CDWs in ARPES

A momentum space picture of Fermi surface instabilities in crystalline solids

Physics 250, UC Davis

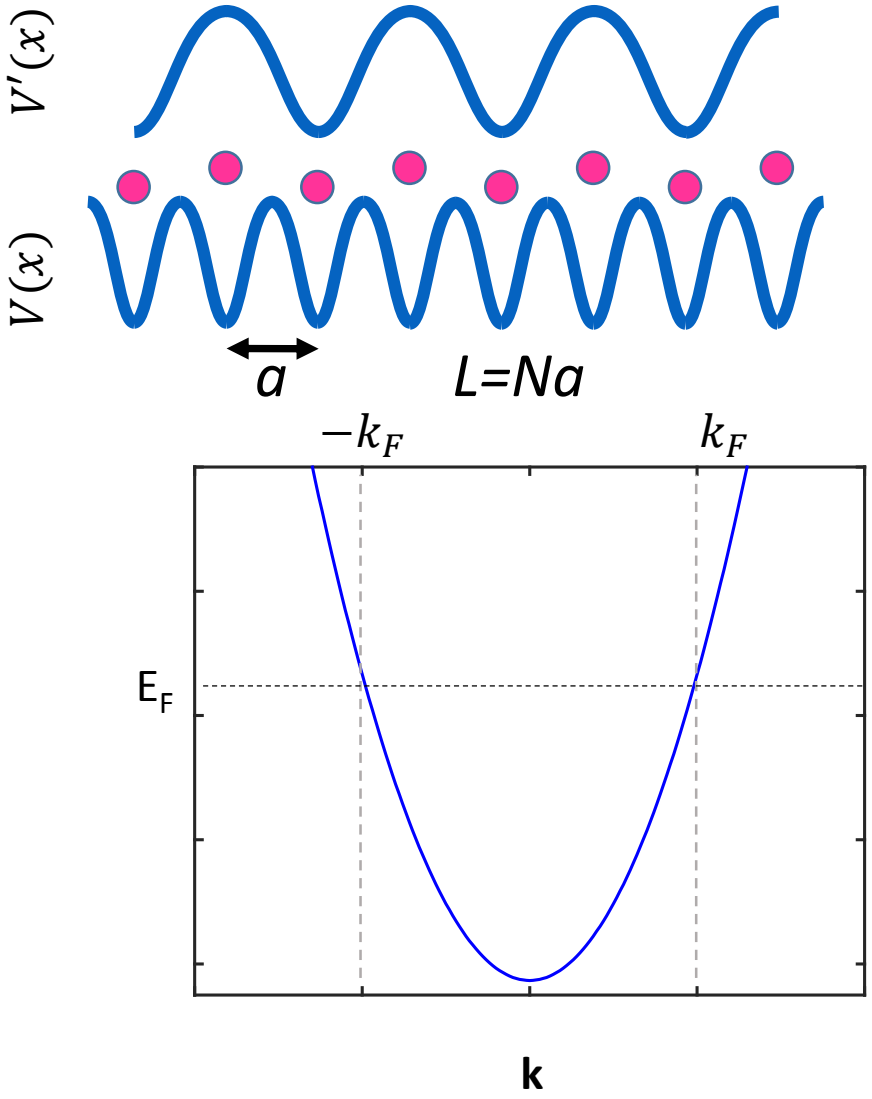
Inna Vishik

Goals of this lecture

- Review CDW concepts from previous lecture
- Practice interpreting ARPES data via ‘textbook’ CDW (RTe_3)
  - Many different types of experiments are required to truly confirm/understand a phenomenon
  - Fermi surface nesting
  - Complex order parameter and spectral gaps
- Time permitting: Kohn Anomaly

CDW Review

Peierls Distortion



- **Begin with 1D metal**
- **Introduce new periodicity into lattice with $q=2k_F$**

