

# Evaluation of cluster expansions and correlated one-body properties of nuclei

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Three different cluster expansions for the evaluation of correlated one-body properties of  $s$ - $p$  and  $s$ - $d$  shell nuclei are compared. Harmonic oscillator wave functions and Jastrow-type correlations are used, while analytical expressions are obtained for the charge form factor, density distribution, and momentum distribution by truncating the expansions and using a standard Jastrow correlation function  $f$ . The harmonic oscillator parameter  $b$  and the correlation parameter  $\beta$  have been determined by a least-squares fit to the experimental charge form factors in each case. The information entropy of nuclei in position space ( $S_r$ ) and momentum space ( $S_k$ ) according to the three methods are also calculated. It is found that the larger the entropy sum,  $S = S_r + S_k$  (the net information content of the system), the smaller the values of  $\chi^2$ . This indicates that maximal  $S$  is a criterion of the quality of a given nuclear model, according to the maximum entropy principle. Only two exceptions to this rule, out of many cases examined, were found. Finally an analytic expression for the so-called ‘‘healing’’ or ‘‘wound’’ integrals is derived with the function  $f$  considered, for any state of the relative two-nucleon motion, and their values in certain cases are computed and compared.

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## I. INTRODUCTION

The effect of short-range correlations (SRC) on the one-body properties of nuclei is an old but challenging and appealing problem. In general, the account of SRC is important for the description of the mean values of some two-body operators, such as the ground-state energy of nuclei, but it is also of interest to investigate the SRC contribution to simpler nuclear quantities related to one-body operators such as the form factor (FF), density distribution (DD), and momentum distribution (MD). It has been shown that mean-field theories cannot correctly describe MD and DD simultaneously [1,2] and the main features of MD depend little on the effective mean field considered [3]. The reason is that MD is sensitive to short-range and tensor nucleon-nucleon correlations that are not included in the mean-field theories. We note however that the choice of a single-particle potential having a short-range repulsion could play a role in improving somehow the values of MD [4].

The experimental evidence obtained from inclusive and exclusive electron scattering on nuclei established the existence of a high-momentum component for momenta  $k > 2 \text{ fm}^{-1}$  [5–8]. It is well known, that the independent-particle model (IPM) fails to reproduce the high-momentum transfer data from electron scattering in nuclei. That is, the IPM is inadequate to reproduce satisfactorily the diffraction minima of the charge FF for high values of momentum transfer. Therefore, theoretical approaches, which take into account SRC due to the character of the nucleon-nucleon forces at small distances, are necessary to be developed.

In this effort, two main problems appear. The first one is the type of SRC that must be incorporated to the mean-field nucleon wave function and the second one is the type of cluster expansion to be used that is connected with the number of simultaneously correlated nucleons.

In the present work we consider central correlations of Jastrow type [9] while three different cluster expansions are considered. The first two types of expansions, named FIY (factor Iwamoto and Yamada) [10] and FAHT (factor Aviles, Hartogh, and Tolhoek) [11] respectively, were developed by Clark and Westhaus [12], Westhaus and Clark [12], and Feenberg [13] while the third one named LOA (low order approximation) was derived by Gaudin, Gillespie, and Ripka [14], and Bohigas and Stringari [1].

The FIY expansion, truncated at the two-body terms was used for the calculation of the charge FF and DD [15] and MD [16] in  $s$ - $p$  and  $s$ - $d$  shell nuclei while the LOA, truncated at the two-body terms and including a part of the three-body term was used for the calculation of the above one-body quantities in the closed shell nuclei  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$  [17] as well as of the bound-state overlap functions, separation energies, and spectroscopic factors in  ${}^{16}\text{O}$  and  ${}^{40}\text{Ca}$  [18]. The FAHT expansion, truncated at the two-body terms, was used for the evaluation of the charge FF [19] and nuclear ground-state energy of  ${}^4\text{He}$  and  ${}^{16}\text{O}$  [20]. In the present paper the FAHT expansion is used in addition for the evaluation of the FF, DD, and MD in  $s$ - $p$  and  $s$ - $d$  shell nuclei.

The present work is, in a way, a generalization of Ref. [21] where a comparison of various cluster expansions for the calculation of the charge FF of  ${}^4\text{He}$  was made. In this generalization, the above mentioned three types of expansions are applied and compared for one-body characteristics of  $s$ - $p$  and  $s$ - $d$  shell nuclei.

The comparison of the three truncated expansions can be made, as usual, by comparing  $\chi^2$  (in computing the FF), i.e., the smaller the  $\chi^2$ , the better the quality of the corresponding expansion. In the present work we use also an information-theoretical criterion in addition to  $\chi^2$ . Information-theoretical methods [22–32] play an important role in the study of quantum many-body systems, mainly through the application of

the maximum entropy principle (MEP) [33,34]. This is done by employing a suitably defined information entropy. A definition of information entropy was given in Ref. [35] based on phase-space considerations. In a previous work [30] this definition was used and it was found that the larger the value of that entropy the better the quality of the nuclear model. Another definition inspired by Shannon's information theory [36] and studied in atomic systems [23–25] is the entropy  $S = S_r + S_k$  (where  $S_r$  is the information entropy in position space and  $S_k$  the corresponding one in momentum space), which is a measure of the net information content of the system. Note also that this sum is scale invariant, i.e., it is independent of the units adopted in measuring position  $r$  and momentum  $k$ . It was demonstrated in atoms [24,25] that the entropy sum  $S$  increases with the quality of atomic distributions. Furthermore, it has been found in Ref. [31] that interesting properties of the information entropy  $S$  hold for a variety of systems. For instance, it was shown that  $S = a + b \ln N$  where  $N$  is the number of particles in nuclei, atomic clusters [31], and atoms [24,25]. Although a rigorous justification of the use of the maximal  $S = S_r + S_k$  as a quality criterion does not exist to our knowledge, the work so far suggests the need to explore further its empirical basis. Here we use this criterion in connection with the study of cluster expansions. We find further support for the contention that the larger the  $S$  the smaller the values of  $\chi^2$ , for various nuclei and expansions, with only two exceptions.

The paper is organized as follows. In Sec. II the general expressions of the one-body density matrix (OBDM) for the three types of expansions are given. Numerical results are reported and discussed in Sec. III, while the summary of the present work is given in Sec. IV. Finally, some details of the FAHT expansion as well as for the calculation of healing integrals are given in Appendices A and B, respectively.

## II. CORRELATED ONE-BODY PROPERTIES

### A. General definitions

The key descriptor of the one-body properties of nuclei is the OBDM  $\rho(\mathbf{r}, \mathbf{r}')$ , which for a system of  $A$  identical particles is defined [37,38] in terms of the complete wave function  $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$  by

$$\begin{aligned} \rho(\mathbf{r}, \mathbf{r}') &= \int \Psi^*(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_A) \Psi(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_A) d\mathbf{r}_2, \dots, d\mathbf{r}_A, \end{aligned} \quad (1)$$

where the integration is carried out over the radius vectors and summation over spin and isospin variables is implied.

In the case where the nuclear wave function  $\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_A)$  can be expressed as a single-Slater determinant depending on the single-particle wave functions we have

$$\rho_{SD}(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^A \phi_i^*(\mathbf{r}) \phi_i(\mathbf{r}'). \quad (2)$$

The diagonal elements of the OBDM give the DD,  $\rho(\mathbf{r}, \mathbf{r}) = \rho(\mathbf{r})$ , while the FF is the Fourier transform of it

$$F(\mathbf{q}) = \int \exp[i\mathbf{q}\mathbf{r}] \rho(\mathbf{r}) d\mathbf{r}, \quad (3)$$

and the MD is given by a particular Fourier transform of the OBDM

$$n(\mathbf{k}) = \frac{1}{(2\pi)^3} \int \exp[i\mathbf{k}(\mathbf{r} - \mathbf{r}')] \rho(\mathbf{r}, \mathbf{r}') d\mathbf{r} d\mathbf{r}'. \quad (4)$$

The second moment of the DD is the mean square radius of the nucleus while the second moment of the MD is related to the mean kinetic energy.

