Measuring Phonons with Neutrons

D. J. Voneshen – Excitations training course

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- One phonon cross section
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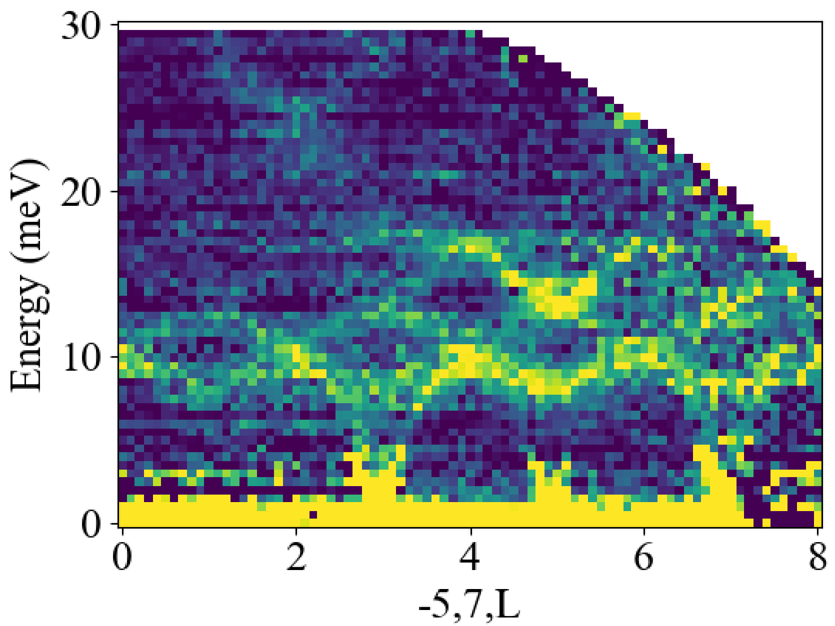
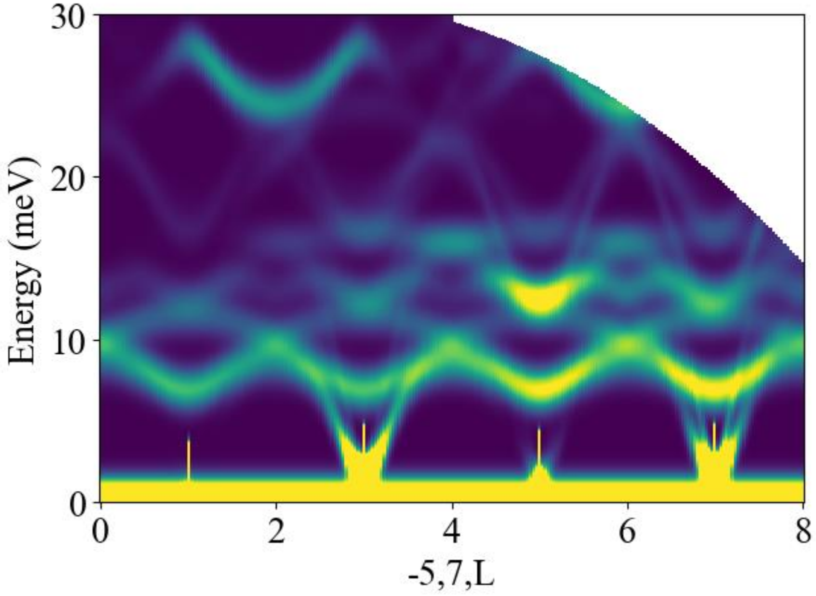
- Measuring powders
- Incoherent approximation





