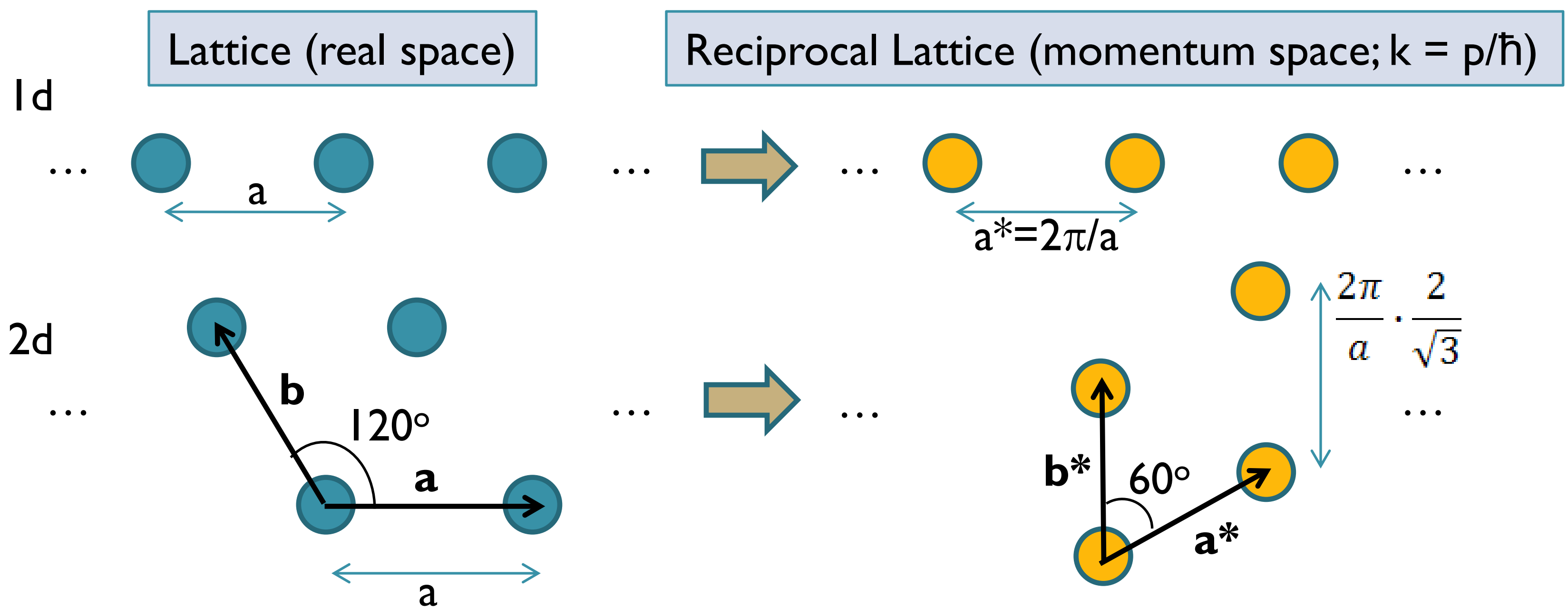
FF ch. 11 – Reciprocal Lattice

- Given the lattice of **a, b, c,** (in 3d; 2d, 1d analogous)

  <u>define reciprocal lattice</u> **a*,b*,c***:

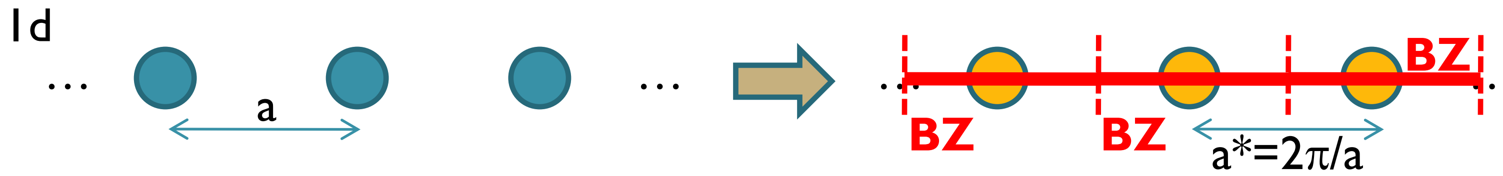
$$\mathbf{a}^*\cdot\mathbf{b} = \mathbf{a}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{c} = \mathbf{b}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{a} = \mathbf{c}^*\cdot\mathbf{b} = 0$$

$$\mathbf{a}^*\cdot\mathbf{a} = \mathbf{b}^*\cdot\mathbf{b} = \mathbf{c}^*\cdot\mathbf{c} = 2\pi$$ (and keep handed-ness)

