

# Quartetizing and pairing effect on pair localization in nuclei

R.-D. Lasserri,<sup>1</sup> J.-P. Ebran,<sup>2</sup> E. Khan,<sup>1</sup> N. Sandulescu,<sup>3</sup> and D. Vretenar<sup>4</sup>

<sup>1</sup>*Institut de Physique Nucléaire, Université Paris-Sud, IN2P3-CNRS, F-91406 Orsay Cedex, France*

<sup>2</sup>*CEA, DAM, DIF, F-91297 Arpajon, France*

<sup>3</sup>*National Institute of Physics and Nuclear Engineering,  
P.O. Box MG-6, Magurele, Bucharest, Romania*

<sup>4</sup>*Physics Department, Faculty of Science, University of Zagreb, 10000 Zagreb, Croatia*

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Correlations play a major part for nuclear structure.

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## I. INTRODUCTION

The correct description of a fermionic system in interaction shall take into account quantum and classical correlations. Nuclear system makes no exception and the impact of two-body correlations, namely pairing, have shown all its importance since Bohr Mottelson and Pines [1]. To describe this phenomenon several theoretical techniques have been developed from the Bardeen Cooper and Schrieffer ansatz [2], to the more advanced Bogoliubov transformations [3]. The physical principle is to explicitly allow two fermions to form a quasi-bosonic pair. These fermions are correlated in momentum space. For example for spin- $\frac{1}{2}$  particles the usual BCS ansatz may be written as.

$$|\Psi_0\rangle = \prod_k (u_k + v_k a_{k,\uparrow}^\dagger a_{-k,\downarrow}^\dagger) |0\rangle \quad (1)$$

Where  $a^\dagger, u_k, v_k$  are respectively the single-particle creation operator, and variational parameter which satisfy the unitary relation  $u_k^2 + v_k^2 = 1$ . This equation translate the fact that a Cooper pair is composed of two fermions of opposite spin and of opposite momenta.

However one can also describe the ground-state including more general, 4-body correlations, which has been already done long ago [5]. Usually the exact treatment of these kinds of correlations is very heavy and almost impossible for realistic interactions. However one can also include the 4-body correlations effects using a very specific ansatz which can be computed in a more convenient way [6]. Nevertheless neither the pairing nor the quartetizing treatment It is necessary to develop others methods which will give direct information on the spatial properties of the pairs. Several studies have been conducted on this purpose in infinite matter [7] and the nuclei [8] in the pairing case. In the quartetizing, spatial studies have also been performed [9] but a systematic analysis of the spatial properties of the pair is an important challenge to get a deeper understanding of the correlated substructures on the nucleus such as clusters [10] or neutron-proton dimers which may have important experimental consequences [11]. Those elements motivate a systematic study of those spatial properties of the pairs. The

following work will use relativistic functional described in ref [12] in an axially symmetric model. In section II we will recall the theoretical foundations of the relativistic mean-field theory, then in section III we will focus on the treatment of 2 and 4 body correlations within the relativistic framework. In section IV we will introduce the necessary tools to study the spatial properties of the pairs in order to present our results and to conclude in section V and VI.

## II. RELATIVISTIC MEAN FIELD

The framework of this study is the one of relativistic energy functional density, describing the nucleus in terms of nucleons considered as pointlike Dirac particles, while the interaction between them is described in term of mesons exchange. The associated phenomenological Lagrangian density is:

$$\mathcal{L} = \bar{\psi} [i\gamma^\mu \partial_\mu - M - g_\sigma \sigma - g_\omega \gamma_\mu \omega^\mu - g_\rho \gamma_\mu \vec{\rho} \cdot \vec{\tau}^\mu - g_\pi \gamma_5 \gamma_\mu \partial^\mu \vec{\pi} \cdot \vec{\tau} - e\gamma_\mu A^\mu \left( \frac{1 - \tau_3}{2} \right)] \psi + \mathcal{L}_k \quad (2)$$

Where  $\mathcal{L}_k$  being the kinetic part of this Lagrangian. The arrows symbolize vectors of the Isospin SU(2) space.  $\psi$  is a Dirac 4-spinor describing a nucleon of mass  $M$ . In Eq (2) the nucleons interacts by the exchange of  $\{\sigma, \rho, \omega$  and  $\pi\}$  mesons. As described in [?] the Dirac equation for a single nucleon can be obtained by variation of (2) with respect of  $\psi$ .