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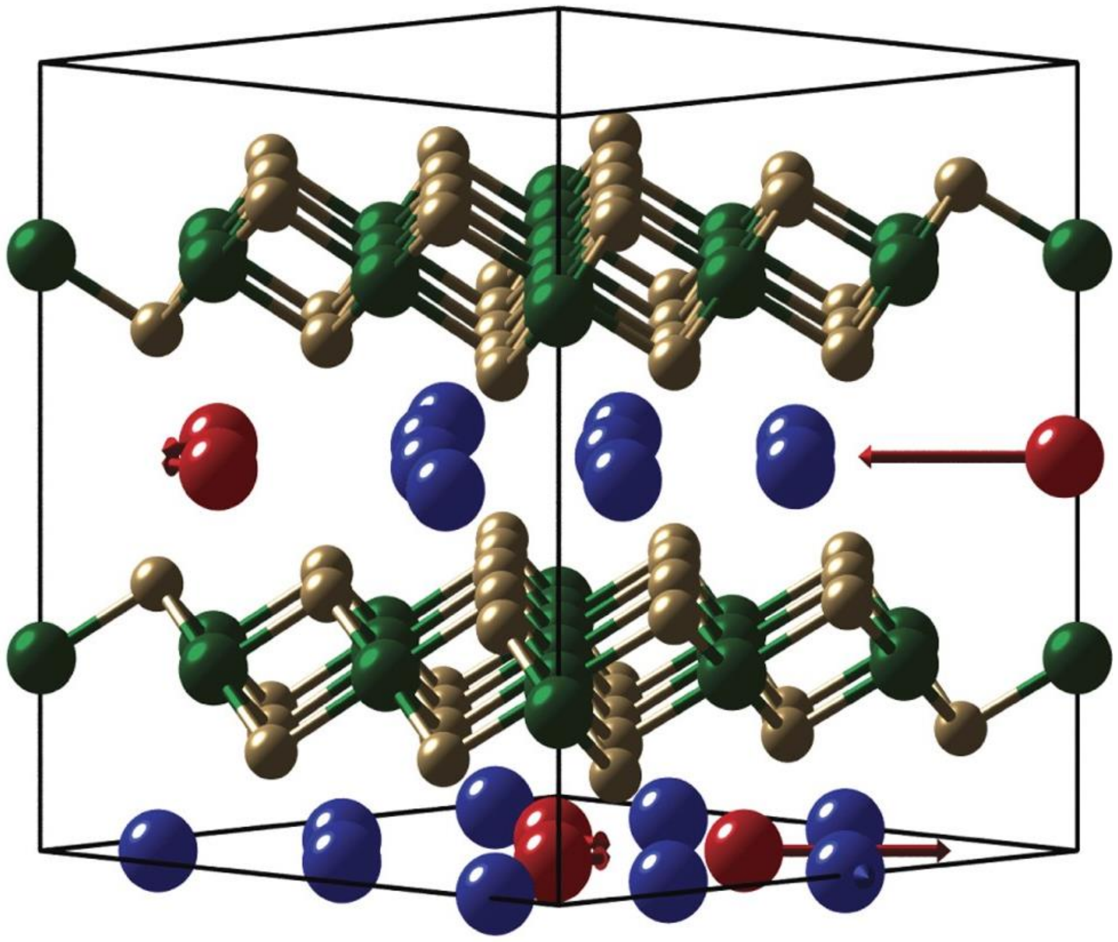
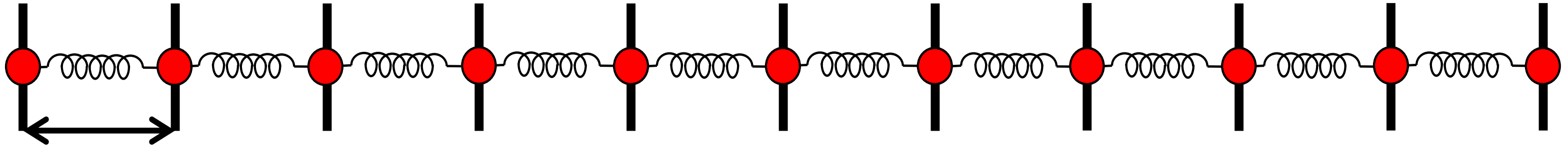
Why Phonons?

- Not just background!
- Lattice dynamics is important for
    - Bonding
    - Heat transfer
    - Phase transitions
    - Some superconductors

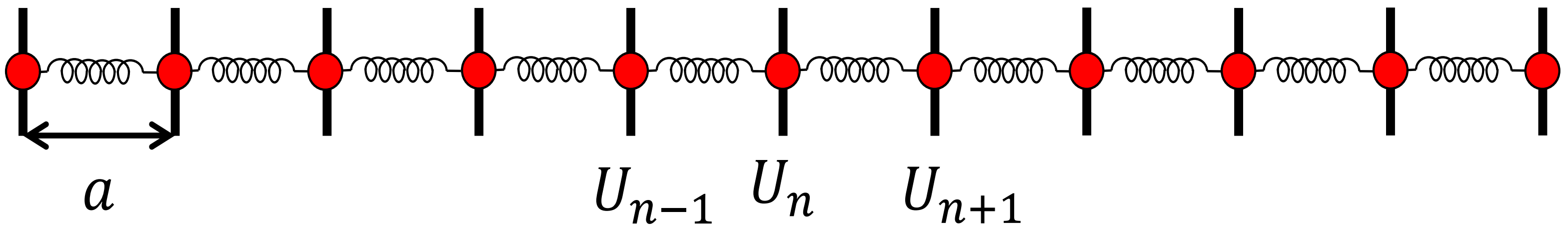


Phonons an overview



- We are going to do everything within the harmonic approximation.
- So, forces on atom n if displaced in x is
$$F = k(U_{n+1} - 2U_n + U_{n-1}).$$

