Alpha-particle condensation: a nuclear quantum phase transition

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When the density of a nuclear system is decreased, homogeneous states undergo the so-called Mott transition towards clusterised states, e.g. alpha clustering, both in nuclei and in nuclear matter. Here we investigate such a quantum phase transition (QPT) by using microscopic energy density functional (EDF) calculations both with the relativistic and the Gogny approaches on the diluted 16O nucleus. The evolution of the corresponding single-particle spectrum under dilution is studied, and a Mott-like transition is predicted at about 1/3 of the saturation density. Complementary approaches are used in order to understand this QPT. A study of spatial localisation properties as a function of the density allows to derive a value of the Mott density in agreement with the one obtained by fully microscopic calculations in 16O and in nuclear matter. Moreover a study of the spontaneous symmetry breaking of the rotational group in 16O, down to the discrete tetrahedral one, provides further insight on the features displayed by the single-particle spectrum obtained within the EDF approach. The content of the tetrahedrally deformed A-nucleon product state in terms of spherical particle-hole configurations is investigated. Finally a study of quartet condensation and the corresponding macroscopic QPT is undertaken in infinite matter.

I. INTRODUCTION

Fermi systems are the host of various phenomena yet to be fully explored. One of the most recent exciting features which has been revealed is the exotic arrangements stabilized by the existence of internal degrees of freedom in N-component Fermi systems with N > 2 [1–4]. Molecular configurations made of bound states of N fermions enrich the celebrated crossover [5] between a Baarden, Cooper and Schrieffer (BCS) superfluid phase to the Bose-Einstein condensation (BEC) of bosonic bound states of two fermions that characterizes 2-component Fermi gases with an attractive s-wave interaction. Nucleons being assigned to spin and isospin SU(2) doublets, atomic nuclei fall in the category of 4-component self-bound Fermi systems. Attractive s-wave interactions in the singlet-even (S = 0, T = 1) and the triplet-even (S = 1, T = 0) channels — S and T stand respectively for the total spin and isospin momenta of the two-nucleon system, with almost similar strength gives rise to various types of superfluid behavior. In the weak coupling regime, the dominant superfluid instability manifests itself through the establishment of a BCS quasi-long range order and involves proton-proton, neutron-neutron or proton-neutron (depending on the matching of neutron and proton Fermi levels) Cooper pairs [6, 7]. Moving towards the strong coupling regime, calculations in infinite symmetric nuclear matter [8] suggested that the dominant superfluid order is not a BEC phase of bosonic dimers (deuterons), but rather a condensation phase of quartets — 4-fermion molecular objects with zero total spin and isospin. Infinite nuclear matter hence undergoes for decreasing densities a phase transition to alpha-particle condensation [8–10]. That is nuclear matter lowers its energy by taking advantage of the nuclear cohesion, i.e. by forming localized clusters that recover saturation density (ρ0 ∼ 0.16 fm−3), rather than remaining in a dilute homogeneous phase. Since this happens at zero temperature, it can be qualified as a Quantum Phase Transition (QPT) where the density is the control parameter.

How such features translate in finite nuclei triggered several research works, see e.g. [11–15]. Unlike homogeneous systems, finite nuclei display large fluctuations of their mass density around the equilibrium value ρ0 either in the ground state of heavy nuclei, where the density near the surface gets shallower, or in excited states. In these local low-density regions, a QPT from a dilute homogeneous phase to a clusterized one is expected to occur, causing a preformation of alphas at the surface of heavy nuclei [16, 17] and endowing the spectroscopy of relatively light nuclei with clusterized excitation modes [18–21]. For instance the famous Hoyle state, important for 12C production in the Universe, could be interpreted as a three-alpha gas state where the alphas occupy with their center of mass (c.o.m.) motion to 70–80 percent the lowest OS wave function while all other states have an occupation probability more than by a factor ten down, see, e.g., [22]. In that sense, the Hoyle state could be qualified as a finite-size alpha-particle condensate. However EDF and geometrical approaches end up with alpha-clusters in a much more robust configuration [23–25], see also [26] for a recent experimental
investigation of this issue and [27] for a discussion of alpha-cluster structures as a manifestation of supersolidity. It should be noted that the action of the Pauli principle is quite similar in both cases (gas or molecular states) so converging results shall be reached from both approaches. Beyond these interpretations, the size of the Hoyle state is extended to 3-4 the volume of the $^{12}$C ground state [28, 29], showing that Hoyle and ground states live in two completely different phases, one dilute, the other dense.

In this work, we want to further substantiate the QPT scenario of alpha-clustering for the case of $^{16}$O through complementary perspectives. Section II first describes how relevant dimensionless quantities such as the localisation and the Brueckner parameters help characterizing the transition from a homogeneous nuclear system towards a localized one. A microscopic analysis based on the energy density functional (EDF) approach is given in section III, where both covariant and Gogny functionals are used. Constrained Hartree-Fock-Bogoliubov (HFB) calculations for $^{16}$O are performed, the constraint being on the radius of $^{16}$O while the system is imposed to stay globally spherical. That is $^{16}$O can break up into clusters while the system still stays spherical on average. The single-particle properties are then addressed in the light of group theory and molecular orbitals. Finally section IV provides an analysis of the occurrence of alpha-condensation in nuclear matter through the explicit treatment of four-nucleon correlations.

II. LOCALISATION AND QUANTUM PHASE TRANSITION IN NUCLEAR SYSTEMS

In contrast with ultra-cold atom physics, it is not possible to directly tweak the effective strength of the interaction between nucleons, for nuclei being self-bound systems. On the other hand, as we shall see below, nucleon density is one of the control parameters driving nuclei from the weak to strong coupling regimes. The nuclear saturation density $\rho_{\text{sat}} \sim 0.16 \text{fm}^{-3}$ is an emergent property [30] setting the characteristic energetic and spatial scales in nuclear systems. Finite nuclei display large fluctuations around $\rho_{\text{sat}}$, such that nucleons evolving in the low-density parts of finite nuclei enter a strong coupling regime and can hence self-arrange into alpha-clusters.

