{T=1} | \gamma \delta, JT \rangle = \sum_{n,N,L} \langle \alpha \beta JT | n^1 S_0, N, L, JT \rangle \langle n^1 S_0, N, L, JT | \gamma \delta, JT \rangle$$

where $|\alpha \beta, JT\rangle$ denotes the antisymmetrized two-nucleon state for oscillator states $\alpha$ and $\beta$ coupled to total angular momentum $J$ and isospin $T$ whereas the quantum numbers $n$...
refers to the radial quantum number for the relative oscillator motion in the $^1S_0$ partial wave while $N$ and $L$ identify the quantum numbers for the center of mass motion. In eq. (2) $\langle \alpha \beta JT | n, ^1S_0, N, L, JT \rangle$ denote the corresponding transformation brackets\[29\].

In the following we will consider the expectation value of this projection operator $\hat{P}^T_{ij}$ for the ground-state of a specific nucleus, $\langle \Psi | \hat{P}^T_{ij} | \Psi \rangle$ divided by the number of antisymmetrized pairs of nucleons $Q^T_{ij}$ of the kind $ij$ and isospin $T$ considered. In the case of 2 neutrons, i.e. $ij = nn$ the total isospin is $T = 1$ and

$$Q^1_{nn} = \frac{N(N - 1)}{2}$$

with $N$ the number of valence neutrons. Note that a projection operator, which corresponds to $\hat{P}^{T=1}$ in eq[2] can also be defined for the $^3S_1$ partial wave and would be applicable for proton-neutron ($pn$) pairs with isospin $T = 0$ and identified as $\hat{P}^0_{pn}$. In the case, $ij = pn$, we have for $Z$ valence protons and $N$ valence neutrons with $Z \leq N$ numbers of pairs with $T = 0$ and $T = 1$:

$$Q^0_{pn} = \frac{1}{2}Z(N + 1)$$

$$Q^1_{pn} = \frac{1}{2}Z(N - 1).$$

This leads to

$$\tilde{S}^T_{ij} = \frac{\langle \Psi | \hat{P}^T_{ij} | \Psi \rangle}{Q^T_{ij}},$$

The average contribution of $^1S_0$ or $^3S_1$ pairs in the two-body density of nucleon type $ij$. This quantity can be normalized dividing it by the average quantity, which is obtained when all orbits of the valence shell are completely filled

$$S^T_{ij} = \frac{\tilde{S}^T_{ij}}{\tilde{S}^T_{ij} (\text{filled shell})}.$$

This will be referred to as the enhancement of the formation of $^1S_0$ or $^3S_1$ pairs in the ground-state of the nucleus under consideration.

Results for the enhancement of $^1S_0$ neutron-neutron pairs in various isotopes of Ne, Na, Mg, and Si isotopes are presented in the left panel of Fig.\[3\] It is obvious that the enhancement factor for the $^1S_0$ component in the $nn$ part of the nuclear wave function decreases with the increasing number of valence neutrons $N$. For $N = 2$ the components of the wave functions for the one pair of neutrons, which contain a large amplitude of the attractive $^1S_0$ partial wave are enhanced by more than a factor 5 as compared to the average content of this partial wave in all pairs which can be formed in the $sd$ shell. For the case of e.g. $N = 5$ one has to consider 10 orthogonal pairs of neutrons. Therefore the enhancement factor drops to a value around 1.5 and is bound to go down to $S_{nn} = 1$ for the maximal number of neutrons $N = 12$ to fill all neutron states in the $sd$ shell.

It is worth noting that the enhancement factor $S^1_{nn}$, which characterizes the $nn$ part of the two-nucleon density is almost independent on the chain of isotopes under consideration despite the strong interaction between protons and neutrons.
Figure 3. (Color online) Enhancement of the $^{1}S_{0}$ pair contribution $S_{nn}^{1}$, defined in eq.6 for various chains of isotopes are displayed in the left panel. The right panel shows the corresponding enhancement $U_{nn}$ of the pairs with $J = 0$ and $T = 1$ as defined in eq.9.

Another feature, which is very evident in Fig.3 is the “odd-even staggering” of $S_{nn}^{1}$ as a function of $N$. This behavior is very similar to the “odd-even staggering” in the binding energy originating from interacting neutrons displayed in Figs.1 and 2. This is a strong indication that these odd-even staggerings are related and indicate the formation of $nn$ pairing correlations due to the attraction in the $^{1}S_{0}$ partial wave in nuclei with an even number of neutrons.

