The best constant of discrete Sobolev inequality on 1812 C60 fullerene isomers

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Abstract

The best constants of discrete Sobolev inequalities corresponding to 1812 isomers of C60 fullerene are found. Classical mechanical models of these isomers with a linear spring on each edge are investigated. The best constants stand for rigidities of these models. We show the best constants of 1812 isomers are distinct rational numbers and among these, Buckyball (or equivalently truncated icosahedron) takes the least. In other words, one can say that the Buckyball is the most rigid among 1812 C60 fullerene isomers.

Keywords

C60 fullerene, Buckyball, discrete Sobolev inequality

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1. Introduction

Our study of Sobolev inequality starts with [1], in which we considered the best constant of Sobolev inequality in an n-dimensional Euclidean space. Afterwards, we treated discrete Sobolev inequalities and found their best constants on polygons [2-5], polyhedra [6-8] and truncated polyhedra [9-11].

Here we note that, if each vertex is regarded as a carbon atom, then truncated icosahedron is equivalent to the C60 Buckyball discovered by Osawa [12] and Kroto et al [13]. Thus we can expect the best constant of Sobolev inequalities have connections with physical properties of materials with crystal structure. The Buckyball has v = 60 vertices, e = 90 edges, and f = 32 faces and consists of 12 pentagons and 20 hexagons. We regard each edge as a linear spring with uniform spring constant. In our work [9], we have found the best constant of the discrete Sobolev inequality on Buckyball. As we noted there, the best constant can be considered to represent the rigidity of this mechanical model. That is, if the best constant is smaller, the model is more rigid.

In order to enumerate distinct fullerenes, several algorithms are proposed in 1990s: for example, Spiral algorithm [14, 15], Yoshida-Osawa’s algorithm [16], Brinkmann-Dress’ algorithm (patch-stitching method) [17]. We note the Spiral algorithm is used in software “fullerenes” [18]. The patch-stitching method is implemented in “fullgen” [19]. In this paper, we employ patch-stitching method [19] to enumerate C60 isomers and obtain all 1812 isomers. The Buckyball is the only isomer which satisfies IPR rule that pentagons are not placed next to each other. In this paper, we calculate all the best constants of the discrete Sobolev inequalities corresponding to these C60 isomers and show that the best constant of the Buckyball is the smallest, which means that the Buckyball is the most rigid among 1812 C60 fullerene isomers.

2. Symmetric C60 fullerene

Hereafter we call the C60 fullerene the C60 for short. If some C60s are expressed in planar graphs, their central horizontal lines are categorized into the three types: zigzag line, zigzag ring and armchair ring shown in Fig. 1 and the planar graphs are symmetric with respect to a certain point on the central horizontal line. We call such types of C60s the symmetric C60s.

Carbon nanotube is found by Iijima [20] and is generated by rolling up a sheet of six-member rings called graphene in a cylindrical form. Geometrically speaking, it is generated by dividing the symmetric C60s with respect to its central line and by arranging hexagons in the crack. The symmetric C60s are regarded as the minimum carbon nanotube. There exists 148 symmetric C60s. We here list up examples which have a specific arrangement
of pentagons and hexagons. The following figures show graph expressions of such C60s. In this figures, the numbers 0, 1, ..., 59 stand for the vertices and the numbers 1, 2, ..., 20 stand for the hexagon faces. In the rest of this section, we give brief descriptions of these figures.

**Buckyball (BB, Figs. 2, 3)** This is a truncated icosahedron. 12 pentagons are apart from each other.

**Twisted Buckyball (TBB, Fig. 4)** This is generated by twisting, or equivalently shifting each face to its neighbor along the zigzag line in Fig. 2.

**Kameball (KB, Fig. 5)** The word “Kame” has two meanings. One stands for a Japanese word meaning turtle. The shape of its graph expression looks like a turtle. The other stands for the name of the first author, who finds this C60.

