The oLJ13_N13IC Cluster Is the Global Minimum Cluster of Lennard Jones' Potential for 13 Particles

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Abstract—The oLJ13_N13IC is the name of the minimal icosahedral cluster with 13 particles where "oLJ" states that it is the global minimum for the Lennard Jones potential, and the suffix "N13IC" represents the family of the particle-centered icosahedral lattice. It is well known from the early work M. R. Hoare and P. Pal (1975, Physical cluster mechanics: statistical thermodynamics and nucleation theory for monatomic systems) and J. A. Northby (1987, Structure and binding of Lennard-Jones clusters: $13 \leq n \leq 147$), and has been found experimentally in xenon clusters (1981, Echt, et al.) and sodium clusters (2005, Haberland, et al.), and is related with so-called magic numbers. It has been considered as a plausible global minimum but not a true global minimum. As far as I know, this is the first formal proof of global optimization of it.

Except for the global optimal clusters of 2, 3 and 4 particles that satisfy the classic strong criterion of global optimality, the clusters with more particles are just putative global minimal clusters due to the lack of criteria or techniques that determine their global optimality. The article proofs the global optimality for the oLJ13_N13IC cluster by using a novel discrete combinatorial approach on the Euler characteristic and a linear prediction of the good pair potential of Lennard Jones.

Index Terms—Optimization, Minimization, Discrete, Formal Methods, Modelling, Operational Research, Combinatorial Optimization, Numerical Methods

I. INTRODUCTION

The global optimality of the clusters with more than five particles under like Van der Waals potentials is an open problem. The research of atomic microclusters is relevant by the scientific and technological applications, even in the emerging fields of nanotechnology, superconductivity, quantum computation, and molecular design by the novel machines based on microscopy by Atomic Forces or Tunneling Effect. There is a huge literature, particularly about Lennard Jones's clusters [27], [19], [18], [28], [24], [25], [2], [8], [22], [34], [10], [37], [23], [16], [3], [36], [17], [6], [20], [7], [33], [21], [21], [30], [39], [38], [31], [1], [32], [9], [11].

The oLJ13_N13IC is well known from the early work of [19], [18], [28] and is experimentally related as the configuration with 13 particles of the so-called magic numbers: 1, 13, 55, 147, 309, ..., $(1/3)(2r + 1)(5r + 5r^2 + 3))$, where $r = 0, 1, 2, 3, ...)$ [12], [13], [15]. It has been considered as a plausible global minimum but not a true global minimum. As far as I know, this is the first proof of the global optimality of it. The global optimality of clusters is related to all the possible geometrical shapes of the clusters, which are unknown, and the classical optimality conditions of nonlinear optimization theory cannot respond to global optimization but local optimization.

The article presents in section II the global optimization problem for clusters under LJ, the section III proofs the global optimality of oLJ13_N13IC, and the last section IV gives the conclusions.

II. THE PROBLEM OF THE GLOBAL MINIMAL CLUSTERS UNDER POTENTIAL OF LENNARD JONES

The well-known properties [29] for a good pairwise potential function PT of the particles' pair distance r are:
1) $\lim_{r \to 0+} \text{PT}(r) = \infty$.
2) $\lim_{r \to \infty} \text{PT}(r) = 0^-$.
3) $\text{PT}'(r*) = 0$ and $\text{PT}''(r*) > 0$.
4) $\text{PT}(r^*) < 0$, it means the potential has a basin.

where r^* is the optimal distance.

The Euclidian distance function $D : \mathbb{R}^3 \times \mathbb{R}^3 \to [0, \infty)$ for any point particles p_i, and p_j is given by $D(p_i, p_j) = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$ where $p_i = (x_i, y_i, z_i)$, $p_j = (x_j, y_j, z_j) \in \mathbb{R}^3$.

The Potential of Lennard Jones is denoted by LJ, hereafter. The pairwise formula of LJ (see [27] and [35]) is

$$\text{LJ}(d) = \frac{1}{d^{12}} - \frac{2}{d^6},$$

where d is the Euclidian distance between a pair of particles, and the optimal distance between a pair of particles is one (see fig. 1).