This conclusion is confirmed by inspecting the enhancement factors $S_{nn}^{1}$ as well as $S_{pp}^{1}$ listed in table 1. In this table we have listed for the example of Mg isotopes enhancement factors resulting from the two-body densities obtained in shell-model calculations and compared them to those evaluated in a Hartree-Fock (HF) calculation. Note that the HF calculations are restricted to the wave functions within the sd shell and that we consider the projection of the HF state $\Phi_{HF}$ to a state with good total angular momentum $J = 0$. Applying the standard tools of angular momentum projection [1, 30], denoting the corresponding projection operator as $\hat{P}(J = 0)$ one obtains

$$|\Psi_{HF}\rangle = \hat{P}(J = 0)|\Phi_{HF}\rangle.$$  

The enhancement factors $S_{ij}^{T}$ are then obtained by replacing the SM wave function by this projected HF state, $|\Psi\rangle \rightarrow |\Psi_{HF}\rangle$ in eq.5. The comparison exhibits a significant enhancement for $S_{nn}^{1}$ derived from the shell-model to the corresponding values obtained in the mean-field approximation. This demonstrates indeed that correlations beyond mean-field are relevant to obtain large components in the two-body density of $nn$ and $pp$ pair densities in the $^{1}S_{0}$ partial wave.

Results for the enhancement of the proton-neutron isovector pairing, $S_{pn}^{1}$, are displayed in the left panel of Fig.4. For the nuclei with an even number of protons, i.e.
Table 1. Results for the enhancement $S_{ij}^{T}$ as defined in eq.6 for various isotope of Mg. Results of shell-model calculations (SM) are compared to those of Hartree-Fock with projection of angular momentum (HF).

|       | $S_{pn}^{0}$ | $S_{pn}^{1}$ | $S_{nn}^{1}$ | $S_{pp}^{1}$ |
|-------|--------------|--------------|--------------|--------------|
| $^{22}$Mg | 1.573        | 2.182        | 5.607        | 2.282        |
| SM     | 1.505        | 2.117        | 4.996        | 1.837        |
| $^{24}$Mg | 1.529        | 2.189        | 2.189        | 2.189        |
| HF     | 1.302        | 1.831        | 1.831        | 1.831        |
| $^{26}$Mg | 1.294        | 1.521        | 1.553        | 2.246        |
| SM     | 1.304        | 1.528        | 1.492        | 1.776        |
| $^{28}$Mg | 1.155        | 1.244        | 1.223        | 2.321        |
| HF     | 1.159        | 1.226        | 1.131        | 1.808        |

For $Ne$, $Mg$ and $Si$, the enhancement factor is maximal for the isotopes with $N = Z$. For the cases of an odd number of protons, $Na$ and $Al$, the enhancement $S_{pn}^{1}$ is suppressed for the isotopes with $N = Z$ as compared to the ones with $N = Z \pm 1$. In these cases the isovector pairing for $N = Z$, which is identical for $nn$, $pp$ and $pn$ pairs, is suppressed because the $pp$ and $nn$ pairing is suppressed for an odd number of the corresponding nucleons.

The definition of the enhancement factors $S_{ij}^{T=-1}$ which we discussed so far are based on the results of the corresponding results for the projection operator $\hat{P}_{ij}^{T}$ defined in eq.2. This definition may be compared to the projection operator

$$\mathcal{N}_{ij} = \sum_{\alpha,\beta} |\alpha \beta, J = 0, T = 1 \rangle \langle \alpha \beta, J = 0, T = 1 |$$

(8)

counting the number of pairs of neutrons ($ij = nn$) or proton-neutron pairs ($ij = pn$) which are coupled to angular momentum $J = 0$ and $T = 1$. The expectation values of this projection operator has been used by Engels et al.\[31]\ to investigate the role of isovector pairing in proton-rich nuclei in the pf-shell.

In analogy to eqs.5 and 6 the expectation values for the operator $\mathcal{N}_{ij}$ can be used to determine enhancement factors

$$\tilde{U}_{ij} = \frac{\langle \Psi | \hat{N}_{ij} | \Psi \rangle}{Q_{ij}^{1}}.$$  

(9)

The normalized enhancement factors $U$ are defined in analogy to eq.6.

