Article

Dynamic Ramsey Theory of Mechanical Systems Forming a Complete Graph and Vibrations of Cyclic Compounds

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Abstract: Ramsey theory influences the dynamics of mechanical systems, which may be described as abstract complete graphs. We address a mechanical system which is completely interconnected with the two kinds of ideal Hookean springs. The suggested system mechanically corresponds to the cyclic molecules, in which functional groups are interconnected with two kinds of chemical bonds, represented mechanically with two springs k_1 and k_2. In this paper, we consider a Cyclic system (molecule) built of six equal masses m and two kinds of springs. We pose the following question: what is the minimal number of masses in the such a system in which three masses are constrained to be connected with spring k_1 or three masses to be connected with spring k_2? The answer to this question is supplied by the Ramsey theory, and it is formally stated as follows: what is the minimal number $R(3,3)$? The result emerging from the Ramsey theory is $R(3,3) = 6$. Thus, in the aforementioned interconnected mechanical system will be necessarily present the triangles (at least one triangle), built of masses and springs. This prediction constitutes the vibrational spectrum of the system. Thus, the Ramsey Theory supplies the selection rules for the vibrational spectra of the cyclic molecules. Symmetrical system built of six vibrating entities is addressed. The Ramsey approach works for 2D and 3D molecules, which may be described as abstract complete graphs.

Keywords: Ramsey theory; complete graph; vibrational spectrum; eigenfrequency; selection rule; cyclic molecule

1. Introduction

Ramsey theory, is a branch of mathematics/combinatorics that focuses on the appearance of ordered substructures within a structure of a known size. Ramsey theory states that any structure will necessarily contain an orderly substructure [1]. Ramsey's theorem, in one of its graph-theoretic forms, states that one will find monochromatic cliques in any edge labelling (with colours) of a sufficiently large complete graph [2]. One more example is supplied by the van der Waerden's theorem: colorings of the integers by finitely many colors must have long monochromatic arithmetic progressions [2]. Problems in Ramsey theory typically ask a question of the form: "how big must some structure be to guarantee that a particular property holds?" More specifically, Ron Graham described Ramsey theory as a "branch of combinatorics"[3-5]. A simple, popular introduction to the Ramsey theory is found in refs. 2-3. More advanced, rigorous mathematical approach is presented in refs. 4-5. Applications of the Ramsey theory for the theory of communication and decision making are discussed in ref. 6. We address the application of the Ramsey theory for the analysis of mechanical systems, which may be represented as complete graphs. Cyclic molecules may be seen as complete graphs [7-8]. Chemical bonds are seen the edges (links) of the graph, which in a very crude approximation may be considered as ideal springs. We demonstrate that the Ramsey theory introduces the "selection rules" for eigenmodes (eigenfrequencies) of the cyclic molecules, treated as completed graphs. Thus, the Ramsey

approach to the vibrational spectra of the cyclic molecules becomes possible. The proposed Ramsey approach predicts the Ramsey modes, which are necessarily present in these spectra.

### 1.1. Ramsey theory and vibrations of cyclic molecules

Consider mechanical system built of six identical masses m shown in **Figure 1**. These masses are connected with two ideal Hookean massless springs k_1 and k_2 as shown in **Figure 1**. The mechanical system depicted in **Figure 1** corresponds to the chemical compound in which two kinds of chemical bonds are present. These bonds are represented by the springs k_1 and k_2. The bonds form the complete graph, i.e. a graph in which each pair of graph vertices (masses) is connected by an edge (spring/chemical bond). We demonstrate that the Ramsey theory supplied predictions related to the eigenvalues of frequencies of vibrations in the system described in **Figure 1**. In other words, the Ramsey theory may predict the peculiarities of the vibrational spectrum of the cyclic chemical compound (molecule) corresponding to the mechanical system, shown in **Figure 1**. For a sake of simplicity, the masses of the vibrating bodies are taken equal.
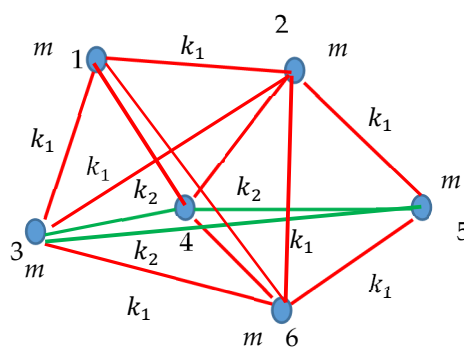
Figure 1. Cyclic chemical compound represented by the mechanical system forming a complete graph. The system is built of identical masses m interconnected by two kinds springs k_1 and k_2.