We also define the information entropy sum

$$S = S_r + S_k, \quad (5)$$

where

$$S_r = - \int \rho(\mathbf{r}) \ln \rho(\mathbf{r}) d\mathbf{r} \quad (6)$$

is the information entropy in position space and

$$S_k = - \int n(\mathbf{k}) \ln n(\mathbf{k}) d\mathbf{k} \quad (7)$$

is the information entropy in momentum space.

$S$  is a measure of quantum-mechanical uncertainty and represents the information content of a probability distribution, in our case of the nuclear density and momentum distributions. In the present work, we employ in calculating  $S$ , a normalization to the number of particles  $A$  for  $\rho(\mathbf{r})$  and  $n(\mathbf{k})$ .

### B. The cluster expansions of the one-body density matrix

The trial wave function  $\Psi$ , which describes a correlated nuclear system, can be written as (e.g., Ref. [39])

$$\Psi = \mathcal{F}\Phi, \quad (8)$$

where  $\Phi$  is a model wave function that is adequate to describe the uncorrelated  $A$ -particle nuclear system and  $\mathcal{F}$  is the operator that introduces SRC.  $\Phi$  is chosen to be a Slater determinant wave function, constructed by single-particle wave functions. Several restrictions can be made on the model operator  $\mathcal{F}$  [40,41]. In the present work  $\mathcal{F}$  is taken to be of the Jastrow type [9]

$$\mathcal{F} = \prod_{i < j}^A f(r_{ij}), \quad (9)$$

where  $f(r_{ij})$  is the state-independent correlation function of the form

$$f(r_{ij}) = 1 - \exp[-\beta(\mathbf{r}_i - \mathbf{r}_j)^2]. \quad (10)$$

### 1. Factor cluster expansion of Iwamoto Yamada

In FIY the OBDM takes the form [16]

$$\rho_{FIY}(\mathbf{r}, \mathbf{r}') = N_0 [\langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1 - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_1) - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_2) + O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_3)], \quad (11)$$

where  $N_0$  is the normalization factor, and the terms  $\langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1$  and  $O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$  ( $l=1,2,3$ ) have the general forms

$$\begin{aligned} \langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1 &= \rho_{SD}(\mathbf{r}, \mathbf{r}') \\ &= \frac{1}{\pi} \sum_{nl} \eta_{nl} (2l+1) \phi_{nl}^*(r) \phi_{nl}(r') P_l(\cos \omega_{rr'}), \end{aligned} \quad (12)$$

and

$$\begin{aligned} O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l) &= \int \mathbf{g}_l(\mathbf{r}, \mathbf{r}', \mathbf{r}_2) [\rho_{SD}(\mathbf{r}, \mathbf{r}') \rho_{SD}(\mathbf{r}_2, \mathbf{r}_2) \\ &\quad - \rho_{SD}(\mathbf{r}, \mathbf{r}_2) \rho_{SD}(\mathbf{r}_2, \mathbf{r}')] d\mathbf{r}_2, \end{aligned} \quad (13)$$

where the various uncorrelated OBDM,  $\rho_{SD}(\mathbf{x}, \mathbf{y})$ , associated with the Slater determinant can be written as in Eqs. (2) and (12). The factors  $\mathbf{g}_l(\mathbf{r}, \mathbf{r}', \mathbf{r}_2)$  ( $l=1,2,3$ ) come from the rearrangement of the operator  $f(r_{12})\mathbf{O}(2)f(r'_{12}) = f(|\mathbf{r}_1 - \mathbf{r}_2|)\mathbf{O}(2)f(|\mathbf{r}'_1 - \mathbf{r}'_2|)$  as described in Ref. [16]. These factors have the forms

$$\begin{aligned} \mathbf{g}_1(\mathbf{r}, \mathbf{r}', \mathbf{r}_2) &= \exp[-\beta(r^2 + r'^2)] \exp[2\beta\mathbf{r}\mathbf{r}_2], \\ \mathbf{g}_2(\mathbf{r}, \mathbf{r}', \mathbf{r}_2) &= \mathbf{g}_1(\mathbf{r}', \mathbf{r}, \mathbf{r}_2), \\ \mathbf{g}_3(\mathbf{r}, \mathbf{r}', \mathbf{r}_2) &= \exp[-\beta(r^2 + r'^2)] \exp[-2\beta r^2] \\ &\quad \times \exp[2\beta(\mathbf{r} + \mathbf{r}')\mathbf{r}_2]. \end{aligned} \quad (14)$$

Performing the spin-isospin summation and the angular integration, the term  $O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$  takes the general form

$$\begin{aligned} O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l) &= 4 \sum_{n_i l_i, n_j l_j} \eta_{n_i l_i} \eta_{n_j l_j} (2l_i + 1)(2l_j + 1) \\ &\quad \times \left[ 4A_{n_i l_i, n_j l_j}^{n_i l_i, n_j l_j, 0}(\mathbf{r}, \mathbf{r}', \mathbf{g}_l) \right. \\ &\quad \left. - \sum_{k=0}^{l_i + l_j} \langle l_i 0 l_j 0 | k 0 \rangle^2 A_{n_i l_i, n_j l_j}^{n_j l_j, n_i l_i, k}(\mathbf{r}, \mathbf{r}', \mathbf{g}_l) \right], \end{aligned} \quad (15)$$

where

$$\begin{aligned} A_{n_1 l_1, n_2 l_2}^{n_3 l_3, n_4 l_4, k}(\mathbf{r}, \mathbf{r}', \mathbf{g}_1) &= \frac{1}{4\pi} \phi_{n_1 l_1}^*(r) \phi_{n_3 l_3}(r') \\ &\quad \times \exp[-\beta r^2] P_{l_3}(\cos \omega_{rr'}) \\ &\quad \times \int_0^\infty \phi_{n_2 l_2}^*(r_2) \phi_{n_4 l_4}(r_2) \\ &\quad \times \exp[-\beta r_2^2] i_k(2\beta r r_2) r_2^2 dr_2, \end{aligned} \quad (16)$$

and the matrix element  $A_{n_1 l_1, n_2 l_2}^{n_3 l_3, n_4 l_4, k}(\mathbf{r}, \mathbf{r}', \mathbf{g}_2)$  can be found from Eq. (16) replacing  $\mathbf{r} \leftrightarrow \mathbf{r}'$  and  $n_1 l_1 \leftrightarrow n_3 l_3$  while the matrix element corresponding to the factor  $\mathbf{g}_3$  can be found from Eq. (16) replacing the factors  $\exp[-\beta r^2]$ ,  $P_{l_3}(\cos \omega_{rr'})$ , and  $i_k(2\beta r r_2)$  by the factors  $\exp[-\beta(r^2 + r'^2)]$ ,  $\Omega_{l_1 l_3}^k(\omega_{rr'})$ , and  $i_k(2\beta|\mathbf{r} + \mathbf{r}'|r_2)$ , respectively [16]. In the expressions of the matrix elements  $A_{n_1 l_1, n_2 l_2}^{n_3 l_3, n_4 l_4, k}(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$ ,  $i_k(z)$  is the modified spherical Bessel function and the factor  $\Omega_{l_1 l_3}^k(\omega_{rr'})$  depends on the directions of  $\mathbf{r}$  and  $\mathbf{r}'$ .

