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On the Normal Modes of Coupled Harmonic Oscillators

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Abstract: We discuss in detail a well known method for obtaining the frequencies of the normal modes of coupled harmonic oscillators that is based on the simultaneous diagonalization of two symmetric matrices. We apply it to some simple illustrative examples recently chosen for the presentation of an alternative approach based on a set of constants of the motion. We show that the traditional method is simpler, even in the case of equal frequencies. We also discuss a problem that commonly appears in elementary courses on quantum mechanics that also requires the diagonalization of two symmetric matrices.

Keywords: keyword 1; keyword 2; keyword 3

1. Introduction

The calculation of the normal modes of coupled harmonic oscillators is commonly discussed in most textbooks on classical mechanics [1] and is of relevance in the analysis of the vibrational spectroscopy of polyatomic molecules in terms of internal nuclear coordinates [2]. The *traditional* treatment of the problem is based on the simultaneous diagonalization of two symmetric matrices for the kinetic an potential energies [2,3]. This approach also applies to the quantum-mechanical version of the problem [4]. In a recent paper, Hojman [5] proposed an alternative method for obtaining the frequencies of the normal modes based on a set of constants of the motion. In our opinion it may be of great pedagogical interest to compare both approaches.

In Section 2 we develop the traditional method in detail and apply it to the models proposed by Hojman in Section 3, where we also discuss an additional three-particle problem with degenerate eigenfrequencies. In Appendix A we outline a problem that commonly appears in elementary courses on quantum mechanics and also requires the simultaneous diagonalization of two symmetric matrices. Finally, in Section 4 we summarize the main results and draw conclusions.

2. Diagonalization of Coupled Harmonic Oscillators

In this paper we consider N coupled harmonic oscillators with kinetic energy T and potential energy V given by

$$T=\frac{1}{2}\dot{\mathbf{Q}}^t\mathbf{A}\dot{\mathbf{Q}},\ \mathbf{V}=\frac{1}{2}\mathbf{Q}^t\mathbf{B}\mathbf{Q}, \tag{1}$$

where $\mathbf{Q}$ and $\dot{\mathbf{Q}}$ are column vectors for the coordinates q_i and velocities $\dot{q}_i$, $i=1,2,\ldots,N$, respectively. The superscript t stands for transpose and $\mathbf{A}$ and $\mathbf{B}$ are time-independent $N\times N$ symmetric matrices. From a physical point of view, we assume that $\mathbf{A}$ is positive definite (all its eigenvalues are positive real numbers).

In order to bring both $\mathbf{A}$ and $\mathbf{B}$ into diagonal form we propose the change of variables $\mathbf{Q}=\mathbf{CS}$, where $\mathbf{C}$ is an $N\times N$ invertible matrix and $\mathbf{S}$ a column vector for the new coordinates s_i, $i=1,2,\ldots,N$. We choose $\mathbf{C}$ to satisfy two conditions, first

$$\mathbf{C}^t\mathbf{B}\mathbf{C}=\mathbf{\Lambda}, \tag{2}$$

where $\mathbf{\Lambda} = (\lambda_i \delta_{ij})$ is a diagonal matrix, second

$$\mathbf{C}^t \mathbf{A} \mathbf{C} = \mathbf{I}, \tag{3}$$

where $\mathbf{I}$ is the $N \times N$ identity matrix. We will show below that this matrix already exists. It follows from Equation (3) that $\mathbf{C}^t = \mathbf{C}^{-1}\mathbf{A}^{-1}$ and Equation (2) thus becomes

$$\mathbf{C}^{-1}\mathbf{A}^{-1}\mathbf{B}\mathbf{C} = \mathbf{\Lambda}. \tag{4}$$

This equation simply represents the diagonalization of the matrix $\mathbf{A}^{-1}\mathbf{B}$. More precisely, the problem reduces to obtaining the eigenvalues λ_i and the column eigenvectors $\mathbf{C}_i$ of the matrix $\mathbf{A}^{-1}\mathbf{B}$. The columns of the matrix $\mathbf{C}$ are precisely such eigenvectors. Since the eigenvectors $\mathbf{C}_i$ are not normalized we use Equation (3) to obtain their norms. Finally, the physical problem reduces to solving the trivial equations of motion for a set of N uncoupled harmonic oscillators:

$$T = \frac{1}{2}\dot{\mathbf{S}}^t\dot{\mathbf{S}} = \frac{1}{2}\sum_{i=1}^{N}\dot{s}_i^2,\ V = \frac{1}{2}\mathbf{S}^t\mathbf{\Lambda}\mathbf{S} = \frac{1}{2}\sum_{i=1}^{N}\lambda_i s_i^2. \tag{5}$$

It only remains to prove that $\mathbf{A}^{-1}\mathbf{B}$ is diagonalizable.