Results for the corresponding enhancement factors $U_{nn}$ and $U_{pn}$ are presented in the right panels of Figs. 3 and 4, respectively. These enhancement factors $U$, which are based on the number of nucleon pairs with $J = 0$ and $T = 1$ show the same features as have been discussed for the corresponding factors $S_{ij}^{1}$ which refer to pairs of nucleons in the $^{1}S_{0}$ partial wave for the relative coordinate. One observes that the features displayed...
Figure 4. (Color online) Enhancement of the $^1S_0$ pair contribution $S_{pn}^1$, defined in eq.6, and the corresponding enhancement factors $U_{pn}$, defined in eq.9, are presented for various chains of isotopes are in the left panel and right panel, respectively.

by the factors $U$ are even more pronounced than those derived from the analysis of the $S^1$ factors.

Below, however we will focus our attention on the factors $S_{ij}^T$ as we are interested in particular in the comparison of isoscalar and isovector pairing. While $S_{pn}^0$, which is based on pairs of nucleons in the $^3S_1$ partial wave and can be interpreted to “measure” the amount of quasi-deuteron pairs, we do not have a corresponding definition for $U$ in the case of isoscalar pairing.

We now return to discuss the results displayed in Figs.1 and 2. It is obvious from this that most attractive contributions to the total energy result from the proton-neutron ($pn$) interaction, in particular from $pn$ pairs with isospin $T = 0$. The results in these figures also indicate that maximal attraction from such pairs is obtained for nuclei with $N = Z$. We want to explore, to which extent this maximal attraction could be identified as a signal for an enhanced formation of quasi-deuterons or $T = 0$ pairing in these nuclei.

For that purpose we inspect the enhancement factors for the $^3S_1$ partial wave in the $pn$ part of the two-body densities. This corresponds to $S_{pn}^0$ in our nomenclature defined in eq.5. Results are displayed in Fig.5.

Similar to the case of $S_{nn}^1$ displayed in Fig.3 also the values for $S_{pn}^0$ decrease with increasing number of valence neutrons $N$. The reason is very similar as discussed above: With increasing $N$ more $pn$ pairs compete for the attraction in the $^3S_1$ partial wave.

At first sight, the enhancement $S_{pn}^0$ seems to be significantly smaller than the results for $S_{nn}^1$. For such a comparison, however, one should notice that e.g. for $N = 2$ only one $nn$ pair has to be optimized and therefore obtains a large contribution from partial wave $^1S_0$. In the $S_{pn}^0$ however, $N = 2$ represents 3 $pn$ pairs with $T=0$ for the case of Ne and 4 pairs in the case of Na isotopes. This means that the enhancement $S_{pn}^0$ yields similar
values as $S_{nn}^1$ if we account for the number of pairs, which share this enhancement.

A very interesting feature for our present discussion is the fact that the enhancement factors $S_{pn}^0$ plotted as a function of $N$ exhibit a kind of “local maximum” for the isotopes with $N = Z$. This means that the maximal gain in the energy contribution from $pn$ pairs is accompanied by a maximum in the enhancement of the $^3S_1$ component in the $pn$ part of the two-body density. Therefore and in line with the discussion of the $T = 1$ pairing between neutrons, it may be appropriate to identify this feature as a formation of quasi-deuterons in $N = Z$ nuclei or as a signal of $T = 0$ pairing.

This argument is supported by the comparison of enhancement factors derived from shell-model calculations to those originating from the Hartree-Fock approach listed in table 1. We find almost no difference between the SM and HF approach comparing $S_{pn}^0$ for the isotopes with $N \neq Z$, whereas a significant increase due to correlations beyond mean field can be observed for the isotope $^{24}$Mg with $N = Z$.

**Figure 5.** (Color online) Enhancement of the $^3S_1$ pair contribution $S_{pn}^0$, defined in eq.6 for various chains of isotopes.

![Figure 5](image_url)

It has been suggested by Matsubara et al.\[32\] that a careful analysis of the Squared Nuclear Matrix Elements (SNME) for isoscalar and isovector M1 transitions should provide direct information for the expectation value for scalar product of the total spin of all protons $\vec{\sigma}_p$ and of all neutrons $\vec{\sigma}_n$

$$
\langle \Psi | \vec{\sigma}_p \cdot \vec{\sigma}_n | \Psi \rangle.
$$

(10)

Since a pair of protons and neutrons in the isovector $^1S_0$ partial wave provides a contribution of $-3/4$ whereas a pair in the isoscalar partial wave $^3S_1$ yields $+1/4$ the
expectation value in eq.10 can be interpreted as a measure for the relative importance of isoscalar and isovector correlations between protons and neutrons[33].