CDW Review

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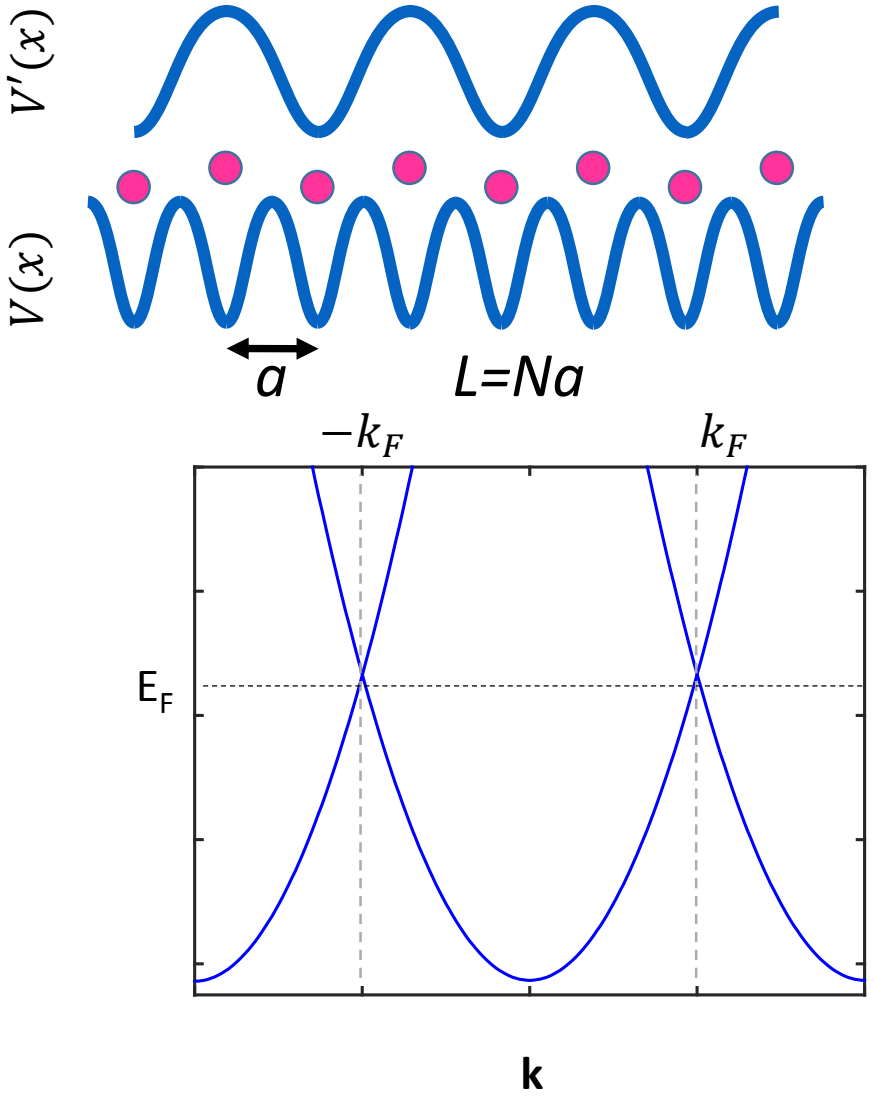

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- **New periodic potential → New Brillouin zone → Need identical dispersion in each Brillouin zone**