Since $\mathbf{A}$ is positive definite, then $\mathbf{A}^{1/2}$ exists and we can construct the new matrix $\mathbf{U} = \mathbf{A}^{1/2}\mathbf{C}$ that is orthonormal ($\mathbf{U}^t = \mathbf{U}^{-1}$) as shown by

$$\mathbf{U}^t\mathbf{U} = \mathbf{C}^t\mathbf{A}\mathbf{C} = \mathbf{I}. \tag{6}$$

If we substitute $\mathbf{C} = \mathbf{A}^{-1/2}\mathbf{U}$ into Equation (2) we obtain

$$\mathbf{U}^t\mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2}\mathbf{U} = \mathbf{\Lambda}. \tag{7}$$

Since $\mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2}$ is symmetric, then it is diagonalizable, the orthogonal matrix $\mathbf{U}$ exists [6] and, consequently, the matrix $\mathbf{C}$ also exists. It is clear that we can always diagonalize the kinetic and potential energies for a system of coupled harmonic oscillators as shown in Equation (5). Present analysis of the problem posed by the simultaneous diagonalization of two symmetric matrices appears to be simpler than the one proposed by Chavda [3] some time ago.

Before discussing suitable illustrative examples, it is convenient to pay attention to the units of the matrices introduced above. The matrix elements of $\mathbf{A}$ and $\mathbf{B}$ have units of mass and energy$\times$length^{-2}, respectively. Consequently, the elements of $\mathbf{C}$ have units of mass$^{-1/2}$ and the new variables s_i have units of mass$^{1/2}\times$length. Finally, the eigenvalues λ_i have units of time^{-2}. If we write $\lambda_i = \omega_i^2$, then ω_i, $i = 1, 2, \ldots, N$, are the frequencies of the normal modes. The new variables s_i can be interpreted as a kind of mass-weighted coordinates for the normal modes.

3. Examples

The first example is the two-dimensional model chosen by Hojman [5]

$$T = \frac{m}{2}\left(\dot{q}_1^2 + \dot{q}_2^2\right),\ V = \frac{1}{2}\left[k_1\left(q_1^2 + q_2^2\right) + k_2\left(q_1 - q_2\right)^2\right], \tag{8}$$

that leads to

$$\mathbf{A} = \mathbb{T}_2 = m\mathbf{I},\ \mathbf{B} = \mathbb{V}_2 = \begin{pmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_1 + k_2 \end{pmatrix}, \tag{9}$$

and

$$\mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2} = \mathbf{A}^{-1}\mathbf{B} = \frac{1}{m}\mathbf{B}. \tag{10}$$

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The two eigenvalues of this matrix are

$$\lambda_1 = \frac{k_1}{m},\ \lambda_2 = \frac{k_1 + 2k_2}{m}, \tag{11}$$

with eigenvectors

$$\mathbf{U}_1 = \alpha \begin{pmatrix} 1 \\ 1 \end{pmatrix},\ \mathbf{U}_2 = \beta \begin{pmatrix} 1 \\ -1 \end{pmatrix}. \tag{12}$$

They are orthogonal and we can choose $\alpha = \beta = 1/\sqrt{2}$ as normalization factors. Therefore, the matrices $\mathbf{U}$ and $\mathbf{C}$ are given by

$$\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},\ \mathbf{C} = \frac{1}{\sqrt{m}} \mathbf{U}. \tag{13}$$

The resulting normal modes

$$\mathbf{U} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} q_1 + q_2 \\ q_1 - q_2 \end{pmatrix}, \tag{14}$$

agree with the ones derived by Hojman [5].