Results for the expectation value of the spin operator of eq.10 are displayed in Fig.6. For all chain of isotopes considered a maximum is obtained for the symmetric case with \( N = Z \). This suggests that the formation of \( T = 0 \) pairs, or quasi-deuterons is maximal in the symmetric case. Note, however, that also the \( ^3P_J \) partial waves with isospin \( T = 1 \) yield positive contributions to the product of the proton and neutron spins.

**Figure 6.** (Color online) Expectation value of the scalar product of proton spin and neutron spin in eq.10 calculated for the ground states of various chains of isotopes.

In the last part of this subsection we would like to discuss the effect of the ingredients of the residual interaction on the various contributions to energy of the ground state of nuclei in the sd-shell listed in tables 2 and 3. The last column of these tables shows the excitation energy of the first excited state. For the isotopes with an even number for protons and neutrons, which are considered in this tables, this first excited states are states with \( J = 2 \), while the ground-states have \( J = 0 \).
For each isotope the first 2 lines with label “SM” and “HF” show results obtained for the G-matrix derived from OBEP A using the diagonalization of the complete shell-model Hamiltonian and the corresponding Hartree-Fock approximation with angular momentum projection. One finds that all excitation energies for the excite states obtained in the HF approach are significantly smaller than those extracted from the SM calculation. This feature may be understood as a consequence of the formation of \( T = 1 \) pairing correlations in the ground-state. At least one of these pairs must be broken to describe the excited state with \( J = 2 \). Consequently, the SM approach accounting for pairing correlations yield a larger excitation energy than the HF approximation. Another interpretation has been given using the rotational picture for the yrast band. In this picture the inclusion of pairing correlation leads to a moment of inertia of a superfluid, which is smaller than the corresponding moment of inertia for a normal liquid. Independent of the underlying interpretation: The increase of the excitation energy by inclusion of correlations going from HF to SM approximation is generally assigned to the formation of \( T = 1 \) pairing correlations in the SM approach.

Other results listed in these tables in the lines with labels “SM1”, “SM2”, and “SM3” have been taken from shell-model calculation using a OBEP interaction in which the contributions due to the exchange of the \( \pi \)-meson (SM1), the scalar-isoscalar \( \sigma \)-meson (SM2), and the \( \omega \) meson has been reduced by 10 percent. This reduction has been achieved by the reduction of the corresponding meson-nucleon coupling constants in the bare interaction. The Bethe-Goldstone equation has been solved for these modified interaction and the calculation of oscillator matrix elements has been done as described above.

From the results displayed in tables 2 and 3 one can see that a reduction of the \( \pi \)-exchange contribution leads to a reduction of total binding energy, which is mainly due to the reduced attraction of \( pn \) pairs with \( T = 0 \). This can be understood from the fact that most of the attractive contributions to the energy of nuclei arises from the iteration of the strong tensor component in the coupled channels of the partial waves \( ^3S_1 - ^3D_1 \). The contributions of the NN interaction for pairs of nucleons with isospin \( T = 1 \) are not very much affected by the reduction of the \( \pi \) exchange.

It is worth noting, that the reduction of the \( \pi \)-exchange has a rather small effect on the excitation energy of the first \( 2^+ \) state. This would be in line with the conclusion that this excitation energy is mainly affected from the pairing effects in the pairs of nucleons \( T = 1 \) (see discussion above).

The reduction of the \( \sigma \)-exchange leads to the reduction of the attractive components resulting from the interaction of \( T = 0 \) pairs as well as pairs with \( T = 1 \). This is accompanied by a decrease of the excitation energy.

Also the reduction of the \( \omega \)-exchange exhibits significant effects on the energy contributions of all kinds of NN pairs. Since the exchange of the vector meson \( \omega \) is responsible for the short-range repulsion of the NN interaction, its reduction leads to an increase in the binding energy for all contributions \( \Delta E \) as well as for the excitation energy \( \Delta E_{J=2} \).
Table 2. Comparison of energy contributions to the total energy obtained in shell-model or Hartree-Fock calculations for various Neon isotopes in the sd-shell. Results are listed for the total energy ($E_{\text{total}}$) the contributions resulting from $T = 0$ pairs and those from the interaction of $pn$, $pp$, and $nn$ pairs with isospin $T = 1$. The last column shows the excitation energy of the first excited state ($J = 2$). The G-matrix derived from the original OBEP A interaction yield the results presented in the lines denoted with SM for shell-model calculations and HF for corresponding Hartree-Fock calculations. The lines denoted with SM1, SM2, and SM3 present the results of shell-model calculations using the OBEP A with reduced $\pi$-exchange, $\sigma$-exchange and $\omega$-exchange, respectively. All energies are listed in MeV.

