2

The Application of Fourier Analysis to the Uncoupling of Lattices

We shall apply here Fourier analysis and other vector space and symmetry concepts introduced in Chapter 1 to the study of certain coupled systems which have simple mechanical realizations as one-dimensional crystalline lattices. In Section 2.1 we define the constituents of such systems and their corresponding solution so that we may pose the problem of uncoupling lattices of such elements in Section 2.2. A rather detailed study of the basic solutions is made in Section 2.3 for a simple lattice and in Section 2.4 for more complicated ones which can be described by second- or farther-neighbor interaction in crystals or as molecular or diatomic chains. We go to a more general setting in studying energy and other phase-space concepts which belong properly to analytical mechanics. Sections 2.5 and 2.6 can be read after the first two sections if the reader so prefers. Although examples drawn from Sections 2.3 and 2.4 are used to illustrate examples of the theory, the reader should be able to follow the general presentation easily.

2.1. Mechanical and Electric Analogies

We shall study here the elements which constitute coupled systems of a rather general type, exemplified by mechanical and electric networks. The former are constituted by masses, restitution forces (springs), driving forces, and viscous damping; the latter will consist of a standard *RLC* circuit plus electromotive forces. The differential equations which describe the time

evolution of these two systems point out analogies between their constituent elements.

2.1.1. Masses, Springs, and Damping

The equation of motion of the simple mechanical system in Fig. 2.1 can be found from the following considerations. The external (time-dependent) force $F(t)$ will produce the following: (a) an acceleration $\ddot{f}(t)$ of the *mass* M, where $\ddot{f}(t) \coloneqq d^2f(t)/dt^2$; (b) a stretching $f(t)$ of the spring with *Hooke's constant* k; and (c) if the system is immersed in a "perfect" viscous fluid, when moving it will experience a *velocity-dependent* drag $c\dot{f}(t)$, where c is the *damping constant* of the medium ($c \geqslant 0$). Setting action equal to reaction, we can write the mechanical equation of motion as

$$M\ddot{f}(t) + c\dot{f}(t) + kf(t) = F(t). \tag{2.1}$$

This is an inhomogeneous second-order *linear* differential equation with constant coefficients, whose solution is quite simple. Of course, actual mechanical systems do not exhibit a constant k for all deformations $f(t)$ since the spring must be finite; the viscous damping does not, for all velocities, have the simple $c\dot{f}(t)$ behavior, and frictional forces—constant and opposite to the direction of motion—can certainly be present. Nevertheless, Eq. (2.1), besides being a good model for actual mechanical situations, lends itself admirably to the modeling of other apparently unrelated systems. It also has the advantage of mathematical simplicity.

2.1.2. Inductances, Capacitors, and Resistance

The electric *RLC* circuit of Fig. 2.2 consists of a series connection of a resistance R, an inductance L, a capacitor C, and an applied electromotive

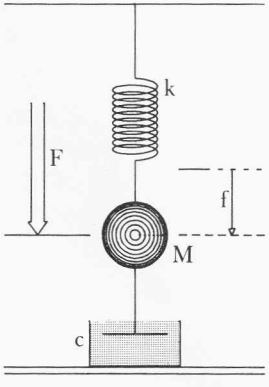


Fig. 2.1. A driven, damped oscillator. An inertial mass M (with elongation f) is subject to a restitution spring with Hooke's constant k, a viscous damping device of constant c, and a driving force F.

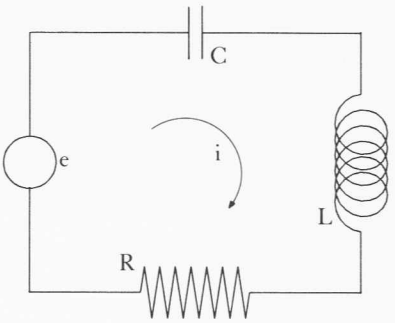


Fig. 2.2. A simple *RLC* circuit. The current i flows through an inertial inductance L, a "spring" capacitor C, and a damping resistance R and is driven by an electromotive source e.

force $e(t)$. If the circulating change is $q(t)$ and the current is $i(t) = dq(t)/dt =: \dot{q}(t)$, Kirchhoff's second law leads to the equations

$$L\ddot{q}(t) + R\dot{q}(t) + C^{-1}q(t) = \dot{e}(t), \tag{2.2a}$$

$$C\ddot{q}(t) + RCL^{-1}\dot{q}(t) + L^{-1}q(t) = CL^{-1}\dot{e}(t), \tag{2.2b}$$

where we have multiplied the first by CL^{-1} to obtain the second. Equations (2.1) and (2.2) are of the same form and lead to analogies between mechanical and electric elements. The spring elongation $f(t)$ and velocity are identified with the circulating charge $q(t)$ and current, while mass, restitution, and viscous drag are identified with either L, C^{-1}, and R or C, L^{-1}, and RC/L. The first analogy is perhaps the more intuitive one, as kinetic and potential mechanical energy are made to correspond with magnetic and electrostatic forms of energy. The second set leads to a correspondence between a class of electric networks and mechanical lattices, as has been presented in the classic book by Brillouin (1946). We shall henceforth refer only to mechanical lattices in illustrating the concepts of complex vector spaces and the Fourier transform. Standing or traveling waves, for instance, are easier to visualize in a mechanical device than in the dials of an array of meters in a circuit. The methods and results can be applied without undue extra effort to the electric case.

2.1.3. Longitudinal and Transverse Mechanical Vibrations

Since many of the models mentioned above make use of longitudinal as well as transverse vibrations of lattices, it is important to point out the difference between the two. Longitudinal vibrations in lattices will be described in the next section and follow the elementary system in Fig. 2.1 and the ensuing solution. For transverse vibrations there is more than Eq. (2.1) to the problem, so we propose the following:

Exercise 2.1. Consider transverse vibrations of the mass M under the action of two springs each of constant $\frac{1}{2}k$ as depicted in Fig. 2.3. Let the *unstretched*

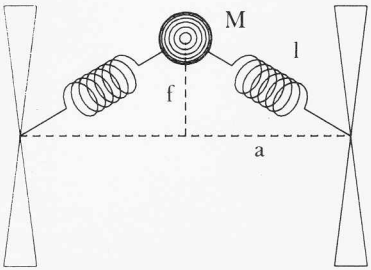


Fig. 2.3. A mass allowed to perform transverse vibrations under the influence of two springs.

length of the springs be a_0. Show that this leads to the *nonlinear* differential equation

$$M\ddot{f}(t) + c\dot{f}(t) + 2kf(t)[1 - a_0(a^2 + f(t)^2)^{-1/2}] = F(t). \tag{2.3}$$

Exercise 2.2. Show that in Eq. (2.3) we can make two approximations: (a) Assume that the stretched length l (Fig. 2.3) is much longer than the natural length a_0. (b) Assume that the oscillations are small, so that $[a^2 + f(t)^2]^{1/2} \simeq a$. In each case one obtains a linear differential equation. They are not identical though.

2.1.4. Solutions to the Equations of Motion with Initial Conditions

In the absence of external forces, Eqs. (2.1)–(2.2) admit solutions of the general type

$$f(t) = a \exp(i\omega t), \tag{2.4}$$

where a is a constant and ω can be found by substituting (2.4) into (2.1):

$$-M\omega^2 + ic\omega + k = 0, \tag{2.5}$$

i.e., we have *two* possible values of ω, given by

$$\omega^{\pm} = \frac{ic}{2M} \pm \left[\frac{k}{M} - \left(\frac{c}{2M}\right)^2\right]^{1/2} =: i\Gamma \pm \omega^e \tag{2.6a}$$

$$\Gamma := \frac{c}{2M}, \qquad \omega^e := (k/M - \Gamma^2)^{1/2}. \tag{2.6b}$$

Hence, the general solution of the homogeneous equation (2.1) can be written as

$$f(t) = \exp(-\Gamma t)[a \exp(i\omega^e t) + b \exp(-i\omega^e t)] \tag{2.7}$$

for a and b arbitrary constants. The latter can be determined from two known data about $f(t)$ and/or its derivatives. Typically, if we know the value and derivative of $f(t)$ at some initial time t_0, $f_0 := f(t_0)$ and $\dot{f}_0 := df(\tau)/d\tau|_{\tau=t_0}$, Eq. (2.7) for $t = t_0$ allows us to solve for a and b as

$$a = -(2\omega^e)^{-1} \exp(-i\omega^+ t_0)(\omega^- f_0 + i\dot{f}_0), \tag{2.8a}$$

$$b = (2\omega^e)^{-1} \exp(-i\omega^- t_0)(\omega^+ f_0 + i\dot{f}_0). \tag{2.8b}$$

Replacement into (2.7) yields

$$f(t) = (2\omega^e)^{-1}\{-\omega^- \exp[i\omega^+(t - t_0)] + \omega^+ \exp[i\omega^-(t - t_0)]\}f_0 + i(2\omega^e)^{-1}\{-\exp[i\omega^+(t - t_0)] + \exp[i\omega^-(t - t_0)]\}\dot{f}_0. \quad (2.9)$$

Reducing further, we can bring the solution to the form

$$f(t) = [\dot{G}(t - t_0) + 2\Gamma G(t - t_0)]f_0 + G(t - t_0)\dot{f}_0, \quad (2.10)$$

where for ω^e real we have defined

$$G(\tau) \coloneqq (\omega^e)^{-1} \exp(-\Gamma\tau) \sin \omega^e\tau \qquad \text{(oscillatory)} \quad (2.11a)$$

and its time derivative

$$\dot{G}(\tau) = -\Gamma G(\tau) + \exp(-\Gamma\tau) \cos \omega^e\tau. \quad (2.11b)$$

As $G(\tau)$ depends on c, M, and k, it will serve us to denote it occasionally by $G^{c,M,k}(\tau)$. Clearly, $G(\tau)$ and $\dot{G}(\tau)$ are themselves solutions of the original differential equation (2.1) with no external forces present.

2.1.5. Critical and Overdamped Cases

The structure of the general solution given by (2.10) is quite transparent. If the damping is small with respect to the restitution spring (more precisely, for $c^2 < 4Mk$), ω^e is a real number, playing the role of the *effective angular frequency,* and the nature of (2.10)–(2.11) is that of a *damped oscillation.* See Fig. 2.4.

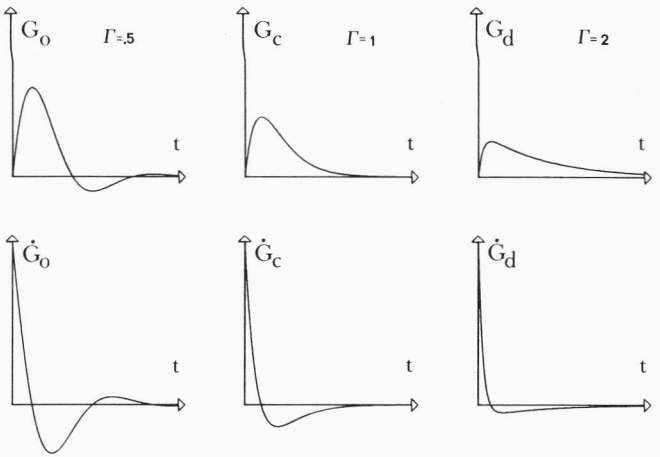


Fig. 2.4. The functions $G(t)$ and $\dot{G}(t)$ for the oscillatory (o), critical (c), and overdamped (d) cases. Time units of $(M/k)^{1/2}$ are used, the t-axis representing the interval from 0 to 10. The vertical axes of the figures have height 1. Damping constants in each case are chosen as $\Gamma = 0.5$, 1, and 2.

If the damping constant increases, the effective angular frequency will decrease and reach zero when $c^2 = 4Mk$. In this case (*critical damping*), the solution (2.10) retains its form, but, as $(\omega^e)^{-1} \sin \omega^e \tau \to \tau$, the function $G(\tau)$ is now given by

$$G(\tau) = \tau \exp(-\Gamma\tau) \qquad \text{(critical)} \tag{2.12}$$

and $\dot{G}(\tau)$ accordingly. See Fig. 2.4 (curves G_c and $\dot{G}_c$). Finally, for $c^2 > k4M$ we have the *overdamped* situation when the solution is (2.9) with

$$G(\tau) = (w^e)^{-1} \exp(-\Gamma\tau) \sinh w^e \tau \qquad \text{(overdamped)}, \tag{2.13a}$$

$$iw^e := \omega^e = i(\Gamma^2 - k/M)^{1/2}. \tag{2.13b}$$

See Fig. 2.4 (curves G_d and $\dot{G}_d$). As $|w^e| < \Gamma$ for all $k > 0$, the solutions fall to zero exponentially, while no proper oscillation takes place.

2.1.6. Some Further Remarks and Exercises

The solution of (2.1) in the presence of an external driving force is a sum of the general solution of the homogeneous part of the differential equation seen above plus a particular solution of (2.1). The general construction of the solution to the inhomogeneous equation (2.1) will be made using the techniques of Fourier and Laplace transforms in Sections 7.4 and 8.1. The methods in this part are not significantly dependent on the presence of external forces so we shall henceforth work only with the *homogeneous* equation (2.1), which represents a damped-oscillator equation of motion with initial conditions.

Among the systems whose models are lattices constituted by such elements we have the oscillations of natural crystals and electric circuits in a larger network; in fact, it is the very model of an elastic ether as conceived in his time by Newton and followed for several centuries which led to Maxwell's equations for the electromagnetic field.

Exercise 2.3. Refer to Exercise 2.2. Denote by ω_a the angular frequency of approximation (a) [simply $\omega_a = \omega^e$ in (2.6b)] and ω_b that of approximation (b) [as above but replacing the spring constant k by $k_b := k(1 - a_0/a)$]. Show that in approximation (b) the longitudinal and transverse oscillation frequencies are not equal but that

$$\omega_a/\omega_b = [(1 - a_0/a) - c^2/2Mk]^{1/2}.$$

Hence, when drawing transverse oscillations and using the mathematical language of longitudinal ones, we are referring to approximation (b).

Exercise 2.4. Follow the developments in this section for the undamped case $c = 0$. Find $G^{0mk}(\tau)$ and the form (2.10).

Exercise 2.5. Consider the case when no spring is present ($k = 0$). In that case $\omega^+ = ic/M$, $\omega^- = 0$, and we are always in the overdamped case with $w = \Gamma = c/2M$. Show that the general solution is (2.10) with

$$G^{cM0}(\tau) = (2\Gamma)^{-1}[1 - \exp(-2\Gamma\tau)], \qquad \dot{G}^{cM0}(\tau) = \exp(-2\Gamma\tau), \tag{2.14}$$

i.e.,

$$f(t) = f_0 + (2\Gamma)^{-1}\{1 - \exp[-2\Gamma(t - t_0)]\}\dot{f}_0. \tag{2.15}$$

Exercise 2.6. Examine the situation where no damping or spring is present. You can solve the problem either directly or by considering (2.14)–(2.15) as $\Gamma \to 0$. Show that the solution can still be written in the form (2.10) with

$$G^{0M0}(\tau) = \tau, \qquad \dot{G}^{0M0}(\tau) = 1, \tag{2.16}$$

so that

$$f(t) = f_0 + (t - t_0)\dot{f}_0, \tag{2.17}$$

i.e., simple inertial motion.

Exercise 2.7. Follow the development in this section when $M = 0$, so the second-derivative term in (2.1) vanishes. The oscillating body looses its inertia, and only restitution and viscous forces act. Show that the solution, in terms of the initial displacement at t_0, is

$$f(t) = f_0 \exp[-k(t - t_0)/c]. \tag{2.18}$$

Exercise 2.8. Verify that the solution (2.18) can also be obtained from (2.10) and (2.13) by letting $M \to 0$. Note that although Γ, $w^e \to \infty$, their difference $\omega^- \to -ik/c$. Similarly, although $G^{c0k}(\tau)$, $\dot{G}^{c0k}(\tau) \to 0$, the term $2\Gamma G^{c0k}(\tau)$ in (2.10) survives and gives rise to the form (2.18).

2.2. The Equation of Motion of Coupled Systems and Solution

A system of N interacting elements will be called a *lattice*. In its simplest one-dimensional mechanical realization, it is a set of N masses interacting through spring-like forces. This interaction can be nonzero for a pair of "nearest neighbors" only or can include "farther" masses as well. Each particle by itself, in addition, can be subject to viscous and external forces. When the nearest-neighbor interaction is the most significant, it is convenient to arrange the mass points on a line where the first-neighbor relation is manifest. Further, as we assume every mass to have two first neighbors, the points in the lattice will close in a circle. See Fig. 2.5. This model is also useful to describe second- and farther-neighbor harmonic oscillator interactions.

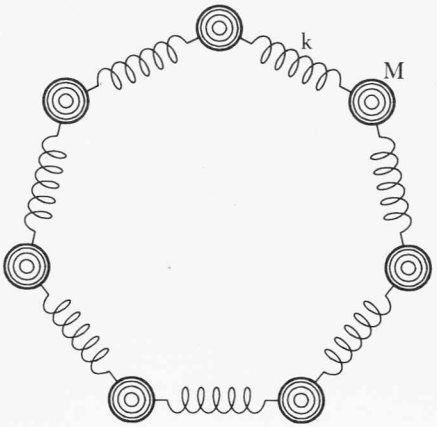


Fig. 2.5. Mechanical lattice composed of masses M and springs k with first-neighbor interaction only.

2.2.1. Inertial, Interaction, and Dissipation Operators

Let f_n denote the displacement of the nth mass M_n relative to its equilibrium position. Unless the lattice is at rest, it will be a function of time: $f_n = f_n(t)$. For the purpose of the model we assume here the vibrations in the lattice to be longitudinal only. Let k_{nm} be the spring constant between particles n and m; then the force acting on the nth mass is $k_{nm}(f_n - f_m)$ in the direction from mass n to mass m. (See Fig. 2.6 for first-neighbor interactions.) If we add the possibility of having a spring k_{nn} between M_n and its equilibrium position, the total force on M_n due to the interaction among the lattice elements is thus

$$\begin{aligned}\sum_{m\neq n} k_{nm}(f_n - f_m) + k_{nn}f_n \\ &= -\sum_{m\neq n} k_{nm}f_m + f_n \sum_m k_{nm} \\ &= \sum_m \left[-k_{nm} + \delta_{n,m}\left(k_{nn} + \sum_r k_{nr}\right)\right] f_m =: \sum_m \kappa_{nm} f_m. \end{aligned} \tag{2.19}$$

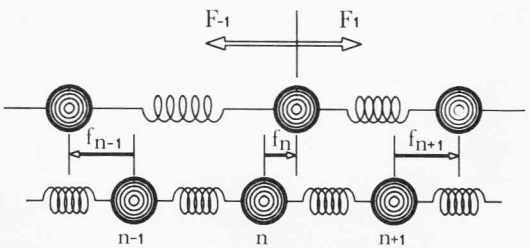


Fig. 2.6. Longitudinal vibrations in a linear lattice. Positions, elongations, and acting forces of the deformed lattice (above) are shown vis-à-vis the undeformed situation (below).

We assume, as in Section 1.6, that the lattice is closed (Fig. 2.5) so that its elements are numbered modulo N. Hence f_k and f_{k+mN} (m integer) describe the same displacement. If, finally, the damping constant for the nth element is c_n and $F_n = F_n(t)$ is the external force, the equation of motion for the nth particle in the lattice is

$$M_n\ddot{f}_n + c_n\dot{f}_n + \sum_m \kappa_{nm} f_m = F_n, \qquad n = 1, 2, \ldots, N. \tag{2.20}$$

2.2.2. Equation of Motion in Operator Form and the Problem of Uncoupling

The N equations (2.20) can be combined into a single vector equation if we identify f_n with the nth coordinate of a vector $\mathbf{f}$ in some (for definiteness, the orthonormal $\boldsymbol{\varepsilon}$-) basis, as was done in Section 1.6, and the same for F_n. The coefficients κ_{nm} can be arranged into a matrix $\mathbf{K} = \|\kappa_{nm}\|$ in the same basis, representing an *interaction* operator $\mathbb{K}$. Similarly, M_n and c_n can be taken to be the elements of diagonal matrices $\mathbf{M} = \|M_n\delta_{nm}\|$ and $\mathbf{C} = \|c_n\delta_{nm}\|$ representing the *inertial* and *dissipation* operators $\mathbb{M}$ and $\mathbb{C}$. Equations (2.20) can then be written as

$$\mathbb{M}\ddot{\mathbf{f}} + \mathbb{C}\dot{\mathbf{f}} + \mathbb{K}\mathbf{f} = \mathbf{F}. \tag{2.21}$$

This form is *basis independent* and in a sense hides the fact that it was obtained from N *coupled* differential equations (2.20): The solution f_n for the nth particle depends through the interaction term on the solution for the other f_m's, which in turn depend on other ones until all N coordinates are involved. This is what Fig. 2.5 tells us. If the interaction operator $\mathbb{K}$ had a basis where it was represented by a diagonal matrix, and in that basis $\mathbb{M}$ and $\mathbb{C}$ also had diagonal representatives, Eq. (2.21) would yield a set of N *uncoupled* equations which could be solved independently, thereby reducing the problem to that of last section. This may not be possible in general, though it will be for the case when $\mathbb{M}$ and $\mathbb{C}$ are multiples of the identity operator—$\mathbb{M} = M\mathbb{1}$, $\mathbb{C} = c\mathbb{1}$—for then they are represented by diagonal matrices in any basis, meaning in particular that all masses and damping constants are equal. In that case we need only direct our efforts toward finding the eigenbasis of $\mathbb{K}$. In that basis, $\mathbb{K}$ will be represented by a diagonal matrix, and the system of equations will uncouple. Such an eigenbasis does exist, as shown through the following.

Exercise 2.9. The action of the mth mass on the nth through the spring with constant k_{nm} should equal the action of the nth on the mth; hence $k_{nm} = k_{mn}$. Show that this implies that $\mathbb{K}$ is a self-adjoint operator. We proved in Section 1.7 that all such operators have a complete eigenbasis. Notice that if $k_{nm} = 0$ and $k_{mn} \neq 0$ this means that mass m is acted upon by but does not influence mass n. This is a "servomechanism" whereby the position of mass n is monitored as an external force on mass m.

