Physics W89 - Introduction to Mathematical Physics - Summer 2023
Problem Set - Module 06 - Diagonalization

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Problem 6.1 - CO_2 Continued

Relevant Videos: Changes of Basis - Transforming Basis Vectors; Transforming Vectors; Transforming Matrices

In Problem 5.2 we started to explore the vibrational modes of carbon dioxide, which we modeled as three masses (m_o, m_c, m_o for the left oxygen, central carbon, and right oxygen, respectively) attached to two springs, each of spring constant k.

The ***mass eigenbasis*** $\{\hat{e}_i\}$ is based on the individual displacements of the atoms, with the three basis vectors $\{\vec{e}_1, \vec{e}_2, \vec{e}_3\}$ representing unit displacements from the equilibrium position for the left oxygen, the central carbon, and the right oxygen, respectively. Let ℓ be the equilibrium lengths of the system so that when the displacement vector is $\vec{x}$ the left-most oxygen is at position $-\ell + x_1$, the carbon is at position x_2, and the right-most oxygen is at position $+\ell + x_3$ relative to the origin. In the mass eigenbasis, the mass matrix is diagonal $\mathsf{M}_{[e]} = \begin{pmatrix} m_o & 0 & 0 \\ 0 & m_c & 0 \\ 0 & 0 & m_o \end{pmatrix}$.

The potential energy $U = \frac{1}{2}\vec{x}\cdot\mathsf{K}\vec{x}$ is determined by the real symmetric matrix K which we found in the mass eigenbasis to be $\mathsf{K}_{[e]} \equiv \begin{pmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{pmatrix}$. The eigenvalues and normalized eigenvectors (expressed in the $\{\hat{e}_i\}$-basis) for K are:

$$\lambda_1 = 0, \quad \hat{s}_{1,[e]} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}; \qquad \lambda_2 = k, \quad \hat{s}_{2,[e]} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \qquad \lambda_3 = 3k, \quad \hat{s}_{3,[e]} = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ -2 \\ 1 \end{pmatrix}.$$

We call this orthonormal basis $\{\hat{s}_1, \hat{s}_2, \hat{s}_3\}$ the ***spring eigenbasis*** because the "spring matrix" K written in this basis is diagonal.

The classical equations of motion for this system are $\ddot{\vec{x}} = -\mathsf{A}\vec{x}$, where $\mathsf{A} = \mathsf{M}^{-1}\mathsf{K}$,

$$\mathsf{A}_{[e]} = \begin{pmatrix} k/m_o & -k/m_o & 0 \\ -k/m_c & 2k/m_c & -k/m_c \\ 0 & -k/m_o & k/m_o \end{pmatrix} = \frac{k}{m_o}\begin{pmatrix} 1 & -1 & 0 \\ -r & 2r & -r \\ 0 & -1 & 1 \end{pmatrix},$$

with $r \equiv m_o/m_c$. It turns out that even though the matrix A is not normal, we can still make an eigenbasis out of the eigenvectors (the eigenbasis will *not* be orthonormal, however). Since A gives the dynamics of the system, we call this the ***dynamics eigenbasis***.

(a) Verify that the eigenvalues and eigenvectors of A (written in terms of the mass eigenbasis) are

$$\lambda_1 = 0, \quad \vec{d}_{1,[e]} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}; \qquad \lambda_2 = \frac{k}{m_o}, \quad \vec{d}_{2,[e]} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}; \qquad \lambda_3 = \frac{k}{\mu}, \quad \vec{d}_{3,[e]} = \begin{pmatrix} 1 \\ -2r \\ 1 \end{pmatrix},$$

where $\mu \equiv m_o/(1+2r)$. *Without* bothering to go through the tedious change-of-basis process or doing any calculations, write down the matrix $\mathsf{A}_{[d]}$ (that is, the matrix expressed in the dynamics eigenbasis).

(b) Sketch and/or describe the displacement of the three atoms in the carbon-dioxide molecule corresponding to the three dynamics eigenvectors. How does the center-of-mass position change under each displacement? How does the potential energy change?

Now let's explore changes of basis! Recall that we have the mass eigenbasis $\{\hat{e}_i\}$, the spring eigenbasis $\{\hat{s}_i\}$, and the dynamics eigenbasis $\{\vec{d}_i\}$.

(c) Construct the change-of-basis matrix $\mathsf{C}_{e\to s}$ that takes us from the mass eigenbasis to the spring eigenbasis. Check explicitly that $\mathsf{C}_{e\to s}$ is an orthogonal matrix.

