Coulomb Energy of $\alpha$-Aggregates on a Soap Bubble Shape

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We study the property of $\alpha$-aggregates on a soap bubble shape within a microscopic framework, which takes full account of the Pauli principle. Our special attention is payed to the Coulomb energy for such an exotic shapes of nuclei, and we discuss the advantage of $\alpha$-clusters with geometric configurations compared with the uniform density distributions in reducing the repulsive effect. We consider four kinds of configurations of $\alpha$ clusters on a soap bubble, which are dual polyhedra composed of a dodecahedron and an icosahedron, octacontahedron and two types of truncated icosahedrons, that is, two kinds of Archimedean solids. The latter two are an icosidodecahedron and a fullerene shape. When putting each $\alpha$-cluster on the vertex of polyhedra, four $\alpha$-cluster aggregates correspond to the following four nuclei; Gd (64 protons), Po (84 protons), Nd (60 protons) and a nucleus with 120 protons, respectively.

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I. INTRODUCTION

This report is written as a series of the study on $\alpha$-cluster structure of heavy nuclei by microscopic aspect. We have already examined the extreme case of hollow configurations and pointed out that the systems have clear energy minimum points when $\alpha$ clusters approach from large distances, and we found that such shapes help very much in reducing the Coulomb repulsion [1]. For such studies, it is also inevitable to quantitatively scrutinize the effect of the Pauli principle with respect to the Coulomb energy, because the contribution of the exchange term works attractively.

The Coulomb energy is one of the main players against the stability of heavy nuclei owing to its strong repulsion. We know that the Coulomb energy is essential in nuclear fission, and also in the nuclear structure, whose quantity appreciably depends on the configuration of the protons. For instance, according to the electrostatics, the Coulomb energy of uniform density of positive point-charges inside a sphere is more repulsive than that on its surface as if they float on a soap bubble. Namely, the former is $\frac{4}{3} \frac{Q^2}{\rho}$, the latter is $\frac{1}{2} \frac{Q^2}{\rho}$, where $Q$ is total charge and $\rho$ is the radius of the sphere. This suggests the possibility that contribution of nonuniform distribution contributes in reducing the Coulomb repulsion. A long standing history of the studies for the shape of heavy nuclei has suggested the existence of special shape called as thin spherical shell nuclei [2], bubble nuclei [2], or torus nuclei [4][5], which prevent drastically the Coulomb repulsion. An appreciable dent in the middle of density distribution of $^{208}$Pb has been observed, which may support the mixing of components of hollowing nuclei [6].

For the proton distribution, it is natural to consider that they are in $\alpha$ clusters, since $\alpha$ clusters are the most stable existence compared with the other nuclear clusters.

With this assumption, it is important to seek for the optimum configurations of $\alpha$-clusters for heavier nuclear systems.

We again take a microscopic $\alpha$-cluster model in Brink-Bloch parameter space [2] and focus on the relation between the geometric configurations of $\alpha$ clusters and Coulomb repulsion more quantitatively. Here geometrical configurations are assumed within the framework, which takes full account of the Pauli principle. We can discuss the Coulomb energy with the Pauli principle extracting the corresponding part from the total binding energy. Therefore, in this report, we focus only upon the Coulomb energy for $\alpha$-clusters on a soap bubble shape and show how they are favored from Coulomb energy point of view.

As examples, we take four kinds of configurations originating in the icosahedron.

1. An Archimedean solid (truncated polyhedron); the 30 $\alpha$ clusters are put on each center of 30 edges of the icosahedron (corresponding to Nd).

2. A dual polyhedron composed of dodecahedron and icosahedron; the 20 $\alpha$-clusters are put on each center of 20 surfaces and 12 $\alpha$-clusters on the 12 vertices of the icosahedron (corresponding to Gd).

3. An octacontahedron; the 12 $\alpha$ clusters are put on the 12 vertices and 30 $\alpha$ clusters on each center of the 30 edges of the icosahedron (corresponding to Po).

