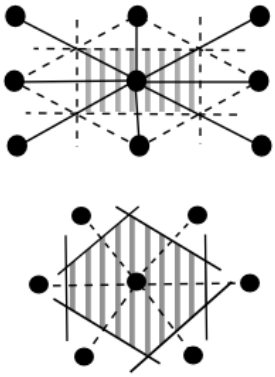
Topic 5-2: Nyquist Frequency and Group Velocity
Kittel Pages: 93, 33, 94

Summary: We begin this video by showing that, while we plotted the dispersion over all *q* it only makes sense to plot it over the range $-\frac{\pi}{a} \leq q \leq \frac{\pi}{a}$. Any *q* outside of this range can be shifted by a reciprocal lattice vector to bring it within this range, called the first brillouin zone. We then introduce the Nyquist frequency as well as the phase and group velocity concepts.

- So far, we have developed a *dispersion relation* which relates our vibrational wave vector q to the frequency of oscillations, ω of the atom
    - Previously plotted ω over all *q*; here we will show that only a subset of *q* values give a physically reasonable solution
- Defined displacement at atom n as $u_n = u_o e^{i(qx_n - \omega t)}$
- Begin by looking at the ratio of displacements $\frac{u_{n+1}}{u_n}$
    - $\frac{u_{n+1}}{u_n} = \frac{u_o e^{i(q(x_n+a)-\omega t)}}{u_o e^{i(qx_n-\omega t)}} = e^{iqa}$
- To cover the whole unit circle qa would have to go from –π to π
    - $-\frac{\pi}{a} \leq q \leq \frac{\pi}{a}$ which is the "first brillouin zone"

Important tangent: Brillouin zones

- The first brillouin zone is constructed in reciprocal space using perpendicular bisectors from near-by lattice points. It is a translatable volume that fills reciprocal space (and it thus has the volume of the reciprocal unit cell); however, it may not have 3 clearly defined axes to form a polyhedron (see the lower image, for example).



End tangent: Back to thinking about physically meaningful displacements between neighboring atoms

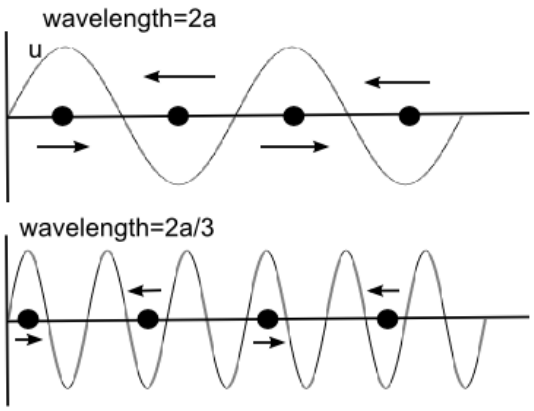
- No point in saying 2 atoms are out of phase by 1.2π because a displacement of -0.8π gives the same position on the unit circle
- If $\vec{q}$ is outside the first brillouin zone we can shift it by $\vec{G}$ to bring it back into the first brillouin zone
    - This is a shift of $\frac{2\pi}{a}$ in 1D
- To see this, consider $\frac{u_{n+1}}{u_n}$. From our definition of u_n, $\frac{u_{n+1}}{u_n} = e^{iqa}$
    - We can multiply by $e^{i2\pi n}e^{-i2\pi n}$
    - This first term is definitely 1, since n is an integer. Let's leave the second term for the moment. $\frac{u_{n+1}}{u_n} = e^{iqa}\, e^{-i2\pi n}$
    - Define $q' = q - \frac{2\pi n}{a} = q - g_{1D}n$
    - Rearranging q and q', we plug into $\frac{u_{n+1}}{u_n} = e^{iqa}\, e^{-i2\pi n}$; this yields $\frac{u_{n+1}}{u_n} = e^{iq'a}$

Conclusion: We obtained $\frac{u_{n+1}}{u_n} = e^{iq'a}$, which indicates q = q'. Recall q' was defined by q, but shifted by a g vector. Thus, the local displacement ratio doesn't care whether or not your using q or q + g. It's identical. However, below, we'll show that using q within the first Brillouin zone makes more physical sense.

