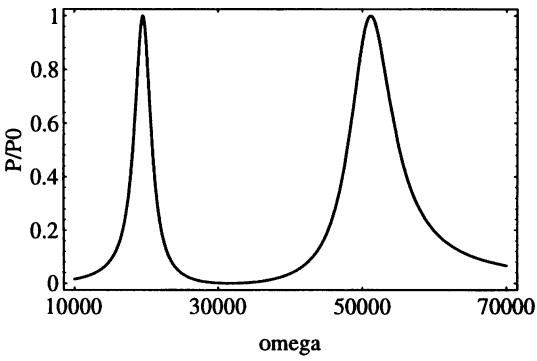


Fig. 2.10. The power $P(\omega)$ dissipated in the ohmic resistance $R = 10\,\Omega$, relative to the power P_0 which is dissipated if the input voltage is connected directly to R

Literature

Crandall R.E. (1991) Mathematica for the Sciences. Addison-Wesley, Redwood City, CA

2.3 Chain Vibrations

It is a well known fact that the motion of a particle in a quadratic potential is described by an especially simple linear differential equation. If several particles interact with each other through such linear forces, their motion can be calculated by linear equations as well. However, one then has several such equations of motion which are coupled to each other. This system of linear equations can be solved by diagonalizing a matrix. A good example of this is the linear chain with different masses. It is a simple model for the calculation of lattice vibrations in a crystal. The eigenvalues of a matrix specify the energy bands of the phonons, while the eigenvectors provide information about the vibration modes of the crystal elements. Every possible motion of the model solid can be represented by superposition of such eigenmodes.

Physics

We consider a chain consisting of pointlike masses m_1 and m_2, which we designate as *light* and *heavy* atoms respectively, for sake of simplicity. The particles are to be arranged in such a way that one heavy atom follows three light ones. The unit cell of length a thus contains four atoms. Only nearest neighbors shall interact with one another. We limit our considerations to small displacements, i.e., the forces are to be linear functions of the shifts of the masses, as indicated in the spring model shown in Fig 2.11.

To describe the longitudinal oscillations, we number the unit cells sequentially and consider the cell with the number n. Within this cell, let r_n, s_n, and t_n be the displacements of the light atoms from their rest positions, and

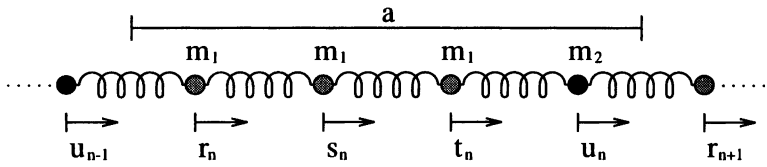


Fig. 2.11. Linear chain consisting of two types of atoms which are connected to each other by elastic forces

let u_n be the displacement of the heavy atom from its rest position. Then the equations of motion are

$$\begin{aligned} m_1\ddot{r}_n &= f(s_n - r_n) - f(r_n - u_{n-1}) \\ &= f(s_n + u_{n-1} - 2r_n) \ , \\ m_1\ddot{s}_n &= f(t_n + r_n - 2s_n) \ , \\ m_1\ddot{t}_n &= f(u_n + s_n - 2t_n) \ , \\ m_2\ddot{u}_n &= f(r_{n+1} + t_n - 2u_n) \ . \end{aligned} \tag{2.17}$$

Here, f is the spring constant. In an infinitely long chain, these equations hold for every unit cell $n \in \mathbb{Z}$. For a finite chain consisting of N unit cells we assume periodic boundary conditions, that is, we think of it as a ringlike arrangement of N identical cells. Since the energy of the chain does not change if it is shifted by the distance a, and consequently the equations of motion are invariant under the translations $\{r_n, s_n, t_n, u_n\} \to \{r_{n+k}, s_{n+k}, t_{n+k}, u_{n+k}\}$, $k = 1, 2, \ldots, N$, (2.17) can be solved by applying a Fourier transformation. Therefore we use the ansatz

$$\boldsymbol{x}_n(t) = \begin{pmatrix} r_n(t) \\ s_n(t) \\ t_n(t) \\ u_n(t) \end{pmatrix} = \boldsymbol{S}(q) \exp(\mathrm{i}qan \pm \mathrm{i}\omega t) \ , \tag{2.18}$$

where, owing to the periodic boundary conditions, q can only take the values $q_\nu = 2\pi\nu/(Na)$, $\nu = -N/2 + 1, \ldots, N/2$. Then

$$\ddot{\boldsymbol{x}}_n = -\omega^2 \boldsymbol{x}_n, \ \boldsymbol{x}_{n\pm1} = \exp(\pm \mathrm{i}qa)\, \boldsymbol{x}_n \ . \tag{2.19}$$