**Large wheel (LW, Fig. 6)** A hexagon is surrounded by six hexagons.

**Hifumikun (H, Fig. 7)** Two sets of one pentagon, two pentagons and three pentagons are arranged. The word “Hi”, “Fu” and “Mi” are Japanese meaning 1, 2
and 3, respectively.

**Triple A (AAA, Fig. 8)** This has three armchair rings.

**Carbon nanotube (CNT, Fig. 9)** This is a special case of carbon nanotubes generated by dividing equally regular dodecahedron into two and by arranging 20 hexagons in the crack.

### 3. Discrete Laplacian

We treat a classical mechanical model of C60s. Its neighboring two atoms are connected by a linear spring with uniform spring constant. Hereafter i (or j) represents the number attached to each vertex in Figs. 2–9. The edge set e is a set of (i, j), where vertices i and j which satisfies (0 ≤ i < j ≤ 59) are connected as an edge. In the case of Buckyball with central zigzag line (Fig. 2), the set e is expressed as

\[ e = \{(i, j) \mid (0, 1), (0, 5), (0, 18), \ldots, (37, 59)\}. \]

The variables u(i) are displacements of the i-th vertex from its equilibrium state and introduce a vector \( u = (u(0), u(5), \ldots, u(59)) \). If the force \( f = (f(0), \ldots, f(59)) \) is acted to the C60, \( u = (u(0), \ldots, u(59)) \) satisfies the equation \( Au = f \), where the matrix A is a discrete Laplacian matrix defined by

\[ A = \begin{pmatrix} a(i, j) \end{pmatrix}, \quad a(i, j) = \begin{cases} 3 & (i = j) \\ -1 & (i, j); (j, i) \in e \\ 0 & \text{otherwise} \end{cases} \]

where 0 ≤ i, j ≤ 59. It should be noted that we have 1812 distinct discrete Laplacian matrices \( A \) corresponding to 1812 C60 isomers. However, each \( A \) is a real symmetric positive-semidefinite matrix and possesses an eigenvalue \( \lambda_0 = 0 \) and eigenvalues \( 0 < \lambda_1 \leq \cdots \leq \lambda_{59} \). The eigenvector corresponding to \( \lambda_0 = 0 \) is \( 1 = (1, \ldots, 1) \in \mathbb{R}^{59} \).

### 4. Discrete Sobolev Inequality

For \( u, v \in C_0^{59} := \{ u \mid u \in C^{59} \text{ and } ^t1u = 0 \} \), we introduce the sesquilinear form

\[ (u, v)_A = v^tAu, \quad ||u||_A^2 = (u, u)_A, \]

where \( u^* \) denotes \( u = ^t\overline{u} \). We rewrite \( ||u||_A^2 \) as

\[ ||u||_A^2 = \sum_{(i,j) \in e} |u(i) - u(j)|^2. \]

In order to describe theorem, we prepare the vector

\[ \delta_j = \begin{cases} \delta(i-j) & 0 \leq i \leq 59, \\ 0 & (i \neq j) \end{cases} \]

**Theorem 1** For any \( u \in C_0^{59} \), there exists a positive constant \( C \) which is independent of \( u \), such that the discrete Sobolev inequality

\[ \left( \max_{0 \leq i \leq 59} |u(j)| \right)^2 \leq C ||u||_A^2 \tag{1} \]

holds. Among such \( C \), the best constant \( C_0 \) is

\[ C_0 = \max_{0 \leq j \leq 59} \delta_j G_j \delta_j = \delta j_0 G_j \delta j_0, \]

where \( j_0 (0 \leq j_0 \leq 59) \) is some number satisfying the equality. The best constants corresponding to 1812 C60 isomers are different rational numbers. We enumerate the best constants \( C_0 \) in an increasing order as \( C_0(1) = 0.63727 \cdots < \cdots < C_0(1812) = 0.85781 \cdots \). If we replace \( C \) by \( C_0 \) in (1), the equality holds if and only if \( u \) is parallel to \( G_j \delta j_0 \).