CDW Review

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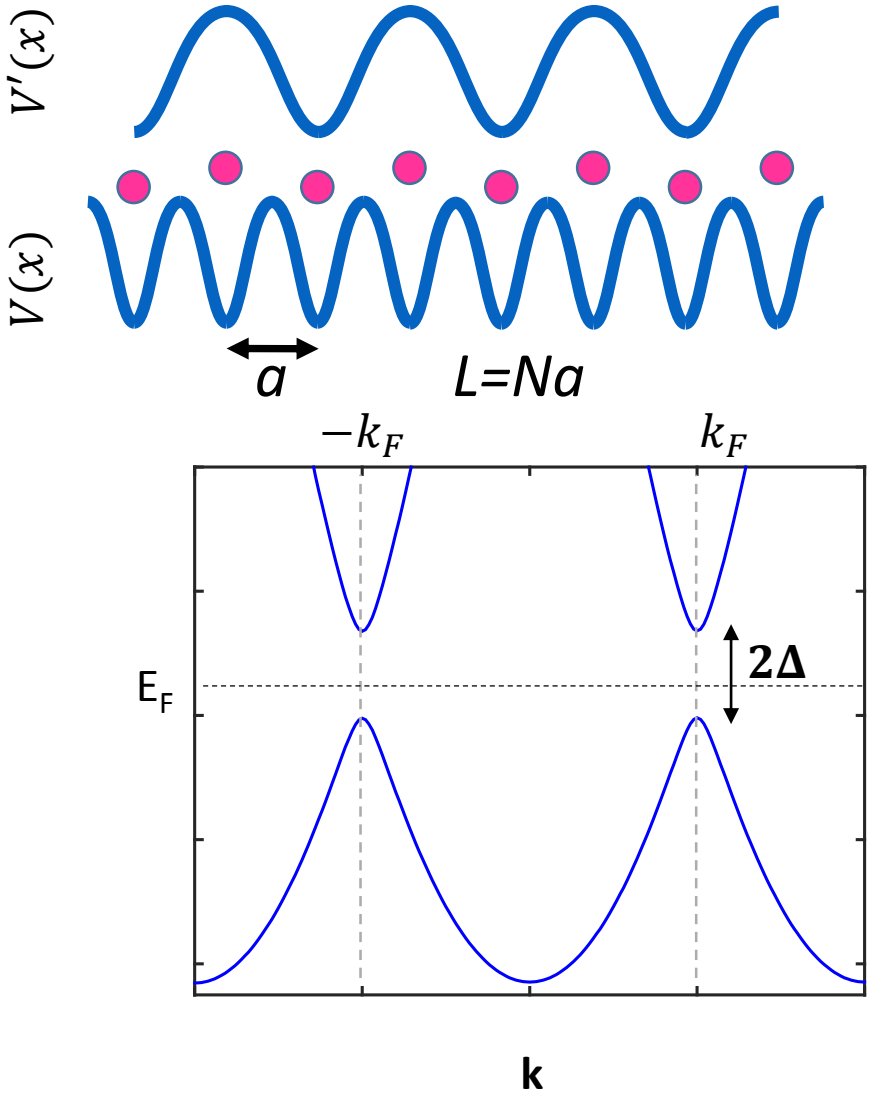