|       | $E_{\text{total}}$ | $\Delta E_{T=0}$ | $\Delta E_{T=1, pn}$ | $\Delta E_{pp}$ | $\Delta E_{nn}$ | $\Delta E_{J=2}$ |
|-------|--------------------|------------------|---------------------|----------------|----------------|-----------------|
| 20Ne  | SM -23.81          | -13.78           | -3.25               | -3.25          | -3.25          | 1.029           |
|       | HF -23.28          | -12.69           | -3.10               | -3.10          | -3.10          | 0.779           |
|       | SM1 -22.75         | -12.33           | -3.31               | -3.31          | -3.31          | 0.984           |
|       | SM2 -20.65         | -12.05           | -2.70               | -2.70          | -2.70          | 0.755           |
|       | SM3 -26.20         | -15.13           | -3.64               | -3.64          | -3.64          | 1.264           |
| 22Ne  | SM -36.46          | -17.40           | -4.76               | -3.28          | -9.05          | 0.737           |
|       | HF -35.06          | -16.47           | -4.73               | -3.06          | -7.86          | 0.394           |
|       | SM1 -35.16         | -15.67           | -4.78               | -3.35          | -9.17          | 0.749           |
|       | SM2 -31.62         | -15.36           | -4.01               | -2.68          | -7.30          | 0.510           |
|       | SM3 -40.08         | -18.97           | -5.30               | -3.73          | -10.33         | 0.933           |
| 24Ne  | SM -49.58          | -20.31           | -5.93               | -3.34          | -16.59         | 1.012           |
|       | HF -47.70          | -20.44           | -6.00               | -2.83          | -14.38         | 0.639           |
|       | SM1 -48.07         | -18.31           | -5.93               | -3.44          | -16.76         | 1.048           |
|       | SM2 -42.81         | -17.87           | -4.96               | -2.68          | -13.45         | 0.735           |
|       | SM3 -54.61         | -22.19           | -6.62               | -3.83          | -18.90         | 0.755           |

3. Correlations beyond one major shell

While the preceding section has been devoted to the role of $NN$ correlations within one major shell, the $1s0d$ shell, we would like to add some remarks about the importance of $NN$ correlations due to excitations across major shells. For that purpose we have performed shell-model calculations assuming a core of $^4He$ and considering configurations of nucleons in the $0p$ and $1s0d$ shell. For the residual interaction we considered matrix elements of the $G$-matrix for the OBEP A interaction discussed before calculated in a basis of oscillator states with an oscillator length $b = 1.76$ fm, which is appropriate for nuclei around $^{16}O$. The single-particle term has been calculated from the interaction with the nucleons in the core of $^4He$. Effects of spurious center of mass motions have been considered by considering an oscillator field for the center of mass motion and subtracting the resulting energy for the c.m. motion.

For the various nuclei listed in the upper part of table 4 we have performed shell-
Table 3. Comparison of energy contributions to the total energy obtained in shell-model or Hartree-Fock calculations for various isotopes of Mg in the sd-shell. Further details see caption of table 2.