The complete graph depicted in **Figure 1** is a graph typical for the Ramsey theory. Let us connect the masses interconnected with the spring k_1 with the red; in turn, let us connect the masses interconnected with the spring k_2 with the green line.

We recognize two triangles in **Figure 1**. The vibrational spectrum of the system shown in **Figure 1** will crucially depend on the presence of the triple of double chains of masses.   Let us pose the following question: what is the minimal number of masses in the system in which three masses are connected with spring k_1 or three masses are connected with spring k_2. The answer to this question is supplied by the Ramsey theory, and it is formulated as follows: what is the minimal number $R(3,3)$? The answer emerging from the Ramsey Theory is: $R(3,3) = 6$. Indeed, we recognize in the example illustrated with **Figure 1**, that in the molecule built of six point masses, in which the relationships "to be connected by spring k_1" and "to be connected by spring k_2" are necessarily present we find triads of masses connected by the same kinds of springs (at least one triangle-shaped ring chain of masses will be necessarily present in the system of masses completely interconnected one to another). Of course, the quantitative prediction of the eigenfrequency corresponding to the triangle-shaped chain of masses, for the asymmetric system, shown in **Figure 1,** presents extremely challenging computational problem. This problem becomes solvable for the symmetric plane distribution of masses depicted in **Figure 2** (the masses form the regular hexagon).
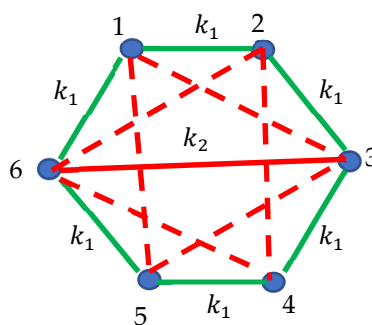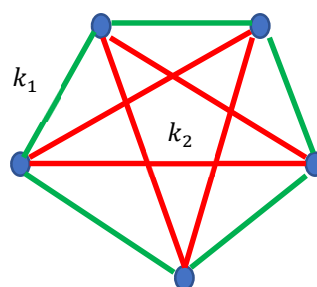
Figure 2. Equal masses *m* forming a regular hexagon are interconnected with two kinds of ideal springs denoted k_1 (green edges) and k_2 (red edges). Two equilateral triangles "153" and "246" are recognized).

Two equilateral triangles, namely "153" and "246" are present within the cyclic "molecule" depicted in Figure 2. These triangles built of the masses m and springs k_2 are shown with the red dashed lines. If harmonic oscillations of the masses connected with the "green" and "red" springs are decoupled (this will take place when $k_1 \gg k_2$ is fulfilled), the eigenvalues of the vibrations occurring within the red dashed triangles are calculated with the standard methods of the classical mechanics [9]. The full spectrum of the eigenfrequencies ω_{eigen} in this case is given by Eq. 1:

$$\omega_{eigen} = \left(0, 0, 0, \sqrt{\frac{3k_2}{2m}}; \sqrt{\frac{3k_2}{2m}}; \sqrt{\frac{3k_2}{m}} \right) \qquad (1)$$

Two of aforementioned trivial zero-eigenfrequencies correspond to the *x* and *y* translations of the entire system in the XY-plane, and the third one corresponds to the uniform rotation of the entire system about its center of mass. The detailed treatment of the eigenmodes is supplied in Appendix A. In addition the modes inherent for the ring of "green" springs k_1 should be considered [10-11]. We call these modes the Ramsey modes. It turns out that the Ramsey theory imposes restrictions on the vibrational spectrum of the cyclic mechanical systems, described by complete graphs. In other words, it supplies the "selection rules" for the vibrational spectra of the cyclic molecules, chemical structure of which may be described with the complete graphs [7-8].). It is noteworthy that $R(2, 6) = 6$. Thus, if we have a molecule, described by a complete graph, which is built of six functional groups, or two or six interconnected groups will necessarily be present in its structure; thus, explaining the formation of the benzene-like ring structures (see Figure 2).

At the same time, eigenfrequencies supplied with Eq. 1 will not necessarily appear in the molecule built of five point masses, shown in Figure 3. Indeed, the triangles built of the springs are not present in these structures, and this conclusion immediately follows from the Ramsey approach: $R(3.3) = 6 > 5$.