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CDW Review

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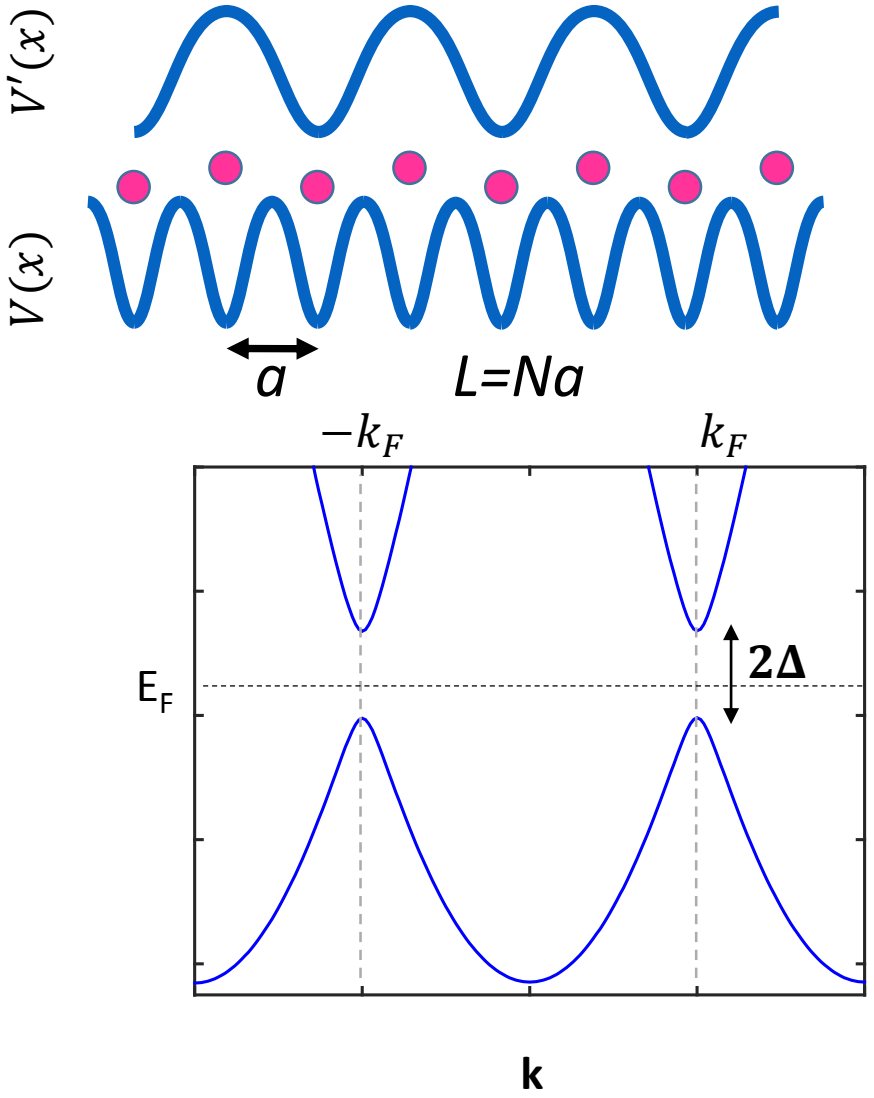
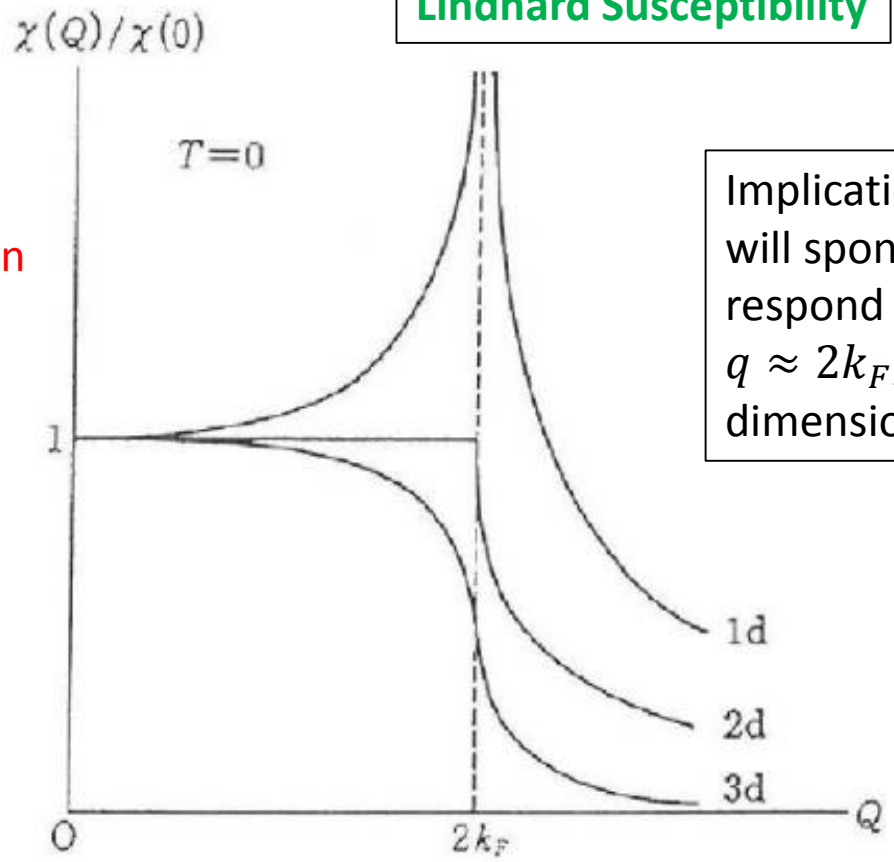


