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Vibrational Normal Modes of an Equilateral Triangular Mechanical Molecule

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Abstract

Three point-like massive particles/atoms are connected with three springs forming an equilateral triangle replicating a prototype triatomic molecule. The triangle is inscribed within a stationary frame via three additional springs confining the vibrations of the molecule to a 2D space. It is the objective of this research flavored investigation to seek the normal vibrational modes for this three-body six-spring structure. The entire analysis including symbolic, numeric, and graphics is carried out by adapting a suitable Computer Algebra System (CAS), *Mathematica*. For a comprehensive understanding, the frequency of the normal mode is used for a visual animation; an actual mechanical replica of the "molecule" for the scenario on hand is fabricated.

Keywords

Triatomic Mechanical Molecule, Vibrating Normal Modes, Computer Algebra System, *Mathematica*

1. Introduction

Depending on personal interests' various aspects of the three-body physics problem have been looked over and explored, and our article falls in the same category. Aiming by analyzing the proposed research-oriented project to contribute to the catalog of knowledge of three-body physics. In achieving our goal and compatible with the growing interest in the Computer Algebra System (CAS) we present our work entirely based on the application of the CAS specifically *Mathematica* [1] fulfilling both aspects of the practice. As briefly mentioned in the abstract the three-body problem of our interest is composed of three point-like massive interactive paired particles. The interaction of the pairs is considered linear distance-dependent forces, imitating inner interaction between the atoms of an equilateral triangulated triatomic molecule. For a more realistic

scenario, one may apply the outlined methodology to various phenomenological interactions. The given scenario forms a 2D structure it is capable of three-dimensional vibrations. To make the scope of the analysis manageable the triangle is placed in a solid frame. In doing so each of the particles is connected by a linear spring to the frame confining the vibrations to a 2D. Considering the assembly that is composed of three masses and six springs representing a mechanical molecular "unit cell" we seek its vibrational modes.

First draft of the schematic of the assembly is shown in Figure 1.

Three point-like masses are shown by 1, 2 and 3, and the stiffness of the inner atomic springs are labeled, k12, k23, and k13, respectively. Points labeled A, B and C are the fixed points of the springs with stiffness-es k1, k2, and k3 to the solid immobile not shown frame. With this structure in hand and mentioned aims, we craft this report that is composed of three sections. In addition to the Introduction, section 2 is the Procedure and the needed mathematics to formulate the problem, it embodies the *Mathematica* codes aiming to identify the frequencies of the normal vibrational modes. This section also includes the relevant graphs making the comprehension of the issues visually understandable. The last section is the Conclusions and Comments summarizing the lesson learned.

2. Procedure

As shown in Figure 1 each of the three masses is subject to three forces. The forces come about from the shown lines representing the springs. All the forces are of the same nature, *i.e.*, they are assumed to be linear with respect to their unstressed relaxed lengths. All the six springs are coplanar as such the vibrations are confined to the same plane [2] [3]. The instantaneous coordinates of each mass in a 2D-horizontal plane are those from their respective equilibria labeled $\{x, y\}$. The mobile status of three masses with the six connecting springs is envisioned to be the solution of a set of six coupled linear equations. This by itself

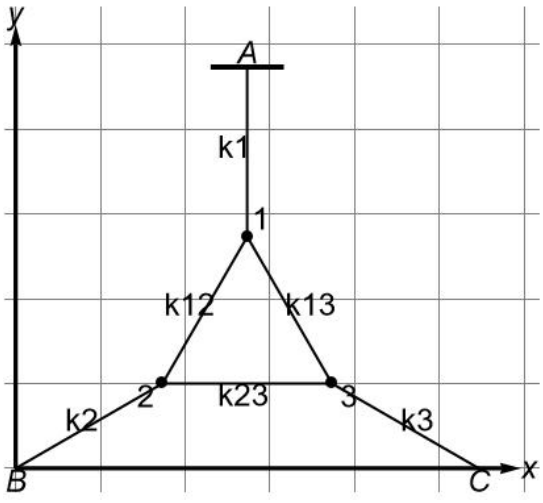

Figure 1. Schematic of the triatomic molecule en-scribed within a solid frame with connecting vertices A, B, and C.

