Gap to hinder the rotational excitation of the ground state of a 13-boson system

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A 13-boson system has been qualitatively studied based on symmetry consideration. The rotational excitation of the ground state is found to be greatly hindered. The geometric feature and some specific modes of internal oscillation of low-lying states have been predicted. An idea for the classification of states has been proposed. A number of rotation bands have been suggested.

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Thirteen is a well known magic number definitely found in nature in the systems composed of various kinds of constituents, e.g., in atomic clusters [1,2]. Even in nuclear systems, the separation energy of a neutron separated from the ^{13}C nucleus was found to be considerably larger [3]. During the past century the magic number has been accounted for by hard-sphere-packing models [4]. However, as quantum-mechanical systems, the physics involved might be much richer. A system with 36 internal degrees of freedom (if the spins are not taken into account) is not able to be quantitatively calculated without approximations at present. This is planned for a work in the future. Nonetheless, a qualitative study might be useful because in this way the underlying physics can be more or less demonstrated, thereby the forthcoming results from theoretical calculations and from experimental observations can be better understood. In this paper a qualitative analysis based on fundamental principles is performed to extract the feature of the low-lying spectrum of a 13-body system of identical bosons with zero spin. The emphasis is placed on the classification of low-lying states.

In coordinate space the wave functions of low-lying states are mainly distributed in the domains with lower potential energy. For a 13-body system with the pairwise interactions containing a repulsive core and an attractive tail, there are three such important domains: (i) the domain surrounding a centered icosahedron (ICO) with an appropriate size as shown in Fig. 1(a), where 42 bonds can be optimized; (ii) the domain surrounding a centered cuboctahedron (CUBO) with an appropriate size as shown in Fig. 1(b), where 36 bonds can be optimized; and (iii) the domain of a shape with a sixfold axis as shown in Fig. 1(c), where the twelve outer particles form two hexagons, where also 36 bonds can be optimized. The other domains are much higher in total potential energy, and therefore are not important.

For the above three important domains, the ICO is the most important (the total potential energy at the ICO is the lowest), and the CUBO is the second most important. For example, for a 13-Ar system, when the pairwise interaction is taken from Ref. [6], the resultant total potential energies at the ICO, CUBO, and the ''sixfold'' shape with optimal sizes are -0.465 eV, -0.428 eV, and -0.398 eV, respectively.

Let us first investigate the behavior of wave functions in the domain of the ICO. It is noted that the existence of an m-fold axis implies that a rotation about the axis by $2\pi/m$ is equivalent to a cyclic permutation of particles. It turns out that this equivalence will impose a constraint. For example, let A denote a geometric configuration with an m-fold axis, let O be an operator of rotation about the axis by the angle $2\pi/m$, and let Ψ be a totally symmetric wave function of spatial coordinates. We then have

$$O\Psi(A)=\Psi(O^{-1}A)=P_{\text{cyclic}}\Psi(A)=\Psi(A), \tag{1a}$$

where P_{cyclic} denotes the cyclic permutations of the particles surrounding the m-fold axis. The last equality holds only for totally symmetric functions of bosonic systems. Thus we have

$$(O-1)\Psi(A)=0. \tag{1b}$$

When Ψ is a basis function of a representation of the rotation and inversion group, Eq. (1b) can be written in a matrix form and appears as a set of homogeneous linear algebra equations (as we shall see). This set of equations must be fulfilled by Ψ at A, thus the behavior of Ψ is constrained. It is noted that the ICO is a highly symmetric shape related to the icosahedral group [5]. It contains six fivefold axes, ten threefold axes, and fifteen twofold axes. Thus, wave functions are definitely strongly constrained at the ICO.

Let us introduce a body frame i'-j'-k' as marked in Fig. 1(a). Let a totally symmetric and translational invariant eigenstate of a 13-boson system with a given total orbital angular momentum L and a given parity Π be expanded as

$$\Psi_M(1,\ldots,13)=\sum_Q D^L_{QM}(-\gamma,-\beta,-\alpha)\Psi_Q(1',\ldots,13'), \tag{2}$$

where M and Q are the projections of L along a fixed Z axis and along the k' axis, respectively; $\alpha\beta\gamma$ are the Euler angles for the rotation of the body frame and D^L_{QM} is the Wigner function. The $(1,\ldots,13)$ and $(1',\ldots,13')$ specify that the coordinates are relative to the fixed frame and to the body frame, respectively. Ψ_Q is called a Q component. Together they form a representation of the rotation, inversion, and permutation groups.

