Clustering in atomic nuclei: a mean field perspective

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Abstract. In this paper the physics of clustering in atomic nucleus as seen from a mean field perspective will be discussed. Special attention is paid to phenomena involving octupole deformation like the α structure of 20Ne or the emission of heavy clusters. The stabilizing role of spin for cluster-like highly deformed states is also discussed in the case of 36Ar.

1. Introduction
Clustering is a fertile field of research in nuclear physics aiming to describe correlation among groups of particles to form aggregates like α particles, the doubly magic nucleus 16O or even 14C [1]. It leads to the understanding of resonances and highly deformed states in light nuclei in terms of cluster aggregates or nuclear molecules as described by the Ikeda diagram [2] of N = Z nuclei, further extended to neutron rich nuclei in Ref [3]. At the heart of clustering is the α particle with it whopping binding energy of 28.3 MeV. However, the binding energy gained by the formation of the α particles inside the nucleus has to compete with an energy loss coming from the increase in the surface of the nucleus as compared to a more compact configuration. It is competition between both effects what determines the cluster nature of a given state. A typical example is the Hoyle state in 12C that is viewed as three α particles located in the vertex of a triangle [4, 5]. Linear chains of α particles lead to hyper-deformed configurations located at a very high excitation energy at low spins. However, at high spins, they get closer to the yrast state and it is easier to characterize them. In heavy systems the existence of clustering is less clear although the phenomenon of cluster emission in the actinides can be regarded as a clustering effect driven by the characteristics of the heavy daughter nucleus.

Among the many theoretical methods used to quantify the physics of clustering we can mention the Anti-symmetrized Molecular Dynamics [6], Fermionic Molecular Dynamics [7] as well as mean field approaches (see [8, 9] for recent applications also dealing with the role of the low density equation of state in clustering). Proposals where the nucleus is depicted as an α particle gas and is described with a simple ansatz for the wave function (THSR wave functions) are also popular [10]. Other alternatives are discussed in the review article in Ref [11]. Last but not least we have to mention the Resonating Group Method of reactions [12]. In this paper, I will use the constrained mean field approach supplemented with some beyond mean field methods (symmetry restoration and configuration mixing) to analyze several physical situations involving clustering: hyper-deformed high spin states in 36Ar with a matter density resembling two 16O plus an α particle, the cluster structure of the first negative parity excited state of 20Ne or the phenomenon of cluster emission characteristic of many actinides.
2. The constrained nuclear mean field

The mean field approach used in the description of the atomic nucleus is based on the Hartree-Fock- Bogoliubov (HFB) approximation [13]. It encompasses in the same framework both the long and short range correlations present in the effective nuclear interaction. In the HFB approximation the elementary excitations are given in terms of the so called Bogoliubov quasiparticles described by creation and annihilation operators which are linear combinations of the creation and annihilation operators of a convenient (typically harmonic oscillator) basis

\[ \beta_\mu = \sum_k U_{k\mu} c_k + V_{k\mu} c_k^+, \quad \beta_\mu^+ = \sum_k U_{k\mu}^* c_k^+ + V_{k\mu}^* c_k \]  

(1)

The Bogoliubov amplitudes \( U \) and \( V \) satisfy unitary constrains in order to make the quasiparticle creation and annihilation operators preserve fermionic canonical commutation relations. This seemingly too technical comment is relevant because the \( U \) and \( V \) amplitudes are determined by using the variational principle on the HFB energy and therefore the unitary constraints prevent their immediate use as variational parameters. A more convenient parametrization of the HFB wave function \( |\Phi\rangle = \prod_\mu \beta_\mu \rangle \) is given by the Thouless theorem [13] that establishes that the most general HFB wave function not orthogonal to a reference one \( |\Phi_0\rangle \) is given by

\[ |\Phi(Z)\rangle = N(Z, Z^*) \exp \left(-\sum_{\mu\mu'} Z_{\mu\mu'} \beta_\mu^+ \beta_{\mu'}^+ \right) |\Phi_0\rangle \]  

(2)

The factor \( N(Z, Z^*) \) is chosen to normalize the wave function to one. There is a well defined way to compute the \( U \) and \( V \) amplitudes above as a function of the \( Z \) parameters that now are true independent complex parameters. They are determined by the variational principle on the energy \( E(Z, Z^*) = \langle \Phi(Z)|\hat{H}|\Phi(Z)\rangle \), where \( \hat{H} \) is the phenomenological nuclear hamiltonian already including short range correlations. Popular choices for \( \hat{H} \) are the Gogny, Skyrme and relativistic families of phenomenological interactions. All of them, in a way or another, include density dependent phenomenological terms that have to be handled with care both at the mean field level and beyond. All the calculations in this paper have been performed with the Gogny D1S parametrization [14].