makes the CAS an ideal investigating tool. With these detailed preliminaries and cumbersome efforts, the net acting forces on each mass are as follows. Meaningful mnemonics are used to label the codes, e.g., **eq1s1x** stands for the **eq**uation for mass **1**, **s**pring **1** along the **x**-axis, etc. For mass1 these are,

$$\{eq1s1x, eq1s1y\} = \{0, -k1y1\};$$

$$eq1s12x = Simplify\left[(-1)k12\cos(60^\circ)\left(\left(x1\cos(60^\circ) + y1\cos(30^\circ)\right) - \left(x2\cos(60^\circ) + y2\cos(30^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$s12y = Simplify\left[(-1)k12\cos(30^\circ)\left(\left(x1\cos(60^\circ) + y1\cos(30^\circ)\right) - \left(x2\cos(60^\circ) + y2\cos(30^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$eq1s13x = Simplify\left[(+1)k13\cos(60^\circ)\left(\left(y1\cos(30^\circ) - x1\cos(60^\circ)\right) - \left(y3\cos(30^\circ) - x3\cos(60^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$eq1s13y = Simplify\left[(-1)k13\cos(30^\circ)\left(\left(y1\cos(30^\circ) - x1\cos(60^\circ)\right) - \left(y3\cos(30^\circ) - x3\cos(60^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

Collecting the above terms, the net force acting on mass1 is:

eq1x = Collect[eq1s12x + eq1s13x + eq1s1x, {x1, y1, x2, y2, x3, y3}]

eq1y = Collect[eq1s12y + eq1s13y + eq1s1y, {x1, y1, x2, y2, x3, y3}]

$$\begin{aligned} &\left(-\frac{k12}{4} - \frac{k13}{4}\right)x1 + \frac{k12x2}{4} + \frac{k13x3}{4} + \left(-\frac{\sqrt{3}k12}{4} + \frac{\sqrt{3}k13}{4}\right)y1 \\ &+\frac{1}{4}\sqrt{3}k12y2 - \frac{1}{4}\sqrt{3}k13y3\left(-\frac{\sqrt{3}k12}{4} + \frac{\sqrt{3}k13}{4}\right)x1 + \frac{1}{4}\sqrt{3}k12x2 \\ &-\frac{1}{4}\sqrt{3}k13x3 + \left(-k1 - \frac{3k12}{4} - \frac{3k13}{4}\right)y1 + \frac{3k12y2}{4} + \frac{3k13y3}{4} \end{aligned} \tag{1}$$

With the same notions, for the second mass these yields,

$$eq2s2x = Simplify\left[(-1)k2\cos(30^\circ)\left(x2\cos(30^\circ) + y2\cos(60^\circ)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$eq2s2y = Simplify\left[(-1)k2\cos(60^\circ)\left(x2\cos(30^\circ) + y2\cos(60^\circ)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$eq2s12y = Simplify\left[(+1)k12\cos(30^\circ)\left(\left(x1\cos(60^\circ) + y1\cos(30^\circ)\right) - \left(x2\cos(60^\circ) + y2\cos(30^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$\{eq2s23x, eq2s23y\} = \{(-1)k23(x3 - x2), 0\};$$

$$\{eq2s23x, eq2s23y\} = \{(-1)k23(x3 - x2), 0\};$$

Similar to the aforementioned procedure the net force on mass2 yields,

eq2x=Collect[eq2s2x+eq2s12x+eq2s23x,{x1,y1,x2,y2,x3,y3}]

eq2y=Collect[eq2s2y+eq2s12y+eq2s23y,{x1,y1,x2,y2,x3,y3}]

