One-, Two- and Three-Dimensional Alpha Lattice Structures of Nuclear Matter

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Alpha-clustering of nuclear matter is studied for the cases of one-, two- and three-dimensional geometry by using a density-dependent two-body effective interaction. We find that in three-dimensional space nuclear matter is more stable without the a-cluster structure at normal densities, while in one-dimensional space, a-structural nuclear matter can be more stable and at lower densities than usual. This has to do with the picture of a-chain structure of excited states of 4N nuclei.

Aglomerados alfa de matéria nuclear são estudados para os casos de geometria uni-, bi- e tri-dimensiional, usando-se uma interação efetiva de dois corpos, dependente da densidade. Nós achamos que a matéria nuclear, em um espaço tri-dimensiional, é mais estável sem a estrutura de aglomerados alfa, a densidades normais, enquanto no espaço uni-dimensi-onal a matéria nuclear estrutural alfa pode ser mais estável e a mais baixas densidades que o usual. Isso se relaciona com a estrutura de cadeia alfa de estados excitados de núcleos 4N.

1. INTRODUCTION

Alpha-clustering of nuclear matter was first investigated by an a-boson gas model. In this model, the internal structure and, therefore, the internal binding energy, of each a-particle are assumed to be kept un-
changed in the many body system. The Pauli principle is taken into account through the repulsive core of the effective a-a potential

Akaishi and the present author proposed an a-cluster lattice model of nuclear matter\(^2\), where nucleons interacting through a nucleon-nucleon interaction are treated explicitly, instead of assuming the rigid \(\alpha\)-particles from the outset. The model wave-function is able to describe the plane wave Fermi gas as a limit of the variational parameter, making it possible to trace the a-clustering. We adopted the simple cubic lattice structure, and studied the a-clustering of nuclear matter with respect to the average density. Based on a similar idea, Brink and Castro employed three different types of cubic structures (simple, body centred, and face centred), and carried out the calculations using two kinds of effective interaction\(^3\). A conclusion common to these works is that nuclear matter, at normal densities, prefers the plane wave Fermi gas structure to the a-cluster; however, the a-cluster lattice structure becomes more stable as the density decreases. From the local density point of view, this result is interpreted as the situation on the nuclear surface of finite nuclei.

Morinaga proposed a linear a-chain model to explain the rotational bands with large moment of inertia which are observed in the excited states of some light nuclei\(^4\). Ikeda, Horiuchi and Suzuki analyzed various observed quantities concerning the bands in \(^{12}\text{C}\) and \(^{16}\text{O}\), and also examined the stability of the linear multi-a-chain structure\(^5\).

Now, in view of the possible reality of the linear a-chain structure, it is interesting to study the a-clustering of nuclear matter with one-, two- and three-dimensional geometry. We make use of the a-cluster lattice model of Ref.\(^2\), with minor modification to account for the deformation of a-clusters. A density-dependent effective interaction, given by Sprung and Banerjee\(^6\), is used. The model is formulated in Sect. 2. Results and discussion are given in Sect. 3.
2. VARIATIONAL WAVE FUNCTION AND ENERGY EXPECTATION VALUE

In order to describe the linear, square and cubic $\alpha$-lattice structures of nuclear matter, we take a variational wave function expressed by a Slater determinant of orthonormal w.f. $\psi_k$:

$$\Psi = A \prod_{i=1}^{A} \psi_k(x_i, \sigma_i, \tau_i),$$

where

$$\psi_k(x_i) = \frac{1}{d_i^{3/2}} N_k^{-1/2} \sum_{n_k} e^{ikn} \phi(x-n).$$

$\chi(\sigma, \tau)$ denotes the spin-isospin function. An orbital state, $\psi_k$, is occupied by two protons, and two neutrons. The function $\phi(x-n)$ is a single particle wave function which characterizes the motion of a nucleon around the $n$-th lattice point. In Eq.(2), $d$ is a periodic distance, and $L$ is the size of the normalization box; $\pi$ takes the values 1, 2 and 3, according to the linear, square and cubic structure, and, correspondingly, the vector $n_k$ is $(0,0,n_z,0,0,n_z)$, $(0,n_z,n_z)$ and $(n_x,n_y,n_z)$, $n_k$ being an integer. The normalization factor $N_k$ is given by