- Begin with 1D metal
- Introduce new periodicity into lattice with $q=2k_F$
- New periodic potential → New Brillouin zone → Need identical dispersion in each Brillouin zone
- Gaps of magnitude 2Δ open where original band crosses replica band
- Energy cost: elastic distortion of lattice
- Energy savings: electrons near E_F lower their energy

1D system are more susceptible to CDW instability

Lindhard Susceptibility

Propensity of an electron gas to distort due to a periodic potential with wavevector **q**



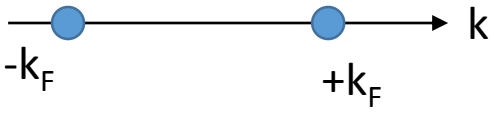
Implication: 1D systems will spontaneously respond to a potential with $q \approx 2k_F$, but higher dimensions will not

Wavevector of periodic potential

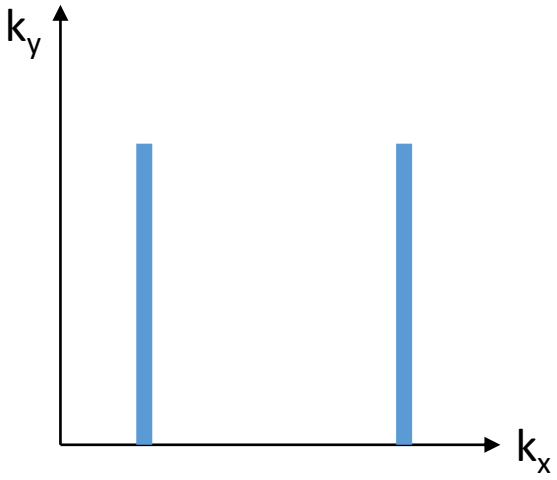
Gruner, *Density waves in solids*

Nesting: how higher dimensional Fermi surfaces can effectively look 1D

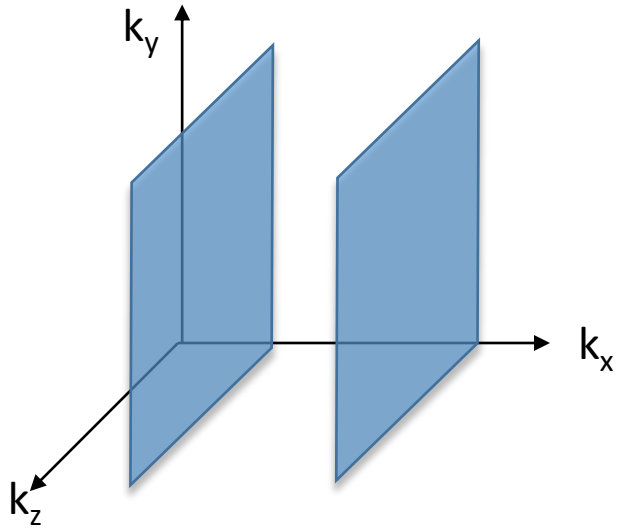
1D FS in 1D space



1D FS in 2D space

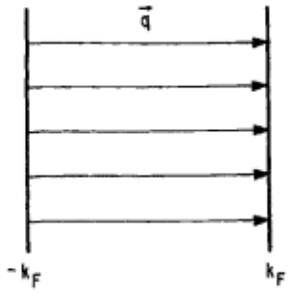


1D FS in 3D space

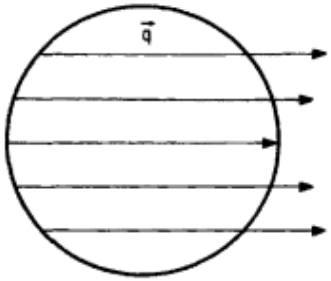


Good candidates for electronically driven CDW have portions of FS which form parallel lines or sheets (i.e. are nested)