4. Another Archimedean solid, the 60 $\alpha$ clusters have a well known fullerene shape.

Note that the second and third cases are adjusted to put all the $\alpha$ clusters on the same sphere (with the radius parameter $\rho$) and they correspond to nuclei, Nd, Gd, Po.
on the quantum mechanics \cite{13,14}. We hope to see analogous structures in a nucleonic world after clarifying the role of neutrons, which may provide a stability against the Coulomb repulsion. In other word, we propose a quantum mechanical $\alpha$ cluster architecture based on full microscopic quantum mechanics.

\section{II. FORMULATION}

We adopt an $\alpha$-clustering standpoint with a microscopic framework. We extract only the Coulomb energy from the total binding energy including kinetic, effective inter-nucleon force. We, here, employ Brink-Bloch type wave function for $n\alpha$ clusters, which takes full account of the Pauli Principle:

$$\Psi(\rho) = \mathcal{A}\{\phi(\rho R_1)\phi(\rho R_2)\cdots\phi(\rho R_n)\},$$

where $\mathcal{A}$ is the antisymmetrization operator among all the nucleons. The $n\alpha$ clusters are on the surface of the sphere with the radius $\rho$ (fin), and the vectors $R_1, R_2, \ldots, R_n$ are the parameters on the dimensionless unit sphere as shown in Fig. 1. The $k$-th $\alpha$ cluster ($k = 1, 2, \ldots, n$) wave function is written by

$$\phi(\rho R_k) = \prod_{i=1,2} \left(\frac{1}{\pi b^2}\right) \frac{1}{2} \exp\left\{-\frac{1}{2b^2}\left(r_{k}^{ij} - \rho R_k \right)^2\right\} \chi_{k}^{ij},$$

where $b$ is the nucleon size parameter, and $\chi_{k}^{ij}$ is a spin isospin wave function. The vector $r_{k}^{ij}$ is the real physical coordinate for the nucleon, and $i$ and $j$ are labels for the spin and isospin, respectively, for the four nucleons in the $k$-th $\alpha$ clusters. The four nucleons in the $k$-th $\alpha$ clusters share the common Gaussian center, $\rho R_k$. We prepare four sets of $\{R_1, \cdots, R_n\}$ corresponding to the configurations in Fig. 1. The norm and energy kernel matrix elements after carrying out the integration with respect to the real physical coordinates $\{r_{k}^{ij}\}$ are functions of variational parameter $\rho$. The Coulomb energy operator is written by

$$V^{(c)} = \frac{1}{2} \sum_{k,\ell, i,j} \frac{e^2}{|r_{k}^{ij} - r_{\ell}^{ij}|},$$

which acts only on the terms with $j=1$, namely, on the protons. Thus the Coulomb energy ($E_{c}(\rho)$) is defined by

$$E_{c}(\rho) = \langle \Psi(\rho)|V^{(c)}|\Psi(\rho)\rangle / \langle \Psi(\rho)|\Psi(\rho)\rangle.$$  

The numerator is given by

$$\langle \Psi(\rho)|V^{(c)}|\Psi(\rho)\rangle = \langle \Psi(\rho)|\Psi(\rho)\rangle \times \sum_{i'k'k''l'} \langle \phi(\rho R_k)\phi(\rho R_l)|\frac{e^2}{|r_{k}^{ij} - r_{\ell}^{ij}|}|\phi(\rho R_{l'})\phi(\rho R_{l''})\rangle \times (2G_{k'k}^{-1}G_{l'l}^{-1} - G_{k'l}^{-1}G_{k'k}^{-1}).$$
which is the sum of direct (proportional to \( G_{kk'}^{-1} G_{kk'}^{-1} \)) and exchange (proportional to \( G_{kk'}^{-1} G_{kk'}^{-1} \)) terms, where \( G_{kk'} \) makes \( n \times n \) matrix of which each element is given by

\[
G_{kk'} = \langle \phi(\rho R_k) | \phi(\rho R_{k'}) \rangle = \exp\{-\frac{\rho^2}{4b^2}(R_k - R_{k'})^2\}. \tag{6}
\]