$$N_k = \sum_{n_k} e^{ikn} \langle \phi(x) | \phi(x-n) \rangle.$$ 

We consider a cubic Fermi surface (-$k_{F.C.} \leq k_x, k_y, k_z \leq k_{F.C.}$) corresponding to the simple cubic lattice structure, similarly square and linear Fermi surface. A nucleons occupy the phase volume $4(2k_{F.C.})^L/(2\pi)^L$ and so the average density $\rho_0$ is related to $k_{F.C.}$ by

$$\rho_0 = 4(k_{F.C.} / \pi)^L.$$
Suppose that each lattice contains four nucleons in average \((\rho_0 a^T = 4)\); we get the relation,

\[ d \cdot k_{F.C.} = \pi \quad , \tag{5} \]

between the lattice distance and the Fermi momentum. The Fermi momentum defined in the Fermi sphere to give the same average density \(\rho_0\) is related to \(k_{F.C.}\) by

\[ k_{F.S.} = \left( \frac{\rho_0}{\pi} \right)^{1/3} k_{F.C.} \quad . \tag{6} \]

We adopt a simple Gaussian wave function for \(\phi(x)\) in Eq. (2):

\[ \phi(x) = \frac{\pi^{-3/4}}{a} \left( \frac{a}{b} \right)^{-1/2} \exp \left\{ -\frac{x^2}{2b^2} - \frac{y^2}{2b^2} - \frac{z^2}{2b^2} \right\} \quad . \tag{7} \]

The size parameters \(b\) are taken as follows:

\[ b_x = b_y = b_0 \quad , \quad b_z = b \quad \text{for 1-dim.} \]

\[ b_x = b_y = b_z = b \quad \text{for 2-dim.} \quad , \tag{8} \]

\[ b_x = b_y = b_z = b \quad \text{for 3-dim.} \]

The Hamiltonian consists of the kinetic energy plus an effective two-body interaction,

\[ H = \sum_i T_i + \sum_{i,j} \nu_{ij} \quad . \tag{9} \]

For \(\nu_{ij}\) we use the GO-force given by Sprung and Banerjee which is expressed as a sum of five Gaussian with different ranges and a \(\rho^{1/6}\) density dependence:

\[ \nu_{ST}^{(p)} = \sum_{\gamma=1}^{5} \left\{ \alpha_{ST}^{\gamma} + \beta_{ST}^{\gamma} \rho^{1/6} \right\} \exp \left( -r^2/k_{F}^{2} \right) \quad , \tag{10} \]

where \(S\) and \(T\) denote spin and isospin, respectively.
Now we present the expression of the energy expectation value with respect to the trial wave function (1) with Eqs. (2)-(8).

\[
E_I (b_0, b, k_{F.C.}) = T_I (b_0, b, k_{F.C.}) + V_I (b_0, b, k_{F.C.}),
\]

where \(E_I\), \(T_I\) and \(V_I\) are the total, kinetic and potential energies per particle, respectively, of the I-dimensional a-lattice nuclear matter. The variational parameters are \(b_0\) and \(b\), characterizing the size of the \(\alpha\)-cluster and the Fermi momentum \(k_{F.C.}\) (or, equivalently, the lattice distance \(d\)). After some algebra, the expressions are obtained as follows:

\[
T_I (b_0, b, d) = \frac{3-\frac{I}{2}}{4} \frac{\hbar^2}{MB_0^2} + \frac{I}{4} \frac{\hbar^2}{MB^2} \left[ 1 - \int_0^1 d\theta \left( \sum_{n \geq 1} \frac{\cos (n\pi \theta) (nd/2b)^2 \exp \left[ -(nd/2b)^2 \right]}{1 + 2 \sum_{n \geq 1} \cos (n\pi \theta) \exp \left[ -(nd/2b)^2 \right]} \right) \right]
\]

