

# 4

## COUPLED OSCILLATORS

**Introduction.** The forces that bind bulk material together have always finite strength. All materials are therefore to some degree deformable, are (as we say of those that—unlike gases and liquids—are able to “hold their shape”) to some degree elastic. When disturbed while at rest in their quiescent state they quiver.<sup>1</sup> In the quiescent state each of the constituent particles was (or is imagined classically to have been) at rest at a local minimum of the in the many-body potential  $U(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ . Injection of a little bit of energy causes the particles to move about in the neighborhood of their respective rest sites, and to begin trading energy amongst themselves. Picture, if you can, of a 3-dimensional multi-particle extension of the situation shown in the first figure of Chapter 3.

The image just presented is most cleanly realized in crystals (and somewhat less perfectly—because they are more essentially quantum mechanical—in molecules). Crystals are macroscopic manifestations of the hidden quantum mechanics of their sub-microscopic parts: that’s why, for instance, a crystallographic configuration that can be assembled from atoms  $A$  and  $B$  sometimes/usually cannot be assembled from atoms  $X$  and  $Y$ . But remarkably many of the essentials of crystal physics can be obtained without reference to quantum mechanics, by thinking of a crystal as an orderly assembly of Newtonian point particles connected to one another (usually only to near neighbors) by springs (see FIGURE 1). The specific details (masses, connection pattern, spring strengths) vary, of course, from case to case. But the analytical principles, and qualitative features of the results to which they lead, are to a very large degree case-independent. They pertain even to structures (ringing bells, vibrating airframes) that we would never be inclined to describe as being “crystalline.”

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<sup>1</sup> If the disturbance is violent enough they fracture/disintegrate, which poses a set of physical problems quite different from the ones that will interest us here.

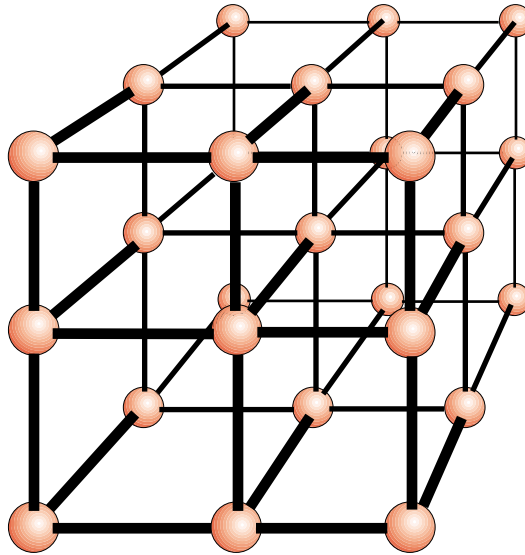


FIGURE 1: A simple “classical crystal,” an arrangement of Newtonian point masses connected to one another by springs. We are interested in the vibrational properties of such systems.

It is to avoid distracting notational complexities and to gain access to various graphic devices that we will, at least initially, abandon two space dimensions, looking to the physics of “one-dimensional crystals.” And we begin with discussion of the simplest of those—a discussion which will serve already to expose all of the most characteristic *general* features of the physics of vibrating multi-particle systems.

**1. A simple “one-dimensional crystal.”** Working from FIGURE 2, we have

$$\begin{aligned} m_1 \ddot{x}_1 &= F_1 + F_{12} = F_1^{\text{net}} \\ m_2 \ddot{x}_2 &= F_2 + F_{21} = F_2^{\text{net}} \end{aligned}$$

where

- $F_i$  refers to the force externally impressed upon  $m_i$
- $F_{ij}$  refers to the interactive force exerted on  $m_i$  by  $m_j$ . Newton’s 3<sup>rd</sup> Law asserts that in all cases  $F_{ij} = -F_{ji}$ .

The forces could, in this instance, be read directly from the figure, but in more complicated cases it would be more efficient to introduce the potential energy function

$$U(x_1, x_2) = \frac{1}{2}k_1x_1^2 + \frac{1}{2}K(x_2 - x_1)^2 + \frac{1}{2}k_2x_2^2$$

and to compute

$$\begin{aligned} F_1^{\text{net}} &= -\frac{\partial U}{\partial x_1} = -k_1x_1 + K(x_2 - x_1) \\ F_2^{\text{net}} &= -\frac{\partial U}{\partial x_2} = -k_2x_2 - K(x_2 - x_1) \end{aligned}$$

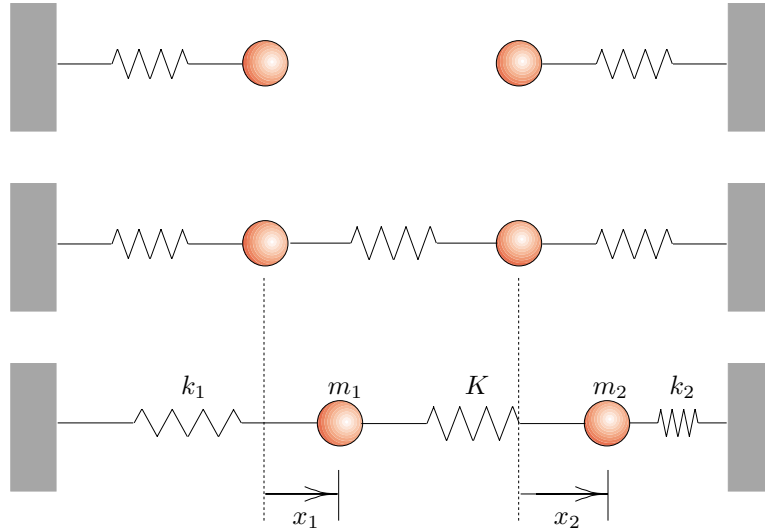


FIGURE 2: The top figure shows a pair of uncoupled oscillators. In the middle figure the oscillators have been coupled. In both figures the masses are shown in their equilibrium positions. The bottom figure establishes the notation we will use to work out the dynamics of such a system. The variables  $x_1$  and  $x_2$  are “excursion variables;” they quantify displacement from equilibrium.

We arrive thus at the coupled linear system of equations

$$\left. \begin{aligned} m_1 \ddot{x}_1 &= -(k_1 + K)x_1 + Kx_2 \\ m_2 \ddot{x}_2 &= Kx_1 - (k_2 + K)x_2 \end{aligned} \right\} \quad (1)$$

Notice that the equations decouple in the limit  $K \downarrow 0$ . And that we can write

$$\mathbb{M} \ddot{\mathbf{x}} + \mathbb{K} \mathbf{x} = \mathbf{0} \quad (2.1)$$

$$\mathbf{x} \equiv \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \mathbb{M} \equiv \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}, \quad \mathbb{K} \equiv \begin{pmatrix} k_1 + K & -K \\ -K & k_2 + K \end{pmatrix} \quad (2.2)$$

Drawing inspiration now from the COMPLEX VARIABLE METHOD as it was described on page 3 of Chapter 3, we proceed from the **Ansatz**

$$\mathbf{z}(t) = \mathbf{Z} e^{i\nu t} : \text{ all particles oscillate with the same frequency } \quad (3)$$

to

$$(\mathbb{K} - \nu^2 \mathbb{M}) \mathbf{Z} = \mathbf{0} \quad (4)$$

This equation will possess non-trivial solutions if and only if  $\det(\mathbb{K} - \nu^2 \mathbb{M}) = 0$ ,

which forces  $\nu^2$  to be one or the other of the roots of a certain second-order polynomial. It is to simplify the writing, and to better expose the essence of what is going on, that we at this point

$$\text{assume } m_1 = m_2 \equiv m \text{ and } k_1 = k_2 \equiv k$$

We agree, in other words, to look to the case in which identical particles are attached to identical springs and to each other. Writing

$$\mathbb{S}(\nu^2) = \begin{pmatrix} k + K & -K \\ -K & k + K \end{pmatrix} - \nu^2 \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}$$

we have

$$\det \mathbb{S}(\nu^2) = m^2 \nu^4 - 2m(k + K)\nu^2 + (k^2 + 2kK)$$

which has roots

$$\left. \begin{aligned} \omega_1^2 &= \frac{k}{m} & : & \text{slow} \\ \omega_2^2 &= \frac{k + 2K}{m} & : & \text{fast} \end{aligned} \right\} \quad (5)$$

*Mathematica* now

responds  $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$  to the command `NullSpace[ $\mathbb{S}(\omega_1^2)$ ]`

responds  $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$  to the command `NullSpace[ $\mathbb{S}(\omega_2^2)$ ]`

We conclude that all instances of

$$\begin{aligned} \mathbf{x}(t) = & \{A_1 \cos \omega_1 t + B_1 \sin \omega_1 t\} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\ & + \{A_2 \cos \omega_2 t + B_2 \sin \omega_2 t\} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \end{aligned} \quad (6)$$

satisfy

$$\left. \begin{aligned} m\ddot{x}_1 &= -(k + K)x_1 + Kx_2 \\ mx_2 &= Kx_1 - (k + K)x_2 \end{aligned} \right\} \quad (7)$$

and that, since (6) contains four arbitrary constants  $\{A_1, B_1, A_2, B_2\}$ , it must provide the *general* solution of that coupled pair of second-order equations. FIGURES 3 provide graphical interpretations of the slow/fast components of (6), of which the general solution is a linear combination. They explain in particular why the slow solution is called the **sloshing mode**, and the fast solution the **breathing mode**.