Figure 3. Five equal masses *m* forming a regular pentagon are interconnected with two kinds of ideal springs denoted k_1 (green edges) and k_2 (red edges). No triangles are formed in the springs network. The Ramsey number $R(3.3) = 6 > 5$.

Again, the Ramsey Theorem works as a selection rule for the vibrational spectra of molecules.

The proposed Ramsey approach is easily extended for the 3D vibrating systems/molecules such as those shown in Figure 4. The molecule shown in Figure 4 is built from two tetrahedrons, denoted "1234" and "1235". Triangle "123" is located in the plane (XOY) (see Figure 4). Masses placed in the vertices of the tetrahedron are connected with two kinds of springs, the green (k_1) and red (k_2) ones.
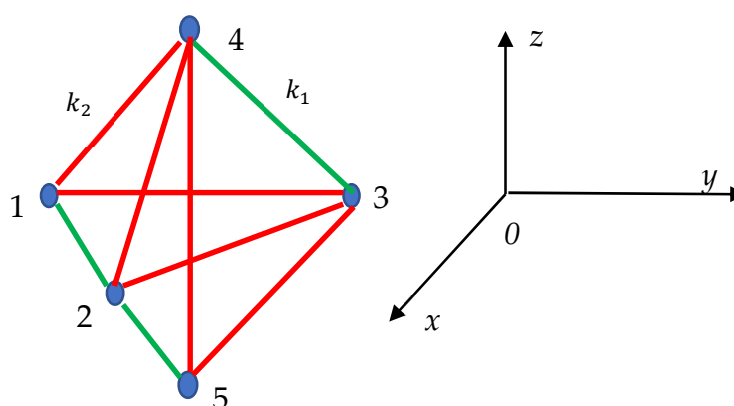
Figure 4. 3D systems built of two tetrahedrons "1234" and "1235" is depicted. Masses placed in the vertices of the tetrahedron are connected with two kinds of springs, the green (k_1) and red (k_2) ones. Triangle "123" is located in the plane (XOY).

Figure 4 depicts coloring of the 3D system in which no monochrome triangle is present. Thus, eigenmodes supplied with Eq. 1 will not appear in the vibrating system/molecule built of five point masses, shown in Figure 4. This result conforms from the Ramsey approach: $R(3,3) = 6 > 5$; and it works for 3D systems. It is noteworthy, that "springs" connecting the masses may be classic or quantum ones [12].

5. Conclusions

Ramsey theory is a branch of combinatorics that predicts the appearance of ordered substructures within a structure of a known size [1-6]. Ramsey theory states, under addressing the properties of complete graphs, that any structure will necessarily contain an orderly substructure [1-6]. We applied the Ramsey theory for the analysis of the cyclic mechanical systems, in which point masses *m* are connected with two kinds of ideal springs. Such systems may be seen as complete graphs, in which vertices (point masses) are connected with the edges colored with two colors (i.e. two kinds of springs). We applied the Ramsey theory for these kinds of graphs. These graphs also represent cyclic molecules, in which functional groups are connected by two kinds of chemical bonds [7-8].

Two kinds of springs/chemical bonds in our case are colored with "green" and "red" correspondingly. The Ramsey number for the aforementioned systems is defined as the smallest value of n such that in a group of n point masses either a group of j masses forms a complete network of "red" springs or i masses form a complete network connected by the "green" springs. We formulated the following question: what is the minimal number of masses in the system in which three masses are connected with spring k_1 or three masses are connected with spring k_2? The answer to this question emerges from the Ramsey Theory, and it is mathematically formalized as follows: what is the minimal Ramsey number $R(3,3)$? The Ramsey Theory states that is $R(3,3) = 6$. Thus, within the interconnected mechanical system built of six point masses the triangles (triangle), comprising masses and springs of the same kind will be necessarily present. This prediction constitutes the vibrational spectrum of the system. Thus, the Ramsey Theory supplies the kind of the selection rules for the vibrational spectra of the mechanical systems/cyclic molecules, which may be described by the complete graph. Consider that also $R(2,6) = 6$. Thus, if we have a molecule, described by a complete graph, which is built of six functional groups, or two or six interconnected groups will necessarily be present in its chemical structure; thus, explaining the formation of the benzene-like ring structures.

The cyclic molecule built of five functional groups interconnected with two kinds of chemical bonds will not necessarily be characterized by the collective modes involving vibration of three point entities. This fact is easily explained within the Ramsey approach $R(3,3) = 6 > 5$. The calculation of the eigen-frequencies of these systems in the general case poses essential mathematical difficulties.

