Researches in Mathematics and Mechanics. — 2020. — V. 25, Is. 1(35). — P. 7–15

UDC 517.9

A. I. Dudko, V. N. Pivovarchik

South Ukrainian National Pedagogical University named after K. D. Ushynsky

SPECTRAL PROBLEM OF FULLERENE VIBRATIONS

Small vibrations of a graph of fullerene (truncated icosahedron) is considered each edge of which is a so-called Stieltjes string (a massless thread bearing finite number of point masses) symmetric with respect to its midpoint. The spectral problem is obtained by imposing the continuity and balance of forces conditions at the vertices. It is shown that when all the edges of the graph are the same then due to the symmetry of the problem there are multiple eigenvalues. The maximal multiplicity of an eigenvalue of such problem is 32, exactly the value which is maximal for cyclically connected graphs, i.e. $\mu + 1$ where μ is the cyclomatic number of the graph.

MSC: 39A70, 39A60, 70J30.

Key words: Stieltjes string, graph, multiplicity, eigenvalue, cyclomatic number, recurrence relations, boundary conditions.

DOI: XXXX.

1. Introduction

Since the time of Plato and Archimedes, it is known that there are only 5 regular polyhedra that are called Platonic solids. There are also Archimedian or so-called semiregular polyhedra.

In our work we will consider a truncated icosahedron. From the point of view of mathematics, this is an old object, which was rediscovered relatively recently. Interest to this object arose unexpectedly again in connection with the discovery by chemists of the third state of aggregation of carbon. It turned out that this state of carbon corresponds to a molecule that consists of 60 atoms, which are located at the vertices of a truncated icosahedron. A fullerene (buckyball) is any molecule composed entirely of carbon, in the form of a hollow sphere, ellipsoid, tube, and many other shapes. In our case, we will consider buckminsterfullerene C_{60}. It was prepared in 1989 by Richard Smalley and was named after Richard Buckminster Fuller, an architect who created a geodesic dome similar to a truncated icosahedron. Buckminsterfullerene is the smallest fullerene molecule containing pentagonal and hexagonal faces in which no two pentagons share an edge. The structure of C_{60} is a truncated icosahedron

Received 04.01.2020

(one of the semiregular or Archimedean solids), which resembles an association football ball of the type made of twenty hexagons and twelve pentagons, with a carbon atom at the vertices of each polygon and a bond along each polygon edge [8] (see Fig.1, [9]).

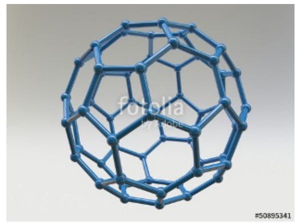

Fig. 1.

In this paper we consider small transverse vibrations of truncated icosahedron the edges of which are so-called Stieltjes strings, i.e. elastic threads of zero density bearing point masses. Transverse vibrations of graphs of such strings were considered in many publications [2], [3], [4].

Spectral problems describing longitudinal vibrations of a graph of springs bearing masses are reduced to the same equations [6].

2. Main Results

1. Fullerine graph. We choose arbitrary orientation of the edges of the graph. Let us consider a Stieltjes string bearing $n \geq 3$ point masses $m_1, m_2, \ldots, m_n$ $(m_k > 0)$, let $l_0, l_1, \ldots, l_n$ $(l_k > 0)$ be the intervals into which the masses divide the total length l of the string $\left(\sum_{k=1}^{n} l_k = l\right)$. We enumerate the point masses m_k $(k = 1, 2, \ldots, n)$ and subintervals l_k $(k = 0, 1, \ldots, n)$ on an edge successively in the direction of the edge. In the sequel we consider Stieltjes strings symmetric with respect to their midpoints. This means that:

1) if n is even then: $m_k = m_{n-k+1}, \;\; k = 1, \ldots, n$; $l_k = l_{n-k}, \;\; k = 0, \ldots, n$;

2) if n is odd then: $m_k = m_{n-k+1}, \;\; k = 1, \ldots, [n]$; $l_k = l_{n-k}, \;\; k = 0, \ldots, [n]$, where $[a]$ denotes the integer part of a.