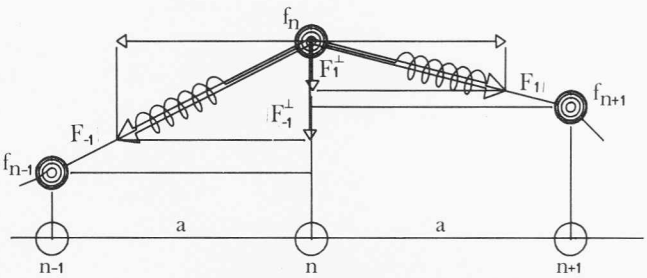


Fig. 2.7. Transverse vibrations in a linear lattice. The longitudinal components of the spring tension forces acting on each mass are equal and opposite. Net force on the mass is the sum of the transverse components.

Exercise 2.10. Consider plane transverse vibrations of the lattice. Show that, within the approximations developed in Exercises 2.1 and 2.2 [(a) and/or (b)], they lead to equations of motion similar to (2.20). Refer to Fig. 2.7.

2.2.3. The Interaction Eigenbasis

Let $\bar{\mathbf{K}} := \|\kappa_n \delta_{nm}\|$ be the diagonal matrix representing $\mathbb{K}$ in its own eigenbasis $\{\boldsymbol{\psi}_n\}_{n=1}^N$, $\{\kappa_n\}_{n=1}^N$ being the eigenvalues. Letting $\bar{f}_n$ be the coordinates of $\mathbf{f}$ in this basis, Eq. (2.21) becomes

$$M\ddot{\bar{f}}_n + c\dot{\bar{f}}_n + \kappa_n \bar{f}_n = \bar{F}_n, \qquad n = 1, 2, \ldots, N, \tag{2.22}$$

which is that of a set of *uncoupled* oscillators with spring constants κ_n, $n = 1, 2, \ldots, N$. As the solution of (2.22) was studied in the last section, we only need to know explicitly the transformation linking the $\boldsymbol{\varepsilon}$- with the $\mathbb{K}$-eigenbasis $\boldsymbol{\psi}$ in order to translate the solutions of (2.22) into the solutions of (2.20). This is easier said than done, so the remainder of Section 2.2 will deal with a simple case where the eigenbasis of $\mathbb{K}$ is one which has been studied before.

2.2.4. The Simple Equal-Mass Lattice

Consider the lattice in Fig. 2.5, where all masses and springs are equal, the viscous and external forces are absent ($\mathbb{C} = \mathbb{0}$, $\mathbf{F} = \mathbf{0}$), and only first-neighbor interactions are considered. As $k_{nm} = k(\delta_{n,m+1} + \delta_{n,m-1})$ and $k_n = 0$, Eq. (2.19) yields

$$\kappa_{nm} = -k(\delta_{n,m+1} + \delta_{n,m-1} - 2\delta_{nm}), \tag{2.23}$$

i.e., *the interaction operator is a multiple k of the second-difference operator* (Section 1.5),

$$\mathbb{K} = -k\mathbb{\Delta}, \tag{2.24}$$

and the vector equation of motion (2.21) then reads

$$M\ddot{\mathbf{f}} - k\Delta\mathbf{f} = \mathbf{0}. \tag{2.25}$$

In the $\boldsymbol{\varepsilon}$-basis, this is represented by the N equations

$$M\ddot{f}_n = k(f_{n+1} - 2f_n + f_{n-1}), \qquad n = 1, 2, \ldots, N, \tag{2.26}$$

which tell us that the acceleration of the nth particle is proportional to the *curvature* of the displacement coordinate around the nth position. In Fig. 2.7 this is manifest: the larger the angle between the $(n-1)-(n)$ and $(n)-(n+1)$ springs, the greater the force and hence the acceleration in the direction of concavity.

2.2.5. Uncoupling and Solution

Equation (2.25) in the $\boldsymbol{\varphi}$-*basis* (see Section 1.4) appears simpler than (2.26), since Δ is diagonal there and the component equations uncouple:

$$M\ddot{\tilde{f}}_m - k\lambda_m\tilde{f}_m = 0, \tag{2.27a}$$

$$\lambda_m := -4\sin^2(\pi m/N), \qquad m = 1, 2, \ldots, N. \tag{2.27b}$$

Equations (1.51) relate the *normal* coordinates $\{\tilde{f}_m\}_{m=1}^N$ to the lattice displacements $\{f_n\}_{n=1}^N$. The general solution of Eqs. (2.27) in terms of the $2N$ initial conditions is thus of the oscillatory type [see Eqs. (2.6)–(2.11) for $c, \Gamma = 0$]:

$$\tilde{f}_m(t) = \dot{\tilde{G}}_m(t - t_0)\tilde{f}_m(t_0) + \tilde{G}_m(t - t_0)\dot{\tilde{f}}_m(t_0), \tag{2.28a}$$

$$\tilde{G}_m(\tau) := \omega_m^{-1}\sin\omega_m\tau, \qquad \dot{\tilde{G}}_m(\tau) = \cos\omega_m\tau, \tag{2.28b}$$

$$\omega_m := (-k\lambda_m/M)^{1/2} = 2(k/M)^{1/2}|\sin(\pi m/N)| = \omega_{N-m}, \tag{2.28c}$$

where $\tilde{f}_m(t_0)$ and $\dot{\tilde{f}}_m(t_0)$ are the $\boldsymbol{\varphi}$-basis coordinates of the initial displacement and velocity vectors $\mathbf{f}_0 := \mathbf{f}(t_0)$ and $\dot{\mathbf{f}}_0 := \dot{\mathbf{f}}(t_0)$. We have given an apparently redundant absolute value to the last member in (2.28c); this will be seen to be convenient when we exploit the identification $m \equiv n \bmod N$. One case we have "overlooked" is the solution of (2.27) for $m = N$, as there $\lambda_N = 0$ so the Nth normal coordinate is that of a springless "oscillator." This case has been referred to before in Exercise 2.6 and leads to a solution of the type (2.17), i.e.,

$$\tilde{f}_N(t) = \tilde{f}_N(t_0) + (t - t_0)\dot{\tilde{f}}_N(t_0), \tag{2.28d}$$

which can still be correctly incorporated into Eq. (2.28a) since for $\omega_N \to 0$ we have $\tilde{G}_N(\tau) \to \tau$ and $\dot{\tilde{G}}_N(\tau) \to 1$.

2.2.6. Green's Operator of Time Evolution

The solutions (2.28) can now be integrated back to vector form as

$$\mathbf{f}(t) = \dot{\mathbb{G}}(t - t_0)\mathbf{f}_0 + \mathbb{G}(t - t_0)\dot{\mathbf{f}}_0, \tag{2.29}$$

where $\mathbb{G}(\tau)$ is *Green's operator*, represented in the $\boldsymbol{\varphi}$-basis by the diagonal matrix $\tilde{\mathbf{G}}(\tau) = \|\delta_{mn}\tilde{G}_m(\tau)\|$, and $\dot{\mathbb{G}}(\tau) = d\mathbb{G}(\tau)/d\tau$ similarly. (Recall Exercise 1.29 where $\mathbb{G}$ explicitly denoted the case $c = 0$, $M = 1$, $k = 1$.)

Exercise 2.11. Show that the Green's operator appearing in (2.29) and its time derivative are *self-adjoint* and that they commute with $\mathbb{A}$.

Exercise 2.12. Using the fact that $\mathbf{f}_0$ and $\dot{\mathbf{f}}_0$ in (2.29) are constant, arbitrary vectors, show that Green's operator $\mathbb{G}(\tau)$ satisfies the lattice equation of motion (2.25):

$$M\ddot{\mathbb{G}}(\tau) = k\mathbb{A}\mathbb{G}(\tau). \tag{2.30}$$

Exercise 2.13. Let Eq. (2.29) give the solution at time t in terms of initial conditions at time t_1. The latter, however, may be due to still earlier conditions at some time $t_0 < t_1$. Show that this implies that the Green's operator must satisfy

$$\mathbb{G}(t - t_0) = \dot{\mathbb{G}}(t - t_1)\mathbb{G}(t_1 - t_0) + \mathbb{G}(t - t_1)\dot{\mathbb{G}}(t_1 - t_0), \tag{2.31a}$$

and, in particular, that

$$\mathbb{G}(0) = \mathbb{0}, \qquad \dot{\mathbb{G}}(0) = \mathbb{1}. \tag{2.31b}$$

The subject of time evolution will be taken up in more detail in Section 2.6.

Equation (2.29), written in the $\boldsymbol{\varepsilon}$-basis, will provide us with the solution of the original equation (2.26) for the displacements. Indeed,

$$f_n(t) = \sum_m \dot{G}_{nm}(t - t_0)f_m(t_0) + \sum_m G_{nm}(t - t_0)\dot{f}_m(t_0), \qquad n = 1, 2, \ldots, N, \tag{2.32}$$

where the coefficients are the elements of *Green's operator* in the $\boldsymbol{\varepsilon}$-basis:

$$\begin{aligned} G_{nm}(\tau) &:= (\boldsymbol{\varepsilon}_n, \mathbb{G}(\tau)\boldsymbol{\varepsilon}_m) = [\mathbf{F}\tilde{\mathbf{G}}(\tau)\mathbf{F}^\dagger]_{nm} \\ &= \sum_k F_{nk}\tilde{G}_k(\tau)F^*_{mk} \\ &= N^{-1}\sum_k \omega_k^{-1} \sin \omega_k\tau \exp[2\pi ik(m - n)/N] \\ &= N^{-1}\sum_k \omega_k^{-1} \sin \omega_k\tau \cos[2\pi k(m - n)/N], \end{aligned} \tag{2.33}$$

$$\dot{G}_{nm}(\tau) = N^{-1}\sum_k \cos \omega_k\tau \cos[2\pi k(m - n)/N]. \tag{2.34}$$

Thus, although in working out the solution we slipped into the field $\mathscr{C}$ of complex numbers and unitary transformations, in the end we see that if the

$2N$ initial conditions are real, since $G_{nm}(\tau)$ and $\dot{G}_{nm}(\tau)$ are real functions, the solutions $f_n(t)$ are real, as one should expect.

Exercise 2.14. Verify that the special expression for $\tilde{G}_N(\tau)$ causes no trouble in (2.32)–(2.34) if we take care to make $\omega_N^{-1} \sin \omega_N \tau = \tau$.

2.2.7. Properties of the Green's Operator

The elements of Green's matrix $G_{nm}(\tau)$ in (2.33) and its time derivative (2.34) have several manifest properties: (a) $G_{nm}(\tau)$ and its time derivative are functions of $|n - m|$. This embodies the principle of *reciprocity*: the effect on mass n of a given initial condition at site m is the same as the effect on mass m of that same initial conditions at n. (b) The effect, moreover, depends only on their *relative* distance $|n - m|$, not on their absolute position n or m. In other words, the system is *translationally invariant*: If $\mathbf{f}(t)$ is a solution with initial conditions $\mathbf{f}_0$ and $\dot{\mathbf{f}}_0$, then the translated initial conditions $\mathbb{R}^k\mathbf{f}_0$ and $\mathbb{R}^k\dot{\mathbf{f}}_0$ give rise to the solution $\mathbb{R}^k\mathbf{f}(t)$, as follows from the observation that $\mathbb{R}^k\mathbb{G}(\tau) = \mathbb{G}(\tau)\mathbb{R}^k$. (In the $\boldsymbol{\varphi}$-basis, both operators are represented by diagonal matrices.) (c) Similarly, inversion through $\mathbb{I}_l$ (and $\mathbb{K}_l$ when N is even) of the initial conditions produces a correspondingly inverted solution, as $\mathbb{I}_l$ (and $\mathbb{K}_l$) also commute with the simple lattice Green's operator. The system is correspondingly *invariant under inversions*. We must emphasize in (b) and (c) that translational invariance and inversion invariance refer to the *simple lattice equations of motion* and *time evolution* embodied by $\mathbb{A}$ and $\mathbb{G}(\tau)$, *not* to the *initial conditions*, which may be arbitrary and not at all invariant under $\mathbb{R}^k$ or $\mathbb{I}_l$. These observations *do* imply, however, that *if* a given set of initial conditions has definite symmetry under some operation (as, i.e., $\mathbb{I}_0\mathbf{f}_0 = \sigma\mathbf{f}_0$ and $\mathbb{I}_0\dot{\mathbf{f}}_0 = \sigma\,\dot{\mathbf{f}}_0$, for $\sigma = 1$ or -1), *then* the resulting solution $\mathbf{f}(t)$ will have the same symmetry [i.e., $\mathbb{I}_0\mathbf{f}(t) = \sigma\mathbf{f}(t)$] for all time. We shall have opportunity to use these facts at the end of next section in order to describe lattices with fixed ends.

Exercise 2.15. Prove the preceding statements in detail.

The solution (2.29) to the simple lattice looks neat and compact. It will serve us, however, to dedicate all of Section 2.3 to describing certain particular solutions in the "physical" $\boldsymbol{\varepsilon}$-basis so as to get a firmer understanding of the processes involved. This will be useful when we extend the treatment of this section to more general lattices.

Exercise 2.16. Repeat the analysis of the simple lattice (Fig. 2.5) to include viscous forces. Assuming they are equal for all particles in the lattice and using the results of Section 2.1, prove that the generalization of (2.29) is

$$\mathbf{f}(t) = [\dot{\mathbb{G}}^\Gamma(t - t_0) + 2\Gamma\mathbb{G}^\Gamma(t - t_0)]\mathbf{f}_0 + \mathbb{G}^\Gamma(t - t_0)\dot{\mathbf{f}}_0, \tag{2.35}$$

where the Green's operator $\mathbb{G}^\Gamma(\tau)$ is represented in the φ-basis by a diagonal matrix with elements

$$\tilde{G}_m{}^\Gamma(\tau) = (\omega_m{}^e)^{-1} \exp(-\Gamma\tau) \sin \omega_m{}^e\tau \qquad \text{(oscillatory)}, \tag{2.36}$$

$$\Gamma := c/2M, \qquad \omega_m{}^e := [4(k/M) \sin^2(\pi m/N) - \Gamma^2]^{1/2}, \tag{2.37}$$

and corresponding expressions for the critical and overdamped cases.

Exercise 2.17. Consider the limit when damping is much larger than inertia, so that $c/2M = \Gamma \to \infty$ while c and k remain finite. Refer to Exercise 2.8. In that case, using the overdamped expression for (2.35)–(2.37), show that $\mathbb{G}^\Gamma(\tau)$, $\dot{\mathbb{G}}^\Gamma(\tau) \to \mathbb{0}$. The operator $2\Gamma\mathbb{G}^\Gamma(\tau)$ remains finite, however, and (2.35) becomes

$$\tilde{f}_m(t) = \exp[-4(t - t_0)kc^{-1} \sin^2(\pi m/N)]\tilde{f}_m(t_0), \tag{2.38a}$$

so that $\tilde{f}_m(t)$ and hence $f_n(t)$ stop depending on the initial velocity. The solutions are exponentially damped and correspond to the vector equation

$$\mathbf{f}(t) = \exp[(t - t_0)kc^{-1}\mathbb{\Delta}]\mathbf{f}(t_0). \tag{2.38b}$$

Compare with Eqs. (1.72). The function (2.38a) appears in Fig. 3.5(a).

Exercise 2.18. As a continuation of Exercise 2.17, define the "total heat" of the damped massless lattice as

$$Q := \sum_n f_n. \tag{2.39}$$

Using (2.38b), show that Q at time t is the same as at time t_0. Refer to Exercise 1.28.

2.3. Fundamental Solutions, Normal Modes, and Traveling Waves

The general solution of a coupled system represented by a simple lattice was obtained in Section 2.2. Here we shall filter out the information which is relevant and extendable to more general cases.

2.3.1. Fundamental Solutions

The expression (2.29) for $t_0 = 0$,

$$\mathbf{f}(t) = \dot{\mathbb{G}}(t)\mathbf{f}_0 + \mathbb{G}(t)\dot{\mathbf{f}}_0, \tag{2.40}$$

gives the state vector for the lattice at time t in terms of the initial displacements $\mathbf{f}_0$ and velocities $\dot{\mathbf{f}}_0$. Assume the lattice starts from rest ($\dot{\mathbf{f}}_0 = \mathbf{0}$) with the mth mass displaced by one unit ($\mathbf{f}_0 = \boldsymbol{\varepsilon}_m$). The ensuing time development of the lattice is then given by the state vector

$$\dot{\boldsymbol{\varepsilon}}^m(t) := \dot{\mathbb{G}}(t)\boldsymbol{\varepsilon}_m \tag{2.41a}$$

with components

$$\dot{\varepsilon}_n{}^m(t) = (\boldsymbol{\varepsilon}_n, \dot{\boldsymbol{\varepsilon}}^m(t)) = \dot{G}_{nm}(t), \qquad n = 1, 2, \ldots, N, \tag{2.41b}$$

given explicitly by Eq. (2.34). Assume now that the initial condition of the lattice is $\mathbf{f}_0 = \mathbf{0}, \dot{\mathbf{f}}_0 = \boldsymbol{\varepsilon}_m$, i.e., the mth mass is moving through its equilibrium position with unit velocity. The corresponding solution state vector is

$$\boldsymbol{\varepsilon}^m(t) \coloneqq \mathbb{G}(t)\boldsymbol{\varepsilon}_m \tag{2.42a}$$

with components

$$\varepsilon_n{}^m(t) = \big(\boldsymbol{\varepsilon}_n, \boldsymbol{\varepsilon}^m(t)\big) = G_{nm}(t), \qquad n = 1, 2, \ldots, N \tag{2.42b}$$

[see Eqs. (2.33)]. We shall refer to (2.41) and (2.42) as the *fundamental solutions* of the N-point lattice. In Figs. 2.8(a) and (b) we have drawn the solutions (2.41) and (2.42) for fixed m. The most general initial condition $\mathbf{f}_0 = \sum_m f_m \boldsymbol{\varepsilon}_m$, $\dot{\mathbf{f}}_0 = \sum_m \dot{f}_m \boldsymbol{\varepsilon}_m$ will then give rise to a state vector

$$\mathbf{f}(t) = \sum_m f_m \dot{\boldsymbol{\varepsilon}}^m(t) + \sum_m \dot{f}_m \boldsymbol{\varepsilon}^m(t), \tag{2.43}$$

which is a *superposition* of the fundamental solutions (2.41) and (2.42). Note that there are $2N$ *parameters* in (2.43): N for the components of $\mathbf{f}_0$ and N for those of $\dot{\mathbf{f}}_0$. The set of solutions (2.43) thus fit a $2N$-dimensional vector space which will be seen in Section 2.6 to be the *phase space* of the system. Meanwhile, we shall only point to the fact that there are $2N$ independent solutions for the N-particle lattice and that the most general solution can be expressed as a linear combination of them.

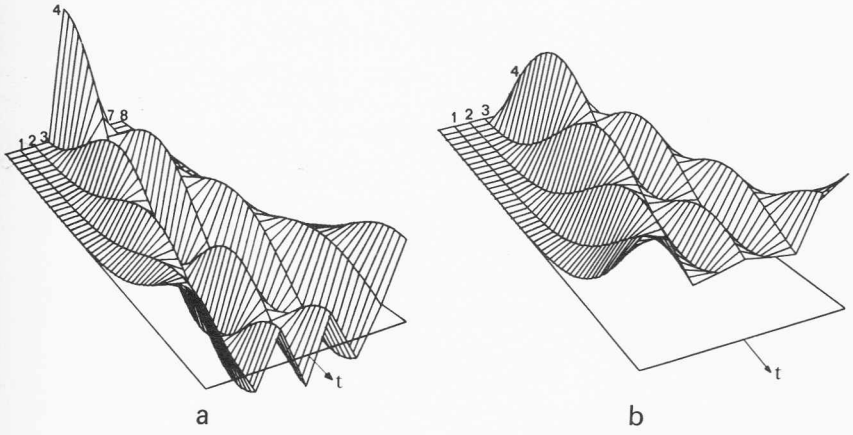


Fig. 2.8. Fundamental solutions for the eight-mass linear closed lattice. (a) The fourth mass starts with unit elongation, and (b) the fourth mass starts with unit velocity. All other fundamental solutions are translated versions of these, numbered modulo 8. Note that for small t a "propagation velocity" for the disturbance can be seen and loosely defined. As the spring mass is zero, however, every mass in the lattice feels the disturbance instantaneously. (Refer to the discussion in Section 5.3 for the infinite lattice.)

Exercise 2.19. Show that the set of fundamental solutions is *not* orthonormal for all t. Green's operator is self-adjoint but *not* unitary.

2.3.2. A Real Orthonormal Basis

Figures 2.8(a) and (b) are neat, but the information they contain is quite structureless. Since the uncoupling of the lattice equations in Section 2.2 was the key step in solving the system and the solutions were those of single harmonic oscillators, we should be asking for fundamental solutions in the $\mathbb{G}$-basis, that is, for the time development of initial conditions given by $\mathbf{f}_0 = \boldsymbol{\varphi}_m$ and/or $\dot{\mathbf{f}}_0 = \dot{\boldsymbol{\varphi}}_{m'}$. The solutions due to such initial conditions would be complex, however, since from (1.52), $(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_m) = F_{mn}$. To have *real* initial conditions still associated with the $\boldsymbol{\varphi}$-basis, we can use the set of vectors ${\boldsymbol{\varphi}_m}^{\pm}$ defined in (1.115), which we write compactly as

$$ {\boldsymbol{\varphi}_m}^{\pm} = {\xi_m}^{\pm} 2^{-1/2}(\boldsymbol{\varphi}_m \pm \boldsymbol{\varphi}_{-m}), \quad m = 0, 1, \ldots, \begin{cases} \tfrac{1}{2}(N-1), & N \text{ odd}, \\ N/2, & N \text{ even}, \end{cases} \tag{2.44a} $$

where we use here and below the convention that the subscripts are considered modulo N, and

$$ \begin{aligned} &{\xi_m}^{-} = i, \quad \text{except } {\xi_0}^{-} = 0, \\ &{\xi_m}^{+} = 1, \quad \text{except } {\xi_0}^{+} = 2^{-1/2}, \quad \text{and, when } N \text{ even}, \quad {\xi^{+}_{N/2}} = 2^{-1/2}. \end{aligned} \tag{2.44b} $$

These vectors also constitute an *orthonormal* basis (see Exercise 1.50), which we shall call the ${\boldsymbol{\varphi}}^{\pm}$*-basis* for short.