### 2. Factor cluster expansion of Aviles, Hartogh, and Tolhoek

In FAHT, truncated at the two-body terms, the OBDM takes the form (details of the calculations are given in Appendix A)

$$\rho_{FAHT}(\mathbf{r}, \mathbf{r}') = \frac{1}{A} \langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1 + (A-1) \left[ \frac{(A-1) \langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1 - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_1) - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_2) + O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_3)}{A(A-1) - \int [O_2(\mathbf{r}, \mathbf{r}, \mathbf{g}_1) + O_2(\mathbf{r}, \mathbf{r}, \mathbf{g}_2) - O_2(\mathbf{r}, \mathbf{r}, \mathbf{g}_3)] d\mathbf{r}} - \frac{1}{A} \langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1 \right], \quad (17)$$

where  $\langle \mathbf{O}_{\mathbf{r}\mathbf{r}'} \rangle_1$  and  $O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$  are given again by Eqs. (12) and (13), respectively. The FAHT expansion has the advantage that the normalization is preserved term by term.

### 3. Low order approximation

In LOA of Gaudin *et al.* [14] the one- and the two-body density matrices of the nucleus were expanded in terms of the functions  $\tilde{g} = f^2(r_{ij}) - 1$  and  $h = f(r_{ij}) - 1$  and were truncated up to the second order of  $h$  and the first order of  $\tilde{g}$ . This expansion contains one- and two-body terms and a part of the three-body term that leads to the normalization of the wave function. In LOA the OBDM takes the form [1,14,17]

$$\rho_{LOA}(\mathbf{r}, \mathbf{r}') = \frac{1}{A} [\langle \mathbf{O}_{rr'} \rangle_1 - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_1) - O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_2) + O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_3) + 2O_3(\mathbf{r}, \mathbf{r}', \beta) - O_3(\mathbf{r}, \mathbf{r}', 2\beta)], \quad (18)$$

where  $\langle \mathbf{O}_{rr'} \rangle_1$  and  $O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$  are given again by Eqs. (12) and (13), respectively, and the three-body term  $O_3(\mathbf{r}, \mathbf{r}', z)$  ( $z = \beta, 2\beta$ ) has the form

$$O_3(\mathbf{r}, \mathbf{r}', z) = \int \mathbf{g}(\mathbf{r}_2, \mathbf{r}_3, z) \rho_{SD}(\mathbf{r}, \mathbf{r}_2) [\rho_{SD}(\mathbf{r}_2, \mathbf{r}') \rho_{SD}(\mathbf{r}_3, \mathbf{r}_3) - \rho_{SD}(\mathbf{r}_2, \mathbf{r}_3) \rho_{SD}(\mathbf{r}_3, \mathbf{r}')] d\mathbf{r}_2 d\mathbf{r}_3, \quad (19)$$

where

$$\mathbf{g}(\mathbf{r}_2, \mathbf{r}_3, z) = \exp[-z(r_2^2 + r_3^2 - 2\mathbf{r}_2 \mathbf{r}_3)], \quad z = \beta, 2\beta. \quad (20)$$

It should be noted that, in Refs. [1,14,17] the three-body term is written

$$O_3(\mathbf{r}, \mathbf{r}') = - \int [f^2(r_{23}) - 1] \rho_{SD}(\mathbf{r}, \mathbf{r}_2) \times [\rho_{SD}(\mathbf{r}_2, \mathbf{r}') \rho_{SD}(\mathbf{r}_3, \mathbf{r}_3) - \rho_{SD}(\mathbf{r}_2, \mathbf{r}_3) \rho_{SD}(\mathbf{r}_3, \mathbf{r}')] d\mathbf{r}_2 d\mathbf{r}_3. \quad (21)$$

If we expand the factor  $f^2(r_{23}) - 1$ ,

$$f^2(r_{23}) - 1 = \exp[-2\beta(\mathbf{r}_2 - \mathbf{r}_3)^2] - 2 \exp[-\beta(\mathbf{r}_2 - \mathbf{r}_3)^2], \quad (22)$$

and insert the right-hand side of this equation into Eq. (21), the three-body term is separated in two terms

$$O_3(\mathbf{r}, \mathbf{r}') = 2O_3(\mathbf{r}, \mathbf{r}', \beta) - O_3(\mathbf{r}, \mathbf{r}', 2\beta), \quad (23)$$

where the term  $O_3(\mathbf{r}, \mathbf{r}', z)$  ( $z = \beta, 2\beta$ ) is given by Eq. (19). The two-body terms  $O_2(\mathbf{r}, \mathbf{r}', \mathbf{g}_l)$  ( $l = 1, 2, 3$ ) of Eq. (18) were calculated from the expression of the two-body term in LOA of Refs. [1,14,17] making similar rearrangements.

Performing the spin-isospin summation and the angular integration, the term  $O_3(\mathbf{r}, \mathbf{r}', z)$  takes the general form

$$O_3(\mathbf{r}, \mathbf{r}', z) = 4 \sum_{n_i l_i, n_j l_j, n_k l_k} \eta_{n_i l_i} \eta_{n_j l_j} \eta_{n_k l_k} (2l_i + 1) \times \left[ 4(2l_k + 1) \delta_{l_i l_j} A_{n_i l_i, n_j l_j, n_k l_k}^{n_j l_j n_i l_i n_k l_k, 0}(\mathbf{r}, \mathbf{r}', z) - (2l_j + 1) \delta_{l_i l_k} \times \sum_{k'=0}^{l_i + l_j} \langle l_i 0 l_j 0 | k' 0 \rangle^2 A_{n_i l_i, n_j l_j, n_k l_k}^{n_k l_k n_i l_i n_j l_j, k'}(\mathbf{r}, \mathbf{r}', z) \right], \quad (24)$$

where

$$A_{n_1 l_1 n_2 l_2 n_3 l_3}^{n_4 l_4 n_5 l_5 n_6 l_6, k'}(\mathbf{r}, \mathbf{r}', z) = \frac{1}{4\pi} \phi_{n_1 l_1}^*(r) \phi_{n_4 l_4}(r') P_{l_1}(\cos \omega_{rr'}) \times \int_0^\infty \phi_{n_2 l_2}^*(r_2) \phi_{n_5 l_5}(r_2) \times \exp[-zr_2^2] r_2^2 dr_2 \times \int_0^\infty \phi_{n_3 l_3}^*(r_3) \phi_{n_6 l_6}(r_3) \times \exp[-zr_3^2] i_{k'}(2zr_2 r_3) r_3^2 dr_3. \quad (25)$$

Expressions (12), (15), and (24) were derived for the closed shell nuclei with  $N=Z$  where  $\eta_{nl}$  is 0 or 1. For the open shell nuclei (with  $N=Z$ ) we use the same expressions where now  $0 \leq \eta_{nl} \leq 1$ . The normalization is preserved for the closed shell nuclei in all the expansions. In the case of the open shell nuclei the normalization is preserved (in the above formalism) for FIY and FAHT expansions. In the case of LOA, in which the number of particles is also conserved [42], particular attention has to be paid in each open shell nucleus.

It is noted that the general expressions of the two- and three-body terms of the density matrix given by Eqs. (15) and (24) are also valid for the expansions of the DD, FF, and MD. The only difference is in the expressions of the matrix elements  $A$  that have to be used. The matrix elements  $A$  of the DD are found from Eqs. (16) and (25) putting  $\mathbf{r}' = \mathbf{r}$ . The corresponding ones of the FF are the Fourier transforms [as defined by Eq. (3)] of  $A(\mathbf{r}, \mathbf{r})$ . Finally, the matrix elements of the MD are the Fourier transforms [as defined by Eq. (4)] of  $A(\mathbf{r}, \mathbf{r}')$ .

In the case when the model wave function  $\Phi$  is constructed from harmonic oscillator (HO) wave functions, analytical expressions of the various terms of the DD, FF, and MD for any  $N=Z$ ,  $s$ - $p$  and  $s$ - $d$  shell nuclei can be found for FIY and FAHT while in the case of LOA analytical expressions of the closed shell nuclei in the same region can be found. These expressions that depend on the HO parameter  $b$  and the correlation parameter  $\beta$  are given in Refs. [15–17] for FIY and LOA while the ones for FAHT can be found easily from the other expansions.

