

5. Normal Modes of a Three-Dimensional Crystal

Consider a face-centered cubic monatomic Bravais lattice in which each ion interacts only with its (twelve) nearest neighbors. Assume that the interaction between a pair of neighboring ions is described by a pair potential ϕ that depends only on the distance r between the pair of ions.

(a) Show that the frequencies of the three normal modes with wave vector \mathbf{k} are given by

$$\omega = \sqrt{\lambda/M} \quad (22.96)$$

where the λ are the eigenvalues of the 3×3 matrix:

$$\mathbf{D} = \sum_{\mathbf{R}} \sin^2 \left(\frac{1}{2} \mathbf{k} \cdot \mathbf{R} \right) [A \mathbf{1} + B \hat{\mathbf{R}} \hat{\mathbf{R}}]. \quad (22.97)$$

Here the sum is over the twelve nearest neighbors of $\mathbf{R} = 0$:

$$\frac{a}{2} (\pm \hat{x} \pm \hat{y}), \quad \frac{a}{2} (\pm \hat{y} \pm \hat{z}), \quad \frac{a}{2} (\pm \hat{z} \pm \hat{x}); \quad (22.98)$$

$\mathbf{1}$ is the unit matrix ($(\mathbf{1})_{\mu\nu} = \delta_{\mu\nu}$), and $\hat{\mathbf{R}} \hat{\mathbf{R}}$ is the diadic formed from the unit vectors $\hat{\mathbf{R}} = \mathbf{R}/R$ (i.e., $(\hat{\mathbf{R}} \hat{\mathbf{R}})_{\mu\nu} = \hat{\mathbf{R}}_\mu \hat{\mathbf{R}}_\nu$). The constants A and B are: $A = 2\phi(d)/d$, $B = 2[\phi''(d) - \phi'(d)/d]$, where d is the equilibrium nearest-neighbor distance. (This follows from Equations (22.59) and (22.11).)

(b) Show that when \mathbf{k} is in the (100) direction ($\mathbf{k} = (k, 0, 0)$ in rectangular coordinates), then one normal mode is strictly longitudinal, with frequency

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} \sin \frac{1}{4}ka, \quad (22.99)$$

and the other two are strictly transverse and degenerate, with frequency

$$\omega_T = \sqrt{\frac{8A + 2B}{M}} \sin \frac{1}{4}ka. \quad (22.100)$$

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