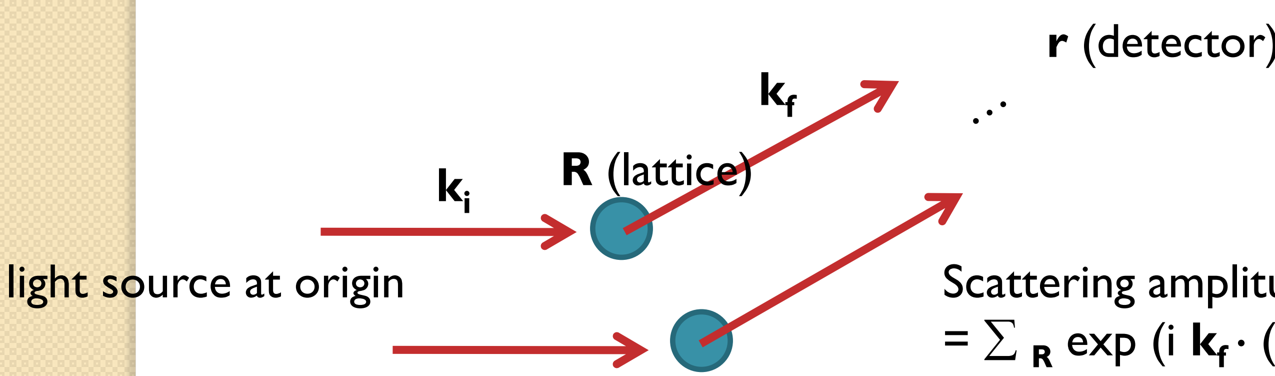


FF ch. 11 – Reciprocal Lattice

- WS cell of R.L.– (first) **<u>Brillouin zone</u>**



- LOTS of Physics, e.g. Bragg's law



Bragg's law: $\mathbf{q} = \mathbf{G}$
$\mathbf{q} = \mathbf{k_f} - \mathbf{k_i}$
$\mathbf{G} = m\,\mathbf{a}^* + n\,\mathbf{b}^* + o\,\mathbf{c}^*$
(m,n,o = integer)

$f \propto$ atomic and structural scattering form factors and spherical wave attenuation factor (1/distance)

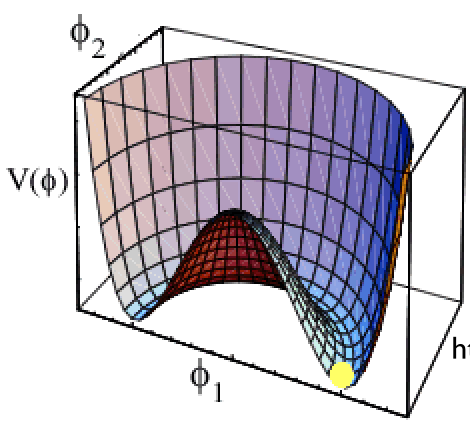
Scattering amplitude
$= \sum_{\mathbf{R}} \exp(i\,\mathbf{k_f}\cdot(\mathbf{r}-\mathbf{R}))\,\exp(i\,\mathbf{k_i}\cdot\mathbf{R})\,f(\mathbf{q})$
$\propto \sum_{\mathbf{R}} \exp(-i\,\mathbf{q}\cdot\mathbf{R})$
= <u>N if **q** is a R.L. vector, 0 otherwise</u>
(N = total number of lattice points)

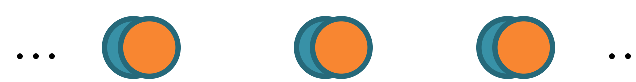
Miller index is (m,n,o) for **G** normal to the plane

Lecture 3

Crystal Dynamics – Phonons

- Phonon = crystal vibration: acoustic (sound), optical
- Sound waves in crystal are Goldstone bosons for the crystal's "spontaneously broken continuous symmetry"



