Week 4

- One-dimensional crystals

One-dimensional crystal

$$V(r) = V(a) + \frac{1}{2}(r-a)^2 K$$

$$K = \frac{\partial^2 V(r=a)}{\partial r^2}$$

$$C = Ka$$

Energy, forces, equations of motion

$$V = const + \sum_n \frac{K}{2}(u_{n+1} - u_n)^2$$

$$F_n = -\frac{\partial V}{\partial u_n} = +(u_{n+1} - u_n) - (u_n - u_{n-1}) = K(u_{n+1} - 2u_n + u_{n-1})$$

Newton's law

$$M\ddot{u}_n = K(u_{n+1} - 2u_n + u_{n-1}), \quad n = 1, 2, \ldots$$

Solution of Newton's equations

$$M\ \ddot{u}_n = K\left(u_{n+1} - 2u_n + u_{n-1}\right),$$

system of N coupled equations

$$u_n = A\exp[i(k\,x_n^{(0)} - \omega t)]$$

$$x_n^{(0)} = na$$

$$-\omega^2 M = K\left(e^{ika} - 2 + e^{-ika}\right)$$

There is no n here, one equation!

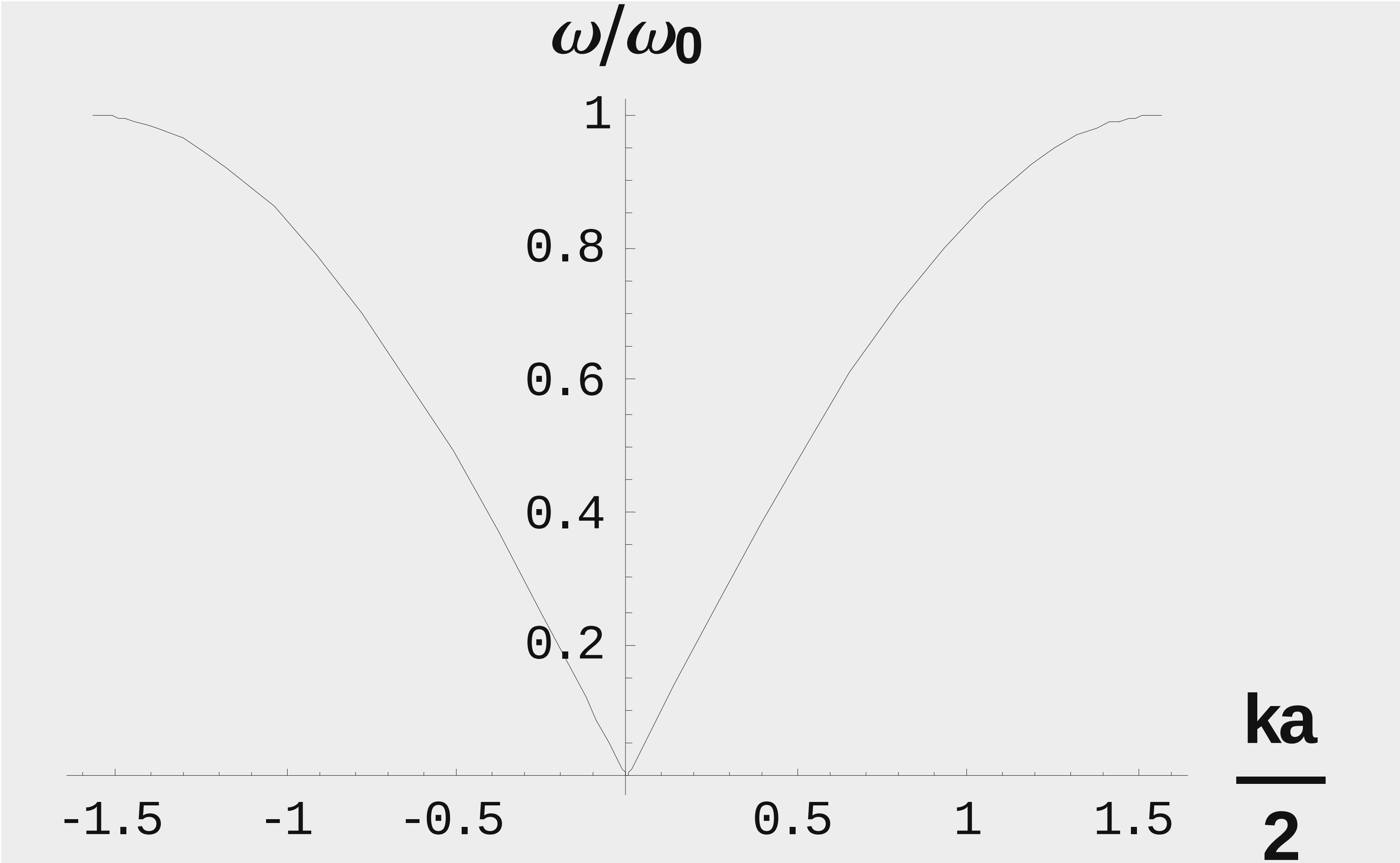
Spectrum

$$-\omega^2 M = K\left(e^{ika} - 2 + e^{-ika}\right)$$

$$\omega^2 = \frac{2K}{M}[1-\cos(ka)] = \frac{4K}{M}\sin^2(ka/2)$$

$$\omega = \omega_0\,|\sin(ka/2)|, \quad \omega_0 = 2\sqrt{\frac{K}{M}}$$

Spectrum



Large-wavelength limit

When $k\,a \ll 1$ then

$$\omega = \mathrm{v}\,k$$

$$\mathrm{v} = \sqrt{\frac{K}{M}}\,a,\;\; C = Ka,\; \rho = M/a \Rightarrow \mathrm{v} = \sqrt{\frac{C}{\rho}}$$

Number of oscillators, Brillouin zone

$n = 1, 2, ...N \quad N$ atoms

Periodic conditions

$$u_n = u_{n+N}$$

$$u_n = A\exp[i(k\,n\,a - \omega t)]$$

$$k\,a\,N = 2\pi m \qquad aN = L \qquad k\,L = 2\pi m$$

$$k = k_m = \frac{2\pi}{L}m, \qquad m = 0, \pm 1, \pm 2, ... \;, \; |m| \leq N/2$$

Number of states

$$\frac{L\,\Delta k}{2\pi} = \Delta m = \text{number of states with momenta}$$

$$\text{between } k \text{ and } k+\Delta k$$

$$\int_{-k_{\max}/2}^{k_{\max}/2} \frac{L\,dk}{2\pi} = N, \qquad k_{\max} = \frac{\pi}{L}$$

Two ways to present the sum over momenta:

$$\sum_{m=-N/a}^{m/2} f(k_m) = \int_{-k_{\max}/2}^{k_{\max}/2} f(k)\frac{L\,dk}{2\pi}$$

Number of states in 3D case

In general 3D case $\frac{Vd^3k}{(2\pi)^3}$ is the number of states,

here V is the volume of the crystal

$$\int_{\mathrm{BZ}} f(\mathbf{k}) \frac{Vd^3k}{(2\pi)^3} = \sum_m f(k_m)$$