Suppose, for example, it were stipulated that initially

$$\mathbf{x}(0) = \begin{pmatrix} A \\ 0 \end{pmatrix} \quad \text{and} \quad \dot{\mathbf{x}}(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

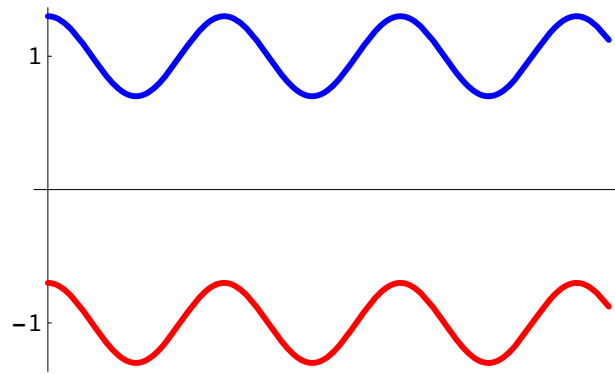


FIGURE 3A: **Sloshing mode**, motion described by the “slow solution” of (7):

$$\mathbf{x}_{\text{slow}}(t) = \{A_1 \cos \omega_1 t + B_1 \sin \omega_1 t\} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (8.1)$$

Note that in this instance the coupling spring  $K$  remains constantly unstretched; the particles move as would mass  $2m$  on a spring of strength  $2k$ .

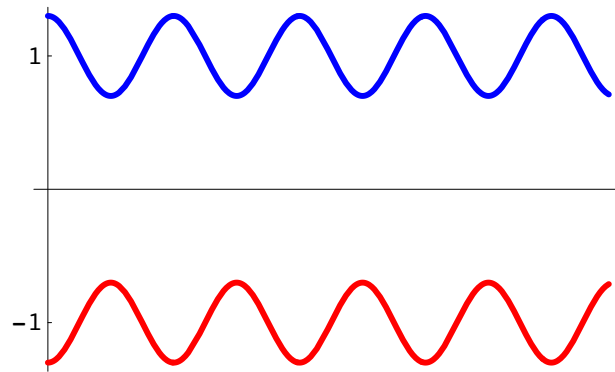


FIGURE 3B: **Breathing mode**, motion described by the “fast solution” of (7):

$$\mathbf{x}_{\text{fast}}(t) = \{A_2 \cos \omega_2 t + B_2 \sin \omega_2 t\} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (8.2)$$

In this instance the  $K$ -spring is stretched maximally during each oscillation.

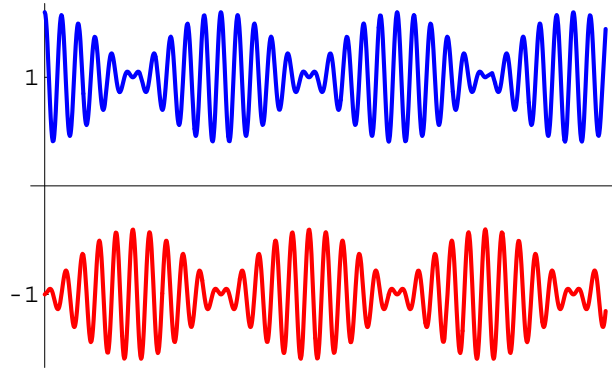


FIGURE 4: Energy is initially invested in the compression of the spring attached to the blue particle, which is in this instance only weakly coupled to the red particle. With the passage of time energy is traded back and forth between the two particles (and their associated springs).

We would then have

$$\begin{aligned} A_1 + A_2 &= A \\ A_1 - A_2 &= 0 \\ \omega_1 B_1 + \omega_2 B_2 &= 0 \\ \omega_1 B_1 - \omega_2 B_2 &= 0 \end{aligned}$$

giving

$$\begin{aligned} A_1 &= \frac{1}{2}A \\ A_2 &= \frac{1}{2}A \\ B_1 &= 0 \\ B_2 &= 0 \end{aligned}$$

The resulting function

$$\mathbf{x}(t) = \frac{1}{2}A \left\{ \cos \omega_1 t \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \cos \omega_2 t \cdot \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right\} \quad (9)$$

is graphed in FIGURE 4.

The pattern evident in the figure can be understood by an argument identical to that which in acoustics serves to account for “beats.” We have (use *Mathematica*’s `TrigFactor` command)

$$\begin{aligned} x_1(t) &= \frac{1}{2}A \{ \cos \omega_1 t + \cos \omega_2 t \} \\ &= A \cos \frac{1}{2}(\omega_2 - \omega_1)t \cdot \cos \frac{1}{2}(\omega_2 + \omega_1)t \end{aligned}$$

where  $\omega_2 = \left[ \frac{k+2K}{m} \right]^{\frac{1}{2}} = \omega_1 [1 + 2K/k]^{\frac{1}{2}} = \omega_1 \{ 1 + (K/k) + \dots \}$ . Weak coupling means that  $K/k \ll 1$ , so we have  $\omega_2 = \omega_1 + \Delta\omega$  with  $\Delta\omega \approx \omega_1 \cdot (K/k)$ , giving

$$\begin{aligned}
x_1(t) &= A \cos[(\Delta\omega)t] \cdot \cos[\bar{\omega}t] \\
&= A \text{ (slow modulation factor)} \\
&\quad \cdot \text{(fast oscillation of mean frequency } \bar{\omega} \equiv \frac{\omega_1 + \omega_2}{2})
\end{aligned}$$

Though technically the “energy exchange frequency” (beat frequency) is  $\Delta\omega$ , the *perceived* exchange frequency is  $2\Delta\omega$ , since it goes waa-waa per period.

The initial-condition-matching calculations that led to (9) are made much easier by the observation that the vectors

$$\mathbf{X}_1 \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathbf{X}_2 \equiv \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (10)$$

are *orthogonal* (are, in fact, *orthonormal*). For it is then immediate that

$$\left. \begin{aligned}
\mathbf{x}_0 &= (\mathbf{x}_0 \cdot \mathbf{X}_1)\mathbf{X}_1 + (\mathbf{x}_0 \cdot \mathbf{X}_2)\mathbf{X}_2 \\
\dot{\mathbf{x}}_0 &= (\dot{\mathbf{x}}_0 \cdot \mathbf{X}_1)\mathbf{X}_1 + (\dot{\mathbf{x}}_0 \cdot \mathbf{X}_2)\mathbf{X}_2
\end{aligned} \right\} \quad (11)$$

from which we obtain

$$\begin{aligned}
\mathbf{x}(t) &= \left\{ (\mathbf{x}_0 \cdot \mathbf{X}_1) \cos \omega_1 t + (\dot{\mathbf{x}}_0 \cdot \mathbf{X}_1) \frac{\sin \omega_1 t}{\omega_1} \right\} \mathbf{X}_1 \\
&+ \left\{ (\mathbf{x}_0 \cdot \mathbf{X}_2) \cos \omega_1 t + (\dot{\mathbf{x}}_0 \cdot \mathbf{X}_2) \frac{\sin \omega_1 t}{\omega_1} \right\} \mathbf{X}_2
\end{aligned} \quad (12)$$

The dynamical motion of  $\mathbf{x}(t)$  is displayed here as a superposition of the excited **normal modes**<sup>2</sup> of the system. We found it initially quite natural to write

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 \quad \text{with} \quad \mathbf{e}_1 \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \mathbf{e}_2 \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

but found that from a dynamical standpoint it is more natural/informative to write

$$\mathbf{x} = \xi_1 \mathbf{X}_1 + \xi_2 \mathbf{X}_2$$

The  $\mathbf{e}_i$  refer to particles individually, the  $\mathbf{X}_i$  refer to them in what have been revealed to be certain dynamically natural collective combinations.

**2. A slightly less simple “one-dimensional crystal.”** Working now from FIGURE 5 we have  $U(x_1, x_2, x_3) = \frac{1}{2}k\{x_1^2 + (x_2 - x_1)^2 + (x_3 - x_2)^2 + x_3^2\}$ . The resulting equations of motion

$$\begin{aligned}
m\ddot{x}_1 &= -k\{2x_1 - x_2\} \\
m\ddot{x}_2 &= -k\{-x_1 + 2x_2 - x_3\} \\
m\ddot{x}_3 &= -k\{-x_2 + 2x_3\}
\end{aligned}$$

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<sup>2</sup> They should more properly be called “orthogonal modes.” Here “normal” refers not to “unit length” but—as in geometry—to perpendicularity.