### III. RESULTS AND DISCUSSION

The three expansions, mentioned in Sec. II, have been used for the analytical calculations of the DD, MD, and charge FF as well as for the calculation of the information entropy sum defined by Eq. (5). The HO parameter  $b$  and the SRC parameter  $\beta$  in the three cases have been determined, for each nucleus separately, by a least-squares fit to the experimental charge FF as in Ref. [15] (using the same expression for  $\chi^2$ ). The choice to determine the parameters in the correlated wave function by fitting the expressions of the FF to the experimental results, which is a customary procedure in phenomenological approaches like the present one, appears to be advisable, in view of also the large amount of the

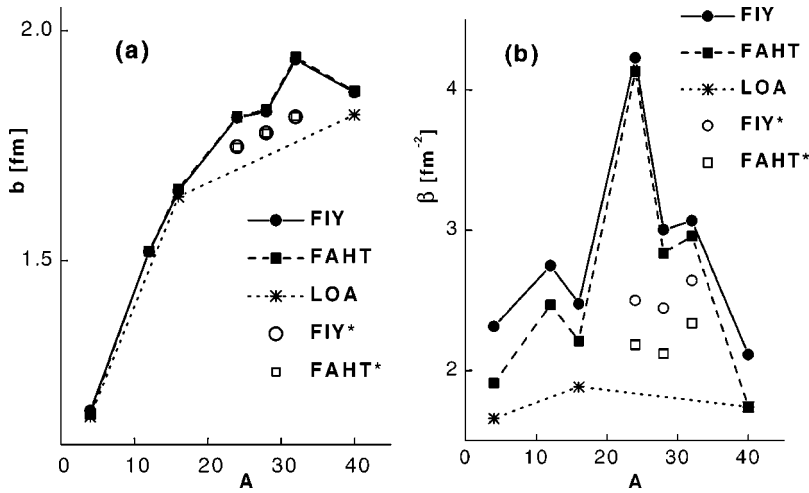


FIG. 1. The harmonic oscillator parameter  $b$  (a) and correlation parameter  $\beta$  (b) vs the mass number  $A$  for the expansions FIY, FAHT, and LOA. Cases FIY\* and FAHT\* (open circles and squares, respectively) correspond to the case when the occupation probability  $\eta_{2s}$  is treated as a free parameter.

existing experimental data. Of course, it would be desirable to determine those parameters also by fitting the expressions of the MD to the corresponding experimental results. These results are, however, very limited and in addition are model dependent and thus not so reliable. The center-of-mass correction has been taken into account by a Tassie-Barker factor [43] while that for the finite proton size and the Darwin-Foldy relativistic correction have been treated by the Chandra and Sauer approximation [44]. These corrections are not taken into account in the calculations of DD and MD to obtain the information entropy sum (and in the plots of MD).

The variation with the mass number  $A$  of the best fit values of the parameters  $b$  and  $\beta$  for each of the three expansions is shown in Fig. 1 where  $b$  and  $\beta$  vs the mass number  $A$  have been plotted for various  $s$ - $p$  and  $s$ - $d$  shell nuclei. It is seen that these parameters have the same behavior in FIY and FAHT expansions. In the case of LOA expansion, which has been used only for  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$  the dependence of the parameters on the mass number seems to have similar behavior. From Fig. 1(b) it is seen also that the SRC parameter  $\beta$  has larger values in the open shell nuclei ( ${}^{12}\text{C}$ ,  ${}^{24}\text{Mg}$ ,  ${}^{28}\text{Si}$ , and  ${}^{32}\text{S}$ ) than in the closed shell ones, indicating that there should be a shell effect in the case of closed shell nuclei.

In this work we compare different expansions in the example of MD for closed and open shell nuclei. The reason for this is that the high-momentum component of  $n(k)$  is very sensitive to the extent to which nucleon correlations are accounted for in a given correlation method and in various approximations. The effect of different expansions on the form factors can be seen comparing the values of  $\chi^2$  for the various expansions and nuclei.

The MD for the closed shell nuclei  ${}^4\text{He}$ ,  ${}^{16}\text{O}$ , and  ${}^{40}\text{Ca}$ , calculated with the best fit values of the parameters and for the three expansions as well as for the HO case, that is, when the SRC are not included, are shown in Fig. 2. It is seen that the inclusion of SRC increases considerably the high-momentum component of  $n(k)$ . It has the same slope up to  $2 \text{ fm}^{-1}$  for the three expansions. In the region,  $2 \text{ fm}^{-1} < k < 5 \text{ fm}^{-1}$ , the slope seems to be a little different. FIY gives a larger contribution in the high-momentum component than FAHT and LOA that give about the same contribution in this region. The same behavior of  $n(k)$  has been observed in the open shell nuclei as can be seen from Fig. 3. Here we would like to note that in general, a more realistic description of MD requires the inclusion of tensor correlations in the theoretical scheme.

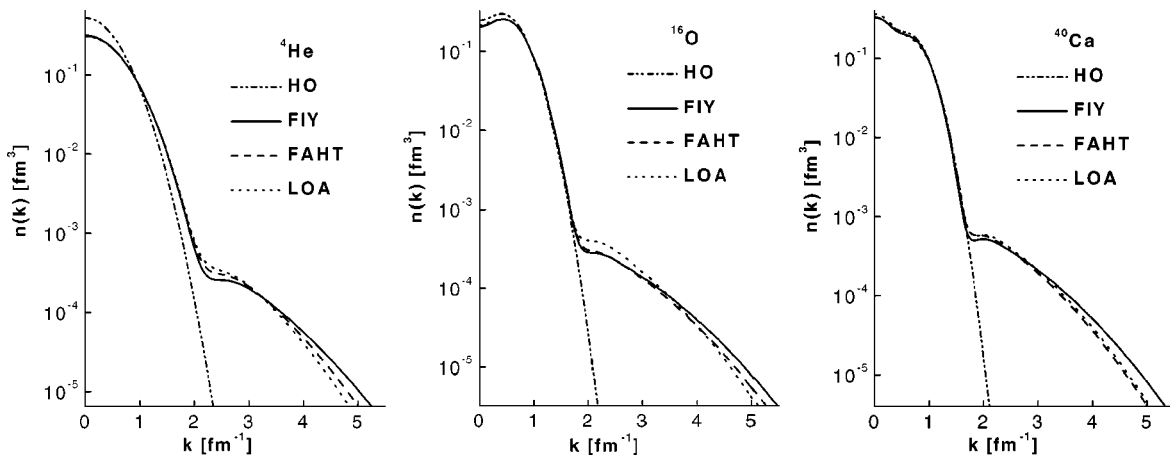


FIG. 2. The momentum distribution of the closed shell nuclei in the three expansions, FIY, FAHT, and LOA as well as of the HO case. The normalization is  $\int n(\mathbf{k}) d\mathbf{k} = 1$ .