In Eq. (4), the internal Coulomb energy of point-charged approximation of each \( \alpha \)-clusters is inevitably included as \( nE_{in} \). The each term for the Coulomb energy operator is given by an analytical form:

\[
\langle \phi(\rho R_k) | \phi(\rho R_l) | e^2 | \psi_{k'} - \psi_{l'}^\dagger | \phi(\rho R_{k'}) | \phi(\rho R_{l'}) \rangle = G_{kk'} G_{ll'} \frac{2e^2}{s_{kk' ll'}} \text{erf}\left(\frac{1}{2s_{kk' ll'}}\right), \tag{7}
\]

where \( s_{kk' ll'} = \frac{1}{\sqrt{2b}}|R_k - R_l + R_{k'} - R_{l'}| \), \( \text{erf} \) is an error function. We should compare the results with those from which the antisymmetrization operator is switched off. Namely, the term without the Pauli principle, so-called direct term, is symbolically denoted by \( E_{c(d)}(\rho) \). Note that the Coulomb energy in microscopic model depends on the size parameter of \( \alpha \). We are also interested in the comparison of results with those of point-charged approximation of each \( \alpha \). The electrostatics teaches us the results:

\[
E_{pc}(\rho) = \frac{4e^2}{\rho} \sum_{k<l} \frac{n}{|R_k - R_l|} + nE_{in}
= C_s(n) \frac{4e^2}{\rho} n(n - 1) + nE_{in}, \tag{9}
\]

where \( n \) is number of \( \alpha \) clusters and \( C_s(n) \) is a constant with respect to the geometric configuration of \( \alpha \) clusters as shown in Table I. We should point out that these values approach \( 1/2 \) corresponding to that of uniform distribution of positive particles on a soap bubble in limiting case of \( n \to \infty \). We, here, know that even such values directly depend on the \( \alpha \)-cluster configurations. In addition to three quantities on the Coulomb energy, \( E_c(\rho) \), \( E_{c(d)}(\rho) \), and \( E_{pc}(\rho) \), we compare two cases:

\[
E_{c(uS)}(\rho) = \frac{1}{2} \frac{4e^2}{\rho} n^2 + nE_{in}, \tag{10}
\]

and

\[
E_{c(uV)}(\rho) = \frac{3}{5} \frac{4e^2}{\rho} n^2 + nE_{in}, \tag{11}
\]

which are those of uniform \( \alpha \) cluster distribution on the surface of the soap bubble and uniform \( \alpha \) cluster distribution inside the sphere. The total charge \( Q \) is given by \( 2ne \). In the following section we discuss these five numerical values for four configurations, where the contribution of the Coulomb energy is divided by \( n \) (half of proton numbers).

### III. NUMERICAL RESULTS AND DISCUSSION

In Figs. 2~5, we show the Coulomb energy for one \( \alpha \) cluster versus the radius \( \rho \) for the four cases, Nd (Fig. 2), Gd (Fig. 3), Po (Fig. 4), and Fullerene (Fig. 5). Here, thick-solid, solid, dotted, dashed, and dash-dotted lines represent the Coulomb energy for one \( \alpha \) defined in Eq. (11) \( (E_{c}(\rho)/n) \), its direct term \( (E_{c(d)}(\rho)/n) \), point charge approximation defined in Eq. (9) \( (E_{pc}(\rho)/n) \), uniform \( \alpha \) cluster distribution on a surface defined in Eq. (10) \( (E_{c(uS)}(\rho)/n) \), and uniform \( \alpha \) cluster distribution in a sphere defined in Eq. (11) \( (E_{c(uV)}(\rho)/n) \), respectively. For the number of neutrons, the Coulomb energy is common for all the isotopes of an individual atom. However, the appropriate \( \rho \) depends on the radius of isotopes with the same proton number, which are related to the neutron number \( N \). In this model, the main part of the neutrons is trapped in the \( \alpha \)-clusters, then the excess of neutrons is estimated as \( N - 2n \). If the excess neutrons exist inside, all the protons in the \( \alpha \)-clusters float on the sphere. On the other hand, they are outside, then the nucleus has an appreciable cavity. Anyhow, the radius \( \rho \) of the sphere is not independent of the number of excess neutrons, in assuming that the nuclear radius is the function of only the mass number \( A = Z + N \). The possible range of \( \rho \) is shown in Figs. 2~5 by a belt with net in assuming the nuclear radius \( r_0 A^{1/3} \) with \( r_0 = 1.2 \) fm and plausible mass numbers, 2.0Z \( \leq A \leq 2.7Z \), where for heavy nuclei, not only many isotopes but also a variety of positions of \( \alpha \)-cluster are imagined.

