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Natural orbital representation in nuclei

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Mean-field approximation results emerging from Hartree-Fock calculations with Skyrme-type forces are compared with those obtained within the natural orbital representation of the Jastrow correlation method in its lowest order approximation for ^{4}He, ^{16}O and ^{40}Ca. The influence of short-range correlations on the single-particle wave functions and occupation probabilities is analyzed. A two part decomposition of the one-body density matrix is achieved which reflects both the low- and high-momentum components of the correlated ground state.

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The effects of short-range correlations (SRC) on single-particle (s.p.) properties of nuclei are currently of great interest in nuclear physics due to recent experimental data that confront the theory with new challenges. On one hand, comparison of the experimental data and theoretical results has demonstrated sizable SRC effects on the nucleon and cluster momentum distributions, the occupation numbers of s.p. states, the spectral functions of deep-hole nuclear states as well as nuclear reaction cross sections [1]. Well known, for example, is the work done in y scaling as an attempt to extract the nuclear momentum distribution from the experimental data on electron-nucleus scattering [2]. The data cannot be explained within the mean-field approximation (MFA) to the nuclear ground state. On the other hand, many experimental data show that the s.p. states that emerge from the MFA are rather close to physical reality. For example, recent $(e,e'p)$ experiments [3] demonstrate that the peak of the s.p. strength is near the energy predicted by the nuclear shell model. These data also yield well-defined s.p. wave functions in coordinate and momentum space [4]. In addition, there has been a great deal of work in (γ,p) reactions having an almost unique sensitivity to high-momentum components of the nuclear wave function and giving information on the single-particle momentum distribution that is complementary to that from electron- and proton-induced reactions [5].

The aim of the present paper is to analyze the s.p. description of nuclei in the framework of the natural orbital representation [6], which is valid also for systems strongly affected by SRC. Instructive conclusions are made about the influence of SRC on the s.p. wave functions and occupation probabilities in nuclei. Some restrictions of the nuclear MFA caused by SRC are revealed.

An important problem arising in correlation methods going beyond the MFA is to define s.p. nuclear states and to calculate s.p. wave functions and occupation probabilities associated with the correlated ground state $\Psi \equiv \Psi(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_A)$ of an A-particle system [7]. The main difficulty comes from the fact that the general representation of the one-body density matrix associated with Ψ

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha,\beta} \rho_{\alpha\beta} \varphi_\beta(\mathbf{r}) \varphi_\alpha^*(\mathbf{r}') \tag{1}$$

does not uniquely define either the set of s.p. wave functions $\{\varphi_\alpha(\mathbf{r})\}$ or the matrix elements $\rho_{\alpha\beta}$, whose diagonal part $0 \le \rho_{\alpha\alpha} \le 1$ is the s.p. occupation probability [6], i.e., the number of particles in a particular s.p. state with wave function $\varphi_\alpha(\mathbf{r})$. Usually, different MFA approaches use additional physically motivated approximations to avoid the arbitrariness of the s.p. set $\{\varphi_\alpha(\mathbf{r})\}$ associated with Ψ or $\rho(\mathbf{r},\mathbf{r}')$. In these cases the resulting set $\{\varphi_\alpha(\mathbf{r})\}$ is clearly model dependent.

The only model - independent way to define a set of s.p. wave functions and occupation probabilities solely from the correlated one-body density matrix $\rho(\mathbf{r},\mathbf{r}')$ is to use its natural orbital representation (NOR), introduced by Löwdin [6]

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha} n_\alpha \psi_\alpha^*(\mathbf{r}) \psi_\alpha(\mathbf{r}') \ . \tag{2}$$

The normalized eigenfunctions $\psi_\alpha(\mathbf{r})$ of $\rho(\mathbf{r},\mathbf{r}')$, called "natural" orbitals, form a complete orthonormal set. The associated eigenvalues n_α, called "natural" occupation numbers, define the probability $(0 \le n_\alpha \le 1)$ that the natural orbital $\psi_\alpha(\mathbf{r})$ is occupied in the ground state Ψ. Usually there are A orbitals $\psi_\alpha(\mathbf{r})$ for which the occupation probabilities n_α are significantly larger than those for the others. As in the MFA, these are called the hole-state orbitals while the others are called particle-state orbitals [8].