When the particles form an ICO as in Fig. 1(a), the k' axis is a fivefold axis. Therefore, a rotation about k' by $2\pi/5$ is equivalent to $p(3,4,5,6,7)p(8,9,10,11,12)$, where $p(i,j,\ldots)$ denotes a cyclic permutation which does not cause a change in bosonic systems. Thus, Eq. (1b) for each Q component is now written as

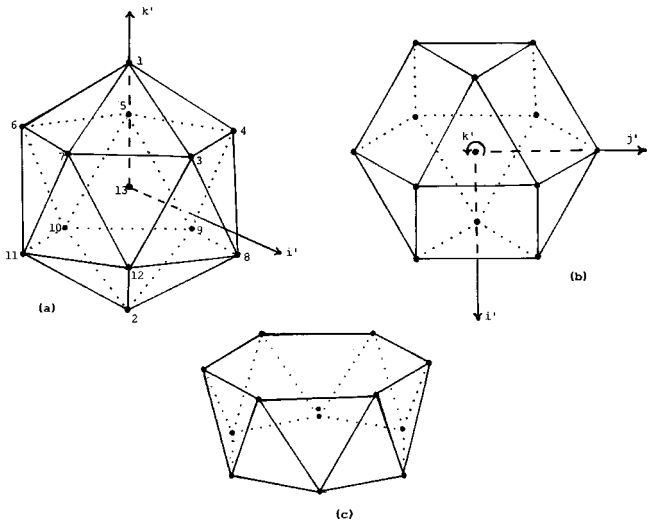

FIG. 1. A regular icosahedron (a) where the i' axis lies on the plane of the particles 1, 3, 2, and 10; a cuboctahedron (b); and a hexagon-pontoon with a sixfold axis (c).

$$(e^{i(2\pi/5)Q}-1)\Psi_Q(ICO)=0 \quad (Q \text{ is from } -L \text{ to } L), \tag{3}$$

where (ICO) denotes that the coordinates form an ICO.

Let B denote the c.m. of the particles 1, 5, and 6; B' denotes the c.m. of the particles 2, 8, and 12. The straight line BB' is a threefold axis which goes through the total c.m. and lies in the i'-k' plane. The angle between BB' and k' is

$$\theta_1=\arcsin[\sqrt{4\sin^2(\pi/5)-1}/\sqrt{3}\sin(\pi/5)]. \tag{4}$$

Let the operator of a rotation about an axis $\vec{n}$ by an angle θ be denoted as $R^{\vec{n}}_{\theta}$. We have

$$R^{BB'}_{2\pi/3}=R^{j'}_{-\theta_1}R^{k'}_{2\pi/3}R^{j'}_{\theta_1}. \tag{5}$$

Thus, for the rotation about BB', Eq. (1b) becomes

$$\sum_{Q'}\left(\sum_K d^L_{Q'K}(-\theta_1)e^{i(2\pi/3)K}d^L_{KQ}(\theta_1)-\delta_{QQ'}\right)\Psi_{Q'}(\mathrm{ICO})=0, \tag{6}$$

where $d^L_{Q'K}(\theta_1)=D^L_{Q'K}(0,\theta_1,0)$.

Let D denote the c.m. of the particles 1 and 3; D' denotes the c.m. of the particles 2 and 10. The straight line DD' is a twofold axis which goes through the total c.m. and lies also in the i'-k' plane. The angle between DD' and k' is

$$\theta_2=\arccos[1/2\sin(\pi/5)]. \tag{7}$$

Similarly, the rotation about DD' leads to

$$\sum_{Q'}\left(\sum_K d^L_{Q'K}(\theta_2)e^{i\pi K}d^L_{KQ}(-\theta_2)-\delta_{QQ'}\right)\Psi_{Q'}(\mathrm{ICO})=0. \tag{8}$$

Equations (3), (6), and (8) are the equations of constraint from a fivefold, threefold, and twofold axis, respectively. It is noted that the ICO has total of 31 m-fold axes ($m=5,\ 3,$ or 2). Each of them will contribute a set of equations of constraint. Fortunately, these equations of constraint are not all independent. For an example, the axis connecting particles 6 and 8 is a fivefold axis denoted as EE'. Since

$$R^{EE'}_{2\pi/5}=R^{BB'}_{-2\pi/3}R^{k'}_{2\pi/5}R^{BB'}_{2\pi/3}, \tag{9}$$

since the constraint caused by the rotations at the right-hand side of Eq. (9) has already been taken into account, the operator $R^{EE'}_{2\pi/5}$ does not cause a new constraint. Consequently, Eqs. (3), (6), and (8) are found to be sufficient to embody the constraints arising from the m-body axes.

