Alpha-like correlations in ^{20}Ne: comparison of quartetting wave function and THSR approaches

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Abstract.
^{20}Ne can be considered as a double-magic ^{16}O core nucleus surrounded by four nucleons, the constituents of an α-like quartet. Similar to other nuclei (^{212}Po, ^{104}Ti, etc.) with a quartet on top of a double-magic core nucleus, significant α-like correlations are expected. The quartetting wave function (QWF) approach predicts a large α-like cluster contribution near the surface of the nuclei. The Tohsaki-Horiuchi-Schuck-Röpke (THSR) approach describes α-like clustering in nuclear systems. The results of the QWF approach in the Thomas-Fermi and shell-model approximation are compared with THSR calculations for the container model.

1 Introduction

Nuclei consist of neutrons (n) and protons (p), which are spin 1/2 fermions. In the simplest approximation, we can describe nuclear systems as an ideal Fermi gas of quasiparticles. The shell model of nuclei considers the independent motion of the nucleons in a mean-field nuclear potential. Due to the strong interaction between the baryons, correlations occur which are not described in the quasiparticle approximation. In particular, cluster and bound states can be formed.

Two-particle correlations lead to pairing, that can also be obtained in mean-field approximation with respect to the interaction with the nuclear medium. Strong correlations are observed for α-like four-nucleon clusters. We consider a quartet $\{n_\uparrow, n_\downarrow, p_\uparrow, p_\downarrow\}$ that forms at zero density a bound state, the α particle, with a binding energy of 28.3 MeV and a point rms radius of 1.46 fm. We are investigating these important quartet correlations in nuclear matter at arbitrary density. A general goal would be to derive a description of quartetting in analogy to pairing, considering the interaction with the nuclear medium in mean-field approximation, i.e. neglecting the correlations between the quartet and the medium.

To model the interaction between the nucleons, we use the separable interaction [1]

$$V_{N-N}(p_1,p_2;p_1',p_2') = -\frac{\lambda}{\Omega} e^{-\frac{(p_2-p_1)^2}{4\gamma^2}} e^{-\frac{(p_2'-p_1')^2}{4\gamma^2}} \times \delta_{p_1+p_2,p_1'+p_2'}\delta_{\sigma\tau,\sigma'\tau'} \quad (1)$$

with Ω the normalization volume, $\lambda = 1449.6$ MeV fm^3, $\gamma = 1.152$ fm^{-1}. After separating the motion of the center of mass (c.m.) with momentum $P = p_1 + p_2 + p_3 + p_4$, we solve the Schrödinger equation for the free α-cluster using a Gaussian variational product approach in momentum space. For the intrinsic motion, we introduce Jacobi-Moshinsky variables $k_{12} = (p_2 - p_1)/2, k_{34} = (p_4 - p_3)/2, k = (p_3 + p_4 - p_1 - p_2)/2$ so that

$$\phi_\alpha^{\rm Gauss}(k,k_{12},k_{34}) = \frac{1}{\rm norm} e^{-(k^2+2k_{12}^2+2k_{34}^2)b^2/4}. \quad (2)$$

The solution for the variational parameter b reproduces the binding energy and the point rms radius of the α particle, $\langle r^2\rangle = (9/16)\, b^2$.

The properties of the quartet change when it is embedded in a nuclear medium. The solution for homogeneous nuclear matter is quite simple because we can use the plane wave representation. For clusters in inhomogeneous matter such as nuclei, the solution is very complex, in particular because of Pauli blocking, which is not local. A recent discussion of this problem and further references can be found in Ref. [1], which is the basis of this contribution, including the figures.

2 The quartet wave function in homogeneous matter

2.1 The quartet wave function in uncorrelated matter

In mean-field approximation where the correlations with the medium are neglected, the quartet wave function (QWF) is obtained from the in-medium Schrödinger equa-