Arbitrary local minimal clusters are denoted as $\text{lLJ}n = \{p_i \in \mathbb{R}^3 | i = 1, \ldots, n\}$, and the putative minimal clusters are denoted as $\text{oLJ}n$.

The complete potential of a cluster is

$$\text{LJ}(\text{pLJ}n) = \sum_{1 \leq i < j \leq n} \text{LJ}(D(p_i, p_j))$$

where $\text{pLJ}n$ is an arbitrary cluster (with or without minimization) with n particles, and $p_i, p_j \in \mathbb{R}^3$.

The open problem is to determine the global minimum cluster of LJ ($\text{oLJ}n$) for $n \geq 5$.
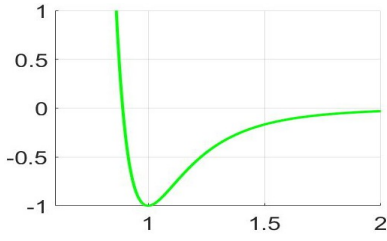
Fig. 1. Lennard Jones Potential vs d.

Any putative global minimal cluster of LJ (pLJn) with $n \geq 5$ satisfies: LJ(lLJn) > LJ(pLJn) where lPTn in a large set of clusters (C).

The set C generally is big and has clusters generated by some method, which is far from being exhaustive or guaranteeing that it corresponds with the one with the lowest potential over all possible clusters, known or unknown, i.e., the mechanism of the algorithms for determining the putative minimal oLJn is as follow:

1) **Creation.** Build randomly cLJn, a cluster with n particles from an ad-hoc Research Space.
2) **Minimization.** lLJn = arg min LJ(cLJn);
3) **Elitism.** if LJ(lLJn)¡LJ(oLJn) then oLJn=lLJn.

However, the global requires:

$$LJ(lLJn) > LJ(oLJn), \forall lLJn. \tag{1}$$

Where $\forall$ demands the result from any clusters.

The difficulties to estimate the optimal clusters are the big number of configurations, and that $\nabla(PT(oLJn))$ is zero for $n = 2, 3$, and 4, meanwhile $\|\nabla(PT(lPTn))\| \approx 0$ for $n \geq 5$. This is because any cluster with more than 5 particles has diagonals, i.e., it is impossible to arrange more than five particles in $\mathbb{R}^3$ with equals size links between all them.

In this work, the center of mass of a cluster is used to detect a 3D convex graph as the nucleus and the seed for structuring the cluster's layers. It is similar to the seed and structures of Hoare [18] and the bonded atom interactions (B set) and the nonbonded atom interactions (NB set) of Maranas [25]. The list of known cores [9], [18], [33], [35]. The tables I and II depict the cores studied in this work. The type of kernel sometimes is added to the name of the minimal clusters, by example, lLJ13_N13IR means the local minimal cluster of LJ with nucleus N13IR and 13 particles.

There is a difference in this work over the sets B and NB of Maranas. Here, they correspond to the one type of particles, therefore the bound to separate them is fixed. The selection of the value 1.3 for defining the set B (bonds) come from the differentiation of the diagonals and the primary links or bonds, i.e., the upper bound 1.3 of the bonds is less than $\sqrt{2} \approx 1.$ 4142, the distance of the diagonal of a square of side 1.

The set B(lLJn) set of the bonds correspond to the pair of particles at distance less than 1.3, and the set NB(lLJn) correspond to the pair of particles at distance greater or

TABLE I
NUCLEUS (I)

Nucleus	Figure
N4T Tetrahedron	
N5QP Quadrangular Pyramid	
N5BT Bi-tetrahedron	
N5T Triangular Star	
N6OC Octahedron	
N6TP Triangular Prism	
N8CB Cube	
N8TBP Triangular Biprism	

TABLE II
NUCLEUS (II)

Nucleus	Figure
N10 Pentagonal Prism IR	
N10 Pentagonal Prism IC	
N12IR Pentagonal Prism, two pentagonal pyramids with central vacancy	
N12IC Icosahedron central vacancy	
N13IR Pentagonal Prism, two pentagonal pyramids with central particle	
N13IC Icosahedron with central particle	
N13CPA close-packed-ABA (hcp)	
N13CPA close-packed-ABC (fcc)	

Fig. 2. lLJ173 with lumps.

