α-Particle Clustering from Expanding Self-Conjugate Nuclei within the Hartree-Fock-Bogoliubov Approach

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The nuclear equation of state (EOS) is explored with the constrained Hartree-Fock-Bogoliubov approach for self-conjugate nuclei. It is found that beyond a certain low, more or less universal density, those nuclei spontaneously cluster into $A/4$ α particles with A the nucleon number. The energy at the threshold density increases linearly with the number of α particles as does the experimental threshold energy. Taking off the spurious c.m. energy of each α particle almost gives agreement between theory and experiment. The implications of these results with respect to α clustering and the nuclear EOS at low density are discussed.

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Introduction.—Cluster phenomena, in particular, α particle clustering in lighter nuclei, is presently a very active field of research. It is highlighted by the famous Hoyle (0_2^+) state in ^{12}C at 7.65 MeV. This state, primordial for the ^{12}C production in the Universe and, thus, for life, has long been believed to be in good approximation formed out of a weakly interacting gas of almost free α particles [1–4]. Since these α particles are all in relative S states, one can qualify this state as an α particle condensate [4], keeping in mind the limitations of this notion for finite systems with small numbers of particles. The research concerning this state has experienced a very vivid revival since about 10 years ago when the hypothesis of the possible existence of α condensates in nuclei was formulated for the first time [4]. The investigations are now extending to heavier self-conjugate nuclei. On the forefront is ^{16}O, where theoretical investigations predict that the sixth 0^+ state at 15.1 MeV is an analog of the Hoyle state but with four α particles instead of three [5]. Similarities between the three α and four α cases are, indeed, being found experimentally [6]. The particularity of those α particle condensate states is that they are spatially extended [7], i.e., at a low average density of $\rho \sim \rho_{\rm eq}/3 - \rho_{\rm eq}/4$, with $\rho_{\rm eq}$ the average density at equilibrium of the nucleus. In this sense the α condensate states can be considered as a continuation of the structure of ^{8}Be which consists of two well-identifiable, separated, weakly interacting α particles with average density in the just-mentioned range [8]. On the other hand, it is also well known that low density nuclear matter is unstable against cluster formation, mainly α particles [9,10]. Theoretical predictions give a critical temperature for macroscopic α condensation as high as $T_c^\alpha \sim 7$–8 MeV at low densities [11]. From this fact, it can be inferred that the Hoyle state and possible heavier Hoyle analog states are precursor states of a macroscopic α condensate phase, very much in analogy with neutron pairing in finite nuclei being a precursor to neutron superfluidity in neutron stars.

The description of α gas states in heavier $n\alpha$ nuclei naturally becomes more and more difficult using, e.g., α condensate wave functions as they are given in [12] by the THSR wave function, coined according to the initials of the authors in [4], which is based on a fully fermionic description. On the other hand, certain 3D Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) calculations of nuclei have recently shown that these mean field approaches can manifest cluster formation [13–15]; they are less affected by size limitations. In this work, we concentrate within the HFB framework, using the Gogny D1S interaction, on constraining the radius of self-conjugate nuclei to larger and larger values, i.e., to lower and lower nuclear densities. In this way, we prevent a transition to strong deformation which would favor clusterization into binaries. Thus, expanding the nucleus, at a critical low density and because of the 3D nature of the code, the system will spontaneously cluster into α particles, eventually also into a heavier compact core with an α gas around it and other cluster formations. Those α particles do not, of course, form a condensate but rather build a lattice. This hinges on the fact that the α's do not have the possibility to move freely with their c.m. coordinate in these HF or HFB calculations. The advantage of the mean field approach is that it can produce many α's in various configurations, still being entirely microscopic. So, qualitatively, the transition of an expanding nucleus passing from the homogeneous density distribution of a Fermi gas (HF) to clusterization can be studied within the mean field approach giving precious insights into the clusterization phenomenon in general and into the formation of α gas phases in particular. For example, as we will show, the energy of the system as a function of the radius first rises from its equilibrium position going over a barrier and entering the cluster phase at around a density $\rho = \rho_{eq}/3$. Among others, this feature is of quite some interest, as will be discussed below.