The analysis of fundamental dimensionless parameters sheds light on how nuclear density drives the coupling regime of its constituents. Indeed, the essential features of nuclear systems are grasped by dimensionless parameters defined in terms of the characteristic energy and length scales of the problem. For instance, the quantum mechanical nature of nuclear systems over a wide range of densities can be justified by expressing a first dimensionless parameter — the localisation parameter $\alpha_{\text{loc}} \simeq \lambda^2$ [31, 32] (with $\lambda$ the typical spatial extension of nucleons and $\bar{r}$ their mean interparticle-distance) in terms of the nuclear density. A value smaller or larger than 1 allows to discuss about localised or delocalized states in quantal systems, whereas the $\alpha_{\text{loc}} \ll 1$ limit corresponds to a classical system. In the zero-temperature case and owing to the fact that nucleons are bound in a nucleus, $\lambda$ is well approximated by the confining length of an harmonic oscillator (HO) potential which parameters are chosen to match the radius $R$ of a given nucleus. We then have in $\hbar = c = 1$ units

$$\lambda \simeq \sqrt{\frac{1}{m\omega}} = \frac{\sqrt{R}}{(2mV_0)^{\frac{1}{4}}},$$

with $\omega$ the typical energy of the HO, $m$ the nucleon mass and $V_0$ the depth of the confining potential. In order to study the behavior of the localisation parameter with the density of the system, and not only at saturation density, let us express the mean-interparticle distance as $\bar{r} = \left(\frac{3}{4\pi\rho}\right)^{\frac{1}{3}}$. One gets in terms of the average density $\rho$

$$\alpha_{\text{loc}} \sim \frac{(A\rho)^{\frac{1}{4}}}{(mV_0)^{\frac{1}{4}}},$$

where $A$ is the number of constituents of the system. Larger densities or a shallower confining potential hence drives the system towards the quantal regime. At saturation density, one typically obtains values of $\alpha_{\text{loc}}$ between $0.8$ and $1.5$ while at one tenth of the saturation density, a factor $0.7$ arises showing that nuclear systems remain quantal over a large range of densities.

It should be noted that behaving quantum-mechanically, the effective strength of nucleons interaction, i.e. the extent to which interactions impact the properties of nuclei and make the latter deviates from the ideal free case, is sometimes measured by another dimensionless ratio between the mean potential $\langle V \rangle$ and the mean quantal kinetic $\langle K \rangle$ energies, or equivalently the ratio between the mean interparticle distance $\bar{r}$ and the generalized Bohr radius $a_B$. This is the so-called Brueckner (also known as the Wigner) parameter (see e.g. [33]) $r_s = \frac{\langle V \rangle}{\langle K \rangle} \sim \frac{\bar{r}}{a_B}$. In the nuclear case, we have

$$r_s = \frac{\omega}{E_F},$$

where the energy of the harmonic oscillator reads $\omega = \frac{m\omega}{\pi} \sqrt{\frac{2}{m}}$ and $E_F = \frac{1}{2m} \left(\frac{\omega^2 \bar{r}^2}{2}\right)^{\frac{1}{2}}$ stands for the Fermi energy. One gets from Eqs. (2) and (3):

$$r_s \sim \alpha_{\text{loc}}^{-2},$$

showing that the localisation parameter captures the relevant effects. Three quantities govern these dimensionless parameters: i) the number of nucleons $A$, ii) the depth of the confining potential $V_0$ and iii) the average density of the system $\rho$. Nuclei are in the strong coupling regime when the Brueckner parameter $r_s$ is large enough (hence the localisation parameter small enough). In other
hedral distribution along \( \beta \) shape along \( \beta \) roughly homogeneously distributed: prolate cigar-like sure in is found at the spherical point, owing to the p-shell clo-
the deformation parameters. The global minimal energy
sic densities are also displayed for values of interest of
and triaxial octupole (\( \lambda, \mu \)) constrained deformation parameters, namely the axial
deformation and clustering by plotting
the alpha-particles. Fig. 1 illustrates the relation between
point group that dictates the geometrical configuration of
Q
alpha-subunits. The multipolar mass moments
field whose fluctuations cause nucleons to gather into
nucleon correlations, it is natural to look for an order pa-
rameter associated to alpha-clustering, i.e. a collective
words, i) fewer nucleons, ii) a deeper confining potential and
and iii) lower densities favor states where quartetting cor-
relations dominate, i.e where clustering is likely to occur.
The first two effects have been studied in [15, 25, 31, 32] and we focus here on the role played by the nucleon density. Because of Pauli blocking effects, alpha-particles in the nuclear medium start dissolving as they overlap with each others. The critical (Mott) density at which this happens can be deduced from the dimensionless parameter \( \alpha_{loc}^\alpha \) where the ratio is now between the size of an alpha-particle \( R_\alpha \sim r_0 A_\alpha^\frac{1}{3} \) and the mean internucleon distance \( \tilde{r} \): it is solution of \( \alpha_{loc}^\alpha = 1 \), that is
\[
\frac{\rho_{\text{Mott}}^\alpha}{\rho_0} = \frac{3}{4\pi r_0^3 A_\alpha^\frac{1}{3} \rho_0} \sim 0.2. \tag{5}
\]
Below \( \sim \rho_0/5 \), quartetting correlations are no more suppressed by Pauli blocking effects and a full alpha-clustering should correspond to the favoured arrangement of alpha-conjugate nuclei. We now wish to further substantiate the broad picture given through the analysis of dimensionless parameters by investigating the QPT in the framework of the EDF approach.