We consider a fullerene graph G each edge of which is the same symmetric Stieltjes string bearing n point masses. The graph is stretched and can vibrate such that each mass moves in the direction orthogonal to the equilibrium position of the edge.

Denote by v_i $(i = 1, 2, \dots, 60)$ the vertices of G, by e_j $(j = 1, 2, \dots, 90)$ the edges of G.

For each i denote by $d(v_i) = 3$ the degree of the vertex v_i, by $d^+(v_i)$ the indegree, i.e. the number of edges incoming into v_i, by $d^-(v_i)$ the outdegree, i.e. the number of edges outgoing from v_i. It is clear that $0 \le d^{\pm}(v_i) \le 3$ and $d^+(v_i) + d^-(v_i) = d(v_i) = 3$.

Let W_i^+ be the set of numbers of edges incoming into v_i and W_i^- be the set of numbers of edges outgoing from v_i $(i = 1, 2, \dots, 60)$.

It should be noticed that the graph of the fullerine belongs to the class of cyclically connected graphs

Definition 1 (see [1], Definition 2)**.** *Two vertices v and w of a connected graph G are said to be cyclically connected if a finite set of cycles $C_1, C_2, ..., C_k$ ($C_j \subset G$, $j = 1, 2, ...k$) exists such that $v \in C_1$, $w \in C_k$ and each neighboring pair of cycles possesses at least one common vertex.*

Definition 2 (see [1], Definition 3)**.** *A graph is said to be cyclically connected if each pair of vertices in it is cyclically connected*

We assume absence of point masses at the vertices. Vibrations of masses on the edges are described by equations (see [5], p. 141 or [11], eq. (0.7.4))

$$\frac{V_k^{(j)}(t) - V_{k-1}^{(j)}(t)}{l_{k-1}} + \frac{V_k^{(j)}(t) - V_{k+1}^{(j)}(t)}{l_k} = m_k \frac{d^2}{dt^2} V_k^{(j)}(t), \tag{1}$$

where $k = 1, 2, \dots, n;$ $j = 1, 2, \dots, g; g$ is the number of edges; $V_k^{(j)}(t)$ is the transverse displacement of the mass m_k lying on the edge e_j; t is the time.

At an interior vertex v_i we impose the continuity conditions

$$\begin{aligned} V_0^{(j_1^-)}(t) &= V_0^{(j_2^-)}(t) = \dots = V_0^{(j^-_{d^-(v_i)})}(t) \\ &= V_{n+1}^{(j_1^+)}(t) = V_{n+1}^{(j_2^+)}(t) = \dots = V_{n+1}^{(j^+_{d^+(v_i)})}(t), \end{aligned} \tag{2}$$

where $\{j_1^-, \dots, j^-_{d^-(v_i)}\} \in W_i^-;$ $\{j_1^+, \dots, j^+_{d^+(v_i)}\} \in W_i^+$ and the balance of forces condition

$$\sum_{m=1}^{d^+(v_i)} \frac{V_{n+1}^{(j_m^+)}(t) - V_n^{(j_m^+)}(t)}{l_n} - \sum_{m=1}^{d^-(v_i)} \frac{V_1^{(j_m^-)}(t) - V_0^{(j_m^-)}(t)}{l_0} = 0. \tag{3}$$

As usually in the linear approach we separate variables by ansatz (see, e.g. eq. (0.7.4), (0.7.5) in [11]) $V_k^{(j)}(t) = U_k^{(j)}(z)e^{i\lambda t}$, $z = \lambda^2$. Substituting it into (1) – (3) we obtain the following spectral problem:

$$\frac{U_k^{(j)}(z) - U_{k-1}^{(j)}(z)}{l_{k-1}} + \frac{U_k^{(j)}(z) - U_{k+1}^{(j)}(z)}{l_k} = -m_k z U_k^{(j)}(z), \tag{4}$$

$$\begin{aligned} U_0^{(j_1^-)}(z) &= U_0^{(j_2^-)}(z) = \cdots = U_0^{(j^-_{d^-(v_i)})}(z) \\ &= U_{n+1}^{(j_1^+)}(z) = U_{n+1}^{(j_2^+)}(z) = \cdots = U_{n+1}^{(j^+_{d^+(v_i)})}(z), \end{aligned} \tag{5}$$