Exercise 2.20. Show that the vectors (1.115) have *real* coordinates in the original $\boldsymbol{\varepsilon}$-basis:

$$ (\boldsymbol{\varepsilon}_n, {\boldsymbol{\varphi}_m}^{+}) = {\xi_m}^{+}(N/2)^{-1/2} \cos(2\pi mn/N), \tag{2.45a} $$

$$ (\boldsymbol{\varepsilon}_n, {\boldsymbol{\varphi}_m}^{-}) = (N/2)^{-1/2} \sin(2\pi mn/N). \tag{2.45b} $$

Note that $(\boldsymbol{\varepsilon}_n, {\boldsymbol{\varphi}_0}^{+}) = N^{-1/2}$ and $(\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}^{+}_{N/2}) = N^{-1/2}(-1)^n$.

2.3.3. Normal Modes

We define state vectors analogous to (2.41)–(2.42) whose initial displacements or velocities at $t_0 = 0$ are the vectors of the ${\boldsymbol{\varphi}}^{\pm}$-basis:

$$ {\dot{\boldsymbol{\varphi}}}^{m\pm}(t) \coloneqq \dot{\mathbb{G}}(t){\boldsymbol{\varphi}_m}^{\pm}, \tag{2.46a} $$

$$ {\boldsymbol{\varphi}}^{m\pm}(t) \coloneqq \mathbb{G}(t){\boldsymbol{\varphi}_m}^{\pm}. \tag{2.46b} $$

Solutions (2.46a) start from rest with maximum displacement, while (2.46b) start with the lattice moving through the equilibrium shape. We can find the form of the lattice vibrations represented by (2.46) by calculating

$$ \begin{aligned} \dot{\varphi}_n^{m\pm}(t) &= \left(\boldsymbol{\varepsilon}_n, {\dot{\boldsymbol{\varphi}}}^{m\pm}(t)\right) = \sum_k (\boldsymbol{\varepsilon}_n, \boldsymbol{\varphi}_k)\left(\boldsymbol{\varphi}_k, \dot{\mathbb{G}}(t){\boldsymbol{\varphi}_m}^{\pm}\right) \\ &= {\xi_m}^{\pm} 2^{-1/2}[F_{nm}\dot{\bar{G}}_m(t) \pm F_{n,-m}\dot{\bar{G}}_{-m}(t)] \end{aligned} \tag{2.47} $$

and similarly for $\varphi_n^{m\pm}(t)$. Now $F_{n,-m} = F_{mn}^*$, and from (2.28b) and (2.28c) we can see that $\tilde{G}_m = \tilde{G}_{-m}$ and similarly for its time derivative. Hence, after a short calculation the lattice solutions (2.46) are obtained as

$$\dot{\varphi}_n^{m+}(t) = \xi_m{}^+(2/N)^{1/2} \cos(2\pi nm/N) \cos \omega_m t, \tag{2.48a}$$

$$\dot{\varphi}_n^{m-}(t) = (2/N)^{1/2} \sin(2\pi nm/N) \cos \omega_m t, \tag{2.48b}$$

$$\varphi_n^{m+}(t) = \xi_m{}^+(2/N)^{1/2} \cos(2\pi nm/N)\omega_m^{-1} \sin \omega_m t, \tag{2.48c}$$

$$\varphi_n^{m-}(t) = (2/N)^{1/2} \sin(2\pi nm/N)\omega_m^{-1} \sin \omega_m t. \tag{2.48d}$$

These have been plotted in Fig. 2.9. In spite of the small complication of the ξ's and the apparent proliferation of indices, the picturing of the solutions—the *normal modes* of the system—is rather simple: they are *standing waves* of the lattice. They are also *separated* functions of n and t; that is, they have the form $\varphi_n(t) = \nu(n)\tau(t)$, the waveform $\nu(n)$ being *modulated* by an oscillating function $\tau(t)$.

Exercise 2.21. Check that there are indeed $2N$ different normal modes in Eqs. (2.48).

Exercise 2.22. Verify that

$$\ddot{\boldsymbol{\varphi}}^{m\pm}(t) = -\omega_m{}^2 \boldsymbol{\varphi}^{m\pm}(t). \tag{2.49}$$

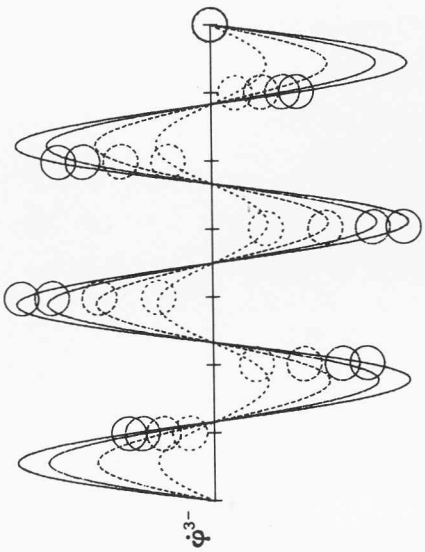
Exercise 2.23. Suppose we had started with the N lattice equations of motion (2.26) and *assumed* that the solutions $f_n(t)$ were separable functions $\nu(n)\tau(t)$. Substituting this ansatz into (2.26) and following the usual procedure of separation of variables, show that one arrives at $\tau(t) = c \exp(i\omega t)$, where the $-\omega^2$ are the separation constants, which are solutions of the eigenvalues problem $k\boldsymbol{\Delta}\boldsymbol{\nu} = -M\omega^2\boldsymbol{\nu}$. If this is solved and linear combinations taken to ensure the reality of the solutions, Eqs. (2.48) will be obtained.

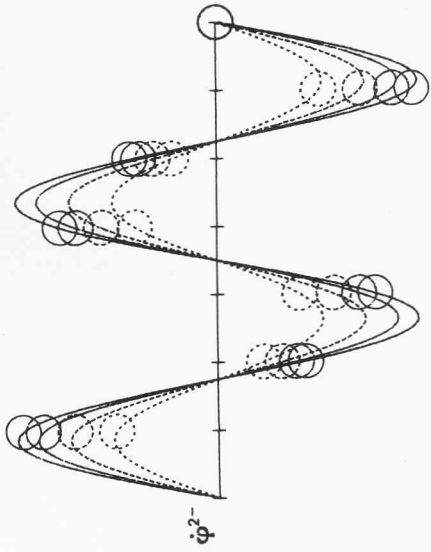
2.3.4. The Brillouin Angular Frequency Diagram

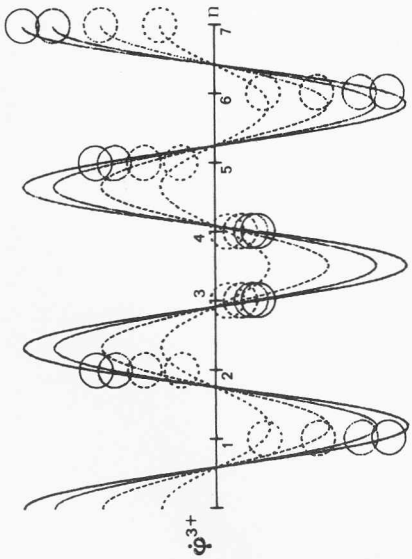
The most general initial condition of a vibrating lattice, in the same form as (2.43), can be expanded in the $\boldsymbol{\varphi}^{\pm}$-basis for displacements and velocities with coefficients $f_m{}^{\pm}$ and $\dot{f}_m{}^{\pm}$, respectively [m and $\pm$ taking the values allowed by (2.44)], giving rise to a state vector

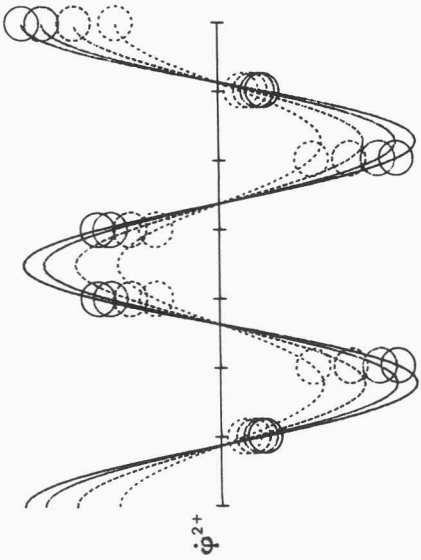
$$\mathbf{f}(t) = \sum_{m,\pm} f_m{}^{\pm} \dot{\boldsymbol{\varphi}}^{m\pm}(t) + \sum_{m,\pm} \dot{f}_m{}^{\pm} \boldsymbol{\varphi}^{m\pm}(t). \tag{2.50}$$

In the form (2.50), the solution $\mathbf{f}(t)$ is decomposed into sinusoidal waves such as those in Fig. 2.9, each set of $\boldsymbol{\varphi}$'s with the same value of m vibrating with its own angular velocity ω_m [Eq. (2.28c)]. The $\boldsymbol{\varphi}^m$'s are one-quarter period behind the $\dot{\boldsymbol{\varphi}}^m$'s so they represent essentially the same waveform of the lattice. A very handy representation of the allowed angular frequencies ω_m, very much used


φ^{3-}


φ^{2-}


n
7
6
5
4
3
2
1
φ^{3+}


φ^{2+}

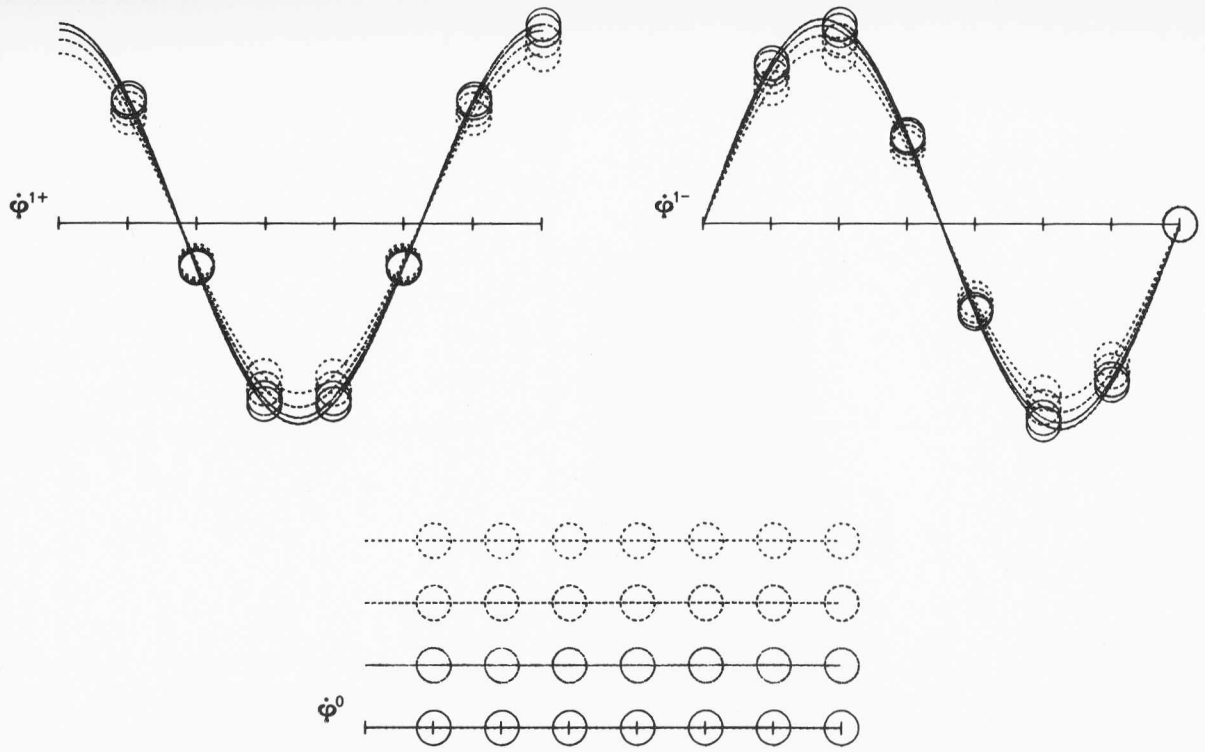


Fig. 2.9. Normal modes $\varphi^{m\pm}$ and φ^{0} (standing waves) for a seven-mass lattice. The lattice shape has been plotted for real n between 0 and 7, actual masses being indicated by circles. Dotted lines and circles refer to subsequent time snapshots spaced by $\frac{1}{8}$ [in units of $(M/k)^{1/2}$]. It is seen that higher-m waves entail an average higher velocity for the masses. The $\varphi^{m\pm}$ normal modes are similar to the ones depicted in the figures, but they start with zero elongation. The zeroth mode describes undeformed rotation for the whole lattice.

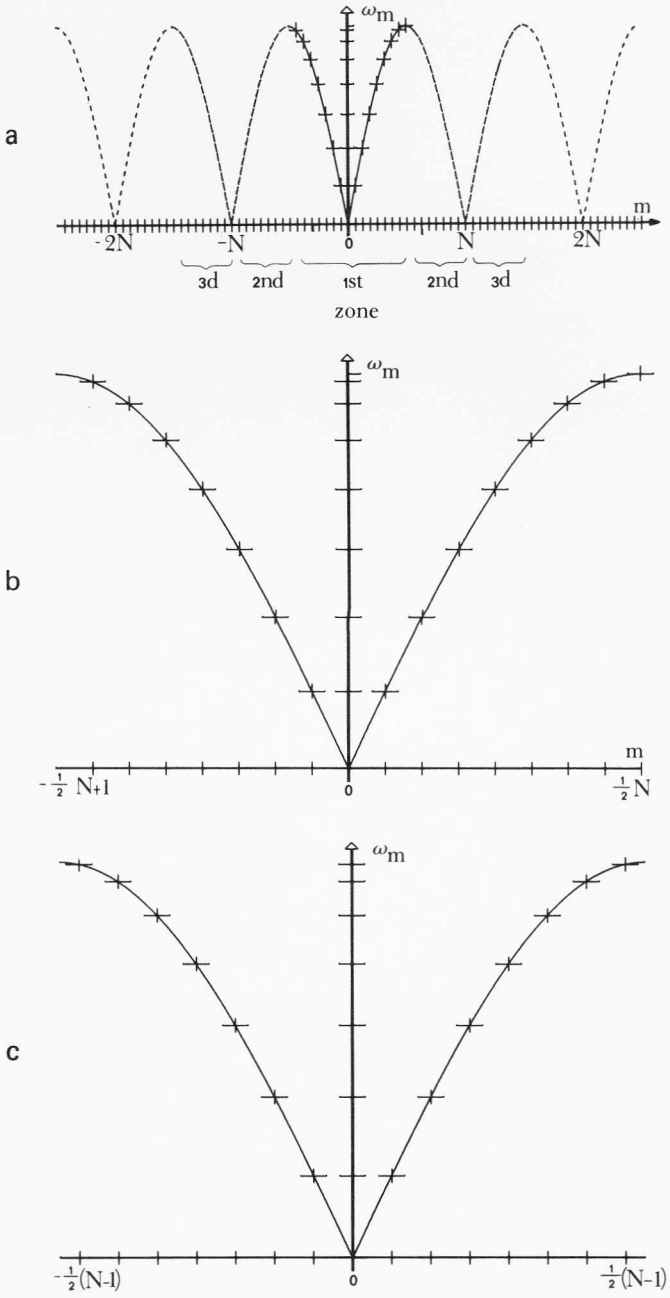


Fig. 2.10. Brillouin frequency diagram plotting the angular frequency ω_m as a function of m: (a) the repeating Brillouin zones; (b) and (c) the central (first) zone for N even and odd. Crosses mark the integer-m allowed frequencies. Note that all ω_m's are doubly degenerate (for $\omega_{\pm m}$) except for ω_0, and, if N is even, $\omega_{N/2}$. This is the difference between (b) and (c).

in solid-state physics, is the *Brillouin* diagram, Fig. 2.10, which plots the ω_m of $\varphi^{m\pm}$ as a function of $\pm m$, taking the interval in m to be centered around $m = 0$. The *first Brillouin zone* for odd $N = 2\nu + 1$ extends over $m = -\nu, -\nu + 1, \ldots, -1, 0, 1, \ldots, \nu - 1, \nu$. When $N = 2\nu'$ is even, it extends over $m = -\nu' + 1, \ldots, -1, 0, 1, \ldots, \nu' - 1, \nu'$. Beyond the ends of these intervals are the second, third, etc., Brillouin zones, which in the case of a one-dimensional lattice are equivalent to the first one. Except for $m = 0$ and $N/2$ (if N is even), two values $\pm m$ correspond to the same value of ω_m, the angular frequency.

Exercise 2.24. Refer to Section 1.7 and note that the $\varphi^{m\pm}(t)$ solutions have *definite parity* under $\mathbb{I}_0$, i.e.,

$$\mathbb{I}_0\varphi^{m\pm}(t) = \pm\varphi^{m\pm}(t) \tag{2.51}$$

for all t. Note that instead of the $\varphi^{\pm}$-basis vectors we could have used any of the eigenbases of $\mathbb{A}$ and $\mathbb{I}_l$ as given in (1.118) and still obtained real solutions. The sine—and cosine—functions of n would have their arguments displaced by $2\pi ln/N$.

2.3.5. Periods and Wavelengths

The period of each set of φ^m's is

$$T_m := 2\pi/\omega_m := (M/k)^{1/2}\pi/|\sin(\pi m/N)|. \tag{2.52}$$

As these periods are in general incommensurable, there will be no periodicity of the total solution $\mathbf{f}(t)$. The normal modes or combinations of the same m-set are the only time-periodic solutions of the vibrating lattice. A representation similar to the Brillouin diagram is shown in Fig. 2.11. Regarding

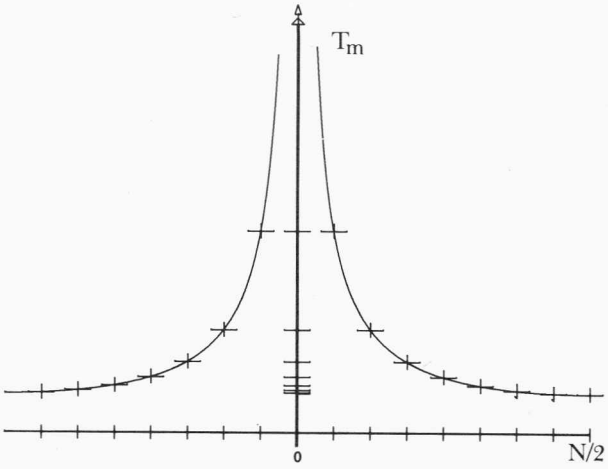


Fig. 2.11. Brillouin diagram for oscillation periods.

the wavelength in units of interparticle separation, it can be seen from (2.48) to be

$$\lambda_m = N/m, \tag{2.53}$$

i.e., there are m wavelengths in the lattice circle. In Fig. 2.12 we plot (2.53) in the Brillouin manner, although λ_m is not a periodic function of m. Had we decided to take $N/(m + N)$, $N/(m \pm 2N)$, etc., we would have been left with the same description of the discrete lattice points; see Fig. 2.13. Some observations on particular normal modes are the following: (a) When N is even, $\varphi^{N/2+}(t)$ and its time derivative [no $\varphi^{N/2-}(t)$ exists] have the largest angular frequency, $\omega_{N/2} = 2(k/M)^{1/2}$, and the smallest period, $T_{N/2} = \pi(M/k)^{1/2}$. The lattice vibrates in such a way that each mass moves in a sense opposite to that of its first neighbors and carries the smallest wavelength: $\lambda_{N/2} = 2$ interparticle separations. (b) When N is odd, the highest frequency corresponds to $m = \pm(N - 1)/2$, as shown in Fig. 2.10. Again, they have the smallest period and wavelength. (c) The "normal mode" $m = 0$ is a bit of a fraud since it does not oscillate at all. Formally, for $\omega_0 = \omega_N$ we had set $(\omega_0)^{-1} \sin \omega_0 t = t$, so, as drawn in Fig. 2.9, $\varphi^0(t) = N^{-1/2}t$, $\dot{\varphi}^0(t) = N^{-1/2}$. It represents a uniform displacement of the full lattice, which by itself is not too interesting. The period and wavelength turn out to be infinite.

Exercise 2.25. When the lattice has an even number of masses one can define an eigenbasis of the $\mathbb{K}_0$ operator proposed in Exercise 1.54 as suggested in (2.51) for $\mathbb{I}_0$—or any $\mathbb{K}_l$ as generalized in Exercise 2.24. Explore the possibilities in this direction. These will be used at the end of this section.

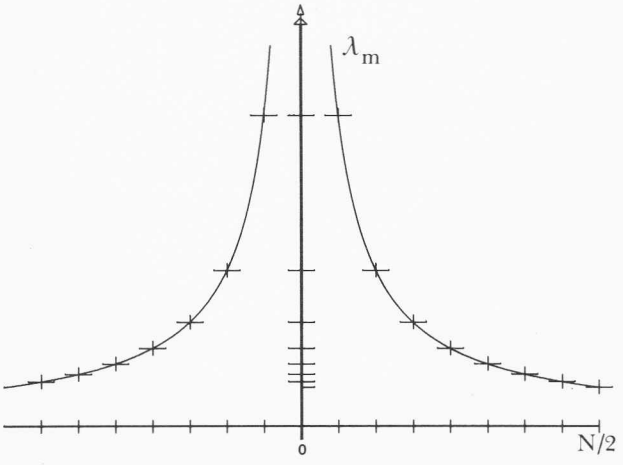


Fig. 2.12. Brillouin diagram for wavelengths.