Clearly, the one-body density matrix and consequently all one-body nuclear characteristics have the simplest form within the NOR, Eq. (2). It is therefore attractive to use the method [9,10] for approximating the correlated density matrix $\rho(\mathbf{r},\mathbf{r}')$ by an expression of the type of Eq. (2),

$$\rho(\mathbf{r},\mathbf{r}') \cong \sum_{\alpha} v_\alpha \varphi_\alpha^*(\mathbf{r}) \varphi_\alpha(\mathbf{r}') \ , \tag{3}$$

where MFA wave functions $\varphi_\alpha(\mathbf{r})$ are used instead of the natural orbitals $\psi_\alpha(\mathbf{r})$ and additional inforamtion is incorporated for the new occupation probabilities v_α.

In the present paper we compare the MFA and the NOR of the correlated ground states of ^{4}He, ^{16}O, and ^{40}Ca. As typical MFA results we consider those for hole- and particle-state wave functions $\{\varphi_\alpha(\mathbf{r})\}$, local densities $\rho(r)$, elastic form factors $F(q)$, nucleon momentum distributions $n(k)$, and related one-body nuclear characteristics obtained within the Hartree-Fock theory with Skyrme SkM* effective forces [11]. The same quantities have been calculated also within the NOR of a one-body density matrix which takes into account SRC using the Jastrow correlation method (JCM) in its low-order approximation (LOA) [12]. A simple choice of harmonic-oscillator wave functions and a Gaussian state-independent correlation factor gives rise [12] to analytical expression for the JCM one-body density matrix in LOA. It depends on two parameters: the oscillator length α and the correlation parameter β. Values $\alpha=(0.82, 0.59,$ and $0.52)$ fm^{-1}, $\beta=(1.23, 1.43,$ and $1.21)$ fm^{-1} have been obtained by fitting the experimental elastic form factor data for the nuclei ^{4}He, ^{16}O, and ^{40}Ca, respectively.

Typical results for both sets $\{\varphi_\alpha\}$ and $\{\psi_\alpha\}$ are shown in coordinate space (Fig. 1) and momentum space (Fig. 2). The natural occupation numbers n_α of ^{40}Ca are compared with recent experimental data in Table I. The comparison leads to the following conclusions concerning the hole-state orbitals:

The NOR hole-state orbitals ψ_α are close to the occupied MFA orbitals φ_α in coordinate space (see, e.g., the 1s-state in Fig. 1) and momentum space (Fig. 2). Thus, the SRC do not affect significantly the hole-state orbitals. Relativistic effects are expected to be important for momenta $k \geq 2$ fm^{-1}; their inclusion would lead to a better agreement with the experimental hole-state momentum distributions (see Fig. 2). The influence of SRC is mainly on the natural hole-state occupation probabilities, which are close to (but less than) unity. Natural hole-state occupation numbers as well as the total depletion of the Fermi sea caused by SRC agree with the available experimental data, as can be seen in Table I.

The conclusions given above justify the MFA as a good approximation to the correlated one-body density matrix

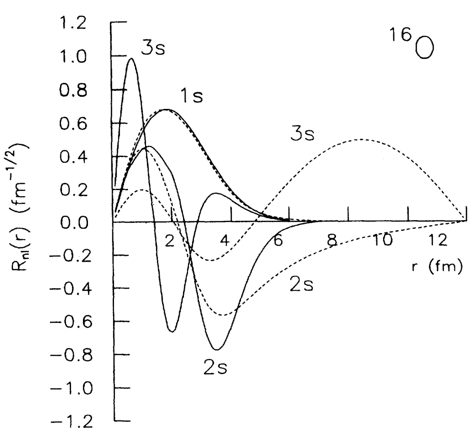

FIG. 1. Particle- and hole-state natural orbitals (solid line) compared with the associated MFA orbitals (dashed line) in ^{16}O (the radial parts multiplied by r).

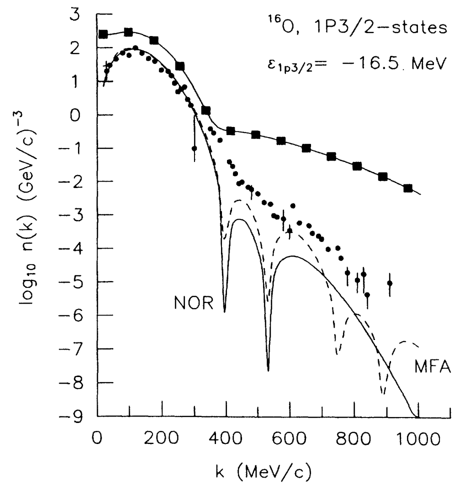

FIG. 2. Nucleon momentum distribution of $1p_{3/2}$ protons in ^{16}O calculated within the NOR (solid line) and MFA (dashed line). Comparison is made with the total JCM momentum distribution $n(k)$ in LOA (solid line with squares) and experimental data [1] (circles).