$$[i\gamma_\mu \partial^\mu - M - \Sigma] \psi(x) = 0 \quad (3)$$

where  $\Sigma$  represent the nucleon self-energy. Performing a Legendre transform of (2) yields the Hamiltonian of the problem

$$\mathcal{H} = \int d^3x \bar{\psi} [i\nabla + M] + \frac{1}{2} \int d^3x \bar{\psi} [g_\sigma \sigma + g_\omega \gamma_\mu \omega^\mu + g_\rho \gamma_\mu \vec{\rho} \cdot \vec{\tau}^\mu + g_\pi \gamma_5 \gamma_\mu \partial^\mu \vec{\pi} \cdot \vec{\tau} + e\gamma_\mu A^\mu \left( \frac{1 - \tau_3}{2} \right)] \psi \quad (4)$$

The nucleonic spinors on a one-body basis  $\{c_i, c_i^\dagger\}$  in interaction representation:

$$\psi(x) = \sum_i (f_i(x) e^{-i\epsilon_i t} c_i) \quad (5)$$

$$\psi^\dagger(x) = \sum_i (\bar{f}_i(x) e^{i\epsilon_i t} c_i^\dagger) \quad (6)$$

Where the  $\epsilon_i$  is the energy of the  $i$ -th state. In this basis the Hamiltonian (4) take the form

$$\begin{aligned} \mathcal{H} = & \sum_{i,j} c_i^\dagger c_j \int d^3x \bar{f}_i[-i\gamma \cdot \nabla + M] f_j \\ & + \frac{1}{2} \sum_{i,j,k,l} c_i^\dagger c_j^\dagger c_k c_l \sum_{m \in \{\sigma, \rho, \omega, \pi, A\}} \int d^3x \int d^3y \bar{f}_i(x) \bar{f}_j(y) \Gamma_m(x, y) \mathcal{D}_m(x, y) f_k(x) f_l(y) \end{aligned} \quad (7)$$

where  $\mathcal{D}_m(x, y)$  is the propagator for the  $m$ -th boson and  $\Gamma_m(x, y)$  is the dressed nucleon-meson interaction vertex. Here the ground state  $\Phi_0$  can be approximated by a Slater determinant.

$$|\Phi_0\rangle = \prod_i c_i^\dagger |0\rangle \quad (8)$$

Where  $|0\rangle$  is the single-particle vacuum. The relativistic energy density is now obtained by taking the mean value of (4) on

$$\mathcal{E}[\rho_b] = \langle \Phi | \mathcal{H} | \Phi \rangle \quad (9)$$

Where  $\rho_b$  is the baryonic density of the system defined as the 1-body operator  $\rho_b = \sum_{i,j} \langle \Phi_0 | c_j^\dagger c_i | \Phi_0 \rangle$ . Expression (9) explicitly contains direct (Hartree) and exchange (Fock) terms. In the present case using the Hartree approximation by neglecting the exchange terms. The minimization of the functional (9) leads to the Relativistic Hartree (RH) equations, solved in a self-consistent way in an axially deformed harmonical oscillator basis.

### III. CORRELATIONS TREATMENT

#### A. Two-body correlations

To include the effect of pairing correlations we use a finite-range interaction [13] which mimic a Gogny pairing, can be written in coordinate space:

$$V(\vec{r}_1, \vec{r}_2, \vec{r}'_1, \vec{r}'_2) = -g\delta(\vec{R} - \vec{R}')G(r)G(r')\frac{1}{2}(1 - P^\sigma) \quad (10)$$

Where  $G(r)$  are gaussian functions that reflect the finite range of the interaction,  $\vec{R}$  and  $\vec{r}$  are respectively the center-of-mass and relative coordinates. The operator

