The best constant of discrete Sobolev inequality on the C60 fullerene buckyball

Yoshinori Kametaka$^1$, Atsushi Nagai$^2$, Hiroyuki Yamagishi$^3$, Kazuo Takemura$^4$ and Kohtaro Watanabe$^5$

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Abstract

The best constants of two kinds of discrete Sobolev inequalities on the C60 fullerene buckyball are obtained. All the eigenvalues of discrete Laplacian $A$ corresponding to the buckyball are found. They are roots of algebraic equation at most degree 4 with integer coefficients. Green matrix $G(a) = (A + aI)^{-1}$ ($0 < a < \infty$) and the pseudo Green matrix $G_* = A^\dagger$ are obtained by using computer software Mathematica. Diagonal values of $G_*$ and $G(a)$ are identical and they are equal to the best constants of discrete Sobolev inequalities.

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1 Introduction

The best constant of discrete Sobolev inequality was obtained for Platon’s regular polyhedra [1, 6] and truncated regular tetra-, hexa- and octa- polyhedra [2]. The purpose of this paper is to extend the above result to the truncated regular icosahedron, that is, the C60 Fullerene Buckyball [3]. The studies of discrete Sobolev inequalities start with [4, 5], where inequalities on a periodic lattice are investigated.

Buckyball, or BB for short, is a polyhedron which consists of 60 carbon atoms, including 12 pentagons and 20 hexagons. The numbers of vertices $v$, faces $f$ and edges $e$ are $v = 60$, $f = 32$, $e = 90$, which satisfies Euler polyhedron theorem $v + f = e + 2$. We use the following two equivalent simplest plane graph expressions in Figs.1.1 and 1.2. Fig.1.1 is called the zigzag type and Fig.1.2 is called the armchair type of BB.

This paper is organized as follows; In section 2, we introduce discrete Laplacian corresponding to BB. In section 3, we present main theorems in this paper. In section 4, we investigate pseudo Green matrix $G_*$ and Green matrix $G(a)$. In section 5, we give the spectral decomposition of $A$ and investigate diagonal values of matrices $G_*$ and $G(a)$. In section 6 and 7, we prove main theorems.
Fig. 1.1. The zigzag type of C60 fullerene Buckyball.

Fig. 1.2. The armchair type of C60 fullerene Buckyball.
Discrete Laplacian

We treat a classical mechanical model of BB. Each neighboring two atoms are connected by a classical linear spring with uniform spring constant. The vertices are labeled by integers $i \ (0 \leq i \leq 59)$ as in Figs. 1.1 and 1.2. The edge set $e$ is a set of $(i, j)$, where $i$ and $j$ are connected by an edge. Discrete Laplacian $A$ is defined by

$$A = \left( a(i, j) \right) \quad (0 \leq i, j \leq 59), \quad a(i, j) = \begin{cases} 3 & (i = j), \\ -1 & ((i, j) \in e), \\ 0 & (\text{else}). \end{cases}$$

$A$ is a $60 \times 60$ real symmetric positive-semidefinite matrix. Although two discrete Laplacians derived from Figs. 1.1 and 1.2 are different, they are similar, they possess a common characteristic polynomial $P(x)$ given by

$$P(x) = \det(xI - A) = x(x - 2)^9(x - 5)^4(x^2 - 5x + 3)^5(x^2 - 7x + 11)^5 \times (x^2 - 7x + 8)^4(x^2 - 9x + 19)^3(x^4 - 9x^3 + 25x^2 - 22x + 4)^3.$$

Each factors of $P(x)$ are a polynomial of $x$ with integer coefficients with degree at most 4. Eigenvalues of $A$, their multiplicities and approximate values, are shown in Fig. 2.1. Fig. 2.2 illustrates a distribution of eigenvalues $\lambda_j$ of $A$. The eigenvector corresponding to $\lambda_0 = 0$ is $1 = (1, \ldots, 1) \in \mathbb{C}^{60}$.