The formation of clusters (or more precisely the existence of cluster-like correlations inside the nucleus) is driven by the nuclear interaction (for instance the huge binding energy of an \( \alpha \) particle) and it is difficult to disentangle in a mean field like wave function like the one depicted above. Therefore, the traditional approach to clustering from the mean field side is to look at the spatial density looking for structures resembling cluster aggregates. As those states are usually excited states a simple ground state mean field calculation is not enough and several constraints on quantities characterizing the mass distribution of the nucleus have to be imposed.

The energy minimization of the HFB now becomes a constrained minimization that involves the introduction of Lagrange multipliers \( \lambda_i \) and replacing the hamiltonian with

\[ \hat{H}' = \hat{H} - \sum_i \lambda_i \hat{C}_i \]  

(3)

where \( \hat{C}_i \) are the operators corresponding to the constrained quantities (plus the constraint on particle numbers). Those are usually taken as the multipoles of the mass distribution \( Q_{\lambda\mu} = r^\lambda Y_{\lambda\mu} \) with \( \lambda = 2 \) (quadrupole) and \( \lambda = 3 \) (octupole) although it may probe convenient to use other quantities like the neck \( n(z_0) = \exp(-\frac{(z-z_0)^2}{a_0^2}) \) or the “slice” \( n(z_0, -\infty) = \theta(z_0-z) \) operators often used in fission calculations. The Lagrange multipliers are fixed by the condition that the gradient of the energy

\[ H'^{20}_{\mu\nu} = H^{20}_{\mu\nu} - \sum_i \lambda_i (C_i)_{\mu\nu}^{20} = \frac{\partial E'(Z, Z^*)}{\partial Z_{\mu\nu}} = \langle \hat{H}' \alpha_\mu^+ \alpha_\nu^+ \rangle \]  

(4)
Figure 1. Left panel: the HFB energy of $^{36}$Ar is shown as a function of the quadrupole moment. Right panels: contour plots of the matter density at two values of $Q_{20}$.

has to be orthogonal to the gradient of the constraints

$$(C_i)^{20}_{\mu \nu} = \frac{\partial c_i(Z, Z^*)}{\partial Z^\mu \nu} = \langle \hat{C}_i \alpha^+_\mu \alpha^+_\nu \rangle. \quad (5)$$

Here lies the strength of the gradient method to solve the HFB equations: the inclusion of additional constraints do not increase the complexity of the calculation. The present formulation of the problem is a simplified version not including second order curvature terms in the gradient required for a fast and uniform convergence in the solution of the non-linear HFB equations. However the extension of the present formalism to handle that situation is straightforward [15].

3. Clusters at high spin

A common way to search for cluster like structures is to perform a HFB constrained calculation with the quadrupole moment as constraint. If axial symmetry is preserved only linear chains are accessible and the breaking of axial symmetry is required to describe more involved structures like the characteristic triangular shapes of the Hoyle state. A typical example of linear chains is provided by the nucleus $^{36}$Ar with $Z = N = 18$ that could show a $^{16}$O$^{16}$O+$^4$He like structure [16]. In Fig 1 we show the most salient results of our HFB constrained calculation for this nucleus. In the left hand side panel the HFB energy is shown as a function of the quadrupole moment. The nucleus $^{36}$Ar shows an oblate ground state but very close in energy to the spherical configuration: this nucleus can be considered as a soft spherical nucleus. At a quadrupole deformation of 1.5 b ($\beta_2 = 0.54$) we have a super deformed minimum which is rather shallow and corresponds to a funny matter distribution that resembles an elongated octagon (see center panel). At even higher quadrupole moments we observe at $Q_{20}$=3b ($\beta_2 = 0.85$) a shoulder in the energy that could be identify (see the right hand side panel) with a $^4$He nucleus surrounded by $^{16}$O at each side. The only problem with this configuration is that it is only a shoulder in the energy and therefore is unstable at zero spin at the HFB level. However, going to high spin the energy landscape gets modified as a consequence of the rotational energy correction $I(I+1)/(2J)$ and the almost linear increase of the moment of inertia $J$ with the quadrupole moment. This modification of the energy landscape helps to stabilize the super-deformed shallow minimum as well as the shoulder.
Figure 2. Left panel: the HFB energy (circles), the positive parity projected energy (bullets) and negative parity projected energy (squares) are shown as a function of the octupole moment. Right panels: contour plots of the matter density of two relevant configurations are shown. Contour levels values are $0.02 fm^{-3}$ apart.

