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P00023529

To be published in *Physical Review C*

Ref: OUNP-94-05

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THE EFFECT OF NUCLEON CORRELATIONS ON NATURAL ORBITALS

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Nucleon correlation effects on the natural orbitals obtained by the generator coordinate method and the coherent density fluctuation model are considered. The single-particle potentials corresponding to the natural orbitals are calculated and discussed.

PACS number(s): 21.10.Gv, 21.60.Cs, 21.60.Jz

The analyses of experimental data from electron-, proton- and heavy ion- scattering on nuclei, from proton pickup and knockout reactions, as well as from photoreactions have shown sizeable nucleon short-range correlation (SRC) effects on the total nucleon and cluster momentum distributions, on the occupation probabilities of the single-particle (s.p.) states, the spectral functions of deep-hole nuclear states and on the cross sections of various nuclear reactions [1–7] which cannot be described within the mean-field approximation (MFA) in the nuclear theory. Though evidence for appreciable high-momentum components in the total nucleon momentum distribution exist, no such components have yet been detected in the momentum distributions of the s.p. states from the exclusive and inclusive electron scattering on complex nuclei [8–18]. This requires detailed studies of s.p. characteristics in nuclei using methods going beyond the limits of MFA. Quantities such as s.p. orbitals and their occupation probabilities have to be introduced in the correlation methods in a model-independent way [19]. This may be done using the natural orbital representation (NOR) [20] (see also [1,2,19]) of the one-body density matrix (OBM) corresponding to the state of the correlated system. The diagonalization of the OBM gives the s.p. functions (natural orbitals (NO)) and occupation numbers in nuclei. Little quantitative information on the NO is available in the nuclear physics literature. The first results have been given in [22] and [23]. Later these quantities were studied by correlation methods, such as the coherent density fluctuation model (CDFM) [1,2,24], the generator coordinate method (GCM) [1,2,25] and the Jastrow correlation method (JCM) [21,26,27].

We emphasize the importance of the study of the SRC effects in the physics of many-body systems. Thus sizeable correlation effects on the characteristics of droplets of liquid ^3He [28] and in the ^4He atom [29] were observed. This mainly causes the strong localization of the PARTICLE-STATE NO and the localized mean-field orbitals in the nuclear interior, while the HOLE-STATE NO turn out not to be very sensitive to the details of the correlations in the wave functions. The main conclusions were confirmed in the studies of NO in ^4He , ^{16}O and ^{40}Ca nuclei within the

JCM [21,26,27]. Due to the importance of correlation effects on the s.p. characteristics in nuclei, and in the light of the results from [28], we give in this work new results which supplement those from [1,2,24,25] concerning the forms of the hole- and particle-state natural orbitals compared with mean-field single-particle functions. The second aim of this work is to calculate and analyse the single-particle potentials corresponding to the NO obtained in both GCM and CDFM correlation methods.

The eigenfunctions $\psi_\alpha(\mathbf{r})$ (“natural orbitals” (NO)) and the associated eigenvalues n_α (“natural occupation numbers”, $0 \leq n_\alpha \leq 1$) of the one-body density matrix $\rho(\mathbf{r}, \mathbf{r}')$ for a correlated state of a system of A particles can be found by solving the equation:

$$\int d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') \psi_\alpha(\mathbf{r}') = n_\alpha \psi_\alpha(\mathbf{r}). \quad (1)$$

The hole-state NO (forming a new Fermi sea F') are those $\psi_\alpha(\mathbf{r})$ for which the numbers n_α are significantly larger than those for the others (“particle-state NO”) [28].

For nuclei with total momentum $J = 0$, the OBM has to be diagonalized within the $\{l, j, m\}$ subspace of the complete space of the NO [23].