Fig. 3. lLJ2054 without noticeable shape.

point for the function arg min LJ.

The good local optimal clusters are minimal clusters that they satisfy:

1) The graph (lPTn, B(lPTn)) is connected, i.e, Vertices of (B(lPTn)) are the vertices of lPTn.
2) The graph (lPTn, B(lPTn)) $\subset K_n$ (complete graph of n vertices) such that $3 \leq \mathrm{grad}(v) \leq 12$, where grad($\cdot$) is the grade of the vertices (v) with respect B(lPTn), and $n \geq 3$.

Remark 2.2: The optimal clusters comply that they stationary points of $\arg \min$LJ(lPTn) where min is a deterministic minimization procedure, such as CGB (Restarted Conjugate gradient [4]) or L-BFGS-B (Limited-memory of the Broyden-Fletcher-Goldfarb-Shanno algorithm (LBFGS-B [5], [26])). Note that the procedures CBG and L-BFGS-B are deterministic because under the same initial data and precision, they give the same answer. There are non-deterministic minimization procedures as The Exponential Tunneling Method see [14]. The minimization of clusters with $n \geq 5$ achieves $\|\nabla(\mathrm{LJ}(\mathrm{lLJ}n))\| \approx 0$ by adjusting the distances of set B around 1, so the gradient of each particle reaches vector equilibrium near 0.

Remark 2.3: The local optimal clusters with vertices of (B(lPTn) less than the vertices lPTn cannot be global optimal cluster, i.e., they have distant particles or particles with less than 3 bonds, by example, clusters with the linear or flat configurations have greater potential than any good minimal clusters, also configurations with lumps or without regularity as in Figure 2, and Figure 3. The potential contribution is significant when a particle is added or adjusted to connect with triangular, rectangular, pentagonal, or hexagonal faces, i.e., its vertex's grade becomes ≥ 3. The upper limit of the grade of a particle is 12, it is because the kissing spherical configuration in 3D is an icosahedron (see fig. 5). Figure 4 depicts examples of good minimal clusters (lLJ13, and lLJ16) and no good minimal cluster (lLJ17).

equals than 1.3. This classification of the links of a cluster allows to divide the contributions to the potential as LJ(lLJn)=LJ(B(lLJn))+LJ(NB(lLJn)).

Definition 2.1: A numerical minimal cluster or minimal cluster complies $\|\nabla(\mathrm{LJ}(\mathrm{lLJ}n))\| \approx 0$ and LJ(lLJn+λd)) > LJ(lPTn)), $\forall \lambda d \in \mathbb{R}^{3n}$, and $0 \neq \lambda \ll 1$. This means that the potential grows in any small direction and lLJn is a fixed
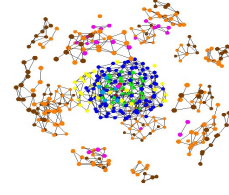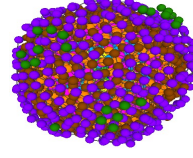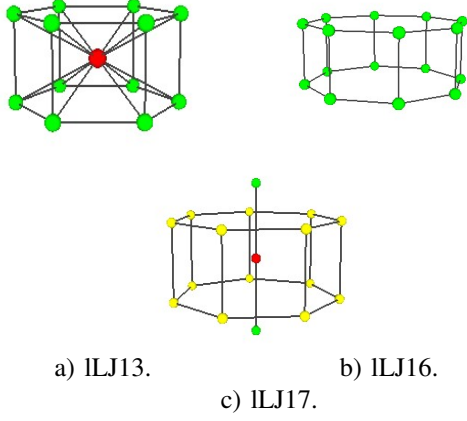
a) lLJ13. b) lLJ16.

c) lLJ17.

Fig. 4. Good minimal clusters: a) Hexagonal Prism with central particle, LJ(lLJ13)=−32.6979, b) Octagonal Prism, LJ(lLJ16)=−29.5174. No good minimal cluster: c) Heptagonal Prism with 3 perpendicular particles at its center, LJ(lLJ17) −43.7004.
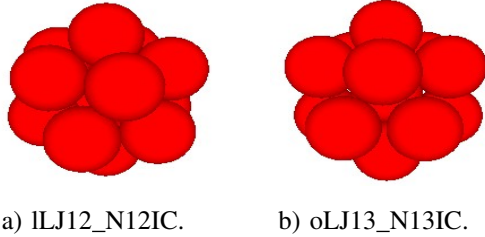

a) lLJ12_N12IC. b) oLJ13_N13IC.