III. EDF APPROACH TO QUANTUM PHASE TRANSITION IN FINITE NUCLEI

A. Clustering and deformation

In the EDF spirit, rather than introducing explicit 4-
body correlations, it is natural to look for an order pa-
rameter associated to alpha-clustering, i.e. a collective
field whose fluctuations cause nucleons to gather into
alpha-subunits. The multipolar mass moments \( Q_\mu \) play such a role. Nuclear deformation indeed provides a necessary (yet not sufficient) condition for localized substructures to emerge in nuclei. The extreme scenario of all nucleons aggregating into alpha degrees of freedom corre-
sponds to a spontaneous breaking of the rotational sym-
metry \( O(3) \) of the nuclear Hamiltonian down to a discrete
point group that dictates the geometrical configuration of the alpha-particles. Fig. 1 illustrates the relation between
nuclear deformation and clustering by plotting \( ^{16}\text{O} \) total
binding energy computed at the Single-Reference (SR)
level of the covariant energy density functional (CEDF)
approach (also referred to as mean field level) against
constrained deformation parameters, namely the axial
quadrupole (\( \lambda, \mu = (2, 0) \)), axial octupole (\( \lambda, \mu = (3, 0) \)) and triaxial octupole (\( \lambda, \mu = (3, 2) \)) modes. \( ^{16}\text{O} \) intrin-
sic densities are also displayed for values of interest of the
deformation parameters. The global minimal energy is found at the spherical point, owing to the p-shell clo-
sure in \( ^{16}\text{O} \). Small values of the deformation parameters
(\( < 1 \)) correspond to deformed shapes where nucleons are roughly homogeneously distributed: prolate cigar-like shape along \( \beta_{20} \), pear-like configuration along \( \beta_{30} \), tetrahe-
drational distribution along \( \beta_{32} \). The energy is rather stiff in the \( \beta_{20} \) direction, contrary to the octupole directions, especially the triaxial one: for \( \beta_{32} \sim 0.3 \) where the tetrahe-
dral shape is already well developed, the energy loss with respect to the spherical configuration is only 3 MeV. Projection on both angular momentum and parity as well as mixing within the generator coordinate method may therefore induce tetrahedral correlations in the ground state of \( ^{16}\text{O} \) and yield several rotation-vibration excited states that can be classified according to the irreducible representations (irreps) of the discrete tetrahedral group \( Td \), along the lines of [24]. For large deformation parameters, Fig. 1 involves binary cluster structures, e.g. \( ^{12}\text{C} + ^{12}\text{C} \), at \( \beta_{30} \sim 1 \), followed by ternary cluster structures (\( ^{6}\text{Be} + 2 \alpha \) at \( \beta_{20} \sim 1.7 \)). For extreme values of the de-
formation parameters where the nuclear radius is large, hence the average density low enough for Pauli blocking effects to be suppressed, \( ^{16}\text{O} \) displays a fully clustered structure with four alphas in linear (\( \beta_{20} \sim 5 \)) or tetrahe-
dral (\( \beta_{32} \sim 6 \)) configurations.

For the sake of completeness, let us recall the link be-
tween deformation and cluster formation before investi-
gating how the mean density drives alpha-clustering. The reason why deformation is intimately related to the occurrence of clusters can already be understood assum-
ing a nuclear confining potential close to a HO one. In the isotropic case (spherical configuration), the de-
genereities of the energy levels of an N-dimensional HO are in one-to-one correspondence with the irreducible to-
tally symmetric representations of \( SU(N) \). Similarly, the quantum states of an N-dimensional anisotropic oscillator (deformed configuration) with commensurate frequencies (i.e. rationally related frequencies \( \omega_i \) such that \( k_i \omega_i = \omega \) and \( k_i \) integral and relatively prime), specified by quan-
tum numbers $n_i$ and possessing energies

$$E_{(n_i)} = \hbar \omega \sum_i \left( n_i + \frac{1}{2} \right) \frac{1}{k_i},$$

(6)

enjoy degeneracy spaces that also correspond to the representations of $SU(N)$, with the important difference that unlike the isotropic oscillator, a given representation occurs not singly but with a multiplicity $\prod_i k_i$ [35, 36]. Indeed, the anisotropic HO with commensurate frequencies is unitarily equivalent to the direct sum of $\prod_i k_i$ isotropic HOs with frequencies $\omega$, such that the phase space of the former can be mapped into the phase space of the isotropic HO at the cost of introducing a foliated (multi-sheeted) structure in the phase space [37]. For instance, a 3-dimensional anisotropic HO with axial symmetry and frequencies in a ratio $\omega_x = \omega_y = \omega_\perp: \omega_z = 2:1$ (superdeformed prolate configuration), i.e. with $k_x = k_y \equiv k_\perp = 1, k_z = 2$, involves $k_\perp^2 k_z = 2$ independent copies of $SU(3)$ irreps. As a consequence, the sym-

mectries of the corresponding many-particle wavefunction can be described by the irreps of two $SU(3)$ groups, suggesting that the shell structure of the superdeformed HO is that of two smaller overlapping spherical HOs [38, 39]. Moreover, the emerging superdeformed magic numbers 2, 4, 10, 16, 28, 40, . . . can be expressed in terms of the spherical ones (2, 8, 20, . . .) either as the sum of two consecutive spherical magic numbers (2 = 2+0, 10 = 8+2, 28 = 20+8, . . .), or as repeating twice a spherical magic number (4 =2+2, 16 = 8+8, 40 = 20+20, . . .), see Fig. 2. From these features, one can infer a susceptibility for nuclei in a superdeformed prolate state to distribute their total mass among two spherical fragments, either in an asymmetric ($^{20}\text{Ne} = \alpha^{16}\text{O}$, $^{56}\text{Ni} = ^{16}\text{O} + ^{40}\text{Ca}$, etc.) or a symmetric ($^8\text{Be} = \alpha + \alpha$, $^{32}\text{S} = ^{16}\text{O} + ^{16}\text{O}$, etc.) way. However, if deformation provides a necessary condition for nuclei to cluster in multiple spherical fragments via the occurrence of dynamical symmetries involving multiple independent copies of the $SU(3)$ irreps, it is not a sufficient one. As explained in Sec. II, other requirements must be met, e.g. a deep enough confining potential or a low enough mean density such that the spherical fragments do not overlap and dissolve by virtue of Pauli blocking effects.

![Graph](image_url)

**Fig. 2:** (Color online) Level diagram of the 3D anisotropic harmonic oscillator in axial symmetry versus the axial quadrupole deformation parameter $\delta$. Degeneracies of the levels (taking into account the spin structure of nucleons) are indicated as well as deformations corresponding to rationally related frequencies $\omega_\perp: \omega_z$.

![Graph](image_url)

**Fig. 3:** (Color online) $^{16}\text{O}$ nucleon radial density for r.m.s. radii constrained (a) from 2.4 to 5.3 fm within symmetry-restricted RMF calculations with the DDME2 parametrization and (b) from 2.5 to 3.8 fm within HFB calculations with the Gogny D1S parametrization [40]. Relativistic calculations (a) are performed in a HO basis with 11 shells and $\hbar \omega = 13$ MeV. Nonrelativistic calculations (b) are also performed in a HO basis with 11 shells but with $\hbar \omega = 15$ (red), 17 (green) and 19 (blue) MeV.
B. Role of the mean density in nuclear clustering

We want to further investigate the impact of the mean density on the occurrence of clusters. Taking the specific case of $^{16}\text{O}$, this can be achieved by inflating isotropically the finite nucleus, i.e. by constraining its r.m.s. radius while imposing a zero global quadrupole mass moment $Q_{20}$ [14, 15], such that the density continuously decreases.

