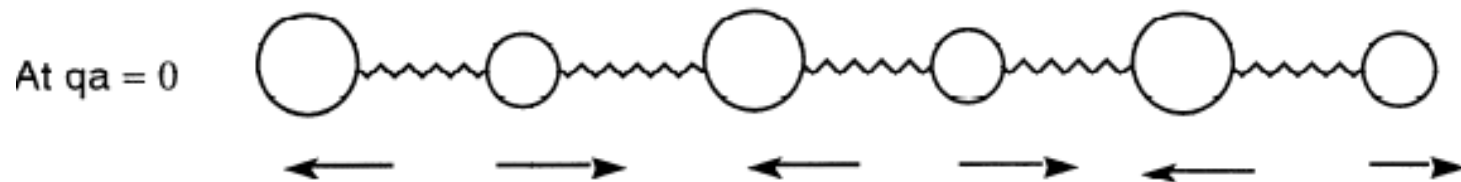
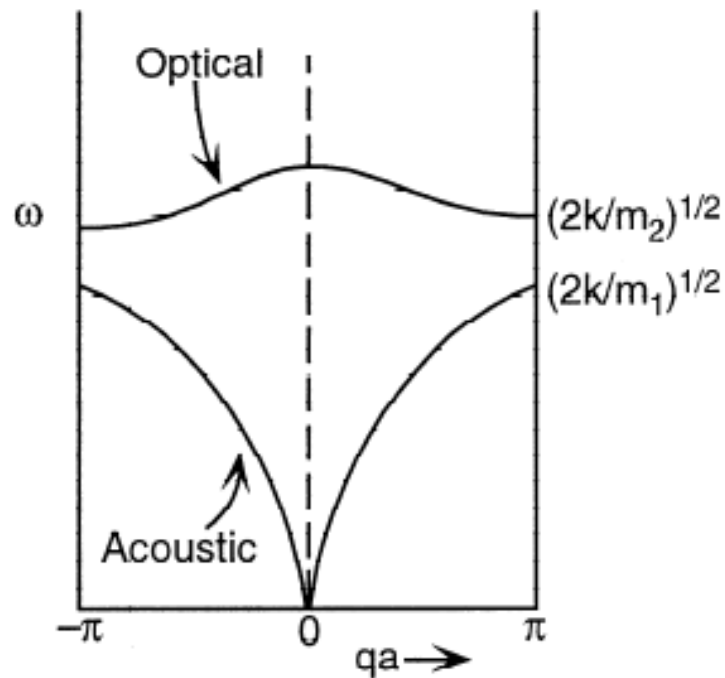
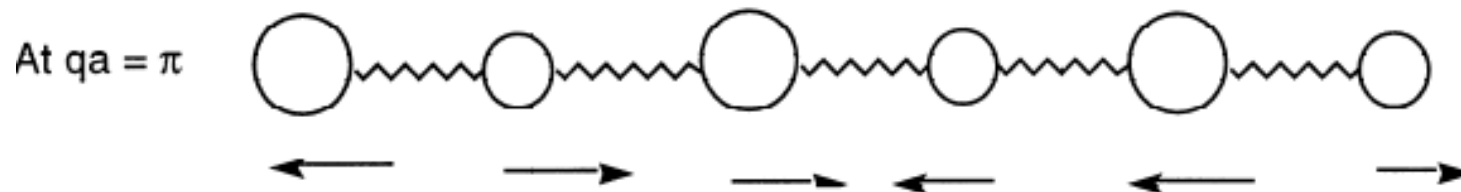


Highest Frequency possible without intra-unit cell motions.

