mathematical methods - week 2

Eigenvalue problems

Georgia Tech PHYS-6124

Homework HW #2 due Wednesday, September 4, 2019

== show all your work for maximum credit,
== put labels, title, legends on any graphs
== acknowledge study group member, if collective effort

Exercise 2.1 *Three masses on a loop* 8 points

Bonus points
Exercise 2.2 *A simple stable/unstable manifolds pair* 4 points

edited September 9, 2019

Week 2 syllabus

Monday, August 26, 2019

- Intro to normal modes: example 2.1 *Vibrations of a classical CO_2 molecule*
- Work through Grigoriev notes 8 Normal modes
- Linear stability : example 2.2 *Stable/unstable manifolds*
- Optional reading: Stone & Goldbart Appendix A; Arfken & Weber Arfken and Weber [1] Chapter 3
- Optional: Work through Grigoriev notes p. 6.6 crankshaft;

The big idea of this is week is *symmetry*: If our physical problem is defined by a (perhaps complicated) Hamiltonian $\mathbf{H}$, another matrix $\mathbf{M}$ (hopefully a very simple matrix) is a symmetry if it commutes with the Hamiltonian

$$[\mathbf{M}, \mathbf{H}] = 0\,. \tag{2.1}$$

Than we can use the spectral decomposition (1.37) of $\mathbf{M}$ to block-diagonalize $\mathbf{H}$ into a sum of lower-dimensional sub-matrices,

$$\mathbf{H} = \sum_i \mathbf{H}_i\,, \qquad \mathbf{H}_i = \mathbf{P}_i \mathbf{H} \mathbf{P}_i\,, \tag{2.2}$$

and thus significantly simplify the computation of eigenvalues and eigenvectors of $\mathbf{H}$, the matrix of physical interest.

2.1 Normal modes

Example 2.1. ***Vibrations of a classical CO_2 molecule:*** *Consider one carbon and two oxygens constrained to the x-axis [1] and joined by springs of stiffness k, as shown in figure 2.1. Newton's second law says*

$$\begin{aligned}
\ddot{x}_1 &= -\frac{k}{M}(x_1 - x_2) \\
\ddot{x}_2 &= -\frac{k}{m}(x_2 - x_3) - \frac{k}{m}(x_2 - x_1) \\
\ddot{x}_3 &= -\frac{k}{M}(x_3 - x_2)\,.
\end{aligned} \tag{2.3}$$

The normal modes, with time dependence $x_j(t) = x_j \exp(it\omega)$, are the common frequency ω vibrations that satisfy (2.3),

$$\mathbf{H}\mathbf{x} = \begin{pmatrix} A & -A & 0 \\ -a & 2\,a & -a \\ 0 & -A & A \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \omega^2 \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}\,, \tag{2.4}$$

where $a = k/m$, $A = k/M$. Secular determinant $\det(\mathbf{H} - \omega^2 \mathbf{1}) = 0$ now yields a cubic equation for ω^2.

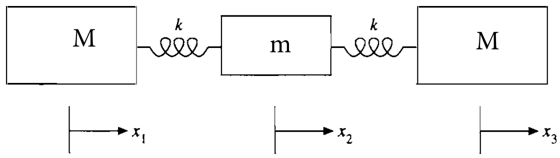

Figure 2.1: A classical colinear CO_2 molecule [1].

You might be tempted to stick this $[3\times3]$ matrix into `Mathematica` *or whatever, but please do that in some other course. What would understood by staring at the output? In this course we think.*

First thing to always *ask yourself is: does the system have a* symmetry*? Yes! Note that the CO_2 molecule (2.3) of figure 2.1 is invariant under $x_1 \leftrightarrow x_3$ interchange, i.e., coordinate relabeling by matrix σ that commutes with our law of motion $\mathbf{H}$,*

$$\sigma = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad \sigma\mathbf{H} = \mathbf{H}\sigma = \begin{pmatrix} 0 & -A & A \\ -a & 2\,a & -a \\ A & -A & 0 \end{pmatrix}. \tag{2.5}$$