It should be noted that even for heavy nuclei, in cluster models, we can correctly obtain numerical values without any round-off errors in the radius parameter region of 1.5 fm \( \geq \rho \). Although the norm kernel, \( \langle \Psi(\rho)|\Psi(\rho) \rangle \), is incredibly small in the small radius of the sphere, the inverse matrix of \( G_{ik} \) is not divergent. We can indicate many interesting features from Figs. 2~5 as follows:

1. The Pauli principle drastically influences the region with small \( \rho \) values of the sphere and decreases the energies in all nuclei. We can know, unlike the curves without the Pauli principle (solid lines), a definite convergence of the Coulomb energy in the case of thick solid lines at small \( \rho \) regions. The exact Coulomb energy in thick solid lines converged to finite values at \( \rho \to 0 \), which cannot be seen in other lines. This effect works in reducing the incompressibility of heavy nuclei.

| \( n \) | \( C_s(n) \) |
|-----|-----|
| 30  | 0.4153 |
| 32  | 0.4156 |
| 42  | 0.4252 |
| 60  | 0.4384 |
On the contrary, in the range of the belt with net corresponding to plausible radii of the isotopes (the left and right edges correspond to \( r_l = r_0(2.0Z)^{1/3} \) and \( r_r = r_0(2.7Z)^{1/3} \), respectively), three curves, \( E_c(\rho)/n \) (thick solid lines), \( E_c(\delta)(\rho)/n \) (dotted lines), and \( E_{pc}(\rho)/n \) (dashed lines), almost coincide with each other in all figures. Surprisingly, even the point-charge model well works in this region. This means that the point charged cluster model, where the Pauli principle is switched off, may be useful for the studies of heavy nuclei based on the cluster models as the first step. For instance, it is possible to employ Ali-Bodmer force between two \( \alpha \)-clusters [15] and phenomenological \( N-\alpha \) force [16].

The curves with geometric \( \alpha \) cluster configurations, \( E_c(\rho)/n \) (thick solid lines), \( E_c(\delta)(\rho)/n \) (dotted lines), and \( E_{pc}(\rho)/n \) (dashed lines), are quite different from that of the uniform density distribution of \( \alpha \) clusters on the surface \( E_c(\rho)/n \), dashed lines) and that in the sphere \( E_{c(\delta)}(\rho)/n \), dash-dotted lines) in all figures. Therefore, the \( \alpha \) clusters with
TABLE II: The \( p(\rho) \) values for the Pauli effect defined in Eq. \( 13 \), and \( p_I = r_0(2.0Z)^{1/3} \) and \( p_r = r_0(2.7Z)^{1/3} \) correspond to the left and right edges, respectively. The quantities \( d_l \) and \( d_r \) mean the nearest neighbor distance of \( \alpha-\alpha \) on the surface obtained with \( \rho = p_I \) and \( p_r \), respectively.

| \( n \) | \( p_I \) (fm) | \( p(p_I) \) | \( d_l \) | \( p(r) \) | \( p(p_r) \) | \( d_r \) |
|---|---|---|---|---|---|---|
| 30 | 5.9 | 0.984 3.7 | 6.5 | 0.870 | 4.1 |
| 32 | 6.1 | 0.947 3.9 | 7.0 | 0.578 | 4.5 |
| 42 | 6.6 | 0.998 3.6 | 7.3 | 0.939 | 4.0 |
| 60 | 7.5 | 1.000 3.0 | 8.2 | 1.000 | 3.3 |

geometric configurations may be responsible for the study of heavy nuclei, when they are on the surface.