(d) Find the matrices $\mathsf{M}_{[s]}$ and $\mathsf{K}_{[s]}$ written with respect to the spring eigenbasis.
[*Note: While this change-of-basis does indeed diagonalize* K*, it "un-diagonalizes"* M*! It turns out that since* K *and* M *don't commute, we can never find a basis in which both matrices will be simultaneously diagonal.*]

Since $\mathsf{A}_{[e]}$ is not a normal matrix, we have no chance of finding an orthonormal eigenbasis. When we write the inverse of our change-of-basis matrix, we have to actually compute an inverse rather than rely on orthogonality or unitary of the matrix. For the change of basis from the mass eigenbasis to the dynamics eigenbasis, we have

$$\mathsf{C}_{e\to d} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -2r \\ 1 & -1 & 1 \end{pmatrix}, \qquad \mathsf{C}_{e\to d}^{-1} = \frac{1}{2(1+2r)} \begin{pmatrix} 2r & 2 & 2r \\ 1+2r & 0 & -(1+2r) \\ 1 & -2 & 1 \end{pmatrix}.$$

Suppose the carbon atom was initially displaced a distance δ to the right, while the two oxygens remained in their original equilibrium position. Call this $\vec{x}(0)$. Let all three atoms initially be at rest, so $\vec{v} = \dot{\vec{x}} = \vec{0}$.

(e) Express the displacement vector $\vec{x}(0)$ as a vector in the mass eigenbasis, $\vec{x}_{[e]}(0)$. Then perform a change-of-basis operation on this vector to find the vector $\vec{x}_{[d]}(0)$ in the dynamics eigenbasis.

Let $\omega_2 \equiv \sqrt{\lambda_2}$ and $\omega_3 \equiv \sqrt{\lambda_3}$. Consider the six time-dependent vectors

$$\begin{aligned} \vec{x}_\alpha(t) &\equiv \vec{d}_1; & \vec{x}_\beta(t) &\equiv t\vec{d}_1; \\ \vec{x}_\gamma(t) &\equiv \cos(\omega_2 t)\vec{d}_2; & \vec{x}_\delta(t) &\equiv \sin(\omega_2 t)\vec{d}_2; \\ \vec{x}_\epsilon(t) &\equiv \cos(\omega_3 t)\vec{d}_3; & \vec{x}_\zeta(t) &\equiv \sin(\omega_3 t)\vec{d}_3. \end{aligned}$$

(f) Show that all six of these vectors solve the equation of motion $\ddot{\vec{x}} = -\mathsf{A}\vec{x}$.
[*Note: Each vector should only take one line of work to show that it's a solution. An example for one of these vectors is given as a spoiler at the end of this problem set and in the spoilers document.*]

The most general solution to our system is a linear combination of these six vectors,

$$\begin{aligned}\vec{x}(t) &= c_\alpha \vec{x}_\alpha(t) + c_\beta \vec{x}_\beta(t) + c_\gamma \vec{x}_\gamma(t) + c_\delta \vec{x}_\delta(t) + c_\epsilon \vec{x}_\epsilon(t) + c_\zeta \vec{x}_\zeta(t) \\ &= \big(c_\alpha + t c_\beta\big)\vec{d}_1 + \big(c_\gamma \cos(\omega_2 t) + c_\delta \sin(\omega_2 t)\big)\vec{d}_2 + \big(c_\epsilon \cos(\omega_3 t) + c_\zeta \sin(\omega_3 t)\big)\vec{d}_3. \end{aligned} \tag{1}$$

We can determine the six coefficients using the initial conditions $\vec{x}_0$ and $\vec{v}(0) = \dot{\vec{x}}(0)$ and the linear independence of the dynamics eigenbasis.

(g) Use the initial conditions from part (e) to find the six coefficients in Eq. 1 displacement vector in the dynamics basis at a later time. Finally, express the displacement vector in the mass eigenbasis as a function of time, $\vec{x}_{[e]}(t)$.

Problem 6.2 - Similarity Ensues

Relevant Videos: Diagonalization; Similarity Transformations

Recall that a ***similarity transformation*** is defined via $\mathsf{M} \to \mathsf{S}^{-1}\mathsf{M}\mathsf{S}$, where S is an invertible matrix. If there exists an invertible S such that $\widetilde{\mathsf{M}}$ and M are connected by a similarity transformation (that is, $\widetilde{\mathsf{M}} = \mathsf{S}^{-1}\mathsf{M}\mathsf{S}$ for some S), then M and $\widetilde{\mathsf{M}}$ are called ***similar***.[1]

Similar matrices have many identical properties, which we explore in this problem. Note that some of these properties will hold for an *arbitrary* similarity transformation and some will only hold for a ***unitary*** or ***orthogonal*** transformation (one in which S is further constrained to be either unitary or orthogonal). If two matrices are similar under a unitary transformation we sometimes call them ***unitarily equivalent***. I will indicate at the start of each part which class of similarity transformations you should be concerned with.

