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Appendix

Longitudinal oscillations of a linear chain with nearest neighbor interactions and free ends

The mechanical system of N mass points of mass M distributed along the x-axis is defined by the Lagrangian ($K = 2b^2$)

$$L(x_n, \dot{x}_n) = \frac{1}{2}M\sum_{n=1}^{N}\dot{x}_n^2 - \frac{1}{2}K\sum_{n=2}^{N}(x_n - x_{n-1} - a)^2.$$

Equilibrium positions of the points are $x_n = na$, $n = 1, 2, \ldots, N$. In terms of longitudinal displacements from equilibrium positions $\psi_n = x_n - na$ the Lagrangian reads

$$L(\psi_n, \dot{\psi}_n) = \frac{1}{2}M\sum_{n=1}^{N}\dot{\psi}_n^2 - \frac{1}{2}K\sum_{n=2}^{N}(\psi_n - \psi_{n-1})^2.$$

The corresponding Lagrange equations are

$$M\ddot{\psi}_n = K[\psi_{n+1} - 2\psi_n + \psi_{n-1}], \quad n = 2, \ldots, N-1, \tag{1}$$

$$M\ddot{\psi}_1 = K[\psi_2 - \psi_1 + 0], \quad M\ddot{\psi}_N = K[0 - \psi_N + \psi_{N-1}].$$

The whole system of equations for $n = 1, 2, \ldots, N$ can be written in the form (1), if fictitious points x_0, x_{N+1} are introduced with the boundary conditions of equal displacements

$$\psi_0 = \psi_1, \qquad \psi_{N+1} = \psi_N,$$

corresponding to free ends, or

$$x_1 - x_0 = a, \qquad x_{N+1} - x_N = a.$$

Summarizing, we are looking for the general solution $\psi_1(t), \ldots, \psi_N(t)$ of the system of N linear ordinary differential equations

$$\ddot{\psi}_n = \frac{K}{M}[\psi_{n+1} - 2\psi_n + \psi_{n-1}], \quad n = 1, 2, \ldots, N, \tag{2}$$

subject to boundary conditions

$$\psi_0 = \psi_1, \qquad \psi_{N+1} = \psi_N \tag{3}$$

Any solution can be written as a linear combination of fundamental solutions — the modes — in which all degrees of freedom oscillate with the same frequency,

$$\psi_n(t) = X_n \cos \omega t, \quad n = 1, 2, \ldots, N,$$

(or $x_n(t) = X_n \cos \omega t + na$). Substitution into (2), (3) leads to the system of linear difference equations for the amplitudes X_n

$$X_{n+1} + X_{n-1} = (2 - \frac{M\omega^2}{K})X_n, \quad n = 1, 2, \ldots, N \tag{4}$$

subject to linear boundary conditions

$$X_0 = X_1, \qquad X_{N+1} = X_N. \tag{5}$$

According to general theory there are N fundamental solutions, each given up to an arbitrary multiplier. These solutions can be determined like the standing waves $A \sin kx + B \cos kx$ on the continuous spring, but restricted to discrete positions $x = na$. Our starting point are the identities

$$\sin k(n+1)a + \sin k(n-1)a = 2 \sin kna \cos ka,$$

$$\cos k(n+1)a + \cos k(n-1)a = 2 \cos kna \cos ka,$$

implying that

$$X_n = A \sin kna + B \cos kna$$

solves (4), if a nonlinear dispersion relation

$$2 - \frac{M\omega^2}{K} = 2 \cos ka$$

holds, i.e.

$$\omega(k)^2 = 2\frac{K}{M}(1 - \cos ka) = 4\frac{K}{M} \sin^2 \frac{ka}{2}. \tag{6}$$

Admissible values of k are determined from the boundary conditions (5). The resulting N modes can be obtained from a simple graphical representation and are given (up to a multiplier) by

$$X_n^{(m)} = \cos k_m(n - \frac{1}{2})a, \quad m = 0, 1, 2, \ldots, N-1, \tag{7}$$

where

$$k_m = \frac{m\pi}{Na}, \tag{8}$$

hence

$$\omega_m^2 = \omega(k_m)^2 = 4\frac{K}{M} \sin^2 \frac{m\pi}{2N}. \tag{9}$$

$A_m = \frac{M}{K}\omega_m^2 \in [0,4$

General solution of (2), (3) depends on $2N$ integration constants $A_1, \ldots, A_{N-1}, \varphi_1, \ldots, \varphi_{N-1}$, V, B:

$$\psi_n(t) = \sum_{m=1}^{N-1} A_m X_n^{(m)} \cos(\omega_m t + \varphi_m) + Vt + B; \tag{10}$$

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here the non-oscillating "zero mode" $\psi_n^{(0)}(t) = Vt + B$ corresponds to free center-of-mass motion of the whole chain.