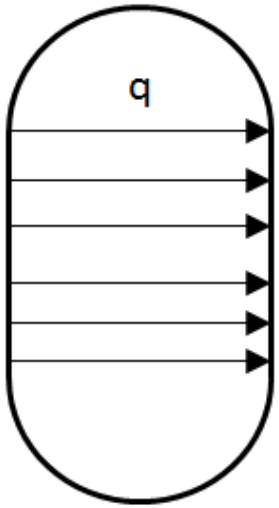
Degrees of nesting



1D: nesting

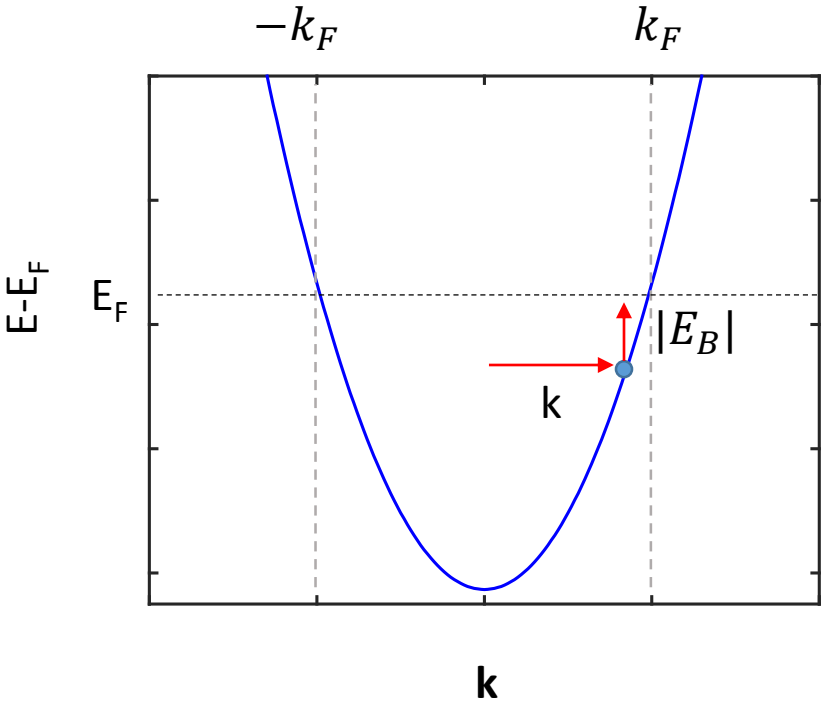


2D: no nesting



2D: partial nesting

Quick review of ARPES



Every electron in band structure has crystal momentum (**k**) and binding energy (E_B)

Photon gives electron energy kick ($h\nu$) and negligible (for this course) momentum kick

(photo)electron loses work function (ϕ) worth of energy upon exiting material

Kinetic energy (E_{kin}) of photoelectron is detected, encoding original binding energy

$$E_{kin} = h\nu - \phi - |E_B|$$

Emission angle (θ) of photoelectron is simultaneously measured, encoding crystal momentum that electron had inside sample