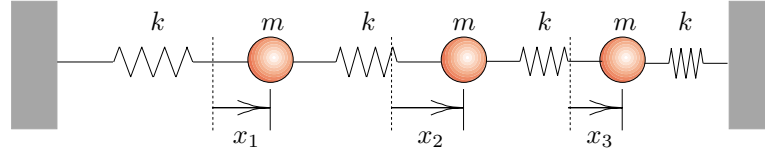


FIGURE 5: One-dimensional crystal assembled from three identical “atoms” connected to one another and to the walls by identical springs.

can be written

$$m \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \ddot{\mathbf{x}} + k \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix} \mathbf{x} = \mathbf{0}$$

and abbreviated<sup>3</sup>  $m \mathbb{I} \ddot{\mathbf{x}} + k \mathbb{S} \mathbf{x} = \mathbf{0}$

Proceeding once again from the Ansatz  $\mathbf{z}(t) = \mathbf{Z}e^{i\nu t}$  we have

$$(\mathbb{S} - \lambda \mathbb{I}) \mathbf{Z} = \mathbf{0} \quad (13)$$

with  $\lambda \equiv (\nu/\omega)^2$  and  $\omega^2 \equiv k/m$ . But (13) presents an instance of the **eigenvalue problem**, in its purest form.<sup>4</sup> Solutions exist only if  $\lambda$  is one of the eigenvalues of  $\mathbb{S}$ . And because  $\mathbb{S}$  is real and symmetric we know that the eigenvalues will be real, and that the associated eigenvectors will be orthogonal. *Mathematica*, in response to the command `Eigensystem`, informs us that

$$\left. \begin{array}{l} \lambda_1 = 2 - \sqrt{2} \quad \text{has normalized eigenvector} \quad \mathbf{X}_1 = \frac{1}{2} \begin{pmatrix} 1 \\ +\sqrt{2} \\ 1 \end{pmatrix} \\ \lambda_2 = 2 \quad \text{has normalized eigenvector} \quad \mathbf{X}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \\ \lambda_3 = 2 + \sqrt{2} \quad \text{has normalized eigenvector} \quad \mathbf{X}_3 = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \end{array} \right\} \quad (14)$$

The modal frequencies are  $\nu_1 = \sqrt{2 - \sqrt{2}}\omega$ ,  $\nu_2 = \sqrt{2}\omega$ ,  $\nu_3 = \sqrt{2 + \sqrt{2}}\omega$  and the characteristic patterns of modal vibration are shown in the following figure:

<sup>3</sup> My notation is intended to emphasize the Symmetry of the Spring matrix.

<sup>4</sup> See again §5 in Chapter 1.



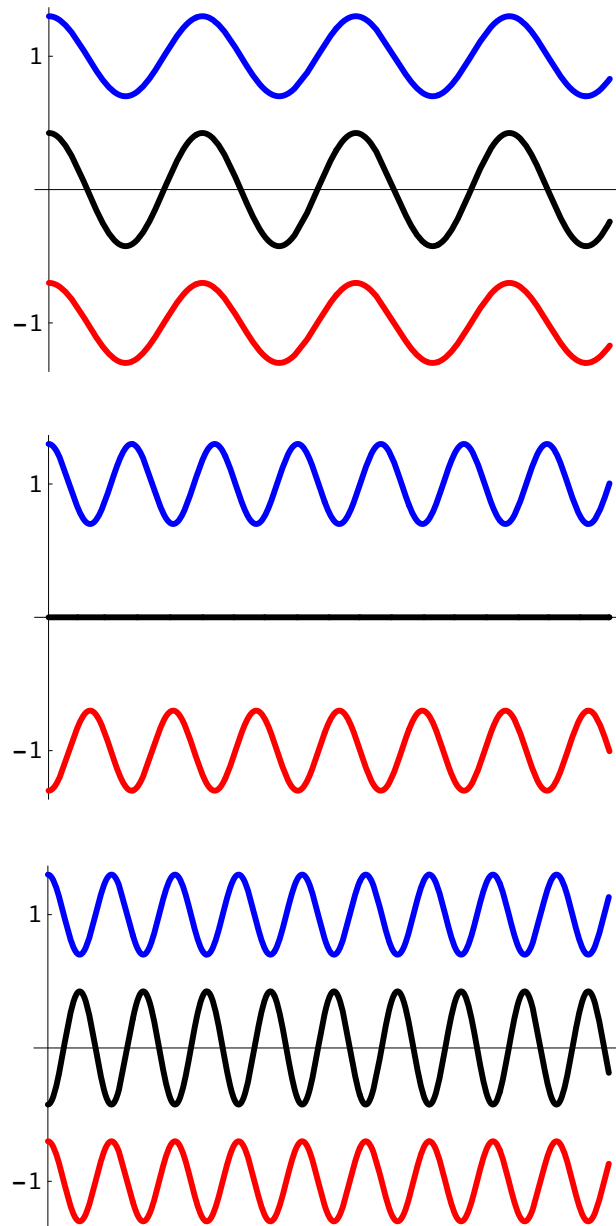


FIGURE 6: *Modal vibration patterns of the tri-atomic system shown in FIGURE 5. The frequencies and relative amplitudes have been drawn in correct proportion.*

**PROBLEM 1 :** Modify the tri-atomic system shown in FIGURE 5 by installation of a fifth spring (spring constant  $k$ , like the other springs) that serves to attach the central particle to its equilibrium point (as shown in the figure it is attached only to its neighbors). Write the new potential  $U(x_1, x_2, x_3)$ , write the new  $\mathbb{S}$  matrix, calculate (*i.e.*, ask *Mathematica* to calculate) the new modal frequencies  $\{\nu_1, \nu_2, \nu_3\}$  and the new normalized eigenvectors  $\{\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3\}$ . Demonstrate that the latter vectors are orthogonal.

**3. One-dimensional diatomic molecule.** *Every* diatomic molecule is 1-dimensional in the sense that “two points determine a line.” But real diatomic molecules can tumble/spin, and that is an important aspect of their physics that we intend here to set aside. We have interest only in the vibrational physics of such structures. Proceeding in reference to FIGURE 7, we confront at the outset this sticky problem:

How—to make the argument as simple as possible—should we proceed to “coordinatize” the molecule? We know from elementary mechanics that in the absence of externally impressed forces its center of mass

$$X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$$

moves uniformly,<sup>5</sup> and can without loss of generality be assumed to be at rest. The implication is that displacements of  $m_1$  relative to the center of mass dictate counterbalancing displacements of  $m_2$ : if  $m_1$  is displaced a distance  $\xi_1$  toward the center of mass then  $m_2$  is displaced a distance  $\xi_2 = -(m_1/m_2)\xi_1$  and the distance between the particles shrinks by

$$[1 + (m_1/m_2)]\xi_1 = \frac{m_1 + m_2}{m_2} \xi_1$$

If the particles sat originally at their equilibrium points (*i.e.*, a molecular length  $a$  from each other) then  $m_1$  has come to feel the opposing spring force that appears on the right side of the following equation:<sup>6</sup>

$$m_1 \ddot{\xi}_1 = -K \frac{m_1 + m_2}{m_2} \xi_1$$

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<sup>5</sup> We have, relative to an inertial frame,

$$\begin{aligned} m_1 \ddot{x}_1 &= F_{12} \\ m_2 \ddot{x}_2 &= F_{21} \\ F_{21} &= -F_{12} \quad \text{by Newton's 3rd Law} \end{aligned}$$

Addition gives  $\ddot{X} = 0$ .

<sup>6</sup> From this equation it follows, by the way, as a redundant corollary, that

$$m_2 \ddot{\xi}_2 = -K \frac{m_1 + m_2}{m_1} \xi_2$$

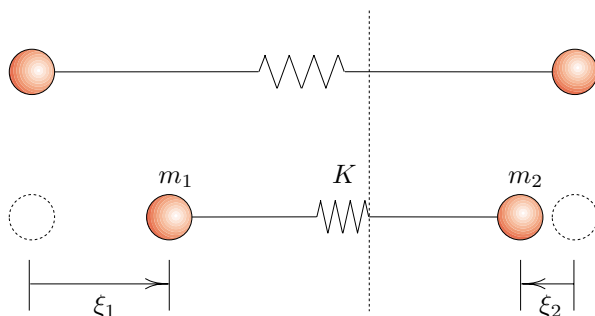


FIGURE 7: Shown above: a relaxed diatomic molecule. Shown below: snapshot of the same molecule in an excited state. The dotted line marks the location of the unmoved center of mass.

We conclude that the two particles “counter-oscillate,” with frequency

$$\nu = \sqrt{K \frac{m_1 + m_2}{m_1 m_2}} \quad (15)$$

and with relative amplitudes fixed by the requirement that the center of mass remain fixed.

