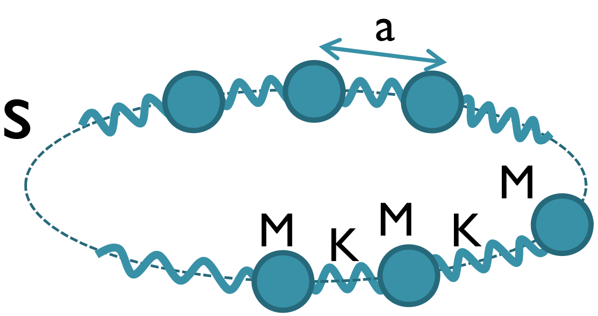
Lecture 5

Crystal Dynamics

Phonons = [acoustic or optical]
crystal vibrations

Monatomic 1d harmonic crystal

- N balls – N normal modes
- By solving Newton's eq.



N balls on a circle

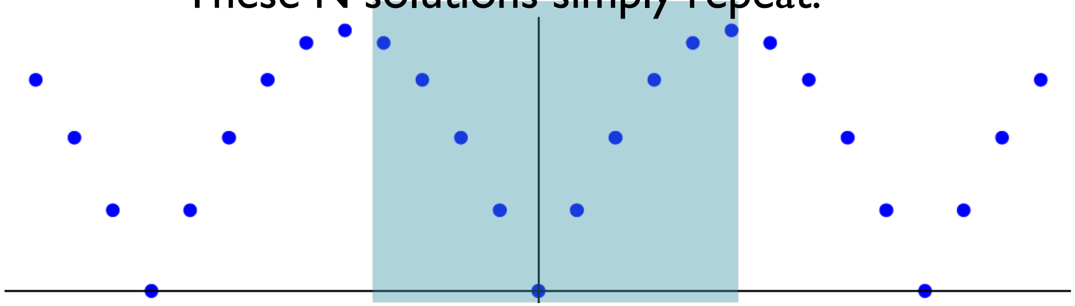
$$M\frac{d^2u_i}{dt^2} = -K\left[(u_i - u_{i-1}) + (u_i - u_{i+1})\right]$$

with a travelling wave form

$$u_n = A\exp[i(kx_n - \omega t)] = A\exp[i(kna - \omega t)]$$

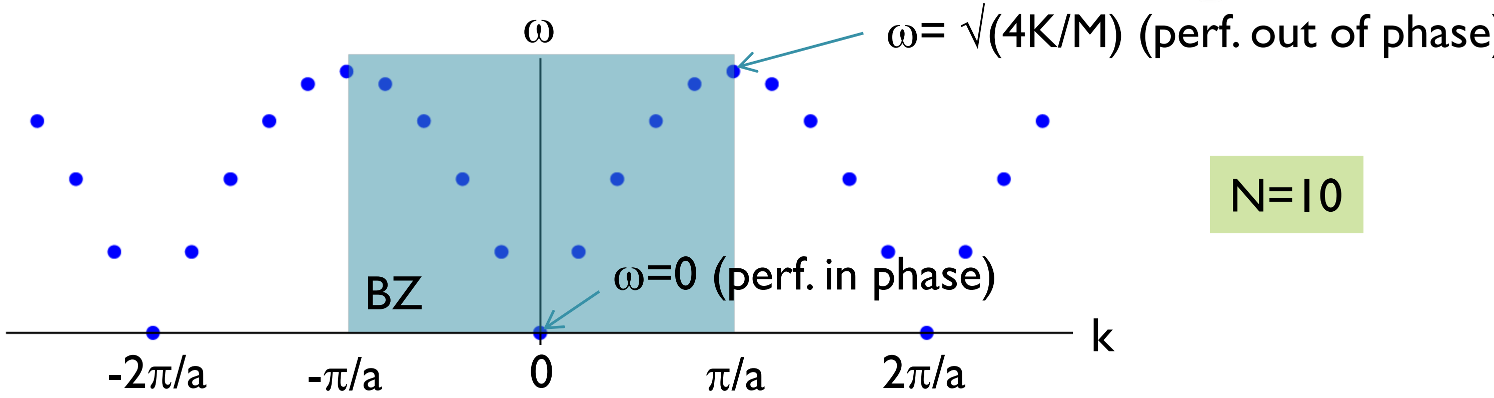
one finds all N normal modes (eq. 2.9).

These N solutions simply repeat.