Phonons an overview



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- So, forces on atom n if displaced in x is

$$F = k(U_{n+1} - 2U_n + U_{n-1}).$$

- $F = ma = m\ddot{U}$. This is a second order differential, if we try

$U = Ae^{-i(Qx_n - \omega t)}$, and work through it

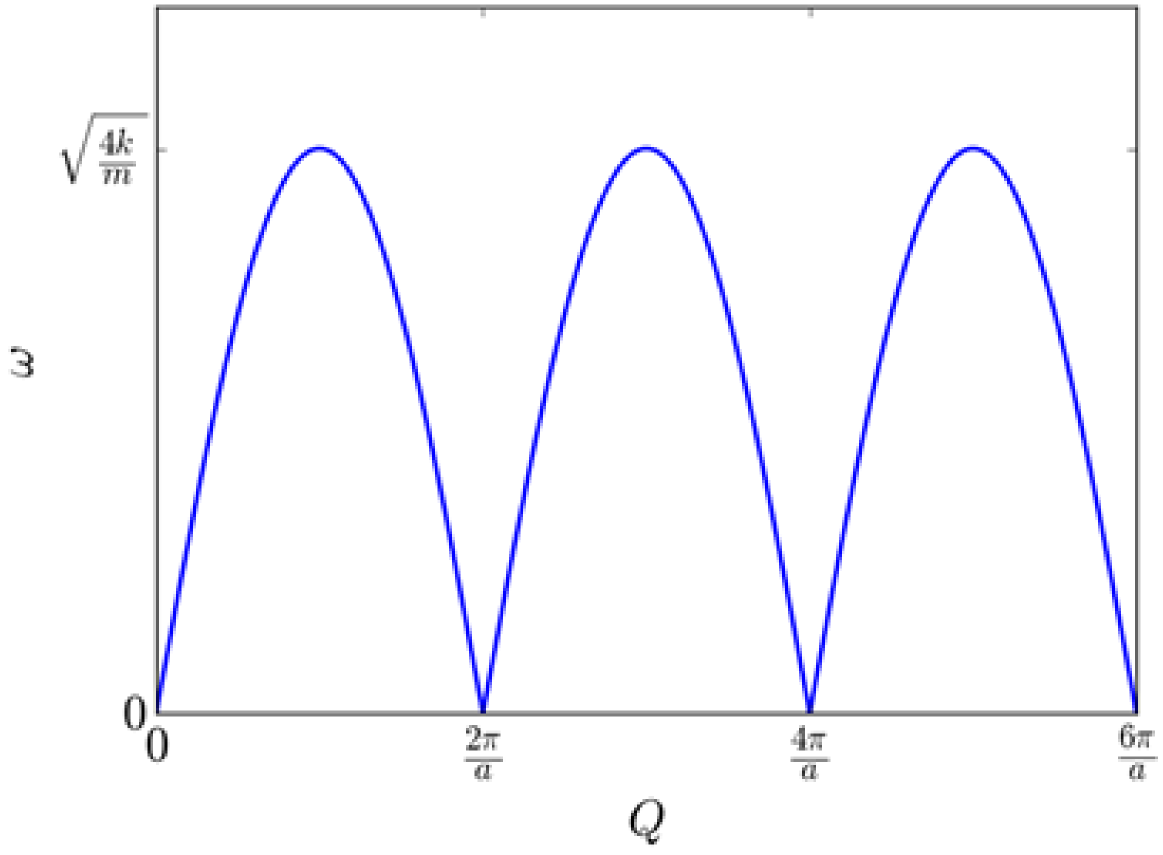
Phonons, an overview

- $\omega = \pm\sqrt{\frac{4k}{m}}\sin\left(\frac{Qa}{2}\right).$

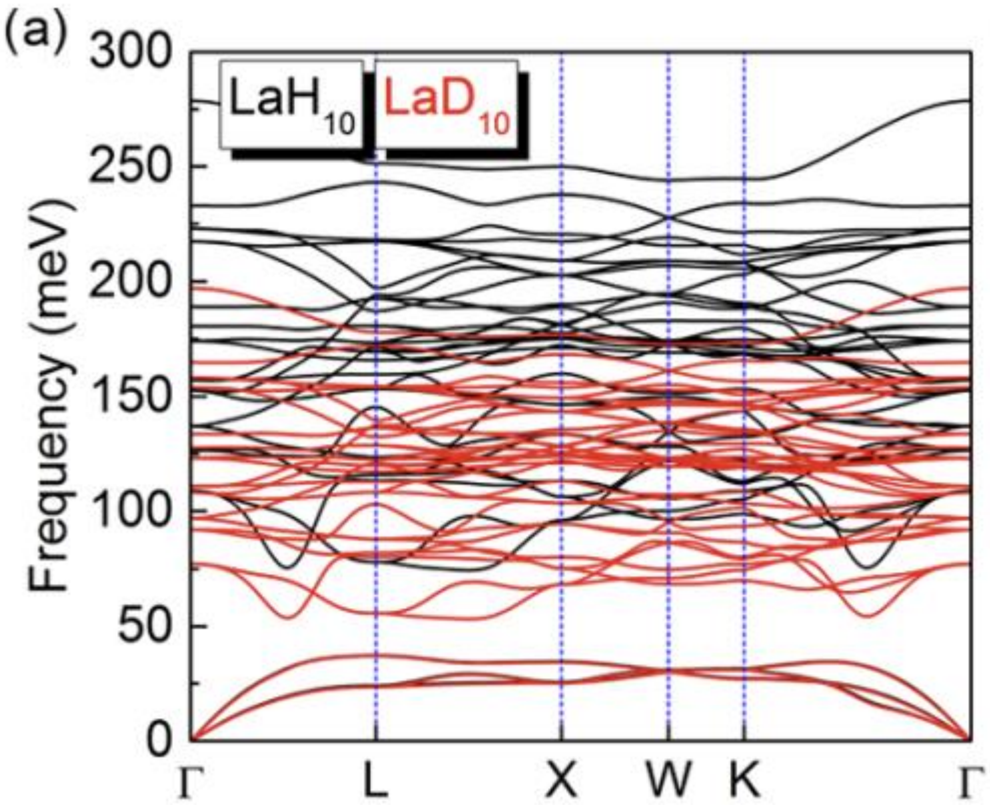
- As we saw in the first practical, our maximum frequency is related to the spring constant and mass.