Formalism and results.—Since the constrained HFB theory is extensively explained in the literature [16–19], here we give only the absolute minimum of formalism. We minimize the HFB ground state energy using the Gogny D1S [19] interaction in constraining the radius of the nucleus, that is,

$$E^{\mathrm{HFB}} = \langle \mathrm{HFB}|H - \lambda r^2|\mathrm{HFB}\rangle / \langle \mathrm{HFB}|\mathrm{HFB}\rangle, \quad (1)$$

where r is the radius. λ is obtained in such way that $\langle \mathrm{HFB}|r^2|\mathrm{HFB}\rangle = r_0^2$. Therefore, choosing values for $r_0 <$ or $> r_{\mathrm{g.s}}$, where $r_{\mathrm{g.s.}}$ is the radius of the ground state, compresses or dilutes the nucleus. In the following, we treat all nuclei in spherical geometry, even though HFB may sometimes yield a deformed solution at the equilibrium position. Since we are interested in the low density (large radius) regime, the precise configuration at the absolute minimum does not matter. It should, however, be stressed that our 3D numerical code allows us to take on any cluster configuration, if this is energetically favorable, but on average the system stays spherical. For our study, we consider self-conjugate $N = Z$ nuclei up to ^{40}Ca [20].

Let us first show in some detail the various α cluster configurations obtained from our constrained HFB calculation (for brevity, we will not show in this work the well-known triangle configuration of ^{12}C; see, e.g., [21,22]). In Fig. 1, we present the ^{16}O case. We see that a tetrahedron of four α particles is formed. Actually, the transition to the cluster state is quite abrupt. In Fig. 2 we show the ^{24}Mg case. The ^{20}Ne case is quite similar, only in the shaded plane three α's are arranged in an equilateral triangle instead of four at the corners of a square. In Fig. 3 we display ^{32}S and in Fig. 4 ^{40}Ca. Going to the heavier systems, it becomes more and more difficult to disrupt the system into α particles only. For example, we show a four ^{8}Be configuration for ^{32}S and a ^{16}O plus six α case for ^{40}Ca. Many more cluster configurations can be obtained progressing, e.g., in smaller steps with the radius increment, but because of space limitations we cannot present this here. Let us also mention that we got an excited ^{36}Ar composed of three ^{12}C nuclei in a bent linear chain configuration. Also ^{48}Cr clustering into four ^{12}C has been found, and many configurations more.

Let us now present the equation of state (EOS) for the energy per particle as a function of density. Expanding (or compressing) a finite spherical nucleus does not, of course, yield the usual equation of state as in infinite nuclear matter, since, in addition to the bulk, the surface and Coulomb energies together with the quantal shell corrections are involved. Therefore, this equation of state which we want to call EOS-A slightly differs from nucleus to nucleus. Even for a given nucleus, in the low density region where clusters are formed, EOS-A may fluctuate, since in this region the energy surface has many different valleys leading to different cluster formations not very much different in energy. In which configuration the calculation gets trapped depends, e.g., on the step size of the expansion and other ingredients. It is important to realize that, once the α particles are formed, in HFB they contain their own spurious c.m. energy which should be eliminated. Since presently no method is available to achieve this in a microscopic way, we follow a heuristic procedure. We perform a HFB calculation of ^{8}Be and constrain the distance between the two forming α's so that they are very well separated. About 14 MeV are then missing to get twice

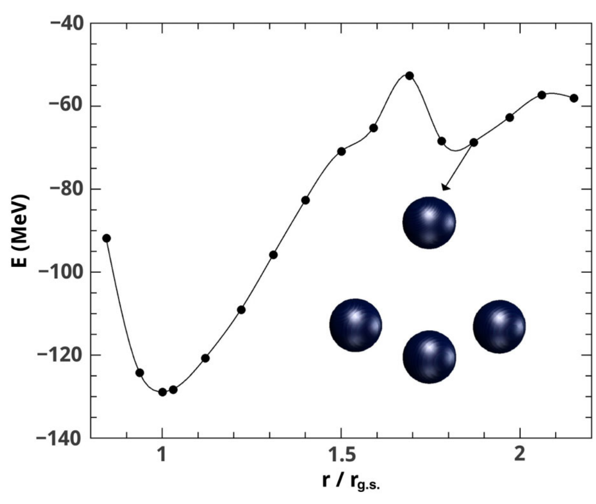

FIG. 1 (color online). Total energy of ^{16}O as a function of the radius scaled with respect to the one of the ground state $r_{\mathrm{g.s.}}$. At $r/r_{\mathrm{g.s.}} = \sim 1.8$, we see that a tetrahedron of four α particles is formed. No c.m. correction for individual α's is applied here. The arrow indicates to which $r/r_{\mathrm{g.s.}}$ value the α configuration corresponds.