(a) For this part, we will consider arbitrary similarity transforms. Prove that two similar matrices have identical traces and determinants.
[*Supplementary Part (Not for Credit): We went over this in lecture, but without looking at the notes, prove that two similar matrices have identical spectra of eigenvalues.*]

(b) **Extra Part** (*Not for Credit*) For this part, we will consider arbitrary similarity transforms. Let $\widetilde{\mathsf{M}} = \mathsf{S}^{-1}\mathsf{M}\mathsf{S}$ and show that S^{-1} is an isomorphism between $\ker \mathsf{M}$ and $\ker \widetilde{\mathsf{M}}$. Use this result to show that similar matrices have identical nullities and ranks.
[*Note: We already know that* $\mathsf{S}^{-1} : \mathsf{M} \to \widetilde{\mathsf{M}}$ *is an isomorphism (since* S^{-1} *is invertible)! To show that* S^{-1} *also provides an isomorphism between* $\ker \mathsf{M}$ *and* $\ker \widetilde{\mathsf{M}}$ *you need to show two properties: 1. If* $\vec{v} \in \ker \mathsf{M}$ *then* $\mathsf{S}^{-1}\vec{v} \in \ker \widetilde{\mathsf{M}}$. *2. If* $\vec{w} \in \ker \widetilde{\mathsf{M}}$ *then there exists a* $\vec{v} \in \ker \mathsf{M}$ *such that* $\vec{w} = \mathsf{S}^{-1}\vec{v}$.]

(c) For this part, we will consider unitary transformations. Let M be unitarily equivalent to $\widetilde{\mathsf{M}}$. Prove that if M is Hermitian then so is $\widetilde{\mathsf{M}}$. Similarly, prove that if M is unitary then so is $\widetilde{\mathsf{M}}$.
[*Note: Unitary transformations also keep symmetric matrices symmetric, orthogonal matrices orthogonal, and, more generally, normal matrices normal.*]

[1] A similarity transformation is an example of a ***equivalence relation***, which we explore in a supplement!

(d) Extra Part (*Not for Credit*) Row reduction does *not* produce similar matrices! Show explicitly that two of the three elementary row operations - flipping two rows and multiplying one row by a non-zero scalar c (let $c \neq 1$ for this part, since that doesn't change the matrix at all) can't be accomplished by a similarity transformation.
[*Spoilers!* How do the row operations affect the determinant? What did we learn in part (a)?]

Now let M be diagonalizable and let $\mathsf{D} = \mathsf{S}^{-1}\mathsf{M}\mathsf{S}$ be the diagonalization of M. Here we are allowing M to be non-normal and allowing S to be non-unitary.

(e) Use the result from part (a) to show $\det(e^{\mathsf{M}}) = e^{\operatorname{tr}\mathsf{M}}$.
[*Spoilers!* Remember Problem 4.4, which foreshadowed all of this!]

Problem 6.3 - Simultaneous Diagonalization

Relevant Videos: Diagonalization; Similarity Transformations

We saw in our CO_2 problem that we couldn't find a basis in which both K and M were diagonal. Given two matrices A and B, when *can* we find a basis in which both A and B are diagonal? Answer: When they ***commute***!

(a) Consider the two Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$. Show that these two matrices don't commute. Find an orthonormal eigenbasis that diagonalizes σ_x and show that σ_y is not diagonal in this basis.

(b) Now consider σ_x and $\mathsf{B} = \begin{pmatrix} 2 & 3 \\ 3 & 2 \end{pmatrix}$. Show that these two matrices *do* commute and show that the basis that diagonalizes σ_x from part (a) also diagonalizes B.

Now let A be any diagonalizable matrix and let B be any matrix that commutes with A.

(c) Let $\vec{v}$ be an eigenvector of A belonging to eigenvalue λ. Show that $\mathsf{B}\vec{v}$ is then *also* and eigenvector of A belonging to the same eigenvalue λ.

Finally, suppose A from part (c) has a non-degenerate spectrum so that all of the eigenspaces are one-dimensional.

(d) Show that $\vec{v}$ must then *also* be an eigenvector for B.
[*Spoilers!* There's some thinking to be done here! The key is that the eigenspaces are one-dimensional, with means that if $\vec{v}$ is an eigenvector of A belonging to eigenvalue λ than any eigenvector of A belonging to a that same eigenvalue λ must be proportional to $\vec{v}$.]

Commentary: This shows that an eigenbasis of A *will* also *be an eigenbasis of* B *and thus in this eigenbasis both* A *and* B *will be diagonal! This of course doesn't prove the general statement that A and B can be simultaneously diagonalized if and only if they commute, but it demonstrates all of the relevant elements of the proof.*

Spoilers! An Example Solution for Problem 6.1(f)

The equations of motion are $\ddot{\vec{x}} = -\mathsf{A}\vec{x}$. We are going to use the fact that $\vec{d}_i$ are eigenvectors. We'll find the left-hand and right-hand side of all six of our forms to show that they are solutions. Note that the vectors $\vec{d}_i$ are constant with respect to time - all the explicit time dependence is in the coefficients.

$$\vec{x}_\delta(t) = \sin(\omega_2 t)\vec{d}_2, \qquad \ddot{\vec{x}}_\delta = -\omega_2^2 \sin(\omega_2 t)\vec{d}_2, \qquad -\mathsf{A}\vec{x}_\delta = -\sin(\omega_2 t)\mathbf{A}\vec{d}_2 = -\lambda_2 \sin(\omega_2 t)\vec{d}_2.$$

Since $\omega_2^2 = \lambda_2$, we have $\ddot{\vec{x}}_\delta = -\mathsf{A}\vec{x}_\delta$ as claimed!

♦