$(1 - P^\sigma)$  projects on the  $^1S_0$  channel while the  $\delta$  insures the translational invariance of this expression, while  $g$  is the coupling constant of the interaction. All the calculations are performed in an axially-deformed oscillator basis this interaction is separable which allows an accurate and a fast numerical treatment. Following the usual textbook approach we have used the usual Bogoliubov transform to take into account two-body correlations in the ground-state wavefunction, which can be written using quasi-particles operators  $\beta_k$

$$|\Phi\rangle = \prod_k \beta_k |0\rangle \quad (11)$$

Which in the single-particle basis can be expanded

$$|\Phi\rangle = \prod_k \left( \sum_\alpha U_{\alpha k}^* a_\alpha + V_{\alpha k}^* a_\alpha^\dagger \right) |0\rangle \quad (12)$$

Where  $\{a_\alpha, a_\alpha^\dagger\}$  are the single-particle ladders operators. The important point in (11) is that we explicitly allow pair formation which cause  $U(1)$  symmetry breaking translated by the fact that

$$\hat{N} |\phi\rangle \neq N |\phi\rangle \quad (13)$$

Where  $\hat{N} = a^\dagger a$  is the usual particle-number operator. Then using the ansatz (12) one can solve the Relativistic-Hartree-Bogoliubov (RHB) equations. To solve this equations a self-coherent mean field algorithm have been adapted from [4] to include pairing and quarteting effects.

#### B. Four-body correlations

##### 1. Quartet wavefunction

A first way to treat 4-body correlations is to construct a new ansatz including this possibility, thus a generalisation of a BCS ground state will take the form:

$$|\Psi_0\rangle = \prod_{k,k'} (u_{kk'} + v_{kk'} a_{k,\uparrow}^\dagger a_{-k,\downarrow}^\dagger a_{k',\uparrow}^\dagger a_{-k',\downarrow}^\dagger) |0\rangle \quad (14)$$

The quarteting model [6] is a convenient way to take into account an import part of the 4-body correlations. The principle is to split the spectra of the considered nucleus in two sets, an inert core including the of lower energy levels and above them, a valence space on which calculations will be performed. But it should be noted that all the states are calculated from a microscopic RH approach. The key point is that the valence space shall be described by a quartet wavefunction  $|\Xi\rangle$ . Defining a pair creation operator

$$P_{i,\tau}^\dagger = a_i^\dagger a_{\bar{i}}^\dagger \quad (15)$$

as usual the  $a_i^\dagger$  create a nucleon on a state  $i$  and  $\bar{i}$  denote the time reversed state and  $\tau$  label the total isospin projection value. From (15) one can construct a collective-pair creation operator.

$$\Gamma_\tau^\dagger = \sum_i x_i P_{i\tau}^\dagger \quad (16)$$

where  $x_i$  is a variational mixing parameter. Adopting two simplifying assumptions[14] i) Isospin symmetry ii) Isovector coupling outweigh isoscalar. These assumptions allow to write the valence wavefunction using (16) as:

$$|\Xi\rangle = (2\Gamma_1^\dagger \Gamma_{-1}^\dagger - \Gamma_0^{\dagger 2})^{n_q} |0\rangle \quad (17)$$

Where  $n_q$  is the number of quartet considered. Equation (17) describes a coherent superposition of collective  $\{nn, pp, np\}$  pairs with a total angular momentum  $J=0$  (This is valid only for a rotationally invariant basis) and a total isospin  $T=0$ . It should be noted that, in opposite to (12), the wavefunction (17) conserves exactly the particle number. The vector state describing the nucleus is

$$|\Psi_{tot}\rangle = |\Psi_{core}\rangle \otimes |\Xi\rangle \quad (18)$$

As in section III A Using (18) to expand (9):

$$\mathcal{E}[\rho_b] = \langle \Psi_{tot} | \mathcal{H} | \Psi_{tot} \rangle = \underbrace{\langle \Psi_{core} | \mathcal{H} | \Psi_{core} \rangle}_{\text{Mean Field}} + \underbrace{\langle \Xi | \mathcal{H} | \Xi \rangle}_{\text{Quartet term}} \quad (19)$$

Thus the minimization of (19) provides the Relativistic Hartree Quarteting (RHQ) equations. Both RHB and RHQ equations have been solved in a fully self-consistent way, meaning that the quartet wavefunction is computed at each mean field iteration until convergence.