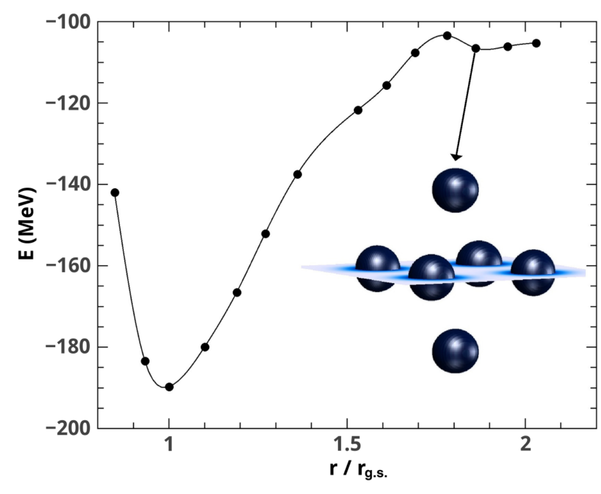

FIG. 2 (color online). Same as Fig. 1 but for ^{24}Mg with six α's. The shaded area only serves to show the three dimensionality of the α arrangement.

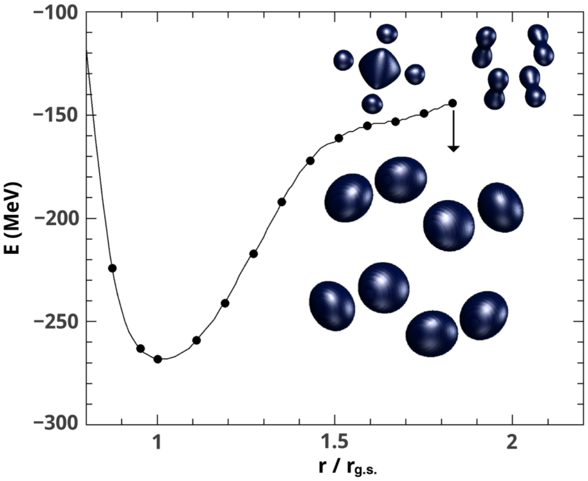

FIG. 3 (color online). Same as Fig. 1 but for ^{32}S with eight α's. Also, configurations with four ^{8}Be and a ^{16}O surrounded by four α's are shown.

the binding energy of a single α particle in the asymptotic limit, as it should be. We attribute this lack of binding to spurious c.m. motion of each α not being correctly treated. Of course, the total kinetic energy is subtracted from the Hamiltonian in all our calculations. So for ^{8}Be we have $\sim$7 MeV extra binding per α particle. We choose the hypothesis that this number stays about the same, even in cases with more α particles. This correction to take off 7 MeV for each α particle is switched on adiabatically from the point of the first clear appearance of the α particle structure which happens around a density $\rho/\rho_{\rm eq} \sim 1/3$. In order to get a global view, we show in Fig. 5 the different EOS-A obtained in this way for various $n-\alpha$ nuclei superposed. With this, we want to put into evidence the general behavior of the nuclear equation of state at low densities when it goes over into an α particle configuration. As can be seen from Fig. 5, there is a clear tendency that the EOS-A goes as a function of decreasing density over a maximum before reaching the zero density limit where the α particles are infinitely far apart and, therefore, the EOS-A reaches the value of an isolated α particle, i.e., -7.5 MeV, which is our theoretical value. Evidently, the numerical HFB code cannot handle configurations with α particles very distant from one another. Therefore, we stopped the calculation, once the α particles are clearly separated, which happens around $\rho \sim \rho_{\rm eq}/5$ (see also the detailed figures noted above). It may seem intriguing that the EOS-A bends down at low densities even for ^{32}S and ^{40}Ca where the energies displayed in Figs. 3 and 4 still show a slight increase in energy. It should, however, be recalled that the energies shown in Figs. 1–4 are uncorrected for spurious α particle c.m. motion. Once this correction is applied, the slight upward trend is converted into a downward trend. In Fig. 5, we show as an artist view lines extrapolating down to zero density just to guide the eye. The existence of a maximum in the nuclear equation of state containing a gas of α particles on the low density side and a Fermi gas (HF) on the higher density side is not evident. It would mean that the α phase is in a metastable state. The transition to the Fermi gas configuration will be strongly different from the scenario when there is no barrier. This may eventually be a question of importance in compact stars where α particle phases may exist in the density-temperature space. This question has been investigated in recent years by several authors, see [23–25], but the existence of a barrier and its height has been discussed, to the best of our knowledge, only in a relatively older paper on nuclear matter by Takemoto *et al.* [10], with similar results to ours. The present investigation seems to indicate the existence of a barrier about 2.5 MeV high, but certainly our procedure is very crude and more investigations have to be performed before a definite conclusion can