| number $j$ | eigenvalue $\lambda_j$ | approximate value | multiplicity |
|------------|-------------------------|-------------------|-------------|
| 0          | 0                       | 0                 | 1           |
| 1~3        | $(9 - \sqrt{5} - \sqrt{38 - 2\sqrt{5}})/4$ | 0.24              | 3           |
| 4~8        | $(5 - \sqrt{13})/2$     | 0.69              | 5           |
| 9~11       | $(9 + \sqrt{5} - \sqrt{38 + 2\sqrt{5}})/4$ | 1.17              | 3           |
| 12~15      | $(7 - \sqrt{17})/2$     | 1.43              | 4           |
| 16~24      | 2                       | 2                 | 9           |
| 25~29      | $(7 - \sqrt{5})/2$      | 2.38              | 5           |
| 30~32      | $(9 - \sqrt{5} + \sqrt{38 - 2\sqrt{5}})/4$ | 3.13              | 3           |
| 33~35      | $(9 - \sqrt{5})/2$      | 3.38              | 3           |
| 36~40      | $(5 + \sqrt{13})/2$     | 4.30              | 5           |
| 41~43      | $(9 + \sqrt{5} + \sqrt{38 + 2\sqrt{5}})/4$ | 4.43              | 3           |
| 44~48      | $(7 + \sqrt{5})/2$      | 4.61              | 5           |
| 49~52      | 5                       | 5                 | 4           |
| 53~56      | $(7 + \sqrt{17})/2$     | 5.56              | 4           |
| 57~59      | $(9 + \sqrt{5})/2$      | 5.61              | 3           |

Fig. 2.1. Eigenvalues of C60 fullerene buckyball.
3 Conclusion

For each vertex \( i \), we attach a complex number \( u(i) \). For vector \( u = (u(0), \cdots, u(59)) \in C^{60} \), we introduce two kinds of Sobolev energies, that is, potential energies.

\[
E(u) = \sum_{(i,j) \in e} |u(i) - u(j)|^2 = u^* Au,
\]

\[
E(a, u) = E(u) + a \sum_{j=0}^{59} |u(j)|^2 = u^* (A + aI) u.
\]

The constant \( a \) (\( 0 < a < \infty \)) stands for a dumping parameter. The relations

\[
AG_* = G_* A = I - E_0, \quad G_* E_0 = E_0 G_* = I - E_0
\]  

(3.1)

determine a unique solution \( G_* \). \( E_0 = (1/60)1^t1 \) is the orthogonal projection matrix to the eigenspace corresponding to eigenvalue 0 of \( A \). We call \( G_* \) the pseudo Green matrix of \( A \). \( G_* \) coincides with a Penrose-Moore generalized inverse matrix \( A^\dagger \) of \( A \). \( G(a) = (A + aI)^{-1} \) (\( 0 < a < \infty \)) is Green matrix of \( A \). In section 4, we show

\[
G_* = \lim_{a \to 0^+} \left( G(a) - a^{-1} E_0 \right).
\]  

(3.2)

The important fact is that diagonal elements of \( G_* \) and \( G(a) \) are all the same, which is observed by direct calculations of Mathematica. Concrete values of these are shown by (3.4) and (3.7) into following two theorems. The above fact reflects high symmetry of BB.
Theorem 3.1. For any \( u \in \mathbb{C}^{60} \) satisfying \( u(0) + \cdots + u(59) = 0 \), there exists a positive constant \( C \) which is independent of \( u \), such that the discrete Sobolev inequality
\[
\left( \max_{0 \leq j \leq 59} |u(j)| \right)^2 \leq CE(u)
\] (3.3)
holds. Among such \( C \), the best (the smallest) constant \( C_0 \) is
\[
C_0 = \frac{239741}{376200} \approx 0.63727 \cdots .
\] (3.4)

Diagonal values of \( G_{\ast} \) take the same value \( C_0 \). In particular, we have
\[
C_0 = \frac{1}{60} \sum_{j=1}^{59} \frac{1}{\lambda_j}.
\] (3.5)

If we replace \( C \) by \( C_0 \) in the above inequality, then the equality holds for any column vector \( u \) of \( G_{\ast} \).

