Influence of 2p-2h ground state correlations on charge distributions of doubly-closed shell nuclei

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Ground state 2p-2h correlations are explicitly calculated in a completely self-consistent way within the framework of the Tamm-Dancoff approximation using a “universal” effective nucleon-nucleon interaction of the Skyrme type. Their influence on the charge distributions of $^{16}$O, $^{40,48}$Ca, and $^{48}$Ca is studied.

NUCLEAR STRUCTURE $^{16}$O, $^{40,48}$Ca; ground state correlations; charge distributions; use of self-consistent methods.

Ground state properties of doubly-closed shell nuclei are generally well described in a spherical Hartree-Fock (HF) approximation. Within this approximation the parameters of the effective interactions (such as zero-range forces, e.g., Skyrme-type interactions,\textsuperscript{1-3} or finite-range forces, e.g., the DI interaction of Gogny\textsuperscript{4}) are adjusted in order to achieve a satisfactory reproduction of binding energies and charge density properties of both light and heavy doubly-closed shell nuclei. Many interactions still encounter difficulties in predicting typical isotopic features (like the $^{48}$Ca-$^{40}$Ca isotope shift), while, on the contrary, some other effective interactions succeed in reproducing those particular features. It should be emphasized that the latter situation is generally the result of specific adjustments of the force parameters, usually giving rise to a worse reproduction of other nonadjusted properties. We can expect that the use of an uncorrelated spherical Hartree-Fock ground state for the doubly-closed shell nuclei is somewhat oversimplified, and that ground state correlations have to be involved, yielding corrections to the self-consistent HF charge distributions. The presence of strongly collective states in the low-energy spectrum of some doubly-closed shell nuclei suggests that such correlations in the ground state (e.g., 2p-2h excitations) could exist.

The problem of describing ground state correlations has been extensively studied by Rowe\textsuperscript{5,6} in the framework of the random phase approximation (RPA). Using the number-operator method\textsuperscript{6} it turns out that the single-particle densities

$$\langle \Psi_0 | c_p^\dagger c_p | \Psi_0 \rangle$$

and

$$\langle \Psi_0 | c_h^\dagger c_h | \Psi_0 \rangle$$

become different from zero, and can be expressed to leading order in $|Y|^2$ by, respectively,

$$\langle \Psi_0 | c_p^\dagger c_p | \Psi_0 \rangle = v_p^2$$

$$= \frac{1}{2(2j_p + 1)} \sum_{a,h} (2J + 1) | Y_{p,j} | (J\alpha) |^2 + 0(|Y|^4)$$

(1)

and

$$\langle \Psi_0 | c_h^\dagger c_h | \Psi_0 \rangle = 1 - v_h^2$$

$$= \frac{1}{2(2j_h + 1)} \sum_{a,j} (2J + 1) | Y_{p,j} | (J\alpha) |^2 + 0(|Y|^4).$$

(2)

Here, we assume $p_i$ and $h_i$ to describe all quantum numbers for the particle and the hole state, respectively. Furthermore, the $Y$ coefficients in (1) and (2) denote the RPA amplitudes of the quasi-boson creation operator $Q_{JM\alpha}$, which creates the excited states with angular momentum $J$:

$$Q_{JM\alpha} | \Psi_0 \rangle = \sum_{(p,h)} [X_{p,h}(J\alpha)A_{p,h}(JM) - Y_{p,h}(J\alpha)(-1)^{J-M}A_{p,h}(J-M)] | \Psi_0 \rangle,$$

(3)
where $A_{\rho,h}^\dagger (JM)$ represents the creation operator of a particle-hole state. In this picture, the Hartree-Fock density $\rho(r)$ is modified, by the single-particle densities (1) and (2), into the expression

$$
\rho_q(r) = \sum_{\alpha \gamma \rho} \langle \Psi_0 | c_{\alpha q}^\dagger c_{\gamma q} | \Psi_0 \rangle \phi_{\alpha q}^*(r) \phi_{\gamma q}(r) \\
= \frac{1}{4\pi} \sum_{h_i} (2j_{h_i} + 1) a_{h_i}^{q^2} \phi_{h_i}^2(r) + \frac{1}{4\pi} \sum_{p_j} (2j_{p_j} + 1) b_{p_j}^{q^2} \phi_{p_j}^2(r) 
$$