## 2. Numerical implementation

To numerically solve the RHQ equations in a reasonable time (less than an hour on a laptop CPU) the valence space  $|\zeta\rangle$  is limited to a finite number of state. The spectrum is then separated into the nearest doubly-magic core and a finite number of state up to the cut-off  $\Lambda$ , in fact the numbers of active states in the valence space above the inert RMF core. The quarteting interaction coupling constant is fitted to the  $N=Z$  binding energies, then for each nuclei the  $\Lambda$  parameter is fine-tuned to reproduce accurately the binding energy. It is important to note that here because of the fact that the only cases to be considered are the  $N=Z$  nuclei, the active valence space considered is symmetric under isospin conjugation.

Nucleus	Core	$\Lambda$ (levels above the core)
$^{20}\text{Ne}$	$^{16}\text{O}$	10
$^{24}\text{Mg}$	$^{16}\text{O}$	14
$^{44}\text{Ti}$	$^{40}\text{Ca}$	12
$^{64}\text{Ge}$	$^{56}\text{Ni}$	10

TABLE I: Parameter used to solve the RHQ equations

## IV. SPATIAL PROPERTIES

### A. Pair Wavefunction

In order to keep the explicit covariance of our theory one shall define the pair wavefunction in the most general way. An usual prescription is (@JP: Ref cond.matt ajouter)

$$\psi_{pair}(\vec{r}_1, \vec{r}_2) = \langle \vec{r}_1, \vec{r}_2 | \hat{\rho}_{pair} \rangle = \sum_{i,j} \bar{\psi}_i^{\tau_i}(\vec{r}_1) \gamma^5 \psi_j^{\tau_j}(\vec{r}_2) \quad (20)$$

where the  $\psi_i^\tau$  is a Dirac 4-Spinor, describing a nucleon at a level  $i$ , of isospin  $\tau$  represented in configuration space.

$$\psi_i^\tau(\vec{r}) = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} f_i^+(\vec{r}) \\ f_i^-(\vec{r}) \\ ig_i^+(\vec{r}) \\ ig_i^-(\vec{r}) \end{pmatrix} \quad (21)$$

$\psi_i^\tau$  is obtained via the time-reversal operation

$$\psi_i^\tau = T\psi_i \quad (22)$$

which for a relativistic model, may be written not only as a spin reversal operator, but in term of the charge conjugation and the generalized Pauli matrix:

$$T = i\Sigma\mathcal{K} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \mathcal{K} \quad (23)$$

where  $\mathcal{K}$  is the complex conjugate operator.

Thus (20) can be expressed directly as a combination of the components of (21).

$$\begin{aligned} \psi_{pair}(\vec{r}_1, \vec{r}_2) = \sum_{(i,j) \in \mathcal{V}} x_i x_j [ & f_i^-(\vec{r}_1) \cdot g_j^+(\vec{r}_2) \\ & - f_i^+(\vec{r}_1) \cdot g_j^-(\vec{r}_2) + g_i^-(\vec{r}_1) \cdot f_j^+(\vec{r}_2) - g_i^+(\vec{r}_1) \cdot f_j^-(\vec{r}_2) ] \end{aligned} \quad (24)$$

With  $\mathcal{V}$  being the valence space. The wavefunction define at equation (20) can be computed after convergence of RHB or RHQ code. This wavefunction will be analysed for the 3 possibles types of pair  $\{nn, pp, np\}$ . In the RHQ case for each quartet a pair density is defined which is a superposition of all possible pair of the same type. This allows a comparison with the pair generated within the Bogoliubov formalism and the one generated by the quarteting model. From this expression one can easily derive an important parameter, the average size of a pair.

$$\langle \xi \rangle = \sqrt{\frac{\int |\vec{r}_2 - \vec{r}_1|^2 \cdot |\psi_{pair}(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2}{\int |\psi_{pair}(\vec{r}_1, \vec{r}_2)|^2 d\vec{r}_1 d\vec{r}_2}} \quad (25)$$

$\langle \xi \rangle$  is the coherence length used to describe Cooper pair [15], up to a normalization factor.