Theorem 3.2. For any \( u \in \mathbb{C}^{60} \), there exists a positive constant \( C \), which is independent of \( u \), such that the discrete Sobolev inequality
\[
\left( \max_{0 \leq j \leq 59} |u(j)| \right)^2 \leq CE(a, u)
\] (3.6)
holds. Among such \( C \), the best constant \( C(a) \) is
\[
C(a) = \frac{N(a)}{D(a)},
\] (3.7)
\[
N(a) = 3344 + 160806a + 1153562a^2 + 3594661a^3 + 6334271a^4 + 7104785a^5 + 5406109a^6 + 2893077a^7 + 1109403a^8 + 306415a^9 + 60463a^{10} + 8315a^{11} + 757a^{12} + 41a^{13} + a^{14},
\]
\[
D(a) = a(2 + a)(5 + a)(3 + 5a + a^2)(8 + 7a + a^2) \times (11 + 7a + a^2)(19 + 9a + a^2)(4 + 22a + 25a^2 + 9a^3 + a^4).
\]

Diagonal values of \( G(a) \) take the same value \( C(a) \). In particular, we have
\[
C(a) = \frac{1}{60} \sum_{j=0}^{59} \frac{1}{\lambda_j + a}.
\] (3.8)

If we replace \( C \) by \( C(a) \) in the above inequality, the equality holds for any column vector \( u \) of \( G(a) \).

From (3.8), it follows that \( C(a) \) is a monotone decreasing function of \( a \). Fig 3.1 is the graph of \( C(a) \) and Fig 3.2 is the graph of \( C(a) - (60a)^{-1} \). From (3.2), (3.5) and (3.8), we have the following theorem.
Fig. 3.1. The graph of $C(a)$.

Fig. 3.2. The graph of $C(a) - (60a)^{-1}$.

**Theorem 3.3.** The relation

$$C_0 = \lim_{a \to 0} (C(a) - (60a)^{-1})$$

holds.

Physical meaning of the above theorems is as follows. If $u(i)$ takes a real value, then $u(i)$ represents a deviation from the steady state. The discrete Sobolev inequalities shows that the square of maximum of deviation $|u(i)|$ is estimated from above by constant multiples of the potential energies $E(u)$ and $E(a, u)$. Hence, it is expected that the best constants $C_0$ and $C(a)$ represent rigidity of the mechanical model.

## 4 Green matrix and pseudo Green matrix

The discrete Laplacian $A$ is written in the following form

$$A = \begin{pmatrix} A_0 & A_1 \\ A_1 & A_0 \end{pmatrix},$$

where $A_0$ and $A_1$ are $30 \times 30$ real symmetric matrices. We introduce a $60 \times 60$ matrix $J$ given by

$$J = \begin{pmatrix} I & I \\ I & -I \end{pmatrix},$$

where $I$ is a $30 \times 30$ identity matrix. We have $J^{-1} = (1/2)J$. Using $J$, we have

$$J^{-1}AJ = \begin{pmatrix} A_0 & O \\ O & A_0 \end{pmatrix}, \quad A_\pm = A_0 \pm A_1.$$

$A_+$ has an eigenvalue 0, corresponding eigenvector is $1 = (1, \cdots, 1) \in \mathbb{C}^{30}$. The other eigenvalues of $A_+$ and $A_-$ are all positive. The pseudo Green matrix $G_*$ of $A$ is

$$G_* = \begin{pmatrix} G_{*0} & G_{*1} \\ G_{*1} & G_{*0} \end{pmatrix} = J \begin{pmatrix} G_{*+} & 0 \\ 0 & G_{*-} \end{pmatrix} J^{-1},$$