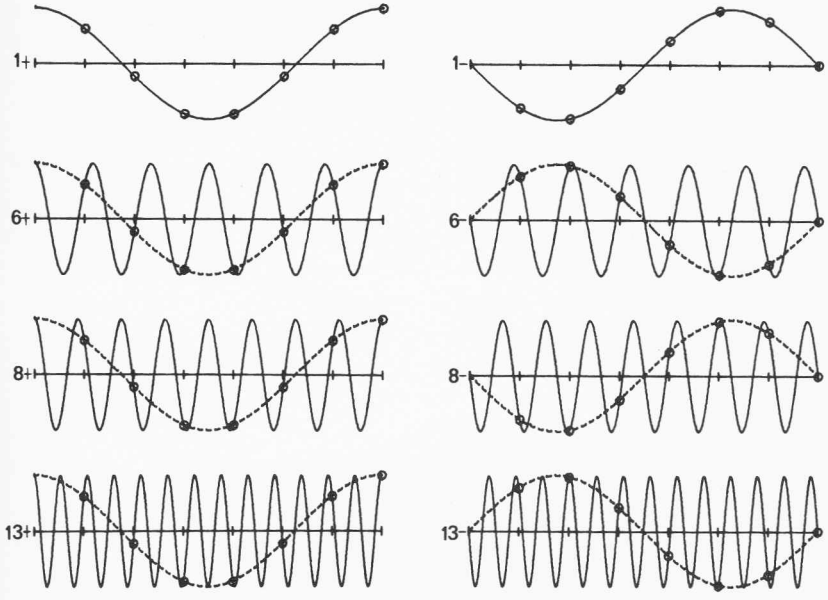


Fig. 2.13. Multiple wavelength degeneracy: $\boldsymbol{\varphi}^{m\pm}$, $\boldsymbol{\varphi}^{N+m\pm}$, ... and $\boldsymbol{\varphi}^{-m\pm}$, $\boldsymbol{\varphi}^{N-m\pm}$, ... describe the same state for the actual lattice masses. All the relevant information is thus contained in the first Brillouin zone.

2.3.6. Traveling Waves

In exploring the fundamental solutions and the normal modes we examined situations in which the initial conditions were either nonzero displacements or nonzero velocities. There is a third set of interesting solutions, *traveling waves*, where both sets of initial conditions are nonzero albeit correlated. From the trigonometric functions appearing in the normal modes (2.48) we can see interesting combinations. Let

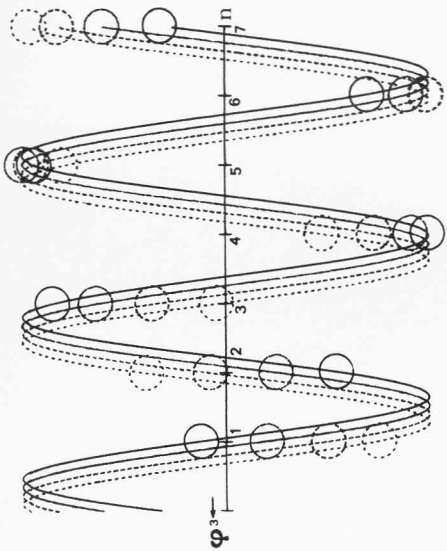
$$\boldsymbol{\varphi}^{m\rightleftarrows}(t) \coloneqq (\omega_m)^{-1}\dot{\boldsymbol{\varphi}}^{m-}(t) \mp \boldsymbol{\varphi}^{m+}(t), \tag{2.54a}$$

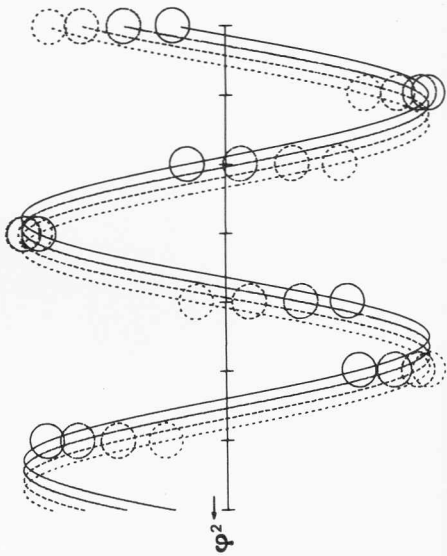
$$\dot{\boldsymbol{\varphi}}^{m\rightleftarrows}(t) \coloneqq \mp\dot{\boldsymbol{\varphi}}^{m+}(t) + \omega_m\boldsymbol{\varphi}^{m-}(t), \tag{2.54b}$$

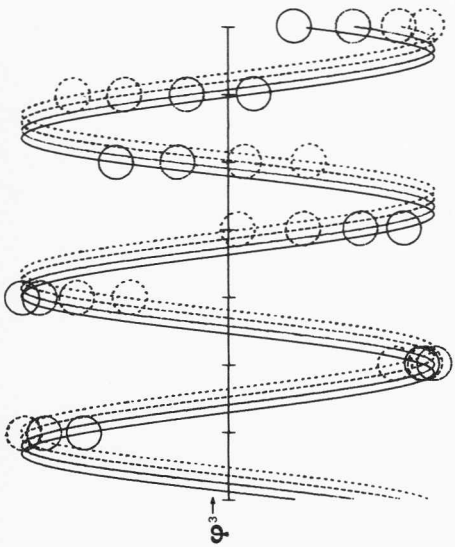
where the ranges of m and $\rightleftarrows$ will be detailed below. The lattice vibrations described by these state vectors (which are solutions of the lattice since the $\boldsymbol{\varphi}^{m\pm}$'s are too) are given by their coordinates in the $\boldsymbol{\varepsilon}$-basis, which can easily be found from (2.48):

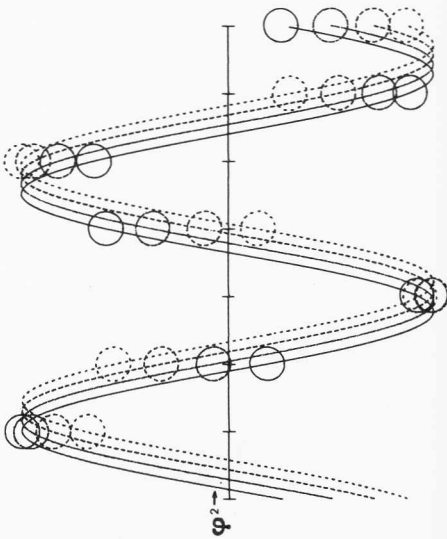
$$\varphi_n^{m\rightleftarrows}(t) = \xi_m{}^{+}(2/N)^{1/2}(\omega_m)^{-1}\sin(2\pi nm/N \mp \omega_m t), \tag{2.55a}$$

$$\dot{\varphi}_n^{m\rightleftarrows}(t) = \mp\xi_m{}^{+}(2/N)^{1/2}\cos(2\pi nm/N \mp \omega_m t). \tag{2.55b}$$


n
7
6
5
4
3
2
1
φ3


φ2


φ3


φ2

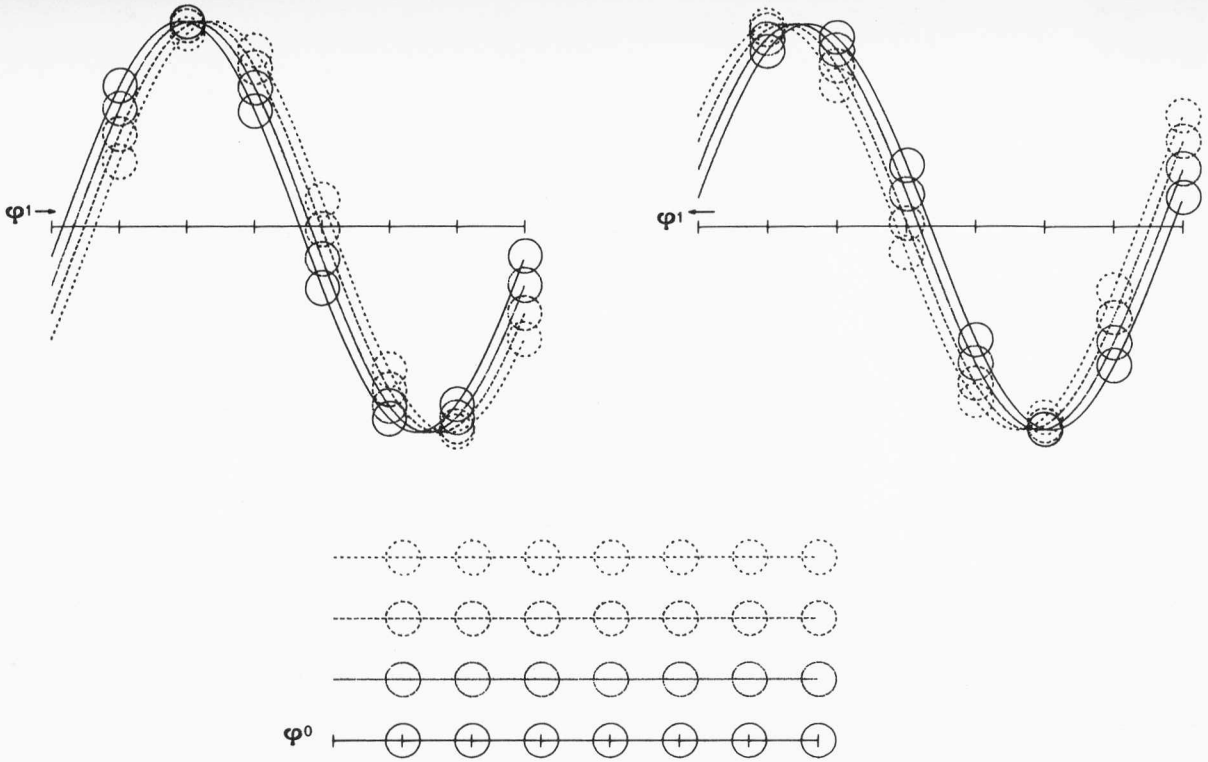


Fig. 2.14. Traveling waves for a seven-mass lattice. As in Fig. 2.9 the lattice shape has been plotted for real n, dotting subsequent time snapshots spaced by $\frac{1}{6}$ [in units of $(M/k)^{1/2}$]. It can be seen that in $\varphi^{m\rightleftarrows}$ the higher values of m entail a greater average movement of the actual masses, although their wave velocity is smaller.

The dependence of $\varphi_n^{m\rightleftarrows}$ on n and t is in the form $2\pi nm/N \mp \omega_m t$, i.e., it is *constant* for

$$n = \pm N\omega_m t/2\pi m. \tag{2.56}$$

With advancing time, the sinusoidal lattice shape represented by $\varphi_n^{m\rightleftarrows}(t)$ will shift to the right and left, respectively, thus describing a right- or left-moving waveform. See Fig. 2.14.

2.3.7. Propagation Velocity

The velocity of this traveling wave is, from (2.56),

$$v_m^{\rightleftarrows} = \pm N\omega_m/2\pi m \tag{2.57}$$

in units of interparticle separation per unit time. The wavelength of the traveling waves is still (2.53), as this is the characteristic of the m-set of states. In Fig. 2.15 we have plotted à la Brillouin the absolute value of the velocities (2.57) as a function of m. This will also clarify the ranges and "extreme" cases of the indices m and $\rightleftarrows$ in (2.54)–(2.55). (a) When N is even, we saw that only $\boldsymbol{\varphi}^{N/2+}$ existed, so here we conclude that $\boldsymbol{\varphi}^{N/2\rightarrow} = -\boldsymbol{\varphi}^{N/2\leftarrow}$. Inspection of (2.55) for this case shows that this "traveling" wave has no definite *sense* of motion, although its velocity (2.57) is $v_{N/2} = 2(k/M)^{1/2}/\pi$. It is the slowest of the waves. (b) When N is odd, the slowest waves correspond to $m = (N-1)/2$. For all other m's down to $m = 1$ both left- and right-traveling waves exist until (c) for $m = 0$, $\boldsymbol{\varphi}^{0\leftarrow} = -\boldsymbol{\varphi}^{0\rightarrow} = \boldsymbol{\varphi}^{0+}$. Again this "wave"

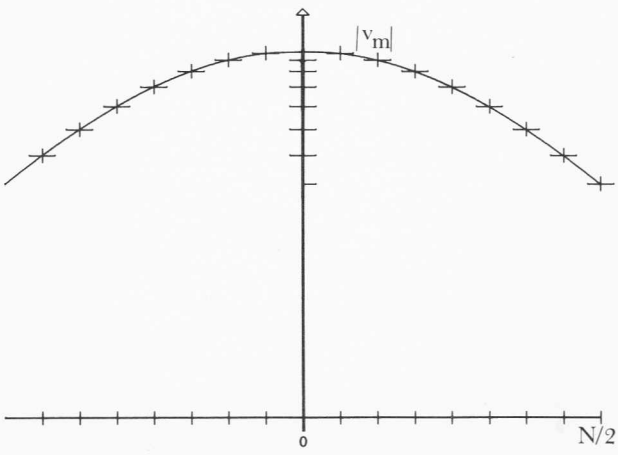


Fig. 2.15. Brillouin diagram for velocities.

is a freak, as it has no sense of motion, although it defines an upper limit for propagation velocities in the lattice. From (2.28c) and for $m \to 0$ this is

$$v_0 = (k/M)^{1/2} \tag{2.58}$$

in units of interparticle separation. Note that this quantity depends only on the lattice parameters of mass and spring.

Exercise 2.26. Show that the traveling waves satisfy

$$\frac{\partial}{\partial t}\boldsymbol{\varphi}^{m\rightleftarrows} = \pm\sigma\omega_m \mathbb{R}^{\sigma N/4m}, \qquad \sigma = \pm 1. \tag{2.59}$$

These are the "square roots" of the second-order differential equation (2.49). Are there "square root" forms for the lattice equation of motion (2.25) for solutions consisting only of right-moving (or left-moving) waves? Why not?

2.3.8. Initial Conditions and Dispersion

Again, the most general state vector describing the lattice can be written in terms of traveling waves as

$$\mathbf{f}(t) = \sum_{m,\rightleftarrows} f_m{}^{\rightleftarrows}\dot{\boldsymbol{\varphi}}^{m\rightleftarrows}(t) + \sum_{m,\rightleftarrows} \mathbf{f}_m{}^{\rightleftarrows}\boldsymbol{\varphi}^{m\rightleftarrows}(t). \tag{2.60}$$

This is the analogue of Eqs. (2.43) and (2.50) for the traveling wave $\boldsymbol{\varphi}^{\rightleftarrows}$-*basis*.

Exercise 2.27. Find explicitly the linear combination coefficients in (2.60) in terms of the initial displacements and velocities of the lattice points.

For any set of linear combination constants, Eq. (2.60) tells us that any vibration state of the lattice can be decomposed into $2N$ traveling waves. As each $m^{\rightleftarrows}$-set of waves travels with its own velocity (2.57), any initial shape of the lattice, even if it is composed only of waves traveling in one direction, will be changed: different constituent waves travel with different velocities. A discrete lattice therefore cannot carry definite "signals" other than pure sinusoidal forms, as their shape is eventually lost. Such media are called *dispersive*.

2.3.9. Lattice Models for Dispersive Media

Since crystals are physical systems modeled by lattices with a very large number of masses N, one can ask how and when the dispersion of signals appears. Note that the velocity diagram, Fig. 2.15, has the same shape for all N, except for the "actual" points corresponding to integer values of m, which come closer together as N increases. The curve v_m, for very small values of m/N, can be approximated by the constant v_0 in Eq. (2.58). If our

signal is composed only of low-m partial waves, whose wavelengths are very much larger than the interparticle separation in the lattice, the signal will propagate, to a good approximation, with no loss of shape, as all constituent waves have the same propagation velocity. In this *linear approximation*, dispersion is absent. The dispersion of signals—mechanical or electromagnetic—gives some information of the "granularity" of the medium. This statement still holds (with the appropriate adaptations) even when the "microscopic" model of a system which "in the large" satisfies the wave equation is not that of a vibrating lattice. Sound propagation in gases or amorphous materials, for instance, can rely on different microscopic models.

As the preceding discussion may suggest, when a mechanical lattice is proposed as a microscopic model for a system, the relevant information is mostly that of the spectrum of oscillation frequencies, transmittable wavelengths, and the like. There is little experimental content in specifying arbitrary initial conditions or following the vibration of individual atoms. In this sense, the Brillouin diagram and its three-dimensional version for various crystalline lattices contain much information, and accordingly we shall time and again cast our results in these terms.

Exercise 2.28. Assume the lattice is damped. Follow the discussion in this section for this case. Note that little is changed except for the fact that the oscillation frequencies ω_m become complex. Generally, there will be overdamped as well as oscillatory solutions, the former ones for small values of m and the latter ones for large m's.

Exercise 2.29. Consider a one-dimensional lattice with *fixed ends*. This can mean that the first and last masses are held fixed [Fig. 2.16(a)] or that the midpoints of two springs are constrained [Fig. 2.16(b)]. Show that the "method of images" appears as a natural way to phrase the problem: Assume that a free N-point lattice (N even) has initial conditions which are *odd* under inversions through $\mathbb{I}_0$ or $\mathbb{K}_0$, as then, for all t, the resulting state vector $\mathbf{f}(t)$ will have the same property. If $\mathbb{I}_0\mathbf{f}(t) = -\mathbf{f}(t)$, masses N and $N/2$ are fixed, while if $\mathbb{K}_0\mathbf{f}(t) = -\mathbf{f}(t)$, the midpoint of the springs joining the mass pairs $(N,1)$ and $(\frac{1}{2}N, \frac{1}{2}N - 1)$ pass through the equilibrium position. The actual lattice (Fig. 2.16) is one-half of the proposed free lattice.

Exercise 2.30. Examine the allowed normal modes which can be present in the above "extended" lattice: In Eq. (2.50) only f_m^- and $\dot{f}_m^-$ can be nonzero for Fig. 2.16(a) and analogously (see Exercise 2.24) for the lattice in Fig. 2.16(b). In terms of traveling waves, show that only combinations of $\varphi^{m\rightarrow} + \varphi^{m\leftarrow}$ are allowed to appear in the former. What about the corresponding combinations in the latter?

Exercise 2.31. What happens with the Brillouin and similar diagrams for the lattice with fixed ends? Show that over the "physical" half-lattice orthogonality and completeness for the odd modes still hold.

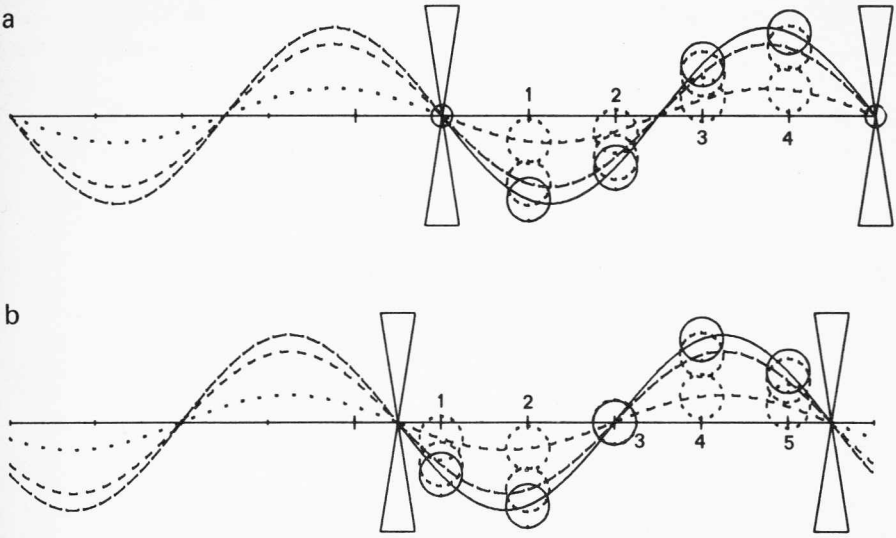


Fig. 2.16. Lattices with two fixed (a) masses, (b) string midpoints. These can be accommodated into a lattice with double the number of masses with restrictions on the allowed vibration modes. Half of the lattice will serve as a "negative mirror image" of the original.

Exercise 2.32. We can consider lattices where the two endpoints are *free*. See that this is well represented, as before, by a closed lattice whose state vectors are *even* under reflection by $\mathbb{I}_0$. A similar analysis follows.

In this part we have for generality concentrated on the description of closed lattices and relegated the study of the fixed-endpoint system to the foregoing exercises. In Part II, the study of the vibrating string will be done almost exclusively on the fixed-endpoint problem.

2.4. Farther-Neighbor Interaction, Molecular and Diatomic Lattices

The concepts developed in Section 2.3 for the simple lattice with only first-neighbor interactions and equal springs and masses will be applied now to systems where each one of these restrictions in turn is lifted in order to examine the features which characterize these extensions.

2.4.1. Farther-Neighbor Interaction and Uncoupling

Lattices with farther-than-first-neighbor interactions (see Fig. 2.17) are certainly relevant in crystallography where the interaction between the

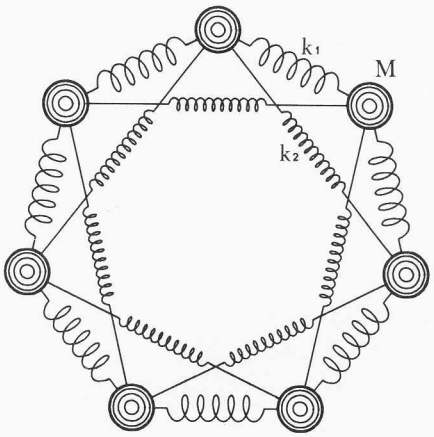


Fig. 2.17. Mechanical model of a linear, closed lattice with first- and second-neighbor interactions.

lattice atoms is electromagnetic and a first-neighbor "spring" model is at best only a good approximation. When describing the interaction term in the lattice equation of motion [Eqs. (2.19)–(2.22)] we allowed for pth neighbor forces through springs of Hooke's constant $k_{n,n\pm p}$ and noted only that $k_{nm} = k_{mn}$ is the requirement of action–reaction equality. Here we shall restrict the lattice to have the same Hooke's constant between all pth neighbors (as shown in Fig. 2.17 for $p = 1$ and $p = 2$) so that $k_p \coloneqq k_{n,n\pm p}$ is independent of n. The simple lattice has only $k_1 \neq 0$, while in the general case we can consider k_p for p from zero (each mass attached to its equilibrium position by a spring k_0) up to $p = \pi(N)$ [$\pi(N) \coloneqq (N-1)/2$ for N odd, and $\pi(N) = N/2$ for N even, taking care to note that in this case *two* springs $k_{N/2}$ join opposite masses]. In this general case, the interaction operator $\mathbb{K}$ of Eq. (2.21) is represented in the $\boldsymbol{\varepsilon}$-basis by a matrix $\mathbf{K}$ with elements

$$\kappa_{nm} = -k_{|n-m|} + 2\delta_{nm} \sum_{p=0}^{\pi(N)} k_p. \tag{2.61}$$

[See Eq. (2.19), recalling that row and column indices are taken modulo N.] The matrix $\mathbf{K}$ therefore has entries $k_0' \coloneqq k_0 + 2\sum_{p=1}^{\pi(N)} k_p$ along the main diagonal and $-k_p$ on diagonals p units on both sides of the main one. For representation purposes it is convenient to write $\mathbf{K}$ in terms of the dihedral matrix representatives [Eq. (1.88)] as

$$\mathbf{K} = k_0'\mathbf{1} - \sum_{p=1}^{\pi(N)} k_p(\mathbf{R}^p + \mathbf{R}^{-p}) \tag{2.62}$$

and correspondingly for the operators themselves. In this way, it is easily

seen that $\mathbb{K}$ is represented by a diagonal matrix in the φ-basis, since the $\mathbb{R}$'s are so represented [Eq. (1.91)]. Quite simply, then,

$$\begin{aligned}\tilde{K}_{mn} &= \delta_{mn}\left\{k_0' - \sum_{p=1}^{\pi(N)} k_p[\exp(2\pi ipm/N) + \exp(-2\pi ipm/N)]\right\} \\ &= \delta_{mn}\left[k_0' - 2\sum_{p=1}^{\pi(N)} k_p \cos(2\pi pm/N)\right] \\ &= \delta_{mn}\left[k_0 + 4\sum_{p=1}^{\pi(N)} k_p \sin^2(\pi pm/N)\right] =: \delta_{mn}\kappa_m. \end{aligned} \tag{2.63}$$

2.4.2. Brillouin Frequency Diagram

The lattice then uncouples into N oscillators with constants $\kappa_m := \tilde{K}_{mm}$ [Eq. (2.22)], and the allowed oscillation frequencies of the system are given by

$$\omega_m = (\kappa_m/M)^{1/2} = 2\left[k_0/4M + \sum_{p=1}^{\pi(N)} (k_p/M)\sin^2(\pi pm/N)\right]^{1/2} \tag{2.64}$$

[compare with Eqs. (2.27) and (2.28)]. The development of Sections 2.2 and 2.3 applies *verbatim* to this lattice with only a change in the values of the allowed angular frequencies (2.64). A Brillouin diagram for this lattice is shown in Fig. 2.18.