## B. Coordinates choice

The pair wavefunction in  $\{\vec{r}_1, \vec{r}_2\}$  space has been derived in section IV A. This wavefunction is a function of the individual position of the nucleons composing of the pair. However to analyse the structure this set of coordinates is not the most adapted. One shall rather use the relative and center-of-mass coordinates to describe the pair.

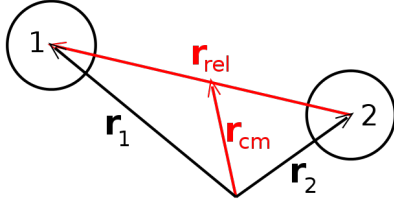


FIG. 1: Definition of the center-of-mass and relative coordinates

As mentioned earlier we expanded the wavefunction on a deformed oscillator basis. To get the expression of this function in the new coordinate system we use Talmi-Moshinsky transformations [16].

Each state is labeled by three quantum numbers (two for the radial dependence, one for the axial), namely,  $\{n_{r\perp}, m_{r\perp}, n_z\}$

Thus the product of two harmonical oscillator wavefunctions can be written in  $\{\vec{r}_1, \vec{r}_2\}$  using the relation:

$$\phi(\vec{r}_{cm}) \cdot \phi(\vec{r}_{rel}) = \sum_{n_1, n_2}^{\infty} \mathcal{M}_{(n_1, m_1)}^{(n_{cm}, m_{cm})(n_{rel}, m_{rel})} \phi_{n_1, m_1}(\vec{r}_1) \phi_{n_2, m_2}(\vec{r}_2) \quad (26)$$

where  $\{\vec{r}_1, \vec{r}_2\}$  and  $\{\vec{r}_{cm}, \vec{r}_{rel}\}$  are respectively the intrinsic and center-of-frame coordinates defined on Fig.1,  $\phi_{n,m}$  is a deformed oscillator wavefunction labelled by the  $\{n, m\}$  quantum numbers. The recurrence relations used to compute the Talmi-Moshinsky Bracket can be found in appendix. Once this transformation achieved one can analyse the properties of the so-defined pair wavefunction in coordinate space.

## V. RESULTS

### A. Impact on the structure

The impact of pairing and quarteting correlations on nuclear structure is important already at a one-body operator level; the density. Fig2 displays the quadrupole deformation map for both cases.

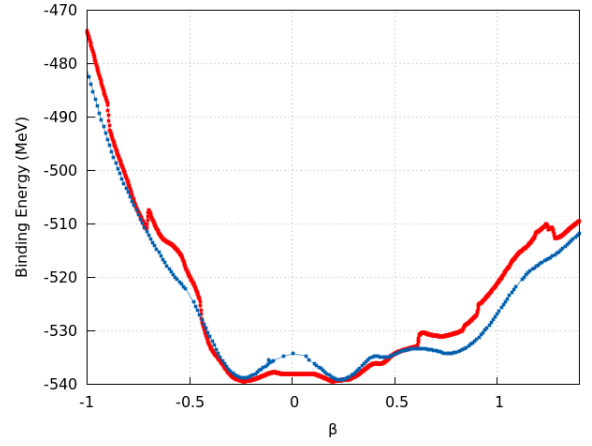


FIG. 2: Quadrupolar deformation map for  $^{64}\text{Ge}$  for pairing (blue) and quarteting (red). The inserts represents the density in the Nucleus reference frame

It is remarkable that for both pairing and quarteting the values of the quadrupole moment which minimize the binding energy are the same, while in average the quartet case is more bound than the pairing case. (@E/JP: Commentaire sur le fait que a "stabilise" les configurations dformes ?)

### B. Size of the pairs

#### 1. Averaged value

To quantify the difference between Bogoliubov and quarteting correlations, a first variable of interest is the size-of-pair defined by (25). The calculation for an identical deformation and a constant correlation energy in order to be sensitive only to the differences between the models is performed. Table II displays  $\langle \xi \rangle$  in the Bogoliubov and quartet case:

Nucleus	$\beta_2$	$E_{corr}$ (MeV)	$\langle \xi_{bogo} \rangle$ (fm)	$\langle \xi_{quart} \rangle$ (fm)
$^{20}\text{Ne}$	0.25	7.53	10.5	12.3
$^{44}\text{Ti}$	0.00	5.21	17.6	13.2
$^{64}\text{Ge}$	0.23	6.61	21.2	14.5