As a three-dimensional example, Hojman chose the toy model

$$\mathbf{A} = \mathbb{T}_3 = \begin{pmatrix} 9 & -23 & -22 \\ -23 & 61 & 58 \\ -22 & 58 & 56 \end{pmatrix},\ \mathbf{B} = \mathbb{V}_3 = \begin{pmatrix} 15 & -37 & -34 \\ -37 & 95 & 86 \\ -34 & 86 & 80 \end{pmatrix}. \tag{15}$$

It is not difficult to verify that the matrix $\mathbf{A}$ is positive definite (its three eigenvalues are positive). The eigenvalues and eigenfunctions of

$$\mathbf{A}^{-1}\mathbf{B} = \begin{pmatrix} 4 & -6 & -6 \\ -1 & 5 & 2 \\ 2 & -6 & -3 \end{pmatrix}, \tag{16}$$

are

$$\begin{aligned} \lambda_1 &= 1,\ \lambda_2 = 2,\ \lambda_3 = 3, \\ \mathbf{C}_1 &= \alpha_1 \begin{pmatrix} 1 \\ 0 \\ \frac{1}{2} \end{pmatrix},\ \mathbf{C}_2 = \alpha_2 \begin{pmatrix} 1 \\ \frac{1}{3} \\ 0 \end{pmatrix},\ \mathbf{C}_3 = \alpha_3 \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}. \end{aligned} \tag{17}$$

It is clear that the matrices $\mathbf{A}$ and $\mathbf{B}$ were purposely chosen to have extremely simple results. It follows from Equation (3) that $\alpha_1 = \pm 1$, $\alpha_2 = \pm 3/2$, $\alpha_3 = \pm 1$. On arbitrarily selecting the positive signs, without loss of generality, we have

$$\mathbf{C} = \begin{pmatrix} 1 & \frac{3}{2} & 0 \\ 0 & \frac{1}{2} & 1 \\ \frac{1}{2} & 0 & -1 \end{pmatrix}, \tag{18}$$

that satisfies both Equations (2) and (3) as one can easily verify.

The mass-weighted coordinates

$$\begin{aligned}
-\frac{1}{2}s_1 &= q_1 - 3\left(q_2 + q_3\right), \\
\frac{1}{2}s_2 &= q_1 - 2\left(q_2 + q_3\right), \\
-\frac{1}{2}s_3 &= \frac{1}{2}\left(q_1 - 3q_2 - 2q_3\right),
\end{aligned} \tag{19}$$

agree with those obtained by Hojman [5] through a lengthier procedure based on the construction of the constants of the motion.

In what follows, we discuss a somewhat more realistic three-dimensional model given by a set of three identical particles with harmonic interactions:

$$T = \frac{m}{2}\left(\dot{q}_1^2 + \dot{q}_2^2 + \dot{q}_3^2\right),\ V = \frac{k}{2}\left[\left(q_1 - q_2\right)^2 + \left(q_1 - q_3\right)^2 + \left(q_2 - q_3\right)^2\right]. \tag{20}$$

The relevant matrices are

$$\mathbf{A} = m\mathbf{I},\ \mathbf{B} = k\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}. \tag{21}$$

The eigenvalues and eigenvectors of $\mathbf{A}^{-1/2}\mathbf{B}\mathbf{A}^{-1/2} = m^{-1}\mathbf{B}$ are

$$\begin{aligned}
\lambda_1 &= 0,\ \lambda_2 = \lambda_3 = \frac{3k}{m}, \\
\mathbf{U}_1 &= \alpha_1\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix},\ \mathbf{U}_2 = \begin{pmatrix} \alpha_2 \\ \alpha_3 \\ -\alpha_2 - \alpha_3 \end{pmatrix},\ U_3 = \begin{pmatrix} \alpha_4 \\ \alpha_5 \\ -\alpha_4 - \alpha_5 \end{pmatrix}.
\end{aligned} \tag{22}$$

In the presentation of his method, Hojman [5] assumed, for simplicity, that all the frequencies were different. In the present case, we appreciate that the application of the traditional approach to the case of equal frequencies is straightforward. The column vector $\mathbf{U}_1$ is orthogonal to the other two and we normalize it by choosing $\alpha_1 = 1/\sqrt{3}$. Without loss of generality we arbitrarily choose $\alpha_3 = 0$ and $\alpha_2 = 1/\sqrt{2}$. From $\mathbf{U}_2^t\mathbf{U}_3 = 0$ we obtain $\alpha_5 = -2\alpha_4$ and $\mathbf{U}_3^t\mathbf{U}_3 = 1$ yields $\alpha_4 = \pm 1/\sqrt{6}$. Finally, the matrix $\mathbf{C}$ becomes