4. The mixing of geometrical configurations drastically reduces the Coulomb repulsion, and as the dent in the middle of \( ^{208}\text{Pb} \) has been observed \[3\], the uniform distribution of protons, the case of \( E_{c(uV)}/n \) may not be plausible, which is a basic idea of Bethe-Weizsacker’s mass formula. This fact may deeply require understanding the distribution of nucleons in nuclei from scratch.

We consider the effect of the Pauli principle with respect to the radius \( \rho \) of the sphere. The diagonal part of the norm kernel has the following property depending on the Pauli principle:

\[
\lim_{\rho \to 0} \langle \Psi(\rho) | \Psi(\rho) \rangle = 0, \tag{12}
\]

and

\[
\lim_{\rho \to \infty} \langle \Psi(\rho) | \Psi(\rho) \rangle = 1. \tag{13}
\]

When we consider only the proton contribution, the index of the Pauli effect is taken as

\[
p(\rho) = 1 - \sqrt{\langle \Psi(\rho) | \Psi(\rho) \rangle}. \tag{14}
\]

The effect coming from the off-diagonal part (different \( \rho \) for bra and ket states) is not considered, which should be taken into account when studying these nuclei dynamically. At both sides of the edges of the belt with net in Fig. 2~5 (the left and right edges correspond to \( p_I = r_0(2.0Z)^{1/3} \) and \( p_r = r_0(2.7Z)^{1/3} \), respectively), we give the quantities of \( p(\rho) \) in Table II. The quantities \( d_l \) and \( d_r \) mean the nearest neighbor distance between two \( \alpha \)-clusters on the surface of the spheres obtained with \( \rho = p_I \) and \( p_r \), respectively. We see from Table II appreciable effect in this region. Nevertheless the three kinds of the Coulomb energies (\( E_c(\rho)/n \), \( E_{c(d)}(\rho)/n \), \( E_{pc}(\rho)/n \)) well coincide with each other as mentioned before, thus we need detailed analysis on the role of the Pauli principle, which can be described in terms of the exchange number of nucleons.

Anyhow, it is natural that the heavier the nucleus is, the stronger the Coulomb energy is. Thus, we should study the stability of \( Z = 120 \), for instance, by applying an effective inter-nucleon force appropriate for the cluster model to account the Coulomb repulsion. We are also waiting for not only the next research taking account of the effective inter-nucleon force but also the consideration of the oozy of excess neutrons.

Our previous report obtained by applying Tohsaki F1 force \[16\] as inter-nucleon force has pointed out that the property of \( \alpha-\alpha \) interaction remains even inside heavy nuclei, such as 60 \( \alpha \) clusters with a fullerene shape \[1\]. Namely, the relative distance of nearest neighbor of \( \alpha-\alpha \) is always around 3.3 fm, which is the optimal distance between \( \alpha \) clusters in the free space. In Figs.2~5, thick arrows show the radius of sphere \( \rho \), in which nearest neighbor corresponds to 3.3 fm. Here the place of arrows for comparably light nuclei (Nd, Gd, Po) is smaller than the belt, on the other hand, the case with \( Z = 120 \), the arrow is inside the belt. As for former three cases, the excess neutrons, which are not contained in \( \alpha \) clusters, may widely exist outside of the sphere. On the other hand, unknown ultra super heavy nucleus with \( Z = 120 \) has 60 \( \alpha \)-clusters floating on surface of the sphere, which enfolds excess neutrons. In Table III, five kinds of energy quantities (\( E_c/n \), \( E_{c(d)}/n \), \( E_{pc}/n \), \( E_{c(uS)}/n \), and \( E_{c(uV)}/n \)) are listed for the fixed nearest neighbor distance with \( d = 3.3 \) fm. We may point out that the former there nuclei, which have arrow positions before the belt regions, have appreciable quantity of the Pauli principle, where the \( E_c/n \) values are slightly lower than \( E_{c(d)}/n \).