(2) for the hole-state orbitals. The MFA and NOR results for both the s.p. wave functions and occupation probabilities are of the same order of magnitude. This explains the observation that whereas clear experimental indications for an appreciable amount of high-momentum components due to the SRC exist in the total nucleon momentum distribution $n(k)$ (solid line with squares in Fig. 2), no such components have been detected with respect to the hole-state momentum distributions (circles in Fig. 2).

However, the situation drastically changes when considering the particle-state orbitals. In this case both the s.p. wave functions and occupation probabilities are strongly affected by SRC:

In coordinate space, the natural particle-state orbitals $\psi_\alpha(\mathbf{r})$ are much more localized than the MFA orbitals $\varphi_\alpha(\mathbf{r})$. The former are concentrated inside the nucleus in the region where the local density $\rho(r)$ is not zero. This feature does not depend on the principal quantum number or the orbital angular momentum of ψ_α (see Fig. 1). The natural particle-state orbitals have significantly smaller rms radii but more than two orders of magnitude

TABLE I. Comparison of MFA and NOR results for the occupation numbers n_α, the depletion of the s.p. states D_α, and the total depletion TD (both D_α and TD in percents) in ^{40}Ca with experimental data [3].

	Occupation numbers				Depletion		
nl	MFA	NOR	Expt.	nl	MFA	NOR	Expt.
1s	1	0.96	0.95	1s	0	4.1	5.0
1p	1	0.93	0.92	1p	0	7.0	8.0
1d	1	0.947	0.892	1d	0	5.3	10.8
2s	1	0.89	0.89	2s	0	11.0	11.0
1f	0	0.013	0.37	TD	0	6.26	9.4
2p	0	0.017	0.12				

larger high-momentum components than the MFA particle-state orbitals. Due to the SRC, small but nonzero occupation probabilities appear for the particle-state orbitals (see Table I). This fact, together with the large high-momentum components of the natural orbitals, suggests that the high-momentum tail in the total distribution $n(k)$ caused by SRC is almost completely determined by the particle-state contributions. The particle-state natural occupation probabilities are about one order of magnitude smaller than the preliminary experimental predictions (see Table I).

The main conclusion concerning the particle-state orbitals is that for these states the natural orbitals are not close to the MFA results nor are the natural occupation numbers close to experimental data. Therefore, the approximation (3) fails to describe properties that are sensitive to large momentum transfer, such as, e.g., the high-momentum components of $F(q)$ or $n(k)$.

Since the approximation (3) is questionable, it is important to find its physically acceptable improvement. This may be done within the present model in which we can decompose the correlated one-body density matrix (2) into two parts,

$$\rho(\mathbf{r},\mathbf{r}')=\rho^{(1)}(\mathbf{r},\mathbf{r}')+\rho^{(2)}(\mathbf{r},\mathbf{r}') . \tag{4}$$

The first part $\rho^{(1)}(\mathbf{r},\mathbf{r}')$ collects all the terms of the JCM one-body density matrix in LOA [12] that are responsible for nuclear characteristics sensitive to low-momentum transfer. The associated part of the total momentum distribution $n^{(1)}(k)$ reproduces almost exactly $n(k)$ up to momentum of about 2 fm^{-1}. In contrast, the second part $\rho^{(2)}(\mathbf{r},\mathbf{r}')$ is responsible for those nuclear properties that are sensitive to SRC or equivalently to the high-momentum components in nuclei. The associated part of the total momentum distribution $n^{(2)}(k)$ reproduces almost exactly $n(k)$ in the high-momentum region.