|         | $E_{total}$ | $\Delta E_{T=0}$ | $\Delta E_{T=1,pn}$ | $\Delta E_{pp}$ | $\Delta E_{nn}$ | $\Delta E_{J=2}$ |
|---------|-------------|-------------------|----------------------|-----------------|-----------------|------------------|
| 24$^\text{Mg}$ |            |                   |                      |                 |                 |                  |
| SM      | -60.62     | -33.31            | -9.06                | -9.06           | -9.06           | 0.951            |
| HF      | -54.88     | -27.35            | -7.76                | -7.76           | -7.76           | 0.371            |
| SM1     | -57.99     | -29.88            | -9.16                | -9.16           | -9.16           | 0.918            |
| SM2     | -52.26     | -29.09            | -7.50                | -7.50           | -7.50           | 0.703            |
| SM3     | -66.87     | -36.59            | -10.18               | -10.18          | -10.18          | 1.16             |
| 26$^\text{Mg}$ |            |                   |                      |                 |                 |                  |
| SM      | -79.39     | -40.01            | -11.59               | -8.95           | -16.93          | 1.005            |
| HF      | -77.01     | -40.35            | -11.59               | -7.48           | -16.30          | 0.580            |
| SM1     | -76.19     | -36.07            | -11.61               | -9.09           | -17.05          | 1.013            |
| SM2     | -68.48     | -35.04            | -9.65                | -7.29           | -13.86          | 0.771            |
| SM3     | -87.50     | -43.80            | -12.98               | -10.16          | -19.16          | 1.189            |
| 28$^\text{Mg}$ |            |                   |                      |                 |                 |                  |
| SM      | -98.31     | -45.98            | -13.92               | -9.06           | -26.46          | 1.144            |
| HF      | -95.59     | -45.52            | -13.61               | -7.46           | -24.95          | 0.748            |
| SM1     | -94.61     | -41.52            | -13.89               | -9.21           | -26.50          | 1.174            |
| SM2     | -84.67     | -40.18            | -11.55               | -7.36           | -21.62          | 0.942            |
| SM3     | -108.43    | -50.40            | -15.62               | -10.31          | -29.99          | 1.305            |

model calculations with two different kinds of truncation schemes. In the first one, we considered configurations with minimal, i.e. $0 \hbar \omega$ excitations in the oscillator model for the single-particle configurations. This means for the nuclei $^{12}\text{C}$, $^{14}\text{N}$, and $^{16}\text{O}$ we suppress all configurations with nucleons occupying states in $1s0d$ shell and consider a closed core of $^{16}\text{O}$ for the nuclei with $A > 16$. In the second truncation scheme we consider all configurations with up to $2 \hbar \omega$ excitations. This means for the nuclei $^{12}\text{C}$, $^{14}\text{N}$, and $^{16}\text{O}$ we consider configurations with up to 2 nucleons in states of the $1s0d$ shell and for the nuclei with $A > 6$ we allow up to 2 holes in the core of $^{16}\text{O}$.

Listed in table 3 is the gain in the energy of the ground state due to the admixture of $2 \hbar \omega$ excitations ($\Delta E_{total}$). Also given are the contributions to this energy difference, which are due to the interaction of $pn$ pairs with isospin $T = 0$ ($\Delta E_{T=0}$), the interaction of nucleons with $T = 1$ ($\Delta E_{T=1}$), and the single-particle term, $\Delta E_{sing}$.

The total gain in energy due to the $2 \hbar \omega$ excitations is remarkable. It is as large as -6.51 MeV in the case of $^{16}\text{O}$. This gain in energy seems to be converging: If one considers configurations up to $4 \hbar \omega$ excitation the gain in energy raises to -7.15 MeV. The gain in energy is largest for the “double-magic” nucleus $^{16}\text{O}$ and decreases if one considers nuclei with more or less nucleons. This is also displayed in Fig. 7 where the gain in energy due to the admixture of $2 \hbar \omega$ excitations is plotted for various isotopes as a function of the nucleon number $A$.

This can be interpreted as a kind of blocking effect: The $2 \hbar \omega$ excitations
**Table 4.** Comparison of energies for shell-model calculations in the $0p + 1s0d$ shells (upper part of the table). Listed is the gain of energy due to the admixture of $2\hbar\omega$ excitations for the total energy, $\Delta E_{\text{total}}$, the contributions from interaction between pairs of nucleons with $T = 0$ and $T = 1$ and the energy difference due to the single-particle term, $\Delta E_{\text{sing}}$ for various nuclei around $^{16}\text{O}$. The lower part of the table shows corresponding results for nuclei around $^{40}\text{Ca}$ obtained in shell-model calculations in the $1s0d + 1p0f$ shells. All energies are given in MeV.