- So strong bonds, high frequency.

- Light isotopes also are at high energy.



Phonons, an overview



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Now to neutrons!

One phonon coherent scattering

$$I(\vec{Q},E) = \frac{N\hbar}{2}\sum_{\nu}\frac{1}{\omega(\vec{Q},\nu)}\left|\sum_{j}\frac{b_j}{m_j^{1/2}}\left[\vec{Q}\cdot\vec{e_j}(\vec{k},\nu)\right]e^{i\vec{Q}\cdot\vec{R_j}}T_j(\vec{Q})\right|^2$$
$$\times\begin{pmatrix}\left[n(\omega(\vec{Q},\nu),T)+1\right]\delta(E+\hbar\omega(\vec{Q},\nu))+\\ \left[n(\omega(\vec{Q},\nu),T)\right]\delta(E-\hbar\omega(\vec{Q},\nu))\end{pmatrix}.$$

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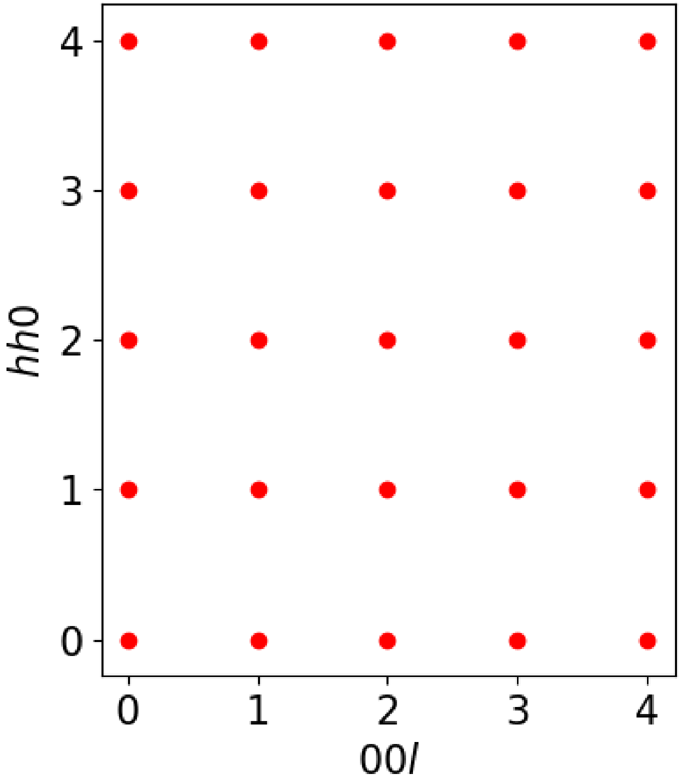
One phonon scattering-key points

- Phonons are strongest when $\vec{Q}$ is parallel to direction of atomic motion.
- Phonon intensity goes up with Q^2.
- Phonons are weaker at high energy.
- Strong Bragg reflections often have strong phonons around them.
- Phonons can be stronger at high temperature (but care needed here).

Measuring a longitudinal acoustic phonon



We want to measure a longitudinal phonon along *00L.*

Which peak would be best to measure around?