Such a program is worked out using both the CEDF and Gogny EDF approaches, where the corresponding constrained mean field equations are solved in a HO basis with 11 major shells. A more careful analysis of the impact of the HO basis parameters, e.g. the frequency $\omega$, must be undertaken when addressing such exotic dilute configurations. Indeed, some values of $\hbar \omega$ may lead to unphysical lower energy configurations where a part of nucleons remains tightly packed at the center of the nucleus while the remaining nucleons are sparsely distributed around this dense core. We retain values of $\hbar \omega$ that minimize the energy of the system and at the same time lead to a regular decrease of the density. These features are illustrated in Fig. 3. The upper panel (a) displays the radial density of $^{16}\text{O}$ for several constrained radii in the relativistic case. The parameter of the HO basis yielding the lowest binding energy for these constrained configurations and a regular decrease of the density is found to be $\hbar \omega = 13 \text{ MeV}$. The lower panel (b) shows the density profile obtained in the non-relativistic case, where the colors distinguish between several values of $\hbar \omega$. For $\hbar \omega < 19 \text{ MeV}$, the constraint on the radius, taken between 2.4 and 3.8 fm, does not lead to a regular decrease of the density at the center of the nucleus. As a matter of fact, the nucleus increases its radius by expanding a low-density nucleon cloud surrounding a quasi constant-density nucleon core (red and green curves). These features do not sound appropriate. A regular decrease of the central density as the radius is constrained to higher values is only obtained for $\hbar \omega \sim 19 \text{ MeV}$ within Gogny D1S calculations, which is the adopted value in the non-relativistic case (as far as spherical configurations are concerned).

Setting the HO basis parameters to their relevant values, $^{16}\text{O}$ binding energy is computed as a function of the constrained r.m.s. radius within both the CEDF and Gogny EDF approaches and displayed in Fig. 4. The relativistic case (Fig. 4 (a)) involves several type of calculations. The curve with red filled circle markers corresponds to a SR-CEDF calculation where we enforce spherical symmetry (i.e. no spatial spontaneous symmetry breaking (SSB) can occur) as well as the global U(1) invariance (i.e. no pairing correlations can develop). We refer to this case as spatial symmetry-restricted relativistic mean field (SSR-RMF). Relaxing the enforcement of U(1) symmetry, i.e. still restricting the spatial symmetry to the spherical one, but letting the system free to break the U(1) invariance signalling the development of pairing correlations, yields the curve with red open circle markers: this is the spatial symmetry-restricted relativistic Hartree Bogoliubov (SSR-RHB) case. For this type of calculation, the green dashed line displays the corresponding pairing energy of the system. Finally, relaxing all the symmetry restrictions, both spatial and internal (with however the constraint $\beta_{20} = 0$ ensuring

FIG. 4: (Color online) Self-consistent binding energy of $^{16}\text{O}$ computed at the SR level of (a) CEDF with the DD-ME2 parametrization and (b) EDF with the Gogny D1S parametrization vs the constrained r.m.s. radius. In (a) curves with red circle symbols correspond to spherical configurations and were obtained in a HO basis with 11 shells and $\hbar \omega = 13 \text{ MeV}$, while the blue square symbol curves correspond to a tetrahedral arrangement and were obtained in a HO basis with 11 shells and $\hbar \omega = 11 \text{ MeV}$. Likewise, in (b) red (circle symbols) and blue (square symbols) correspond to spherical and tetrahedral configuration respectively and were obtained in a HO basis with 11 shells and $\hbar \omega = 19$ and $12 \text{ MeV}$ respectively. In both cases, the blue open square symbol curve corrects the mean field energy with the zero-point energy contribution, and the inserts display $^{16}\text{O}$ intrinsic density at the corresponding constrained radii. See text for detailed explanations.
an isotropic inflation of the nucleus) yields the curves with blue square markers (filled and open markers). This case is referred to as spatial symmetry-unrestricted relativistic Hartree Bogoliubov (SSU-RHB). In the curve with the square open symbols, the zero-point energy, computed as in ref. [14], is subtracted from the SSU-RHB energy.

Let us first analyse the SSR-RMF case. Fig. 5 displays the neutron single-particle (sp) levels for three different constrained radii, namely the radius of the equilibrium configuration \( R = 2.6 \) fm, a radius belonging to the interval where the three type of calculations (SSR-RMF, SSR-RHB and SSU-RHB) yield the same result \( R = 3.4 \) fm, and an extreme radius of \( R = 6.0 \) fm. Diluting \(^{16}\)O causes a drastic reduction of the valence neutron gap from 10.71 MeV at \( R = 2.60 \) fm to 4.63 MeV at \( R = 3.40 \) fm and 2.36 MeV at \( R = 6.0 \) fm. The sp spectrum gets shrunk and all spin-orbit partners eventually become degenerate. These features can be understood by looking at the radial dependence of two combinations of the scalar and time-like nucleon self-energies \( S \) and \( V \) (Fig. 6). The combination \( V+S \) defines the mean potential where independent nucleons evolve in the mean field picture. From a typical depth of \(-75\) MeV at the equilibrium configuration, the confining potential become shallower as the constrained radius increases until reaching \(-10\) MeV at \( R = 6.0 \) fm. Likewise, the other combination \( V-S \), whose derivative (with a prefactor \( 1/M^2 \) and \( M \) the nucleon mass) governs the spin-orbit splitting, gets weaker as the radius increases, restoring the spin \( SU(2) \) symmetry of the Dirac Hamiltonian, and therefore causing spin-orbit partners to be degenerate.