| nucleus  | $\Delta E_{\text{total}}$ | $\Delta E_{T=0}$ | $\Delta E_{T=1}$ | $\Delta E_{\text{sing}}$ |
|---------|----------------|----------------|----------------|----------------|
| $^{12}\text{C}$ | -3.71 | -5.07 | -0.85 | 2.21 |
| $^{14}\text{N}$ | -4.82 | -6.83 | -0.84 | 2.85 |
| $^{16}\text{O}$ | -6.52 | -7.80 | -1.75 | 3.04 |
| $^{18}\text{O}$ | -5.50 | -5.97 | -1.49 | 1.95 |
| $^{18}\text{F}$ | -5.68 | -6.71 | -1.14 | 2.16 |
| $^{19}\text{O}$ | -4.86 | -4.85 | -0.22 | 0.21 |
| $^{20}\text{O}$ | -4.43 | -4.63 | -1.04 | 1.23 |
| $^{20}\text{Ne}$ | -4.75 | -5.61 | -1.07 | 1.93 |
| $^{21}\text{Ne}$ | -4.11 | -4.64 | 0.02 | 0.51 |
| $^{22}\text{Ne}$ | -3.68 | -3.96 | -0.88 | 1.16 |
| $^{23}\text{Ne}$ | -3.22 | -3.60 | -0.89 | 1.28 |
| $^{24}\text{Ne}$ | -2.91 | -2.89 | -0.76 | 0.74 |
| $^{36}\text{Ar}$ | -7.11 | -8.62 | -2.65 | 4.16 |
| $^{38}\text{Ar}$ | -7.65 | -8.48 | -3.10 | 3.93 |
| $^{40}\text{Ca}$ | -8.93 | -9.85 | -3.37 | 4.29 |
| $^{42}\text{Ca}$ | -8.30 | -9.09 | -3.19 | 3.98 |
| $^{42}\text{Sc}$ | -8.40 | -9.55 | -3.06 | 4.21 |

correspond to excitations two-particle two-hole excitations of the core nucleus $^{16}\text{O}$. These configurations are partially “blocked” when additional particle and hole-states are occupied by adding or subtracting nucleons with respect to $N = Z = 8$.

The gain in energy due to inter-shell excitations is dominated by the $T = 0$ contributions. This dominance of $T = 0$ correlations is much larger than in the case of correlations within one major shell. As an example we consider the energy contributions to the energy of $^{20}\text{Ne}$ listed in the first line of table 2. The contribution resulting from interaction in nucleon pairs with $T = 0$, -13.78 MeV, is by a factor of 1.41 larger than the energy contribution from $T = 1$ pairs. This may be compared to the case of inter-shell correlations with a ratio for $^{20}\text{Ne}$ of 5.24. This dominance of $T = 0$ inter-shell configurations also explains that the correlation energies are large in particular for the isotopes with $N = Z$ as can be seen from the results displayed in Fig. 7.

This is in line with the results from studies of quasi-nuclear systems in [25], which demonstrated that the formation of quasi-deuterons or $T = 0$ pairing is much more robust against the density of single-particle states around the Fermi energy. Therefore it also occurs for closed-shell nuclei. This robustness, however, is also the reason that it does not show such a clear signature as the odd-even mass difference in the case of $T = 1$ pairing.
Figure 7. (Color online) Gain in energy due to the admixture of $2\hbar\omega$ configurations for nuclei around $^{16}O$.

Table 5. Comparison of energies and ratio of energies as defined in the text and eq.11 calculated for $^{16}O$

|        | OBEPA    | SM1      | SM2      | SM3      |
|--------|----------|----------|----------|----------|
| $\langle V \rangle$ | -159.94  | -152.35  | -139.58  | -174.88  |
| $\Delta V_{2\hbar\omega}$ | -9.56    | -8.60    | -8.57    | -10.47   |
| $\Delta \Omega$       | 2.18     | 0.81     | 1.02     |          |

Finally, we would like to explore the question, which components of the $NN$ interaction lead to the inter-shell correlations discussed in this subsection. For that purpose we present in table 5 for the example of the nucleus $^{16}O$ the expectation value for the $NN$ interaction determined in the shell-model calculations with the inclusion of $2\hbar\omega$ configurations, $\langle V \rangle$ and compare this quantity with the change in this expectation value if the $2\hbar\omega$ configurations are suppressed

$$\Delta V_{2\hbar\omega} = \langle V \rangle - \langle V \rangle_{0\hbar\omega}.$$ 

These calculations have been repeated using the interactions SM1, SM2 and SM3 mentioned above, i.e. the interactions in which the exchange of $\pi$-, the $\sigma$, and the $\omega$ exchange are suppressed by 10 percent. We than compare the effect of the change in
the interaction in the quantity $\Delta V_{2\hbar\omega}$,

$$\Delta \chi_{SM1} = \frac{[\Delta V_{2\hbar\omega}]_{OBEP A} - [\Delta V_{2\hbar\omega}]_{SM1}}{[\Delta V_{2\hbar\omega}]_{OBEP A}}$$

and compare this with the effect in the total energy

$$\chi_{SM1} = \frac{\langle V \rangle_{OBEP A} - \langle V \rangle_{SM1}}{\langle V \rangle_{OBEP A}}.$$