(spherical symmetry), where $\phi_{h_i}(r)$ and $\phi_{p_j}^q(r)$ describe the radial single-particle wave functions. The normalization is such that

$$
4\pi \int \rho_q(r) r^2 dr = Z \text{ or } N,
$$

depending on the nature of $q$ (proton or neutron). The nucleon density (4) can be calculated from the knowledge of the $Y$ amplitudes in the RPA wave functions by means of Eqs. (1) and (2). It is important to note that use of the quasi-boson approximation gives rise to single-particle densities (1) and (2) which are twice as large. This double-counting of the ground state correlations is inherent in the quasi-boson approximation, and has been involved in the calculation of Faessler et al. with applications to the Ca isotopes and $^{208}$Pb. Even the exact number-operator method can easily overestimate the effect of ground-state correlations on the HF density. Furthermore, the calculations performed in Refs. 7 and 8 are not completely self-consistent since the structure of the collective states has been obtained using an interaction different from the interaction used to obtain the HF basis. We also mention a recent self-consistent calculation of the Montrouge group using the DI force. Their method is also based upon the quasi-boson approximation, but a more sophisticated RPA ground state has been used, compared with earlier studies.

In this work, we try to construct the correlated ground state in a completely different way, avoiding such double-counting problems. In order to get a reliable estimate of the admixture of 2p-2h excitations in the ground state, we consider the intrinsic ground state $|\Psi_0\rangle$ of a doubly-closed shell nucleus as being the lowest $J^\pi=0^+$ eigenstate in a Tamm-Dancoff approximation (TDA) diagonalization procedure. We construct and diagonalize the energy matrix in a Hilbert space composed of the spherical Hartree-Fock ground state $|\text{HF}\rangle$ and an orthonormal set of 2p-2h configurations (after elimination of all spurious center-of-mass excitations):

$$
|\Psi_0\rangle = a^{(0)} |\text{HF}\rangle + \sum_i a_i^{(2)} |(2p-2h)_i;0^+\rangle.
$$

The orthonormal basis states

$$
|(2p-2h)_i;0^+\rangle
$$

constitute linear combinations of 2p-2h configurations according to the Schmidt orthogonalization procedure:

$$
|(2p-2h)_i;0^+\rangle = \sum_j c_{ij}^f [A_{\rho,h}^\dagger (J) A_{p_j,h_j}^\dagger (J)]_{0^+,i} |\text{HF}\rangle.
$$

With the explicit knowledge of the 2p-2h correlated ground state, the single-particle densities (1) and (2) are evaluated in a more straightforward way. This leads finally to a nucleon density expressed by (spherical symmetry)

$$
\rho_q(r) = \rho_{q_{\text{HF}}}(r) + \frac{1}{4\pi} \sum_{ij} a_i^{(2)} a_j^{(2)} c_{ij}^f \left[ \delta_{J_{h_i} J_{h_j}} (\delta_{p_j p_i} \delta_{h_j h_i} + \delta_{h_j p_i} \delta_{h_j h_i}) \\
+ \tilde{J} \cdot \begin{pmatrix} j_{p_i} & j_{h_i} \\ j_{p_j} & j_{h_j} \end{pmatrix} \delta_{h_i h_j} (\delta_{p_j p_i} \delta_{h_i h_j} + \delta_{h_j p_i} \delta_{h_j h_i}) \right] \\
\times [\delta_{q_{p_i}}^2 (r) - \delta_{q_{h_i}}^2 (r)] \delta_{q_i q} + [\delta_{q_{p_j}}^2 (r) - \delta_{q_{h_j}}^2 (r)] \delta_{q_j q},
$$

where $q_i$ and $q_j$ denote the nature (proton or neutron) of the $p_i/h_i^{-1}$ and $p_j/h_j^{-1}$ excitation, respectively. The notation $i$, used in the summation symbols, stands for $[p_i/h_i; p_j/h_j]$. The charge density is derived from the pointlike proton density after incorporating the standard corrections for center-of-mass motion, finite nucleon size, and electromagnetic neutron effects, and for effects due to the spin-orbit interaction in spin unsaturated shells.

When carrying out such calculations in a self-consistent way, the only remaining problem is the choice of the effective nucleon-nucleon interaction, which is required to be used both in the Hartree-Fock and TDA calculations. In a detailed and extensive study (Ref. 3 and 11, hereafter referred to as I and II, respectively), a “universal”
Skryrne-type interaction SkE suitable for describing both ground state (see I) and excited state (see II) properties for finite nuclei throughout the whole nuclear mass table, has been determined. Its behavior as a particle-hole interaction has been extensively studied, resulting in good overall experimental agreement. It turned out that the force parametrization SkE4 serves as a highly appropriate nucleon-nucleon interaction in reproducing charge properties of nuclei in a quantitative way. Moreover, even within the spherical Hartree-Fock approximation, good saturation of the density is generally obtained in the inner part of the nucleus. This is in contrast to many nucleon-nucleon forces yielding density fluctuations which are too pronounced in the nuclear interior.