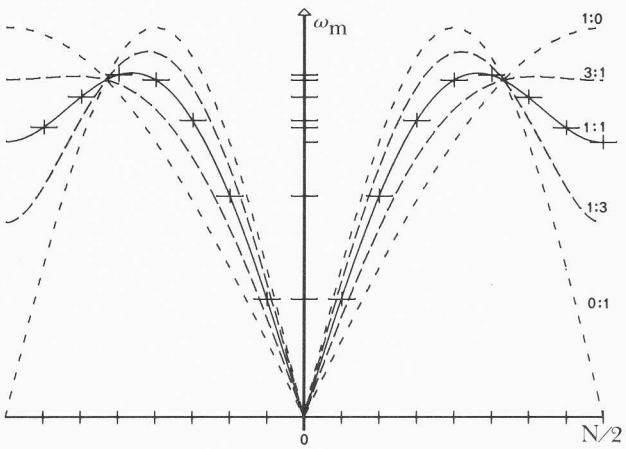


Fig. 2.18. Brillouin frequency diagram for a lattice with first- and second-neighbor interactions through spring constants k_1 and k_2. Curves are plotted for various ratios $k_1:k_2$. If $k_1:k_2 :: 1:0$, we obtain the first-neighbor case (Fig. 2.10). In the other extreme, if $k_1:k_2 :: 0:1$, we obtain two uncoupled lattices of the former type, which results in a doubling of the simple lattice first Brillouin zone.

Exercise 2.33. Note that if $k_0 \neq 0$ the zeroth mode becomes a true oscillation mode. What is the effect on the Brillouin diagram in Fig. 2.18?

Exercise 2.34. Describe the fundamental solutions, elements of Green's matrix, and normal modes of this lattice.

Exercise 2.35. Find the propagation velocities of the traveling waves.

Exercise 2.36. Note that instead of expanding $\mathbf{K}$ in powers of $\mathbf{R}$ as was done in Eq. (2.62), one could expand it in powers of $\boldsymbol{\Delta}$. For the case of first- and second-neighbor interaction only, this leads to $\mathbf{K} = -(k_1 + 4k_2)\boldsymbol{\Delta} - k_2\boldsymbol{\Delta}^2$. Arrive at the result (2.64) for this case and the more general pth-neighbor interaction case.

Exercise 2.37. Suppose only $k_2 \neq 0$. Show that if N is even the lattice uncouples into two $N/2$-mass lattices. What if N is odd?

Exercise 2.38. Introduce viscous damping into the problem.

2.4.3. Molecular Lattices

We consider now a lattice with two kinds of first-neighbor interaction: one with Hooke's constant k_1 between masses N and 1, 2 and 3, etc., up to $N - 2$ and $N - 1$ (note that N is even) and another with k_2 between 1 and 2, etc., up to $N - 1$ and N, as in Fig. 2.19. Such a system is said to be a *molecular* lattice.

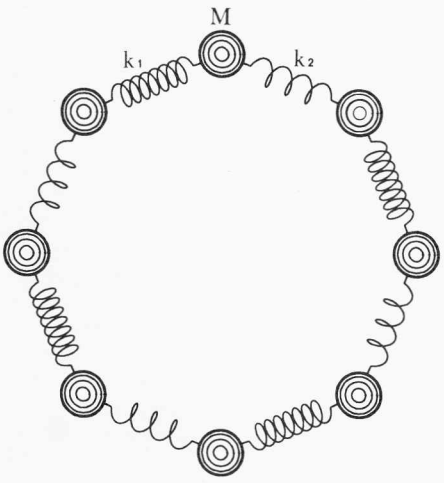


Fig. 2.19. Molecular lattice. Springs with constants k_1 and k_2 alternate between the masses.

The interaction operator will no longer be represented by a matrix constant along the diagonals as in (2.62) but, from (2.19), by

$$\mathbf{K} = \begin{pmatrix} k_1 + k_2 & -k_2 & & & 0 & -k_1 \\ -k_2 & k_1 + k_2 & -k_1 & & & 0 \\ & -k_1 & k_1 + k_2 & -k_2 & & \\ & & -k_2 & \ddots & \ddots & -k_2 \\ 0 & & & \ddots & k_1 + k_2 & -k_2 \\ -k_1 & & 0 & & -k_2 & k_1 + k_2 \end{pmatrix}. \tag{2.65}$$

In terms of simpler matrices which have appeared before [Eqs. (1.67a) and (1.88a)], we can write (2.65) as

$$\mathbf{K} = (k_1 + k_2)\mathbf{1} - k_1(\mathbf{E}_1\mathbf{R} + \mathbf{R}^{-1}\mathbf{E}_1) - k_2(\mathbf{E}_1\mathbf{R}^{-1} + \mathbf{R}\mathbf{E}_1) \tag{2.66}$$

and correspondingly for the represented operators. Manifestly, (2.65) is a hermitian matrix, while in (2.66) the hermiticity is also evident, as $\mathbf{E}_1$ is hermitian and $\mathbf{R}$ unitary. The dihedral symmetry D_N of the original simple lattice is broken, and we are left only with invariance transformations which are powers of $\mathbb{R}^2$ and the $\mathbb{K}$'s (Section 1.6) which by themselves form a subgroup of D_N. The odd powers of $\mathbb{R}$ and the $\mathbb{I}$'s will exchange springs k_1 and k_2.

2.4.4. The Interaction Matrix and First Uncoupling

Following earlier treatments of the D_N-symmetric lattices, let us write the equation of motion $\mathbb{M}\ddot{\mathbf{f}} + \mathbb{K}\mathbf{f} = 0$ in the $\boldsymbol{\varphi}$-basis. In this we can aid ourselves with Eqs. (1.67), which have four diagonal blocks, and (1.91), which is completely diagonal, in order to arrive, after some calculation, at

$$\tilde{\mathbf{K}} = \begin{pmatrix} 2(k_1 + k_2)\|\delta_{mn}\sin^2(\pi m/N)\| & i(k_2 - k_1)\|\delta_{mn}\sin(2\pi m/N)\| \\ -i(k_2 - k_1)\|\delta_{mn}\sin(2\pi m/N)\| & 2(k_1 + k_2)\|\delta_{mn}\cos^2(\pi m/N)\| \end{pmatrix}, \tag{2.67}$$

where $\|\delta_{mn}\nu(n)\|$ are $N/2 \times N/2$ diagonal submatrices with $\nu(n)$, $n = 1, 2, \ldots, N/2$, along the diagonal. The matrix (2.67) is thus hermitian, as it should be, and composed of *four diagonal blocks*. The Fourier transform has failed here to produce a completely diagonal matrix. It has, however, considerably simplified the problem since the original equations of motion $M\ddot{f}_n = -\sum_k K_{nk}f_k$ were fully coupled, whereas now $M\ddot{\tilde{f}}_m = -\sum_k \tilde{K}_{mk}\tilde{f}_k$, due to the form (2.67) of $\tilde{\mathbf{K}}$, consists of $N/2$ uncoupled pairs of equations. These are

$$M\ddot{\tilde{f}}_m = -2(k_1 + k_2)\sin^2(\pi m/N)\tilde{f}_m - i(k_2 - k_1)\sin(2\pi m/N)\tilde{f}_{m+N/2}, \tag{2.68a}$$

$$M\ddot{\tilde{f}}_{m+N/2} = i(k_2 - k_1)\sin(2\pi m/N)\tilde{f}_m - 2(k_1 + k_2)\cos^2(\pi m/N)\tilde{f}_{m+N/2}, \quad m = 1, 2, \ldots, N/2 - 1, \tag{2.68b}$$

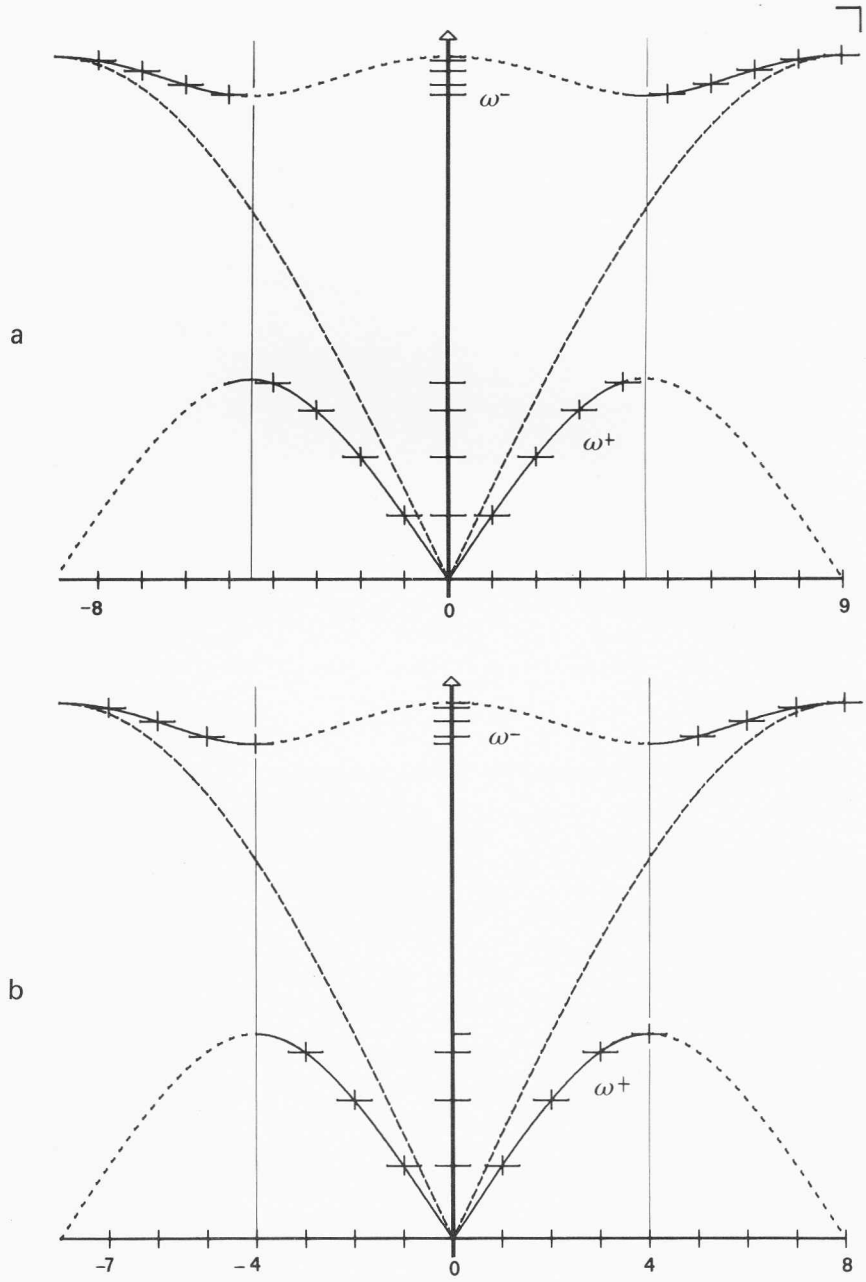


Fig. 2.20. "Extended" Brillouin diagram for the frequencies of a molecular lattice of N masses where (a) $N/2$ is odd ($N = 18$) and (b) $N/2$ is even ($N = 16$) for a ratio $k_\delta/k_\sigma = \frac{1}{2}$. The dotted line represents the Brillouin diagram of an equal-spring lattice. The allowed frequencies, roots of Eq. (2.70) [$\omega_m{}^\pm \sim (-\alpha_m{}^\pm)^{1/2}$; see Eq. (2.80)], thus become the double-period "optic" and "acoustic" branches of the diagram.

and

$$M\ddot{\tilde{f}}_{N/2} = -2(k_1 + k_2)\tilde{f}_{N/2}, \qquad M\ddot{\tilde{f}}_N = 0. \tag{2.68c}$$

Notice first that Eqs. (2.68c) correspond exactly to (2.27) for $m = N/2$ and $m = N$ *for a simple lattice with spring constant* $k_\sigma := (k_1 + k_2)/2$. The solutions will be given then by Eqs. (2.28) for these values of m and k, so we can start drawing our new Brillouin diagram for the molecular lattice by fixing these two values of λ'_m, eigenvalues of $-k_\sigma^{-1}\mathbb{K}$. See Fig. 2.20 for $m = 0$ and $m = N/2$, the dotted line representing the simple lattice with $k_\sigma := (k_1 + k_2)/2$.

2.4.5. Complete Uncoupling

For Eqs. (2.68a)–(2.68b), some further uncoupling is necessary: using the λ_m, $m = 1, 2, \ldots, N$, eigenvalues of $\mathbb{A}$, we can write them as

$$M\ddot{\tilde{\mathbf{f}}}^{(m)} = k_\sigma \tilde{\mathbf{A}}^{(m)} \tilde{\mathbf{f}}^{(m)} \tag{2.69a}$$

with

$$\tilde{\mathbf{f}}^{(m)} := \begin{pmatrix} \tilde{f}_m \\ \tilde{f}_{m+N/2} \end{pmatrix},$$

$$\tilde{\mathbf{A}}^{(m)} := \begin{pmatrix} \lambda_m & i(k_\delta/k_\sigma)(\lambda_m \lambda_{m+N/2})^{1/2} \\ -i(k_\delta/k_\sigma)(\lambda_m \lambda_{m+N/2})^{1/2} & \lambda_{m+N/2} \end{pmatrix}, \tag{2.69b}$$

where $k_\delta := (k_2 - k_1)/2$ and k_σ as before. The 2×2 hermitian matrix $\tilde{\mathbf{A}}^{(m)}$ can be diagonalized exactly [see Eqs. (1.119) and (1.120)], obtaining for its eigenvalues

$$\begin{aligned} \alpha_m{}^{\pm} &:= (\lambda_m + \lambda_{m+N/2})/2 \pm \{[(\lambda_m - \lambda_{m+N/2})/2]^2 + (k_\delta/k_\sigma)^2 \lambda_m \lambda_{m+N/2}\}^{1/2} \\ &= -2 \pm 2[\cos^2(2\pi m/N) + (k_\delta/k_\sigma)^2 \sin^2(2\pi m/N)]^{1/2} \\ &= \alpha^{\pm}_{N/2-m}. \end{aligned} \tag{2.70}$$

Comparing with the equal-spring system ($k_\delta \to 0$), we recognize that $\alpha_m{}^+ \to \lambda_m = \lambda_{N-m}$ and $\alpha_m{}^- \to \lambda_{N/2-m} = \lambda_{N/2+m}$. Reflection symmetry under the exchange $m \leftrightarrow N/2 - m$ holds from (2.70). For $m = 0$, the cases (2.68c) are also correctly reproduced in (2.70). We can thus denote the eigenvalues of $-\mathbb{K}$ as $k_\sigma \lambda'_m$, $m = 1, 2, \ldots, N$ [in analogy with those of $\mathbb{A}$; see Eq. (2.27b)], where

$$\lambda'_m = \lambda'_{N-m} = \alpha_m{}^+ = \alpha^+_{N/2-m}, \tag{2.71a}$$

$$\lambda'_{N/2-m} = \lambda'_{N/2+m} = \alpha_m{}^- = \alpha^-_{N/2-m},$$

$$m = 0, 1, 2, \ldots, \begin{cases} N/4 - 1 & \text{for } N/2 \text{ even}, \\ (N-2)/4 & \text{for } N/2 \text{ odd}, \end{cases} \tag{2.71b}$$

and

$$\lambda'_{N/2} = \alpha^{+}_{N/4}, \qquad \lambda'_{3N/4} = \alpha^{-}_{N/4} \quad \text{when } N/2 \text{ even.} \tag{2.71c}$$

2.4.6. Oscillation Frequencies and Shifts

The meaning of the rather involved numbering used above should be apparent in Figs. 2.20(a) and (b) for odd and even $N/2$, respectively. The spectrum of $\mathbb{K}$ modifies that of $-k\mathbb{\Delta}$ in that (a) the eigenvalues λ'_m divide into two sets: those due to the α^{+}'s and those due to the α^{-}'s, as

$$0 = \lambda'_0 \leqslant |\alpha_m{}^{+}| \leqslant 2 - 2|k_\delta/k_\sigma| \leqslant 2 + 2|k_\delta/k_\sigma| \leqslant |\alpha_m{}^{-}| \leqslant |\lambda'_{N/2}| = 4; \tag{2.72}$$

in between, there is a *gap* of height $4|k_\delta/k_\sigma|$; (b) the α^{-}'s raise "wings," while the α^{+}'s lower them by the same amount:

$$\alpha_m{}^{+} - \lambda_m = \lambda_{N/2-m} - \alpha_m{}^{-} \geqslant 0. \tag{2.73}$$

The slope of the curve for λ'_m in Fig. 2.20 remains positive for m between 0 and $N/2$ and vanishes for $m = 0$, $N/4$ and $N/2$. The inequality (2.72) holds for all values of $|k_\delta/k_\sigma|$, preventing the "wings" from topping $\lambda'_{N/2}$.

Exercise 2.39. Show that for small $|k_\delta/k_\sigma|$

$$\alpha_m{}^{+} - \lambda_m \simeq (k_\delta/k_\sigma)^2 \sin^2(2\pi m/N). \tag{2.74}$$

Exercise 2.40. When one of the springs vanishes ($k_2 \to 0$) we are left with $N/2$ simple oscillators. What happens with the spectrum of $\mathbb{K}$?

2.4.7. Optic and Acoustic Modes

The eigenvectors of the submatrix $\tilde{\mathbf{A}}^{(m)}$ which involves the m and $(N/2 + m)$ rows and columns of the interaction matrix $\tilde{\mathbf{K}}$ will now be found. For

$$\tilde{\mathbf{A}}^{(m)}\mathbf{x}^{m\pm} = \alpha_m{}^{\pm}\mathbf{x}^{m\pm}, \qquad \mathbf{x}^{m\pm} = \begin{pmatrix} x_{1_l}^{m\pm} \\ x_2^{m\pm} \end{pmatrix}, \tag{2.75}$$

the ratios of the components can be conveniently written, using (2.69b), (2.70), (2.73), and identities between the λ's, as

$$-i\rho_m := \frac{x_2^{m+}}{x_1^{m+}} = -i\frac{k_\sigma}{k_\delta}\frac{\alpha_m{}^{+} - \lambda_m}{2\sin(2\pi m/N)} = -i\frac{k_\sigma}{k_\delta}\frac{\lambda_{N/2-m} - \alpha_m{}^{-}}{2\sin(2\pi m/N)} = \frac{x_1^{m-}}{x_2^{m-}}, \tag{2.76}$$

where $0 \leqslant \rho_m < 1$. In this form it is manifest that as the springs become equal ($k_\delta \to 0$, $\rho_m \to 0$), $\mathbf{x}^{m+}$ has a vanishing lower component and $\mathbf{x}^{m-}$ a vanishing upper one. In this case $\tilde{f}_m\boldsymbol{\varphi}_m$ and $\tilde{f}_{m+N/2}\boldsymbol{\varphi}_{m+N/2}$ in (2.69) give, for

their coefficients $\tilde{f}_m(t)$ and $\tilde{f}_{m+N/2}(t)$, uncoupled differential equations. In general, however, the eigenvectors of the molecular lattice will be a superposition of $\boldsymbol{\varphi}_m$ and $\boldsymbol{\varphi}_{m+N/2}$ with the ratio (2.76). We can thus define, corresponding to the eigenvalues $-k_\sigma \alpha_m{}^{\pm}$ of the interaction operator,

$$\boldsymbol{\psi}_m{}^{+} \coloneqq x_1^{m+}\boldsymbol{\varphi}_m + x_2^{m+}\boldsymbol{\varphi}_{m+N/2} = x_1^{m+}(\boldsymbol{\varphi}_m - i\rho_m\boldsymbol{\varphi}_{m+N/2}) \qquad \text{for } \alpha_m{}^{+}, \quad (2.77a)$$

$$\boldsymbol{\psi}_m{}^{-} \coloneqq x_1^{m-}\boldsymbol{\varphi}_m + x_2^{m-}\boldsymbol{\varphi}_{m+N/2} = x_2^{m-}(-i\rho_m\boldsymbol{\varphi}_m + \boldsymbol{\varphi}_{m+N/2}) \qquad \text{for } \alpha_m{}^{-}, \quad (2.77b)$$

which constitute an orthonormal basis for $\mathscr{V}^N$ once the proper coefficients x_1^{m+} and x_2^{m-} are determined:

$$|x_1^{m+}| = (1 + \rho_m{}^2)^{-1/2} = |x_2^{m-}|. \quad (2.77c)$$

[To keep the index bureaucracy straight, we remark that the range of indices in (2.77) follows that in (2.71) and that in the case $m = 0$ or $N/2$, ρ_m is undefined, as we have only $\boldsymbol{\psi}_0{}^{+} = \boldsymbol{\varphi}_N$ and $\boldsymbol{\psi}_{N/2}^{-} = \boldsymbol{\varphi}_{N/2}$.] Expanding now the sought for solution $\mathbf{f}(t)$ in terms of the $\boldsymbol{\psi}^{\pm}$-basis (2.77),

$$\mathbf{f}(t) = \sum_{m,\pm} \bar{f}_{m,\pm}(t)\boldsymbol{\psi}_m{}^{\pm}, \quad (2.78)$$

the equation of motion for the molecular lattice [Eq. (2.21) with the interaction matrix (2.65)] uncouples completely as

$$M\ddot{\bar{f}}_{m,\pm} + k_\sigma \alpha_m{}^{\pm}\bar{f}_{m,\pm} = 0. \quad (2.79)$$

Its solutions were worked out before in Section 2.1 and are of the purely oscillating type (2.7), with angular frequencies

$$\omega_m{}^{\pm} = (k_\sigma/M)^{1/2}(-\alpha_m{}^{\pm})^{1/2}. \quad (2.80)$$

2.4.8. Brillouin Diagrams

We have drawn the Brillouin diagram corresponding to (2.80) in Fig. 2.21, where, as is customary, only the range of m between $\pm N/4$ is represented. Figure 2.21 shows that the oscillator frequencies divide into two sets: the so-called *acoustical band* for the ω^{+}'s, which involves low frequencies, and the *optical band* for the ω^{-}'s, which involves a range of higher frequencies. They are separated by the gap which is called the *stopping* band. This nomenclature stems from solid-state physics and refers to the fact that in actual crystals the frequencies correspond, respectively, to mechanical acoustic vibrations and electromagnetically induced oscillating fields in the optical range which the crystal is able to carry or transmit. It is opaque for frequencies outside these bands. Electric circuits acting as low-pass or high-pass filters work on the same principles.