In the GCM [30,2] the OBM has the form [25]:

$$\rho(\mathbf{r}, \mathbf{r}') = \iint dx dx' f(x) f(x') \mathcal{N}(x, x') \rho(x, x', \mathbf{r}, \mathbf{r}'), \quad (2)$$

where $f(x)$ is the ground state solution of the Hill-Wheeler integral equation:

$$\int [\mathcal{H}(x, x') - E \mathcal{N}(x, x')] f(x') dx' = 0 \quad (3)$$

with

$$\mathcal{H}(x, x') = \left\langle \Phi(\{\mathbf{r}_i\}; x) \left| \hat{H} \right| \Phi(\{\mathbf{r}_i\}; x') \right\rangle, \quad i = 1, \dots, A, \quad (4)$$

$\hat{H}$ being the nuclear Hamiltonian and $\Phi(\{\mathbf{r}_i\}; x)$ the GCM generating function (taken to be a Slater determinant constructed by a complete set of s.p. functions $\varphi_\lambda(x, \mathbf{r})$ corresponding to a given construction potential),

$$\rho(x, x', \mathbf{r}, \mathbf{r}') = 4 \sum_{\lambda, \mu=1}^{A/4} [N^{-1}(x, x')]_{\mu\lambda} \varphi_\lambda^*(x, \mathbf{r}) \varphi_\mu(x', \mathbf{r}'), \quad (5)$$

where N^{-1} is the inverse of the matrix

$$N_{\lambda\mu}(x, x') = \int \varphi_\lambda^*(x, \mathbf{r}) \varphi_\mu(x', \mathbf{r}) d\mathbf{r} \quad (6)$$

and

$$\mathcal{N}(x, x') = [\det(N_{\lambda\mu})]^4. \quad (7)$$

Skyrme-effective forces with parameter values fitted to give the binding energies of ${}^4\text{He}$, ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$ and two types of construction potentials (harmonic oscillator (GCHO case) and square-well with infinite walls (GCSW case)) were used in the GCM calculations. In the GCHO case the binding energies of the nuclei considered are in agreement with the results of GCM calculations in [31]. In the GCSW case they are (without the Coulomb energy) [32,2]: $E_0 = -37.06$ MeV, -144.58 MeV and -402.92 MeV for ${}^4\text{He}$, ${}^{16}\text{O}$ and ${}^{40}\text{Ca}$, respectively. The calculated proton density distributions have the correct asymptotic form [32,2].

In the CDFM [33,1,2] (which is related to the delta-function limit of GCM [30]) the OBM has the form:

$$\rho(\mathbf{r}, \mathbf{r}') = \int_0^\infty |f(x)|^2 \rho_x(\mathbf{r}, \mathbf{r}') dx, \quad (8)$$

where

$$\rho_x(\mathbf{r}, \mathbf{r}') = 3\rho_0(x) \frac{j_1(k_F(x)|\mathbf{r} - \mathbf{r}'|)}{k_F(x)|\mathbf{r} - \mathbf{r}'|} \theta\left(x - \frac{|\mathbf{r} + \mathbf{r}'|}{2}\right), \quad (9)$$

$$\rho_0(x) = 3A/4\pi x^3; \quad k_F(x) = \left(\frac{3}{2}\pi^2\rho_0(x)\right)^{1/3} \equiv \frac{\alpha}{x}; \quad \alpha = (9\pi A/8)^{1/3} \quad (10)$$

and

$$|f(x)|^2 = - \frac{1}{\rho_0(x)} \frac{d\rho(r)}{dr} \Big|_{r=x} \quad (11)$$

for monotonically decreasing density distributions $\left(\frac{d\rho}{dr} \leq 0\right)$.

The results for the NO in the GCM and CDFM are obtained by solving Eq.(1) and using Eqs.(2-7) and (8-11), respectively. Some results for hole- and particle-state NO are given in Figs.1 and 2, compared with the s.p. wave functions (which correspond to the given construction potential) calculated for the values of the generator coordinate for which the diagonal part of the GCM energy kernel (4) has a minimum. It can be seen that: i) The correlations included in the GCHO case change both hole- and particle- state natural orbitals. The NO are more localized in the coordinate space than the uncorrelated harmonic-oscillator single-particle wave functions for both hole- and particle-states. The localization of the NO in the coordinate space is connected with the presence of high-momentum components of the NO in momentum space (e.g. Fig.1c). ii) The correlations in the GCSW case change weakly the hole-state NO and affect more strongly the particle-state NO.