$$\sum_{m=1}^{d^+(v_i)} \frac{U_{n+1}^{(j_m^+)}(z) - U_n^{(j_m^+)}(z)}{l_n} - \sum_{m=1}^{d^-(v_i)} \frac{U_1^{(j_m^-)}(z) - U_0^{(j_m^-)}(z)}{l_0} = 0 \tag{6}$$

where $k = 1, 2, \ldots, n$; $i = 1, 2, \ldots, 60$; $j_m^- \in W_i^-$, $m = j_1^-, \ldots, j^-_{d^-(v_i)}$; $j_m^+ \in W_i^+$, $m = j_1^+, \ldots, j^+_{d^+(v_i)}$ and $U_k^{(j)}$ is the amplitude of vibrations of the mass m_k located on the edge e_j, z is the spectral parameter. Here equations (5) are the continuity conditions and (6) describe the balance of forces.

2. Graph of Stieltjes strings vibrations.

Following [5] we look for a solution in the form $U_k^{(j)}(z) = R_{2k-2}(z, c)U_1^{(j)}$, $k = 1, 2, \ldots, n+1$, where $R_{2k-2}(z, c)$ is a polynomials of degree $k-1$. In the sequel, we use $R_k(c)$ instead of $R_k(z, c)$ to shorten the notation.

The polynomials $R_k(c)$ satisfy the following recurrence relations:

$$R_{2k}(c) = l_k R_{2k-1}(c) + R_{2k-2}(c), \tag{7}$$

$$R_{2k-1}(c) = R_{2k-3}(c) - m_k z R_{2k-2}(c)$$

with the initial conditions

$$R_{-1}(c) \equiv \frac{1-c}{l_0}, \quad R_0(c) \equiv 1.$$

For a symmetric string

$$R_{2n-1}(0) = \frac{1}{l_0} R_{2n}(1) \tag{8}$$

and due to the Lagrange identity

$$R_{2n-1}(0)R_{2n}(1) - R_{2n-1}(1)R_{2n}(0) = \frac{1}{l_0}$$

(see, e.g. [7], Lemma 3.5) we obtain

$$\frac{1}{l_0}\left(R_{2n}(1)\right)^2 - \frac{1}{l_0} = R_{2n}(0)R_{2n-1}(1). \tag{9}$$

Now we use the procedure described in [10]. It is convenient to introduce the following solution of (4):

$$U_k^{(j)}(z) = \frac{B^{(j)} - A^{(j)}R_{2n}(1)}{R_{2n}(0)}R_{2k-2}(0) + A^{(j)}R_{2k-2}(1), \tag{10}$$

where $A^{(j)}, B^{(j)}$ are constants independent of k and z. These solutions exist for all z which are not zeros of $R_{2n}(0)$. In view of (1), (2), equation (7) for $k = 0$ implies $R_{-2}(0) = 0, \quad R_{-2}(1) = 1$.

Substituting these into (10) we have

$$U_0^{(j)}(z) = \frac{B^{(j)} - A^{(j)}R_{2n}(1)}{R_{2n}(0)}R_{-2}(0) + A^{(j)}R_{-2}(1) = A^{(j)}. \tag{11}$$

In the same way, for $k = n + 1$

$$U_{n+1}^{(j)}(z) = \frac{B^{(j)} - A^{(j)}R_{2n}(1)}{R_{2n}(0)}R_{2n}(0) + A^{(j)}R_{2n}(1) = B^{(j)}. \tag{12}$$

Continuity conditions (5) look now as

$$A^{(j_1^-)} = A^{(j_2^-)} = \cdots = A^{(j^-_{d^-(v_i)})} = B^{(j_1^+)} = B^{(j_2^+)} = \cdots = B^{(j^+_{d^+(v_i)})} := \Phi(v_i). \tag{13}$$