and

\[
V_I (b_0, b, d) = \frac{1}{8} \sum_{\gamma=1}^{5} \sum_{ST} 3^{S+T} \left( 1 + \frac{2b_0^2}{k_\gamma^2} \right) \left( 1 + \frac{2b^2}{k_\gamma^2} \right) \left( \alpha^{ST}_\gamma (\mathcal{D}^{ST}_\gamma (-)^{S+T}E^{ST}_\gamma^{I}) + \beta^{ST}_\gamma \xi^{I}_I (\mathcal{D}^{ST}_\gamma (-)^{S+T}E^{ST}_\gamma^{I}) \right)
\]

where the direct and exchange contributions, \(\mathcal{D}^0\) and \(E^0\) elevated to the \(I\)-th power in the previous equation, are given by

\[
\mathcal{D}^0 = \frac{1}{4} \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta_1 \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta_2 \left[ f_0 (\theta_1) f_0 (\theta_2) (g_0 (0) \xi_0 + g_2 (0) \xi_2) + f_1 (\theta_1) f_1 (\theta_2) (g_0 (0) \xi_2 + g_2 (0) \xi_0) + f_0 (\theta_1) f_1 (\theta_2) (g_1 (0) \xi_3 + g_3 (0) \xi_1) \right]
\]

\[+ f_1 (\theta_1) f_0 (\theta_2) (g_0 (0) \xi_3 + g_2 (0) \xi_1) + f_0 (\theta_1) f_0 (\theta_2) (g_1 (0) \xi_0 + g_3 (0) \xi_1) \]

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\[ E^0 = \frac{1}{4} \int_{-1}^{1} d\theta_1 \int_{-1}^{1} d\theta_2 \left\{ \left[ g_{012} (\theta_1, \theta_2) \right] \left[ g_{112} (\theta_1, \theta_2) \right] \right\} \left\{ \left[ g_{012} (\theta_1, \theta_2) \right] \left[ g_{112} (\theta_1, \theta_2) \right] \right\} \]

and

\[ F.\text{C.} \]

In Eqs. (14) and (15), the subscript \( \gamma \) specifying the force range is omitted for conciseness. Expressions of \( \mathcal{D} \) and \( E \) for the \( p \)-independent part of Eq. (13) are obtained by putting all \( \zeta \) equal to 1 in Eqs. (14) and (15). The various functions in Eqs. (14) and (15) are defined as

\[ f_j (\theta) = \sum_{n \geq 0} (2-\delta_j \delta_{n0}) \cos \left( (2n+j+1) \pi \theta \right) \exp \left[ -(2n+j+1)^2 \sigma^2 \right] , \quad j = 0, 1, \]

\[ g_{12} (\theta) = \sum_{n \geq 0} (2-\delta_j \delta_{n0}) \cos \left( (2n+j+1) \pi \theta \right) \exp \left[ -(2n+j+1)^2 \sigma^2 \right] , \quad j = 0, 1, \]

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where the integration variable \( k/k_{\text{F.C.}} \) is denoted by \( \theta \).

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\( \xi_I \) in Eq. (13) concerns the matrix element of \( \rho^{1/6} \) with respect to the center-of-mass wave functions of two interacting nucleons in an \( \alpha \)-cluster:

\[
\xi_I = 4^{1/6} \eta(b_0)^3 \eta(b)^I ,
\]

(19)

where

\[
\eta(b) = \left( \frac{2}{\pi b^2} \right)^{1/2} \int_{-\infty}^{\infty} \exp(-2z^2/b^2) \rho_\alpha(z)^{1/6} dz ,
\]

(20)

with \( \rho_\alpha(z) = (\sqrt{\pi b})^{-1} \exp(-z^2/b^2) \), \( z \) being one of the Cartesian coordinates, and hence \( \eta(b) = (12/13)^{1/2} (\sqrt{\pi b})^{-1/6} \).