The correlations included in the GCM using both construction potentials lead to small depletions of the Fermi sea [25,2]. It was shown in [32] that the nucleon momentum distribution in the GCSW case has high-momentum

components at $k > 2 \text{ fm}^{-1}$ and differs significantly from that calculated with the Hartree-Fock method, while the momentum distribution in the GCHO case differs less.

The NO within the CDFM were calculated by using in Eq.(11) the nuclear charge density distributions obtained from the experiments on electron elastic scattering by nuclei. Results for hole- and particle-state NO in CDFM are given in Fig.3. It can be seen that the NO in the CDFM strongly deviate from the harmonic-oscillator and square-well shell-model s.p. wave functions for both hole- and particle-states. The NO are more strongly localized in coordinate space and this is related to the existence of high-momentum components of the NO in momentum space. The correlations in CDFM also strongly affect the occupation numbers [24,2] and both these lead to the strong high-momentum components of the total nucleon momentum distribution $n(k)$ in nuclei within the CDFM [33,1,2]. We note that the root-mean-square radii calculated in the present work for some particle-states in NO become smaller with increasing quantum number n (e.g., in ^{16}O : $r(3p) < r(2p)$ and in ^{40}Ca : $r(3d) < r(2d)$; $r(3f) < r(2f)$). We remark that a similar effect with a stronger localization of the s.p. wave functions in coordinate space when n increases has been observed for a system of 70 atoms of ^3He considered in [28].

The results of the present work are in accord with those for the NO obtained in [21] within the JCM. It was shown that the SRC in the JCM do not affect significantly the hole-state NO but they do affect mainly the occupation probabilities and the particle-state NO. The high-momentum components of the total momentum distribution $n(k)$ are almost completely determined by the particle-state contributions. This is the case in our work within the GCSW calculations. In the case of the GCHO and in the CDFM the correlations affect both hole- and particle-state natural orbitals and they both give contributions to the high-momentum components of the total momentum distribution. The results for the NO of the present work are also in agreement with those for other many-particle systems, such as the Fermi-liquid drop of 70 ^3He atoms [28] and the ^4He atom [29]. This concerns particularly the localization of the particle-state NO in the ^3He system.

The methods considered in this work go beyond the limits of the MFA. In this case there is no one common potential corresponding to all the natural orbitals for a given nucleus. It is important, however, to investigate the single-particle potentials corresponding to the NO of various states.

Using the Schrödinger equation and the results for the NO ($\psi_\alpha(r)$) obtained in this work for ^4He , ^{16}O and ^{40}Ca nuclei, we calculated the s.p. potentials corresponding to the radial parts of their NO ($R_\alpha(r)$) using

$$U_\psi(r) = \frac{\hbar^2}{2m} \left[\frac{(rR_\alpha(r))''}{(rR_\alpha(r))} - \frac{l_\alpha(l_\alpha + 1)}{r^2} \right] + \varepsilon_\alpha, \quad (12)$$

where $(rR_\alpha(r))''$ means the second derivative of the function with respect to r and ε_α are the s.p. energies (taken

for ^{16}O and ^{40}Ca states from [34]). Some examples of the s.p. potentials corresponding to the NO calculated in the cases of GCHO, GCSW and CDFM are given in Fig.4. The results can be summarized as follows: i) There exist good average s.p. potentials corresponding to the hole-state NO. Their forms are similar to those of the corresponding construction potentials and have similar behaviour (particularly in GCM) for different states; ii) Generally, there exist s.p. potentials corresponding to the particle-state NO, that are different from those of the hole-states. Some of them are similar to each other (particularly in CDFM). The results are in agreement with those obtained with the Jastrow correlation method in [21], where it was found that there is no common s.p. potential associated with the NO corresponding to the OBM. The s.p. potentials related to the eigenfunctions of the two parts of the OBM in JCM are grouped in two types of harmonic-oscillator-like potentials, the first one being of MFA-type, while the second is completely different from it.