Balance of forces equation (6) with account of (10), (13) attains the form

$$\sum_{m=1}^{d^+(v_i)}\left(l_n B^{(j_m^+)}R_{2n-1}(0) - A^{(j_m^+)}\right) - \sum_{m=1}^{d^-(v_i)}\left(B^{(j_m^-)} - A^{(j_m^-)}R_{2n}(1)\right) = 0. \tag{14}$$

$$\sum_{m=1}^{d^+(v_i)}\left(l_n B^{(j_m^+)}R_{2n-1}(0) - A^{(j_m^+)}\right) - \sum_{m=1}^{d^-(v_i)}\left(B^{(j_m^-)} - A^{(j_m^-)}R_{2n}(1)\right)$$

$$= \sum_{m=1}^{d^+(v_i)} l_n B^{(j_m^+)}R_{2n-1}(0) + \sum_{m=1}^{d^-(v_i)} A^{(j_m^-)}R_{2n}(1) - \left(\sum_{m=1}^{d^+(v_i)} A^{(j_m^+)} + \sum_{m=1}^{d^-(v_i)} B^{(j_m^-)}\right)$$

$$= \sum_{m=1}^{d^+(v_i)} B^{(j_m^+)}R_{2n}(1) + \sum_{m=1}^{d^-(v_i)} A^{(j_m^-)}R_{2n}(1) - \sum_{v_j\sim v_i}\Phi(v_j)$$

$$= R_{2n}(1)\left(\sum_{m=1}^{d^+(v_i)}\Phi(v_i)+\sum_{m=1}^{d^-(v_i)}\Phi(v_i)\right)-\sum_{v_j\sim v_i}\Phi(v_j)$$

$$= R_{2n}(1)d(v_i)\Phi(v_i)-\sum_{v_j\sim v_i}\Phi(v_j).$$

or

$$R_{2n}(1)d(v_i)\Phi(v_i)-\sum_{v_j\sim v_i}\Phi(v_j)=0.$$

Here the sum is taken over all the vertices v_j adjacent with v_i.

Finally, we obtain using the notation $\zeta = 3R_{2n}(1)$, $F = \{\Phi(v_1),\dots,\Phi(v_{60})\}^T$, and denoting by A the adjacency matrix of our graph:

$$\zeta F - AF = 0. \tag{15}$$

Let z_0 be not a zero of $R_{2n}(0)$, then it is an eigenvalue of problem (4)–(6) if and only if $\zeta_0 := 3R_{2n}(1)$ is an eigenvalue of matrix equation (15). This means that the spectrum of problem (4)–(6) consists of zeros of $R_{2n}(0)$ and of zeros of the polynomials $3R_{2n}(1)-\zeta_s$, where ζ_s $(s=1,2,\dots,60)$ are the eigenvalues of (15).

Theorem 1. *The characteristic polynomial of problem (4)–(6) is*

$$\phi(z) = (R_{2n}(z,0))^{30}P_{60}(3R_{2n}(z,1))$$

where P_{60} is the characteristic polynomial of matrix A.

Proof. We have already shown above that if z_0 is an eigenvalue of problem (4)–(6) and $R_{2n}(z_0,0)\neq 0$ then ζ_0 is a zero of $P_{60}(\zeta)$. This gives $60n$ (with account of multiplicities) eigenvalues of problem (4)–(6). The total number of eigenvalues is $90n$ since 90 is the number of edges in the fullerene. Therefore, there are $30n$ (with account of multiplicities) eigenvalues more. They are the zeros of $R_{2n}^{30}(z,0)$ because for each eigenvalue there exist 30 linearly independent eigenvectors which are composed by the vectors $R_2(z,0), R_4(z,0), ..., R_{2n-2}(z,0)$ on the edges of the hexagonal faces of the graph. Theorem is proved.