Furthermore, the parity will cause an additional constraint on the wave function. When the particles form an ICO, a space inversion is equivalent to particle interchanges. Thus we have

$$(\Pi-1)\Psi_Q(\mathrm{ICO})=0. \tag{10}$$

Evidently, the Q components Ψ_Q depend also on the choice of the body frame. When the body frame is adopted as in Fig. 1(a), a rotation about j' by π is also equivalent to particle interchanges. Thus we have

$$\sum_{Q'}[(-1)^{L+Q}\delta_{\overline{QQ'}}-\delta_{QQ'}]\Psi_{Q'}(\mathrm{ICO})=0. \tag{11}$$

Equations (3), (6), (8), (10), and (11) are the equations that Ψ_Q must fulfill at ICO configurations irrespective of the sizes of the ICO. It is well known that homogeneous equations do not always have nonzero solution. Therefore, it is very possible that the above five sets of equations do not have a common nonzero solution, depending on the coefficients of these equations. The coefficients depend on L and Π. For odd-parity states, it is obvious that all the Ψ_Q must be zero at the ICO due to Eq. (10). Thus the ICO is inaccessible to odd parity states. For even parity states with specific L, these sets of equations might have one (or more) common nonzero solution(s). These specific states are ICO-accessible. The other states are ICO-inaccessible, where all the Ψ_Q (Q is from $-L$ to L) must be zero at the ICO, and therefore $\Psi_M(ICO)$ is zero irrespective of the size and orientation of the ICO [cf. Eq. (2)]. Thus, all the ICO-inaccessible states contain a nodal surface at ICO configurations. This surface is called an inherent nodal surface [7,8]. Since in general the appearance of a nodal surface implies an excitation of oscillation, the above nodal surface will cause an excited oscillation back and forth around the ICO as an equilibrium shape resulting in a great increase in energy.

Since the search of solutions of linear algebra equations is trivial, we shall give directly the results. Owing to Eq. (11) the wave function as expanded in Eq. (2) can be rewritten at the ICO as

$$\Psi_M(\mathrm{ICO})=C\left\{\sum_{Q>0}[D^L_{QM}+(-1)^{L+Q}D^L_{-Q,M}]f_Q+D^L_{0M}f_0\right\}, \tag{12}$$

where C is an unknown number and f_Q and f_0 are numbers obtained from solving the sets of equations. The arguments

TABLE I. The ICO-accessible states of a 13-boson system and their wave functions given in a body frame at the ICO [cf. Eq. (12)]. The body frame is plotted in Fig. 1(a). The values of the f_Q not listed in the table are zero.

L^{Π}	f_0	f_5	f_{10}	f_{15}
0^+	1			
6^+	$\sqrt{\frac{11}{25}}$	$-\sqrt{\frac{7}{25}}$		
10^+	$\sqrt{\frac{247}{1875}}$	$\sqrt{\frac{209}{625}}$	$\sqrt{\frac{187}{1875}}$	
12^+	$\sqrt{\frac{1071}{3125}}$	$-\sqrt{\frac{286}{3125}}$	$\sqrt{\frac{741}{3125}}$	
15^+		$-\sqrt{\frac{667}{2500}}$	$-\sqrt{\frac{957}{6250}}$	$\sqrt{\frac{1001}{12500}}$

$\alpha\beta\gamma$ contained in D^L_{QM} are not explicitly written. It was found that there are only five ICO-accessible states with $L \leqslant 15$; they are listed in Table I. Those states with $L \leqslant 15$ but not in the table are ICO-inaccessible.

Let L_i^{Π} denote the ith state of a series having the same L and Π. The L_1^{Π} is the lowest one of the series and is called a first state. Let the eigenenergy of a state be approximately divided as

$$E = E_{\text{int}} + E_{\text{rot}}, \tag{13}$$

where E_{int} is the internal oscillation energy and E_{rot} is the energy of collective rotation. Obviously, if the wave function can peak at the ICO and be smoothly distributed surrounding it, E_{int} would be minimized . Only ICO-accessible states are allowed to make this favorable choice. Evidently, all the first states will do their best to lower the E_{int}. Thus the ICO-accessible first states, namely the 0_1^+, 6_1^+, 10_1^+, 12_1^+, 15_1^+, ..., definitely will make this favorable choice. Consequently, they have the same kind of internal structure (having the ICO as the most probable shape), and thereby constitute the lowest rotation band, the ICO band. Its bandhead, namely the 0_1^+, is just the ground state. It is noted that not only have the quantum numbers of each member of this band been determined, but also the wave functions at the ICO have been determined before solving the Schrödinger equation (except the common number C). This fact demonstrates the decisive effect of symmetry. Since the $L=1$ to 5 states are excluded from the band, the rotational excitation of the ground state is greatly hindered.