(4.1)
where \( G_{s+} = A_+^\dagger \) is a Penrose-Moore generalized inverse matrix of \( A_+ \) and \( G_{s-} = A_-^{-1} \) is an inverse matrix of \( A_- \). We have

\[
G_{s\pm} = G_{s0} \pm G_{s1} \iff \begin{cases} G_{s0} = (G_{s+} + G_{s-})/2, \\ G_{s1} = (G_{s+} - G_{s-})/2. \end{cases}
\]

It is easy to see that

\[
A + aI = J \begin{pmatrix} A_+ + aI & O \\ O & A_- + aI \end{pmatrix} J^{-1}.
\]

If we put \( G_{\pm}(a) = (A_{\pm} + aI)^{-1} \), Green matrix \( G(a) = (A + aI)^{-1} \) is given by

\[
G(a) = (A + aI)^{-1} = J \begin{pmatrix} G_+ & O \\ O & G_- \end{pmatrix}(a) J^{-1} = \begin{pmatrix} G_0 & G_1 \\ G_1 & G_0 \end{pmatrix}(a),
\]

where

\[
G_{\pm}(a) = G_0(a) \pm G_1(a) \iff \begin{cases} G_0(a) = (G_{\pm}(a) + G_{\mp}(a))/2, \\ G_1(a) = (G_{\pm}(a) - G_{\mp}(a))/2. \end{cases}
\]

Using the above expressions (4.1) and (4.2), one can reduce the number of computations in finding explicit forms of \( G_* \) and \( G(a) \).

## 5 The spectral decomposition of \( A \)

For \( 0 \leq j \leq 59 \), we introduce

\[
\delta_j = \delta(-j), \delta(1-j), \cdots, \delta(59-j), \quad \delta(k) = \begin{cases} 1 & \text{(Mod}(k, 60) = 0), \\ 0 & \text{(Mod}(k, 60) \neq 0). \end{cases}
\]

The discrete Laplacian \( A \) is a \( 60 \times 60 \) real symmetric matrix. Using unitary matrix \( Q \), \( A \) is diagonalized as \( Q^*AQ = \tilde{A} = \text{diag}\{\lambda_0, \cdots, \lambda_{59}\} \). \( E_k = q_k^* q_k \) (\( 0 \leq k \leq 59 \)) are orthogonal projection matrices which satisfy

\[
E_k^* = E_k, \quad E_k E_l = \delta(k-l)E_k \quad (0 \leq k, l \leq 59).
\]

The spectral decomposition of \( 60 \times 60 \) unit matrix \( I \) and the discrete Laplacian \( A \) are rewritten as

\[
I = QQ^* = \sum_{k=0}^{59} E_k, \quad A = \tilde{Q} \tilde{A} Q^* = \sum_{k=0}^{59} \lambda_k E_k = \sum_{k=1}^{59} \lambda_k E_k.
\]

For \( 0 < a < \infty \), we have

\[
G(a) = (A + aI)^{-1} = \sum_{k=0}^{59} (\lambda_k + a)^{-1} E_k \quad (5.1)
\]

\[
G_* = \lim_{a \to +0} (G(a) - a^{-1} E_0) = \sum_{k=1}^{59} \lambda_k^{-1} E_k. \quad (5.2)
\]
It is easy to see that (5.2) satisfies (3.1).

The rest of this section is devoted to the proof of (3.5) and (3.8) in the main theorems.

**Proposition 5.1.** For any \( j_0 \) \((0 \leq j_0 \leq 59)\), we have

\[
C_0 = ^t \delta_{j_0} G \delta_{j_0} = \frac{1}{60} \sum_{k=1}^{59} \lambda_k^{-1}.
\]

**Proof of Proposition 5.1**

First of all, we have

\[
\sum_{j=0}^{59} \delta_j E_k \delta_j = \sum_{j=0}^{59} \delta_j q_k^+ \delta_j = \sum_{j=0}^{59} |q_k^+ \delta_j|^2 = q_k^+ q_k = 1 \quad (0 \leq k \leq 59).
\]

We note that diagonal values of \( G \) are identical. For any \( j_0 \) \((0 \leq j_0 \leq 59)\), using (5.2) and (5.3), we have

\[
C_0 = ^t \delta_{j_0} G \delta_{j_0} = \frac{1}{60} \sum_{j=0}^{59} \delta_j G \delta_j = \frac{1}{60} \sum_{j=0}^{59} \lambda_k^{-1} E_k \delta_j = \frac{1}{60} \sum_{k=1}^{59} \lambda_k^{-1}.
\]

Thus we have Proposition 5.1. That is to say, we have (3.5).