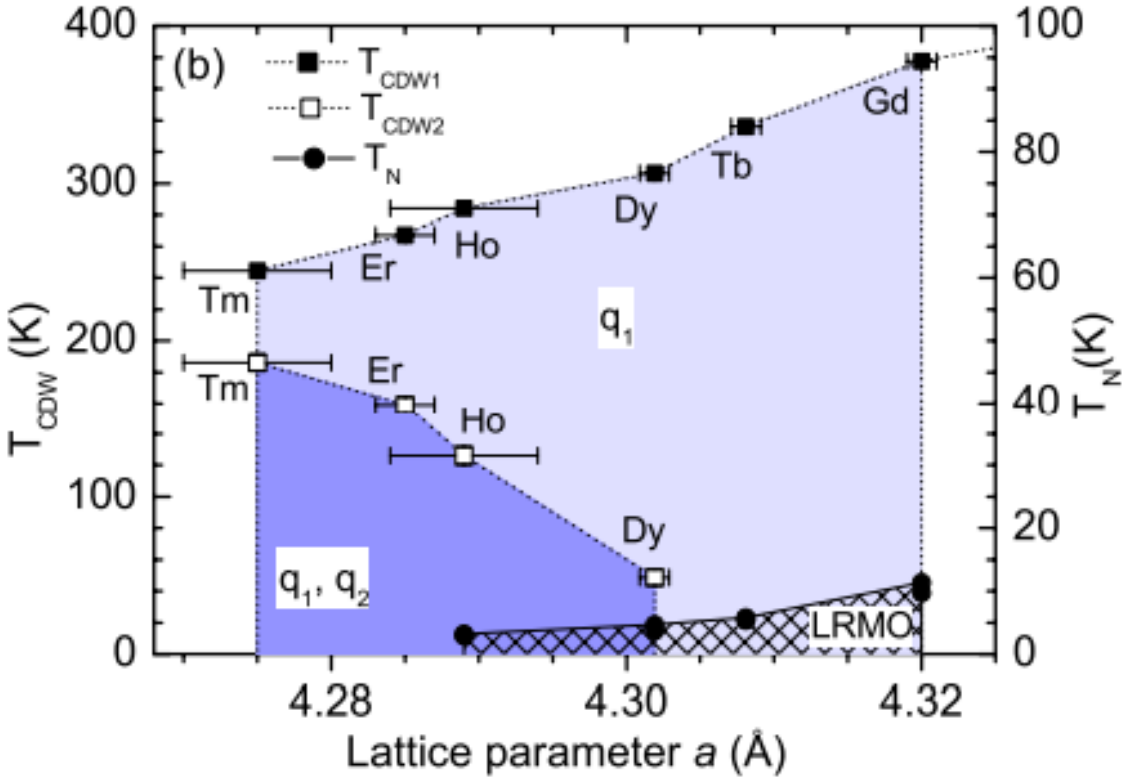
$$\hbar \boldsymbol{k} = \sqrt{2 \boldsymbol{m_e E_{kin}}} \boldsymbol{sin\theta}$$

ARPES resources

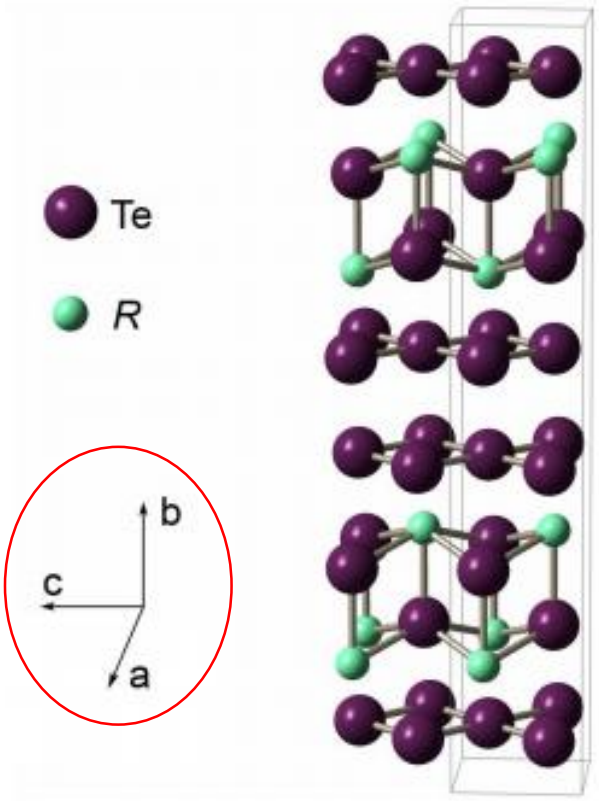
- Campuzano, Norman, Randeria. *Photoemission in the high-Tc superconductors.* https://arxiv.org/pdf/cond-mat/0209476.pdf
  Good for: matrix elements
- Damascelli, Hussain, Shen. *Angle-resolved photoemission studies of the cuprate superconductors.* Rev. Mod. Phys. **75** 473 (2003)
  Good for: short review of formalism
- Damascelli. *Probing the Electronic Structure of Complex Systems by ARPES.* Physica Scripta. Vol. T109, 61–74, 2004 (https://www.cuso.ch/fileadmin/physique/document/Damascelli_ARPES_CUSO_2011_Lecture_Notes.pdf)
  Good for: information about kz and quantifying quasiparticle lifetimes
- Hufner, *Photoelectron Spectroscopy, Springer (2003)*
  Good for: Historical overview; formalism; broad review of technique