Fig. 5. Spheres of influence for LJ(lLJ12_N12IC)=-33.5975, 12 red spheres with ratio 0.4954, and LJ(oLJ13_N13IC)=-44.3268, 13 red spheres with ratio 0.4819.
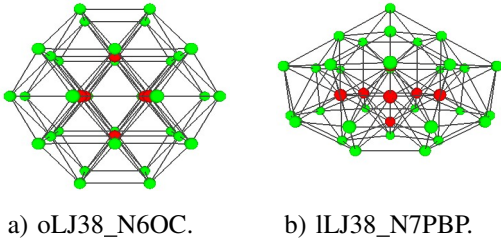

a) oLJ38_N6OC. b) lLJ38_N7PBP.

Fig. 6. LJ(oLJ38_N6OC)=-173.9284, |B(oLJ38_N6OC)| = 144, and LJ(lLJ38_N7PBP)=-173.2524, |B(lLJ38_N7PBP)| = 147.

a) lLJ13_N4T. b) lLJ13_N8CB.
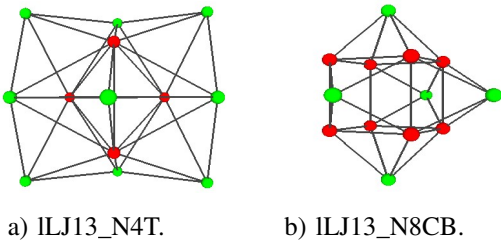
Fig. 7. LJ(lLJ13_N4T)=-40.7585, |B(lLJ13_N4T)| = 38, and LJ(lLJ13_N8CB)=-36.9739, |B(oLJ13)| = 32.

a) lLJ13_N12HEXPRISC. b) lLJ13_N6TP.
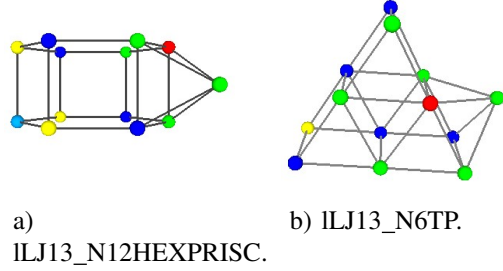
Fig. 8. LJ(lLJ13_N12HEXPRISC)=-26.5658, |B(lLJ13_N12HEXPRISC)| = 22, and LJ(lLJ13_N6TP)=-33.8578, |B(lLJ13_N6TP)| = 28.

TABLE III
EULER CHARACTERISTIC AND THE REGULAR POLYHEDRONS WITH 12 VERTICES

figure	V	E	F	LJ
Icosahedro (N12IC)	12	30	20	-33.5975
N12IR	12	25	15	-41.5552
N12CPA_ABA	12	24	14	-28.9988
N12CPA_ABA	12	24	14	-28.9544
N12HEXPRIST	12	24	14	-26.3282*
N12HEXPRISC	12	18	8	-22.5729

* Unstable, not minimizing

III. THE GLOBAL OPTIMALITY OF THE oLJj13_N13IC

The equation 1 with $n = 13$ by the remark 2.3 can focus on good local minimal cluster of LJ. For any clusters the number of links correspond to the number of links of K_n, i.e. $\binom{n}{2}$ links. For any cluster with 13 particles the numbers of links is 78. The oLJ13_N13IC has LJ(oLJ13)= -44.3268, with LJ(B(oLJ13))= -41.0877, and LJ(NB(oLJ13))= -3.2391, where |B(oLJ13)|=42 (bonds), and |NB(oLJ13)|=78-42=36 (diagonals).

The following condition is necessary but sufficient, for a putative global minimal cluster oLJn, there is not a good minimal cluster (lLJn) such that |B((lLJn))| > |B(oLJn)|.