The preceding argument was elementary but tedious. It felt improvisatory. And it appeared on its face to favor  $m_1$ , discriminate against  $m_2$ , though no such asymmetry is presented by the molecule itself. All those defects, it is pretty clear, will become instantly more serious the moment we turn our attention to more complicated molecules. I describe now an alternative, more symmetrical line of argument: it proceeds from the observation that the crystal of FIGURE 2 turns into the molecule of FIGURE 7 when the endsprings are turned off:  $k_1 \downarrow 0$  and  $k_2 \downarrow 0$ . The equations of motion (1) then become

$$\left. \begin{aligned} m_1 \ddot{x}_1 &= -Kx_1 + Kx_2 \\ m_2 \ddot{x}_2 &= Kx_1 - Kx_2 \end{aligned} \right\} \quad (16)$$

Arguing now precisely as we argued on page 3—the only difference being that now

$$\mathbb{K} = \begin{pmatrix} +K & -K \\ -K & +K \end{pmatrix}$$

—we arrive again at the requirement that

$$\det(\mathbb{K} - \nu^2 \mathbb{M}) = \nu^2 \cdot [m_1 m_2 \nu^2 - K(m_1 + m_2)] = 0$$

So necessarily  $\nu^2$  has one or the other of the values

$$\nu_0^2 = 0 \quad \text{or} \quad \nu_1^2 = \sqrt{K \frac{m_1 + m_2}{m_1 m_2}} \quad (17.1)$$

Only in those cases can the equation  $(\mathbb{K} - \nu^2 \mathbb{M})\mathbf{Z} = \mathbf{0}$  be solved. *Mathematica's* `NullSpace` command supplies

$$\mathbf{Z}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \text{or} \quad \mathbf{Z}_1 = \begin{pmatrix} 1 \\ -(m_1/m_2) \end{pmatrix} \quad (17.2)$$

respectively. The first solution describes a *non-oscillatory drift of the center of mass*, the second describes precisely the counter-oscillatory internal vibration that we encountered before.

**PROBLEM 2 :** Mimic the preceding argument as it pertains to the linear tri-atomic molecule that is formed by removal of the endsprings from the 3-atom crystal shown in FIGURE 5. Retain the simplifying assumption that all three particles have the same mass  $m$ , and that the remaining springs both have strength  $k$ . Construct figures in the style of FIGURE 6 that illustrate the modes of internal vibration of such a molecule.

Why are the vectors  $\mathbf{Z}_0$  and  $\mathbf{Z}_1$  not orthogonal unless  $m_1/m_2 = 1$ ? Because only in that case (*i.e.*, only when  $m_1 = m_2 \equiv m$ ) does  $(\mathbb{K} - \nu^2 \mathbb{M})\mathbf{Z} = \mathbf{0}$  provide an instance of the eigenvalue problem: only then can that equation be written

$$(\mathbb{K} - \lambda \mathbb{I})\mathbf{Z} = \mathbf{0} \quad : \quad \lambda \equiv \nu^2 m$$

A true eigenvalue problem does, however, lie always close at hand. I show now how to get there.

Suppose  $\mathbb{M}$  could be written  $\mathbb{M} = \mathbb{N}\mathbb{N}$ . We would then have

$$\mathbb{N}(\mathbb{N}^{-1}\mathbb{K}\mathbb{N}^{-1} - \lambda \mathbb{I})\mathbb{N}\mathbf{Z} = \mathbf{0}$$

which when multiplied on the left by  $\mathbb{N}^{-1}$  becomes

$$(\tilde{\mathbb{K}} - \lambda \mathbb{I})\tilde{\mathbf{Z}} = \mathbf{0}$$

(here  $\tilde{\mathbb{K}} \equiv \mathbb{N}^{-1}\mathbb{K}\mathbb{N}^{-1}$  and  $\tilde{\mathbf{Z}} \equiv \mathbb{N}\mathbf{Z}$ ), which *does* present a true eigenvalue problem. From  $\det(\mathbb{A}\mathbb{B}) = \det \mathbb{A} \cdot \det \mathbb{B}$  it follows moreover that

$$\det(\tilde{\mathbb{K}} - \lambda \mathbb{I}) = \frac{\det(\mathbb{K} - \lambda \mathbb{M})}{(\det \mathbb{N})^2}$$

so the roots of  $\det(\tilde{\mathbb{K}} - \lambda \mathbb{I}) = 0$  (eigenvalues of  $\tilde{\mathbb{K}}$ ) coincide with the roots of  $\det(\mathbb{K} - \lambda \mathbb{M}) = 0$ .

Observe finally that if  $\mathbb{M}$  is symmetric then so also are each of its square roots  $\mathbb{N}$ . And that if  $\mathbb{N}$  is symmetric then so also is  $\mathbb{N}^{-1}$ . And that if  $\mathbb{K}$  is symmetric then so also is  $\tilde{\mathbb{K}}$ . So the eigenvectors  $\tilde{\mathbf{Z}}_i$  of  $\tilde{\mathbb{K}}$ —at least those associated with distinct eigenvalues—are necessarily orthogonal in the familiar sense

$$\tilde{\mathbf{Z}}_i^T \tilde{\mathbf{Z}}_j = 0 \quad \text{if} \quad i \neq j$$

The vectors  $\mathbf{Z}_i$  are therefore orthogonal in the unfamiliar sense

$$\mathbf{Z}_i^T \mathbb{M} \mathbf{Z}_j = 0 \quad \text{if} \quad i \neq j$$

**EXAMPLE:** Returning with these ideas to the case at hand, from

$$\mathbb{M} = \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix}$$

we obtain

$$\mathbb{N} = \begin{pmatrix} \sqrt{m_1} & 0 \\ 0 & \sqrt{m_2} \end{pmatrix} \quad \text{and} \quad \mathbb{N}^{-1} = \begin{pmatrix} \frac{1}{\sqrt{m_1}} & 0 \\ 0 & \frac{1}{\sqrt{m_2}} \end{pmatrix}$$

From

$$\mathbb{K} = K \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

it therefore follows that

$$\tilde{\mathbb{K}} = \begin{pmatrix} \frac{1}{m_1} & -\frac{1}{\sqrt{m_1 m_2}} \\ -\frac{1}{\sqrt{m_1 m_2}} & \frac{1}{m_2} \end{pmatrix}$$

The command `Eigensystem[ $\tilde{\mathbb{K}}$ ]` supplies eigenvalues

$$\lambda_0 = 0 \quad \text{and} \quad \lambda_1 = \frac{m_1 + m_2}{m_1 m_2}$$

and associated (not-yet-normalized) eigenvectors

$$\tilde{\mathbf{Z}}_0 = \begin{pmatrix} \sqrt{m_1} \\ \sqrt{m_2} \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{Z}}_1 = \begin{pmatrix} \sqrt{m_2} \\ -\sqrt{m_1} \end{pmatrix}$$

which are clearly orthogonal in the standard sense:  $\tilde{\mathbf{Z}}_0^\top \tilde{\mathbf{Z}}_1 = 0$ . The vectors

$$\mathbf{Z}_0 = \mathbb{N}^{-1} \tilde{\mathbf{Z}}_0 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\mathbf{Z}_1 = \mathbb{N}^{-1} \tilde{\mathbf{Z}}_1 = \begin{pmatrix} \sqrt{m_2/m_1} \\ -\sqrt{m_1/m_2} \end{pmatrix} = \sqrt{m_2/m_1} \begin{pmatrix} 1 \\ -(m_1/m_2) \end{pmatrix}$$

are “orthogonal relative to the  $\mathbb{M}$ -metric”:  $\mathbf{Z}_0^\top \mathbb{M} \mathbf{Z}_1 = 0$ .

It is to expose an important respect in which the preceding discussion is restricted/specialized, and to motivate discussion of how that specialization might be relaxed, that I turn now to study of some simple

**4. Coupled electrical circuits.** Proximate electrical circuits interact magnetically, by “mutual induction.” For the circuits shown in FIGURE 8 we have

$$L_1 \ddot{q}_1 + M \ddot{q}_2 + C_1^{-1} q_1 = 0$$

$$L_2 \ddot{q}_2 + M \ddot{q}_1 + C_1^{-1} q_2 = 0$$

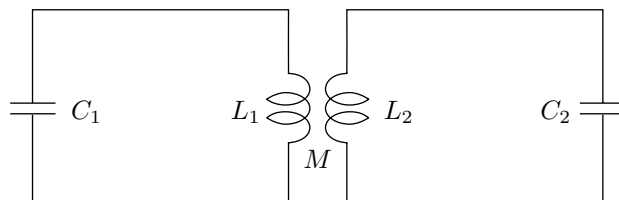


FIGURE 8: A pair of LC circuits. Each is responsive to the changing magnetic fields generated by time-dependent currents in the other. The mutual inductance  $M$  quantifies the strength of the interaction.

which can be written

$$\begin{pmatrix} L_1 & M \\ M & L_2 \end{pmatrix} \begin{pmatrix} \ddot{q}_1 \\ \ddot{q}_2 \end{pmatrix} + \begin{pmatrix} C_1^{-1} & 0 \\ 0 & C_2^{-1} \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and abbreviated<sup>7</sup>

$$\mathbb{M}\ddot{\mathbf{x}} + \mathbb{K}\mathbf{x} = \mathbf{0} \quad (18.1)$$

$$\mathbf{x} \equiv \begin{pmatrix} q_1 \\ q_2 \end{pmatrix}, \quad \mathbb{M} \equiv \begin{pmatrix} L_1 & M \\ M & L_2 \end{pmatrix}, \quad \mathbb{K} \equiv \begin{pmatrix} C_1^{-1} & 0 \\ 0 & C_2^{-1} \end{pmatrix} \quad (18.2)$$