at higher quadrupole moments. In order to analyze the high spin behavior of the nucleus we used in Ref [16] the technique of angular momentum projection to compute the energy as a function of both the quadrupole moment of the intrinsic state and the spin. In addition a Generator coordinate method calculation using the intrinsic quadrupole moment as collective coordinate was carried out on top of the angular momentum projected states. As discussed in Ref [16] the low spin states have an almost spherical intrinsic state. However, at angular momentum $I = 8\hbar$ the lowest state gets shifted to the intrinsic super-deformed configuration. The hyper-deformed intrinsic state corresponding to the exotic linear chain at $Q_{20}=3\hbar$ becomes the lowest energy at $I = 16\hbar$. From these results we conclude that indeed going to high spins helps stabilizing the exotic cluster like structures often observed as shoulders at zero spin in mean field calculations. The same effect is also observed in other nuclei in the region like $^{32}\text{S}$ [17].

4. Cluster structure of $^{20}\text{Ne}$

The nucleus of $^{20}\text{Ne}$ with its 10 protons and neutrons is a firm candidate to show clustering because it could be portrayed as a $^{16}\text{O}$ plus $^{4}\text{He}$ nuclei. It turns out that this structure is manifest in the matter density of the first negative parity excited state of $^{20}\text{Ne}$. To describe negative parity states one usually resorts to the octupole degree of freedom [18] due to its breaking of reflection symmetry. The restoration of this symmetry leads to two states, one of positive parity and the other of negative parity that are usually associated to the correlated ground state and the first negative parity excited state, respectively. Extensive studies using this concept lead to the conclusion that just in a handful of nuclei in the actinide and rare earth regions there is a unique intrinsic state for both parities [18]. For the other nuclei each parity has a different optimal intrinsic state that has to be computed using the Variation After Projection
Figure 3. Same as Figure 2 but for $^{52}$Fe.

(VAP) method [13] of symmetry restoration. In [18] we implemented the VAP method for parity restoration by first obtaining a set of HFB wave functions with different values of the (axially symmetric) octupole moment $|\Phi(Q_{30})\rangle$ and then computing the energy of the parity projected states $E^\pi=\frac{\langle \Phi(Q_{30})|\hat{H}\hat{P}_\pi|\Phi(Q_{30})\rangle}{\langle \Phi(Q_{30})|\hat{P}_\pi|\Phi(Q_{30})\rangle}.$

The intrinsic configurations (i.e. the intrinsic $Q_{30}$ values) for each parity are determined by looking at the minimum of the projected energies $E^\pi(Q_{30})$. The procedure is exemplified in the left hand side panel of Fig 2 for $^{20}$Ne. There we observe three curves that represent the HFB and parity projected energies as a function of the octupole moment computed with the Gogny D1S force. The positive parity curve has a minimum at $\beta_3 = 0.4$ whereas the minimum of the negative parity curve lies at a much higher octupole deformation of $\beta_3 = 0.95$. The excitation energy of the negative parity state is 6.7 MeV and the E3 transition strength to the $0^+\rightarrow 0^+$ ground state computed with the rotational formula is 12 W.u. The matter distribution of the two intrinsic configurations is depicted in the right hand side panels of Fig 2. For the positive parity intrinsic state we observe the typical density distribution of octupole deformed nuclei with moderate deformation. However, for the negative parity state the intrinsic state has a density that clearly resembles the $^{16}$O plus $^4$He matter distribution. A more quantitative assessment can be obtained by computing the number of particles $N(z,-\infty)$ obtained by integrating the matter distribution from $-\infty$ up to $z$. This definition takes advantage of the axial symmetry imposed in the calculation.