Some detailed isotopic effects, such as the isotopic $^{48}$Ca-$^{40}$Ca shift [$r_c^{\exp}(^{40}$Ca) = 3.478 fm; $r_c^{\exp}(^{48}$Ca) = 3.481 fm (Ref. 12)] constitute a highly sensitive test for the interaction. Self-consistent spherical Hartree-Fock calculations, using SkE4, closely approach the experimental data [$r_c^{HF}(^{40}$Ca) = 3.455 fm; $r_c^{HF}(^{48}$Ca) = 3.469 fm], but still a discrepancy remains. The electromagnetic spin-orbit coupling, arising from the presence of unsaturated $Jf_{7/2}$ neutrons, already reduces the $^{48}$Ca-$^{40}$Ca isotopic shift in an important way ($\Delta r_c = -0.015$ fm). We expect the remaining discrepancy to be removed when including 2p-2h correlations in the $J^* = 0^+$ ground state.

We now apply the method outlined above, using SkE4, in evaluating 2p-2h correlations in the ground states of $^{16}$O, $^{40}$Ca, and $^{48}$Ca in order to test detailed charge density properties as discussed before. Moreover, the whole calculation is carried out in a completely self-consistent way as follows:

(i) a spherical Hartree-Fock calculation yielding single-particle wave functions and energies (and resulting in a correct total binding energy of the considered nucleus), and thereafter

(ii) construction and diagonalization of the energy matrix in the Hilbert space of 0p-0h + 2p-2h configurations with the use of the same SkE4 interaction. The model space of 2p-2h excitations has been restricted to four or five major shells. It has been found that further enlargement of the configuration space has no significant effect on the final 2p-2h admixture in the ground state.

The resulting charge radii for $^{16}$O, $^{40}$Ca, and $^{48}$Ca are summarized in Table I. We remark that the most important ground state correlations occur in $^{40}$Ca (34.7%), while the ground state of $^{48}$Ca is the most stable against an admixture of 2p-2h excitations (only 23.9%), indicating a stronger shell closure in the latter nucleus than in the former. This obviously results in a larger correction for the charge radius in $^{40}$Ca than in $^{48}$Ca, removing in this way the discrepancy which is still present in explaining the experimental isotopic shift, to a high degree of accuracy.

It should be noted that the influence of the ground state correlations on the charge density turns out to be not as significant as could be expected from the large 2p-2h admixture. Some disagreement with the calculations of Faessler et al. occurs, where an increase of the charge rms radius in $^{40}$Ca of about 0.080 fm is obtained. We get a value of 0.016 fm (see Table I). This large difference obviously originates from the double-counting involved in the calculation of Ref. 7. However, after correcting for this double-counting effect, reducing the corrections to the densities and to all related quantities by about 25%, one still encounters an increase of the $^{40}$Ca charge rms radius which is much larger than the very weak correction of 0.016 fm obtained in this work. This may be partly due to the force SkE4 and not only to the method used in this work when evaluating the correlated ground state. It is a general feature of the SkE4 force that the self-consistent Hartree-Fock charge distributions, without taking into account ground state correlations, already show a less smaller central bump and less pronounced density oscillations in the inner part of the nucleus (see I), in contrast to most other effective nucleon-nucleon interactions. This behavior of the SkE4 force is best visualized when comparing the charge distributions of $^{40}$Ca and $^{208}$Pb, where the central bump is mainly due to the $2s_{1/2}$ and $3s_{1/2}$ pro-
TABLE II. Charge distribution of $^{40}$Ca. Recent experimental data from the Mainz-Saclay collaboration were taken (Ref. 12). $\Delta \rho_e$ stands for the total experimental uncertainty including statistical and completeness errors.

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<th>$\rho_e$ ($10^{-2}$ fm$^{-3}$)</th>
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<th>$\rho_e$(0p-0h) ($10^{-2}$ fm$^{-3}$)</th>
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(|$r_e^2$|)$^{1/2}$ (fm) 3.478 0.007 3.455 3.471

In case the self-consistent Hartree-Fock wave functions for the $2s_{1/2}$ and $3s_{1/2}$ proton orbitals are already more spread out over larger distances, one might expect the influence of ground state correlations (even when they are large) on the charge distribution to be not necessarily of noticeable magnitude.