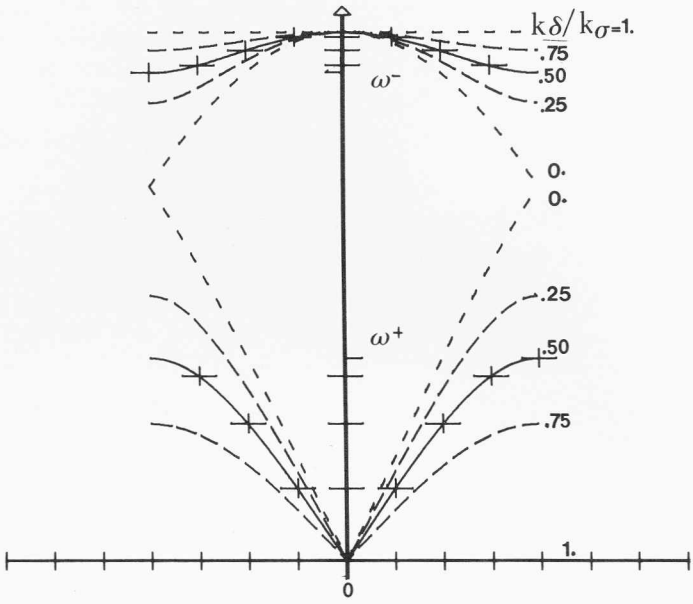


Fig. 2.21. Usual Brillouin frequency diagram for a molecular (and diatomic) lattice extending on integer values within $\pm N/4$. It has been plotted for various values of k_δ/k_σ. If this ratio is zero, the simple lattice diagram is regained; on the other extreme, if $k_1 = 0$, the lattice breaks up into $N/2$ two-mass dumbbells. As each has only zero and its natural oscillation frequency, we obtain two clusters of $N/2$-fold degenerate frequencies.

2.4.9. General Description of the Solutions

In spite of the rather lengthy derivation, the orthonormal $\boldsymbol{\psi}^{\pm}$-basis in Eqs. (2.77) is clearly the "natural" basis for the description of the molecular lattice. Most of the developments of Section 2.2 and 2.3 follow unchanged as follows: (a) Once the solution for the coordinates $\bar{f}_m(t)$ is found in terms of initial conditions, it assumes precisely the form (2.28) in terms of functions $\bar{G}_m(\tau)$ and their time derivatives, where the proper oscillation frequencies (2.80) appear. These constitute the $\boldsymbol{\psi}^{\pm}$-basis representative of the self-adjoint *Green's operator* $\mathbb{G}(\tau)$, whose expression in other bases—notably the "physical" $\boldsymbol{\varepsilon}$-basis—can be calculated leading to the general form (2.29) of the solution. (b) *Fundamental solutions*, for initial conditions of single vectors in the $\boldsymbol{\varepsilon}$-basis, can be found. (c) The basis vectors $\boldsymbol{\psi}_m{}^{\pm}$ do not have purely real coordinates in the $\boldsymbol{\varepsilon}$-basis, so in order to produce *normal modes* we must find a more appropriate basis. We can consider an eigenbasis of $\mathbb{K}_0$ (the dihedral operator, using the results of Exercises 1.54 and 1.57) and replace the $\boldsymbol{\varphi}_m$'s in (2.77) by the $\boldsymbol{\varphi}'^{\pm}_m$'s of that basis. We can also build *real* eigenvectors out of (2.77), recalling that complex conjugation in the $\boldsymbol{\varphi}$-basis is defined through

$\varphi_m^* \coloneqq \varphi_{N-m}$. Consideration of initial conditions given by single vectors in this real basis will lead to normal modes as (2.48) with the new ω_m's and two trigonometric summands in place of one.

Exercise 2.41. Find explicitly the unitary transformation linking the ε- and the $\psi^{\pm}$-bases.

Exercise 2.42. When obtaining the nth coordinate in the ε-basis of $\psi_m{}^{\pm}$, you will notice that they behave like $\exp(-2\pi imn/N)$ times $[1 - (-1)^n i\rho_m]$ for the acoustical band eigenvectors and like the same function times $[-i\rho_m + (-1)^n]$ for the optical band eigenvectors. In the latter modes, then, first neighbors oscillate—on the average—on opposite sides of the equilibrium line, while for the acoustical modes they tend to be on the same side. See Fig. 2.22.

Exercise 2.43. Will the Green's matrix in the ε-basis be an even function of $|n - m|$ as it was in (2.33)? What should be its main characteristics?

Exercise 2.44. Can you find an eigenbasis related to (2.77) which is also an eigenbasis of $\mathbb{I}_0$? Why not?

Exercise 2.45. Consider finding *traveling* wave solutions for the molecular lattice.

Exercise 2.46. Introduce viscous damping into the problem.

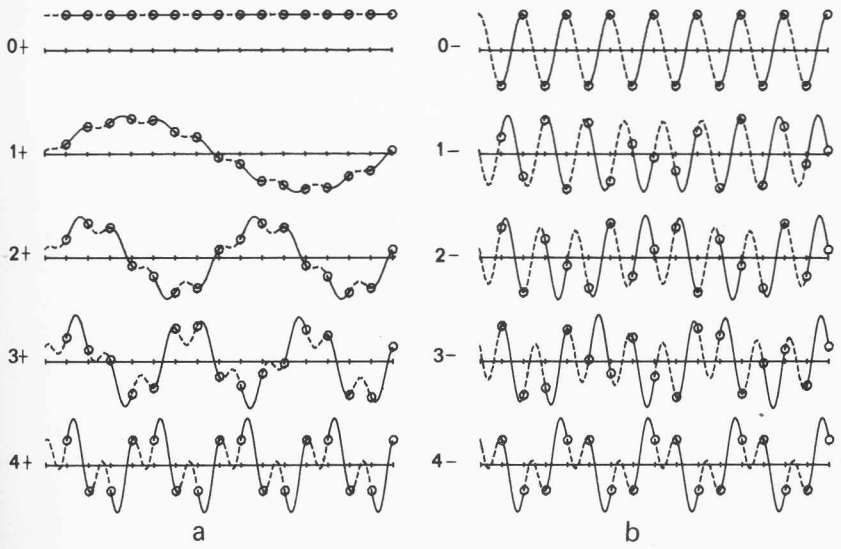


Fig. 2.22. (a) Acoustic, and (b) optic oscillation modes for a molecular lattice with 16 masses (circles). Springs k_1 and k_2 are represented by broken and unbroken lines, plotted for real values of the abscissa. The spring ratio is $k_\delta/k_\sigma = \frac{1}{2}$.

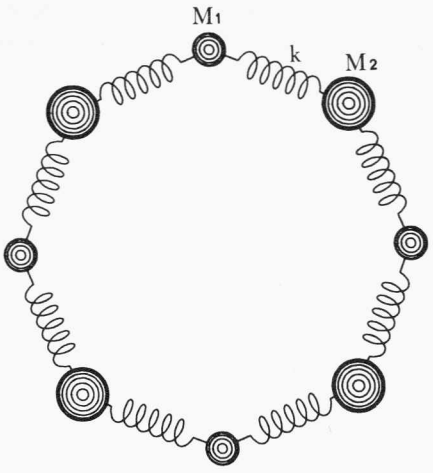


Fig. 2.23. Diatomic lattice. Masses M_1 and M_2 alternate.

2.4.10. Diatomic Lattices

The *diatomic* lattice (see Fig. 2.23) is a lattice with two alternating masses M_1 and M_2. It has several features in common with the molecular lattice and some differences as well. The intertial operator was up to now a multiple M of the unit operator [Eq. (2.21)]. For the diatomic lattice, it will be represented in the $\boldsymbol{\varepsilon}$-basis by a diagonal $N \times N$ matrix (N even) with M_1 in the odd and M_2 in the even position. In terms of matrices we have introduced before [Eqs. (1.67)], we can write

$$\mathbf{M} = \begin{pmatrix} M_1 & & & & 0 \\ & M_2 & & & \\ & & M_1 & & \\ & & & \ddots & \\ 0 & & & & M_2 \end{pmatrix} = M_1\mathbf{E}_1 + M_2\mathbf{E}_2, \tag{2.81}$$

and the (undamped) equation of motion can be written as

$$\ddot{\mathbf{f}} + \mathbb{M}^{-1}\mathbb{K}\mathbf{f} = 0. \tag{2.82}$$

2.4.11. Diagonalization of a Nonhermitian Matrix

Our procedure up to now has been to find the eigenvectors and -values of the interaction operator in order to find a basis of $\mathscr{V}^N$ where the lattice equations uncouple. The problem with Eq. (2.82) is that $\mathbb{M}^{-1}\mathbb{K}$ is *not* a hermitian operator. Although the two factors *are* hermitian, they do not

commute. Yet $\mathbb{M}^{-1}\mathbb{K}$ is not too "far" from being hermitian; in the φ-basis it is represented by

$$(M_1\tilde{\mathbf{E}}_1 + M_2\tilde{\mathbf{E}}_2)^{-1}\tilde{\mathbf{K}} = (M_1^{-1}\tilde{\mathbf{E}}_1 + M_2^{-1}\tilde{\mathbf{E}}_2)\tilde{\mathbf{K}}$$

$$= \begin{pmatrix} \mu_\sigma \| \delta_{mn}\kappa_m \| & \mu_\delta \| \delta_{mn}\kappa_{m+N/2} \| \\ \mu_\delta \| \delta_{mn}\kappa_m \| & \mu_\sigma \| \delta_{mn}\kappa_{m+N/2} \| \end{pmatrix}, \qquad \begin{cases} \mu_\sigma := (\mu_1^{-1} + \mu_2^{-1})/2, \\ \mu_\delta := (\mu_2^{-1} - \mu_1^{-1})/2, \end{cases} \tag{2.83}$$

where we have used the result (1.67) on the $\tilde{\mathbf{E}}_i$ and Eq. (2.63) for the form of the general pth-neighbor equal-spring interaction matrix. We are representing an $N/2 \times N/2$ diagonal matrix with elements $\nu(n)$ by $\| \delta_{nm}\nu(m) \|$ as in Eq. (2.67). All 2×2 submatrices formed by taking the intersections of the nth and mth row and column are diagonal and hermitian except when $m = n + N/2$.

Exercise 2.47. Show that $\mathbb{M}^{-1}\mathbb{K}$, in its ε-basis representation, has two $N/2 \times N/2$ hermitian submatrices: those constituted by the even- or odd-rowed and -columned elements of the original matrix.

The nondiagonal 2×2 submatrices are

$$\tilde{\mathbf{K}}^{(m)} := \begin{pmatrix} \mu_\sigma\kappa_m & \mu_\delta\kappa_{m+N/2} \\ \mu_\delta\kappa_m & \mu_\sigma\kappa_{m+N/2} \end{pmatrix} =: \mu_\sigma k_1 \tilde{\mathbf{B}}^{(m)}. \tag{2.84}$$

Their eigenvalues can be found by applying (1.120) and extracting the factor $\mu_\sigma k_1$:

$$k_1\beta_m{}^{\pm} = (\kappa_m + \kappa_{m+N/2})/2 \pm \{[(\kappa_m - \kappa_{m+N/2})/2]^2 + (\mu_\delta/\mu_\sigma)^2\kappa_m\kappa_{m+N/2}\}^{1/2}. \tag{2.85}$$

The spectrum of (2.84) and (2.85) looks very much like the molecular lattice spectrum (2.70). Indeed, for first-neighbor interactions only, we have $\kappa_m = k_1\lambda_m$, and the expressions for $\beta_m{}^{\pm}$ in the two-mass case and $\alpha_m{}^{\pm}$ for the molecular case in (2.70) become *identical* under the formal substitution

$$\frac{k}{M_1} \to \frac{k_1}{M}, \qquad \frac{k}{M_2} \to \frac{k_2}{M}, \qquad \text{i.e.,} \quad \frac{\mu_\delta}{\mu_\sigma} \to \frac{k_\delta}{k_\sigma}. \tag{2.86}$$

2.4.12. Oscillation Frequencies

The Brillouin diagram for the diatomic first-neighbor interaction lattices is then given by Fig. 2.21 with the same eigenvalue numbering and the appropriate label changes: for $M_2 \to M_1$, $\mu_\delta \to 0$ and $k_1\beta_m{}^{+} \to \kappa_m$, $k_1\beta_m{}^{-} \to \kappa_{m+N/2}$. For the pth-neighbor interacting lattice another property of the

molecular case carries over: the raising of the optical band "wings" equals the lowering of the acoustical band ones,

$$k_1\beta_m^{+} - \kappa_m = \kappa_{m+N/2} - k_1\beta_m^{-} \geqslant 0. \tag{2.87}$$

For the general diatomic lattice, the Brillouin diagram can thus be constructed based on the monatomic one in Fig. 2.18.

2.4.13. Optic and Acoustic Modes

Finding the eigenvectors $\mathbf{y}^{m\pm}$ of (2.84) corresponding to $\beta_m^{\pm}$ is an exercise parallel to (2.75)–(2.76). Indeed, using analogous notation,

$$\begin{aligned} \rho_m^{+} &:= \frac{y_2^{m+}}{y_1^{m+}} = \frac{\mu_\sigma}{\mu_\delta}\frac{k_1\beta_m^{+} - \kappa_m}{\kappa_{m+N/2}} \geqslant 0, \\ \rho_m^{-} &:= \frac{y_1^{m-}}{y_2^{m-}} = \frac{\mu_\sigma}{\mu_\delta}\frac{k_1\beta_m^{-} - \kappa_{m+N/2}}{\kappa_m} \geqslant 0. \end{aligned} \tag{2.88}$$

It follows that the eigenvectors of $\mathbb{M}^{-1}\mathbb{K}$ are

$$\hat{\boldsymbol{\psi}}_m^{+} := y_1^{m+}\boldsymbol{\varphi}_m + y_2^{m+}\boldsymbol{\varphi}_{m+N/2} = y_1^{m+}(\boldsymbol{\varphi}_m + \rho_m^{+}\boldsymbol{\varphi}_{m+N/2}), \tag{2.89a}$$

$$\hat{\boldsymbol{\psi}}_m^{-} := y_1^{m-}\boldsymbol{\varphi}_m + y_2^{m-}\boldsymbol{\varphi}_{m+N/2} = y_1^{m-}(\rho_m^{-}\boldsymbol{\varphi}_m + \boldsymbol{\varphi}_{m+N/2}), \tag{2.89b}$$

where we still have to fix y_1^{m+} and y_2^{m-} adequately for normalization. Now, the set of vectors (2.89) constitutes a basis for $\mathscr{V}^N$, but not a completely orthonormal one. From the remarks on the "not far from hermitian" matrix (2.83) it follows that $(\hat{\boldsymbol{\psi}}_m, \hat{\boldsymbol{\psi}}_{m'}) = 0$ for $m \neq m'$. When $m = m'$ the acoustical and optical modes (2.89a) and (2.89b), although linearly independent, are *not* orthogonal. The natural description of the diatomic lattice is thus in terms of a nonorthogonal basis. This is not too inconvenient from the point of view of a good qualitative picture of the workings of such lattices, in particular the two-band structure of the frequency spectrum and the identification of "optical" (or "acoustical") modes with vibrations where the two unequal masses are preferentially on opposite sides (or on the same side) of the equilibrium position.

Exercise 2.48. Starting from the equation of motion of the diatomic lattice in the $\boldsymbol{\varepsilon}$-basis $\mathbf{M}\ddot{\mathbf{f}} = -\mathbf{K}\mathbf{f}$, perform a *nonunitary* transformation $\mathbf{f} = \mathbf{M}^{-1/2}\mathbf{g}$, where $\mathbf{M}^{-1/2}$ is a well-defined diagonal matrix, and multiply the whole equation by $\mathbf{M}^{-1/2}$. Thus arrive at $\ddot{\mathbf{g}} = -\mathbf{K}'\mathbf{g}$, $\mathbf{K}' = \mathbf{M}^{-1/2}\mathbf{K}\mathbf{M}^{-1/2}$ *hermitian*. Note that for first-neighbor interactions in $\mathbf{K}$, $\mathbf{K}'$ represents a first-neighbor interaction plus two different zero-order interaction springs.

Exercise 2.49. A nonunitary transformation linking the two-band and diatomic lattices can also be set up comparing the eigenvectors $\mathbf{x}^{m\pm}$ in (2.75) and $\mathbf{y}^{m\pm}$ for (2.84). The question is to find a 2×2 matrix $\mathbf{T}^{(m)}$ (for fixed m) such that

$\mathbf{x}^{m\pm} = \mathbf{T}^{(m)}\mathbf{y}^{m\pm}$, i.e., $\tilde{\mathbf{A}}^{(m)}\mathbf{T}^{(m)} = \mathbf{T}^{(m)}\tilde{\mathbf{B}}^{(m)}$. Show that such a matrix is diagonal with elements $t_m := \exp(i\pi/4)\tan^{1/2}(\pi m/N)$ and t_m^{-1}, $m = 1,2, \ldots, N/2 - 1$.

Exercise 2.50. Find the most general solution vector $\mathbf{f}(t)$ for the diatomic lattice expressed in terms of the nonorthogonal eigenbasis (2.89). Identify Green's matrix in the ψ-basis. See that upon transforming back to the "physical" ε-basis the Green's operator matrix representative becomes *nonhermitian.*

2.4.14. Short Survey of Other Lattice Systems

Having worked on different sample cases in this section, we can see that, generally speaking, the Fourier transform takes us from the fully coupled "physical" basis to a mathematically simpler one. Immediate extensions involve lattices with q different springs or masses which repeat a pattern r times (so $N = qr$). These can be treated and the problem reduced to diagonalizing $q \times q$ matrices, which in turn divide the spectrum into q bands which raise and lower "wings" with respect to the equal-spring or -mass case. For an overall view and physical application we warmly recommend the classic book by Brillouin (1946). This book is mainly concerned with actual three-dimensional crystals of infinite extent. Very readable articles dealing with finite lattices with different types of constraints and characteristics have been written by Louck (1962), Merchant and Brill (1973), and Chaturvedi and Baijal (1974). A very interesting problem whose treatment departs from our line of work but which nevertheless is important in the physics of semiconductors is that of a *mass defect* in the lattice, i.e., one mass being different from the others. Articles on this subject have been written by Weinstock (1970, 1971) and Maradudin *et al.* (1963). Variants of this problem include molecular lattices with atomic or bond defects: See Dettmann and Ludwig (1965), Dean (1967), and Munn (1969). A qualitative description of the behavior of a linear crystal when mass defects are introduced one at a time is given by Alonso *et al.* (1973) and, for the threshold oscillation frequencies of a diatomic lattice, by Valladares (1975). On the more philosophical aspects of lattice couplings in very general systems, an article and book by Capra (1974a, 1974b) are a must for the interested reader.

2.5. Energy in a Lattice

In this section we shall describe the energy present in a vibrating N-mass lattice. In the absence of damping we expect the total energy to be conserved. Moreover, when we uncouple the system in its eigenbasis, we shall find that the individual energies associated with the normal modes are conserved as well.

2.5.1. Kinetic and Potential Energy in Each Particle

Consider an N-element lattice described by the vector equation

$$\mathbb{M}\ddot{\mathbf{f}} + \mathbb{C}\dot{\mathbf{f}} + \mathbb{K}\mathbf{f} = \mathbf{0}, \tag{2.90}$$

where, as detailed in Section 2.2, $\mathbb{M}$, $\mathbb{C}$, and $\mathbb{K}$ are the inertial, dissipation, and interaction operators. In the "physical" $\boldsymbol{\varepsilon}$-basis the coordinates of $\mathbf{f}$, $f_n(t)$ describe the displacements of the lattice points, while $\mathbb{M}$ and $\mathbb{C}$ are represented by diagonal matrices $\|M_n\|$ and $\|c_n\|$, M_n being the mass and c_n the damping constant of the nth lattice element. The interaction operator $\mathbb{K}$ is self-adjoint and represented by $\|\kappa_{mn}\|$ [see Eq. (2.19)].