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tion

$$[E_4-\hat{h}_1-\hat{h}_2-\hat{h}_3-\hat{h}_4]\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3,\mathbf{r}_4)$$
$$= \int d^3\mathbf{r}'_1\, d^3\mathbf{r}'_2\langle\mathbf{r}_1\mathbf{r}_2|\hat{B}(1,2)\ \hat{V}_{N-N}|\mathbf{r}'_1\mathbf{r}'_2\rangle\Psi(\mathbf{r}'_1,\mathbf{r}'_2,\mathbf{r}_3,\mathbf{r}_4)$$
$$+ \int d^3\mathbf{r}'_1\, d^3\mathbf{r}'_3\langle\mathbf{r}_1\mathbf{r}_3|\hat{B}(1,3)\ \hat{V}_{N-N}|\mathbf{r}'_1\mathbf{r}'_3\rangle\Psi(\mathbf{r}'_1,\mathbf{r}_2,\mathbf{r}'_3,\mathbf{r}_4)$$
+four further permutations, (3)

with the single-quasiparticle Hamiltonian (single-nucleon shell states $|n,\nu\rangle$)

$$\hat{h}_i = \frac{\hbar^2\hat{p}_i^2}{2m} + [1-\hat{f}_{\nu_i}]\,V^{\rm mf}_{\nu_i}(\hat{r}), \qquad \hat{f}_\nu = \sum_n^{\rm occ.} |n,\nu\rangle\langle n,\nu| \quad (4)$$

denoting the phase space which, according to the Pauli principle, cannot be used for an interaction process of a nucleon with an intrinsic quantum state $\nu = \sigma, \tau$. In addition to the nucleon-nucleon potential $\hat{V}_{N-N}$, the nucleon-nucleon interaction terms also contain the blocking operator $\hat{B}(1,2) = [1-\hat{f}_1-\hat{f}_2]$ for the first term on the r.h.s. of Eq. (3) and corresponding expressions for the other 5 terms. The mean-field potential $V^{\rm mf}_{\nu_i}(\hat{r})$ contains the strong core-nucleon interaction $V^{\rm ext}(r)$ as well as the Coulomb potential of the core nucleus. Note that the occupation $\hat{f}_\nu$ contains not only the quasiparticle orbitals, but also the contribution of the bound states if they occur in the medium.

It can be shown that the QWF is decomposed in a unique way in a factor which describes the c.m. motion and a factor which describes the intrinsic motion, but depends also parametrically on the c.m. variables. We are interested in the QWF of the c.m. motion in coordinate space. The intrinsic part of the wave function characterises the structure of the quartet, being a bound state with medium dependent point rms radius, or being an extended state in the continuum.

For a homogeneous system, the in-medium wave equation (3) becomes simple in momentum ($\hbar\mathbf{k}$) representation. If the density takes a finite value, due to the Pauli blocking the binding energy is shifted. If we assume uncorrelated matter, the phase space occupation $\hat{f}_\nu(k)$ is given by the Fermi distribution function. The solution is shown in Fig. 1 where (for symmetric matter at $T = 0$) the bound state energy and the edge of the continuum is given as a function of the nucleon density. Bound states appear for $n_B \leq 0.03$ fm^{-3}. To give a simple relation for the dependence on the baryon density, the fit formula derived within a variational approach to solve the in-medium four-nucleon wave equation,

$$\Delta E^{\rm Pauli}(n_B) = 4515.9\, n_B - 100935\, n_B^2 + 1202538\, n_B^3 \quad (5)$$

can be used, $n_n = n_p = n_B/2$. For $n_B \geq 0.03$ fm^{-3}, no bound state is formed, and the four nucleons added to the nuclear matter are implemented each on top of the Fermi energy.

Of interest is the behavior near the so-called Mott point [2], baryon density $n_B^{\rm Mott} = 0.03$ fm^{-3}. Within the variational approach, the Gaussian trial function (2) was taken with the width parameter b, and excluding the states within