The basic idea for the best constant of the discrete Sobolev inequality can be seen in, for example, [2–11]. However, for the sake of self-containment we give a proof.

**Lemma 2** For any \( u \in C_0^{59} \) and fixed \( j \) (0 ≤ j ≤ 59), we have the following reproducing relations:

\[ u(j) = (u, G_j)A, \tag{2} \]

\[ ^t\delta_j G_j \delta_j = \|G_j \delta_j\|_A^2. \tag{3} \]

**Proof of Lemma 2** Noting \( G^*_j = G_j \), we have

\[ (u, G_j)A = \delta_j G_j Au = \delta_j (I - E_0)u = \delta_j u - \frac{1}{60} ^t1u = u(j). \]

Putting \( u = G_j \delta_j \) in (2), we obtain (3).

**QED**

**Proof of Theorem 1** For any \( u \in C_0^{59} \), applying the Schwarz inequality to (2) and using (3), we have

\[ |u(j)|^2 \leq ||u||_A^2 \|G_j \delta_j\|_A^2 = \delta_j G_j \delta_j ||u||_A^2. \]

Taking the maximum with respect to \( j \) on both sides, we obtain the discrete Sobolev inequality

\[ \left( \max_{0 \leq j \leq 59} |u(j)| \right)^2 \leq C_0 ||u||_A^2, \tag{4} \]

\[ C_0 = \max_{0 \leq j \leq 59} \delta_j G_j \delta_j = \delta j_0 G_j \delta j_0. \]

From the above inequality (4), \( ||u||_A^2 = 0 \) holds if and only if \( u = 0 \). This shows that the sesquilinear form
\( (u, v)_A \) is an inner product of vector space \( \mathbb{C}^n_0 \). We note that in the case of Buckyball the diagonal values \( \delta_j G \cdot \delta_j \) do not depend on \( j \), which implies the symmetry of the Buckyball. If we take \( u = G \cdot \delta_{j_0} \) in (4), then we have

\[
\left( \max_{0 \leq j \leq 59} |\delta_j G \cdot \delta_{j_0}| \right)^2 \leq C_0 \| G \cdot \delta_{j_0} \|_A^2 = (C_0)^2.
\]

Combining this with the trivial inequality

\[
(C_0)^2 = |\delta_{j_0} G \cdot \delta_{j_0}|^2 \leq \left( \max_{0 \leq j \leq 59} |\delta_j G \cdot \delta_{j_0}| \right)^2,
\]

we have

\[
\left( \max_{0 \leq j \leq 59} |\delta_j G \cdot \delta_{j_0}| \right)^2 = C_0 \| G \cdot \delta_{j_0} \|_A^2.
\]

Hence \( C_0 \) is the best constant of (4) and the equality holds for \( j_0 \)-th column of \( G \).

(*** QED ***)

The approximate values of \( C_0(n) \) (\( n = 1, 2, \ldots, 1812 \)) are as follows.

| \( n \) | \( C_0(n) \) |
|---|---|
| 1 | 0.6372700691 |
| 2 | 0.6577294008 |
|   |   |
| 12 | 0.6594161135 |
|   |   |
| 42 | 0.6669694342 |
|   |   |
| 166 | 0.6719601465 |
|   |   |
| 387 | 0.6839200228 |
|   |   |
| 1811 | 0.8325592565 |
| 1812 | 0.8578134657 |

Fig. 10 shows the best constant \( C_0(n) \). Horizontal and vertical lines stand for \( n \) and \( C_0(n) \), respectively. Comparing the best constants \( C_0(n) \), especially their two decimal places, \( C_0(1) \) is much less than the other \( C_0(n) \) (\( n = 2, 3, \ldots, 1812 \)). This fact shows that the Buckyball is by far the most rigid among 1812 C60s. We can also observe from Fig. 10 that \( C_0(1810) < C_0(1811) < C_0(1812) \) are much larger than the other best constants. This fact shows that the best constant \( C_0(1812) \) of the carbon nanotube with dodcachadra on its both sides is the softest.

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