We can now use the symmetry operator σ to simplify the calculation. As $\sigma^2 = \mathbf{1}$, its eigenvalues are ±1, and the corresponding symmetrization, anti-symmetrization projection operators *(1.43) are*

$$\mathbf{P}_+ = \frac{1}{2}(\mathbf{1}+\sigma), \qquad \mathbf{P}_- = \frac{1}{2}(\mathbf{1}-\sigma). \tag{2.6}$$

The dimensions $d_i = \mathrm{tr}\,\mathbf{P}_i$ of the two subspaces are

$$d_+ = 2, \qquad d_- = 1. \tag{2.7}$$

As σ and $\mathbf{H}$ commute, we can now use spectral decomposition (1.37) to block-diagonalize $\mathbf{H}$ to a 1-dimensional and a 2-dimensional matrix.

On the 1-dimensional antisymmetric subspace, the trace of a $[1\times1]$ matrix equals its sole matrix element equals it eigenvalue

$$\lambda_- = \mathbf{H}\mathbf{P}_- = \frac{1}{2}(\mathrm{tr}\,\mathbf{H} - \mathrm{tr}\,\mathbf{H}\sigma) = (a+A) - a = \frac{k}{M},$$

so the corresponding eigenfrequency is $\omega_-^2 = k/M$. To understand its physical meaning, write out the antisymmetric subspace projection operator (2.7) explicitly. Its non-vanishing columns are proportional to the sole eigenvector

$$\mathbf{P}_- = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \Rightarrow \mathbf{e}^{(-)} = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}. \tag{2.8}$$

In this subspace the outer oxygens are moving in opposite directions, with the carbon stationary.

On the 2-dimensional symmetric subspace, the trace yields the sum of the remaining two eigenvalues

$$\lambda_+ + \lambda_0 = \mathrm{tr}\,\mathbf{H}\mathbf{P}_+ = \frac{1}{2}(\mathrm{tr}\,\mathbf{H} + \mathrm{tr}\,\mathbf{H}\sigma) = (a+A) + a = \frac{k}{M} + 2\,\frac{k}{m}.$$

We could disentangle the two eigenfrequencies by evaluating $\mathrm{tr}\,\mathbf{H}^2\mathbf{P}_+$*, for example, but thinking helps again.*

There is still another, translational symmetry, so obvious that we forgot it; if we change the origin of the x*-axis, the three coordinates* $x_j \to x_j - \delta x$ *change, for any continuous translation* δx*, but the equations of motion (2.3) do not change their form,*

$$\mathbf{H}\,\mathbf{x} \;=\; \mathbf{H}\,\mathbf{x} + \mathbf{H}\,\delta\mathbf{x} \;=\; \omega^2\mathbf{x} \quad\Rightarrow\quad \mathbf{H}\,\delta\mathbf{x} \;=\; 0\,. \tag{2.9}$$

So any translation $\mathbf{e}^{(0)} = \delta\mathbf{x} = (\delta x, \delta x, \delta x)$ *is a nul, 'zero mode' eigenvector of* $\mathbf{H}$ *in (2.5), with eigenvalue* $\lambda_0 = \omega_0^2 = 0$*, and thus the remaining eigenfrequency is* $\omega_+^2 = k/M + 2\,k/m$*. As we can add any nul eigenvector* $\mathbf{e}^{(0)}$ *to the corresponding* $\mathbf{e}^{(+)}$ *eigenvector, there is some freedom in choosing* $\mathbf{e}^{(+)}$*. One visualization of the corresponding eigenvector is the carbon moving opposite to the two oxygens, with total momentum set to zero.*

2.2 Stable/unstable manifolds

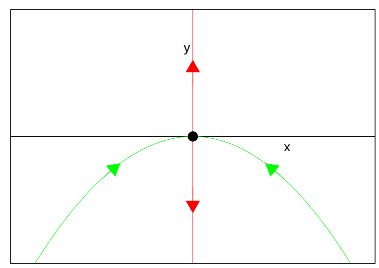

Figure 2.2: The stable/unstable manifolds of the equilibrium $(x_q, x_q) = (0,0)$ of 2-dimensional flow (2.10).