\( \xi_J \) in Eqs. (14) and (15) are defined as the ratio of the matrix element of \( \rho^{1/6} \) of nuclear matter to that of a-particle:

\[
\xi_J = \eta(b)^{-1} \left( \frac{2}{\pi b^2} \right)^{1/2} \int_{-\infty}^{\infty} \exp(-2z^2/b^2) \rho(z + \frac{5d}{4})^{1/6} dz ,
\]

(21)

\( J = 0,1,2,3. \)

The density distribution \( \rho(Z) \) in the direction of extended matter is given by

\[
\rho(Z) = (\sqrt{\pi b})^{-1} \int_0^1 d\theta \left[ f_0(\theta) \sum_n e^{-(Z-n\theta)^2/b^2} + f_1(\theta) \exp(-Z(\theta)^2/b^2) \right] \times
\]

\[
\times \left[ f_0(\theta) + f_1(\theta) \right]^{-1}.
\]

(22)

The density distribution \( \rho(Z) \) is clearly periodic:

\[
\rho(Z+d) = \rho(Z)
\]

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and hence

$$\zeta_{j} = \eta(b)^{-1} (2/\pi b^2)^{1/2} \int_{0}^{d} \rho(z)^{1/6} \sum_{n=-\infty}^{\infty} \exp(-2(z - nd - jd/4)/b^2) \, dz,$$

$$j = 0, 1, 2, 3. \quad (23)$$

As seen in Eqs. (14), (15) and (23), the density dependence of the effective interaction works through only four numbers $\zeta_{j} (j=0, 3)$ (actually three because $\eta_{1} = \eta_{4}$) in the present model.

We have three variational parameters: the lattice distance (distance between closest two a-clusters), $d$ (or equivalently the Fermi momentum $k_{F.C.}$) and $b_{0}$ and $b$ characterizing the size of a-clusters in the direction perpendicular and parallel, respectively, to the extended matter. The ratio $b/d$ is an important measure of $\alpha$-clustering. If the ratio $b/d$ increases, the wave functions of a-clusters overlap each other and the nuclear matter is supposed to tend to the ordinary plane wave Fermi gas. In fact, we can prove that the expressions (22), (12) and (13) tend to the following forms in the limit of $b/d \to \infty$:

$$\rho(z) \to 1/d, \quad (24)$$

$$T_{I} \to \frac{3-I}{4} \frac{\eta_{0}^{2}}{M b_{0}^{2}} + \frac{I}{4} \frac{\eta_{0}^{2} k_{F.C.}^{2}}{M} \quad (25)$$

and

$$V_{I} \to \frac{1}{8} \sum_{r=1}^{5} \sum_{ST} 3^{S+T} \left\{ 1 + \frac{2b_{0}^{2}}{\kappa_{r}^{2}} \right\}^{3-3} \left\{ \frac{b_{0}^{2}}{r_{r}^{2} + \eta_{0}^{2}} \right\}^{4/6} \eta(b_{0})^{3-I} \left( \frac{k_{F.C.}}{\pi} \right)^{I-6} \right\}^{I} \times \left( \frac{\kappa_{F.C.} \kappa_{r}^{2}}{\sqrt{\pi}} \right)^{I} \left\{ 1 - (-)^{S+T} \left( \frac{1}{4} \int_{-1}^{1} d\theta_{1} \int_{-1}^{1} d\theta_{2} \exp \left( -\frac{1}{4} k_{F.C.}^{2} (\theta_{1} - \theta_{2})^{2} \right) \right)^{I} \right\}^{I} \quad (26)
By putting \( b' = 3 \), we can see that Eqs. (25) and (26) are just those of plane wave nuclear matter with cubic Fermi surface. On the other hand, in the limit of \( b/d \to 0 \), Eqs. (12) and (13) tend to

\[
T = \frac{3}{4} \frac{\hbar^2}{M b_0^2} + \frac{1}{4} \frac{\hbar^2}{M b^2}
\]

(27)

and

\[
V_I = \frac{1}{8} \sum_{r=1}^{5} \sum_{ST} \left[ 1 + \frac{2b_0^2}{\kappa_r^2} \right]^{\frac{I-3}{2}} \left[ 1 + \frac{2b^2}{\kappa_r^2} \right] \frac{1}{2} \times (\alpha_{ST}^r + \xi_{ST}^r)
\]

(28)

which corresponds to the energy per particle of an a-cluster (including the c.m. motion) confined around one of the lattice points.