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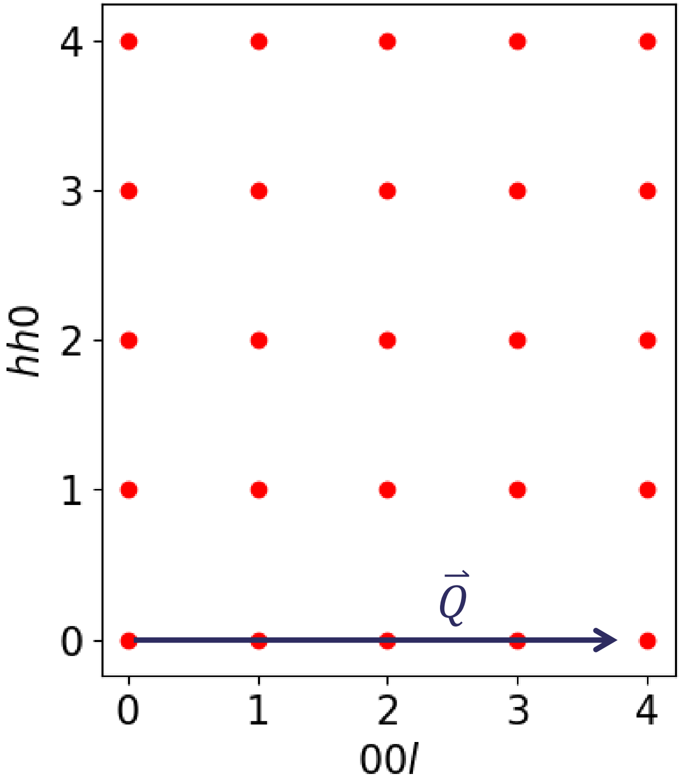
Measuring a longitudinal acoustic phonon



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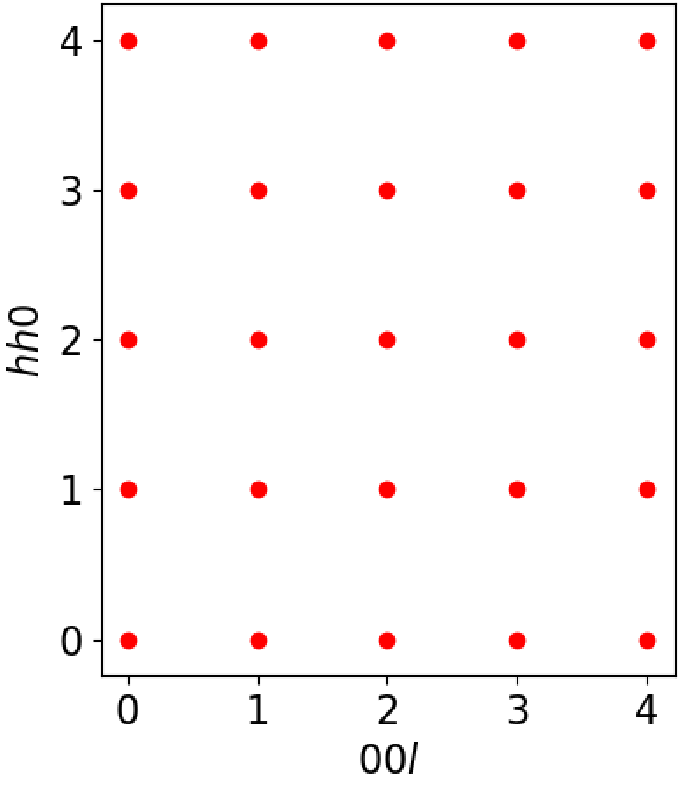
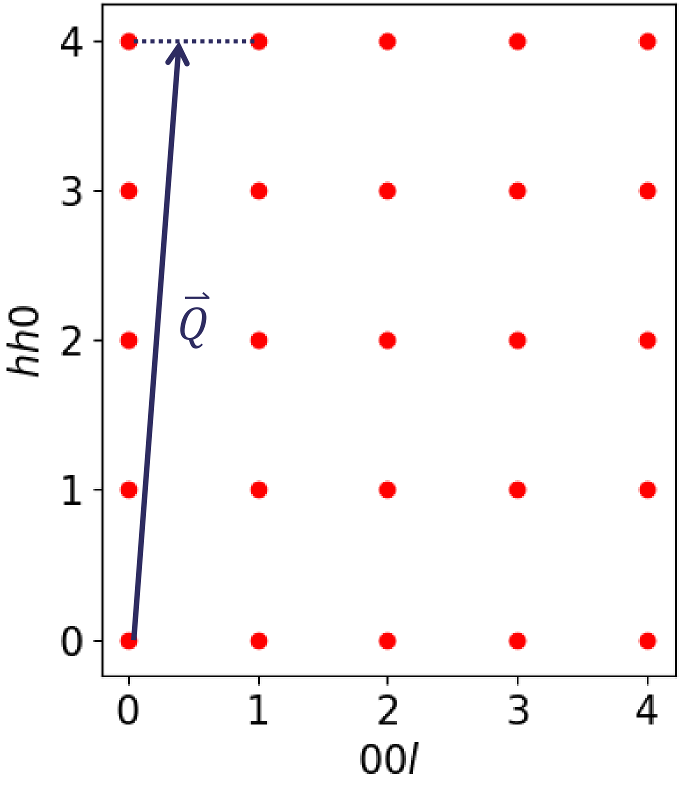
Measuring a transverse acoustic phonon



What about a transverse phonon along 00l?