This inserted into (2.17) yields

$$\begin{pmatrix} 2f & -f & 0 & -f\mathrm{e}^{-\mathrm{i}qa} \\ -f & 2f & -f & 0 \\ 0 & -f & 2f & -f \\ -f\mathrm{e}^{\mathrm{i}qa} & 0 & -f & 2f \end{pmatrix} \boldsymbol{S}(q) = \omega^2 \begin{pmatrix} m_1 & 0 & 0 & 0 \\ 0 & m_1 & 0 & 0 \\ 0 & 0 & m_1 & 0 \\ 0 & 0 & 0 & m_2 \end{pmatrix} \boldsymbol{S}(q) \ , \tag{2.20}$$

which is a generalized eigenvalue equation of the type

$$\mathsf{F}\boldsymbol{S} = \lambda \mathsf{M} \boldsymbol{S} \ . \tag{2.21}$$

Here, M is the mass matrix, and we are looking for the eigenvalues $\lambda(q) = \omega^2(q)$ and the corresponding normal modes $\boldsymbol{S}(q)$ for a given value of q. In our

case, the mass matrix can easily be inverted and (2.21) is obviously equivalent to

$$\mathsf{M}^{-1}\mathsf{F}\boldsymbol{S} = \lambda \boldsymbol{S} \,. \tag{2.22}$$

$\mathsf{M}^{-1}\mathsf{F}$ is not a Hermitian matrix, however. The following transformation of (2.21) shows that the eigenvalues are real and nonnegative in spite of this. We multiply this equation from the left by $\mathsf{M}^{-1/2}$, the inverse of the matrix $\mathsf{M}^{1/2}$, and obtain

$$\mathsf{M}^{-1/2}\mathsf{F}\mathsf{M}^{-1/2}\mathsf{M}^{1/2}\boldsymbol{S} = \lambda \mathsf{M}^{1/2}\boldsymbol{S} \,. \tag{2.23}$$

This is an ordinary eigenvalue equation for the positive semidefinite Hermitian matrix $\mathsf{M}^{-1/2}\mathsf{F}\mathsf{M}^{-1/2}$ with the eigenvector $\mathsf{M}^{1/2}\boldsymbol{S}$.

The eigenmodes $\boldsymbol{x}_n(t) = \boldsymbol{S}_\ell(q_\nu)\exp(\mathrm{i}q_\nu an \pm \mathrm{i}\omega_{\nu\ell}t)$ thus obtained are particular complex-valued solutions of the equations of motion (2.17). Analogously to the electrical filters (Sect. 2.2), the general solution can be obtained by a superposition of the eigenmodes. From the complex conjugate of (2.20) and the substitution $q \to -q$ we see that, along with $\boldsymbol{S}(q)$, $\boldsymbol{S}(-q)^*$ is an eigenvector as well, with the same eigenvalue. Therefore, the general real solution of (2.17) has the form

$$\begin{aligned}\boldsymbol{x}_n(t) = \sum_{\nu,\ell} & \boldsymbol{S}_\ell(q_\nu)\exp(\mathrm{i}q_\nu an) \\ & \times \left[c_{\nu\ell}\exp(\mathrm{i}\omega_{\nu\ell}t) + c^*_{-\nu\ell}\exp(-\mathrm{i}\omega_{\nu\ell}t)\right] \,.\end{aligned} \tag{2.24}$$

The coefficients $c_{\nu\ell}$, which are not yet determined, are fixed by the initial conditions.

Algorithm and Results

The 4×4 matrix (2.22) does not represent any particular challenge to an analytical solution of the eigenvalue equation. If we consider several different types of atoms, or the corresponding two-dimensional problem, however, the matrices become so large that only a numerical determination of the vibration modes is possible. We want to demonstrate the latter using our simple example.