3. RESULTS AND DISCUSSIONS

In order to visualize the a-clustering of nuclear matter, we show the density \( \rho(z) \) of Eq. (22) in Fig. 1 for different values of the ratio \( b/d \). We see that \( b/d \approx 1 \) already produces almost constant density distribution. In connection with this, we evaluate the overlap of the wave function (2) with the plane wave. The overlap for the three-dimensional case is given by

\[
e^{i k r} \frac{1}{2} |\psi_{\nu}(r)| = \prod_{i=1}^{3} O(b/d, k_x/k_{F.C.})
\]

(29)

\[
O(b/d, k/k_{F.C.}) = (2\pi b/d)^{1/2} \exp \left\{ -\frac{\pi^2}{2} \left( b/d \right)^2 \left( k/k_{F.C.} \right)^2 \right\}
\]

\[
/\{f_0(k/k_{F.C.}) + f_1(k/k_{F.C.})\}^{1/2}
\]

(30)
Fig. 1 - The density distribution $\rho(Z)$ in the direction of one of the Cartesian coordinates for some values of the ratio of the size of a-cluster $b$ to the lattice distance $d$.

Fig. 2 - The overlap between the single particle lattice wave function and the plane wave.
The function $O$ is shown in Fig. 2. As is expected, only the states close to the Fermi surface deviate appreciably from the plane wave and, for $b/d \approx 1$, the $\alpha$-lattice wave function (1) almost coincides with the ordinary Fermi gas wave function. Note that the normal density of nuclear matter ($k_{F,C} = 1.36 \text{ fm}^{-1}$) corresponds to $k_{F,C} = 1.10 \text{ fm}^{-1}$ and $\bar{d} = 2.86 \text{ fm}$. The value of $b$ is about $1.4 \text{ fm}$ in the free $\alpha$-particle.

Calculated energies for various $k_{F,C}$ are drawn in Fig. 3, as functions of the size parameter $b$. The parameter $b_0$ is fixed to $1.75 \text{ fm}$ for both the one- and two-dimensional cases. In the three-dimensional nuclear matter with $k_{F,C}$ above $0.7 \text{ fm}^{-1}$, the binding energy increases with $b$, indicating that the plane wave structure corresponding to $b = \infty$ is more stable than the $\alpha$-cluster lattice structure. For $k_{F,C}$ less than $0.7 \text{ fm}^{-1}$, the energy minimum appears at finite values of $b$, showing that the $\alpha$-cluster structure tends to be more stable. This result is consistent with the previous ones\textsuperscript{2,3}. By comparing the three-, two- and one-dimensional cases, we see that the critical $k_{F,C}$ is almost common to all cases, however the energy curves become flat wrt $b$ even at high density. In the one-dimensional case of $k_{F,C} = 0.9 \text{ fm}^{-1}$, the energy difference between the plane wave structure and the $\alpha$-cluster structure with $b = 1.75$ is only $0.3 \text{ MeV}$. This indicates that both structures are easily transferable with each other.

In our lattice model, the $\alpha$-clusters are always confined around the lattice points and therefore the energy expectation value includes the zero point oscillation energy of the c.m. of the $\alpha$-clusters, as can be typically seen in Eq. (27) for the low density limit. This is not quite realistic in such situations that the average density is low and the overlap between the $\alpha$-clusters is small, because the $\alpha$-clusters are considered to be able to move around with a smaller zero point energy. It is beyond the scope of the present approach to estimate precisely how much energy can be released from the c.m. kinetic energy of the $\alpha$-clusters included in the values of Fig. 3. However, it can be $I/16.\pi^2/Mb^2$ at maximum. Therefore, if this possibility is taken into consideration, the $\alpha$-cluster structure is probably more stable than the plane wave structure, at least in the one-dimensional case.
Fig. 3 - Total energies per particle for the one-, two- and three-dimensional cases plotted as a function of the size parameter of the α-cluster \( b \). The Fermi momentum \( k_{F,C} \) characterizing the average density is varied from 0.5 fm\(^{-1}\) to 1.1 fm\(^{-1}\). \( b_0 \) is fixed to 1.75 fm\(^{-1}\).
Fig. 4 shows the energies versus $k_{F,C}$ (or $d$) for two values of $b$: 1.75 and 2.5 fm; $b_0$ is fixed again to 1.75 fm. The energy minimum is obtained at $k_{F,C} = 1.05$, $0.95$ and $0.85$ fm$^{-1}$ for the three-, two- and one-dimensional cases, respectively. The value $k_{F,C} = 1.05$ fm$^{-1}$ corresponds to the normal density of nuclear matter. The corresponding binding energy is less by 3 MeV than that of the usual Fermi sphere, for which the GO-force is adjusted to give 16 MeV per particle. This is because of the cubic form of the Fermi surface. The value $k_{F,C} = 0.85$ fm$^{-1}$ in the one-dimensional case corresponds to the lattice distance $d = 3.7$ fm. This suggests the picture that the $\alpha$-particles are in line in contact with the neighbours, since the r.m.s. radius of $\alpha$-particle is about 1.6 fm. This fact indicates that the $\alpha$-particle-chain structure should appear, if the linear geometry is realized due to some physical effects.