Physical interpretation:

Example 1: If I have $q = \frac{\pi}{a}$ which has a wavelength of 2a and $q = \frac{3\pi}{a}$ which is a wavelength of 2a/3 how are these equivalent?

- Remember our lattice is a discrete set of points



- One can see that the atoms sit at either a peak or a trough in both waves and it is the ***same*** in both waves (ignore differences in amplitude, that's just bad artistry)
- This demonstrates how two different waves give the same physical result
- This is a visual representation of the Nyquist frequency
    - Nyquist frequency: In communication theory, the Nyquist frequency is an upper bound on the measurable frequency for a given sampling frequency.
        - Sampling failure would involve trying to measure a wave, but sampling it too slowly to correctly resolve the frequency. In short, the wave frequency is so high you miss peaks and troughs, resulting in an incorrect measurement
- In our case, atoms in the crystal can only support wavelengths greater than or equal to 2a. We can think of the atoms as "sampling" the vibrational wave moving through them.
    - A wave with a shorter wavelength than 2a (eg figure above) will have no meaning but can be shifted to an equivalent q in the first brillouin zone where it does have meaning
- This is why dispersions are only plotted from $-\frac{\pi}{a}$ to $\frac{\pi}{a}$ in 1D, and within the 1st Brillouin zone in 3D.

Part two: Phase and group velocity

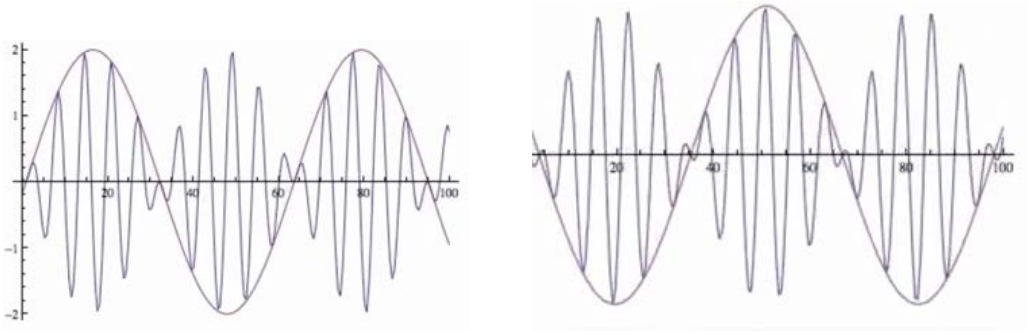
Phase velocity

- Phase velocity, v_p, is the distance a single wave peak travels over time (single wave refers to a single plane wave that is infinite in size and can be described with the usual complex exponential form)

- For one oscillation this is $\frac{\lambda}{t}$
- Knowing that k = q= $\frac{2\pi}{\lambda}$ and t= $\frac{2\pi}{\omega}$ we get $v_p = \frac{\omega}{k} = \frac{\omega}{q}$

Group Velocity

- Consider adding two waves of the following form
  - $\psi = \cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega_2 t)$
- Let $k_1 = k - \Delta k, \;\; \omega_1 = \omega - \Delta\omega$ and $k_2 = k + \Delta k, \;\; \omega_2 = \omega + \Delta\omega$
- Then $\psi = \cos((k - \Delta k)x - (\omega - \Delta\omega)t) + \cos((k + \Delta k)x - (\omega + \Delta\omega)t)$
- With the powers of trigonometry, we get $\psi = 2\cos(kx - \omega t)\cos(\Delta kx - \Delta\omega t)$ where the first term describes the ***inner wave*** and the second describes the **traveling wave packet**
- Phase velocity corresponds to the first cosine term. The second, with $\frac{\Delta\omega}{\Delta k}$, is the group velocity



- In the above figure, captured at two different times where the left is an earlier time than the right, the motion of the large sine wave is the group velocity
- The motion of the inner wave, the one with more peaks and troughs, is the phase velocity
- Going back to the dispersion q(ω), this means that all of our phonons could have different group velocities
  - Each phonon mode's group velocity is directly determined by the dispersion


Can you have a group velocity if there is only one frequency present?

Questions to Ponder

1. Plot two waves with a frequency higher than the Nyquist frequency and show how the same result can be obtained with a wave shifted by $\frac{2\pi}{a}$.