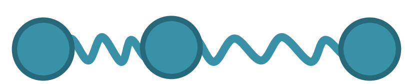


http://cosmicvariance.com/2005/10/24/hidden-symmetries

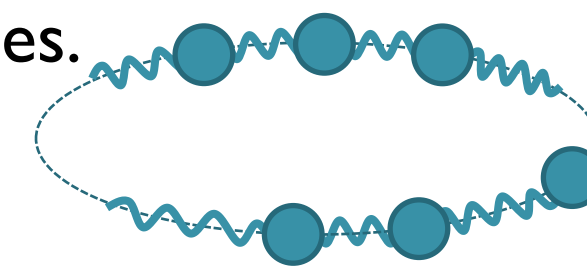
Just a warm-up

- Let’s recall some classical mechanics – **coupled harmonic oscillator problem** in one dimension (for simplicity, but without losing essence).
- For the following three cases, enumerate the total number of degrees of freedom. For the first case, sketch normal modes. For the low energy normal mode, find equivalent normal modes for the right two cases.

2 balls

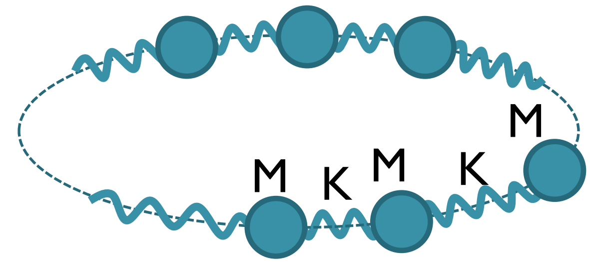


3 balls



N balls on a ring/circle

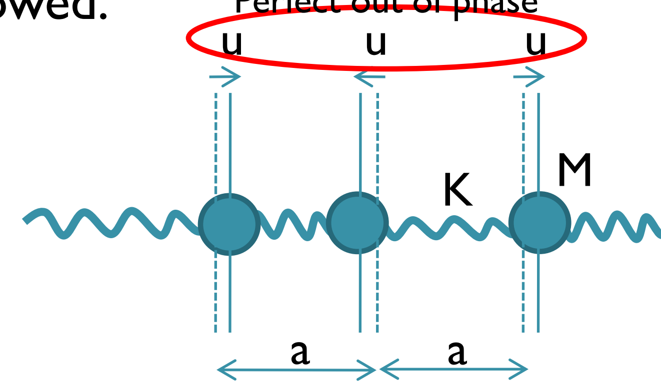
More warm-ups



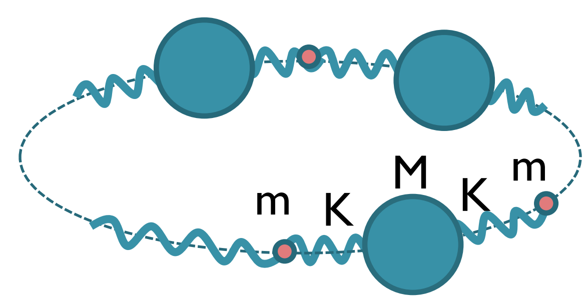
N balls on a circle

- Consider the "ring" problem which is model for 1d crystal (why?).

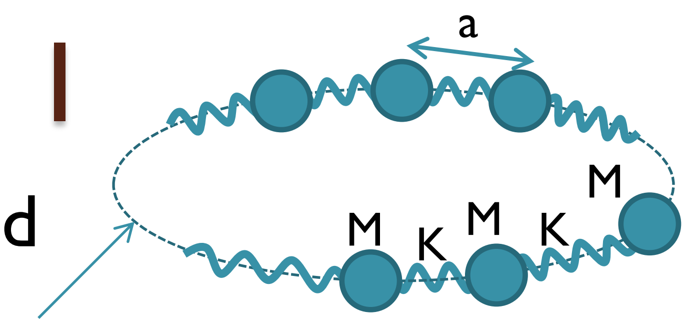
1) State the lowest ω mode and its k (wave vector).
2) Suppose the following mode was allowed. What is k? Obtain ω from Newton's eq. for u. Explain why this is the hardest or "stiffest" mode. (maximum frequency)



3) Now, consider two atoms per unit cell. Consider the limit M >> m. Discuss (k, ω) for the following three physical modes.
(i) lowest energy mode,
(ii) M's move perfectly out of phase and m just follows,
(iii) m's move and M is fixed