$$\begin{aligned}&\frac{k12x1}{4} + \left(-\frac{k12}{4} - \frac{3k2}{4} + k23\right)x2 - k23x3 + \frac{1}{4}\sqrt{3}k12y1\\&+\left(-\frac{\sqrt{3}k12}{4} - \frac{\sqrt{3}k2}{4}\right)y2\frac{1}{4}\sqrt{3}k12x1 + \left(-\frac{\sqrt{3}k12}{4} - \frac{\sqrt{3}k2}{4}\right)x2\\&+\frac{3k12y1}{4} + \left(-\frac{3k12}{4} - \frac{k2}{4}\right)y2\end{aligned} \tag{2}$$

And for the third mass, we have,

$$\{eq3s23x, eq3s23y\} = \{(+1)k23(x3 - x2), 0\};$$

$$eq3s13x = Simplify\left[(-1)k13\cos(60^\circ)\left(\left(y1\cos(30^\circ) - x1\cos(60^\circ)\right) - \left(y3\cos(30^\circ) - x3\cos(60^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$eq3s13y = Simplify\left[(+1)k13\cos(30^\circ)\left(\left(y1\cos(30^\circ) - x1\cos(60^\circ)\right) - \left(y3\cos(30^\circ) - x3\cos(60^\circ)\right)\right) /.\left\{\cos(30^\circ) \to \frac{\sqrt{3}}{2}, \cos(60^\circ) \to \frac{1}{2}\right\}\right];$$

$$\{eq3s23x, eq3s23y\} = \{(+1)k23(x3 - x2), 0\};$$

eq3x=Collect[eq3s3x+eq3s13x+eq3s23x,{x1,y1,x2,y2,x3,y3}]

eq3y=Collect[eq3s3y+eq3s13y+eq3s23y,{x1,y1,x2,y2,x3,y3}]

$$\begin{aligned}&\frac{k13x1}{4} - k23x2 + \left(-\frac{k13}{4} + k23 - \frac{3k3}{4}\right)x3 - \frac{1}{4}\sqrt{3}k13y1 + \left(\frac{\sqrt{3}k13}{4} + \frac{\sqrt{3}k3}{4}\right)y3\\&-\frac{1}{4}\sqrt{3}k13x1 + \left(\frac{\sqrt{3}k13}{4} + \frac{\sqrt{3}k3}{4}\right)x3 + \frac{3k13y1}{4} + \left(-\frac{3k13}{4} - \frac{k3}{4}\right)y3\end{aligned} \tag{3}$$

Equation (1), (2), and (3) is a set of the entangled coordinate-dependent component of the forces acting on each particle. One of the objectives of our study is to put the system in motion and analyze the movement of each mass. In doing so we envision applying Newton's dynamic law, $\vec{F}_i = m_i\ddot{\vec{r}}_i$ with $\vec{r}_i = \{x_i, y_i\}$ for $i = 1$, 2, 3. According to shown equations component of each force is a linear combination of the six coordinates. E.g., $F_{1x} = \sum_{i=1}^{3}\tilde{k}_i x_i + \sum_{i=1}^{3}\tilde{\tilde{k}}_i y_i$ where $\tilde{k}$ and $\tilde{\tilde{k}}$ are stiffness related coefficients these are forthcoming. Putting all these pieces together yields a set of coupled six algebraic linear equations. By introducing K, a 6x6 matrix the dynamic equation yields the master equation,