Example 2.2. ***A simple stable/unstable manifolds pair:*** *Consider the 2-dimensional ODE system*

$$\frac{dx}{dt} = -x, \quad \frac{dy}{dt} = y + x^2\,, \tag{2.10}$$

The flow through a point $x(0) = x_0, y(0) = y_0$ *can be integrated*

$$x(t) = x_0\,e^{-t}, \quad y(t) = (y_0 + x_0^2/3)\,e^t - x_0^2\,e^{-2t}/3\,. \tag{2.11}$$

Linear stability of the flow is described by the stability matrix

$$\mathbf{A} = \begin{pmatrix} -1 & 0 \\ 2x & 1 \end{pmatrix}. \tag{2.12}$$

The flow is hyperbolic, with a real expanding/contracting eigenvalue pair $\lambda_1 = 1$*,* $\lambda_2 = -1$*, and area preserving. The right eigenvectors at the point* (x, y)

$$\mathbf{e}^{(1)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \qquad \mathbf{e}^{(2)} = \begin{pmatrix} 1 \\ -x \end{pmatrix}. \tag{2.13}$$

can be obtained by acting with the projection operators (see example 1.2 Decomposition of 2-dimensional vector spaces*)*

$$\mathbf{P}_i = \frac{\mathbf{A} - \lambda_j \mathbf{1}}{\lambda_i - \lambda_j} : \qquad \mathbf{P}_1 = \begin{bmatrix} 0 & 0 \\ x & 1 \end{bmatrix}, \quad \mathbf{P}_2 = \begin{bmatrix} 1 & 0 \\ -x & 0 \end{bmatrix} \tag{2.14}$$

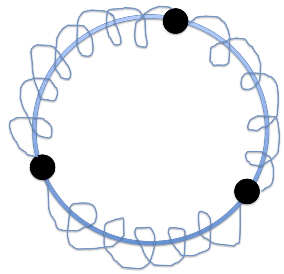

Figure 2.3: Three identical masses are constrained to move on a hoop, connected by three identical springs such that the system wraps completely around the hoop. Find the normal modes.

on an arbitrary vector. Matrices $\mathbf{P}_i$ are orthonormal and complete.

The flow has a degenerate pair of equilibria at $(x_q, y_q) = (0, 0)$, with eigenvalues (stability exponents), $\lambda_1 = 1$, $\lambda_2 = -1$, eigenvectors $\mathbf{e}^{(1)} = (0, 1)$, $\mathbf{e}^{(2)} = (1, 0)$. The unstable manifold is the y axis, and the stable manifold is given by (see figure 2.2)

$$y_0 + \frac{1}{3}x_0^2 = 0 \Rightarrow y(t) + \frac{1}{3}x(t)^2 = 0\,. \tag{2.15}$$

(N. Lebovitz)

References

[1] G. B. Arfken and H. J. Weber, *Mathematical Methods for Physicists: A Comprehensive Guide*, 6th ed. (Academic, New York, 2005).

Exercises

2.1. **Three masses on a loop.** Three identical masses, connected by three identical springs, are constrained to move on a circle hoop as shown in figure 2.3. Find the normal modes. Hint: write down coupled harmonic oscillator equations, guess the form of oscillatory solutions. Then use basic matrix methods, i.e., find zeros of a characteristic determinant, find the eigenvectors, etc.. See also Exercise 13.1. (Kimberly Y. Short)

2.2. **A simple stable/unstable manifolds pair.** Integrate flow (2.10), verify (2.11). Check that the projection matrices $\mathbf{P}_i$ (2.14) are orthonormal and complete. Use them to construct right and left eigenvectors; check that they are mutually orthogonal. Explain why is (2.15) the equation for the stable manifold. (N. Lebovitz)