TABLE II: Pair size in fm

However, one can see that there is not a systematic difference between the models while studying only this variable for different nuclei. This is related to the fact that we are computing an averaged value which don't allow us to gather all the physical information contained in (24). We shall then go a step further and use (26) to study the 2-body operators in an adapted reference frame, using center-of-mass coordinates. Performing the corresponding transformation yields (20) in the center of mass reference frame. Which allows to compare the pair

size at each point of the nucleus using either Bogoliubov model or the quarteting model Fig.3 to show the corresponding results for the  $^{64}\text{Ge}$ , which have a non-vanishing pairing energy ( $E_{\text{pair}} \simeq 5.6$  MeV) in the ground-state, this is the first time in this framework that this computation is done. One shall be really clear about the physics lying beyond 3 which represent along the symmetry axis of the nucleus the relative distance between two nucleons correlated in momentum. This does not give information about the exact localization of the pair, but instead state give, for a fixed position on this axis, the distance between the two paired nucleons. Hence one can see that for the ground-state of  $^{64}\text{Ge}$  the pair embedded within a quartet are smaller than the usual Bogoliubov pair.

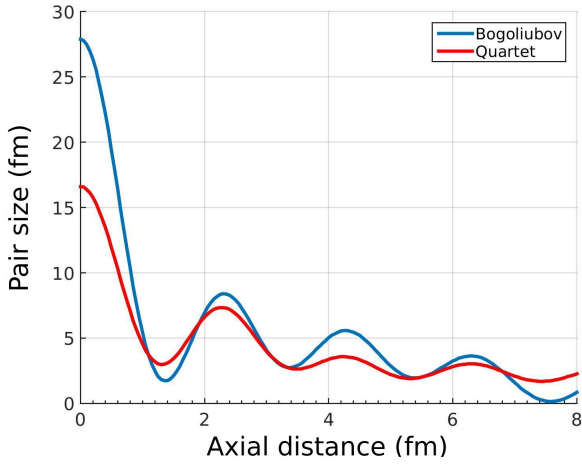


FIG. 3: Size of the pair in the  $^{64}\text{Ge}$  ground-state for Bogoliubov and Quarteting model

## 2. Spatial repartition

Fig.6 display on the left side, the ground-state density of  $^{20}\text{Ne}$ ,  $^{40}\text{Ca}$  and  $^{64}\text{Ge}$  while on the right side is shown in the same basis the pair size as a function of the position of the considered pair. At the surface of the nuclei the size of the correlated pair is very small while at the center of the nucleus the size between the nucleons constituting the pair is maximal in agreement with [8]. For  $^{20}\text{Ne}$  the pair distance is significantly decreasing at the position of the clusters. These result generalize the current understanding of pair localisation in nuclei, showing that the finite size constrain, because of the Pauli principle, the pairs to be localized at the surface, but show also that at the positions of clusters the pairs are also localised. (@El/JP: Je retravaille ce paragraphe)

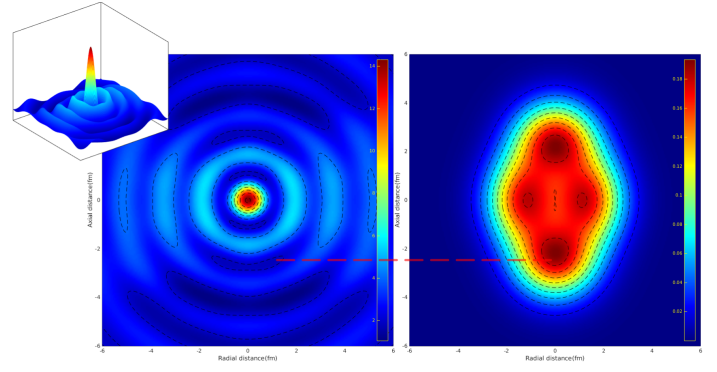


FIG. 4: (Left) Pair size in  $\text{fm}$  (Right)  $^{20}\text{Ne}$  Density in  $\text{fm}^{-3}$ . Dashed red line indicate the position of a cluster.