$$K\vec{r} = m\ddot{\vec{r}}, \tag{4}$$

where k is,

$$k=\begin{pmatrix} -\frac{k12}{4}-\frac{k13}{4} & \frac{\sqrt{3}k13}{4}-\frac{\sqrt{3}k12}{4} & \frac{k12}{4} & \frac{\sqrt{3}k12}{4} & \frac{k13}{4} & -\frac{1}{4}\left(\sqrt{3}k13\right) \\ \frac{\sqrt{3}k13}{4}-\frac{\sqrt{3}k12}{4} & -k1-\frac{3k12}{4}-\frac{3k13}{4} & \frac{\sqrt{3}k12}{4} & \frac{3k12}{4} & -\frac{1}{4}\left(\sqrt{3}k13\right) & \frac{3k13}{4} \\ \frac{k12}{4} & \frac{\sqrt{3}k12}{4} & -\frac{k12}{4}-\frac{3k2}{4}+k23 & -\frac{\sqrt{3}k12}{4}-\frac{\sqrt{3}k2}{4} & -k23 & 0 \\ \frac{\sqrt{3}k12}{4} & \frac{3k12}{4} & -\frac{\sqrt{3}k12}{4}-\frac{\sqrt{3}k2}{4} & -\frac{3k12}{4}-\frac{k2}{4} & 0 & 0 \\ \frac{k13}{4} & -\frac{1}{4}\left(\sqrt{3}k13\right) & -k23 & 0 & -\frac{k13}{4}+k23-\frac{3k3}{4} & \frac{\sqrt{3}k13}{4}+\frac{\sqrt{3}k3}{4} \\ -\frac{1}{4}\left(\sqrt{3}k13\right) & \frac{3k13}{4} & 0 & 0 & \frac{\sqrt{3}k13}{4}+\frac{\sqrt{3}k3}{4} & -\frac{3k13}{4}-\frac{k3}{4} \end{pmatrix}; \quad (5)$$

The first two rows of the K are the x and y coefficients of particle 1 given by (3). The K_{11} and K_{12} are the coefficients of x_1 and y_1, etc., respectively. The meaning of the rest of the elements in K follows the same trend.

The 36 elements of K are composed of the stiffness es of the springs shown in Figure 1. The elements are real numbers making the matrix real. The K is a symmetric matrix, meaning the elements about the diagonal are mirrors of each other. The diagonal elements are shown on a yellow background and a few of the mirror elements are colored. The K is Hermitian, meaning $K = K^{\dagger}$, where † stands for conjugate-transpose. Noticed, the careful analysis of the components of the forces acting on each mass shown in Figure 1 has led to the symmetrized formation of K.

Equation (4) given (5) being a set of six coupled ODEs with some initial conditions can be solved symbolically conducive to explicit time-dependent coordinates of the masses. This makes the problem on hand an ideal candidate to be handled by a CAS. Likewise, it can be solved numerically. However, our objective is different. We envision a scenario in which all three masses would be oscillating with the same frequencies about their respective equilibria; in other words, we seek the normal modes. The steps leading to our goal follow.

For the normal modes, the time-dependent position vector of each mass is subject to $\vec{r}(t)=\vec{r}_0 e^{\pm i\omega t}$, where ω is the angular frequency of the normal mode. Substituting this in (4) utilizing (5) yields,

$$\left(m^{-1}K\right)\vec{r}_0=\omega^2\vec{r}_0, \quad (6)$$

This eigenvector equation gives,

$$\omega=\sqrt{m^{-1}K}, \quad (7)$$

with the term underneath the radical being the eigenvalue of (6) with m^{-1} the inverse of the 6 × 6 diagonal mass-matrix,

$$m=\begin{pmatrix} m1 & 0 & 0 & 0 & 0 & 0 \\ 0 & m1 & 0 & 0 & 0 & 0 \\ 0 & 0 & m2 & 0 & 0 & 0 \\ 0 & 0 & 0 & m2 & 0 & 0 \\ 0 & 0 & 0 & 0 & m3 & 0 \\ 0 & 0 & 0 & 0 & 0 & m3 \end{pmatrix}, \quad (8)$$

This concludes the formal solution conducive to the normal modes. For a practical exercise, we consider a set of reasonable values for the stiffness es and masses; units are MKS.