First, we write the matrices F and M in a form suited for *Mathematica*, choosing $a = 1$:

```
mat1 = { {          2f, -f,  0, -f*Exp[-I q]},
         {          -f, 2f, -f,            0},
         {           0, -f, 2f,           -f},
         {-f*Exp[I q],  0, -f,           2f} }

massmat = DiagonalMatrix[{m1, m1, m1, m2}]
```

From this we form the product `mat2 = Inverse[massmat].mat1`. In this case, *Mathematica* is still capable of specifying the eigenvalues in a general

form in response to the command `Eigenvalues[mat2]`. The calculation is complex, however, and the result consists of nested square and cube roots; therefore we prefer a numerical calculation.

```
eigenlist = Table[{x, Chop[Eigenvalues[
            mat2 /.{f->1.,m1->0.4,m2->1.0,q->x}]]},
                  {x,-Pi,Pi,Pi/50}]
```

In a short time this command yields a list of q values and the four corresponding squares of the frequencies.

```
Flatten[ Table[
         Map[{#[[1]],Sqrt[#[[2,k]]]}&, eigenlist],
         {k,4}], 1]
```

turns this result into a list of $(q$–$\omega)$ pairs, which were plotted with `ListPlot` in Fig. 2.12. As we can see, the allowed frequencies of the lattice vibrations form four bands. The lowest branch represents the so-called acoustic phonons, for which adjacent atoms almost always oscillate in the same direction. For $q = 0$, the entire chain is just shifted as a whole, which does not require any energy ($\omega = 0$). The three upper branches, the optical phonons, have many atoms oscillating against each other which requires energy even at $q = 0$.

The individual displacements can be determined from the eigenvectors of the matrix $\mathsf{M}^{-1}\mathsf{F}$. Figure 2.13 shows the four eigenmodes for $q = 0$. Surpris-

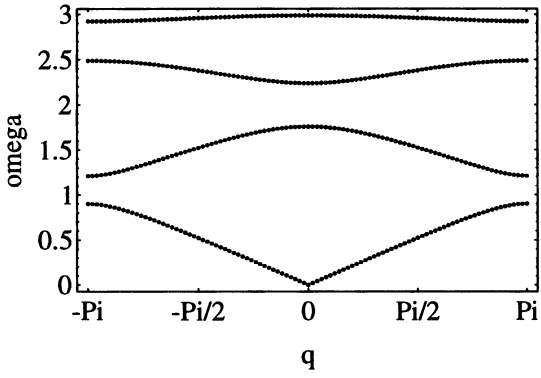


Fig. 2.12. The frequencies of the four eigenmodes of the linear chain from Fig. 2.11 as a function of the wave number q

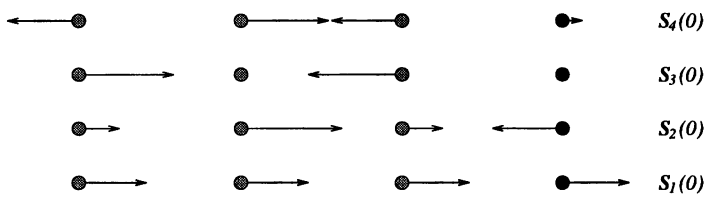
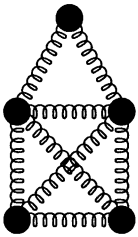


Fig. 2.13. Eigenmodes of the chain for $q = 0$

ingly the heavy atom and one of the light ones are at rest in the third branch, while the two other masses oscillate against each other.

Exercise

Investigate the two-dimensional vibrations of your single-family home. Five equal masses m are coupled by springs, and the potential between neighboring masses is



$$V(\boldsymbol{r}_i, \boldsymbol{r}_j) = \frac{D}{2}\left(|\boldsymbol{r}_i - \boldsymbol{r}_j| - a_{ij}\right)^2 \ ,$$

where the a_{ij} are the distances between the masses at rest, i.e., $a_{ij} = l$ for the sides and the roof, and $a_{ij} = \sqrt{2}l$ for the two diagonals.

Calculate the frequencies of the vibrations for small displacements and plot the eigenmodes. It is especially impressive if you produce an animation of the eigenmodes.

Literature

Goldstein H. (1980) Classical Mechanics. Addison-Wesley, Reading, MA
Kittel C. (1996) Introduction to Solid State Physics. Wiley, New York

2.4 The Hofstadter Butterfly

Linear equations can have intriguing solutions. This becomes especially apparent in the case of a crystal electron in a homogeneous magnetic field. The electron's energy spectrum as a function of the strength of the magnetic field has a complicated structure reminiscent of a butterfly. This problem was investigated in 1976 by Douglas Hofstadter. Amazingly, the differences between rational and irrational numbers become evident in this spectrum. We want to derive the quantum-mechanical equation for the energies of the electron and solve it numerically. A small computer program produces the intriguing butterfly.