Let us see finally the subtle point of the dependence on the parameter $b_0$. The energies versus $b_0$ are shown in Fig. 5; $b$ and $k_{F,C}$ are fixed to 1.75 fm and 0.9 fm$^{-1}$, respectively. The energies in Fig. 5 include the c.m. kinetic energy of each $\alpha$-cluster. We see that the energy minimum shifts to the smaller $b_0$ values for larger dimensional case as indicated by the arrows, showing that the $\alpha$-cluster tends to be compressed in the direction perpendicular to the extended matter. In some sense this must be a consequence of the saturation property of nuclei.

The main result of this paper is summarized as follows. Although the plane wave Fermi gas structure is favoured in the three-dimensional nuclear matter which is supposed to correspond to the ground states of nuclei, the linear $\alpha$-chain structure with the $\alpha-\alpha$ distance of about 3.5 fm is expected to appear as the most stable, if the one-dimensional geometry is realized in the excited states of nuclei.

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Fig. 4 - Total energies per particle plotted as a function of the Fermi momentum $k_{F,C}$ for two values of the size parameter of the a-cluster $b$. $b_0$ is fixed to 1.75 fm$^{-1}$. 
APPENDIX

The orthogonality of the basis function $\psi_k(x)$ (Eq. (2)) is proved generally from its periodic symmetry. For simplicity, proof is given for the one-dimensional case.

Equation (2) can be written as

$$\psi_k(x) \sim e^{ikx} u_k(x),$$  \hspace{1cm} (A.1)

$$u_k(x) = \sum_n e^{-ik(x-nd)} \phi(x-nd).$$  \hspace{1cm} (A.2)

The function $u_k(x)$ is clearly periodic, satisfying

$$u_k(x+d) = u_k(x).$$  \hspace{1cm} (A.3)

The following proof can be done by using only the functional form (A.1) and the periodic symmetry (A.3), without reference to the specific function (A.2).

\[
\int_{-\infty}^{\infty} \psi_k^*(x) \psi_k^*(x) \, dx = \int_{-\infty}^{\infty} e^{ik't-x} \, u_k^*(x) u_k, x \, dx
\]

\[
= \sum_n \int_{nd}^{(n+1)d} e^{ik't-x} \, u_k^*(x) u_k, x \, dx
\]

\[
= \sum_n \int_0^d e^{ik't-x} (y+nd) \, u_k^*(y+nd) u_k, (y+nd) \, dy
\]

\[
= \sum_n e^{ik't-x} \int_0^d e^{ik't-y} \, u_k^*(y) u_k, (y) \, dy
\]

\[
\sim \delta_{k',k} \int_0^d e^{ik't-y} \, u_k^*(y) u_k, (y) \, dy.
\]

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Fig. 5 - Total energies per particle for the one- and two- dimensional cases plotted as a function of the parameter $b_0$ are compared with the single a-particle. The parameters $k_{F,C}$ and $b$ are fixed to 0.9 fm$^{-1}$ and 1.75 fm, respectively. See text for further explanations.

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