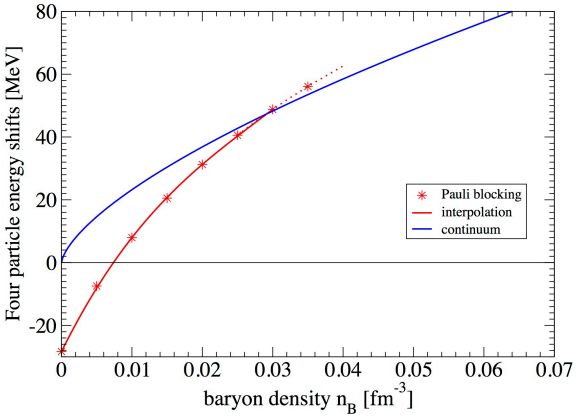

Figure 1. Intrinsic four-nucleon energy in a medium with baryon density $n_B = n_n + n_p$ (zero temperature). The continuum edge of free single-particle states is given by $4E_{\rm Fermi}$. At zero baryon density, the four-nucleon energy is given by the binding energy of the α particle, $E^0_\alpha = -B^0_\alpha = -28.3$ MeV. With increasing density, the binding energy B^0_α is decreasing due to the Pauli blocking. The four-nucleon bound state disappears at $n_B \approx 0.03$ fm^{-3}. A fit (interpolation) to the calculated values $\Delta E^{\rm Pauli}(n_B)$, Eq. (5), is also shown.

the Fermi sphere. The wave function at the minimum of the intrinsic energy of the quartet at finite b approximates the bound state solution of Eq. (3). A second local minimum appears at $b = \infty$ which describes an extended state, the edge of the continuum of the intrinsic states of the quartet. This solution is given by the product of four orbitals, zero angular momentum, at Fermi wave number k_F. At the critical density $n_B^{\rm Mott}$, the minimum of the energy jumps from a finite value of b to $b = \infty$. This means a sharp change of the intrinsic wave function of the α-like quartet from a localized state with a large overlap with the free α wave function to an uncorrelated product of free wave functions, where the overlap becomes zero.

So far, the question remains open whether the resolution of the bound state is associated with a jump in the form of the eigenstate of the nuclear system. Using a variational approach to solve the in-medium quartet wave equation (3) in a certain approximation may cause the jump of the solution. Near the Mott point, where the bound state merges with the continuum states, the variational approach should consider more flexible wave functions. An exact solution of the four-particle problem with the Faddeev-Yakubovski approach [3] argues for a sharp transition. The discussion of the consequences of this problem is a main topic of the present work.

2.2 The quartet wave function in correlated matter

A self-consistent description of a quartet in nuclear matter should allow that the medium also exhibits correlations. This requirement is fulfilled in the BCS theory of superfluidity, in which Cooper pairs move in a paired medium, the BCS state. Similarly, at low densities we expect a gas of alpha particles forming a Bose condensate ($T = 0$). While

the exact treatment of Pauli blocking is achieved with the BCS wave function, the Pauli principle is not easy to realize for α matter.

Within a simple model, calculations for periodic α-like structures were performed in [4]. Orthonormal Bloch states were introduced so that Pauli blocking by nucleons bound in α-clusters is strictly realized. One problem is the separation of the c.m. contribution to the kinetic energy, which is solved by a simple ansatz based on the energy gap at zero momentum. As a result, in Ref. [4] it was shown that the bound state merges with the continuum at about 0.03 fm^{-3}. Calculations with a separable potential adapted to reproduce the free-α properties mass and rms radius, have been performed in [1]. The difference between the energy per nucleon in the uncorrelated free-nucleon state (E_F) and the α-matter state is shown in Fig. 2. A value $\rho_{\rm Mott} = 0.04$ fm^{-3} was found for the dissolution of the bound state.

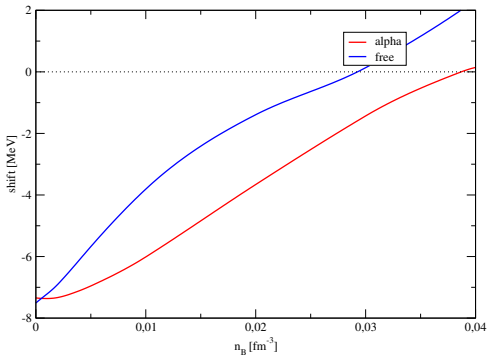

Figure 2. Shift of the binding energy per nucleon for an α-cluster as function of the nucleon density n_B. The difference of the energy per nucleon in α-matter and in momentum eigenstates (red) is compared with the shift (blue) in uncorrelated matter, Eq. (6).