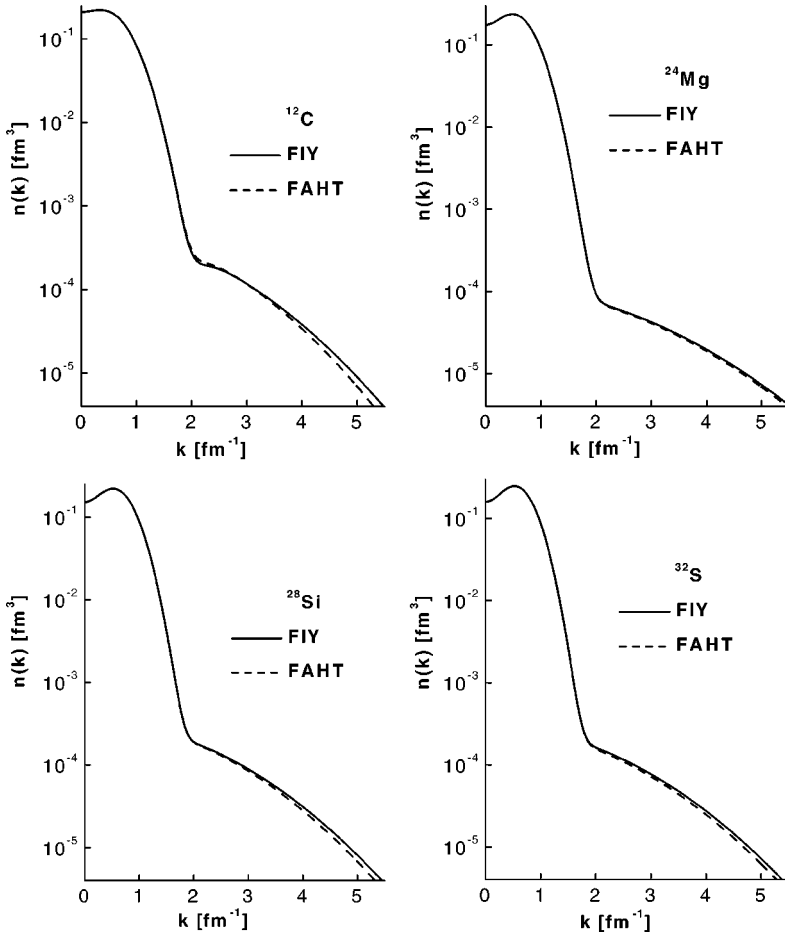


FIG. 3. The momentum distribution of the open shell nuclei in the two expansions, FIY and FAHT. The normalization is as in Fig. 2.

In the previous analysis, the nuclei  $^{24}\text{Mg}$ ,  $^{28}\text{Si}$ , and  $^{32}\text{S}$  were treated as  $1d$  shell nuclei, that is, the occupation probability of the  $2s$  state was taken to be zero. The formalism of the expansions FIY and FAHT has the advantage that the occupation probabilities of the various states can be treated as free parameters in the fitting procedure of the charge FF. Thus, the analysis can be made with more free parameters. For that reason we considered, as in Ref. [16], the cases FIY\* and FAHT\* in which the occupation probability  $\eta_{2s}$  of the nuclei  $^{24}\text{Mg}$ ,  $^{28}\text{Si}$ , and  $^{32}\text{S}$  was taken to be a free parameter together with the parameters  $b$  and  $\beta$ . We found that in both expansions the  $\chi^2$  values become smaller, compared to those of cases FIY and FAHT and the  $A$  dependence of the parameter  $\beta$ , as can be seen from Fig. 1(b), is not so strong as before. Also the values of  $\eta_{2s}$  found in the fit and the values of  $\eta_{1d}$  found through the relation  $\eta_{1d} = [(Z-8) - 2\eta_{2s}]/10$ , are very close for both expansions in each nucleus.

Our best fit values of the parameters and the values of  $\chi^2$  for the various nuclei under consideration and for the three expansions as well as for the HO case are shown in Table I. From the values of  $\chi^2$  we conclude that the three expansions give similar values of  $\chi^2$ . The FIY and FAHT expansions have almost the same  $\chi^2$  values. They differ less than 2% in the two expansions in each nucleus. In most cases the  $\chi^2$  values corresponding to FIY (or FIY\*) are smaller. There are two cases ( $^{12}\text{C}$  and  $^{28}\text{Si}$ ) when the FAHT or FAHT\*

expansion gives smaller  $\chi^2$  value and one case ( $^{16}\text{O}$ ) when LOA gives smaller  $\chi^2$  value.

In addition, we verify the information-theoretic criterion for comparing the quality of the three expansions. It is seen in Table I that almost in all the cases, the smaller the  $\chi^2$  the larger the  $S$ . Both methods of comparison ( $S$  and  $\chi^2$ ) show that the FIY (or FIY\*) expansion is better than the FAHT and LOA for  $^4\text{He}$ ,  $^{24}\text{Mg}$ ,  $^{32}\text{S}$ , and  $^{40}\text{Ca}$ . For  $^{16}\text{O}$  the LOA is the best. There are only two exceptions to this rule, i.e., in  $^{12}\text{C}$  for cases FIY and FAHT and in  $^{28}\text{Si}$  for cases FIY\* and FAHT\*. In  $^{12}\text{C}$   $\chi^2$  is smaller in FAHT and we expect  $S$  to be larger than in FIY while in  $^{28}\text{Si}$   $\chi^2$  is smaller in FIY\* and we expect  $S$  to be larger than in FAHT\*. These are two exceptions to our rule. It should also be noted that in these two exceptions the difference in the  $\chi^2$  values for the two expansions in both nuclei is less than 1%.

We consider also the so-called ‘‘healing’’ or ‘‘wound’’ integrals, denoted here as  $w_{nl}^2$  [41,45] for the various states of the relative two-nucleon motion, pertinent to the closed shell nuclei of Table I and in each case, that is, in each of the cluster expansions FIY, FAHT, and LOA. The values of these integrals express in a way the ‘‘amount of correlations’’ introduced to each state of the relative two-nucleon motion. The healing integrals [for a state-independent correlation function  $f(r)$ , such as the one given by Eq. (10)] are defined as follows:

TABLE I. The values of the parameters  $b$  (fm) and  $\beta$  (fm<sup>-2</sup>), the  $\chi^2$ , the rms charge radii  $\langle r_{ch}^2 \rangle^{1/2}$  (fm), the mean kinetic energy per nucleon  $\langle T \rangle$  (MeV), and the nuclear information entropy in position space ( $S_r$ ) and momentum space ( $S_k$ ) and their sum  $S$  for various  $s$ - $p$  and  $s$ - $d$  shell nuclei. The various cases have been ordered according to increasing values of  $\chi^2$ . For the various cases see the text.