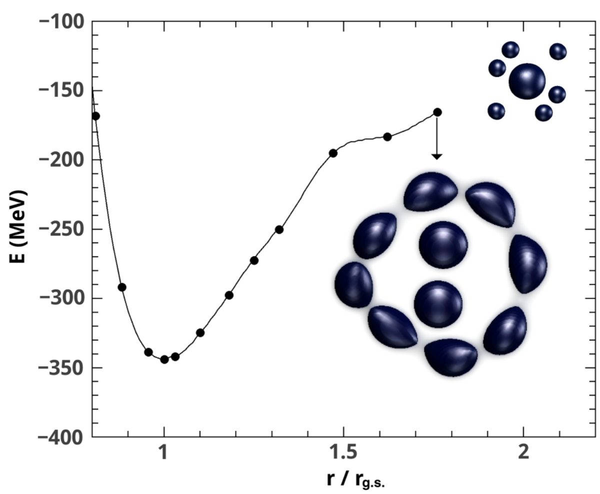

FIG. 4 (color online). Same as Fig. 1 but for ^{40}Ca with ten α's. Also, configurations with a ^{16}O surrounded by six α's are shown.

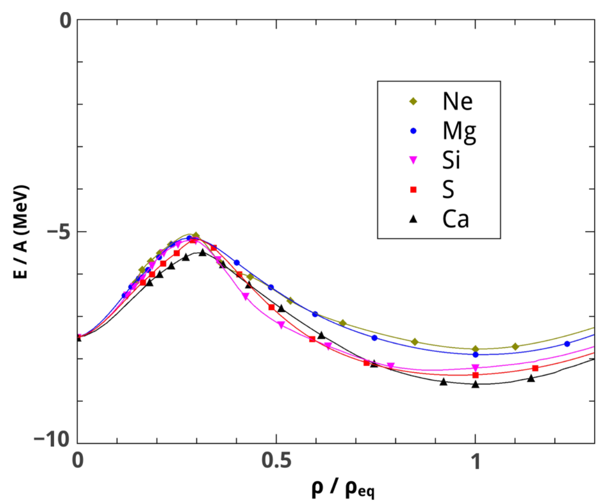

FIG. 5 (color online). Equation of state for a choice of self-conjugate nuclei (EOS-A) as a function of average density scaled by the one at equilibrium; see text for detailed definition.

be made. It should, however, be observed that at $\rho/\rho_{eq} \sim 1/3$, where the α's start to appear, the EOS-A are already well above the asymptotic limit of -7.5 MeV, so that in any case the systems have to go over a substantial barrier. This is the important point. The existence and height of the barrier are, of course, of great importance for the coalescence process of α particles into heavier nuclei in such star scenarios.