**Proposition 5.2.** For any \( j_0 \) \((0 \leq j_0 \leq 59)\), we have

\[
C(a) = ^t \delta_{j_0} G(a) \delta_{j_0} = \frac{1}{60} \sum_{k=0}^{59} (\lambda_k + a)^{-1}.
\]

**Proof of Proposition 5.2**

We note that the diagonal values of \( G(a) \) are identical. For any \( j_0 \) \((0 \leq j_0 \leq 59)\), using (5.1) and (5.3), we have

\[
C(a) = ^t \delta_{j_0} G(a) \delta_{j_0} = \frac{1}{60} \sum_{j=0}^{59} \delta_j G(a) \delta_j = \frac{1}{60} \sum_{j=0}^{59} \delta_j \sum_{k=0}^{59} (\lambda_k + a)^{-1} E_k \delta_j = \frac{1}{60} \sum_{k=0}^{59} (\lambda_k + a)^{-1} \sum_{j=0}^{59} \delta_j E_k \delta_j = \frac{1}{60} \sum_{k=0}^{59} (\lambda_k + a)^{-1}.
\]

Thus we have Proposition 5.2. That is to say, we have (3.8).
6 Proof of Theorem 3.1

For \( u, v \in C^{60} \), we attach an inner product \((u, v)\) defined by
\[
(u, v) = v^* u, \quad \| u \|^2 = (u, u).
\]
For \( u, v \in C_0^{60} := \{ u \mid u \in C^{60} \text{ and } u(0) + \cdots + u(59) = 0 \} \), we also define \((u, v)_A\) by
\[
(u, v)_A = (Au, v) = v^* Au, \quad \| u \|^2_A = (u, u)_A = E(u).
\]

Lemma 6.1. For any \( u \in C_0^{60} \), we have the following reproducing relation.
\[
u(j) = (u, G^* \delta_j)_A \quad (0 \leq j \leq 59).
\]

The proof of Lemma 6.1 We first note that \( G^* \) is an Hermitian matrix and that \( E_0 u = 60^{-1} \cdot 1 u = 0 \). For any \( u \in C_0^{60} \) and any fixed \( j = 0, 1, \ldots, 59 \), we have
\[
(u, G^* \delta_j)_A = (Au, G^* \delta_j) = \delta^*_j G^*_A u = \delta^*_j (I - E_0) u = \delta^*_j u = u(j).
\]

This completes the proof of Lemma 6.1. \(\blacksquare\)

Putting \( u = G^* \delta_j \) in (6.1), we have
\[
C_0 = \delta_j G^*_A \delta_j = \| G^* \delta_j \|^2_A = E(G^* \delta_j).
\]

Applying Schwarz inequality to (6.1) and using (6.2), we have
\[
| u(j) |^2 \leq \| u \|^2_A \| G^* \delta_j \|^2_A = C_0 E(u).
\]
Taking the maximum with respect to \( j \) on both sides, we obtain discrete Sobolev inequality
\[
\left( \max_{0 \leq j \leq 59} | u(j) | \right)^2 \leq C_0 E(u).
\]
If we take \( u = G^* \delta_{j_0} \) in (6.3), then we have
\[
\left( \max_{0 \leq j \leq 59} | \delta_j G^* \delta_{j_0} | \right)^2 \leq C_0 E(G^* \delta_{j_0}) = C_0^2.
\]
Combining this and a trivial inequality
\[
C_0^2 = (\delta_{j_0} G^* \delta_{j_0})^2 \leq \left( \max_{0 \leq j \leq 59} | \delta_j G^* \delta_{j_0} | \right)^2,
\]
we have
\[
\left( \max_{0 \leq j \leq 59} | \delta_j G^* \delta_{j_0} | \right)^2 = C_0 E(G^* \delta_{j_0}).
\]
This shows that if we replace \( C \) by \( C_0 \) in an inequality (3.3), the equality holds for \( G^* \delta_{j_0} \). (3.4) follows from (3.5) by simple calculation. (3.4) is also confirmed by the observation of the diagonal values of \( G^* \). This completes the proof of Theorem 3.1. \(\blacksquare\)
7 Proof of Theorem 3.2