Such a reduction of the Fermi gap opens the room for the development of non-dynamical correlations. Indeed, \(^{16}\)O become a near degenerate system, i.e. excited particle-hole (ph) configurations have close to the fundamental one, such that the system will rearrange itself in a non perturbative way to lift the (near) degeneracies. A possible strategy consists in developing pairing correlations that can be accounted for, at the SR level, through the spontaneous breaking of the global \( U(1) \) group associated to the conservation of nucleon number. From the corresponding SSR-RHB calculations displayed Fig. 4, the normal to superfluid QPT occurs at \( R = 3.8 \) fm, even if a sensible effect on the binding energy has to wait for radii greater than \( R = 5.5 \) fm. Such a QPT translates into the opening of a gap in the quasi-particle (qp) spectrum of \(^{16}\)O and the strength of the corresponding correlations is measured by the pairing energy. At \( R = 6.0 \) fm, the gap in the neutron qp spectrum jumps from 2.2 MeV in the SSR-RMF case to 4.1 MeV in the SSR-RHB one, with a pairing energy of \(-8\) MeV. As one can see from the small impacts on \(^{16}\)O binding energy (Fig. 4), rearranging itself by developing pairing correlations seem rather ineffective because of the large energy splitting between the \( d \) and \( f \) levels that hinders the scattering of Cooper pairs, as shown by the occupation numbers of the canonical neutron sp spectrum in Fig. 7. A more effective strategy to

![FIG. 5: (Color online) \(^{16}\)O neutron single-particle levels associated to SSR-RMF calculations with the DD-ME2 parametrization constrained at \( R = 2.6, 3.4, 6.0 \) fm.](image)

![FIG. 6: (Color online) Radial evolution of combinations (a : \( V+S \), b: \( V-S \)) of the scalar (\( S \)) and time-like (\( V \)) nucleon self-energies in \(^{16}\)O for radii constrained at \( R = 2.6, 3.4, 6.0 \) fm.](image)
lift the degeneracies is to develop angular correlations. From the SSU-RHB calculations, a Mott-like QPT is observed at a critical radius \( R_c = 3.7 \) fm, that is a mean density \( \rho_{\text{Mott}}/\rho_0 = (R_{\text{eq}}/R_c)^3 \sim 0.35 \), or \( \rho_{\text{Mott}} \sim \rho_0/3 \), in relatively good agreement with the estimation based on dimensionless ratios of characteristic variables of the problem in Sec. II. The transition occurs between a phase where nucleons are delocalized in a dilute spherical volume (the maximal value of the nucleon density is 0.046 fm\(^{-3}\) at \( R = 3.40 \) fm) and a phase where nucleons are localized in four alpha-like degrees of freedom which recover a density equals to the saturation one and are arranged according to a tetrahedral configuration. For such a tetrahedral configuration, no pairing correlations develop.

The robustness of these results can be tested by performing similar calculations with the non-relativistic Gogny EDF. The corresponding binding energy versus the constrained r.m.s. radius is displayed in Fig. 4 (b) and shows remarkable similarities with the relativistic case (Fig. 4 (a)). Here the transition happens slightly later, at \( R_c = 3.9 \) fm, that is a mean density \( \rho_{\text{Mott}}/\rho_0 = (R_{\text{eq}}/R_c)^3 \sim 0.33 \), i.e. again \( \rho_{\text{Mott}} \sim \rho_0/3 \). In the non-relativistic calculations, a break is observed between the curve related to the spherical configurations (in red) and those for the tetrahedral configurations (in blue). The discontinuity occurs at the radius beyond which the spherical density evolves into a four alpha-like configuration and stems from different values for the optimal \( \hbar \omega \) in the spherical configuration case (\( \hbar \omega = 19 \) MeV) and in the tetrahedral one (\( \hbar \omega = 12 \) MeV). For the latter, the nucleus increases its radius by placing the alphas further apart, as illustrated in the inserts.

C. Analysis of non-axial octupolar correlations

The non-dynamical correlations grasped though the spatial SSB trigger the formation of alpha-clusters, allowing the dilute system to lower its energy by taking advantage of the nuclear cohesion. The corresponding neutron sp spectrum of the SSU-RHB calculation (Fig. 7) displays a band-like structure, i.e. neutron sp levels assemble into two bunches of four near degenerate orbitals separated by a huge gap of 17.4 MeV. We can further investigate the features of the tetrahedrally-deformed sp spectrum by considering the SSB of the rotational group \( O(3) \) down to the (double) point group \( T_d \), whose character table is shown in Table I. As spin-1/2 fermions, nucleon wavefunctions can be classified along the \( \Gamma_6, \Gamma_7 \) and \( \Gamma_8 \) irreps of the \( T_d \) group. The correlations grasped through the SSB of \( O(3) \) down to \( T_d \) can be translated in the language of ph excitations on top of a symmetry-preserving reference state by computing the overlaps \( \langle \Phi^{\text{sphe}}_i | \Phi^{\text{tetra}}(\beta_{32}) \rangle \) (the tetrahedral closed-shell configuration involving the \( \Gamma_6, \Gamma_7 \) and \( \Gamma_8 \) states) and spherical SDs \( \langle \Phi^{\text{sphe}}_i | \Phi^{\text{tetra}}(\beta_{32}) \rangle \) (both ground (\( i = 0 \)) and ph excitations (\( i > 0 \)) in a valence space spanning the 1s1/2 to the 1f5/2 states) for various values of the order parameter \( \beta_{32} \) (Fig. 8). The contribution of the spherical closed-shell configuration (0p-0h state) drops rapidly as the tetrahedral deformation increases. Collective excitations, in particular 2p-2h and 6p-6h ones, quickly become dominant, meaning that the amplitude excitations from the p-shell to sd-shells do not describe the total correlated wavefunction in a satisfactory manner, but one eventually needs to account for pf-shell states as well as holes in the s state. It should be noted that the probabilities displayed in Fig. 8 do not add up to one because of the too small valence space. The role played by the orbitals beyond the p- and sd-shells can be understood by comparing the shape of the spherical canonical orbitals with the tetrahedral ones (Fig. 9). The four near degenerate tetrahedral orbitals \( \Gamma_6, \Gamma_7 \) and \( \Gamma_8 \) (doubly degenerate) share the same partial density that resembles four alphas arranged in a tetrahedral configuration. To illustrate how spherically-symmetric nucleonic shell combine in such tetrahedrally-deformed orbitals, let us

![FIG. 7: (Color online) \(^{16}\)O neutron canonical single-particle levels computed at \( R = 6.0 \) fm with the DD-ME2 parametrization in the SSR-RMF, SSR-RHB and SSU-RHB cases.]