On the strength once again of the Ansatz  $\mathbf{z}(t) = \mathbf{Z}e^{i\omega t}$  we are led to an equation

$$(\mathbb{K} - \nu^2\mathbb{M})\mathbf{Z} = \mathbf{0} \quad (19)$$

that is structurally identical to the mechanical equation (4), the difference being that in (4) the coupling was accomplished by the off-diagonal elements of the  $\mathbb{K}$ -matrix (which is to say: with the aid of springs), but in (19) is accomplished by off-diagonal elements of the  $\mathbb{M}$ -matrix. This detail requires us to introduce a preliminary step to our analytical procedure:

We know from (25.2) in Chapter 1 that the real symmetric matrix  $\mathbb{M}$  can be developed

$$\mathbb{M} = \mathbb{R} \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \mathbb{R}^{-1} \quad : \quad \mathbb{R}^{-1} = \mathbb{R}^T$$

where the  $m_i$  are the (assuredly real) eigenvalues of  $\mathbb{M}$ , and the rotation matrix  $\mathbb{R}$  has been assembled from its eigenvectors. Equation (19) can therefore be written

$$\mathbb{R} \left[ \mathbb{R}^{-1}\mathbb{K}\mathbb{R} - \nu^2 \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \right] \mathbb{R}^{-1}\mathbf{Z} = \mathbf{0}$$

and from here on we can proceed as before: takng  $\mathbb{N}$  to be any one of the  $2^2$

<sup>7</sup> My notation—electrically quite unnatural as it admittedly is—has been designed to underscore parallelism with our previous mechanical work.

square roots of  $\mathbb{M}$

$$\mathbb{N} = \begin{pmatrix} \pm\sqrt{m_1} & 0 \\ 0 & \pm\sqrt{m_2} \end{pmatrix}$$

we write

$$\mathbb{R}\mathbb{N} \left[ \underbrace{\mathbb{N}^{-1}\mathbb{R}^{-1}\mathbb{K}\mathbb{R}\mathbb{N}^{-1}}_{\tilde{\mathbb{K}}} - \nu^2 \cdot \underbrace{\mathbb{N}^{-1} \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \mathbb{N}^{-1}}_{\tilde{\mathbb{I}}} \right] \underbrace{\mathbb{N}\mathbb{R}^{-1}\mathbf{Z}}_{\tilde{\mathbf{Z}}} = \mathbf{0}$$

From the symmetry of  $\mathbb{K}$  and  $\mathbb{N}^{-1}$  and the fact that  $\mathbb{R}$  is a rotation matrix ( $\mathbb{R}^{-1} = \mathbb{R}^\top$ ) we readily deduce the symmetry of  $\tilde{\mathbb{K}}$ . It is clear moreover that

$$\det(\mathbb{K} - \lambda\mathbb{M}) = 0 \iff \det(\tilde{\mathbb{K}} - \lambda\tilde{\mathbb{I}}) = 0$$

The plan, therefore, would be to compute the eigenvalues  $\lambda_i = \nu_i^2$  and the associated eigenvectors  $\tilde{\mathbf{Z}}_i$ . The vectors  $\mathbf{Z}_i = \mathbb{R}\mathbb{N}^{-1}\tilde{\mathbf{Z}}_i$  will serve then to describe (in variables of direct physical significance) the vibrational modes of the system.

From the vectors  $\tilde{\mathbf{Z}}_i$  one can assemble the rotation matrix  $\tilde{\mathbb{R}}$  that serves (see again (25.1) in Chapter 1) to diagonalize  $\tilde{\mathbb{K}}$

$$\tilde{\mathbb{R}}^\top \tilde{\mathbb{K}} \tilde{\mathbb{R}} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

while at the same time preserving the already-achieved diagonalization of  $\tilde{\mathbb{M}} = \tilde{\mathbb{I}}$ :

$$\tilde{\mathbb{R}}^\top \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tilde{\mathbb{R}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The argument is seen therefore to hinge on the possibility of *simultaneously diagonalizing two symmetric matrices*—the point of the simultaneous diagonalization being to **decouple the equations of motion**.

An interesting problem is brought to light when (as would be physically quite natural) one introduces resistance into the circuits. The coupled equations of motion (18) then read

$$\mathbb{M}\ddot{\mathbf{x}} + 2\mathbb{G}\dot{\mathbf{x}} + \mathbb{K}\mathbf{x} = \mathbf{0} \quad \text{with} \quad 2\mathbb{G} \equiv \begin{pmatrix} R_1 & 0 \\ 0 & R_2 \end{pmatrix}$$

Proceeding as above, one achieves  $\{\mathbb{M}, \mathbb{G}, \mathbb{K}\} \mapsto \{\tilde{\mathbb{I}}, \tilde{\mathbb{G}}, \tilde{\mathbb{K}}_{\text{diagonal}}\}$ . But the process will, in general, destroy the initial diagonality of  $\mathbb{G}$ . And any effort to diagonalize  $\tilde{\mathbb{G}}$  will, in general, de-diagonalize  $\tilde{\mathbb{K}}_{\text{diagonal}}$ .

It is, in general, not possible to simultaneously diagonalize three or more symmetric matrices.

All, however, is not lost: one can still

- complexify;
- assume  $\mathbf{z}(t) = \mathbf{Z} e^{i\nu t}$  to obtain

$$(\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M})\mathbf{Z} = 0$$

which is a polynomial of order four in  $\nu$ ;

- use `Solve[Det[ $\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}$ ]==0,  $\nu$ ]` to evaluate  $\nu_1, \nu_2, \nu_3$  and  $\nu_4$ ;
- use `NullSpace[ $\mathbb{K} + 2i\nu_j\mathbb{G} - \nu_j^2\mathbb{M}$ ]` to discover the associated vectors  $\mathbf{Z}_j$ .

**EXAMPLE:** Define  $\mathbb{F}(\nu) \equiv \mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}$  with

$$\mathbb{K} = \begin{pmatrix} 4 & 0 \\ 0 & 5 \end{pmatrix}, \quad \mathbb{G} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}, \quad \mathbb{M} = \begin{pmatrix} 8 & 1 \\ 1 & 9 \end{pmatrix}$$

Command `Solve[Det[ $\mathbb{F}(\nu)$ ]==0]` and obtain roots

$$\nu_1 = +0.734 + 0.220i$$

$$\nu_2 = -0.734 + 0.220i$$

$$\nu_3 = +0.680 + 0.132i$$

$$\nu_4 = -0.680 + 0.132i$$

Command `NullSpace[ $\mathbb{F}(\nu_i)$ ]`//Transpose//MatrixForm and get

$$\mathbf{Z}_1 = \begin{pmatrix} +0.442 + 0.069i \\ -0.604 - 0.660i \end{pmatrix}$$

$$\mathbf{Z}_2 = \begin{pmatrix} +0.442 - 0.069i \\ -0.604 + 0.660i \end{pmatrix}$$

$$\mathbf{Z}_3 = \begin{pmatrix} -0.459 - 0.807i \\ -0.358 - 0.098i \end{pmatrix}$$

$$\mathbf{Z}_4 = \begin{pmatrix} -0.459 + 0.807i \\ -0.358 + 0.098i \end{pmatrix}$$

Command `ComplexExpand[Exp[ $i\nu_p t$ ] $\mathbf{Z}_p$ ]` and obtain

$$\mathbf{z}_1(t) = \mathbf{x}_1(t) + i\mathbf{y}_1(t)$$

$$\mathbf{z}_2(t) = \mathbf{x}_2(t) + i\mathbf{y}_2(t)$$

and their complex conjugates, with

$$\mathbf{x}_1(t) = e^{-0.220t} \begin{pmatrix} +0.442 \cos(0.734t) - 0.069 \sin(0.734t) \\ -0.604 \cos(0.734t) + 0.660 \sin(0.734t) \end{pmatrix}$$

$$\mathbf{y}_1(t) = e^{-0.220t} \begin{pmatrix} +0.069 \cos(0.734t) + 0.442 \sin(0.734t) \\ -0.660 \cos(0.734t) - 0.604 \sin(0.734t) \end{pmatrix}$$

$$\mathbf{x}_2(t) = e^{-0.132t} \begin{pmatrix} -0.459 \cos(0.680t) + 0.807 \sin(0.680t) \\ -0.358 \cos(0.680t) + 0.098 \sin(0.680t) \end{pmatrix}$$

$$\mathbf{y}_2(t) = e^{-0.132t} \begin{pmatrix} -0.807 \cos(0.680t) - 0.459 \sin(0.680t) \\ -0.098 \cos(0.680t) - 0.358 \sin(0.680t) \end{pmatrix}$$



By calculation we confirm that each of those vector-valued functions satisfies the coupled differential equation of motion

$$\mathbb{M}\dot{\mathbf{x}} + 2\mathbb{G}\dot{\mathbf{x}} + \mathbb{K}\mathbf{x} = \mathbf{0}$$

To discover the general solution

$$\mathbf{x}(t) = a_1\mathbf{x}_1(t) + b_1\mathbf{y}_1(t) + a_2\mathbf{x}_2(t) + b_2\mathbf{y}_2(t)$$

that conforms to prescribes initial data  $\mathbf{x}_0$  and  $\dot{\mathbf{x}}_0$  one has to discover the  $\{a_1, b_1, a_2, b_2\}$ -values that satisfy a quartet of simultaneous linear equations (which I will not trouble to spell out), the point being that orthonormality is no longer available as a computational tool: the “normal modes” are no longer normal!