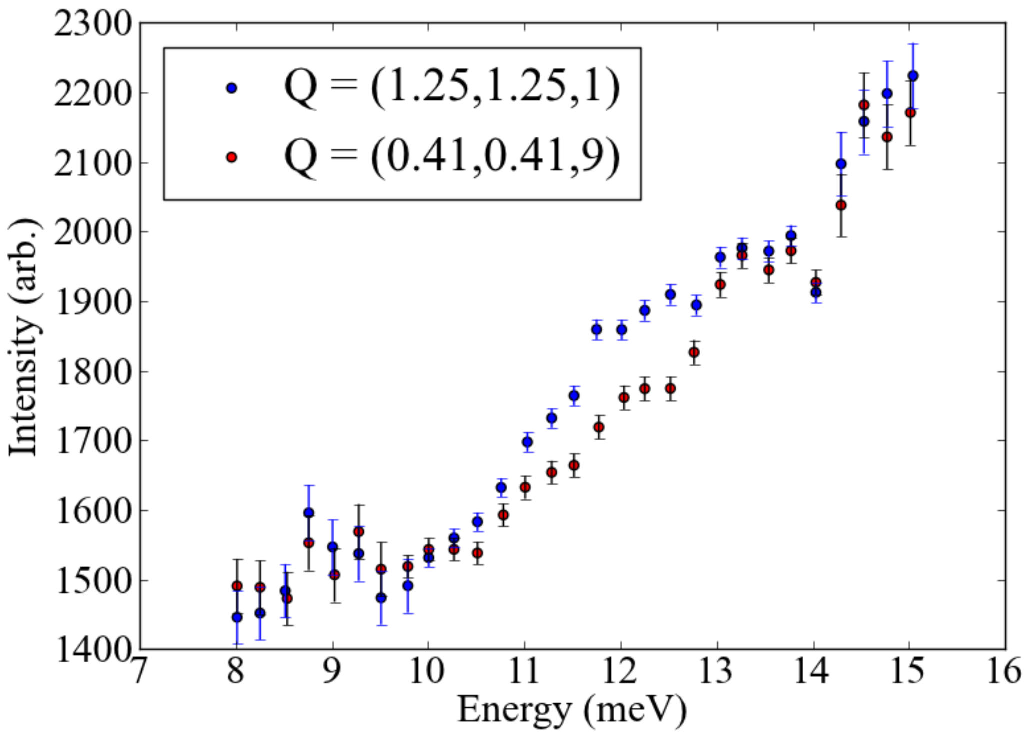
Measuring a transverse acoustic phonon



What about a transverse phonon along 00l?

Exploiting $Q \cdot e$, an example

- We were looking for a phonon around 12 meV.
- However, the background from the cryostat/mount was huge.
- Rotate sample 90°. Suppresses, phonon but background unchanged