For \( u, v \in \mathbb{C}^{60} \), we introduce

\[
(u, v)_H = ((A + aI)u, v) = v^*(A + aI)u, \quad \| u \|_H^2 = (u, u)_H = E(a, u).
\]

In this section, we use the simpler notation \( G = G(a) \).

**Lemma 7.1.** For any \( u \in \mathbb{C}^{60} \), we have the following reproducing relation.

\[
 u(j) = (u, G\delta_j)_H \quad (0 \leq j \leq 59). \tag{7.1}
\]

The proof of Lemma 7.1: We note that \( G \) is an Hermitian matrix. For any \( u \in \mathbb{C}^{60} \) and any fixed \( j = 0, 1, \cdots, 59 \), we have

\[
(u, G\delta_j)_H = ((A + aI)u, G\delta_j) = t\delta_j G(A + aI)u = t\delta_j u = u(j).
\]

This completes the proof of Lemma 7.1. ■

Putting \( u = G\delta_j \) in (7.1), we have

\[
 C(a) = t\delta_j G\delta_j = \| G\delta_j \|_H^2 = E(a, G\delta_j). \tag{7.2}
\]

Applying Schwarz inequality to (7.1) and using (7.2), we have

\[
| u(j) |^2 \leq \| u \|_H^2 \| G\delta_j \|_H^2 = C(a)E(a, u).
\]

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

\[
 \left( \max_{0 \leq j \leq 59} | u(j) | \right)^2 \leq C(a)E(a, u). \tag{7.3}
\]

If we take \( u = G\delta_{j_0} \) in (7.3), then we have

\[
 \left( \max_{0 \leq j \leq 59} | t\delta_j G\delta_{j_0} | \right)^2 \leq C(a)E(a, G\delta_{j_0}) = C(a)^2.
\]

Combining this and a trivial inequality

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

we have

\[
 \left( \max_{0 \leq j \leq 59} | t\delta_j G\delta_{j_0} | \right)^2 = C(a)E(a, G\delta_{j_0}).
\]

This shows that if we replace \( C \) by \( C(a) \) in an inequality (3.6), the equality holds for \( u = G\delta_{j_0} \). (3.7) follows from (3.8) by simple calculation. (3.7) also follows from the observation of the diagonal value of \( G \) after calculating \( G \) by Mathematica. This completes the proof of Theorem 3.2.
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1 Faculty of Engineering Science, Osaka University
1-3 Machikaneyama-cho, Toyonaka 560-8531, Japan
E-mail address: kametaka@sigmath.es.osaka-u.ac.jp

2 Liberal Arts and Basic Sciences, College of Industrial Technology
Nihon University, 2-11-1 Shin-ei, Narashino 275-8576, Japan
E-mail address: nagai.atsushi@nihon-u.ac.jp

3 Tokyo Metropolitan College of Industrial Technology
1-10-40 Higashi-oi, Shinagawa Tokyo 140-0011, Japan
E-mail address: yamagisi@s.metro-cit.ac.jp

4 General Education, College of Science and Technology
Nihon University, 7-24-1 Narashinodai, Funabashi 274-8501, Japan
E-mail address: takemura.kazuo@nihon-u.ac.jp
Department of Computer Science, National Defense Academy
1-10-20 Yokosuka 239-8686, Japan
E-mail address: wata@nda.ac.jp