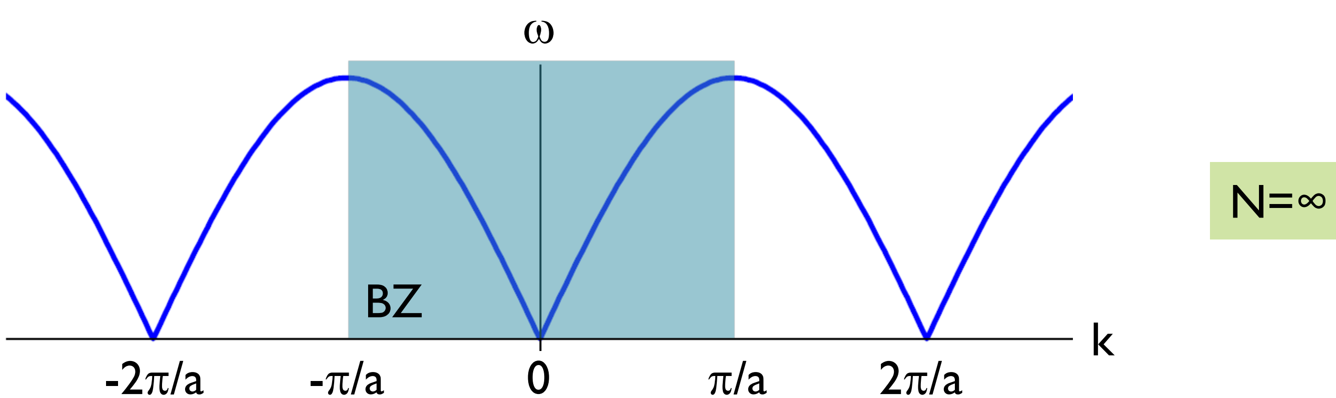


$$\omega = \sqrt{\frac{4K}{M}}\left|\sin\left(\frac{ka}{2}\right)\right|$$

Monatomic 1d harmonic crystal



- k period = 2π/a, N solutions in one period (i.e. complete)
- k step = 2π/(Na) =2π/L (L=length of crystal=circumference of ring)
- ω = vk for small k, with v = a√(K/M)   (sound velocity)



A diatomic 1d harmonic crystal

- Always remember that the solution is of the form (by Bloch's theorem – will do it later)

  $\exp(i(kna - \omega t))$

  where a is the unit cell size of the Bravais lattice (here a is NOT the inter-atomic distance)
- In the diatomic case write (note: difference from H&H)

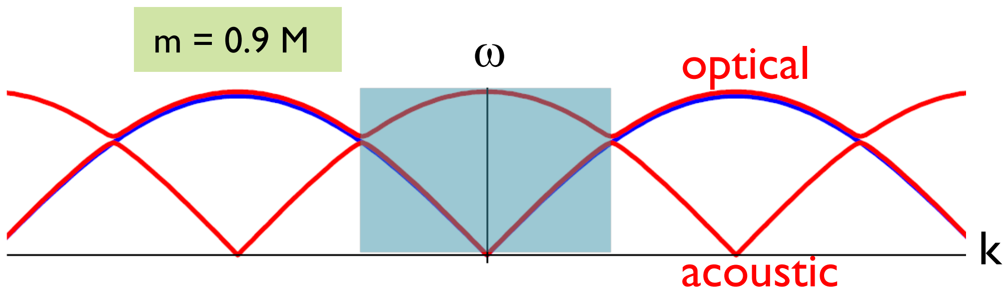
  $u_n = u \exp(i(kna - \omega t))$ for atom 1

  $v_n = v \exp(i(kna - \omega t))$ for atom 2

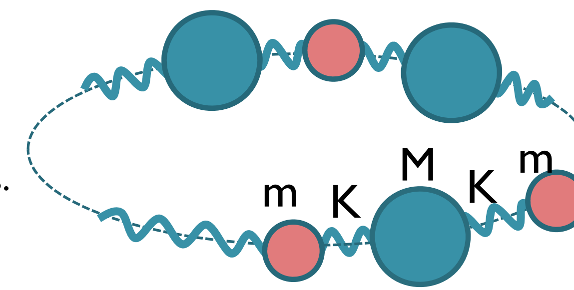
  Eq. (2.21): $$\omega = \sqrt{\frac{K(M+m)}{Mm}\left[1 \pm \sqrt{1 - 4\frac{Mm}{(M+m)^2}\sin^2(ka/2)}\right]}$$
- Always think "periodicity" and "inner dynamics" separately!

A diatomic 1d harmonic crystal

Change mass at every other atom from M to m



Blue: before
Red: after change



- Real space periodicity doubles, and so k space periodicity halves.
- k spacing ($2\pi/L$) is unchanged.
- Number of branches doubles (2 – acoustic and optical – now).
- Total number of modes = total number of atoms N = unchanged

- Acoustic branch: $\omega \to 0$ as $k \to 0$
- Optical branch: others