Symmetrical systems/molecules in turn may be analyzed explicitly. Symmetrical system built of six entities is addressed. The eigenfrequencies inherent for the vibrations of triangles are reported. We call these modes the Ramsey modes of the systems described by complete graphs [7-8]. The introduced approach is easily extended for 3D vibrating systems interconnected by classical/quantum springs, which may be described as abstract complete graphs. Future work should consider k-partite-graph extensions of Ramsey theory, which correspond to graphs with k sets of nodes which cannot self-interact.

APPENDIX A

Calculation of eigenmodes of system built of the point masses interconnected with ideal springs forming an equilateral triangle

Consider three equal masses connected with ideal springs k_2. Springs form an equilateral triangle (the side of the triangle is a), as shown in **Figure 1A**. The center of the masses of the entire system is in rest, considering this fact yields:

$$x_1 + x_2 + x_3 = 0; \; y_1 + y_2 + y_3 = 0 \;, \tag{1A}$$

where x_i and y_i denote the displacement of i-body from equilibrium.
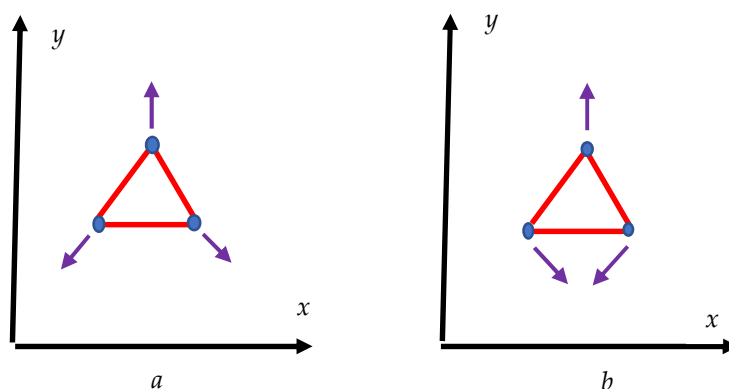
Figure 1. A. Modes of the vibrations occurring within a system built from three equal masses m and springs k_2. Springs form an equilateral triangle.

The addressed planar system is characterized by six degrees of freedom; hence, it necessarily has six eigenfrequencies; three of these eigenfrequencies equal zero (see Eq. 1). Two of these trivial eigenfrequencies correspond to the x and y translations of the entire system in the XY-plane, and the third one corresponds to the uniform rotation of the entire system about its center of mass. The non-trivial modes are depicted in **Figure 1A**. The mode shown in inset (a) corresponds to the situation when all of the bodies move along the bisectors of the triangle. The Lagrange function corresponding to this mode is supplied by Eq. 2A:

$$L(x, \dot{x}) = \frac{3m\dot{x}^2}{2} - \frac{9k_2 x^2}{2} \qquad (2A)$$

Eq. 2A immediately yields (see Eq. 1):

$$\omega_{1eigen} = \sqrt{\frac{3k_2}{m}} \qquad (3A)$$

One more mode, shown in inset (b) is found from the symmetry considerations. One of the nodes (the upper one in the inset (b)) moves along the bisector of the triangle. The movements of the remaining nodes in this case will be a mirror image of each other in the plane of symmetry of the triangle. The Lagrange function corresponding to this mode is supplied by Eq. 4A ($x_1, y_1 \ll a$ is adopted):

$$L(x_1, y_1, \dot{x}_1) = 4m\dot{x}_1^2 - \frac{9}{4}k_2 x_1^2 - \frac{27k_2 y_1^2}{4} + \frac{3\sqrt{3}k_2 x_1 y_1}{2} \qquad (4A)$$

The eigenfrequency emerging from this Lagrange function is given by Eq. 5A:

$$\omega_{2eigen} = \sqrt{\frac{3k_2}{2m}} \qquad (5A)$$

The symmetry considerations yield (see Eq. 1):

$$\omega_{3eigen} = \omega_{2eigen} = \sqrt{\frac{3k_2}{2m}} \qquad (6A)$$

Author Contributions: For research articles with several authors, a short paragraph specifying their individual contributions must be provided. The following statements should be used "Conceptualization, N. S. and E. B.; methodology, N. S. and E. B.; formal analysis, N. S.; M. F.; S. S. and E. B.; investigation, N. S.; M. F.; S. S. and E. B.;   writing—original draft preparation, N. S.; M. F.; S. S. and E. B.

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