| \( E \) | \( \bar{E} \) | \( 8C_3 \) | \( 8C_3 \) | \( 3C_2 \) | \( 3C_2 \) | \( 6S_4 \) | \( 6S_4 \) | \( 6\sigma_d \) |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| \( \Gamma_1 \) | 1 1 1 1 1 1 1 1 1 1 |
| \( \Gamma_2 \) | 1 1 1 1 -1 -1 -1 -1 -1 -1 |
| \( \Gamma_3 \) | 2 2 -1 -1 2 0 0 0 |
| \( \Gamma_4 \) | 3 3 0 0 -1 1 1 -1 -1 -1 |
| \( \Gamma_5 \) | 3 3 0 0 -1 -1 -1 1 1 1 |
| \( \Gamma_6 \) | 2 -2 1 -1 0 \( \sqrt{2} \) - \( \sqrt{2} \) 0 |
| \( \Gamma_7 \) | 2 -2 1 -1 0 - \( \sqrt{2} \) 0 0 |
| \( \Gamma_8 \) | 4 -4 -1 1 0 0 0 0 |

TABLE I: Character table of the double \( T_d \) group detailing its 8 classes and irreps. See [41] for further details.
focus on the $\Gamma_6$ level. From Table II that details the decompositions of the irreps of the full rotation group into irreps of the group $T\bar{d}$, the irreps compatible with $\Gamma_6$ are $D^+_0$, $D^+_1$, etc. for the positive parity case and $D^-_5$, $D^-_6$, etc. for the negative parity one. The corresponding lowest energy levels at $R = 3.4$ fm can be read from Fig. 9: the occupied $1s1/2$, $1p3/2$, $1p1/2$, $2s1/2$ and $1f7/2$ orbitals (the p and d shells are not compatible with $\Gamma_6$). Superpositions of these (at least) four spherically-symmetric orbitals are needed to yield a tetrahedrally-shaped $\Gamma_6$ orbital. The latter having a zero contribution at the center of the nucleus, one first need a mixture between the $1s1/2$ and $2s1/2$, which belong to the $\Gamma_6$ subspace, to cancel the density at the origin. The resulting density is still isotropically distributed in space. To localize the nucleons occupying the $\Gamma_6$ orbital into alphas in a tetrahedral configuration, superposition with f states are also needed (since the p and d shells only involve the $\Gamma_7$ and $\Gamma_8$ irreps). Fig. 10 illustrates this statement by splitting the $1f7/2$ partial density into its magnetic $m = 1/2, 3/2, 5/2, 7/2$ degenerate components.

The tetrahedral shape of the four $\Gamma_i$ ($i = 6, 7, 8$) orbitals can be analysed by employing the language of quantum chemistry. These states resemble 'molecular' orbitals that have the structure of a linear combination of localized 'atomic' orbitals, here is orbitals associated to the alpha-particle ground state. In the LCAO-MO picture [42], the molecular orbitals $\psi_i$ ($i=1,2,3,4$) read

$$ \psi_i = \sum_{j=1}^{4} f^j_i \phi_j, \quad (7) $$

where the $\phi_j$'s stand for the original Gaussian-type atomic orbitals. The unknown coefficients $f^j_i$ follow from the resolution of an eigenvalue equation involving the norm and energy kernels $N_{ij}$ and $H_{ij}$ between the atomic orbitals. In the Hückel approximation, $N_{ij} = 0, \forall i, j$ while all $H_{ij} = 0$ except when the ith and jth atomic sites are adjacent. Denoting $\epsilon \equiv H_{ij} \forall i$ and $-\mu \equiv H_{ij}$ for all the other adjacent i and j, the Hückel eigenvalue equation for 4 alphas located on the vertices of a tetrahedron
These results hence account for the structure of the symmetry-broken sp spectrum. The SSB of $O(3)$ down to the point group $Td$ translates into the clusterization of the nucleon in four alphas arranged according to a tetrahedral configuration. The latter brings into play four nearly degenerate (up to the value of $\mu$ for the first orbital) molecular-like orbitals that can be expressed as linear combinations of four $1s$ alpha states. At $R = 6.0$ fm the energies of the $I_i$ ($i = 6, 7, 8$) $E_1 = -18.090$ MeV and $E_2 = E_3 = E_4 = -18.004$ MeV (see Fig. 9) lead to identify the energy of the $1s$ alpha state $\epsilon = -18.004$ MeV as well as the non-diagonal energy kernel $\mu = 0.086$ MeV. Taking into account the $\sim 10$ MeV correction coming from the zero-point energy contribution (blue open square curve in Fig. 4), the energy of the $1s$ alpha state drops to $\sim -28$ MeV, in agreement with the binding energy of $^4$He. It should be noted that the energy gap of 17.4 MeV between occupied and unoccupied states of the tetrahedrally deformed sp spectrum is of the order of the lowest excitation energy of the alpha-particle (20.2 MeV), suggesting an exclusion property that acts among the nucleons sharing the same intrinsic state when embedded in an alpha-cluster.

FIG. 10: (Color online) $1f7/2$ partial density (a) and its decomposition on $m = 1/2, 3/2, 5/2, 7/2$ (b).

The resolution of Eq. (8) yields the four LCAO-MO’s:

$$\begin{pmatrix} \epsilon & -\mu & -\mu & -\mu \\ -\mu & \epsilon & -\mu & -\mu \\ -\mu & -\mu & \epsilon & -\mu \\ -\mu & -\mu & -\mu & \epsilon \end{pmatrix} \begin{pmatrix} f'_1 \\ f'_2 \\ f'_3 \\ f'_4 \end{pmatrix} = E_i \begin{pmatrix} f_i \\ f_i \\ f_i \\ f_i \end{pmatrix}.$$  

Equation (8) reads

$$\left( \begin{array}{cccc} \epsilon & -\mu & -\mu & -\mu \\ -\mu & \epsilon & -\mu & -\mu \\ -\mu & -\mu & \epsilon & -\mu \\ -\mu & -\mu & -\mu & \epsilon \end{array} \right) \begin{pmatrix} f'_1 \\ f'_2 \\ f'_3 \\ f'_4 \end{pmatrix} = E_i \begin{pmatrix} f_i \\ f_i \\ f_i \\ f_i \end{pmatrix}. \quad (8)$$

with energy $E_1 = \epsilon - 3\mu$;

$$\psi_1 = \frac{1}{2} (\phi_1 + \phi_2 + \phi_3 + \phi_4), \quad (9)$$

with energy $E_2 = \epsilon + \mu$;

$$\psi_2 = \frac{1}{\sqrt{2}} (-\phi_1 + \phi_2), \quad (10)$$

with energy $E_3 = E_2$;

$$\psi_3 = \frac{1}{\sqrt{2}} (-\phi_1 + \phi_3), \quad (11)$$

with energy $E_4 = E_3 = E_2$. Being degenerate, the three last orbitals are not uniquely defined. Any linear combination involving a $3 \times 3$ unitary transformation yields a triplet of different but equivalent orbitals, e.g.