Defining $\rho = \rho_{eq}/3$ ($r/r_{g.s.} \sim 1.45$) as the theoretical threshold for α formation, we display in Fig. 6 the energy progression with the number n of α particles at that density. It is seen that this progression is about linear with n, increasing by ~16 MeV per α particle. Taking off 7 MeV of spurious c.m. energy for each α particle strongly improves the agreement with experiment; see the broken line in Fig. 6. The experimental threshold energies follow rather well a 7.6 MeV increase per α particle. It is, however, clear that this procedure can only yield a very rough estimate of the real situation. It is encouraging that the overall picture seems to be quite reasonable. Since it is clear by now that the α particles form a quantum gas rather than a crystal, see [26] where a Brink-type, i.e., crystal-like, approach is put into competition with the THSR approach with the latter the clear winner, it will be important in the future to find less heuristic ways to take off the spurious c.m. energies from the clusters, once they are formed in the mean field approach.

Summary and discussion.—In this work, for the first time, a rather systematic study for quite a number of self-conjugate nuclei is presented within mean field theory (HFB) concerning the formation of α particles when the nuclei are expanding, that is, at low density. Here, we adopted a static approach revealing rich scenarios of α cluster configurations and other heavier clusters, such as ^{8}Be and ^{12}C. However, for the lighter nuclei α clusters are

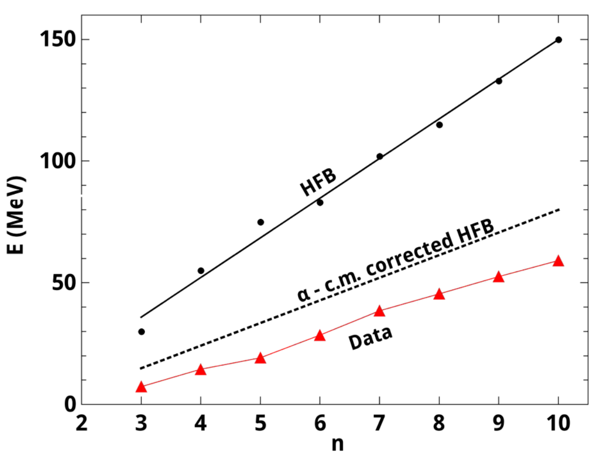

FIG. 6 (color online). Threshold energies as a function of the number n of α particles. Triangles: Experimental values; dots: values from HFB calculations, see text for precise definition; full line: best straight line fit to HFB results; broken line: α particle c.m. corrected HFB values.

largely dominant. The mean field approach has a great advantage over other cluster models to be entirely microscopic, employing a realistic energy density functional, and to be able to describe the formation of quite a large number of α particles and eventually other clusters. It can cover within the same approach all density regions going in a continuous way from stable nuclei to highly excited ones at low density where the clusters form. It is found in this work that by expanding an n-α nucleus the corresponding EOS-A goes over a maximum before reaching the asymptotic very low density limit of the α gas. This may be of importance in stabilizing an α phase. In principle there is no restriction for our 3D mean field approach to produce any kind of shapes and clusters in which the systems want to go. We also have checked that a single α particle is well described in HF with the Gogny force. Indeed, we have demonstrated in this work that there can exist a great variety of rather surprising and unexpected cluster configurations when the nucleus is expanding.

The disadvantage of the mean field approach is that it fixes the clusters to certain spatial positions as, e.g., on the corners of a tetrahedron in the case of ^{16}O, whereas it is predicted in recent work with the so-called THSR wave function that α particles rather form a (degenerate quantum) gas than a crystal [1–4,27]. To overcome this drawback, we applied in this work a purely heuristic procedure in eliminating "by hand" the spurious c.m. energy of each α particle. It is shown that in this way the theoretical threshold energies for n α's get rather close to the experimental values; see Fig. 2. Let us mention that other approaches have also been used before for the description of cluster formation [21,22]. This was mostly done within the antisymmetrized molecular dynamics [28] or fermionic molecular dynamics [21] approaches. We are not aware of any work that uses HF or HFB wave functions in a systematic study for clustering at low densities. The correct microscopic treatment of the spurious c.m. motion of clusters formed in a mean field approach remains an important task of nuclear many body physics for the future. Our work opens a variety of further investigations. Most interesting is the cluster formation as a function of neutron excess. Repeating our study with relativistic mean field may also be interesting, since it has recently been shown that relativistic mean field favors cluster formation [15]. We believe that the rich cluster scenarios found in this work are very inspiring, and we hope that this will trigger more experimental and theoretical work along this line in the future.

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