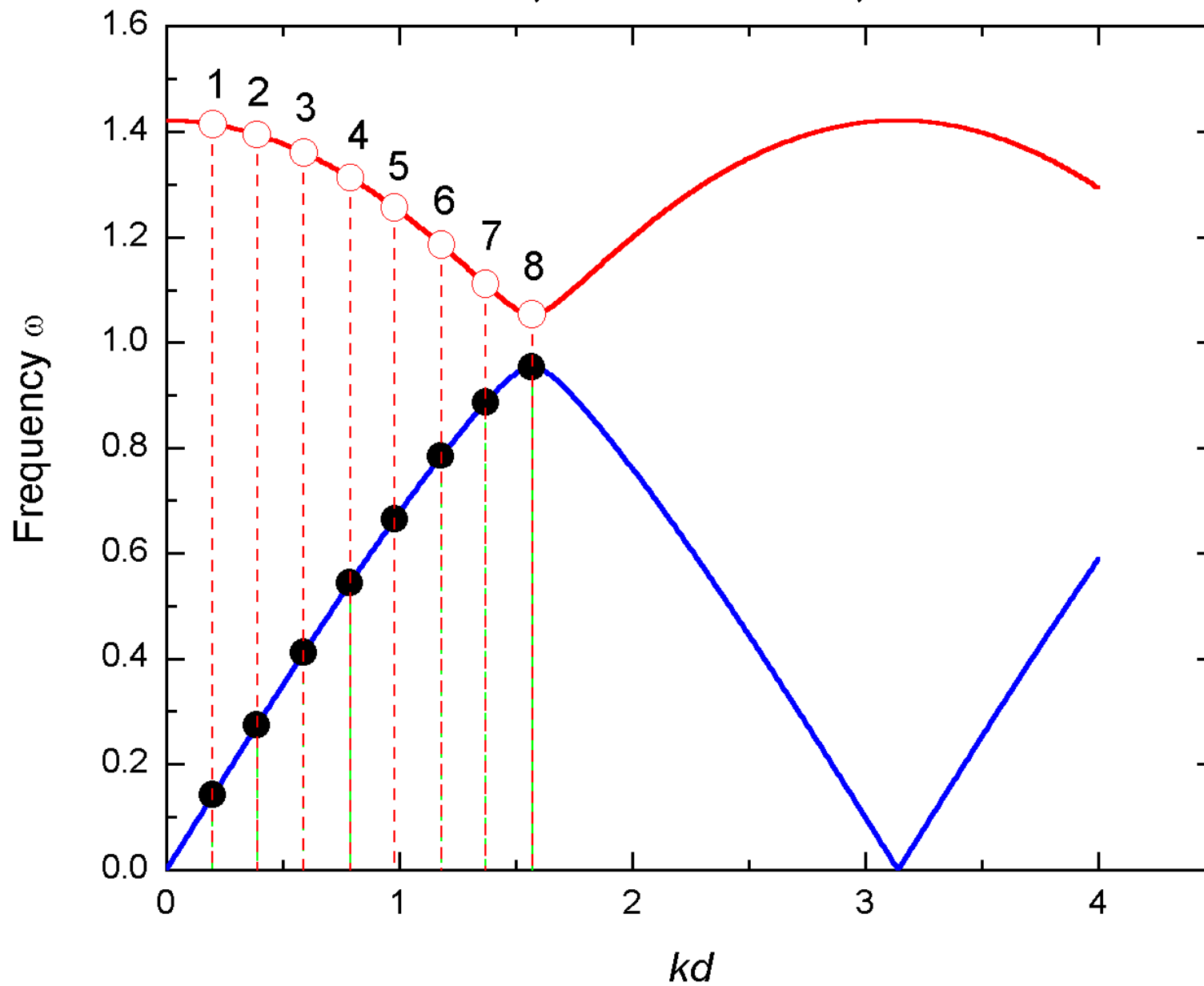


Atoms within each unit cell move out of phase but phases within each cell are identical