$$\begin{align*} 
\psi'_1 &= \frac{1}{2} (\phi_1 - \phi_2 - \phi_3 + \phi_4), \\
\psi'_2 &= \frac{1}{2} (\phi_1 + \phi_2 - \phi_3 - \phi_4), \\
\psi'_3 &= \frac{1}{2} (-\phi_1 + \phi_2 - \phi_3 + \phi_4). 
\end{align*} \quad (12)$$

IV. QUARTET QUANTUM PHASE TRANSITION IN INFINITE MATTER

So far, we have considered a QPT in $^{16}$O as a function of the density where the nucleus changes from a homogeneous mean-field density spontaneously into a tetrahedral configuration of four $\alpha$ particles. However, those crystalline structures, imposed by the mean-field, come too high in energy. It is, for example, known that it is difficult to describe in detail the famous Hoyle state in $^{12}$C at 7.65 MeV in this way. However effects of the Pauli principle and the density are already well given in mean field theory.

We here want to study quartet condensation and the corresponding QPT in infinite matter and make a link with the preceding mean-field study of $^{16}$O concerning the typical densities at which the QPT occurs in nuclear systems. Quartet condensation is described following very closely the usual procedure of pairing with the BCS approach. For the latter the BCS equations can be written in the following way

$$(e_{p_1} + e_{p_2})\kappa_{p_1p_2} + (1 - n_{p_1} - n_{p_2}) \sum_{p'_1p'_2} v_{p_1p_2p'_1p'_2} \kappa_{p'_1p'_2} = 2\mu\kappa_{p_1p_2}, \quad (14)$$

with the occupation numbers given by

$$n_k = \frac{1}{2} \left[ 1 - \frac{e_k - \mu}{\sqrt{(e_k - \mu)^2 + \delta_k^2}} \right], \quad (15)$$

with the gap
\[ \Delta_k = g \kappa_{kk}, \]

where \( \tilde{k} \) is the time reversed state of \( k \) and we used as pairing force a delta interaction \( g\delta(r_1 - r_2) \). Finite range forces can be treated accordingly.

In above equations \( e_k \) are the kinetic energies, eventually with inclusion of a Hartree-Fock (HF) shift, and \( \mu_1 \) is the chemical potential. The indices \( p \) include momenta and spin, \( \kappa_{p_1p_2} = \langle c_{p_1}c_{p_2} \rangle \) is the pairing tensor, and \( \nu_{p_1p_2p_3p_4} \) is the matrix element of the pairing force. Equations (14) and (15) are the BCS equations in their general form. Usually one considers the Cooper pairs at rest, what makes that the momenta of the two particles are opposite and one considers spin singulet pairing.

For quartetting, one proceeds in a completely analogous way: one writes the in medium four body equation [43]

\[
(e_1 + e_2 + e_3 + e_4)\kappa_{1234} + \sum_{1'2'3'4'} V_{1234;1'2'3'4'}\kappa_{1'2'3'4'} = 4\mu \kappa_{1234},
\]

with

\[
V_{1234;1'2'3'4'} = (1 - n_1 - n_2)\nu_{121'2'}\delta_{33'}\delta_{44'} \\
+ (1 - n_1 - n_3)\nu_{131'3'} + \text{permutations},
\]

where we used an obvious short hand notation. In the case of quartetting the expressions for the occupation numbers \( \alpha_k \) are quite a bit more complicated with respect to the pairing case and we refer the reader to the literature [43]. To ease the numerical solution of the quartet equation, in Ref. [43], the four nucleon order parameter was approximated by a mean-field ansatz projected to good total center of mass momentum \( K = 0 \) in the following way

\[
(\psi_{1}^{+} \psi_{2}^{+} \psi_{3}^{+} \psi_{4}^{+}) = \delta(k_1 + k_2 + k_3 + k_4)\varphi(k_1)\varphi(k_2)\varphi(k_3)\varphi(k_4),
\]

where \( \psi_k^+ \) creates a nucleon with momentum \( k \) (obvious spin-isospin indices are suppressed as well as the total scalar spin-isospin part of the wave function) and \( \varphi(k) \) is a 0S single particle wave function in momentum space. The selfconsistent equation for the order parameter then boils down to a nonlinear equation for \( \varphi(k) \) and it turned out that this approximation reproduces very well a full solution of the in medium four body equation [44]. The point now is that this order parameter only exists below a critical density of \( \sim \rho_0/5 \) [45] which is a value similar to what found in the preceding study for \( ^{16}\text{O} \). In infinite matter, this can then be qualified as a macroscopic QPT for quartets (\( \alpha \) particles) with the density as control parameter.

This breakdown was studied with the calculation of the single nucleon occupation numbers \( \alpha_k \) in the \( \alpha \)-condensate as a function of the chemical potential \( \mu \). We see in Fig.11 that as \( \mu \) increases, \( \alpha_k \) naturally also increase. However, beyond \( \mu \sim 0.55 \text{ MeV} \) the solution ceases to exist, that is the \( \alpha \) order parameter has disappeared and the system has turned over into a standard nuclear superfluid very analogous to what we have seen happening in \( ^{16}\text{O} \). It should be pointed out that this behavior is in strong contrast to pairing, for instance deuteron pairing, where the density can be increased without breakdown of superfluidity, the decrease of the gap being only connected with the finite range of the pairing force. The corresponding \( \alpha_k \) steadily increase from negative to positive values of \( \mu \) without interruption. Of course the Pauli principle forbids that \( \alpha_k \) overshoots the value of one (disregarding spin and iso-spin degeneracies) reaching the typical BCS-like behavior at nuclear saturation densities. This behavior is shown in Fig. 12 in a qualitative way. We see the strong difference with the behavior of \( \alpha_k \) in the quartet case. It should be noted that the distributions below and around \( \mu \approx 0 \) should be compared with the ones of the quartet case.