Using (15) we obtain the characteristic equation for Buckminsterfullerene graph by program MAPLE

$P_{60}(\zeta) = 2985984+54743040\zeta+186416640\zeta^2-1566501120\zeta^3-7440712560\zeta^4+$

$$+26034025632\zeta^5+108565938200\zeta^6-310065067080\zeta^7-831616531095\zeta^8+$$

$$+2527365617120\zeta^9+3576552321006\zeta^{10}-13627897407360\zeta^{11}-8131429397135\zeta^{12}+$$

$$+49433493646080\zeta^{13}+4679380503120\zeta^{14}-126428882536240\zeta^{15}+$$

$$+29617003666920\zeta^{16}+238553091055200\zeta^{17}-112654402736360\zeta^{18}-$$

$$-344185906596720\zeta^{19}+228227031040884\zeta^{20}+390055074762240\zeta^{21}-$$

$$-324375523213200\zeta^{22}-354145195147200\zeta^{23}+351861389316780\zeta^{24}+$$

$$+261359090670624\zeta^{25}-303315997028160\zeta^{26}-158412719276240\zeta^{27}+$$

$$+212712221820840\zeta^{28}+79417625268960\zeta^{29}-123163094844616\zeta^{30}-$$

$$-33076275953760\zeta^{31}+59443188508110\zeta^{32}+11466942645600\zeta^{33}-$$

$$-24056403184260\zeta^{34}-3308173115904\zeta^{35}+8189116955350\zeta^{36}+$$

$$+792175427520\zeta^{37}-2346799508400\zeta^{38}-156652575440\zeta^{39}+$$

$$+565407465144\zeta^{40}+25376437920\zeta^{41}-114118295000\zeta^{42}-$$

$$-3327625680\zeta^{43}+19180834020\zeta^{44}+347208896\zeta^{45}-2661033600\zeta^{46}-$$

$$-28113600\zeta^{47}+300906380\zeta^{48}+1700640\zeta^{49}-27244512\zeta^{50}-$$

$$-72240\zeta^{51}+1925160\zeta^{52}+1920\zeta^{53}-102160\zeta^{54}-24\zeta^{55}+$$

$$+3825\zeta^{56}-90\zeta^{58}+\zeta^{60},$$

and, consequently, (this is given by MAPLE)

$$P_{60}(\zeta)=(\zeta-3)(\zeta^2+3\zeta+1)^3(\zeta^4-3\zeta^3-2\zeta^2+7\zeta+1)^3*$$

$$*(\zeta+2)^4(\zeta^2+\zeta-4)^4(\zeta^2-\zeta-3)^5(\zeta^2+\zeta-1)^5(\zeta-1)^9.$$

Thus we obtain the following set of zeros of P_{60}: $\zeta_1=\zeta_2=\zeta_3\approx-2.618$, $\zeta_4=\zeta_5=\zeta_6=\zeta_7\approx-2.562$, $\zeta_8=\zeta_9=\zeta_{10}=\zeta_{11}=-2$, $\zeta_{12}=\zeta_{13}=\zeta_{14}=\zeta_{15}=\zeta_{16}\approx-1.6818$, $\zeta_{17}=\zeta_{18}=\zeta_{19}\approx-1.438$, $\zeta_{20}=\zeta_{21}=\zeta_{22}=\zeta_{23}=\zeta_{24}\approx-1.303$, $\zeta_{25}=\zeta_{26}=\zeta_{27}\approx-0.382$, $\zeta_{28}=\zeta_{29}=\zeta_{30}\approx-0.139$, $\zeta_{31}=\zeta_{32}=\zeta_{33}=\zeta_{34}=\zeta_{35}\approx0.618$, $\zeta_{36}=\zeta_{37}=\zeta_{38}=\zeta_{39}=\zeta_{40}=\zeta_{41}=\zeta_{42}=\zeta_{43}=\zeta_{44}=1$, $\zeta_{45}=\zeta_{46}=\zeta_{47}=\zeta_{48}\approx1.562$, $\zeta_{49}=\zeta_{50}=\zeta_{51}\approx1.820$, $\zeta_{52}=\zeta_{53}=\zeta_{54}=\zeta_{55}=\zeta_{56}\approx2.303$, $\zeta_{57}=\zeta_{58}=\zeta_{59}\approx2.757$, $\zeta_{60}=3$.

3. Conclusion

The graph C_{60} is cyclically connected (see Definition 2). The maximum multiplicity of an eigenvalue of the problem on such graph is $\mu+1$ where μ is the cyclomatic number of the graph [1], Theorem 3.2. Since $\mu = q - p + 1$, where p is the number of vertices and q is the number of edges, in our case $\mu + 1 = 32$. We see that in our problem the maximum possible multiplicity is 32 when the eigenvalue is a (simple) zero of $R_{2n}(z, 0)$ and a double zero of $R_{2n}(z, 1) - 1$.