Let us study the ICO-inaccessible states. Since they contain an inherent nodal surface at the ICO, their energies are in general much higher. Would this nodal surface extend from the ICO to its neighborhood? When an ICO is prolonged (or shortened) along a fivefold axis, let the deformed shape be called a P5 shape. At this shape a wave function is constrained only by Eqs. (3), (10), and (11), but not by Eqs. (6) and (8). Therefore, an ICO-accessible state must be P5-accessible. However, an ICO-inaccessible state is either P5-accessible or P5-inaccessible. In the latter case the inherent nodal surface extends from the ICO to the P5. The P5-accessibility can be easily identified as listed in the third row of Table II.

TABLE II. Accessibility of the regular shapes. A block with an *a* implies that the associated shape is accessible to the associated states; an empty block denotes inaccessibility.

	10^+	9^+	8^+	7^+	6^+	5^+	4^+	3^+	2^+	1^+	0^+
ICO	*a*				*a*						*a*
P5	*a*	*a*	*a*	*a*	*a*	*a*	*a*		*a*		*a*
T5	*a*		*a*		*a*		*a*		*a*		*a*
P3	*a*	*a*	*a*	*a*	*a*	*a*	*a*	*a*	*a*		a
T3	*a*	*a*	*a*	*a*	*a*		*a*		*a*		*a*
CUBO	*a*	*a*	*a*		*a*		*a*				*a*
sixfold	*a*		*a*		*a*		*a*		*a*		*a*
	10^-	9^-	8^-	7^-	6^-	5^-	4^-	3^-	2^-	1^-	0^-
ICO											
P5											
T5		*a*	*a*	*a*	*a*	*a*					
P3											
T3		*a*	*a*	*a*	*a*	*a*	*a*	*a*			
CUBO											
six-fold		*a*	*a*	*a*	a						

When an ICO is twisted about a fivefold axis [e.g., when the particles 3 to 7 in Fig. 1(a) rotate as a whole by the angle $\pi/10$, while the particles 8 to 12 rotate as a whole by $-\pi/10$ about the k' axis], the deformed shape is called a T5 shape. Similarly, P3 and T3 shapes can be likewise defined, where, instead of a fivefold axis, a threefold axis is contained. The P5, T5, P3, and T3 are regular shapes in the domain of the ICO. A slight deformation of the ICO will lead to these shapes. The accessibility of these shapes is essential to ICO-inaccessible states and is summarized in Table II. When some of these shapes are accessible, the wave function of an ICO-inaccessible state may peak at them.

It is quite often that the structure of a higher state would have a number of competing choices allowed by symmetry. For example, the ICO-inaccessible states may also peak at the CUBO and/or the ''sixfold'' shape. Since higher states are less constrained by symmetry, we shall neglect the general discussion on them. Instead, some series of states with specific structures will be pointed out.

The accessibility of shapes is associated with the inherent nodal structure of wave functions. For an example, the 5^+ state is not only ICO-inaccessible, but also T5- and T3-inaccessible. Thus, the inherent nodal surface existing at the ICO will extend to the T5 and T3. It is clear from Table II that each ICO-inaccessible state has its own inherent nodal structure. This structure affects seriously the feature of the wave function, therefore it is an objective base for the classification of states.

Based on the inherent nodal structure, the ICO-inaccessible states can be further classified into four groups. The first group contains the 2^+, 4^+, 8^+, ... states. They all contain an inherent nodal surface at the ICO, but this surface does not extend to the neighborhood. Thus, while the wave functions can be freely distributed in the neighborhood of the ICO, the node at the ICO (the minimum of the total potential energy) would cause a number of modes of oscillation back and forth around the ICO as an equilibrium shape

TABLE III. The CUBO-accessible states (refer to Table I). The body frame is given in Fig. 1(b).