The term underneath the radical in (7) *i.e.*, yields the eigenvalues. Noted, various approaches are searching for the eigenvalues, here we show one. We define an identity matrix with diagonal elements λ that stands for the eigenvalues. Then we solve its corresponding eigenvalue equation. An alternative is to apply the Eigensystem command.

The eigenvalues are shown in **Figure 2**.

Noticing, the eigenvalue equation is a 6th-order polynomial. One of its roots is always zero as shown in **Figure 2**. Since the eigenvalues correspond to the vibration frequency of the normal mode, this means the system stays motionless. The rest of the modes come about by solving a 5th-order quintic polynomial with five distinct roots. **Figure 2** shows the case in hand has four negative and only one positive root. This general characteristic holds for the exhaustively tested set of values searched for the stiffness es and masses. Meaning, for the proposed triangular triatomic molecule there is only one normal mode.

Knowing the value of the unique frequency of the normal mode, $f = 55$ mHz we craft animation to help visualize the case on hand. A snapshot of the case is shown in **Figure 3**.

The black dots are the initial static positions of the masses, they form an equilateral triangle. The blue dots are their maximum displaced positions. The red dots are the mobile vibrating black dots. If the animation could be run that would show oscillations of the masses. The zoomed image of **Figure 3** is not included here and shows the maximum distance of the blue dots from their corresponding blacks these are different for each. This is because these distances are given by the eigenvectors. Despite these differences, they oscillate at the same frequency, emphasizing the character of the normal mode.

Each mass oscillates in the 2D horizontal plane. Oscillations of each mass along the x and y axis are different. For a better understanding, these are depicted in **Figure 4**.

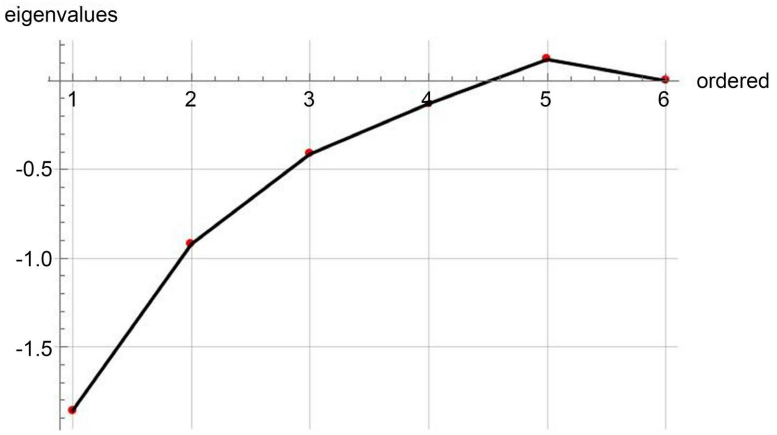

Figure 2. The display of the numbered eigenvalues of (7).

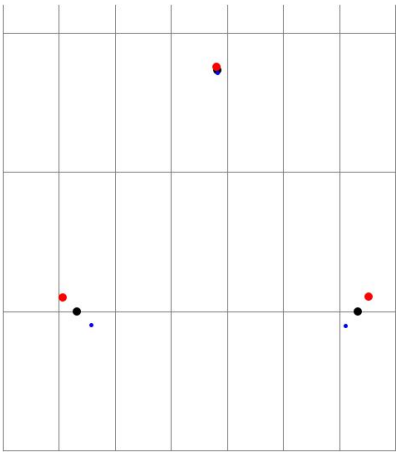

Figure 3. A snapshot of the animation. The colored dots are the instantaneous positions of the particles. Horizontal and vertical axes are $x(t)$ and $y(t)$ positions of the masses.