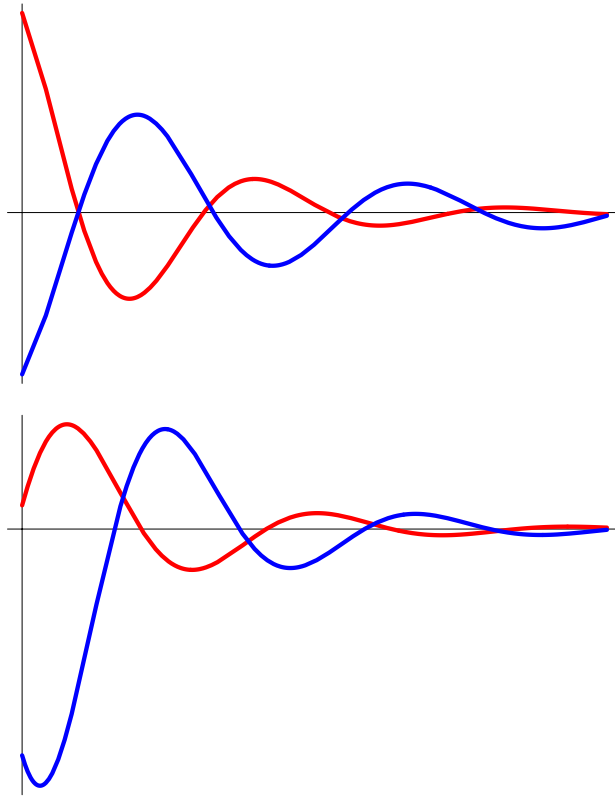


FIGURE 9A: *Shown above: graphs of the top and bottom components of  $\mathbf{x}_1(t)$ . Shown below: graphs of  $\mathbf{y}_1(t)$ , color coded in the same way. In each case one component is a bit out of phase with respect to the other.*

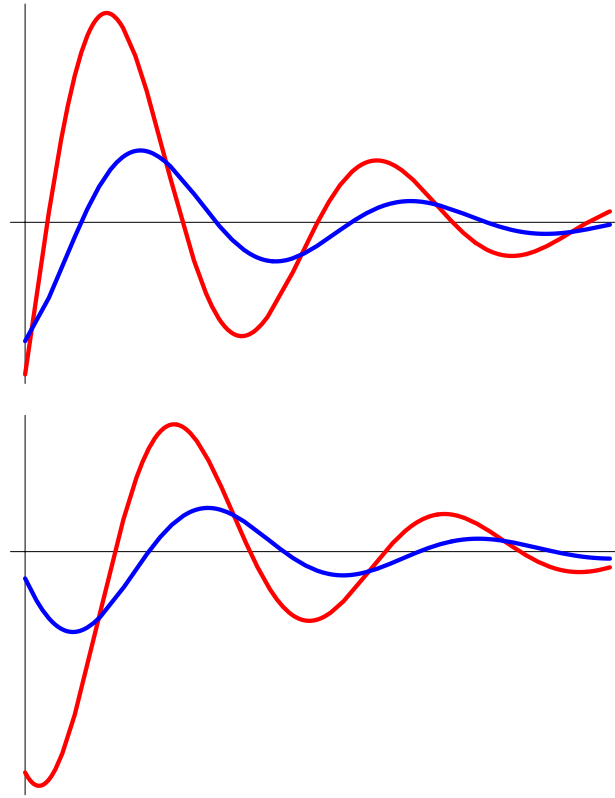


FIGURE 9B: Shown above: graphs of the *top* and *bottom* components of  $\mathbf{x}_2(t)$ . Shown below: graphs of  $\mathbf{y}_2(t)$ , color coded in the same way.

In constructing the example I have honored the electro-dynamical principle which asserts that in all cases  $L_1 L_2 - M^2 = \det \mathbb{M} > 0$ .<sup>8</sup> The computational method just described works in *all* cases (though it is my experience that in cases that violate the condition just described it leads sometimes to absurd results)—whether or not damping terms are present—and in practical situations is arguably superior to the more formal/abstract/theoretical method described earlier.

**PROBLEM 3 :** Report how the preceding example would read after the definitions of  $\mathbb{M}$  and  $\mathbb{K}$  are interchanged (an adjustment that puts the coupling in what in mechanics we would call the “spring matrix”).

<sup>8</sup> This is one consequence of the more general statement that the energy stored in a magnetic field is never negative: see ELECTRODYNAMICS (2001/2002), Chapter 1, pages 86 & 99. When looks to the theory of coupled *mechanical* oscillators the the statement  $\det \mathbb{M} > 0$  becomes simply a statement of the non-negativity of kinetic energy—than which nothing could be more obvious!

**5. Response of molecules to harmonic stimulation.** Many of the vibrating structures of greatest physical interest are too small to be examined directly. Valuable circumstantial information can be obtained in such cases by “buzzing” the structure—usually with tunable microwave, infrared or optical radiation—and measuring the enthusiasm with which the structure drinks incident energy. We look now into the physics of the matter, which is of direct relevance also to such macroscopic phenomena as the collapse (1940) of the Tacoma Narrows bridge.<sup>9</sup>

To describe the damped vibration of a linear system with  $n$  degrees of freedom we have learned to write

$$\mathbb{M}\ddot{\mathbf{x}} + 2\mathbb{G}\dot{\mathbf{x}} + \mathbb{K}\mathbf{x} = \mathbf{0}$$

where  $\mathbf{x}$  is an  $n$ -vector, where  $\{\mathbb{M}, \mathbb{G}, \mathbb{K}\}$  are real  $n \times n$  matrices, and where  $\mathbb{M}$ ,  $\mathbb{K}$  and usually also  $\mathbb{G}$  are symmetric. If the system is subject to external stimulation we have

$$\mathbb{M}\ddot{\mathbf{x}} + 2\mathbb{G}\dot{\mathbf{x}} + \mathbb{K}\mathbf{x} = \mathbf{F}(t) \quad \text{with} \quad \mathbf{F}(t) = \begin{pmatrix} F_1(t) \\ F_2(t) \\ \vdots \\ F_n(t) \end{pmatrix}$$

We will restrict our attention here to cases of the harmonic form

$$\mathbf{F}(t) = \mathbf{F}e^{i\nu t} \quad \text{with} \quad \mathbf{F} = \begin{pmatrix} F_1 \\ F_2 \\ \vdots \\ F_n \end{pmatrix}$$

and will look for solutions of the form  $\mathbf{z}(t) = \mathbf{Z}(\nu)e^{i\nu t}$ . Immediately

$$\mathbf{Z}(\nu) = [\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}]^{-1}\mathbf{F}$$

In the absence of damping ( $\mathbb{G} = \mathbb{O}$ ) the matrix  $[\mathbb{K} - \nu^2\mathbb{M}]^{-1}$  would fail to exist whenever  $\nu$  becomes equal to one or another of the (necessarily real!) zeros of  $\det[\mathbb{K} - \nu^2\mathbb{M}]$ . But as the damping term is turned on—this we have on the evidence of the  $\nu_i$ s reported on page 16 (see FIGURE 10), but is, for the most fundamental of reasons,<sup>10</sup> true quite generally—the zeros drift off the real axis onto the upper half (never the lower half) of the complex plane. With this consequence: as we tune the  $\nu$ -dial on our stimulus machine (*i.e.*, as we range on the real axis in  $\nu$ -space) we never hit a frequency at which  $[\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}]^{-1}$

<sup>9</sup> <http://www.enm.bris.ac.uk/research/nonlinear/tacoma/tacoma.html#file>.

<sup>10</sup> Those “fundamental reasons” have to do with causality: effects do not precede their causes, response does not precede stimulus. In which connection we note that energy dissipation assigns an arrow to time.