The ratio of these 2 quantities

$$\Delta \Omega = \frac{\Delta \chi}{\chi},$$

is listed in table 5 and shows a value of $\Delta \Omega = 2.18$ for the case of the interaction SM1. This demonstrates that a modification of the $\pi$-exchange contribution in the $NN$ interaction leads to an effect in the correlation energy, which is by a factor 2.18 larger than the effect in the total energy. Modifications of the $\omega$ or $\sigma$-exchange yield values for $\Delta \Omega$ of 1.02 and 0.81, respectively. This leads to the conclusion that the effect of the $\omega$ meson on the correlation energy is very close to its effect on the total energy, while the effect of the $\sigma$ exchange is even weaker in the correlation energy. One should recall that in our discussion of inner shell correlations in the preceding section we observed a connection between the $\sigma$ exchange and isovector pairing, whereas the $\pi$-exchange had larger impact on the formation of quasi deuterons in the $T = 0$ pairing.

In table 5 we display results for the nucleus $^{16}O$. Results for other nuclei are different if one looks at $\langle V \rangle$ or $\Delta V_{2\hbar\omega}$, but are essentially identical for the ratio $\Delta \Omega$.

The conclusions drawn from the study of inter-shell correlations in the neighborhood of $^{16}O$ are supported by the results for nuclei around $^{40}Ca$. These results have been obtained from shell-model calculations assuming a core of $^{16}O$ and allowing for configurations of valence nucleons in the $1s0d$ and $1p0f$ shells. The matrix elements for the G-matrix of OBEP A have been calculated using an oscillator length of $b = 2.06$ fm.

4. Conclusions

The role of two-nucleon correlations for pairs of nucleons with isospin $T = 0$ and $T = 1$ has been investigated by analyzing the results of shell-model calculations (SM) for nuclei in the mass region $12 \leq A \leq 42$ considering configurations in one or two major shells. For that purpose the contributions of the $pp$, $nn$, and $pn$ pairs with $T = 0$ and $T = 1$ to the energy of the ground states of such nuclei have been analyzed and compared to a decomposition of the corresponding two-nucleon densities in terms of partial waves of relative motion.

One finds that the gain in energy for nuclei with even number of protons or neutrons is correlated with an enhancement of the components in the two-body density with two nucleons in the $1S_0$ partial wave. This is interpreted as a strong signal for the occurrence of $T = 1$ pairing for such nuclei.
This interpretation is supported by a comparison of shell-model calculations and Hartree-Fock calculations with angular momentum projection: The two-nucleon densities derived from HF calculations show a smaller amount of components in the $^1S_0$ partial wave.

In a very similar way a strong correlation is also observed between the energy-contributions from $pn$ pairs with $T = 0$ and the components of the $^3S_1$ partial wave in the two-body density. Consequently, such large contributions to the energy and a corresponding enhancement of the $^3S_1$ in the two-body density are interpreted as a signal for the formation of quasi-deuterons or $T = 0$ pairing in those nuclei.

One finds that $T = 0$ pairing is maximal for symmetric nuclei with $N = Z$ but is important also for neighbored nuclei. The occurrence of $T = 0$ pairing is not so sensitive to the density of single-particle states at the Fermi surface and therefore one does not observe a phenomenon comparable to the blocking effect and the “odd-even” staggering of $pp$ and $nn$ pairing.

This “robustness” can also be seen from the fact that correlations due to excitations across shell-closures are dominated by $T = 0$ correlations, while the effect of $T = 1$ excitations are significantly smaller. This is in line with the studies of [25] investigating quasi-nuclear systems in the transition from nuclear matter to finite nuclei.

The results seem to be rather insensitive to the interaction considered for the SM calculation. Most of the results presented here are based on a $G$-matrix calculated for a realistic One-Boson-Exchange model for the $NN$ interaction[26]. Using the meson-exchange picture for the $NN$ interaction allows to explore the contributions of the various mesons to the structure of nuclei. Such investigations show that pion-exchange has a strong effect on the formation of $T = 0$ pairing but is almost negligible for $T = 1$ pairing. On the other hand, the exchange of isoscalar meson ($\sigma$ and $\omega$ mesons) effect $T = 0$ and $T = 1$ pairing.

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