A second explanation for the large rms-radius corrections obtained in previous calculations$^7$ and$^9$ could be found in the replacement of the true ground state $|\Psi_0\rangle$ by the uncorrelated HF ground state in the standard RPA approximation.$^6$ So, $\rho_e$ amplitudes which are too large are obtained for the collective levels which are used in evaluating $\Delta \rho_e (r)$ [Eqs. (1) and (2)]. In II, we have shown that the standard RPA method turns out to be inadequate for describing strongly collective low-lying vibrations (overestimation of the collective properties) when using effective forces adjusted for Hartree-Fock calculations.

This inadequacy is assumed to be a direct consequence of the neglect of explicit ground state correlations (2p-2h admixtures) in the derivation of the RPA secular equation. Such correlated RPA calculations on doubly-closed shell nuclei are in progress.

In light of the very accurate recent Mainz-Saclay (e,e) measurements on the Ca isotopes, a detailed comparison between the experimental and theoretical charge density is very instructive. We tabulate both charge distributions (Table II) instead of displaying the results in a figure (we refer to Fig. 3 of I), since the experimental data are of extremely high accuracy. We remark on an obvious movement of the charge from the interior to the surface region of the nucleus (r > 4 fm), giving rise to a slight increase in the radius. The overall agreement achieved in both descriptions is quantitatively fairly good. Although not strikingly large, a slightly better agreement is provided by the 0p-0h + 2p-2h calculation in reproducing the tail of
the density slope. This is best visualized in Fig. 1, where the charge distribution differences per radial element $r^2 \Delta \rho_e$ for $^{40}$Ca and $^{48}$Ca are displayed. The broken line represents the HF result; the 2p-2h admixture (full line) tends to shift the curve towards the experimental uncertainty band. The depletion of the density near 2 fm is correctly reproduced, as well as the peak observed at 4 fm. The only discrepancy is the shift of the maximum of $r^2 \Delta \rho_e^{2h}$ to some higher radius as compared to $r^2 \Delta \rho_e^{\text{exp}}$.

A comparative study with theoretical results using other effective interactions would be very instructive but is hard to realize, as reproduction of the $r^2 \Delta \rho_e$ curve at the nuclear surface region needs sufficiently accurate values for both $^{40}$Ca and $^{48}$Ca charge densities, which are not given explicitly in the literature. Some general conclusions may still be drawn. In most microscopic calculations the central density exhibits too much central peaking, especially in $^{40}$Ca, certainly not leading to a satisfactory reproduction of $r^2 \Delta \rho_e$ for $r < 3$ fm. Very recently, Skyrme-type forces have been presented which have been adjusted to more than 20 nuclei by rigorously fitting binding energies and radii within the spherical HF approximation [plus Bardeen-Cooper-Schrieffer (BCS) for taking into account pairing correlations]. Using these forces, one succeeds in almost correctly reproducing the above quantities, but fails in describing nuclear features not taken into account in the fitting procedure. We likely refer to such a force, presented by Tondeur, reproducing experimental masses for spherical nuclei within an rms deviation of 1 MeV. When evaluating $r^2 \Delta \rho_e$ with this force, the maximum is obtained at 3.8 fm, corresponding with a value of $2.6 \times 10^{-2}$ fm$^{-1}$, which is in excellent agreement with experiment (Fig. 1).

In Fig. 2 we display the charge distribution of $^{16}$O. The charge distribution per radial element $\Delta \rho_e$ for $^{16}$O shows a similar trend to $^{40}$Ca and $^{48}$Ca. The broken line represents the HF result; the 2p-2h admixture (full line) tends to shift the curve towards the experimental uncertainty band. The depletion of the density near 2 fm is correctly reproduced, as well as the peak observed at 4 fm. The only discrepancy is the shift of the maximum of $r^2 \Delta \rho_e^{2h}$ to some higher radius as compared to $r^2 \Delta \rho_e^{\text{exp}}$.