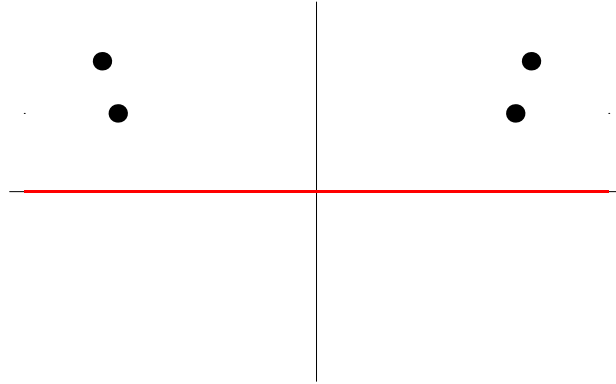


FIGURE 10: The complex zeros  $\{\nu_1, \nu_2, \nu_3, \nu_4\}$  encountered in our recent EXAMPLE are symmetrically positioned on the upper half of the complex  $\nu$ -plane, and are in this respect—and for the most fundamental of reasons—quite typical.

blows up. Resolve  $[\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}]^{-1}$  into its real and imaginary parts

$$[\mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}]^{-1} = \mathbb{S}(\nu) + i\mathbb{T}(\nu)$$

where the symmetry of  $\mathbb{K}$ ,  $\mathbb{G}$  and  $\mathbb{M}$  is readily seen to imply that of the real matrices  $\mathbb{S}$  and  $\mathbb{T}$ . We conclude that harmonic stimulation  $\mathbf{F} \cos \nu t$  of the system produces the harmonic response

$$\mathbf{x}_\nu(t) = [\mathbb{S}(\nu) \cos \nu t - \mathbb{T}(\nu) \sin \nu t] \mathbf{F} \quad (20)$$

The energy of the system is given by

$$\begin{aligned} E(t) &= \frac{1}{2} \dot{\mathbf{x}}^\top \mathbb{M} \dot{\mathbf{x}} + \frac{1}{2} \mathbf{x}^\top \mathbb{K} \mathbf{x} \\ &= \frac{1}{2} \nu^2 \mathbf{F}^\top [\sin^2 \nu t \cdot \mathbb{S} \mathbb{M} \mathbb{S} + \sin \nu t \cos \nu t \cdot (\mathbb{S} \mathbb{M} \mathbb{T} + \mathbb{T} \mathbb{M} \mathbb{S}) + \cos^2 \nu t \cdot \mathbb{T} \mathbb{M} \mathbb{T}] \mathbf{F} \\ &\quad + \frac{1}{2} \mathbf{F}^\top [\cos^2 \nu t \cdot \mathbb{S} \mathbb{K} \mathbb{S} - \sin \nu t \cos \nu t \cdot (\mathbb{S} \mathbb{K} \mathbb{T} + \mathbb{T} \mathbb{K} \mathbb{S}) + \sin^2 \nu t \cdot \mathbb{T} \mathbb{K} \mathbb{T}] \mathbf{F} \end{aligned}$$

which ripples with frequency  $2\nu$ . Averaging over a period we get

$$\begin{aligned} \langle E \rangle &= \frac{1}{2} \nu^2 \mathbf{F}^\top \left[ \frac{1}{2} \mathbb{S} \mathbb{M} \mathbb{S} + \frac{1}{2} \mathbb{T} \mathbb{M} \mathbb{T} \right] \mathbf{F} \\ &\quad + \frac{1}{2} \mathbf{F}^\top \left[ \frac{1}{2} \mathbb{S} \mathbb{K} \mathbb{S} + \frac{1}{2} \mathbb{T} \mathbb{K} \mathbb{T} \right] \mathbf{F} \end{aligned} \quad (21)$$

which presents  $\langle E \rangle$  as a complicated function of  $\nu$ .

**EXAMPLE:** Consider the 2-particle system with

$$\mathbb{M} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathbb{G} = \frac{1}{80} \begin{pmatrix} 9 & 1 \\ 1 & 9 \end{pmatrix}, \quad \mathbb{K} = \begin{pmatrix} 2 & -1 \\ -1 & 2 \end{pmatrix}$$

Construct  $\mathbb{R}[\nu] = \mathbb{K} + 2i\nu\mathbb{G} - \nu^2\mathbb{M}$ , command

$$\text{Solve}[\text{Det}[\mathbb{R}[\nu]] = 0, \nu] // \mathbb{N}$$

and get

$$\begin{aligned}\nu_1 &= \pm 0.992 + 0.125i \\ \nu_2 &= \pm 1.729 + 0.100i\end{aligned}$$

[REMARK: I have concocted the example so as to make the real parts of these complex roots fairly widely spaced, and the imaginary parts relatively small.] Now enter serially the commands

```
Inverse[R[ν]]
ComplexExpand[%]
Re[%]
ComplexExpand[%]
Simplify[%]
S=%
T=-i(Inverse[R[ν]]-S)//Simplify
```

One has only to execute these commands to discover why I have not committed the results to paper! Let us now, in the interest of simplicity, assume that the stimulus acts only upon particle #1:

$$F = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Command

```
 $\frac{1}{4}\nu^2$ Transpose[F].(S.M.S+T.M.T).F
 $+\frac{1}{4}$ Transpose[F].(S.K.S+T.K.T).F//Simplify
```

and obtain

$$\langle E \rangle_\nu = \frac{4000 + 1641\nu^2 - 3909\nu^4 + 1600\nu^6}{8(3600 - 9359\nu^2 + 8619\nu^4 - 3159\nu^6 + 400\nu^8)} \quad (22)$$

which is plotted in FIGURE 11. It should be noted that the peaks occur at frequencies near the real parts of  $\nu_1$  and  $\nu_2$ , and are broad or narrow according as the imaginary part of the  $\nu_i$  in question is large or small. It would not be difficult, working from the unreported details, to speak quantitatively about the fact that the constituent “atoms,” though they oscillate with the same frequency as the stimulus, move out of phase not only with the stimulus but also with each other.

It will also be appreciated that the information conveyed by such a spectrum is far less from definitive, in the sense that it is pretty obviously insufficient to permit one to reconstruct the matrices  $\mathbb{M}$ ,  $\mathbb{G}$  and  $\mathbb{K}$  and on that basis to attempt to reconstruct the design of the molecule.

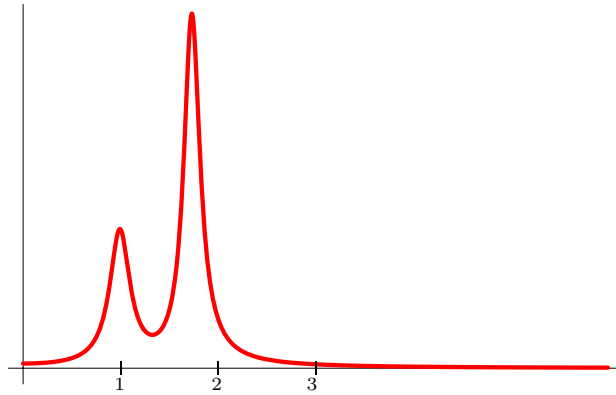


FIGURE 11: *Graph of the molecular energy spectrum (22) that was latent in the most recent EXAMPLE. Specifically: one atom receives unit stimulus of frequency  $\nu$ ; the graph shows the  $\nu$ -dependence of the steady mean energy  $\langle E \rangle_\nu$  of the thus-stimulated molecule.*

To summarize: The physical objects of interest move as described by the coupled linear equations of motion

$$[\mathbb{M}\partial^2 + 2\mathbb{G}\partial + \mathbb{K}]\mathbf{x}(t) = \mathbf{F}(t) \quad (23.1)$$

where the matrices are symmetric, and  $\partial \equiv \frac{d}{dt}$ . It is always possible to write

$$\begin{aligned} \mathbb{W}[\mathbb{M}\partial^2 + 2\mathbb{G}\partial + \mathbb{K}]\mathbb{W}^{-1} \cdot \mathbb{W}\mathbf{x}(t) &= \mathbb{W}\mathbf{F}(t) \\ \Downarrow \\ [\tilde{\mathbb{M}}\partial^2 + 2\tilde{\mathbb{G}}\partial + \tilde{\mathbb{K}}]\tilde{\mathbf{x}}(t) &= \tilde{\mathbf{F}}(t) \end{aligned} \quad (23.2)$$

If one of the matrices ( $\tilde{\mathbb{G}}$ , let us say) is absent (because we have “turned of the damping”) then one can always choose  $\mathbb{W}$  in such a way that the remaining matrices are **diagonal**: the equations of motion will then be uncoupled, each presenting a copy of the equation

$$[\tilde{m}_i\partial^2 + \tilde{k}_i]\tilde{x}_i(t) = \tilde{F}_i(t) \quad : \quad i = 1, 2, \dots, n \quad (24)$$

familiar from the theory of single (driven but undamped) oscillators (see again §5 in Chapter 3). It becomes natural in such cases to write  $\tilde{\mathbf{x}}(t) = \sum_i \tilde{x}_i(t)\mathbf{e}_i$  and to speak of independently stimulated non-interactive “normal modes.” But if all three matrices are present then we confront the full force of the fact that it is not in general possible to diagonalize three matrices simultaneously: it is, for that reason, generally not possible to decouple the equations of motion, and the “non-interactive mode” concept loses not only its utility but also its very

meaning. One might elect, in place of (24), to write

$$[\tilde{m}_i \partial^2 + 2\tilde{g}_i \partial + \tilde{k}_i] \tilde{x}_i(t) = \tilde{F}_i(t) \quad : \quad i = 1, 2, \dots, n$$

but to do so—to introduce “modal damping” parameters—is to assume that the system-matrices  $\{\mathbb{M}, \mathbb{G}, \mathbb{K}\}$  can—exceptionally—be simultaneously diagonalized ... and this is an assumption that would in most instances have no physical justification.<sup>11</sup> The method described just above proceeds, however, without reference either to matrix diagonalization or to the modal concept. And it works just as efficiently when the  $\mathbb{G}$  term is present as when it is absent. To illustrate these points we look to a final

**EXAMPLE: The 3-atom crystal, revisited:** We look first, by way of orientation, to the

**UNDAMPED CRYSTAL IN NATURAL COORDINATES** We set both  $m$  and  $k$  equal to unity and have

$$\mathbb{M} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbb{G} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathbb{K} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{pmatrix}$$

We construct  $\mathbb{R}(\nu)$  and find that  $\det \mathbb{R}(\nu)$  has roots

$$\left. \begin{array}{l} \nu_1 = \pm 0.765 \\ \nu_2 = \pm 1.414 \\ \nu_3 = \pm 1.847 \end{array} \right\} \quad (25.1)$$

Running this data through our algorithm we obtain

$$\langle E \rangle_\nu = \frac{14 - 16\nu^2 - 9\nu^4 + 26\nu^6 - 13\nu^8 + 2\nu^{10}}{(2 - \nu^2)^2(2 - 4\nu^2 + \nu^4)^2} \quad (25.2)$$

when the stimulus vector has been taken to be

$$\mathbf{F} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

This spectrum is displayed as FIGURE 12A. From (14) we are led to the observation that

$$\mathbb{W} \mathbb{K} \mathbb{W}^{-1} = \begin{pmatrix} 2 - \sqrt{2} & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 + \sqrt{2} \end{pmatrix} \equiv \begin{pmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{pmatrix}$$

<sup>11</sup> This train of thought is developed in the final pages of SECOND COURSE IN CLASSICAL MECHANICS (2004), Chapter 3, §10.