$$\mathbf{C} = \frac{1}{\sqrt{m}}\mathbf{U},\ \mathbf{U} = \frac{1}{6}\begin{pmatrix} 2\sqrt{3} & 3\sqrt{2} & \sqrt{6} \\ 2\sqrt{3} & 0 & -2\sqrt{6} \\ 2\sqrt{3} & -3\sqrt{2} & \sqrt{6} \end{pmatrix}, \tag{23}$$

that yields

$$\begin{aligned}
s_1 &= \sqrt{\frac{m}{3}}\left(q_1 + q_2 + q_3\right), \\
s_2 &= \sqrt{\frac{m}{2}}\left(q_1 - q_3\right), \\
s_3 &= \sqrt{\frac{m}{6}}\left(2q_2 - q_1 - q_3\right).
\end{aligned} \tag{24}$$

The occurrence of the eigenvalue $\lambda_1 = 0$ tells us that the center of mass of the system moves freely at constant velocity. Note that the variable s_1 is proportional to the coordinate of the center of mass $q_{CM} = \left(q_1 + q_2 + q_3\right)/3$.

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4. Conclusions

The approach proposed by Hojman [5] is interesting in itself. However, from a practical point of view the traditional approach [2,3] is more convenient because it appears to be simpler. Although this approach is well known, we think that its detailed application to particular simple examples may be of pedagogical value to students of classical mechanics. For this reason, we have applied it to all the models chosen by Hojman and also to the case of equal frequencies that he avoided for simplicity.

The problem discussed in Appendix A may also be of pedagogical interest because it shows that two problems that students commonly face in completely different courses (classical mechanics and quantum mechanics) may be expressed in terms of identical mathematical equations.

Appendix A. Analogy: Hermitian operator on a finite real vector space

In this appendix we discuss a well known mathematical problem that also requires the simultaneous diagonalization of two matrices. Consider an Hermitian operator H defined on an N-dimensional real vector space endowed with an inner product $\langle f | g \rangle = \langle g | f \rangle$, for any f and g that belong to the vector space. Such operator has a complete set of eigenfunctions ψ_i with eigenvalues E_i,

$$H\psi_i = E_i\psi_i, \; i = 1, 2, \ldots, N, \tag{A.1}$$

that we may choose to be orthonormal $\langle \psi_i | \psi_j \rangle = \delta_{ij}$. Suppose that $B = \{f_1, f_2, \ldots, f_N\}$ is a complete set of non-orthogonal vectors f_i. Since each ψ_i can be written as a linear combination of the basis vectors

$$\psi_i = \sum_{j=1}^{N} c_{ji} f_j, \tag{A.2}$$

then we have

$$\begin{aligned} \langle f_k | H | \psi_i \rangle &= \sum_{j=1}^{N} \langle f_k | H | f_j \rangle c_{ji} = E_i \sum_{j=1}^{N} \langle f_k | f_j \rangle c_{ji} \\ &= \sum_{j=1}^{N} \sum_{m=1}^{m} E_m \delta_{mi} \langle f_k | f_j \rangle c_{jm}, \end{aligned} \tag{A.3}$$

that can be written in matrix form as

$$\mathbf{HC} = \mathbf{SCE}, \tag{A.4}$$

where $(\mathbf{H})_{kj} = \langle f_k | H | f_j \rangle$, $(\mathbf{S})_{kj} = \langle f_k | f_j \rangle$ and $\mathbf{E} = (E_i \delta_{ij})$. Therefore,

$$\mathbf{C}^{-1}\mathbf{S}^{-1}\mathbf{HC} = \mathbf{E}. \tag{A.5}$$

The orthonormality of the eigenfunctions leads to

$$\langle \psi_i | \psi_j \rangle = \sum_{k=1}^{N} \sum_{m=1}^{N} c_{ki} c_{mj} \langle f_k | f_m \rangle = \delta_{ij}, \tag{A.6}$$

that in matrix form reads

$$\mathbf{C}^t\mathbf{SC} = \mathbf{I}. \tag{A.7}$$

Note that the matrix $\mathbf{H}$ is symmetric and $\mathbf{S}$ is symmetric and positive definite as in the case of the diagonalization of coupled harmonic oscillators. In fact, Equations (A.7) and (A.5) are identical, from a mathematical point of view, to Equations (3) and (4), respectively. It is clear that the problem posed by the diagonalization of two symmetric matrices is not uncommon in mathematical physics.

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