Learning question 1



N balls on a circle

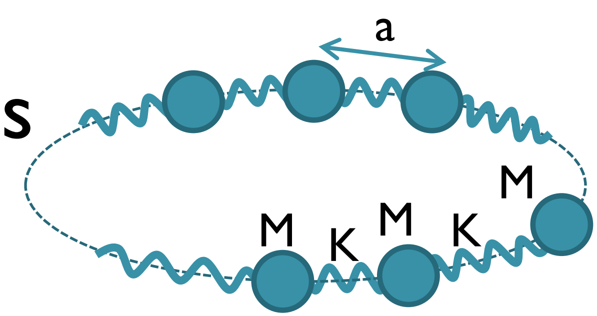
- Derive (2.9) and (2.11) and Figure (2.4) (i.e. solve this problem) by assuming a travelling wave form (2.8) for Newton's equation (2.7).
- Show that corresponding to <u>real space periodicity of a</u>, there is a <u>momentum space periodicity of $2\pi/a$</u> in (2.9) and there are N distinct values of k by (2.11) (i.e. the solution is complete).
- Show that at long wave length $\omega = v\,k$. Prove (2.13) and (2.14) for v.

Learning question 2

- Use (2.21), Figure 2.7 and 2.8 to explain what happens to the dispersion when a …-M-M-M-M-… ring is changed to a …-M-m-M-m-… ring. In so doing, address what changes are happening in (1) the real space periodicity, (2) the k space periodicity, (3) the step of k, (4) the total number of modes, (5) the number of branches, and (6) the sound velocity (page 44). Also, (7) verify that (2.21) in the limit of M >> m is indeed correct when compared against our previous considerations.
- <u>Qualitatively</u> sketch (cf. Fig. 2.8 and 2.7) what would happen for an …-M-m-m'-M-m-m'-… ring.
- How many acoustic phonons are present for 2d and 3d crystals?

Monatomic 1d harmonic crystal

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



N balls on a circle

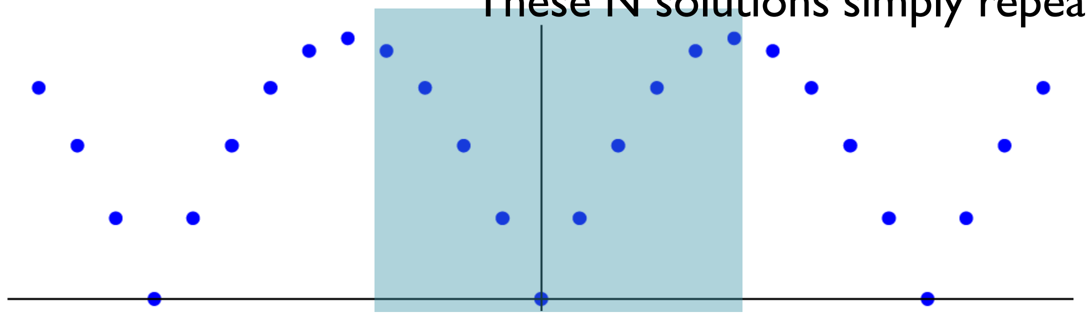
$$M\frac{d^2u_i}{dt^2} = -K\left[(u_i - u_{i-1}) + (u_i - u_{i+1})\right]$$

with a travelling wave form

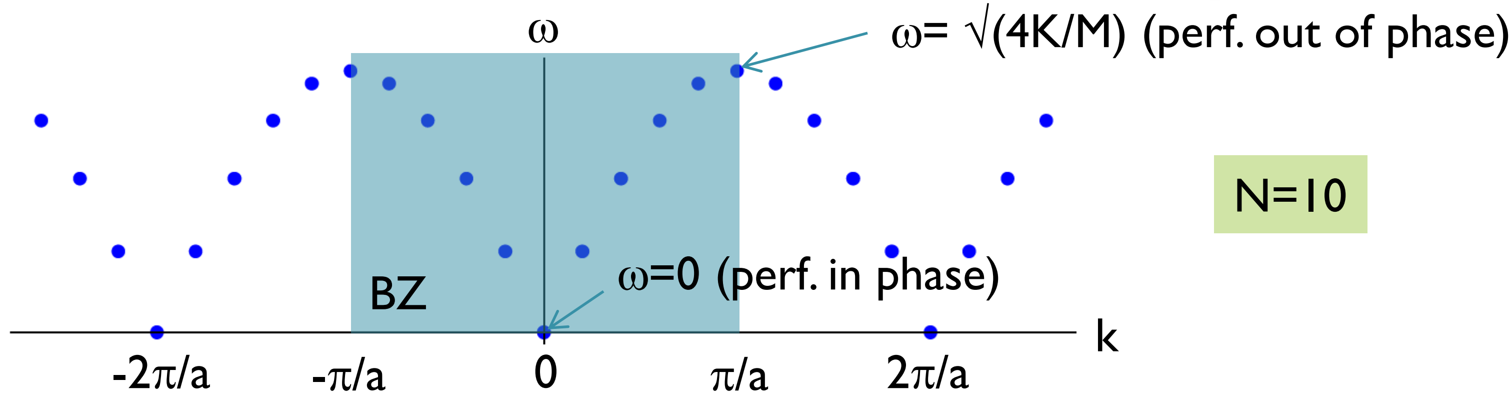
$$u_n = A\exp[i(kx_n - \omega t)] = A\exp[i(kna - \omega t)]$$