IV. SOME REMARKS

Following our previous report \[1\], we studied the Coulomb energy of the \( \alpha \)-clusters on a soap bubble. We, here, indicated the advantage of the geometric configurations of \( \alpha \)-clusters in reducing the Coulomb repulsion by comparing with two types of uniform distributions of \( \alpha \) clusters, namely, an uniform distribution inside the sphere and that on the surface of the sphere. We also have shown that the Pauli principle drastically influences the region with small radius parameter \( \rho \) of the sphere and decreases the energies in all nuclei. A definite convergence of the Coulomb energy has been shown at \( \rho \to 0 \).

TABLE III: The energies of \( E_c/n \), \( E_{c(d)}/n \), \( E_{pc}/n \), \( E_{c(uS)}/n \), and \( E_{c(uV)}/n \) (all in MeV) for the four geometric configurations shown in Fig. 1, where \( n \) is number of \( \alpha \) cluster. The energies are calculated at the radius parameter \( \rho \), which gives 3.3 fm for the nearest neighbor distance. The \( \alpha-\alpha \) distance of 3.3 fm is the optimal one in the free space.

| \( n \) | \( \rho \) | \( E_c/n \) | \( E_{c(d)}/n \) | \( E_{pc}/n \) | \( E_{c(uS)}/n \) | \( E_{c(uV)}/n \) |
|---|---|---|---|---|---|---|
| 30 | 5.34 | 6.76 | 6.87 | 6.90 | 8.50 | 10.11 |
| 32 | 5.15 | 7.44 | 7.57 | 7.61 | 9.35 | 11.14 |
| 42 | 6.04 | 8.56 | 8.69 | 8.72 | 10.42 | 12.42 |
| 60 | 8.18 | 9.43 | 9.49 | 9.51 | 10.87 | 13.08 |
unlike the curves without the Pauli principle. On the contrary, in the range of plausible radii of the isotopes even the point-charge model well works. This means that the point charged cluster model, where the Pauli principle is switched off, may be useful for the studies of heavy nuclei based on the cluster models as the first step.

However, in this model, it is indispensable to investigate the distribution of the excess neutrons. Uniform distribution of excess neutrons, otherwise di-neutron pairing, and inside or outside, there are various kinds of possibilities. Before that, we should find out the most reliable inter-nucleon force including many-body terms for cluster model due to the guarantee of the saturation property of nuclear matter. In our previous study for the geometric configurations [1], we have utilized Tohsaki F1 force [17], which guarantees the saturation properties and also reproduces the $\alpha$-$\alpha$ scattering phase shift. This interaction should be more examined in neutron-rich side, as we have introduced for light neutron-rich nuclei [18, 19]. In order to step in the world of fundamental phenomena in heavy nuclei, which contain $\alpha$-decay, $\beta$-decay, fission and so on, it is necessary for us to clarify the role of excess neutrons within the microscopic cluster model. This is because the microscopic cluster model, which naturally includes the ground state of the shell model, can exactly evaluate the Pauli principle.

In this article, we discussed the geometric configurations; however the opposite aspect is gas-like behavior of the $\alpha$ clusters. We have previously introduced the Tohsaki Horiuchi Schuck Röpke (THSR) wave function for the studies of gas-like nature of $\alpha$ clusters in various nuclei including the so-called Hoyle state of $^{12}\text{C}$ [20]. Therefore, the next step should go to the study for heavy nuclei within a microscopic cluster model by using the THSR model, which is most suitable for the gas-like cluster structure with a microscopic aspect. Description of $\alpha$ distribution on the surface or inside the sphere based on this approach is on going, and we compare with the results of the geometric configurations.

Acknowledgments

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