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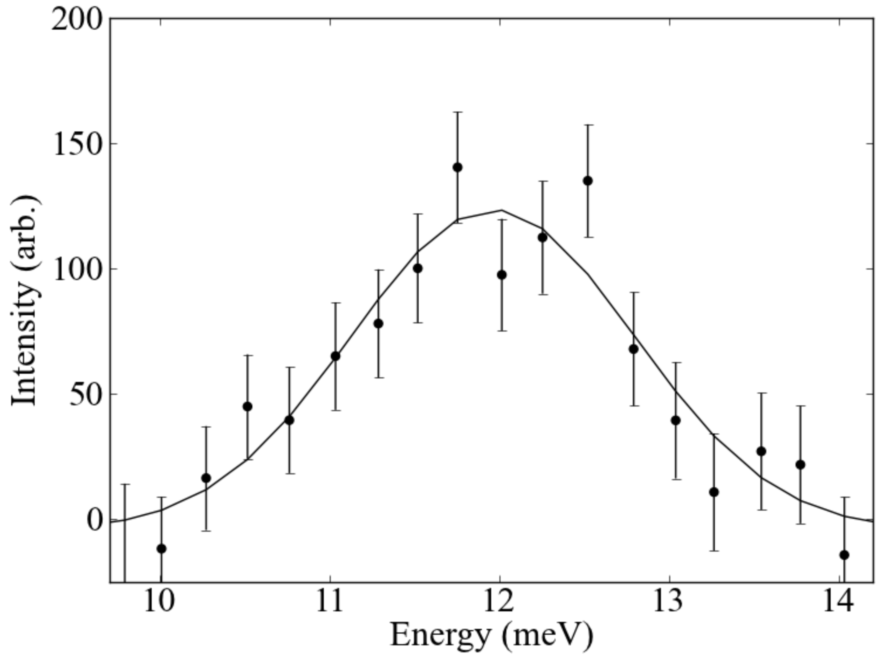
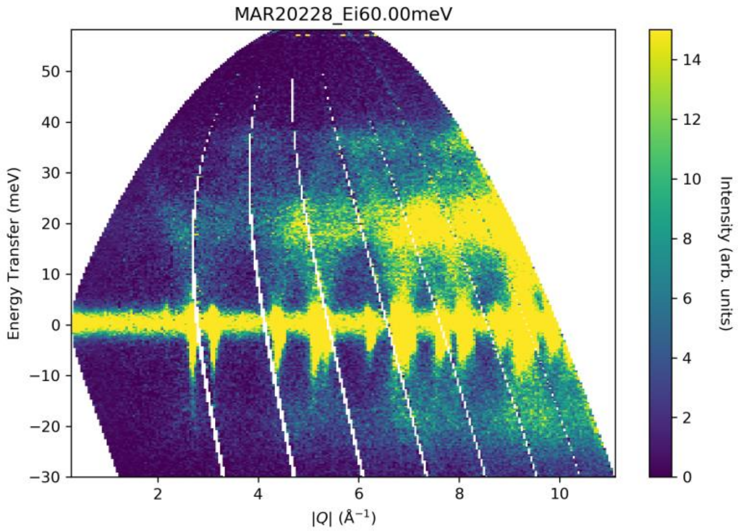
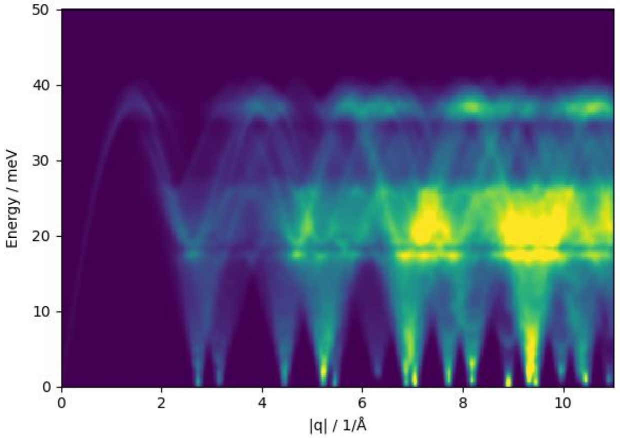


Powders!

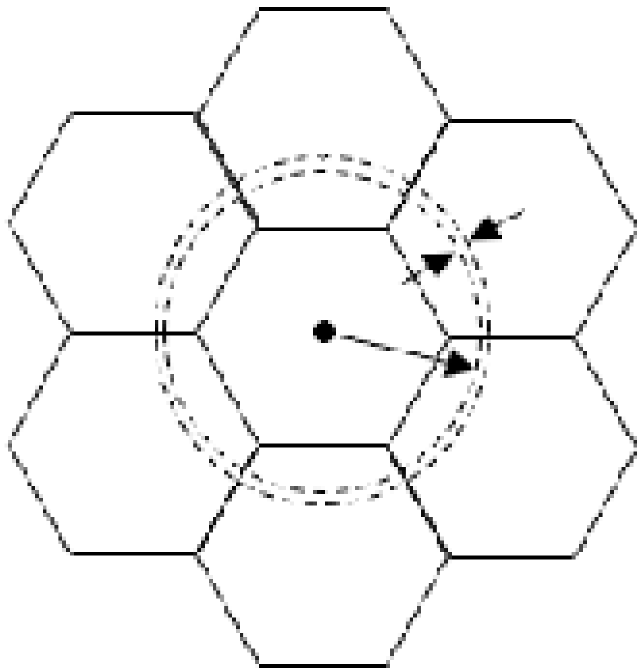
- Good news, powder experiments are simpler!
- Much simpler.
- With them we can extract the neutron weighted phonon density of states.
- But, going beyond that is hard.





Powders, what are we doing?

- We are averaging over a sphere at some $|Q|$.
- So, for small values of $|Q|$ we are covering just a few (or even 1) Brillouin zones.
- But, for large $|Q|$ we are covering many zones, essentially capturing everything in 1 shot.
- This means for high $|Q|$ we can no longer see the effect of $\boldsymbol{Q} \cdot \boldsymbol{e}$ and the signal is the same as incoherent scattering.