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

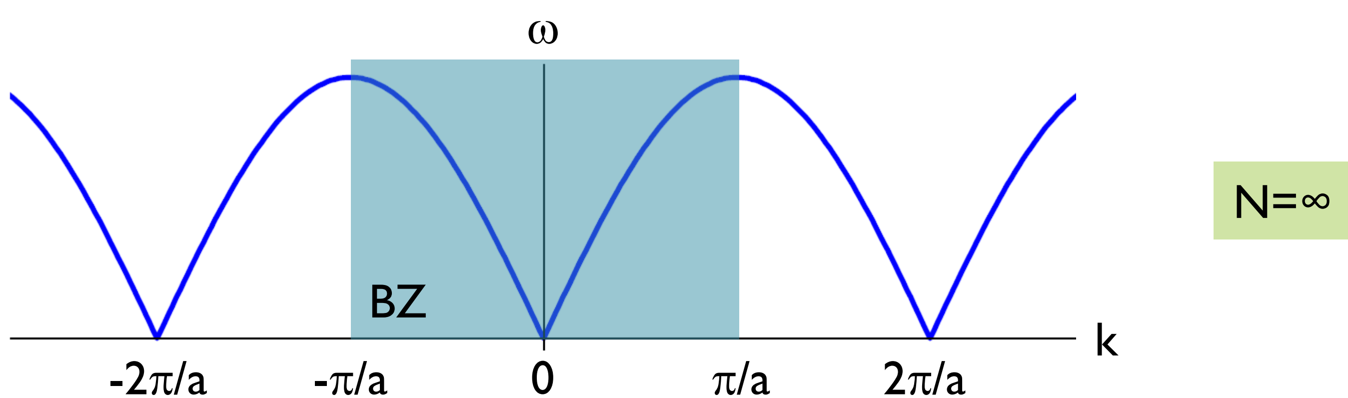
These N solutions simply repeat.



Monatomic 1d harmonic crystal

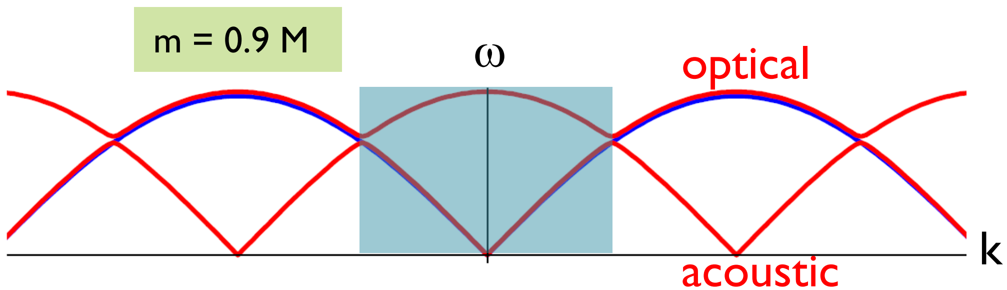


- k period = $2\pi/a$, N solutions in one period (i.e. complete)
- k step = $2\pi/(Na) = 2\pi/L$ (L=length of crystal=circumference of ring)
- $\omega = vk$ for small k, with $v = a\sqrt{(K/M)}$ (sound velocity)