For comparison, in Fig. 2 also shown is the shift of the binding energy for uncorrelated matter where the surrounding nuleons occupy free single-particle states,

$$E^{\rm uncorr}_{\rm bound}(n_B) = -7.07\,{\rm MeV} + \Delta E^{\rm Pauli}(n_B) - E_F(n_B). \quad (6)$$

Compared to the Pauli blocking by free nucleons considered in Eq. (5), the blocking in α matter is smaller because the distribution in momentum space is spreed out, and the blocking is less efficient. As a consequence, the critical density at which bound states are dissolved is larger when clustering in the environment is taken into account. However, the Mott effect also appears as a sharp transition for the periodic α matter model. The jump in the intrinsic structure of the quartet from a finite value of b, which changes only slightly with increasing density ($b = 1.934$ fm at zero density), to the delocalized value $b = \infty$ at the Mott density for this model matter is shown. Note that the energy per nucleon at zero density does not approach the free α value (-7.07 MeV) because the c.m. motion of the quartets, localized on the lattice, remains finite. The energy per nucleon, where the c.m. energy has been subtracted in some approximation, is shown in Ref. [1].

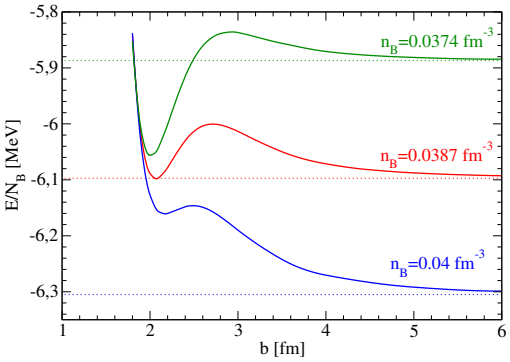

Figure 3. Energy per nucleon as function of the width parameter b at different nucleon density n_B. The result for the uncorrelated nuclear matter is shown as dotted line.

3 The quartet wave function in nuclei

Nuclei are inhomogeneous nuclear matter systems. Instead of plane waves, the quasiparticle approximation leads to the shell model where the orbits are calculated self-consistently within a mean field approach. A local density approach is difficult to perform because Pauli blocking is a non-local phenomenon. A simple approximation is the Thomas-Fermi model, where results for the homogeneous matter are used. Since the formation of correlations is important at low nucleon densities compared to the Mott density, α-like clusters can only exist in the low-density tails of the density distribution of nuclei. First steps have been taken [6–9] to start from the shell-model orbitals, but the formation of quartets needs further investigations. Pauli blocking, i.e. the antisymmetrization of the fermion wave function, is fully taken into account in the THSR approach, but the wave functions are assumed to be Gaussian, and the number of nucleons is limited. We present these three versions in the following subsections.

We use the theorem that the four-particle wave is decomposed uniquely in a c.m. part and an intrinsic part. For nucleons in an external potential, corresponding in-medium wave equations can be derived [5]. Solutions are found after performing several approximations. For the application to the α decay see Refs. [6–14]. We discuss here the application to ^{20}Ne [15]. The number of nucleons is not too large so that the various approximations can be performed.

3.1 Thomas-Fermi model with quartetting

The nucleons are moving in an mean-field potential $V(r)$ formed by the Coulomb interaction and the strong nucleon-nucleon interaction. We consider the double-magic core nucleus ^{16}O as a Thomas-Fermi gas of nucleons, chemical potential $\mu_\nu = V(r) + E_F[n_\nu(r)]$ for the

four components, and add the for nucleons of the quartet. The c.m. wave equation contains the mean-field potential $V(r)$ and an additional contribution given by the binding energy of the quartet, with the shift (5) given by the density of the core nucleons. The resulting potential has a pocket structure, see Fig. 4. In the range where the core nucleon density $n(r)$ exceeds the Mott density $n^{\rm Mott}$, the quartet is approximated by free states in the continuum, and these four additional nucleons are introduced at the chemical potential μ_ν. This gives the Thomas-Fermi condition $E_{\alpha,\rm bound} = E_{\rm c.m.} = 4\mu_\nu$ to solve the c.m. wave equation.

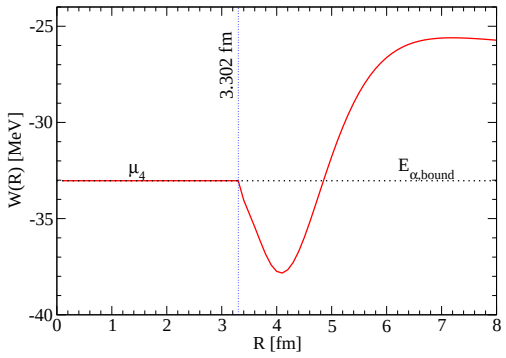

Figure 4. Effective potential for the c.m. motion of the quartet in ^{20}Ne. The Mott density of the ^{16}O core nucleus appears at $R = 3.302$ fm. Thomas-Fermi condition: The chemical potential μ_4 coincides with the bound state energy $E_{\alpha,\rm bound}$ of the α cluster.