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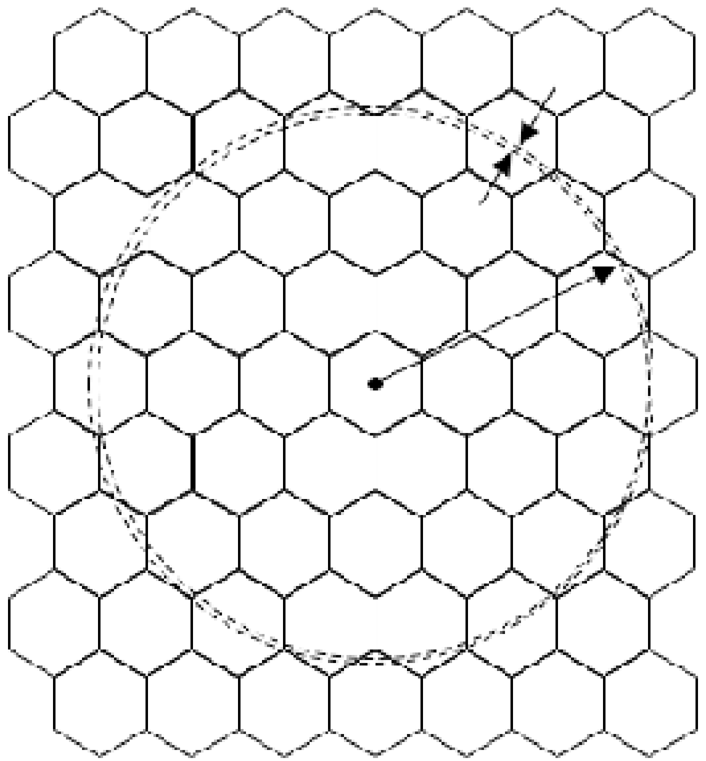

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The neutron weighted phonon density of states

$$PDOS_{neut}(E) = A\sum_j \left(\frac{b_j^2}{m_j}\right) PDOS_j(E),$$

- We normally correct the data for the effects of Bose statistics, ${}^{1}/_{\omega}$ and Q^2.
- Then, in the incoherent approximation, the real Phonon Density of States (PDOS) is related to the PDOS we see via the above.
- This means we cannot obtain the true PDOS for anything other than a monoatomic system.

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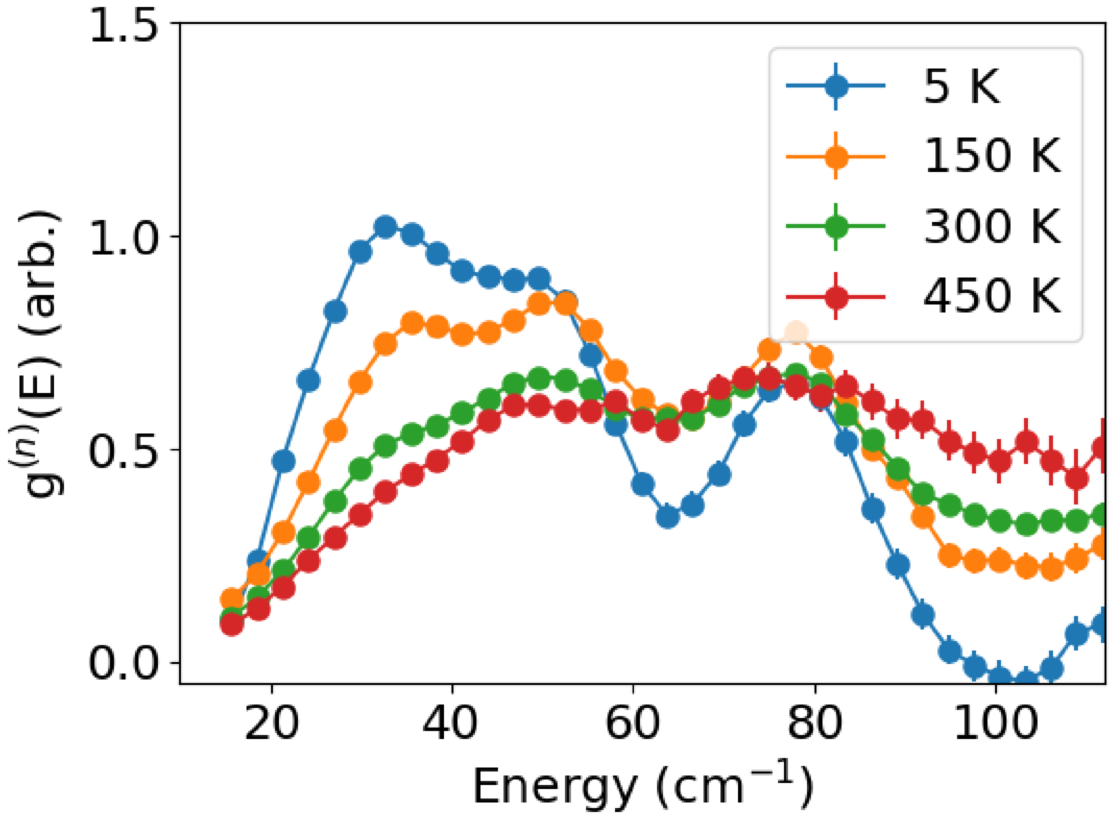
Beyond the harmonic approximation

- This is where all the interesting stuff happens
- But, it gets tricky fast.
- Phonon-phonon scattering (broadening)
- Multiphonon signals (signal above the top of the dispersion)

Beyond the harmonic approximation



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Thank you

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