| Nucleus          | Case  | $b$    | $\beta$  | $\chi^2$ | $\langle r_{ch}^2 \rangle^{1/2}$ | $\langle T \rangle$ | $S_r$   | $S_k$   | $S$    |
|------------------|-------|--------|----------|----------|----------------------------------|---------------------|---------|---------|--------|
| <sup>4</sup> He  | FIY   | 1.1732 | 2.3127   | 3.50     | 1.623                            | 29.904              | 9.978   | 5.985   | 15.963 |
|                  | FAHT  | 1.1661 | 1.9092   | 3.70     | 1.621                            | 29.048              | 9.943   | 6.013   | 15.955 |
|                  | LOA   | 1.1605 | 1.6584   | 3.88     | 1.620                            | 28.543              | 9.917   | 6.034   | 15.951 |
|                  | HO    | 1.4320 | $\infty$ | 30.94    | 1.765                            | 15.166              | 11.632  | 3.014   | 14.646 |
| <sup>12</sup> C  | FAHT  | 1.5204 | 2.4683   | 90.19    | 2.427                            | 24.779              | 31.455  | 1.989   | 33.444 |
|                  | FIY   | 1.5190 | 2.7468   | 90.87    | 2.426                            | 25.580              | 31.436  | 2.142   | 33.578 |
|                  | HO    | 1.6251 | $\infty$ | 176.54   | 2.490                            | 17.010              | 32.714  | -2.2484 | 30.465 |
| <sup>16</sup> O  | LOA   | 1.6387 | 1.8825   | 115.50   | 2.674                            | 23.006              | 42.083  | -4.393  | 37.690 |
|                  | FIY   | 1.6507 | 2.4747   | 120.19   | 2.680                            | 23.614              | 42.237  | -4.557  | 37.680 |
|                  | FAHT  | 1.6554 | 2.2097   | 122.49   | 2.684                            | 22.518              | 42.313  | -4.939  | 37.374 |
|                  | HO    | 1.7610 | $\infty$ | 199.45   | 2.738                            | 15.044              | 43.655  | -10.667 | 32.988 |
| <sup>24</sup> Mg | FIY*  | 1.7473 | 2.4992   | 140.37   | 3.064                            | 24.614              | 63.532  | -14.334 | 49.198 |
|                  | FAHT* | 1.7468 | 2.1833   | 140.40   | 3.064                            | 23.742              | 63.536  | -14.603 | 48.933 |
|                  | FIY   | 1.8103 | 4.2275   | 177.51   | 3.095                            | 21.109              | 64.452  | -19.228 | 45.224 |
|                  | FAHT  | 1.8120 | 4.1322   | 177.91   | 3.096                            | 20.818              | 64.483  | -19.410 | 45.073 |
|                  | HO    | 1.8496 | $\infty$ | 188.01   | 3.117                            | 16.162              | 65.124  | -23.429 | 41.695 |
| <sup>28</sup> Si | FAHT* | 1.7773 | 2.1193   | 103.39   | 3.184                            | 24.184              | 72.901  | -20.844 | 52.057 |
|                  | FIY*  | 1.7774 | 2.4440   | 103.47   | 3.184                            | 25.205              | 72.888  | -20.438 | 52.450 |
|                  | FIY   | 1.8236 | 3.0020   | 126.33   | 3.216                            | 22.933              | 73.889  | -24.115 | 49.774 |
|                  | FAHT  | 1.8279 | 2.8372   | 127.84   | 3.219                            | 22.110              | 73.987  | -24.645 | 49.342 |
|                  | HO    | 1.8941 | $\infty$ | 148.28   | 3.257                            | 16.099              | 75.288  | -32.022 | 43.266 |
| <sup>32</sup> S  | FIY*  | 1.8121 | 2.6398   | 166.11   | 3.282                            | 24.916              | 82.100  | -28.343 | 53.758 |
|                  | FAHT* | 1.8131 | 2.3358   | 166.31   | 3.283                            | 23.961              | 82.129  | -28.827 | 53.302 |
|                  | FIY   | 1.9368 | 3.0659   | 304.96   | 3.443                            | 20.867              | 86.921  | -36.707 | 50.214 |
|                  | FAHT  | 1.9417 | 2.9585   | 306.46   | 3.446                            | 20.252              | 87.045  | -37.316 | 49.729 |
|                  | HO    | 2.0016 | $\infty$ | 320.45   | 3.483                            | 14.878              | 88.361  | -44.881 | 43.480 |
| <sup>40</sup> Ca | FIY   | 1.8660 | 2.1127   | 160.44   | 3.516                            | 26.617              | 101.501 | -42.710 | 58.791 |
|                  | FAHT  | 1.8685 | 1.7397   | 161.13   | 3.517                            | 24.643              | 101.558 | -44.172 | 57.387 |
|                  | LOA   | 1.8164 | 1.7404   | 188.36   | 3.397                            | 25.586              | 97.611  | -42.121 | 55.490 |
|                  | HO    | 1.9453 | $\infty$ | 229.32   | 3.467                            | 16.437              | 100.987 | -58.709 | 42.278 |

$$w_{nl}^2 = \int_0^\infty |\psi_{nl}(r) - \phi_{nl}(r)|^2 dr, \quad (26)$$

where  $\phi_{nl}(r)$  is the (normalized to unity) uncorrelated (HO) radial relative wave function and  $\psi_{nl}(r)$  the corresponding, normalized to unity, correlated one:  $\psi_{nl}(r) = N_{nl} f(r) \phi_{nl}(r)$ , where  $N_{nl}$ , the normalization factor of  $\psi_{nl}(r)$ , is given by

$$N_{nl} = \left[ \int_0^\infty f^2(r) \phi_{nl}^2(r) dr \right]^{-1/2}. \quad (27)$$

It is interesting to note that with the correlation function (10) the healing integrals can be calculated analytically for

every state  $nl$ . Some details are given in Appendix B. As one expects, these integrals depend on both, the HO parameter  $b$  and the correlation parameter  $\beta$ . We may note, however, that their dependence on them is only through the dimensionless product  $y = 2\beta b^2$  [see expression (B6) of Appendix B].

In Table II the values of the parameters  $b$ ,  $\beta$ , and  $\tilde{y} = \beta b^2$  for each closed shell nucleus and cluster expansion considered are displayed along with the corresponding values of  $w_{nl}^2$  for certain relative states in the  $s$ - $p$  and  $s$ - $d$  closed shell nuclei. It is seen from the results in this table that the values of  $w_{nl}^2$  for each of the relative states ( $nl$ ) involved in each nucleus are smaller when  $w_{nl}^2$  is obtained with the FIY expansion and larger when obtained with the LOA. Further-

TABLE II. The values of the parameters  $b$  (fm),  $\beta$  (fm<sup>-2</sup>), and  $\tilde{y} = \beta b^2$  and the values of the healing integral  $w_{nl}^2$  for various states and for the closed shell nuclei <sup>4</sup>He, <sup>16</sup>O, and <sup>40</sup>Ca and the three expansions FIY, FAHT, and LOA.

| Nucleus          | Case | $b$    | $\beta$ | $\tilde{y} = \beta b^2$ | $w_{00}^2$ | $w_{01}^2$ | $w_{02}^2$           | $w_{10}^2$ | $w_{03}^2$           |
|------------------|------|--------|---------|-------------------------|------------|------------|----------------------|------------|----------------------|
| <sup>4</sup> He  | FIY  | 1.1732 | 2.3127  | 3.1832                  | 0.01874    |            |                      |            |                      |
|                  | FAHT | 1.1661 | 1.9092  | 2.5961                  | 0.02450    |            |                      |            |                      |
|                  | LOA  | 1.1605 | 1.6584  | 2.2335                  | 0.02971    |            |                      |            |                      |
| <sup>16</sup> O  | FIY  | 1.6507 | 2.4747  | 6.7431                  | 0.00664    | 0.00024    | $8.6 \times 10^{-6}$ | 0.00925    |                      |
|                  | FAHT | 1.6554 | 2.2097  | 6.0554                  | 0.00773    | 0.00031    | $1.2 \times 10^{-5}$ | 0.01069    |                      |
|                  | LOA  | 1.6387 | 1.8825  | 5.0552                  | 0.00996    | 0.00048    | $2.3 \times 10^{-5}$ | 0.01359    |                      |
| <sup>40</sup> Ca | FIY  | 1.8660 | 2.1127  | 7.3563                  | 0.00586    | 0.00020    | $6.4 \times 10^{-6}$ | 0.00821    | $2.1 \times 10^{-7}$ |
|                  | FAHT | 1.8685 | 1.7397  | 6.0738                  | 0.00770    | 0.00031    | $1.2 \times 10^{-5}$ | 0.01065    | $4.8 \times 10^{-7}$ |
|                  | LOA  | 1.8164 | 1.7404  | 5.7421                  | 0.00833    | 0.00035    | $1.5 \times 10^{-5}$ | 0.01148    | $6.2 \times 10^{-7}$ |

more, for each nucleus and expansion the values of  $w_{nl}^2$  of the nodeless ( $n=0$ ) states decrease as the value of  $l$  increases, the correlations having less effect to these higher  $l$  states, because of the existing centrifugal (repulsive) term of the HO potential. The values of  $w_{n0}^2$  increase when  $n=1$  or  $n=2$  in comparison with those of  $w_{00}^2$ .

From the analysis in Sec. II we may observe that the three truncated expansions have common basic ingredients in their structure. Their main difference is in the way one takes into account the normalization. In the FIY this is done by the overall normalization factor  $N_0$ . In the FAHT, the normalization is preserved term by term, while in LOA is done by taking into account, suitably, a part of the three-body term. The close agreement of the numerical results obtained with the three expansions suggests that the way of performing the normalization does not influence much these results. The existing small differences, however, indicate that there should be some difference in the magnitude of the higher-order terms. More specifically, we note that the values of the healing integral  $w_{nl}^2$  are smaller in FIY than in the other two expansions indicating that the magnitude of the higher-order terms is smaller in this expansion.