We evaluate in the present work the effect of the nucleon-nucleon correlations in a given correlation method on single-particle characteristics, namely natural orbitals and the single-particle potentials corresponding to them. This is of importance because, as shown in [35], a knowledge of the one-body density matrix of the correlated ground state of the A -particle system (and the related quantities, such as the natural orbitals and the occupation probabilities) gives information on the single-particle overlap functions used for the description of direct one-nucleon transfer and $(e, e'p)$ knock-out reactions, as well as the spectroscopic factors and the separation energies of the bound eigenstates of the $(A - 1)$ -particle system.

Two of the authors (A.N.A. and D.N.K.) thank the Bulgarian National Science Foundation for the partial support of this work under the Contract Nr.Φ-32. One of them (A.N.A.) is grateful to the ECC for the partial support of this work under the Contract No. ERB-CIPA-CT-92-2159 and to the Nuclear Physics Laboratory of Oxford University for hospitality.

¹ A.N. Antonov, P.E. Hodgson and I.Zh. Petkov, *Nucleon Momentum and Density Distributions in Nuclei* (Clarendon Press, Oxford, 1988).

² A.N. Antonov, P.E. Hodgson and I.Zh. Petkov, *Nucleon Correlations in Nuclei* (Springer-Verlag, Berlin-Heidelberg-New York, 1993).

³ B. Frois, C. Papanicolas, *Ann. Rev. Nucl. Sci.* **37**, 133 (1987).

- ⁴ L. Lapikás, in *Proceedings of 6th International Conference on Nuclear Reaction Mechanisms, Varenna, June 10-15, 1991*, Ed. by E. Gadioli, 1991, p.610.
- ⁵ L. Lapikás, Preprint EMIN 92-06, Amsterdam, 1992.
- ⁶ M. Jaminon, C. Mahaux, H. Ngô, Phys. Lett. **158B**, 103 (1985).
- ⁷ O. Bohigas, S. Stringari, Phys. Lett. **95B**, 9 (1980).
- ⁸ K. Allaart, H.P. Blok, I. Bobeldijk, M.N. Harakeh, C.W. de Jager, E. Jans, L. Lapikás, R.W. Lourie, A. Saha, G. van der Steenhoven, H. de Vries, NIKHEF-K Report Nr:91-E19, 1991.
- ⁹ D.B. Day, J.S. McCarthy, Z.E. Meziani, R.C. Minehart, R.M. Sealock, S.T. Thornton, J. Jourdan, I. Sick, B.W. Filippone, R.D. McKeown, R.G. Milner, D.H. Potterveld, Z. Szalata, Phys. Rev. Lett. **59**, 427 (1987); Phys. Rev. C **40**, 1011 (1989); D.B. Day, J.S. McCarthy, T.W. Donnelly and I. Sick, Ann. Rev. Nucl. Part. Sci. **40**, 357 (1990).
- ¹⁰ C. Ciofi degli Atti, E. Pace, G. Salmè, Phys. Rev. C **43**, 1155 (1991); Nucl. Phys. **A497**, 349c (1989); **A497**, 361c (1989).
- ¹¹ S. Fantoni, V.R. Pandharipande, Nucl. Phys. **A473**, 234 (1987).
- ¹² R. Schiavilla, A. Fabrocini, V.R. Pandharipande, Nucl. Phys. **A473**, 290 (1987).
- ¹³ G. Orlandini, M. Traini, Rep. Progr. Phys. **54**, 257 (1991).
- ¹⁴ X. Ji, J. Engel, Phys. Rev. C **40**, R497 (1989).
- ¹⁵ V.R. Pandharipande, C.N. Papanicolas, J. Wambach, Phys. Rev. Lett. **53**, 1133 (1984).
- ¹⁶ L. Lapikás, in *Proceedings of 4th Workshop on Perspectives in Nuclear Physics at Intermediate Energies (Trieste, 1989)*, World Scientific, Singapore, 1989, p.419.
- ¹⁷ P.K.A. de Witt Huberts, J. Phys. G: Nucl. Part. Phys. **16**, 507 (1990).
- ¹⁸ A.E.L. Dieperink, P.K.A. de Witt Huberts, Ann. Rev. Nucl. Part. Sci. **40**, 239 (1990).
- ¹⁹ C. Mahaux, R. Sartor, Adv. Nucl. Phys. **20**, 1 (1991).
- ²⁰ P.-O. Löwdin, Phys. Rev. **97**, 1474 (1955).
- ²¹ M.V. Stoitsov, A.N. Antonov, S.S. Dimitrova, Phys. Rev. C **47**, R455 (1993); Phys. Rev. C **48**, 74 (1993).
- ²² M. Gaudin, J. Gillespie, G. Ripka, Nucl. Phys. **A176**, 237 (1971).