We have diagonalized independently both parts $\rho^{(1)}(\mathbf{r},\mathbf{r}')$ and $\rho^{(2)}(\mathbf{r},\mathbf{r}')$ entering Eq. (4). In this way the JCM one-body density matrix in LOA takes the form

$$\rho(\mathbf{r},\mathbf{r}')\equiv\sum_\alpha n_\alpha\psi_\alpha^*(\mathbf{r})\psi_\alpha(\mathbf{r}')=\sum_\alpha v_\alpha\varphi_\alpha^*(\mathbf{r})\varphi_\alpha(\mathbf{r}') + \sum_\alpha \eta_\alpha\chi_\alpha^*(\mathbf{r})\chi_\alpha(\mathbf{r}') , \tag{5}$$

where (n_α,ψ_α) are the natural orbitals and occupation numbers of the complete density matrix $\rho(\mathbf{r},\mathbf{r}')$, while $(v_\alpha,\varphi_\alpha)$ and $(\eta_\alpha,\chi_\alpha)$ are the eigenvalues and eigenfunctions of the matrices $\rho^{(1)}(\mathbf{r},\mathbf{r}')$ and $\rho^{(2)}(\mathbf{r},\mathbf{r}')$, respectively.

Typical results for the eigenvalues n_α, v_α, and η_α in ^{16}O are given in Table II. Unphysical negative values for some occupation probabilities n_α arise due to breaking of the A representability of $\rho(\mathbf{r},\mathbf{r}')$ in the LOA [12]. The negative values of n_α are obviously related to the states φ_α having negative eigenvalues v_α. In this sense, our next conclusion is that the decomposition (5) gives a method for restoring the A representability of the JCM one-body density matrix in LOA.

Simply, one has to exclude from Eq. (5) all states φ_α with negative v_α and eventually to renormalize the resulting new A-representable matrix $\rho(\mathbf{r},\mathbf{r}')$. Its associated new natural orbitals and occupation numbers (the completely non-negative values $\bar{n}_\alpha$ in Table II) do not significantly change since the breaking of the A representability is small.

TABLE II. Eigenvalues entering Eq. (5) for ^{16}O. Natural occupation numbers before (n_α) and after ($\bar{n}_\alpha$) restoring the A representability are also given.

nl	n_α	v_α	η_α	$\bar{n}_\alpha$
1s	0.9495	0.9409	0.0113	0.9495
2s	−0.0016	−0.0053	0.0044	0.0057
3s	0.0038	0.0	0.0015	0.0026
4s	0.0013	0.0	0.0004	0.0001
1p	0.9646	0.9603	0.0079	0.9646
2p	−0.0018	−0.0056	0.0027	0.0053
3p	0.0032	0.0	0.0008	0.0018
4p	0.0009	0.0	0.0002	0.0005
1d	0.0057	0.0	0.0057	0.0057
2d	0.0017	0.0	0.0017	0.0017
3d	0.0005	0.0	0.0005	0.0005
1f	0.0035	0.0	0.0035	0.0035
2f	0.0010	0.0	0.0010	0.0010
3f	0.0003	0.0	0.0003	0.0003

The most important result from the two-part decomposition (5) is the following. Whereas there is no single potential associated with the natural orbitals $\psi_\alpha(\mathbf{r})$ there are just two different harmonic-oscillator-like potentials associated with $\varphi_\alpha(\mathbf{r})$ and $\chi_\alpha(\mathbf{r})$: $U^{(1)}(\mathbf{r})$ for all the states $\varphi_\alpha(\mathbf{r})$ and $U^{(2)}(\mathbf{r})$ for all the states $\chi_\alpha(\mathbf{r})$. It turns out that $U^{(1)}(\mathbf{r})$ is of the same type as the MFA potentials ($\hbar\omega\cong 14.4$ MeV), while the second potential $U^{(2)}(\mathbf{r})$ is completely different from that of the MFA and has $\hbar\omega\cong 62.14$ MeV.

Extrapolating the above results to the general correlated one-body density matrix $\rho(\mathbf{r},\mathbf{r}')$, we expect that its decomposition as in Eq. (5) should be more realistic than the approximation (3). The first term $\rho^{(1)}(\mathbf{r},\mathbf{r}')$ may come from the MFA for $\varphi_\alpha(\mathbf{r})$ and some additional information about the eigenvalues v_α, while the second term $\rho^{(2)}(\mathbf{r},\mathbf{r}')$ is associated with "another MFA" responsible for the high-momentum components of the nuclear ground state Ψ.

Concluding, it should be noted that the present results are in agreement with those for the NOR in other systems, such as the ^{4}He atom [13], as well as with "the best" wave functions used so far in describing Fermi liquid drops [8]. This gives us confidence that the present conclusions reflect some general properties that are relevant for the exact correlated ground states of many-fermion systems.

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