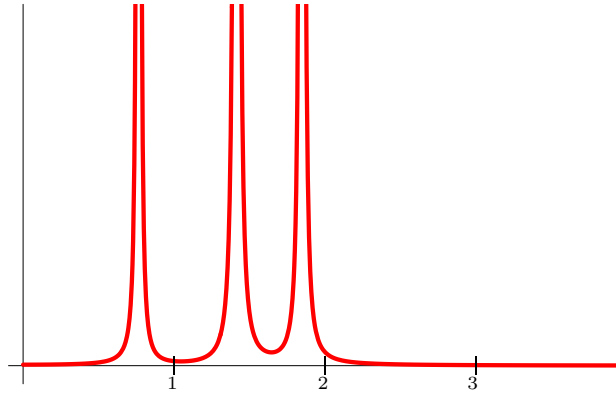


FIGURE 12A: Graph of the undamped spectrum (25.2).  
The singularities stand at the frequencies (25.1).

where

$$\mathbb{W} = \frac{1}{2} \begin{pmatrix} 1 & -\sqrt{2} & 1 \\ +\sqrt{2} & 0 & -\sqrt{2} \\ 1 & +\sqrt{2} & 1 \end{pmatrix}$$

is a proper rotation matrix:  $\mathbb{W}^{-1} = \mathbb{W}^T$  and  $\det \mathbb{W} = 1$ . In the present instance it is the matrix that describes how natural coordinates must be combined to produce modal coordinates.

**WEAK MODAL DAMPING IN NATURAL COORDINATES** All matrices of the form

$$\mathbb{G} = \mathbb{W}^{-1} \begin{pmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & g_3 \end{pmatrix} \mathbb{W}$$

can—by contrivance—be diagonalized simultaneously with  $\mathbb{M}$  and  $\mathbb{K}$ , and therefore achieve what I have called “modal damping.” Setting  $g_1 = \frac{1}{8}$ ,  $g_2 = \frac{1}{12}$  and  $g_3 = \frac{1}{10}$  we find

$$\left. \begin{aligned} \nu_1 &= \pm 0.758 + 0.100i \\ \nu_2 &= \pm 1.412 + 0.083i \\ \nu_3 &= \pm 1.844 + 0.125i \end{aligned} \right\} \quad (25.3)$$

and are led to the spectrum shown in FIGURE 12B, the analytical description of which is much too complicated to write out. Notice that

$$\begin{aligned} \text{imaginary part of } \nu_1 &= g_3 i \\ \text{imaginary part of } \nu_2 &= g_2 i \\ \text{imaginary part of } \nu_3 &= g_1 i \end{aligned}$$



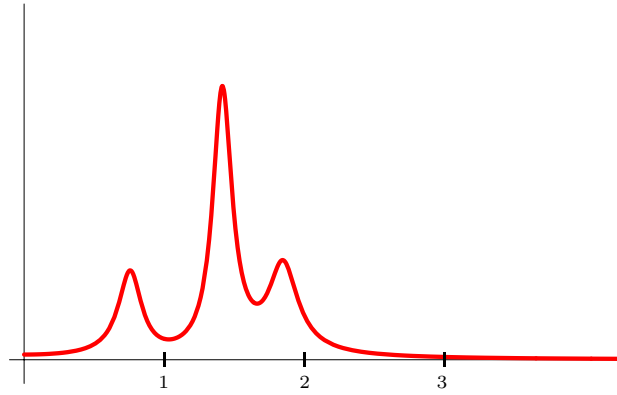


FIGURE 12B: *Graph of the modally damped spectrum developed in the text. The peaks stand at the slightly depressed frequencies (25.3).*

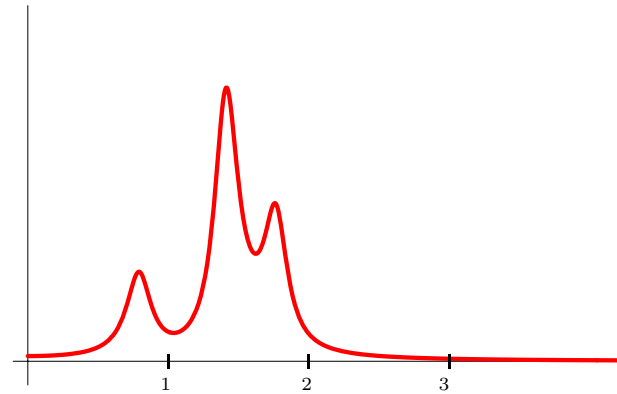


FIGURE 12C: *Graph of the non-modally damped energy spectrum developed in the text. Imaginary parts of the  $\nu_i$  can no longer be described in a simple way.*

**NON-MODAL DAMPING IN NATURAL COORDINATES** Matrices of the form

$$\mathbb{G} = \mathbb{W}^{-1} \begin{pmatrix} g_1 & h_3 & h_2 \\ h_3 & g_2 & h_1 \\ h_2 & h_1 & g_3 \end{pmatrix} \mathbb{W}$$

—by contrivance—cannot be diagonalized simultaneously with  $\mathbb{M}$  and  $\mathbb{K}$ , and therefore achieve what I call “non-modal damping.” Retaining the former values of  $g_1 = \frac{1}{8}$ ,  $g_2 = \frac{1}{12}$  and  $g_3 = \frac{1}{10}$ , we set

$h_1 = h_3 = \frac{1}{7}$ ,  $h_2 = \frac{1}{8}$  and find

$$\left. \begin{aligned} \nu_1 &= \pm 0.792 + 0.105i \\ \nu_2 &= \pm 1.408 + 0.103i \\ \nu_3 &= \pm 1.769 + 0.099i \end{aligned} \right\} \quad (25.4)$$

The resulting spectrum is shown in FIGURE 12C.

NON-MODAL DAMPING IN “MODAL COORDINATES” Just above we studied an instance of (23.1)

$$[\mathbb{M}\partial^2 + 2\mathbb{G}\partial + \mathbb{K}]\mathbf{x}(t) = \mathbf{F}(t)$$

in which

$$\begin{aligned} \mathbb{M} &= \begin{pmatrix} m & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & m \end{pmatrix} \\ \mathbb{K} &= \mathbb{W}^{-1} \begin{pmatrix} k_1 & 0 & 0 \\ 0 & k_2 & 0 \\ 0 & 0 & k_3 \end{pmatrix} \mathbb{W} \\ \mathbb{G} &= \mathbb{W}^{-1} \begin{pmatrix} g_1 & h_3 & h_2 \\ h_2 & g_2 & h_1 \\ h_2 & h_1 & g_3 \end{pmatrix} \mathbb{W} \end{aligned}$$

Passing—as indicated at (23.2)—to coordinates that are *normal with respect to the undamped crystal* we obtain

$$\left[ m \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \partial^2 + 2 \begin{pmatrix} g_1 & 0 & 0 \\ 0 & g_2 & 0 \\ 0 & 0 & g_3 \end{pmatrix} \partial + 2\mathbb{H} \right] \tilde{\mathbf{x}} = \tilde{\mathbf{F}}$$

with 
$$\mathbb{H} = \begin{pmatrix} 0 & h_3 & h_2 \\ h_3 & 0 & h_1 \\ h_2 & h_1 & 0 \end{pmatrix}$$

The point I would emphasize is that the  $\mathbb{H}$ -matrix serves to couple those equations. One could diagonalize  $\mathbb{H}$ , but that effort would serve to de-diagonalize the matrices that have  $g_i$ s and  $h_i$ s on their diagonals. Such systems of equations **cannot be decoupled: one cannot, in such a context, speak meaningfully of “normal modes,”** though it does remain meaningful/useful to speak of “resonances.”

Notable features of the preceding discussion are that it proceeds in *natural* coordinates, makes no use of the modal concept (so pertains to situations in which that concept is not available), yet does permit one to construct detailed descriptions of particle motions at resonance.