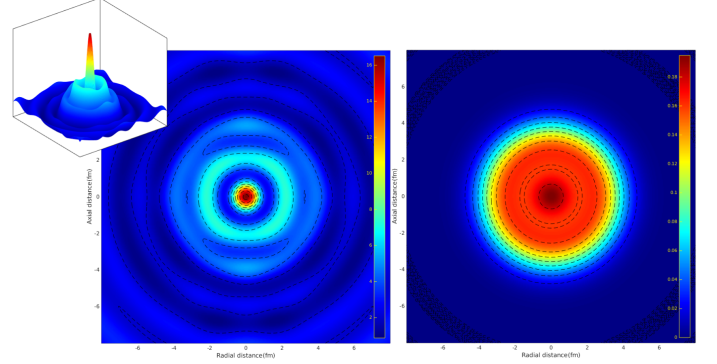


FIG. 5: (Left) Pair size in  $\text{fm}$  (Right)  $^{40}\text{Ca}$  Density in  $\text{fm}^{-3}$

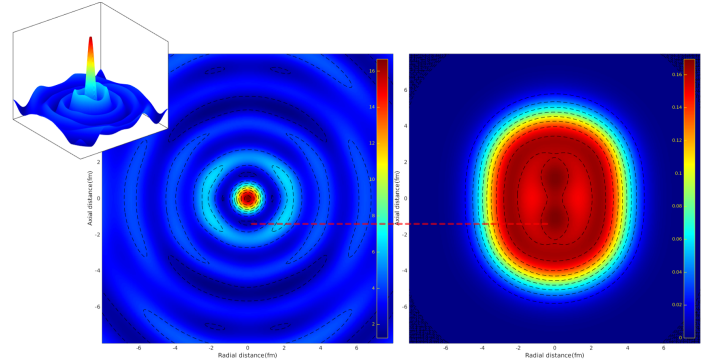


FIG. 6: (Left) Pair size in  $\text{fm}$  (Right)  $^{64}\text{Ge}$  Density in  $\text{fm}^{-3}$ . Dashed red line indicate the position of a cluster.

## VI. CONCLUSIONS

In this work we propose the first treatment of quartets correlations within the framework of relativistic mean-field theory. Four-body-like correlations have a direct incidence on one-body operators such as the baryonic density. This impact is quantitatively different from the usual effect of pairing correlations treated within the Hartree-Bogoliubov formalism even at the density level. The quarteting approach displays several advantages with respect to the Bogoliubov one. First of all

this quarteting model allows momentum correlations of a system of 4-nucleons, this is suited to the study of the apparition of  $\alpha$ -like clusters. Moreover by preserving  $U(1)$  gauge symmetry this model conserves the exact particle number. The drawbacks are mostly of numerical origin. The choice of the core and the cutoff, even if optimized, introduces two new parameters to the model, but progress on the implementation can be expected to allow no-core calculations at least for light nuclei. The Talmi-Moshinsky transformations used to study the two-body operators allowed us to have a direct insight on the spatial structure of the correlated pairs. This systematic study of the differences between pairing and quarteting models have shown another deep difference of the two approaches. While Bogoliubov theory predicts very-delocalised pairs as shown in Fig.3 the quartet model predicts for most of the nuclei smaller inter-nucleonic distance within the correlated structures. This statement explains that for systems which present important pairing the global structures tends to get homogenized while this trend is less apparent while considering quartets correlations. As it has been shown in previous sections where a nuclei present clusterised structures, the

correlated nucleons at the position of the clusters are localized. This leads to an interesting remark, are the nucleons contributing to cluster formation, spatially localized within the so-formed cluster ? This study tends to indicate that this is indeed the case, however to get a complete answer one have to study the 4-body wavefunctions constructed by generalizing (20). This so-defined wavefunction will contain all the information to study quartet localization and would then be comparable to other well-known clusters model as THSR [17] model. This work can also be one of the starting point to give a microscopic justification to algebraic model of the nuclei.

## Appendix A: Talmi-Moshinsky coefficients

Imposing axial symmetry we may write any variable as

$$\psi(\vec{r}) = \psi(\vec{r}_\perp) \cdot \psi(z) \quad (A1)$$

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