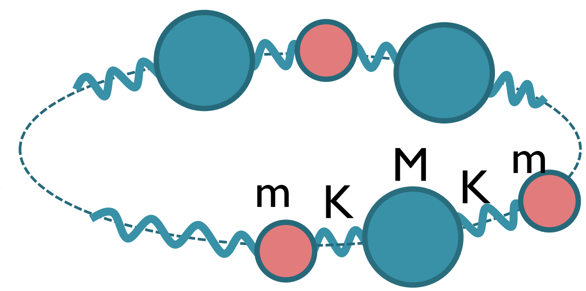


Diatomic 1d harmonic crystal

Change mass at every other atom from M to m

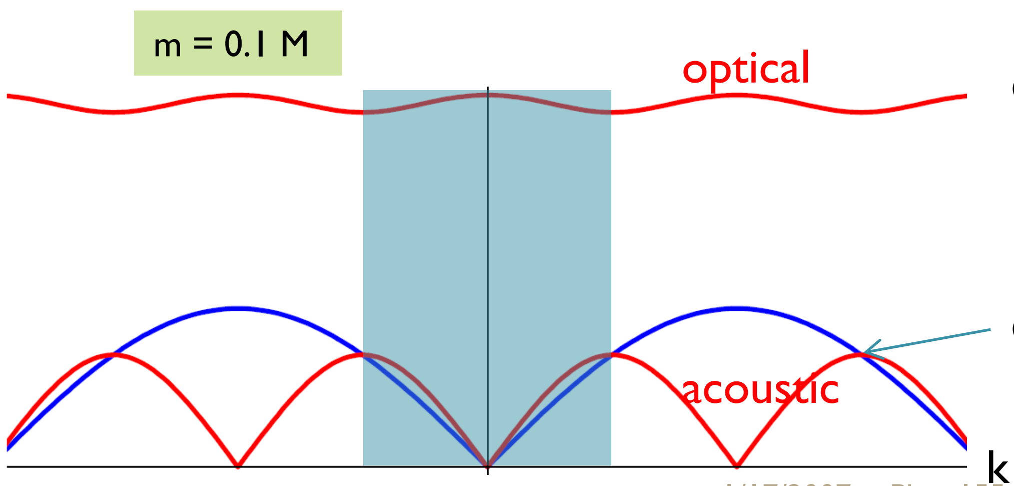


Blue: before
Red: after change



- 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



$\omega \approx \sqrt{(2K/m)}$

$\omega \approx \sqrt{(2K/M)}$

Acoustic and Optical Branches

- # of branches = Dh

  D = spatial dimension

  h = # of atoms in the <u>primitive</u> basis

  (Consider k=0 only, as the number of branches should be indep. of k. Number of possible branches = number of possible normal modes for each primitive basis = Dh.)