Дудко А. І., Пивоварчик В. М.
Спектральна задача, пов'язана з коливаннями фулеріну

Резюме

Розглянуті малі поперечні коливання графу фулеріну (усіченого ікосаедру), кожне ребро якого — стільтьєсівська струна (безмасова нитка, що несе на собі скінчену кількість зосереджених мас), симетрична відносно своєї середини. Спектральна задача отримана накладанням умов неперервності та балансу сил у вершинах. Показано, що якщо всі ребра однакові, то завдяки симетрії задачі виникають кратні власні значення. Максимальна кратність такого власного значення становить 32, що є максимальним можливим для циклічно зв'язного графу, тобто $\mu+1$, де μ — це цикломатичне число графу.
Ключові слова: Стільтьєсівська струна, граф, кратність, власне значення, цикломатичне число, рекурентні співвідношення, крайові умови.

Дудко А. И., Пивоварчик В. Н.
Спектральная задача, связанная с колебаниями фулерина

Резюме

Рассмотрены малые поперечные колебания графа фулерина (усеченного икосаэдра), каждое ребро которого — стильтьесовская струна (безмассовая нить, несущая на себе конечное количество сосредоточенных масс), симметричная относительно своей середины. Спектральная задача получена наложением условий непрерывности и баланса сил в вершинах. Показано, что если все ребра одинаковые, то благодаря симметрии задачи возникают кратные собственные значения. Максимальная кратность такого собственного значения 32, что является максимальным возможным для циклически связного графа, т.е. $\mu+1$, где μ — это цикломатическое число графа.
Ключевые слова: Стильтьесовская струна, граф, кратность, собственное значение, цикломатическое число, рекуррентные соотношения, краевые условия.

References

1. Boyko O., Martynyuk O., Pivovarchik V. (2019) *On maximal multiplicity of eigenvalues of finite-dimensional spectral problem on a graph*. Methods of Functional Analysis and Topology, Vol. 25, no. 2, p. 104–117.
2. Genin J., and Maybee J. S. (1974). Mechanical vibrations trees. *J. Math. Anal. Appl.*, Vol. 45, p. 746–763.
3. Gladwell G. (2004).*Inverse problems in vibration* Kluwer Academic Publishers, Dordrecht, 457 p.
4. Gladwell G., A. Morassi. (2011). Matrix inverse eigenvalue problems.[Dynamical Inverse Problems: Theory and Applications]. *CISM Courses and Lectures*, Vol. 529, p. 1–29.
5. Gantmakher F.R., Krein M.G.(2002) *Oscillating matrices and kernels and vibrations of mechanical systems*. AMS Chelsea Publishing, Providence, RI, 310 p.
6. Marchenko V.A. (2005) *Introduction to the theory of inverse problems of spectral analysis (in Russian)*. Kharkov: Acta, 141 p.
7. Pivovarchik V., Rozhenko N., Tretter C. (2013) Dirichlet—Neumann inverse spectral problem for a star graph of Stieltjes strings. *Linear Algebra and Applications*, Vol. 439, P. 2263–2292.
8. Qiao R., Roberts A., Mount A., Klaine S., Kleine P. C. (2007) Translocation of C60 and Its Derivatives Across a Lipid Bilayer. *Nano Letters*, Vol. 7, no. 3, p. 614–619.
9. https://blog.biolinscientific.com/hs-fs/hubfs/fullereneC60.jpeg?width=900 name=fullereneC60.jpeg.
10. Pivovarchik V., Taystruk O. (2014) Spectral problem for a graph of symmetric Stieltjes strings. *Methods of Functional Analysis and Topology*, Vol. 20, no. 2, p. 164–174.
11. Atkinson F.V. Discrete and continuous boundary problems. Academic Press, NY, London (1964). Russian translation. Аткинсон Ф.В. *Дискретные и непрерывные граничные задачи*, Москва, “Мир”, (1968), 749 с.