A final comment is appropriate. The problem of finding the proper trial density matrices for an  $A$ -particle system at given symmetry is known as the  $A$ -representability problem [46]. It includes the determination of general necessary and sufficient conditions ensuring that a trial density matrix is derivable from a full  $A$ -particle density matrix (the so-called ensemble  $A$ -representability) or from an existing  $A$ -particle state  $\Psi$  (the so-called  $A$ -representability by pure states). The one-body density matrix  $\rho(\mathbf{r}, \mathbf{r}')$  has the simplest form in the natural orbital representation [38],

$$\rho(\mathbf{r}, \mathbf{r}') = \sum_a \eta_a \chi_a^*(\mathbf{r}) \chi_a(\mathbf{r}'), \quad (28)$$

where  $\{\chi_a(\mathbf{r})\}$  are single-particle wave functions (called natural orbitals) that diagonalize the one-body density matrix

at the associated eigenvalues (called natural occupation numbers)  $\eta_a$ . The natural occupation numbers satisfy the general conditions [38]

$$0 \leq \eta_a \leq 1, \quad \sum_a \eta_a = A. \quad (29)$$

The  $A$ -representability problem has been solved for the one-body density matrix. It turns out that the ensemble  $A$  representability for fermions is ensured by the relations (29) [47], which are only a necessary condition for the  $A$ -representability of the OBDM in the case of pure fermion states. The first investigation of the  $A$ -representability problem with respect to the variational Jastrow correlation method (JCM) in LOA has been performed by Stoitsov *et al.* [17]. They showed that the  $A$ -representability condition (29) is violated in LOA of JCM leading to negative values (very small in absolute value) of some of the occupation numbers. Such values of  $\eta_a$  appear for the states with a given multipolarity  $l$  that lie just above the states belonging to the Fermi sea and have the same multipolarity. Stoitsov *et al.* suggested an approach to restore the  $A$  representability by omitting the negative values and then diagonalizing the remaining reduced OBDM [17]. The LOA  $A$ -representability violation has been also noted in Ref. [42]. The  $A$ -representability problem with respect to the variational JCM in FIY and FAHT (as well as in FIY\* and FAHT\*) is not investigated in the present work, e.g., it is not clear that the OBDM used in the present work, especially for FIY\* and FAHT\*, corresponds to an existing wave function. Calculations of the natural orbitals and the natural occupation numbers, with the imposed conditions concerning the violation of the  $A$  representability, are in progress. This analysis could be another comparison test of the three expansions examined in the present work.

#### IV. SUMMARY

In the present work, a systematic study of the effect of SRC on one-body properties of  $s$ - $p$  and  $s$ - $d$  shell nuclei has



been made evaluating three different cluster expansions. The HO parameter  $b$  and the SRC parameter  $\beta$  have been determined by a least-squares fit to the experimental charge FF.

The comparison of the three expansions in the example of the MD and the FF shows that they can be considered as equivalent expansions. It is found that, when the calculations are made with the best fit values of the parameters, these expansions reproduce the diffraction minima of the FF in the correct place and they give similar MD for all the nuclei we have considered. The inclusion of SRC increases considerably the high-momentum component of  $n(k)$ .

The FIY and FAHT expansions have been used for both closed and open shell nuclei while the occupation probabilities can be treated as free parameters together with the parameters  $b$  and  $\beta$  in the fitting procedure of the FF. In LOA, calculations for open shell nuclei are in progress.

In addition, the information entropy sum has been calculated according to the three methods compared in the present work. It was found almost in all of the numerous cases (different expansions and nuclei), that the larger the  $S$ , the smaller the  $\chi^2$ . That is maximal  $S$  could be used as a criterion for the quality of a given nuclear model. We found only two exceptions to this rule. In these two exceptions the difference of the  $\chi^2$  values is less than 1%.

Finally, attention was paid to the ‘‘healing’’ or ‘‘wound’’ integrals  $w_{ni}^2$  of the relative two-nucleon states. A convenient analytic expression of  $w_{ni}^2$  with correlation function (10) was derived for any relative state  $nl$ . Their values were computed in a number of states with that expression and were also discussed.

## APPENDIX A

In this appendix, we give some details about the FAHT expansion. We define the correlated wave function as

$$\Psi = \prod_{i < j}^A f(\mathbf{r}_i, \mathbf{r}_j) \Phi, \quad (\text{A1})$$

where  $f(\mathbf{r}_i, \mathbf{r}_j)$  is the Jastrow correlation function and  $\Phi$  is a Slater determinant wave function. To buildup the cluster expansion, we start, following Ref. [20], from the  $A$ -body integrals  $J_A(\lambda)$  defined as

$$J_A(\lambda) = \frac{1}{A(A-1)\cdots 1} \times \sum_{i_1 \dots i_A}^A \left\langle \phi_{i_1} \dots \phi_{i_A} \left| \prod_{i < j}^A f(\mathbf{r}_i, \mathbf{r}_j) \mathbf{O}_1(A) e^{\lambda \mathbf{O}_2(A)} \right. \right. \\ \left. \left. \times \prod_{i < j}^A f(\mathbf{r}'_i, \mathbf{r}'_j) \right| \phi'_{i_1} \dots \phi'_{i_A} \right\rangle_a, \quad (\text{A2})$$

where the sum over the states  $i_1, i_2, \dots, i_A$  has no restrictions and extends over all one-particle states and  $a$  stands for the antisymmetrization. The operators  $\mathbf{O}_1(A)$  and  $\mathbf{O}_2(A)$  have the forms

$$\mathbf{O}_1(A) = \prod_{i=1}^A \delta(\mathbf{r}_i - \mathbf{r}'_i), \\ \mathbf{O}_2(A) = \frac{1}{\prod_{i=1}^A \delta(\mathbf{r}_i - \mathbf{r}'_i)} \sum_{i=1}^A \delta(\mathbf{r}_i - \mathbf{r}) \delta(\mathbf{r}'_i - \mathbf{r}') \prod_{j \neq i}^A \delta(\mathbf{r}_j - \mathbf{r}'_j). \quad (\text{A3})$$

The OBDM  $\rho_{FAHT}(\mathbf{r}, \mathbf{r}')$ , normalized to  $A$ , is defined as

$$\rho_{FAHT}(\mathbf{r}, \mathbf{r}') = \left[ \frac{d \ln J_A(\lambda)}{d \lambda} \right]_{\lambda=0}. \quad (\text{A4})$$

We introduce the  $n$ -body integrals  $J_n(\lambda)$  defined as

$$J_n(\lambda) = \frac{1}{A(A-1)\cdots(A-n+1)} \times \sum_{i_1 \dots i_n}^A \left\langle \phi_{i_1} \dots \phi_{i_n} \left| \prod_{i < j}^n f(\mathbf{r}_i, \mathbf{r}_j) \mathbf{O}_1(n) e^{\lambda \mathbf{O}_2(n)} \right. \right. \\ \left. \left. \times \prod_{i < j}^n f(\mathbf{r}'_i, \mathbf{r}'_j) \right| \phi'_{i_1} \dots \phi'_{i_n} \right\rangle_a. \quad (\text{A5})$$

The cluster integrals  $\mathcal{J}_n (n=1, 2, \dots, A)$  are defined through the successive application of the equation

$$J_n = \prod_{k=1}^n \mathcal{J}_k^{(n)} = \mathcal{J}_1^{(n)} \mathcal{J}_2^{(n)} \dots \mathcal{J}_n^{(n)}, \quad n=1, 2, \dots, A. \quad (\text{A6})$$

For example, for  $n=1$  and  $n=2$  it gives

$$\mathcal{J}_1 = J_1, \quad \mathcal{J}_2 = \frac{J_2}{J_1^2}. \quad (\text{A7})$$