- # of acoustic branches = D

  i.e. 1 in 1d, 2 in 2d, 3 in 3d

  1 LA – longitudinal acoustic,

  and the rest are TA – transverse

- # of optical branches = Dh – D

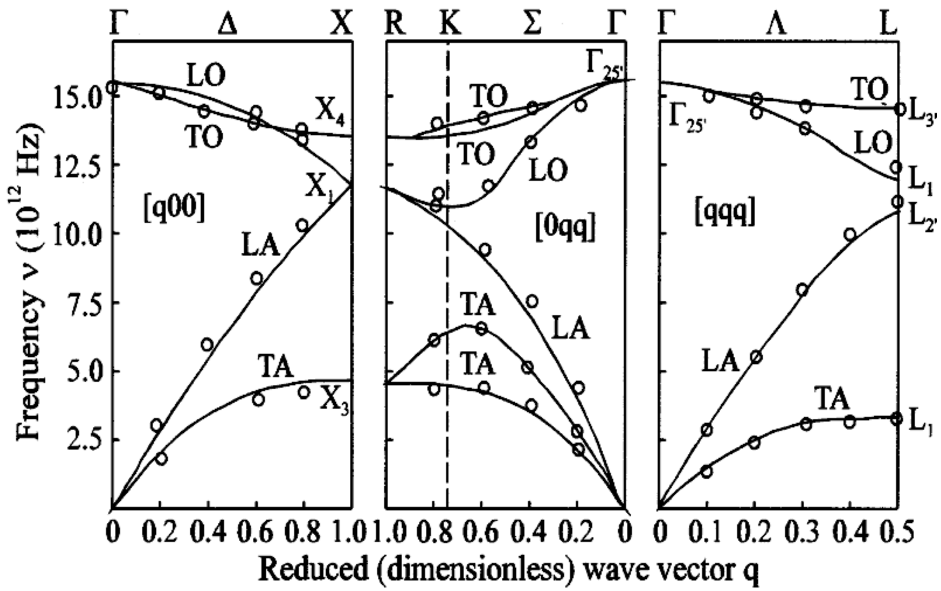
A and O Branches – example

Material = Si

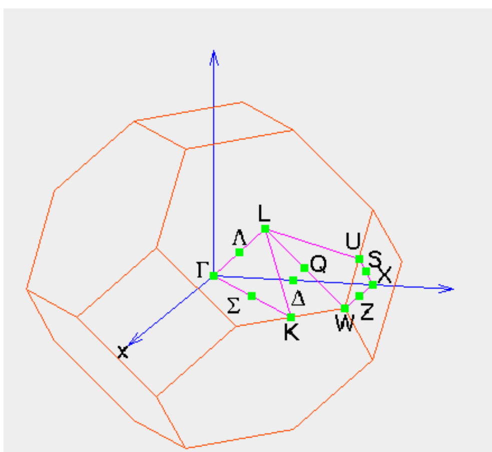
(note: 10^{12} Hz = THz = 4.1 meV)

Diamond structure

2 atom basis in fcc



http://www.ioffe.rssi.ru/SVA/NSM/Semicond/SiGe/mechanic.html



http://cst-www.nrl.navy.mil/~mehl/phonons/fcczone.png

Generally, TA has lower energy than LA, and tends to be degenerate.

Phonons

- So far, we used only classical mechanics. But, once we find classical normal modes, it is trivial to treat the problem in quantum mechanics, since each normal mode is described by an independent harmonic oscillator Hamiltonian (by definition of a normal mode).
- Energy levels for each normal mode is then given by