- ²³ F. Malaguti, A. Uguzzoni, E. Verondini, P. E. Hodgson, Riv. Nuovo Cim. **5**, 3 (1982).
- ²⁴ A.N. Antonov, Chr.V. Christov, E.N. Nikolov, I.Zh. Petkov, P.E. Hodgson, Nuovo Cim. **A102**, 1701 (1989).
- ²⁵ A.N. Antonov, I.S. Bonev, Chr.V. Christov, E.N. Nikolov, I.Zh. Petkov, Nuovo Cim. **A103**, 1287 (1990).
- ²⁶ M.V. Stoitsov, A.N. Antonov, Z. Phys. **A345**, 259 (1993).
- ²⁷ M.V. Stoitsov, A.N. Antonov, S.S. Dimitrova, Z. Phys. **A345**, 359 (1993).
- ²⁸ D.S. Lewart, V.R. Pandharipande, S.C. Pieper, Phys. Rev. B **37**, 4950 (1988).
- ²⁹ C.F. Fischer, *The Hartree-Fock Method for Atoms* (Wiley, New York, 1977).
- ³⁰ J.J. Griffin, J.A. Wheeler, Phys. Rev. **108**, 311 (1957).
- ³¹ H. Flocard, D. Vautherin, Phys. Lett. **55B**, 259 (1975); Nucl. Phys. **A264**, 197 (1976).
- ³² A.N. Antonov, I.S. Bonev, Chr.V. Christov, I.Zh. Petkov, Nuovo Cim. **A100**, 779 (1988).
- ³³ A.N. Antonov, V.A. Nikolaev, I.Zh. Petkov, Bulg. J. Phys. **6**, 151 (1979); Z. Phys. **A297**, 257 (1980); Z. Phys. **A304**, 239 (1982).
- ³⁴ S. Boffi, F.D. Pacati, Nucl. Phys. **A204**, 485 (1973).
- ³⁵ D. Van Neck, M. Waroquier, K. Heide, Phys. Lett. **B314**, 255 (1993).

FIG. 1. Single-particle wave functions of $1p(\text{hole})$ - and $2p(\text{particle})$ -states of ^{40}Ca in r -space (a,b) and of $2p(\text{particle})$ -state of ^{16}O in k -space (c). Dashed line: natural orbitals in GCHO; solid line: harmonic-oscillator shell-model wave functions.

FIG. 2. Single-particle wave functions of $1s(\text{hole})$ -state (a) and $2s(\text{particle})$ -state (b) of ^{16}O in r -space. Dashed line: natural orbitals in GCSW; solid line: square-well shell-model wave functions.

FIG. 3. Single-particle wave functions of $1p(\text{hole})$ -state (a) and $2p(\text{particle})$ -state (b) of ^{16}O in r -space. Short-dashed line: natural orbitals calculated in the CDFM; long-dashed line: square-well shell-model wave functions; solid line: harmonic-oscillator shell-model wave functions.

FIG. 4. Single-particle potentials in ^{40}Ca corresponding to natural orbitals calculated with GCHO and GCSW for $1s$ -, $1p$ -, $1d$ -, $2s(\text{hole})$ - and $2p(\text{particle})$ - states (a) and with CDFM for $1s$ -, $1p$ -, $1d$ -, $2s(\text{hole})$ - and $2p$ - and $1f(\text{particle})$ -states (b).

Fig. 1

Fig. 2

Fig. 3

Fig. 4