The last of Eqs. (A6), which corresponds to  $n=A$  is the quantity we are interested in

$$J_A = \prod_{n=1}^A \mathcal{J}_n^{(A)} \equiv \mathcal{J}_1^{(A)} \mathcal{J}_2^{(A)} \mathcal{J}_3^{(A)} \dots \mathcal{J}_A. \quad (\text{A8})$$

If the factor-cluster expansion is limited to the two-body term (assuming that the remaining cluster integrals are equal to unity [20]), then

$$J_A \approx \mathcal{J}_1^{(A)} \mathcal{J}_2^{(A)}. \quad (\text{A9})$$

From Eqs. (A4) and (A9) we have

$$\rho_{FAHT}(\mathbf{r}, \mathbf{r}') = \binom{A}{1} \left[ \frac{1}{J_1} \frac{dJ_1}{d\lambda} \right]_{\lambda=0} \\ + \binom{A}{2} \left[ \frac{1}{J_2} \frac{dJ_2}{d\lambda} - 2 \frac{1}{J_1} \frac{dJ_1}{d\lambda} \right]_{\lambda=0}, \quad (\text{A10})$$

where

$$J_1(\lambda) = \frac{1}{A} \sum_{i_1=1}^A \langle \phi_{i_1}(\mathbf{r}_1) | \mathbf{O}_1(1) e^{\lambda \mathbf{O}_2(1)} | \phi_{i_1}(\mathbf{r}'_1) \rangle, \quad (\text{A11})$$

and

$$J_2(\lambda) = \frac{1}{A(A-1)} \sum_{i_1, i_2}^A \langle \phi_{i_1}(\mathbf{r}_1) \phi_{i_2}(\mathbf{r}_2) | f(\mathbf{r}_1, \mathbf{r}_2) \times | \mathbf{O}_1(2) e^{\lambda \mathbf{O}_2(2)} f(\mathbf{r}'_1, \mathbf{r}'_2) | \times \phi_{i_1}(\mathbf{r}'_1) \phi_{i_2}(\mathbf{r}'_2) \rangle_a. \quad (\text{A12})$$

After some algebra we obtain

$$J_1(0) = 1,$$

$$J_2(0) = \frac{1}{A(A-1)} \left[ A(A-1) - \int [O_2(\mathbf{r}, \mathbf{r}, g_1) + O_2(\mathbf{r}, \mathbf{r}, g_2) - O_2(\mathbf{r}, \mathbf{r}, g_3)] d\mathbf{r} \right],$$

$$\left[ \frac{dJ_1}{d\lambda} \right]_{\lambda=0} = \frac{1}{A} \langle \mathbf{O}_{rr'} \rangle_1,$$

$$\left[ \frac{dJ_2}{d\lambda} \right]_{\lambda=0} = \frac{2}{A(A-1)} [(A-1) \langle \mathbf{O}_{rr'} \rangle_1 - O_2(\mathbf{r}, \mathbf{r}', g_1) - O_2(\mathbf{r}, \mathbf{r}', g_2) + O_2(\mathbf{r}, \mathbf{r}', g_3)], \quad (\text{A13})$$

where the terms  $\langle \mathbf{O}_{rr'} \rangle_1$  and  $O_2(\mathbf{r}, \mathbf{r}', g_i)$  have been defined in Sec. II.

Finally, the  $\rho_{FAHT}(\mathbf{r}, \mathbf{r}')$ , normalized to unity, becomes

$$\rho_{FAHT}(\mathbf{r}, \mathbf{r}') = \frac{1}{A} \langle \mathbf{O}_{rr'} \rangle_1 + (A-1) \left[ \frac{(A-1) \langle \mathbf{O}_{rr'} \rangle_1 - O_2(\mathbf{r}, \mathbf{r}', g_1) - O_2(\mathbf{r}, \mathbf{r}', g_2) + O_2(\mathbf{r}, \mathbf{r}', g_3)}{A(A-1) - \int [O_2(\mathbf{r}, \mathbf{r}, g_1) + O_2(\mathbf{r}, \mathbf{r}, g_2) - O_2(\mathbf{r}, \mathbf{r}, g_3)] d\mathbf{r}} - \frac{1}{A} \langle \mathbf{O}_{rr'} \rangle_1 \right]. \quad (\text{A14})$$

## APPENDIX B

The healing integral defined by Eq. (26) is written as follows [47]:

$$w_{nl}^2 = 2[1 + N_{nl}(I_{nl}(b, \beta) - 1)], \quad (\text{B1})$$

where

$$I_{nl}(b, \beta) = \int_0^\infty \exp[-\beta r^2] \phi_{nl}^2(r) dr, \quad (\text{B2})$$

and the normalization factor  $N_{nl}$  is given by Eq. (27). This factor can be easily expressed in terms of the integrals  $I_{nl}(b, \beta)$  and  $I_{nl}(b, 2\beta)$  by means of expression (10)

$$N_{nl} = [1 - 2I_{nl}(b, \beta) + I_{nl}(b, 2\beta)]^{-1/2}. \quad (\text{B3})$$

Thus, the analytical calculation of any healing integral  $w_{nl}^2$  is reduced to the calculation of two integrals of type (B2). The expression of  $I_{nl}(b, 2\beta)$  follows immediately from the expression of  $I_{nl}(b, \beta)$ .

We use the general expression of the radial HO wave function (normalized to one as  $\int_0^\infty \phi_{nl}^2 dr = 1$ ) in the form

$$\phi_{nl}(r) = \left( \frac{2n!}{\Gamma\left(n+l+\frac{3}{2}\right) b_r} \right)^{1/2} \times \left( \frac{r}{b_r} \right)^{l+1} L_n^{l+1/2} \left( \frac{r^2}{b_r^2} \right) \exp\left[ \frac{-r^2}{2b_r^2} \right], \quad (\text{B4})$$

where  $b_r$  is the HO parameter of the relative motion, which is related to the usual HO parameter  $b$  by  $b_r = \sqrt{2}b$  [ $b = (\hbar/m\omega)^{1/2}$ ].

Substituting expression (B4) into Eq. (B2) and using the transformation  $r^2/b_r^2 = \xi$ ,  $I_{nl}$  is written as

$$I_{nl}(b, \beta) = \frac{n!}{\Gamma[n+l+3/2]} \int_0^\infty e^{-(1+y)\xi} \xi^{l+1/2} [L_n^{l+1/2}(\xi)]^2 d\xi, \quad (\text{B5})$$

where  $y = \beta b_r^2 = 2\beta b^2$ .

Using formula (13) of § 7.414 of Ref. [48]  $I_{nl}$  takes the form

$$I_{nl}(b, \beta) = (y-1)^n (y+1)^{-n-l-3/2} P_n^{[l+1/2, 0]} \left( \frac{y^2+1}{y^2-1} \right), \quad (\text{B6})$$

where  $P_n^{(a_1, a_2)}(z)$  are the Jacobi polynomials. These may be easily expressed in terms of the hypergeometric function

(see, e.g., § 8.962 of Ref. [48]). In the case of the nodeless states [because  $P_0^{(a_1, a_2)}(z) = 1$ ]  $I_{nl}$  takes the simple form

$$I_{0l}(b, \beta) = (y + 1)^{-l - 3/2}. \quad (\text{B7})$$

By substituting  $\beta \rightarrow 2\beta$ , the expression of  $I_{nl}(b, 2\beta)$  fol-

lows immediately and therefore the analytic expression of the  $w_{nl}^2$  by means of the formulas (B1) and (B6). It is thus clear that the healing integral  $w_{nl}^2$  for any state depends on the correlation parameter  $\beta$  and the HO one, only through the product  $y = 2\beta b^2$ . The expressions of  $w_{nl}^2$  for the lower  $n$  states follow also very easily.

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