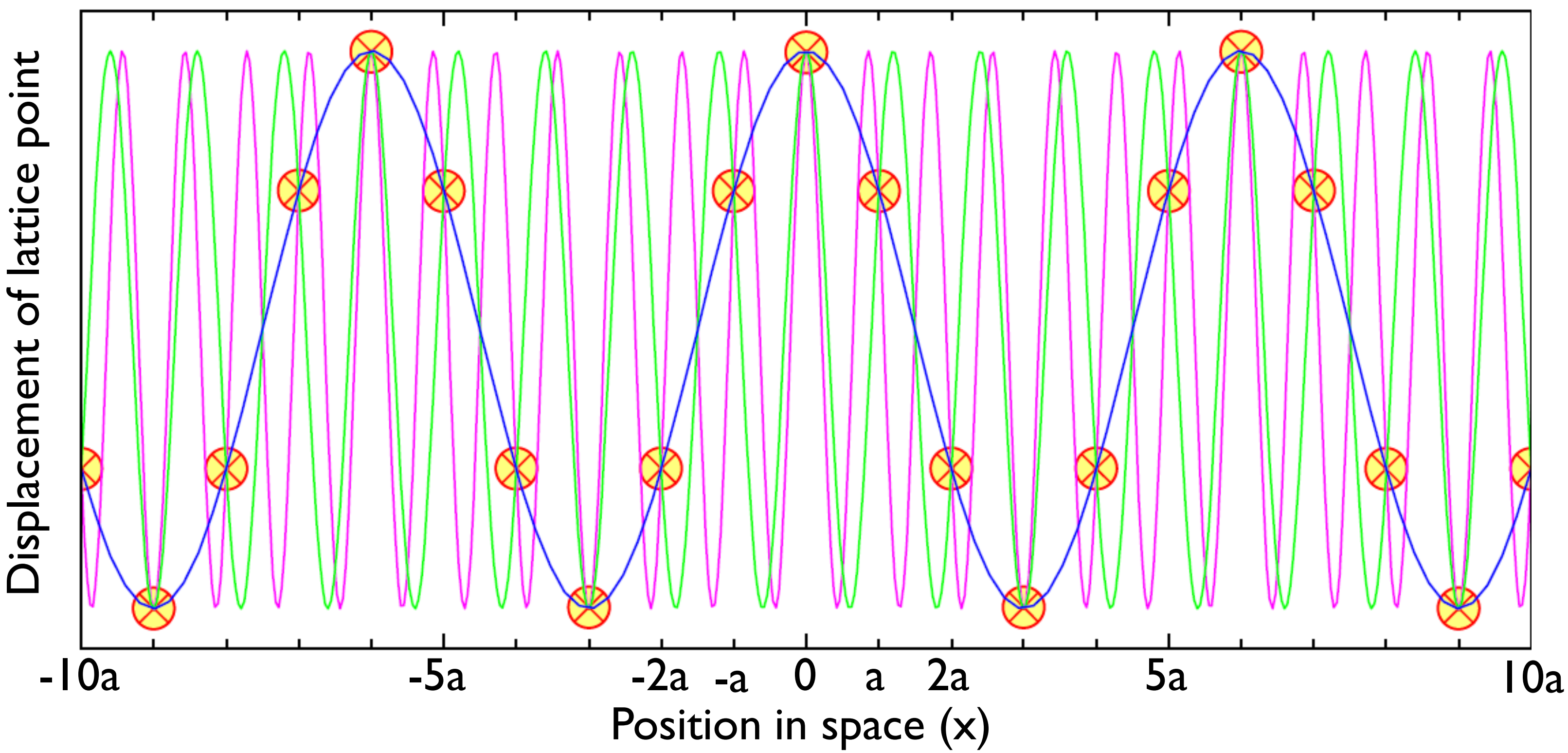
  $$(n + \tfrac{1}{2})\,\hbar\omega$$

  where $\omega = \omega$(k, other quantum numbers), and

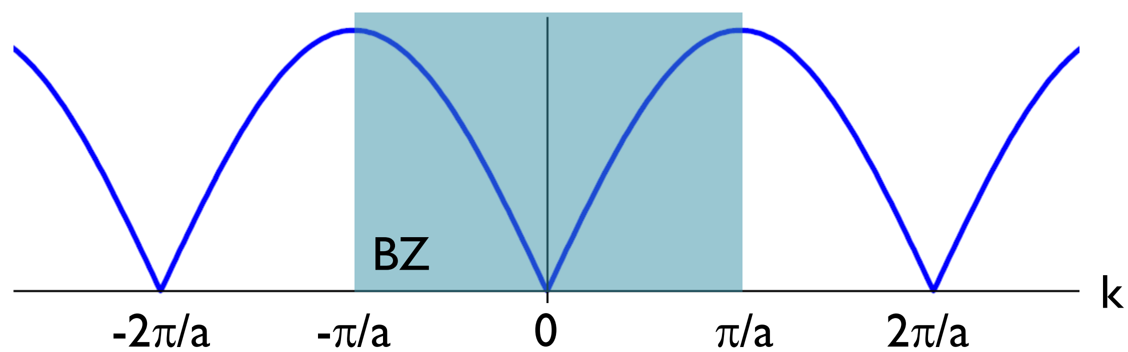
  $n = 0, 1, 2, \ldots$
- Quantum of these (vibrational) normal modes is called **phonon**, i.e. n describes the number of phonons.
- As we have seen, k is a good quantum number for describing phonons. Other good quantum numbers are polarizations, i.e. T or L – transverse or longitudinal.

Crystal Momentum

The following shows examples of waves associated with lattice displacement u, $\propto$ cos(kx) with k = $\pi/(3a)$ (blue), $\pi/(3a)-2\pi/a$ (green), $\pi/(3a)+2\pi/a$ (magenta). While these waves would be distinct if they existed in free space (curves), in 1d crystal with periodicity a, the physical displacement u is defined only at lattice points, x=na, i.e. <u>only those values at yellow circles are physically observable</u>. Note that <u>these waves</u> (and any other with k = $\pi/(3a)$ + integer x $2\pi/a$) are identical at the positions of yellow circles and thus <u>are indistinguishable from each other in the crystal</u>.



Crystal Momentum



- k is a good quantum number (i.e. eigenvalue $\omega=\omega(k)$), but is ambiguous up to wave vector $2\pi/a$, or **G** (R.L. vector) in general.
- $\hbar k$ (or sloppily just k) is called "**crystal momentum**"
- A continuous translational symmetry is broken but there is a discrete translational symmetry. Symmetry implies a conserved quantity, which in this case is the crystal momentum.
- It is as though the "new vacuum," i.e. the lattice, is able to impart momentum $\hbar$**G** to any wave (phonon, electron, neutron, photon, …) that exist in it (remember Bragg's law **q**=**G**).