It is straightforward to verify that our solutions (7), (8) satisfy the boundary conditions (5) for all $m = 0, 1, 2, \ldots, N-1$:

$$\begin{aligned}
X_1^{(m)} - X_0^{(m)} &= \cos k_m(1 - \frac{1}{2})a - \cos k_m(0 - \frac{1}{2})a = 0, \\
X_{N+1}^{(m)} - X_N^{(m)} &= \cos k_m(N + 1 - \frac{1}{2})a - \cos k_m(N - \frac{1}{2})a = \\
&= \cos(m\pi + \frac{m\pi}{2N}) - \cos(m\pi - \frac{m\pi}{2N}) = \\
&= -2\sin m\pi \sin\frac{m\pi}{2N} = 0.
\end{aligned}$$

If ψ denotes the column vector with components ψ_n, $n = 1, \ldots, N$, equations of motion (2) can be written in matrix form

$$\ddot{\psi} + \mathbb{B}\psi = 0.$$

The matrix $\mathbb{B}$ with matrix elements $B_{jk} = \frac{1}{M}\frac{\partial^2 V}{\partial\psi_j\partial\psi k}|_{\psi=0}$ describes the interaction,

$$\mathbb{B} = \frac{K}{M}\begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}.$$

For the modes $\psi(t) = X\cos\omega t$, where X is the column vector with components X_n, equations (4) take the matrix form

$$(\mathbb{B} - \omega^2\mathbb{I})X = 0$$

or the form of the eigenvalue problem

$$\mathbb{B}X^{(m)} = \omega_m^2 X^{(m)}.$$

It is a well-known fact that the eigenvectors $X^{(m)}$, $X^{(m')}$ belonging to different eigenvalues $\omega_m^2 \neq \omega_{m'}^2$ are orthogonal in the sense of the inner product

$$(X^{(m)}, X^{(m')}) = \sum_{n=1}^{N} X_n^{(m)} X_n^{(m')} = 0.$$

After normalization $\sum_{n=1}^{N}(X_n^{(m)})^2 = 1$ we have

$$(X^{(m)}, X^{(m')}) = \delta_{mm'}.$$

In order to diagonalize $\mathbb{B}$, the matrix $\mathbb{X}$ is introduced, whose columns are the normalized eigenvectors, $X_{nm} = X_n^{(m)}$. This matrix is orthogonal, $\mathbb{X}^T\mathbb{X} = \mathbb{I}$, and the eigenvalue problem takes the form

$$\mathbb{B}\mathbb{X} = \mathbb{X}\mathbb{L},$$

where $\mathbb{L} = \mathrm{diag}(\omega_0^2 = 0, \omega_1^2, \ldots, \omega_{N-1}^2)$, implying diagonalization of $\mathbb{B}$ by $\mathbb{X}$,

$$\mathbb{X}^T\mathbb{B}\mathbb{X} = \mathbb{X}^T\mathbb{X}\mathbb{L} = \mathbb{L}.$$

$\psi = Xy$

References

[1] W.V. Houston: *Principles of Mathematical Physics*, McGraw-Hill, New York 1948

[2] M. Born, K. Huang: *Dynamical Theory of Crystal Lattices*, Clarendon Press, Oxford 1954

[3] D.E. Rutherford, *Proc. Roy. Soc. (Edinburgh)*, Ser. A, **62** (1947), 229, **63** (1951), 232

[4] H. Puszkarski, On the approximation of real boundary conditions in a linear finite chain by cyclic conditions, *Acta Phys. Polon.* **36** (1969), 675–696

[5] Ch. Jordan: *Calculus of Finite Differences*, Chelsea Publ. Comp., New York 1950