The clear identification of an $\alpha$ particle in the matter distribution is only possible in light nuclei. For heavier systems it is only possible to look for heavier fragments. To explore this

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1 See Ref [19] for a discussion of the difficulties in computing projected energies with density dependent forces.
Isosurface plot of the matter density of $^{224}\text{Ra}$ in its evolution from a near ground state configuration with $Q_{30} = 4000\text{fm}^3$ up to a very elongated configuration with $Q_{30} = 52000\text{fm}^3$ in steps of $Q_{30} = 6000\text{fm}^3$. Calculations are performed with the Gogny D1S force.

possibility I have performed calculations in $^{52}\text{Fe}$ which is a $^{12}\text{C}$ away from $^{40}\text{Ca}$. The results for the parity projected calculations are presented in Fig 3. The main difference is that now the negative parity state lies at a much lower $\beta_3$ value than in the $^{20}\text{Ne}$ case and, as a consequence, the matter distribution of the negative parity state has a structure where the $^{12}\text{C}$ is not as prominent as before and therefore it is more difficult to characterize as a cluster structure.

5. Cluster emission

In 1984 Rose and Jones [20], following a prediction by Sandulescu and collaborators [21], reported the results of an experiment where the emission of $^{14}\text{C}$ nuclei by $^{223}\text{Ra}$ was observed for the first time. Since then, the emission of $^{14}\text{C}$, $^{20}\text{O}$, $^{23}\text{F}$, $^{24,26}\text{Ne}$, $^{28,30}\text{Mg}$ and $^{32}\text{Si}$ light fragments by several isotopes of the actinides Fr, Ra, Ac, Th, U and Pu has been observed -see [22] for a review. This new kind of "radioactivity" lies in between traditional fission and $\alpha$ decay and its energy balance is mostly due to the heavier daughter being close to the doubly magic $^{208}\text{Pb}$.

Cluster emission, a name coined soon after its discovery, was successfully described theoretically by extending models of $\alpha$ decay to handle the emission of heavier clusters - by modifying the pre-formation factor. Before scission the parent nucleus is made of a heavy fragment and a touching lighter one. The mass distribution of such configuration closely resembles the shape of an octupole deformed nucleus with very large deformation parameter $\beta_3$. This is the main motivation to attempt the description of "cluster emission" by using the same mean field techniques applied to traditional fission but replacing the quadrupole moment constraint of fission by a constraint on the octupole moment. With this in mind, axially symmetric HFB calculations constraining the shape of the nucleus to have very large values of $Q_{30}$ were carried out. The details are thoroughly described in Ref [23] and section I above. A typical sequence of the evolution of the matter density distributions with increasing octupole moment is depicted in Fig 4 in the $^{224}\text{Ra}$ case.

As a typical example we will consider the nucleus $^{226}\text{Ra}$. Its HFB energy as a function of the octupole moment is shown in the left panel of Fig 5. The energy sharply increases as a function of $Q_{30}$ until a point at $Q_{30} = 35b^{3/2}$ where the nucleus breaks apart and the energy starts to decrease as a consequence of Coulomb repulsion (Path 1). The mass split corresponds to the emission of a $^{20}\text{O}$ nucleus. At this point it is also possible to find other configurations with two fragments like the one shown as Path 2. For large octupole moments this is the lowest energy solution and it corresponds to the emission of a $^{14}\text{C}$ cluster. In order to make sure that no additional two fragment solutions are available we carried out a calculation constraining $Q_{30}$ to $50b^{3/2}$ and the number of particles in the smallest fragment (denoted $A_R$). The energies obtained are depicted in the right hand side panel of Fig 5 as a function of $A_R$. We observe the presence of only two minima corresponding to the $^{14}\text{C}$ and $^{20}\text{O}$ fragments, being the $^{14}\text{C}$ the lowest in energy. As discussed in [23] it is possible to compute not only the energy of the nucleus in its path to cluster emission but also the collective inertias (associated with the
octupole degree of freedom) what allows the use of the standard techniques in fission to compute lifetimes for spontaneous emission using a WKB like formula. The results for the spontaneous cluster emission half life computed for many actinides are discussed in [23] where it is possible to observe a good agreement with experimental data that extends over several decades.

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