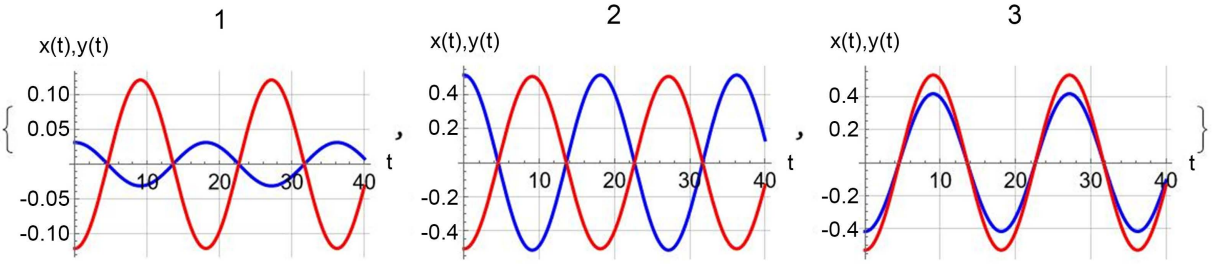

Figure 4. The plot labels correspond to the mass numbers. The blue and red curves are their corresponding plots of $x(t)$ and $y(t)$, respectively.

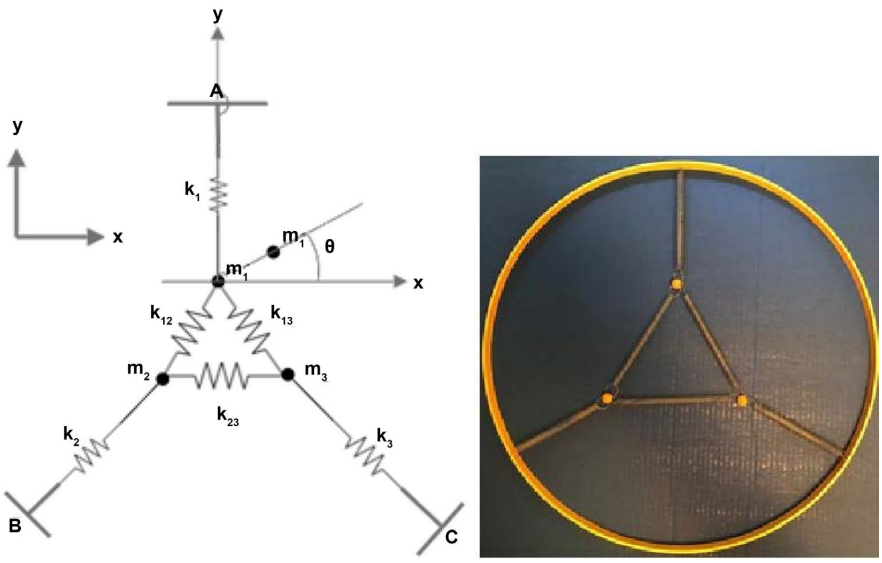

Figure 5. The left graph is the display of the triatomic molecule with six connecting springs. The right panel is its manufactured mechanical replica.

As shown in each of the plots the amplitudes of the blue and the red oscillatory functions are different. This is because the amplitudes are the eigenvectors. Despite these differences as shown the period of the oscillations meaning their

frequencies are indicative of the normal mode is the same. A refined sketch of the assembly along with a photo of the actual replica is shown in Figure 5.

3. Conclusion and Comments

The dynamic aspect of the inner interaction of the atoms in a given triatomic molecule is due to the temperature variation. We envisioned a scenario where the interactions are modeled as if the atoms are connected with linear springs. The scenario on hand deals with a framed triatomic molecule confining the vibrations to a 2D planar plane. A specific mode of vibrations namely the normal mode is considered where all three atoms oscillate with the same frequency. A mechanical replica of the molecule is fabricated and for a set of reasonable practical parameters, the vibrations are videotaped. Analysis of the entire problem is done by applying a CAS. The entire computation is done numerically making the CAS an indefensible computational tool. Utilizing the numeric output an animation code is crafted making the dynamic visual, its snapshot is included. For programming, animation, and coding the interested reader may find [4] and [5] resourceful. Although we considered a specific structure the applied methodology and the analysis may easily be applied to the structure of interest.

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Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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