The reason for this breakdown has a simple physical interpretation. It seems clear that in a four-body problem the in medium four-body level density plays a dominant role. It is defined by [46]

\[
g_4(\omega) = \sum_{k_1,k_2,k_3,k_4} [\delta(\omega - e_1 - e_2 - e_3 - e_4) - \delta(\omega - e_1 - e_2 - e_3 - e_4)],
\]

where \( \tilde{f} = 1 - f \) and \( f = f(e_i) \) is the Fermi-Dirac function equal to \( \Theta(\mu - e_i) \) at zero temperature. The \( e_i \) are the kinetic energies \( p_i^2/(2m) \). One easily verifies that for positive chemical potential \( \mu \), this four-body level density goes through zero at \( \omega = 4\mu \). Where there is no level density at the Fermi surface no correlations can develop and, thus, the order parameter goes to zero very
FIG. 12. Schematic (non-selfconsistent) view of BCS occupation numbers as the chemical potential varies from positive to negative (binding) values.

soon after $\mu$ has turned from negative values (binding) to positive ones (scattering). Actually for the calculation of the $n_k$ shown in Fig. 11, one needs the three hole level density [43, 47]

$$g_{3h}(\omega) = \sum_{k_1k_2k_3} [\bar{f}_1\bar{f}_2\bar{f}_3 + f_1f_2f_3] \delta(\omega + e_1 + e_2 + e_3),$$

(20)

and for convenience we show that level density here for three values of the chemical potential, see Fig. 13. Actually all many-particle level densities besides the one for two particles, where the pair is at rest, go through zero at the Fermi level, see [46] and below. For the case of negative $\mu$ the Fermi-Dirac functions at zero temperature are zero and then there is no qualitative difference for any of the multiparticle level densities, since the phase space factors reduce to unity.

Actually the disappearance of the $\alpha$-particle condensate does not coincide with the appearance of an uncorrelated Fermi gas as we here supposed. Rather, as already mentioned, there will appear a superfluid Fermi gas. However, a superfluid Fermi gas shows a gap at the Fermi level (chemical potential) and thus the level densities are even more suppressed around the Fermi level than without pairing.

The critical density coincides with the Mott density at zero temperature [45]. Actually the critical density is just the one where the alphas start to overlap with their tails to some appreciable extent (see, e.g., the two alphas in $^8$Be [48]) and, thus, the Pauli principle becomes active. For the pairing case, for two particles at rest with their c.o.m., one verifies that the two-body level density is finite at $\omega = 2\mu$, this being the reason why pairing also exists for positive $\mu$, or at high densities. For example the two-body level density for two particles below two times the chemical potential is given by

$$g(\omega)_{2p} = \sum_{k_1k_2} \Theta(\mu - e_{k_1})\Theta(\mu - e_{k_2})\delta(\omega - e_{k_1} - e_{k_2}).$$

(21)

For the particle pair at rest $k_1 = k_2$, one easily verifies that for $\omega = 2\mu$ the level density is finite. On the contrary, if the two nucleons are moving with a finite center of mass momentum, also a hole develops at the Fermi level similar to what we have seen for the three-particle case. The width of this hole increases with increasing center of mass momentum until the gap disappears. This signals the critical center of mass momentum. The finiteness of the level density at the Fermi level for two particles at rest is unique for the case of many-body level densities.
densities. This being the reason why pairing is such a unique phenomenon.

In conclusion, we have seen in this section that the density dependence of alpha condensation in infinite matter is somewhat lower but still in line with the mean field studies in finite nuclei presented above. This means in particular that the action of the Pauli principle on the existence of alpha clusters is similar in infinite matter and finite nuclei. As mentioned above the density of the Hoyle state is \( \rho_0/3 - \rho_0/4 \), very close to the mean field values in this study. In [49] for the hypothetical four-alpha condensate state in \( ^{16}\text{O} \) at 15.1 MeV the calculation yields quite a bit a lower density close to \( \rho_0/6 \). However, the four-alpha calculation is more involved and the density of the condensate may not be equivalent to the critical density which can be higher. Also the four-alpha calculation may be more sensitive to small perturbations like the increased (with respect to the \( ^{12}\text{C} \) case) Coulomb repulsion.

V. CONCLUSIONS

In conclusion, we have studied in nuclear systems the transition from a Fermi gas to alpha-clustering as a function of density at zero temperature. A first study based on dimensionless ratios of characteristic length- and energy-scales of the nuclear many-body problem lead to a Mott-like transition from a delocalized phase to an alpha-clustered one at the critical density \( \sim \rho_0/5 \), under which the Pauli principle does not prevent anymore the formation of 4-nucleon bound states. Very satisfactorily, these results are consistent with calculations in infinite matter, where the phase transition from the Fermi-gas to alpha-particle condensation happens at the critical density \( \rho_{\text{Mott}} = 0.03 \text{fm}^3 \sim \rho_0/5 \) [43, 45]. On the other hand, we also made constrained HFB calculations, both with RMF and Gogny EDFs, where the radius of \( ^{16}\text{O} \) is increased under the constraint that on average the system stays spherical, that is that the mean-value of the quadrupole operator remains zero. Also in this way the system shows a critical radius, i.e., low density where the homogeneously inflated \( ^{16}\text{O} \) nucleus abruptly goes over into a tetrahedral configuration of four alphas. This happens consistently with the relativistic and non-relativistic approaches at practically the same critical density \( \sim \rho_0/3 \), slightly higher than in the infinite matter calculation as well as the analysis of dimensionless parameters of the nuclear many-body problem. This shows that the Pauli-principle which triggers this QPT-transition acts rather similarly independently of whether the system goes over into a condensate or a lattice configuration as this happens with the constrained mean field calculation for \( ^{16}\text{O} \). We further investigated the transition to four alphas in \( ^{16}\text{O} \). We expressed the non-dynamical correlations grasped through the SSB of the \( O(3) \) rotation group down to the point group \( Td \) in terms of ph excitations on top of a symmetry-preserving SD, and discussed the crucial role played by orbitals beyond the p- and sd-shells to localize nucleons into alphas at the corners of a tetrahedron. All in all, \( ^{16}\text{O} \) provides a rather spectacular example of a quantum phase transition in nuclear physics.

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