Finally, we discuss the 2p-2h ground state correlations in detail. Therefore, we decompose in Fig. 3 the total 2p-2h admixture in the ground state with respect to the intermediate 1p-1h spin $J^\pi$ [see Eq. (6)]. We readily observe that almost half the total admixture arises from 2p-2h configurations with $J^\pi = 3^-$ as the intermediate 1p-1h spin. Further important contributions result from the $J^\pi = 1^-$ and $5^-$ spins. The low-energy spectrum of doubly-closed shell nuclei are predominantly governed by 1p-1h excitations. Obviously some excited states are more involved in the ground state correlations than others. In order to gain more insight into the various contributions to the entire ground state admixture, we transform the orthogonal basis of 2p-2h configurations to an orthonormal basis of two-phonon coupled states: Expansion (5) can be rewritten as

$$\Psi_0 = a^{(0)} | \text{HF} \rangle + \sum_{j\alpha} d_{j\alpha \beta} (Q^\dagger_{j\alpha} Q^\dagger_{\beta})_{0+} | \text{HF} \rangle,$$

where $Q^\dagger_{j\alpha}$ represents the creation operator of a 1p-1h excited state in the TDA [all $Y_{j\alpha} (\hat{J} \alpha) = 0$ in Eq. (3)]. After

In Fig. 1, we display the difference of the charge distribution per radial element of $^{40}$Ca and $^{48}$Ca. The dashed area represents the experimental result (Ref. 12) including the statistical and completeness error. The broken line is the spherical HF result using SkE4, while the full line includes the 2p-2h ground state correlations.

In Fig. 2, we display the charge distribution of $^{16}$O. (a) from Ref. 16; (b) from Ref. 14.

In Fig. 3, we display the decomposition of the 2p-2h ground state correlations, according to the intermediate 1p-1h spin $J^\pi$. 

$$r \rightarrow 0$$ seems to have been reproduced. The 0p-0h + 2p-2h prediction for the $^{16}$O charge rms radius is apparently somewhat too large (Table I), which is also the case in the calculation of Tondeur. It should be emphasized that in $^{16}$O the correction to the point-proton radius arising from the center-of-mass motion is large and the method to treat this problem is far from unique.
TDA diagonalizations in a 1p-1h model space, applied on the nuclei $^{16}$O and $^{40}$Ca, we dispose of the TDA wave functions $X_{p,h}(J\alpha)$ defining the $Q_{1\alpha}$ excited state. Thus, the $d$ coefficients of Eq. (8) can be deduced from the additional knowledge of the $a_{\alpha}^{(2)}$ amplitudes [Eq. (5)]. It turns out, as could be expected, that in $^{16}$O almost half the total $J^\pi=3^-$ contribution to the 2p-2h ground state correlations is induced by the low-lying collective octupole $J^\pi=3^-$ state (44%). The remaining part mainly arises from three isovector octupole resonances (50%) with reasonably good isospin purity $T=1$. Concerning the $J^\pi=1^-$ contributions, 74% can be accounted for by the giant dipole resonance ($T=1$) in $^{16}$O.

Similar conclusions can be drawn for $^{40}$Ca. The collective octupole $T=0$ state takes 55% of the total $J^\pi=3^-$ contribution, while 29% arises from the dominant isovector resonance. A similar behavior is found for the $J^\pi=5^-$ contributions: 45% arises from the low-lying collective $J^\pi=5^-$ state, while 48% is due to those states supporting strong E5 isovector transitions to the ground state. The giant dipole resonance is responsible for 63% in the $J^\pi=1^-$ admixture.

If we carry out the calculation, but start from a basis of the type (8), composed of some selected $Q_{3\alpha}$ excitations, we get a drastically reduced configuration space without losing important correlations. In Fig. 4 we display for $^{16}$O and $^{40}$Ca the result of such a space truncation. The various contributions to the total 2p-2h admixture of the ground state are given, resulting from a model space $Q_{3\alpha} \times Q_{1\beta}$ restricted to those configurations, showing good isospin purity and large ground state transition probability. The lack of admixture is in essence not noticeably large.

We would like to stress that the binding energy corresponding with the correlated ground state no longer agrees with the experimental mass. Due to the 2p-2h admixture the ground state is lowered by several MeV's (Table I). In the case of $^{16}$O this lowering constitutes almost 10% of the total binding energy. The SkE4 interaction has been adjusted to reproduce masses within the framework of the spherical Hartree-Fock approximation. One might indeed question the validity of using SkE4 in the evaluation of the 2p-2h ground state correlations, as now the binding energies are no longer reproduced. It is a common feature of all Skyrme-type forces that the final HF ground state energy is the result of cancellation between large attractive and repulsive contributions, corresponding to the various terms of the force. We have found that small adjustments of the force parameters are sufficient to obtain a lower value for the binding energy in the HF calculation, so that when corrected for 2p-2h ground state correlations a correct reproduction of the binding energies would be possible. Moreover, such small force adjustment would not cause appreciable changes in the particle-hole matrix elements. Hence, the obtained results remain quantitatively valid and so do the conclusions.

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