At some time t, the kinetic energy of the nth mass is

$$E_n^{\,k}(t) := \tfrac{1}{2}M_n(\dot{f}_n)^2, \tag{2.91}$$

while its potential energy can be found by integrating the force to which the particle is subject, Eq. (2.19), along a segment from its equilibrium position to its actual position $f_n(t)$, all other lattice elements being fixed:

$$E_n^{\,p}(t) := \int_0^{f_n} dx\Big(\sum_{m\neq n}\kappa_{nm}f_m + \kappa_{nn}x\Big) = \sum_{m\neq n}\kappa_{nm}f_nf_m + \tfrac{1}{2}\kappa_{nn}f_n^{\,2}. \tag{2.92}$$

No other forms of energy being present in the lattice, the total energy of the nth particle is

$$E_n(t) = E_n^{\,k}(t) + E_n^{\,p}(t). \tag{2.93}$$

Substitution of a solution $\mathbf{f}(t)$ as found in the last sections into (2.91)–(2.93) should give $E_n(t)$ for each of the individual particles. The description obtained in this fashion, however, is not too illuminating. Since the particles are coupled, as the lattice motion proceeds in time, potential energy is exchanged between the lattice constituents so that none of the individual $E_n(t)$'s is constant. As before, a simpler description of the quantities involved is obtained through writing them in a vector-basis-independent form applied to the whole lattice.

2.5.2. Total Energy and Its Conservation

The total kinetic energy can be written as

$$E^k(t) := \sum_n E_n^{\,k}(t) = \tfrac{1}{2}\sum_n \dot{f}_n^{*}M_n\dot{f}_n = \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}), \tag{2.94}$$

using the inner product defined in Section 1.2. The $E^k(t)$ thus defined is positive even for complex $\dot{f}_n(t)$.

The total potential energy will be the sum of the $E_n^p(t)$ in (2.93) over all n. In setting up this expression we have to be careful in order not to double-count the cross terms $f_n f_m$ which appear twice. Halving these, we obtain the sum

$$E^p(t) \coloneqq \sum_n E_n^p(t) = \tfrac{1}{2} \sum_{m,n} f_n^* \kappa_{nm} f_m = \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\mathbf{f}), \tag{2.95}$$

where again we have used the inner product form. The total energy present in the lattice is thus the sum of (2.94) and (2.95):

$$E = \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}) + \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\mathbf{f}). \tag{2.96}$$

This expression is both compact and useful, as we can find the effect of dissipation on the expected conservation of total energy. Indeed, using the hermiticity of $\mathbb{M}$, $\mathbb{K}$, and $\mathbb{C}$, the reality of (2.94) and (2.95), and Eq. (2.90), we find that

$$\begin{aligned} \frac{d}{dt} E &= \tfrac{1}{2}(\ddot{\mathbf{f}}, \mathbb{M}\dot{\mathbf{f}}) + \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{M}\ddot{\mathbf{f}}) + \tfrac{1}{2}(\dot{\mathbf{f}}, \mathbb{K}\mathbf{f}) + \tfrac{1}{2}(\mathbf{f}, \mathbb{K}\dot{\mathbf{f}}) \\ &= (\dot{\mathbf{f}}, \mathbb{M}\ddot{\mathbf{f}} + \mathbb{K}\mathbf{f}) = -(\dot{\mathbf{f}}, \mathbb{C}\dot{\mathbf{f}}). \end{aligned} \tag{2.97}$$

The conclusion of (2.97) is that *in the absence of dissipation, the total energy (2.96) of the lattice is conserved.*

2.5.3. Energy in the Normal Modes

Our original description in terms of the energy in each lattice element was inconvenient because potential energy exchange is taking place. As we saw in the last sections, however, the more natural description of the lattice is in terms of the eigenvectors of the operator $\mathbb{M}^{-1}\mathbb{K}$. In what follows, as in Section 2.2, we shall consider all masses equal $\mathbb{M} = M\mathbb{1}$ and similarly for all dissipation coefficients $\mathbb{C} = c\mathbb{1}$. Let $\{\boldsymbol{\psi}_n\}_{n=1}^N$ be the orthonormal eigenbasis of the self-adjoint interaction operator. Then, for

$$\mathbf{f}(t) = \sum_n \bar{f}_n(t)\boldsymbol{\psi}_n, \qquad \mathbb{K}\boldsymbol{\psi}_n = \kappa_n \boldsymbol{\psi}_n, \tag{2.98}$$

Eq. (2.90) leads to

$$M\ddot{\bar{f}}_n + c\dot{\bar{f}}_n + \kappa_n \bar{f}_n = 0, \tag{2.99}$$

and the solutions for $\bar{f}_n(t)$ were given in Section 2.1. Now, substitution of (2.98) into the expression for the total energy (2.96) yields

$$\begin{aligned} E &= \tfrac{1}{2} \sum_{m,n} \dot{\bar{f}}_m^* \dot{\bar{f}}_n (\boldsymbol{\psi}_m, \mathbb{M}\boldsymbol{\psi}_n) + \tfrac{1}{2} \sum_{m,n} \bar{f}_m^* \bar{f}_n (\boldsymbol{\psi}_m, \mathbb{K}\boldsymbol{\psi}_n) \\ &= \tfrac{1}{2} \sum_m (M|\dot{\bar{f}}_m|^2 + \kappa_m |\bar{f}_m|^2) = \sum_m E_m^{\psi}, \end{aligned} \tag{2.100}$$

where we have defined the energy associated with the mth mode (relative to the ψ-basis):

$$E_m^{\psi} := \tfrac{1}{2}(M|\dot{\bar{f}}_m|^2 + \kappa_m|\bar{f}_m|^2). \tag{2.101}$$

As this depends only on the mth component of the state vector $\mathbf{f}$ and cross terms are absent, we conjecture (and prove below) that *there is no energy exchange between the different modes of the interaction operator eigenbasis.* Moreover, *in the absence of dissipation, each of the mode energies (2.101) is conserved.* Parallel to our proof of (2.97) from (2.96) and (2.90), we can show that the energy loss of the mth mode (2.101) is due only to its own dissipation term. Using the equation of motion (2.99) for each mode, we obtain

$$\frac{d}{dt}E_m^{\psi} = \tfrac{1}{2}M(\ddot{\bar{f}}_m\dot{\bar{f}}_m^* + \dot{\bar{f}}_m\ddot{\bar{f}}_m^*) + \tfrac{1}{2}\kappa_m(\dot{\bar{f}}_m\bar{f}_m^* + \bar{f}_m\dot{\bar{f}}_m^*) = -c|\dot{\bar{f}}_m|^2. \tag{2.102}$$

Exercise 2.51. In the expression for the total energy (2.96), assume that not all masses are equal, so $\mathbb{M}$ is not a multiple $M\mathbb{1}$ and does not commute with $\mathbb{K}$. Then, in finding the eigenbasis of $\mathbb{M}^{-1}\mathbb{K}$ [as in the case of the diatomic lattice, Eq. (2.82)] we have $\mathbb{K}\psi_n = \gamma_n\mathbb{M}\psi_n$ for the eigenbasis, and the expression for the total energy analogous to (2.100) becomes

$$E = \tfrac{1}{2}\sum_{m,n}(\dot{\bar{f}}_m^*\dot{\bar{f}}_n + \gamma_n\bar{f}_m^*\bar{f}_n)(\psi_m, \mathbb{M}\psi_n), \tag{2.103}$$

which shows there is energy exchange between modes. Examine the options for defining conserved "partial" energies in cases when $(\psi_m, \mathbb{M}\psi_n)$ is zero except for subsets of ψ's.

2.6. Phase Space, Time Evolution, and Constants of Motion

In our description of the time evolution of a lattice of mechanical elements we have seen that both $\mathbf{f}(t)$ and its time derivative $\dot{\mathbf{f}}(t)$ entered as initial conditions, basically because the equations of motion are differential equations of second order. Our account of the lattice energy, moreover, suggests that $\mathbf{f}(t)$ and $\dot{\mathbf{f}}(t)$ should be taken on equal footing. The appearance of two (or more) quantities intertwined in this way strongly indicates that vector space concepts give the most economical description of the system. That this is so will be seen in this section. The concept to be developed is that of the *phase space* of a system and the insight it gives into its time evolution and conservation laws.

2.6.1. Phase Space of a System

In our mechanical representation of a coupled system by mass-and-spring lattices, $\mathbf{f}(t) \in \mathscr{V}^N$ stands for the displacement vector. We define the *momentum vector*,‡ closely related to the velocity vector $\dot{\mathbf{f}}(t)$, as

$$\mathbf{g}(t) \coloneqq \mathbb{M}\dot{\mathbf{f}}(t), \tag{2.104}$$

where $\mathbb{M}$ is, as before, the inertia operator. In the "physical" $\boldsymbol{\varepsilon}$-basis, where $f_n = (\boldsymbol{\varepsilon}_n, \mathbf{f})$ are the individual mass displacements, $\mathbb{M}$ is represented by a diagonal matrix $\mathbf{M} = \|M_n\|$, where $\{M_n\}_{n=1}^N$ are the N particle masses. We now construct the $2N$-dimensional *phase space* of N-mass systems, $\mathscr{V}_{\text{II}}^N$, as a vector space with elements

$$\boldsymbol{\zeta} = \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}, \qquad \mathbf{f}, \mathbf{g} \in \mathscr{V}^N. \tag{2.105}$$

In the canonical column-vector realization, $\boldsymbol{\zeta} \in \mathscr{V}_{\text{II}}^N$ is represented by $2N$ components, the first being those of $\mathbf{f}$ and the second those of $\mathbf{g}$; $\mathscr{V}_{\text{II}}^N$ is then said to be the *direct sum* of two $\mathscr{V}^N$ spaces ($\mathscr{V}_{\text{II}}^N = \mathscr{V}^N \oplus \mathscr{V}^N$).

2.6.2. The Simple Harmonic Oscillator

It will help us to get a better grasp of the phase space $\mathscr{V}_{\text{II}}^N$ if we consider the one-dimensional oscillator problem examined in Section 2.1 whose complete solution is (2.10) and, to start with, disregard damping. As there, phase space is two-dimensional, $\mathscr{V}_{\text{II}}^1 = \mathscr{V}^2$. We can plot the motion of the oscillator in this plane as in Fig. 2.24. If the appropriate scales are chosen for f and g, the system is described by a point which moves clockwise in a circle. The radius of this circle is proportional to the energy $(\frac{1}{2}M^{-1}g^2 + \frac{1}{2}kf^2)$, while the angular velocity is $(k/M)^{1/2}$, the same for all radii. The initial position of the phase-space point is f_0, g_0. In Fig. 2.25 we have represented a similar but damped oscillator.

2.6.3. The Lattice Equations of Motion in Phase Space

The free lattice equation of motion, Eq. (2.90), may be written as a *vector* equation in $\mathscr{V}_{\text{II}}^N$ as

$$\begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & -\mathbb{C}\mathbb{M}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} \mathbf{f} \\ \mathbf{g} \end{pmatrix}. \tag{2.106}$$

Indeed, the first row is only (2.104), which identifies $\mathbf{g}$ as the momentum

‡ Note that in the presence of viscous drag, $g_n(t)$ is *not* the momentum *canonically conjugate* to $f_n(t)$ as defined, for instance, in Goldstein (1950, Chapter 6).

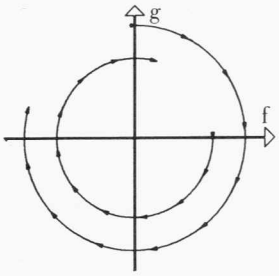


Fig. 2.24. Motion in phase space of harmonic oscillators with nonzero elongation and velocity. Distances between arrows represent equal time intervals.

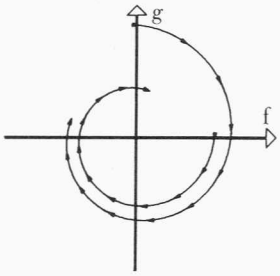


Fig. 2.25. Motion in phase space of damped harmonic oscillator. Distances between arrows represent equal time intervals.

associated to **f**, while the second row rewrites the original Eq. (2.90) using both **f** and **g**. Equation (2.106) has the simple structure

$$\mathbb{H}_{II}\zeta = \frac{d}{dt}\zeta, \qquad \text{where } \mathbb{H}_{II} := \begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & -\mathbb{C}\mathbb{M}^{-1} \end{pmatrix}; \tag{2.107}$$

i.e., it is a system of differential equations which are of *first order* in time. We shall refer to $\mathbb{H}_{II}$ as the *generator* of the equation of motion.

2.6.4. Time-Evolution Operator

The simplification inherent in the reduction of order of the differential equation of motion is considerable. The reason for this is that *the time evolution becomes a Taylor expansion*:

$$\zeta(t + t_0) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{d^n}{dt'^n} \zeta(t') \Big|_{t'=t_0} =: \exp\left(t \frac{d}{dt'}\right) \zeta(t') \Big|_{t'=t_0}, \tag{2.108}$$

where we can define the exponential of the operator td/dt' in terms of the series expansion of the exponential function. This is in line with our description of functions of operators in terms of functions of the representing matrices in Section 1.5, although here we have exponentiated a *differential* operator. The validity of the definition depends here on the validity of the Taylor expansion of $\zeta(t)$: we must assume $\zeta(t)$ to be a set of $2N$ *analytic* functions of t, i.e., to have a convergent Taylor expansion for all finite t. The explicit solutions obtained from Section 2.1 onward indicate that this is valid. Now, the vector $\zeta(t)$ must satisfy the equation of motion (2.107), which states that $(d/dt')^n \zeta(t') = \mathbb{H}_{II}^n \zeta(t')$. The linear combination of such powers of d/dt' in (2.108) thus yields

$$\zeta(t + t_0) = \exp(t\mathbb{H}_{II})\zeta(t_0) \tag{2.109}$$

as the general solution of the equation of motion with initial conditions $\zeta(t_0)$.

2.6.5. The Simple Lattice Case

Equation (2.109) is not only simple-looking but useful as well; it leads to the explicit expressions of time evolution through the Green's operator discussed in Sections 2.2–2.4. Indeed, consider first the case of the simple lattice of Section 2.2; $\mathbb{M} = M\mathbb{1}$, $\mathbb{C} = \mathbb{0}$, and $\mathbb{K} = -k\mathbb{\Delta}$. The operator $\mathbb{H}_{II}$ takes the form

$$\mathbb{H}_{II} = \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} \qquad \text{(simple lattice)}. \tag{2.110}$$

Its square is already diagonal,

$$\mathbb{H}_{II}^2 = \begin{pmatrix} M^{-1}k\mathbb{\Delta} & \mathbb{0} \\ \mathbb{0} & M^{-1}k\mathbb{\Delta} \end{pmatrix}, \tag{2.111a}$$

and its even powers can be written as

$$\mathbb{H}_{II}^{2m} = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} (M^{-1}k\mathbb{\Delta})^m. \tag{2.111b}$$

The exponential series can be then evaluated as

$$\begin{aligned} \exp(t\mathbb{H}_{II}) &= \left(\sum_{n=0\,\text{even}}^{\infty} + \sum_{n=1\,\text{odd}}^{\infty} \right) \frac{t^n}{n!} \mathbb{H}_{II}^n \\ &= \sum_{m=0}^{\infty} \frac{t^{2m}}{(2m)!} \mathbb{H}_{II}^{2m} + \mathbb{H}_{II} \sum_{m=0}^{\infty} \frac{t^{2m+1}}{(2m+1)!} \mathbb{H}_{II}^{2m} \\ &= \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} \sum_{m=0}^{\infty} \frac{[t(M^{-1}k\mathbb{\Delta})^{1/2}]^{2m}}{(2m)!} \\ &\quad + \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} [M^{-1}k\mathbb{\Delta}]^{-1/2} \sum_{m=0}^{\infty} \frac{[t(M^{-1}k\mathbb{\Delta})^{1/2}]^{2m+1}}{(2m+1)!}. \end{aligned} \tag{2.112}$$

In the last member we have arranged things so that the cosh x and x^{-1} sinh x power series are manifest, noting that only integer powers of the operator $\mathbb{\Delta}$ are actually involved. This allows us to write

$$\begin{aligned} \mathbb{G}_{II}(t) \coloneqq \exp(t\mathbb{H}_{II}) &= \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} \cosh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \\ &\quad + \begin{pmatrix} \mathbb{0} & M^{-1}\mathbb{1} \\ k\mathbb{\Delta} & \mathbb{0} \end{pmatrix} (M^{-1}k\mathbb{\Delta})^{-1/2} \sinh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \\ &= \begin{pmatrix} \dot{\mathbb{G}}(t) & M^{-1}\mathbb{G}(t) \\ k\mathbb{\Delta}\mathbb{G}(t) & \dot{\mathbb{G}}(t) \end{pmatrix}, \end{aligned} \tag{2.113}$$

having defined

$$\mathbb{G}(t) \coloneqq (M^{-1}k\mathbb{\Delta})^{-1/2} \sinh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \tag{2.114a}$$

and

$$\dot{\mathbb{G}}(t) = \cosh[t(M^{-1}k\mathbb{\Delta})^{1/2}] \tag{2.114b}$$

as its time derivative [see Eqs. (1.76)–(1.79)]. The definition (2.114) is not new: it has already appeared in Eq. (1.73) for $M = 1 = k$ and corresponds exactly to the $\mathscr{V}^N$ Green's operator and its time derivative for the simple lattice. We can then write Eqs. (2.109) and (2.113) as

$$\boldsymbol{\zeta}(t) = \mathbb{G}_{II}(t - t_0)\boldsymbol{\zeta}(t_0). \tag{2.115}$$

In terms of the **f**- and $\dot{\mathbf{f}}$-components and initial conditions,

$$\begin{pmatrix} \mathbf{f}(t) \\ \dot{\mathbf{f}}(t) \end{pmatrix} = \begin{pmatrix} \dot{\mathbb{G}}(t - t_0) & \mathbb{G}(t - t_0) \\ \ddot{\mathbb{G}}(t - t_0) & \dot{\mathbb{G}}(t - t_0) \end{pmatrix} \begin{pmatrix} \mathbf{f}_0 \\ \dot{\mathbf{f}}_0 \end{pmatrix}. \tag{2.116}$$

In the last expression we have used (2.104) and introduced $\ddot{\mathbb{G}}(t - t_0)$ through differentiation of (2.114b) in order to replace the 1-2 element of the matrix (2.113). This is only a restatement of the time-evolution equation (2.29) and its derivative.

2.6.6. Group Properties

Several relations in $\mathscr{V}^N$ between the equation of motion and the Green's operator become simplified in $\mathscr{V}^N_{II}$ where $\mathbb{G}_{II}(t)$ is the sole time-evolution operator. From (2.113) and the composition of two exponential functions of the same operator, Eq. (1.70), it follows that

$$\mathbb{G}_{II}(t_1)\mathbb{G}_{II}(t_2) = \mathbb{G}_{II}(t_1 + t_2) \tag{2.117}$$

as well as

$$\mathbb{G}_{II}(0) = \mathbb{1}, \tag{2.118}$$

where here $\mathbb{1}$ is the unit operator in $\mathscr{V}^N_{II}$. Writing $\mathbb{G}_{II}$ in 2×2 matrix form, we reproduce Eqs. (2.31).

The foregoing two equations and the obvious property of associativity show that the time-evolution operators have the first three properties of a *group* (Section 1.4). The fourth defining property, that of the existence of an *inverse* operator $\mathbb{G}_{II}^{-1}(t)$ for every $\mathbb{G}_{II}(t)$, is also true here. In fact,

$$\mathbb{G}_{II}^{-1}(t) = \mathbb{G}_{II}(-t), \tag{2.119}$$

as can be seen from its definition (2.113), (2.117), or explicit calculation. The set of time-evolution operators $\mathbb{G}_{II}(t)$ for $t \in (-\infty, \infty)$ thus forms a *one-parameter continuous* group of time translations *generated* by $\mathbb{H}_{II}$. As the group elements *commute* [this can be seen by exchanging t_1 and t_2 in (2.117)], the group is said to be *abelian*. Thus far in this section we have been speaking in basis-independent vector and operator language. The physical displacements of the lattice elements and their momenta are the coordinates of $\boldsymbol{\zeta}$ in $\boldsymbol{\varepsilon}$-bases for the displacement and momentum $\mathscr{V}^N$'s in $\mathscr{V}^N_{II} = \mathscr{V}^N \oplus \mathscr{V}^N$. We shall assume that the two $\mathscr{V}^N$'s are described by the same basis.

2.6.7. Evolution Operator in Normal Mode Basis

When it comes to the explicit expression for the time-evolution operator we can make good use of the Fourier transform since $\mathbb{G}_{II}(t)$ is the exponential of $\mathbb{H}_{II}$ and thus will be represented by a matrix with four diagonal blocks whenever $\mathbb{H}_{II}$ is likewise represented. As the operators in the 2×2 matrix form of $\mathbb{H}_{II}$ are, in the simple case (2.110), only multiples of $\mathbb{\Delta}$ and $\mathbb{1}$, this happens in the Fourier $\boldsymbol{\varphi}$-basis. The matrix equation then uncouples into N separate 2×2 matrix equations each of the form

$$\begin{pmatrix} \tilde{f}_m(t) \\ \dot{\tilde{f}}_m(t) \end{pmatrix} = \begin{pmatrix} \tilde{G}_m(t - t_0) & \tilde{G}_m(t - t_0) \\ \dot{\tilde{G}}_m(t - t_0) & \dot{\tilde{G}}_m(t - t_0) \end{pmatrix} \begin{pmatrix} \tilde{f}_m(t_0) \\ \dot{\tilde{f}}_m(t_0) \end{pmatrix}.$$

$$m = 1, 2, \ldots, N, \quad (2.120a)$$

where, from (2.114),

$$\tilde{G}_m(t - t_0) = (M^{-1}k\lambda_n)^{-1/2} \sinh[t(M^{-1}k\lambda_n)^{1/2}]. \quad (2.120b)$$

Of course, this is precisely Eqs. (2.28): Recall that the elements of diagonal $\tilde{\mathbf{\Delta}}$ are λ_n [see Eqs. (1.62)], and use the identity $(ix)^{-1} \sinh ix = x^{-1} \sin x$.

In terms of $2N$-dimensional phase-space diagrams, the motion in the $\boldsymbol{\varphi}$-basis (2.120) appears as in Fig. 2.24 in each of the N Fourier component phase-space planes. The oscillation frequencies are different for different m's.