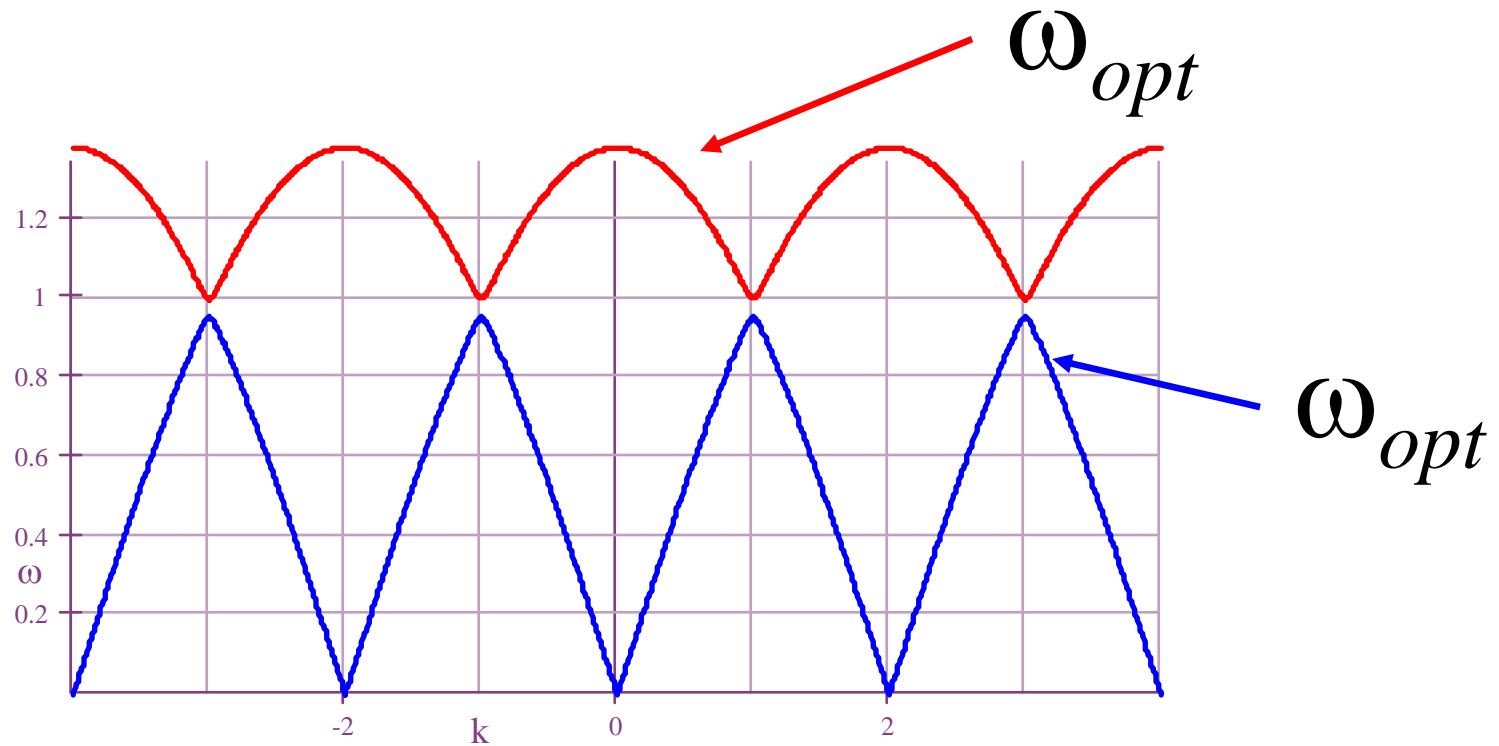


Atoms in each cell are out of phase and phase changes from cell to cell

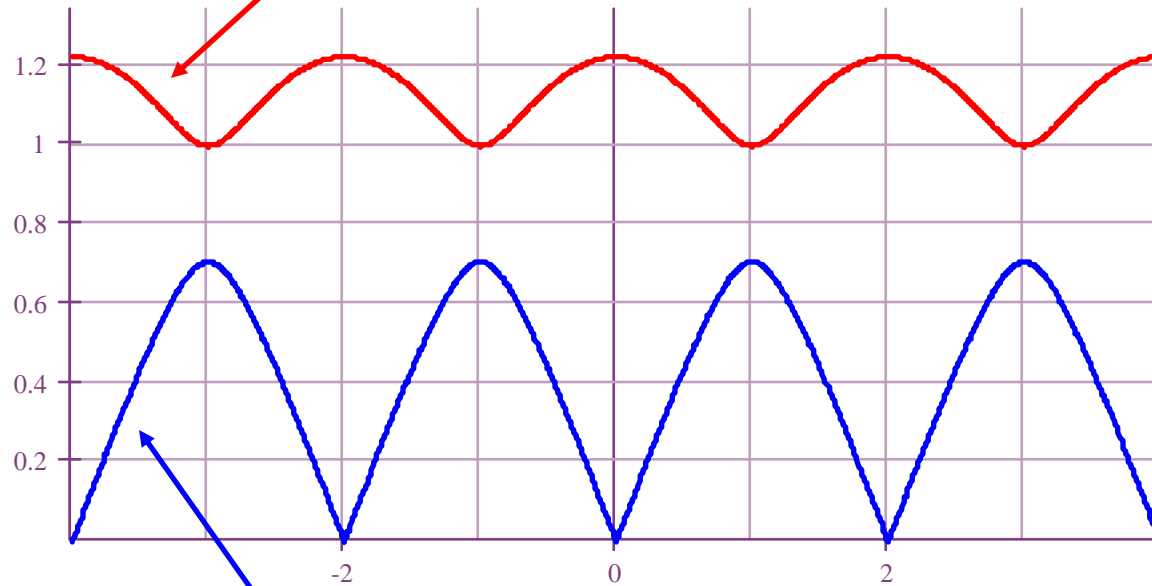
Diatomic chain, 16 masses, 8 unit cells



Dispersion Relation: diatomic

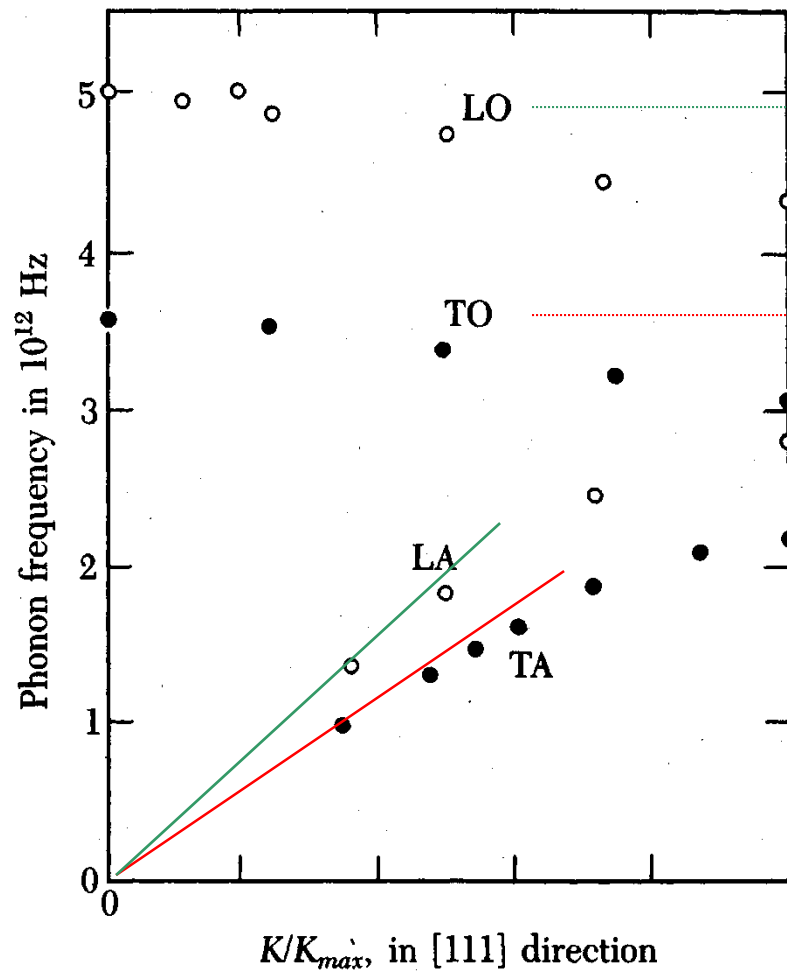


$$\omega_{opt} = \sqrt{\kappa \left(\frac{1}{M} + \frac{1}{m} \right) + \kappa \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \left(\sin \left[k \frac{a}{2} \right] \right)^2}}$$



$$\omega_{ac} = \sqrt{\kappa \left(\frac{1}{M} + \frac{1}{m} \right) - \kappa \sqrt{\left(\frac{1}{M} + \frac{1}{m} \right)^2 - \frac{4}{Mm} \left(\sin \left[k \frac{a}{2} \right] \right)^2}}$$

Dispersion Relation for KBr (measured by neutron scattering)



$\omega_{\text{opt}}/2\pi$ (longitudinal)

$\omega_{\text{opt}}/2\pi$ (transverse)

From C. Kittel, *Solid State Physics*
after Woods, Brockhouse, Cowley
and Cochran, *Phys. Rev.* **131**, 1025-1029
(1963)

Classical vibrations of atoms in a crystal

Normal modes involve *every* atom in the crystal

One natural frequency is associated with each normal mode

each $k=2\pi/\lambda$ describes the normal mode

Quantum wavefunctions of electrons in a crystal

eigenstate wavefunctions spread the probability density over the entire crystal

Each normal mode has a discrete vibrational frequency ω_k

each k describes the eigenstate wavefunction