We describe the formation of a cluster in the surface region of ^{20}Ne, and can calculate the overlap if the intrinsic wave function with the free α wave function. The rms radius of the ^{20}Ne nucleus is also well described.

3.2 Shell model with quartetting

Since nuclei are finite systems, the energy levels are discrete. The shell model provides quasiparticle states, which are occupied from the lowest energies until all nucleons of the core nucleus are inserted. An additional nucleon can occupy the lowest free state, which is separated by a gap. If we add a quartet of without mutual interaction, the four components of the quartet occupy the lowest free shell states so that the quartet energy $E_{\rm quartet,free}$ is higher than the sum of the four highest quasiparticle energies of the core nucleus. This gap is obtained from the shell model calculation for the nucleus.

If we have the four free quasiparticle states with the lowest possible energy available, we can construct the c.m. wave function and the intrinsic wave function of the quartet for this quartet of uncorrelated quasiparticle states. For the c.m. wave function we obtain the corresponding c.m. potential. Now we consider the mutual interaction of the components of the quartet. If the density of the nucleus is low, the c.m. potential is lowered by the free α binding energy. This shift is reduced by the Pauli shift and becomes zero when the density of the core nucleus approaches the Mott density.

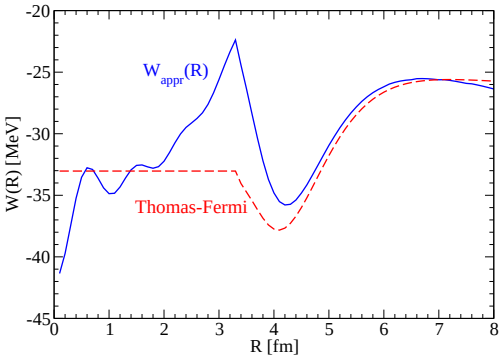

Figure 5. Effective potential for the c.m. motion of the quartet in ^{20}Ne. The shell model approach is compared with the Thomas-Fermi approach. At $R_{\rm Mott} = 3.302$ fm the nucleon density of the core nucleus takes the value of the Mott density.

Using this concept, the quartet was calculated within the shell model approach. A corresponding result for ^{20}Ne is shown in Fig. 5. The c.m. potential $W_{\rm appr}(R)$ is constructed from the four nucleons in the $2s$ orbitals which are orthogonal to the occupied $1s, 1p$ orbitals of the the ^{16}O core nucleus. This potential is not constant as in the case of the Thomas-Fermi model but increases with R, becoming zero at $R \to \infty$ if the intrinsic interaction is neglected.

For $R \geq R_{\rm Mott}$, a bound state can be formed, and we get a corresponding shift of the c.m. potential $W_{\rm appr}(R)$. A pocket is formed, and $W_{\rm appr}(R)$ approaches the Thomas-Fermi value at large R. The solution of the c.m. wave equation with the c.m. potential $W_{\rm appr}(R)$ gives the energy level of the quartet as well as the overlap with the free α wave function, see [1].

This solution of the shell model with quartetting has the shortcoming that at $R_{\rm Mott}$ a sharp peak for $W_{\rm appr}(R)$ occurs, which does not appear to be physical, but is due to the local treatment of the Pauli blocking shift. For larger nuclei such as ^{212}Po this effect is less dominant. One has to improve the local treatment of the Pauli blocking. In addition, the construction of the c.m. potential using free nucleon orbitals is not self-consistent. For a better approximation, the intrinsic wave function including mutual interaction must be solved in the space orthogonal to the occupied core states, and the construction of the c.m. potential $W(R)$ must be improved. Also for $R \leq R_{\rm Mott}$, correlations within the quartet owing to the mutual interaction are present. The non-local character of the Pauli blocking would also smear out the sharp peak at $R_{\rm Mott}$.