The counter example is the well-known oLJ38_N6OC versus lLJ38_N7PBP where |B(oLJ38_N6OC)|=144 and |B(lLJ38_N7PBP)|=147 (see fig. 6).

The set B(oLJ13_N13IC) consists of 12 bonds of 0.96381 (towards the central particle) with LJ(0.96381)= -0.93873 and 30 bonds of 1.0134 (for the faces of the icosahedron) with LJ(1.0134)= -0.99411. The set NB(oLJ13_N13IC) consists of 30 diagonals of 1.6397 with LJ(1.6397)= -0.10026 and 6 diagonals of 1.9276 with LJ(1.9276)=-0.03861.

Taking the distances that contribute more to the potential, LJ(B(oLJ13)) ≈ 42*(LJ(1.0134))(=-41. 753) and LJ(NB(oLJ13)) ≈ 36*(LJ(1.6397)) (= -3. 6094). From this a linear model to approximate LJ for clusters with 13 particles using the (b=|B|) is

$$J(b) = -0.89384b - 7.8203. \qquad (2)$$

The linear model (eq.2) predicts that there is a cluster with 41 bonds, such that J(41)= -44. 468 < LJ(oLJ13).

There is no a good minimal cluster of LJ with 41 bonds. The icosahedron is the regular polyhedron with the great number

TABLE IV
CLUSTERS OF LJ WITH 13 VERTICES

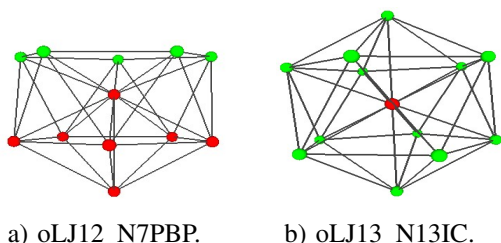| LJ(Cluster)	E
LJ(oLJ13_N13IC)=-44.3268	42
LJ(lLJ13_N13IR) = -41.5552	37
LJ(lLJ13_N13CPA_ABA= -40.9215	36
LJ(lLJ13_N13CPA_ABC=-40.8845	36
LJ(lLJ_N13HEXPRIST)=-37.3292	36
LJ(lLJ_N13HEXPRISC)=-32.6979	30

a) oLJ12_N7PBP.   b) oLJ13_N13IC.

Fig. 9.   LJ(oLJ12_N7PBP)=-37.9676, |B(oLJ12)| = 36, and LJ(oLJ13_N13IC)=-44.3268, |B(oLJ13)| = 42.

of faces. The Euler characteristic ($V - E + F = 2$) depicts the configuration of the regular polyhedrons with 12 particles in the table III. Adding a particle at the center of the regular polyhedron in table III, the local good minimal clusters of LJ with the great number of bonds are obtained (see table IV). oLJ13_N13IC is the cluster with the putative global minimal LJ.

Taking any particle from the icosahedral surface of the oLJ13_N13IC, the oLJ12_N13IC with 36 bonds is obtained (see fig. 9). The upper pentagonal face (green) offers 5 bonds if a particle is added to it, but in reality, if a particle is added, it has 6, not 5 bonds, and the global optimal cluster oLJ13_N13IC is recovered after minimization. The other good minimal cluster configurations with 13 particles (see table IV) do not have the possibility to create a cluster of 41 bonds. On the other hand, figures 7, and 8 depicts good minimal clusters that were created by adding particles to the cores of table I or II that do not have 42 bonds because they have quadrangular faces. The cluster lLJ13_N4T has 38 bonds which is greater than the number of bonds of the cluster lLJ13_N13IR, i.e., there are no good minimal clusters with more than 38 bonds, but oLJ13_N13IC. Finally, the Euler characteristic has no other solutions with a larger number of edges for 12 vertices on an spherical surface and there is no other way to accommodate 13 vertices to obtain a figure with more than 42 bonds with minimal potential. Therefore, oLJ13_N13IC is the unique and true global minimal of LJ with 13 particles.

IV. CONCLUSIONS

The global optimization of the clusters has just started. The oLJ13_N13IC is now the unique and true global optimal cluster of LJ with 13 particles. More clusters with other good pairwise potential, as the Morse Potential, will study in the future.

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