L^{Π}	f_0	f_3	f_6	f_9
0^+	1			
4^+	$\sqrt{\frac{7}{27}}$	$\sqrt{\frac{10}{27}}$		
6^+	$\sqrt{\frac{32}{81}}$	$-\sqrt{\frac{35}{243}}$	$\sqrt{\frac{77}{486}}$	
8^+	$\sqrt{\frac{11}{243}}$	$\sqrt{\frac{140}{729}}$	$\sqrt{\frac{208}{729}}$	
9^+		$-\sqrt{\frac{221}{729}}$	$\sqrt{\frac{119}{1458}}$	$\sqrt{\frac{28}{243}}$
10^+	$\sqrt{\frac{8320}{19683}}$	$\sqrt{\frac{44}{6561}}$	$-\sqrt{\frac{1331}{13122}}$	$\sqrt{\frac{3553}{19683}}$

(e.g., a prolongation and shortening along one of its m fold axes). Among these modes the softest mode (having the least excitation energy) would be chosen by the first states 2_1^+, 4_1^+, 8_1^+, ... When the rotation-oscillation coupling is weak (this case is quite usual for atomic clusters because they have a large moment of inertia), these first states dominated by the softest mode will be similar in structure. Thus they would form another rotation band, the ICO* band. Here, the ICO* implies the specific excited oscillation with one node.

The second group of ICO-inaccessible states contains the odd parity L^- states with $L \geqslant 5$. They are T5- and T3-accessible but P5- and P3-inaccessible. They may have the T5 and/or T3 as their most probable shape(s). In addition to the oscillation caused by the node at the ICO, the nodal surface at the P5 and P3 would spoil greatly the stability of the T5 and T3, and cause an excitation of the twist motion (e.g., the upper half and the lower half of an ICO would rotate back and forth in reverse directions about a fivefold or a threefold axis). Thus, the excited twist mode as an inherent mode exists in this group. The first states of this group would constitute a rotation band characterized by having the twist motion. This band is called the odd parity twist band. Since more inherent nodal surfaces are contained in this band, its internal energy is remarkably higher than the ICO* band.

The third group of ICO-inaccessible states contains the 5^+, 7^+, 9^+, ... Their first states might form an even parity twist band.

The fourth group of ICO-inaccessible states contains the 1^+ and 3^+ states, together with all the L^- states with $L \leqslant 4$. These states contain a number of inherent nodal surfaces. Thus, very strong and complicated internal motions are involved, and therefore their energies are very high.

Let us investigate the domain of the CUBO, which is also important to higher states. The CUBO is also a highly symmetric shape related to the octahedral group [5]. It has three fourfold axes, four threefold axes, and six twofold axes. By using the above approach, the CUBO-accessible states can be identified as listed in Table III and summarized in Table II. They might form a rotation band, namely the CUBO band. The L^{Π} states with $L \leqslant 10$ not listed in Table III (including all odd parity states) are CUBO-inaccessible.

TABLE IV. Possible rotation bands of 13-boson systems.

Band	L^{Π} states
ICO band	$0^+,6^+,10^+,\ldots$
ICO* band	$2^+,4^+,8^+,\ldots$
twist-band (even)	$5^+,7^+,9^+,\ldots$
twist-band (odd)	$5^-,6^-,7^-,\ldots$
CUBO band	$0^+,4^+,6^+,8^+,\ldots$
sixfold band (even)	$0^+,2^+,4^+,6^+,\ldots$
sixfold band (odd)	$6^-,7^-,8^-,\ldots$

Since the ''sixfold'' as plotted in Fig. 1(c) is also associated with a local minimum, the ''sixfold''-accessible states, namely the 0^+, 2^+, 4^+, 6^+, ... states, together with the L^- states with $L \geqslant 6$ might also form rotation bands higher than the CUBO band. The possible bands of a 13-boson system are summarized in Table IV.

Among the above suggested bands, the members of the ICO band are pure in structure, because their structure is superior and no other structures can compete with them. However, higher states usually have many competing choices; we do not know how pure the other bands are. It is probable that some members of the higher bands are not well defined, in which different structures are mixed up strongly. How the mixing would be is an open problem.

Nonetheless, although the ''sixfold'' shape is higher in potential energy, it has a larger moment of inertia resulting in having a reduction in $E_{\rm rot}$. When L is larger than a critical value L_c, the reduction of $E_{\rm rot}$ can overcompensate for the increase in potential energy. In this case, the ''sixfold'' shape is more superior than the other shapes. Thus, the L_1^{Π} states with $L \geqslant L_c$ will be dominated by this shape; they would constitute the higher members of the sixfold band pure in geometric feature. Since the moment of inertia and the total potential energy associated with a shape can be evaluated, the L_c can be thereby evaluated. It turns out that L_c is a big number. In the case of the 13-He cluster, L_c is about 45.

In summary, the analysis presented in this paper is based on the inherent nodal structure of wave functions associated with the accessibility of regular shapes. This approach can be generalized to study other few-body systems [7,8].

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