Exercise 2.52. Differentiating (2.113), show that

$$\mathbb{H}_{II}\mathbb{G}_{II}(t) = \mathbb{G}_{II}(t)\mathbb{H}_{II} = \dot{\mathbb{G}}_{II}(t), \quad (2.121)$$

i.e., the time-evolution operator commutes with its generator and is a solution of the lattice equation of motion. Compare with (2.30).

Exercise 2.53. Write out explicitly the time-evolution operator for a general interaction operator $\mathbb{K}$ (when $\mathbb{M} = M\mathbb{1}$ and $\mathbb{C} = \mathbb{0}$, covering the cases of the farther-neighbor interaction and molecular lattices). Show that you need only replace $k\mathbb{\Delta}$ by $-\mathbb{K}$ in (2.113) and (2.114). All the subsequent equations follow without change; in particular, the Fourier transform continues to provide a basis, where Green's operator is represented by a block-diagonal matrix.

Exercise 2.54. Consider the case of the diatomic lattice in Section 2.4. There, we saw, $\mathbb{M}$ and $\mathbb{K}$ are self-adjoint but do not commute. Carry out the exponentiation of the generator (2.107) (for $\mathbb{C} = \mathbb{0}$) with due care. Show that

$$\mathbb{H}_{II}^{2n} = \begin{pmatrix} (-\mathbb{M}^{-1}\mathbb{K})^n & \mathbb{0} \\ \mathbb{0} & (-\mathbb{K}\mathbb{M}^{-1})^n \end{pmatrix} \quad \text{(general, undamped).} \quad (2.122)$$

Following (2.111)–(2.113), one arrives at the expression

$$\mathbb{G}_{II}(t) = \begin{pmatrix} \dot{\mathbb{G}}(t) & \mathbb{M}^{-1}\mathbb{G}(t)^\dagger \\ -\mathbb{K}\mathbb{G}(t) & \dot{\mathbb{G}}(t)^\dagger \end{pmatrix}, \quad (2.123a)$$

which generalizes (2.113) for noncommuting operators. Here,

$$\mathbb{G}(t) = (-\mathbb{M}^{-1}\mathbb{K})^{-1/2} \sinh[t(-\mathbb{M}^{-1}\mathbb{K})^{1/2}] \quad \text{(general, undamped).} \quad (2.123b)$$

Note that for any well-defined function P,

$$\mathbb{M}^{-1}P(\mathbb{M}^{-1}\mathbb{K})^{\dagger} = \mathbb{M}^{-1}P(\mathbb{K}\mathbb{M}^{-1}) = P(\mathbb{M}^{-1}\mathbb{K})\mathbb{M}^{-1}, \tag{2.124a}$$

$$\mathbb{K}P(\mathbb{M}^{-1}\mathbb{K}) = P(\mathbb{K}\mathbb{M}^{-1})\mathbb{K} = \mathbb{M}P(\mathbb{M}^{-1}\mathbb{K})\mathbb{M}^{-1}\mathbb{K}. \tag{2.124b}$$

This allows one to generate various identities. In particular, it should be noticed that if we have found a basis where $\mathbb{M}^{-1}\mathbb{K}$ is represented by a diagonal matrix, as in the treatment of the diatomic lattice in Section 2.4, Green's operator $\mathbb{G}(t)$ in $\mathscr{V}^N$ and its time derivatives will also be diagonal and easily calculable from (2.123b). However, the block entries of the time-evolution operator (2.123a) involve operators $\mathbb{M}^{-1}\mathbb{G}(t)^{\dagger}$ and $\mathbb{K}\mathbb{G}(t)$ which are *not* diagonal. Not all is lost, however, since the expressions for $\mathbb{M}^{-1}$ and $\mathbb{K}$ are usually simple to calculate if we know the basis explicitly. This is the case for the diatomic lattice, where the basis in which $\mathbb{M}^{-1}\mathbb{K}$ is diagonal is given by (2.89). Try implementing this program in detail.

Exercise 2.55. Allow for damping. One can solve exactly the case when $\mathbb{M} = M\mathbb{1}$ and $\mathbb{C} = c\mathbb{1}$ using the results in Exercises 1.55 and 1.56, transforming $\mathbb{H}_{II}$ to diagonal form, exponentiating, and transforming back [i.e., Eq. (1.71)]. Show that this leads to the time-evolution operator in $\mathscr{V}^N_{II}$ given by

$$\mathbb{G}^{cM}_{II}(t) = \begin{pmatrix} \dot{\mathbb{G}}^{cM}(t) + 2\Gamma\mathbb{G}^{cM}(t) & M^{-1}\mathbb{G}^{cM}(t) \\ -\mathbb{K}\mathbb{G}^{cM}(t) & \dot{\mathbb{G}}^{cM}(t) \end{pmatrix}, \tag{2.125a}$$

where

$$\mathbb{G}^{cM}(t) = \exp(-\Gamma t)\mathbb{U}^{-1/2}\sinh t\mathbb{U}^{1/2} \qquad \text{(damped)}, \tag{2.125b}$$

$$\mathbb{U} = \Gamma^2\mathbb{1} - M^{-1}\mathbb{K}, \qquad \Gamma = c/2M. \tag{2.125c}$$

Compare with the results of Exercise 2.16. Notice that here, too, the Fourier φ-basis allows for the explicit solution of the problem.

Exercise 2.56. Following Exercise 2.17, consider the limit of (2.125) when the masses are very small, so damping overwhelms inertia and $\Gamma = c/2M \to \infty$, while c remains finite. The phase-space description breaks down; $\mathbf{f}$ and $\dot{\mathbf{f}}$ become uncoupled as the time-evolution operator (2.125) written in the form (2.116) becomes diagonal. Here again the Fourier φ-basis is the appropriate one.

Exercise 2.57. Given the time-evolution operator $\mathbb{G}^{cM}(t)$ in (2.123) and (2.125), verify that, indeed, it is generated by $\mathbb{H}_{II}$ of Eq. (2.107). To this end, refer to Eqs. (1.76) and (1.79), which are independent of the adjunction properties of the operators involved.

There is another area we should like to present in our study of vector analysis in phase space: the role of the symmetry of a system in finding its constants of motion.

2.6.8. Energy as a Sesquilinear Form

The expression for the energy, Eq. (2.96), can be generalized to a *sesquilinear form* in $\mathscr{V}_{II}^{N}$. Indeed, we can write for the undamped case

$$\begin{aligned} E(\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2) &:= \tfrac{1}{2}(\mathbf{f}_1, \mathbb{K}\mathbf{f}_2) + \tfrac{1}{2}(\mathbf{g}_1, \mathbb{M}^{-1}\mathbf{g}_2) \\ &= (\mathbf{f}_1^\dagger \quad \mathbf{g}_1^\dagger)\begin{pmatrix} \frac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \frac{1}{2}\mathbb{M}^{-1} \end{pmatrix}\begin{pmatrix} \mathbf{f}_2 \\ \mathbf{g}_2 \end{pmatrix} =: \boldsymbol{\zeta}_1^\dagger \mathbb{E}_{II} \boldsymbol{\zeta}_2. \end{aligned} \tag{2.126}$$

We shall call $\mathbb{E}_{II}$ the *energy operator*. The adjunction of $\mathscr{V}_{II}^{N}$ vectors and operators is defined in terms of the corresponding adjunction of vectors and matrix representatives in $\mathscr{V}^{N}$: $\boldsymbol{\zeta}^\dagger$ is the row vector whose elements are the complex conjugates of those of $\boldsymbol{\zeta}$ in (2.105), and for $\mathscr{V}_{II}^{N}$ operators we transpose the 2×2 matrix and adjoin the $\mathscr{V}^{N}$ operator elements. Clearly, $E(\boldsymbol{\zeta}, \boldsymbol{\zeta})$ (note $\boldsymbol{\zeta}_1 = \boldsymbol{\zeta} = \boldsymbol{\zeta}_2$) is the energy corresponding to the phase-space state vector $\boldsymbol{\zeta}$. The conservation of the quantity (2.126) under time evolution of the undamped lattice can be proven through calculating

$$\begin{aligned} E(\boldsymbol{\zeta}_1(t), \boldsymbol{\zeta}_2(t)) &= \boldsymbol{\zeta}_1^\dagger(t)\mathbb{E}_{II}\boldsymbol{\zeta}_2(t) \\ &= \boldsymbol{\zeta}_1^\dagger(t_0)\mathbb{G}_{II}^\dagger(t - t_0)\mathbb{E}_{II}\mathbb{G}_{II}(t - t_0)\boldsymbol{\zeta}_2(t_0) \end{aligned} \tag{2.127}$$

and showing that this equals $E(\boldsymbol{\zeta}_1(t_0), \boldsymbol{\zeta}_2(t_0))$, i.e., that

$$\mathbb{G}_{II}^\dagger(t - t_0)\mathbb{E}_{II}\mathbb{G}_{II}(t - t_0) = \mathbb{E}_{II}. \tag{2.128}$$

One can verify directly that (2.128) is true by replacing the expressions for $\mathbb{G}_{II}^\dagger$, $\mathbb{G}_{II}$, and $\mathbb{E}_{II}$ as 2×2 matrices with operator elements from (2.123) and (2.126). It is more illuminating, however, to use an alternative proof which makes use of $\mathbb{H}_{II}$, the generator of $\mathbb{G}_{II}$. Consider infinitesimal time evolution, letting $\delta t := t - t_0$ be as small as we please. We can then use the exponential series in writing

$$\mathbb{G}_{II}(\delta t) = \exp(\delta t \mathbb{H}_{II}) \simeq \mathbb{1} + \delta t \mathbb{H}_{II}, \tag{2.129}$$

where we disregard terms of second and higher order in δt. Substitution into (2.128) yields

$$\mathbb{E}_{II} = (\mathbb{1} + \delta t \mathbb{H}_{II}^\dagger)\mathbb{E}_{II}(\mathbb{1} + \delta t \mathbb{H}_{II}). \tag{2.130}$$

Collecting terms in δt, we obtain

$$\mathbb{H}_{II}^\dagger \mathbb{E}_{II} + \mathbb{E}_{II}\mathbb{H}_{II} = \mathbb{0}. \tag{2.131}$$

This equation is easier to verify than (2.128), as it only involves products of two operators at a time:

$$\begin{aligned} \mathbb{H}_{II}^\dagger \mathbb{E}_{II} &= \begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix}^\dagger \begin{pmatrix} \frac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \frac{1}{2}\mathbb{M}^{-1} \end{pmatrix} = \begin{pmatrix} \mathbb{0} & -\mathbb{K}^\dagger \\ \mathbb{M}^{-1\dagger} & \mathbb{0} \end{pmatrix}\begin{pmatrix} \frac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \frac{1}{2}\mathbb{M}^{-1} \end{pmatrix} \\ &= \begin{pmatrix} \mathbb{0} & -\frac{1}{2}\mathbb{K}\mathbb{M}^{-1} \\ \frac{1}{2}\mathbb{M}^{-1}\mathbb{K} & \mathbb{0} \end{pmatrix} = -\begin{pmatrix} \frac{1}{2}\mathbb{K} & \mathbb{0} \\ \mathbb{0} & \frac{1}{2}\mathbb{M}^{-1} \end{pmatrix}\begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix} \\ &= -\mathbb{E}_{II}\mathbb{H}_{II}. \end{aligned} \tag{2.132a}$$

Now, the validity of (2.131) implies the validity of the original equation (2.128), since for any power n,

$$(\mathbb{H}_{\text{II}}^{\dagger})^n\mathbb{E}_{\text{II}} = -(\mathbb{H}_{\text{II}}^{\dagger})^{n-1}\mathbb{E}_{\text{II}}\mathbb{H}_{\text{II}} = \cdots = (-1)^n\mathbb{E}_{\text{II}}\mathbb{H}_{\text{II}}^n, \tag{2.132b}$$

and similarly for any sum of powers. Thus, for any well-defined function P of $\mathbb{H}_{\text{II}}$ (see Section 1.5),

$$P(\mathbb{H}_{\text{II}}^{\dagger})\mathbb{E}_{\text{II}} = \mathbb{E}_{\text{II}}P(-\mathbb{H}_{\text{II}}). \tag{2.132c}$$

When $P = \exp$, Eq. (2.128) is proven.

We would like to stress that the invariance of the sesquilinear form for the energy is a consequence of the *operator* equation (2.131). If we can find a basis $\{\boldsymbol{\psi}_n\}_{n=1}^N$ in $\mathscr{V}^N$ such that $\mathbb{H}_{\text{II}}$ be represented by a 2×2 matrix of diagonal $N \times N$ blocks, then $\mathbb{E}_{\text{II}}$ will be similarly represented since it is constituted by the same operators. It follows that we will have N conserved "partial" energies since the analogue of Eqs. (2.128)–(2.131) holds for each 2×2 submatrix involving the mth and $(N + m)$th rows and columns. These are the E_m^{ψ} in Eq. (2.101).

2.6.9. Other Conserved Sesquilinear Forms and Symmetry

We can now turn the tables and investigate how to construct conserved sesquilinear forms in $\mathscr{V}_{\text{II}}^N$, i.e., to find operators $\mathbb{F}_{\text{II}}$ such that

$$F(\boldsymbol{\zeta}_1, \boldsymbol{\zeta}_2) \coloneqq \boldsymbol{\zeta}_1^{\dagger}\mathbb{F}_{\text{II}}\boldsymbol{\zeta}_2, \qquad \mathbb{F}_{\text{II}} = \begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix} \tag{2.133}$$

is a constant of the motion. The form (2.133) will be conserved if and only if Eq. (2.131) holds, $\mathbb{F}_{\text{II}}$ replacing the energy operator $\mathbb{E}_{\text{II}}$; that is,

$$\begin{pmatrix} \mathbb{0} & -\mathbb{K} \\ \mathbb{M}^{-1} & \mathbb{0} \end{pmatrix}\begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix} = -\begin{pmatrix} \mathbb{F}_a & \mathbb{F}_b \\ \mathbb{F}_c & \mathbb{F}_d \end{pmatrix}\begin{pmatrix} \mathbb{0} & \mathbb{M}^{-1} \\ -\mathbb{K} & \mathbb{0} \end{pmatrix}. \tag{2.134}$$

This embodies the four equations

$$\mathbb{M}^{-1}\mathbb{F}_a = \mathbb{F}_d\mathbb{K}, \tag{2.135a}$$

$$\mathbb{K}\mathbb{F}_d = \mathbb{F}_a\mathbb{M}^{-1}, \tag{2.135b}$$

$$\mathbb{K}\mathbb{F}_c = -\mathbb{F}_b\mathbb{K}, \tag{2.135c}$$

$$\mathbb{M}^{-1}\mathbb{F}_b = -\mathbb{F}_c\mathbb{M}^{-1}. \tag{2.135d}$$

Note that if we have two operators $\mathbb{F}_{\text{II}}^{(1)}$ and $\mathbb{F}_{\text{II}}^{(2)}$ satisfying (2.134)–(2.135), any linear combination of them will also be an operator leading to a conserved sesquilinear form. We thus need only look for a *basis* of $\mathbb{F}_{\text{II}}$'s satisfying these equations. If we set $\mathbb{F}_b = \mathbb{0} = \mathbb{F}_c$ in (2.135) so that the last two equations are trivially satisfied, one solution to the two first ones is $\mathbb{F}_a = c\mathbb{K}$, $\mathbb{F}_d = c\mathbb{M}^{-1}$ for any constant c. This yields, for $c = \frac{1}{2}$, the energy operator $\mathbb{E}_{\text{II}}$.

Consider next setting $\mathbb{F}_a = \mathbb{0} = \mathbb{F}_d$ and $\mathbb{F}_c = -\mathbb{F}_b$. This leaves then the requirement that $\mathbb{F}_b$ *commute* with $\mathbb{K}$ and $\mathbb{M}$. In light of Sections 1.6, 2.3, and 2.4 we see that $\mathbb{F}_b$ may be *any of the operators of the dihedral group which are symmetries of the lattice.*

2.6.10. All Constants of Motion for the Simple Lattice

For definiteness, consider the simple lattice (equal masses and springs) where the symmetry group is constituted by rotations $\mathbb{R}^k$ and inversions $\mathbb{I}_l$ and $\mathbb{K}_m$, letting $\mathbb{D}$ stand for any linear combination of these operators.

The operators we are examining here will thus have the form

$$\mathbb{F}_{II} = \begin{pmatrix} \mathbb{0} & \mathbb{D} \\ -\mathbb{D} & \mathbb{0} \end{pmatrix}, \tag{2.136a}$$

$$\mathbb{D} = \sum_k a_k \mathbb{R}^k + \sum_l b_l \mathbb{I}_l + \sum_m c_m \mathbb{K}_m. \tag{2.136b}$$

The associated conserved quantity for a particular lattice state is the form (2.133) for $\boldsymbol{\zeta}_1 = \boldsymbol{\zeta} = \boldsymbol{\zeta}_2$:

$$\begin{aligned} F(\boldsymbol{\zeta}, \boldsymbol{\zeta}) &= \boldsymbol{\zeta}^\dagger \mathbb{F}_{II} \boldsymbol{\zeta} = (\mathbf{f}, \mathbb{D}\mathbf{g}) - (\mathbf{g}, \mathbb{D}\mathbf{f}) \\ &= \sum_{m,n} D_{mn}(f_m^* g_n - g_m^* f_n) \\ &= \sum_{m,n} \tilde{D}_{mn}(\tilde{f}_m^* \tilde{g}_n - \tilde{g}_m^* \tilde{f}_n). \end{aligned} \tag{2.137}$$

If we now ask the physical displacements and momenta to be real, the next to last member in (2.137) tells us that unless $D_{mn} = -D_{nm}$, the constant (2.137) will vanish. If we look up the matrix elements of the dihedral operators [Eqs. (1.89) and (1.99)],we see that the inversions $\mathbb{I}_l$ and $\mathbb{K}_m$ are symmetric; hence they cannot be in $\mathbb{D}$, which can only consist then of combinations of $\mathbb{R}^k - \mathbb{R}^{-k}$, i.e.,

$$\begin{aligned} F_k^R &\coloneqq \sum_{m,n} (\delta_{m,n+k} - \delta_{m,n-k})(f_m g_n - g_m f_n) \\ &= \sum_n (f_n g_{n-k} - g_n f_{n-k}). \end{aligned} \tag{2.138}$$

This form is reminiscent of angular momentum. Out of the constant of motion (2.133) we can also find "partial" conserved quantities. In the $\boldsymbol{\varphi}$-basis the operator $\mathbb{R}^k - \mathbb{R}^{-k}$ is represented by a diagonal matrix [Eq. (1.91)] which, when substituted into (2.137), leads to

$$F_k^R = -4 \sum_m \sin(2\pi km/N)\, \mathrm{Im}(\tilde{f}_m^* \tilde{g}_m). \tag{2.139}$$

Since $\mathbb{F}_{II}$ has diagonal blocks in the φ-basis, it follows that (for k not a divisor of N) the members of the sum (2.139) are separately conserved, that is,

$$F_m \coloneqq \mathrm{Im}(\tilde{f}_m^* \tilde{g}_m), \qquad m = 1, 2, \ldots, N, \tag{2.140}$$

are N constants of motion which arise because of the invariance of the lattice under rotations. These, together with the partial-wave energies E_m^{ψ} in (2.101), give $2N$ constants of motion. The lattice with real displacements is expected to have no more constants of motion than the parameters needed to specify its initial condition: a total of $2N$ numbers. (See Exercise 2.60.) In terms of the N-dimensional phase-space diagram in the φ-basis (Fig. 2.24), the partial energies E_m^{ψ} fix the radii of the circles, while the F_m are related to the angular coordinates of the initial conditions.

Exercise 2.58. Verify directly, using the explicit lattice solutions (2.28), that (2.140) are indeed independent of time.

Exercise 2.59. Using the vector form of the equations of motion, show from the third member of (2.137) that $dF/dt = 0$. The derivation is parallel to (2.97).

Exercise 2.60. When we examined the choice $\mathbb{F}_b = \mathbb{0} = \mathbb{F}_c$ in (2.134) we glossed over pointing out a more general solution to the remaining operators: $\mathbb{F}_a = \mathbb{K}\mathbb{D}$, $\mathbb{F}_d = \mathbb{M}^{-1}\mathbb{D}$, where $\mathbb{D}$ is any operator (2.136b) embodying the symmetry group of the lattice. Follow the argument starting from (2.136) to show that for real constants of motion one needs $\mathbb{D}$'s such that $\tilde{D}_{mn} = \tilde{D}_{nm}^*$. This excludes rotations but allows operators of the kind $\mathbb{I}_l + \mathbb{I}_{-l}$ [see Eq. (1.92)] or $\mathbb{K}$'s when permitted. Show that, as in finding (2.140), this does not bring in new independent constants of motion.

Exercise 2.61. The sesquilinear form $E(\zeta_1, \zeta_2)$ in (2.126) can be thought of as defining an inner product (see Section 1.2) with *metric* $\mathbb{E}_{II}$. Note, however, that this is not a *positive* inner product, since there exists a nonzero vector $\zeta_0 \coloneqq \binom{\varphi_N}{0}$ such that $E(\zeta_0, \zeta_0) = 0$. This represents the energy of a lattice at rest with all masses having equal displacements. Such a *nonnegative* inner product does not allow for the unique definition of the adjoint of an operator. Nevertheless, one can help oneself with the adjunction in $\mathscr{V}^N$ in order to define a unique adjoint under $E(\zeta_1, \zeta_2)$. The conceptual advantage of this point of view is that Eq. (2.128) becomes the statement that *time evolution is a unitary transformation of phase space*. The generator of this transformation, $\mathbb{H}_{II}$, is such that $i\mathbb{H}_{II}$ is self-adjoint under $E(\zeta_1, \zeta_2)$: Eq. (2.131). In this connection, recall Exercise 1.33.

To sum up, we would like to emphasize the role which the Fourier transform played in the reduction of the description of coupled systems to that of its uncoupled elements. Since *a posteriori* we see that the solutions always involve superpositions of sine waves, it stands to reason that a sine-wave basis of solutions should be the proper approach to the problem. The vector space version of this constitutes the essence of the foregoing sections. Sine waves are not only periodic but have the property that all their deriva-

tives—or even finite differences—are also functions of the same kind. We can expect them to appear in most problems which involve linear difference equations with constant coefficients. When the coefficients are not constant, other functions appear—the special functions of mathematical physics—which lend themselves to analyses which parallel Fourier analysis. We shall have a taste of this in the sections on circular membrane vibration modes and oscillator wave functions.