3.3 The THSR approach

Similar to the discussion in Sec. 2.2, a consistent approach would also take into account the quartet correlation in the core nucleus. In particular, if the quartet energy $E_{\rm quartet}$ is

lower than the quartet energy $E'_{\text{quartet,free}}$ of the highest core states, a reconstruction of the state function of the core with respect to quartetting occurs, similar to the discussion of pairing above.

A consistent description of a quartet in the medium, which also exhibits quartetting correlations, is obtained with the THSR (Tohsaki-Horiuchi-Schuck-Röpke) approach [16, 17]. The wave function of the core system is reconstructed in analogy to the BCS ground state. Quartets with intrinsic wave functions approximated by α-like Gaussian's, move in reference to the c.m. motion in a harmonic oscillator-like container potential. Since the c.m. motion of all clusters follows the same wave function, the analogy to the Bose-Einstein condensate was used. Of course, the entire nucleon wave function is completely antisymmetrized to satisfy the Pauli principle.

This approach has currently been generalized to describe ^{20}Ne using a two-parameter container model with different Gaussian c.m. wave functions for the ^{16}O core and the additional quartet in Ref. [18–21], where further references can also be found. We refrain from a detailed discussion of this approach. We only mention that the use of Gaussian factors makes the antisymmetrization of the wave function possible, but this variational approach could be improved to obtain more general forms for the wave functions.

To compare with the other approaches to introduce quartetting, we would like to derive a wave function for the c.m. motion of the valence quartet outside the ^{16}O-nucleus. However, due to the antisymmetrization of the full wave function, we cannot select a valence cluster. As in Ref. [1], a parameter can be introduced that is related to the effective radius and characterizes the distance between the valence cluster and the nucleus. The effective potential is shown in Fig. 6. For $R > R_{\text{Mott}}$ the behavior is similar to the Thomas-Fermi approach and a pocket is also formed. For $R \leq R_{\text{Mott}}$, the concept of a separate valence cluster in the THSR approach becomes problematic, and the c.m. potential cannot be determined with this approach.

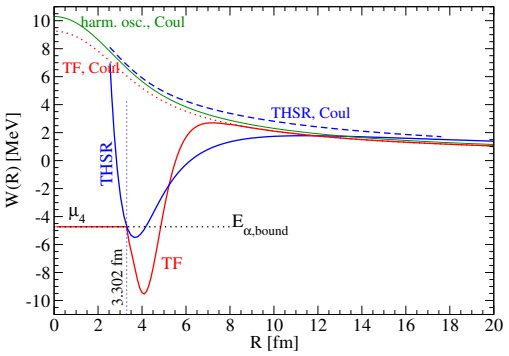

Figure 6. Effective ^{16}O - α interaction potential as function of the c.m. distance R. The THSR calculations (blue full line) are compared with the Thomas-Fermi approximation of the QWF (red full line). The total potential (TF, THSR) is shown as well as the Coulomb contribution (dashed lines). In addition, the Coulomb interaction for the harmonic oscillator density of the ^{16}O-core is also shown. At $R_{\text{Mott}} = 3.302$ fm the nucleon density of the core nucleus takes the value of the Mott density.

4 Discussion

To go beyond a quasiparticle approach for nuclear matter, correlations must be included. For two-particle correlations, pairing is well understood in the framework of a two-particle mean-field approximation. A similar treatment of quartetting, which describes the important α-like correlations in nuclear matter, remains to be worked out.

In this work, we discuss several examples, homogeneous matter and finite nuclei, without and with correlations in the medium surrounding the α-like quartet. A main effect is the dissolution of the bound state due to Pauli blocking when the density of the surrounding matter exceeds the Mott density. The bound state merges with the continuum of delocalised scattering states.

The main problem is the correct accounting of the Pauli blocking. In particular, the combination of quartetting with shell-model calculations would be of great interest. In the framework of the THSR approach, which was primarily developed to describe Hoyle-like nuclear states, Pauli blocking was strictly taken into account. This approach was further developed to be applicable to more complex nuclei. A closer connection to shell model calculations would be highly desirable.

The QWF approach was used in particular to describe the α decay of nuclei with a well-defined core nucleus and a valence α particle. Further applications are the formation of clusters on the surface of nuclei as seen in quasi-free α cluster-knockout reactions. The formation of α clusters is of interest in heavy ion collisions, ternary fission and astrophysical processes, which are not covered in this work.

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