Case study: RTe_3 (R=Tm, Er, Ho, Dy, Tb, Gd)

Some members have two CDWs
and some become
superconducting under pressure

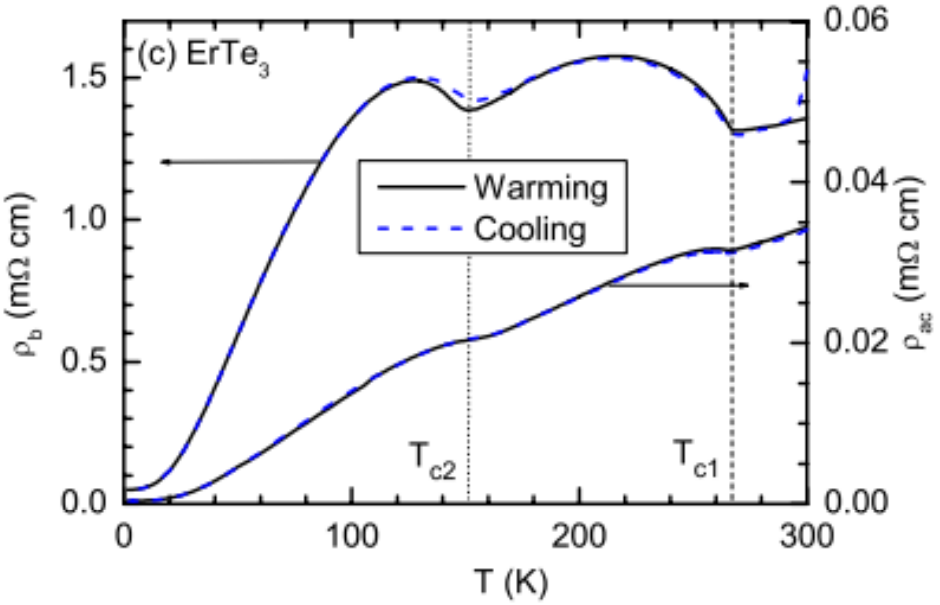


Ru *et al.* PRB **78**, 012410 (2008)



N. Ru thesis
http://web.stanford.edu/group/fisher/people/Nancy_Ru_thesis.pdf

How are CDWs usually discovered?



Ru *et al.* PRB **77**, 035114 (2008)

(not the first resistivity measurement on this material)

Often discovered by transport

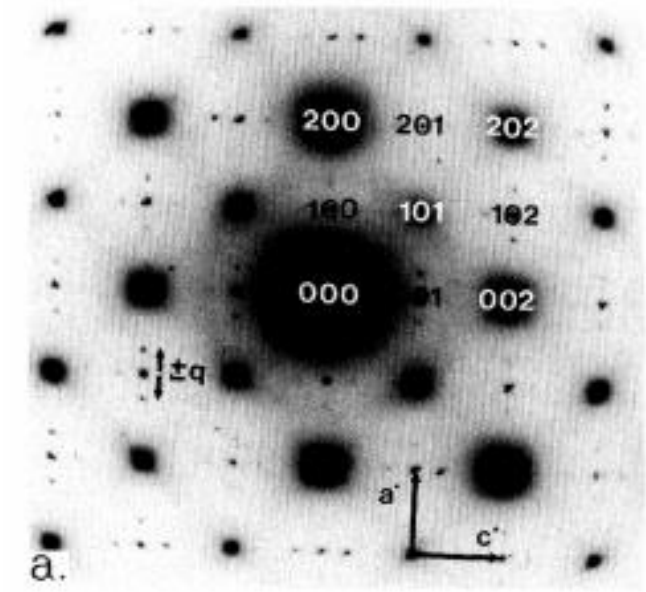
Why does resistivity show upturn just below T_{CDW}?

Why is there metallic resistivity at low temperature?

How are CDWs confirmed to be CDWs?

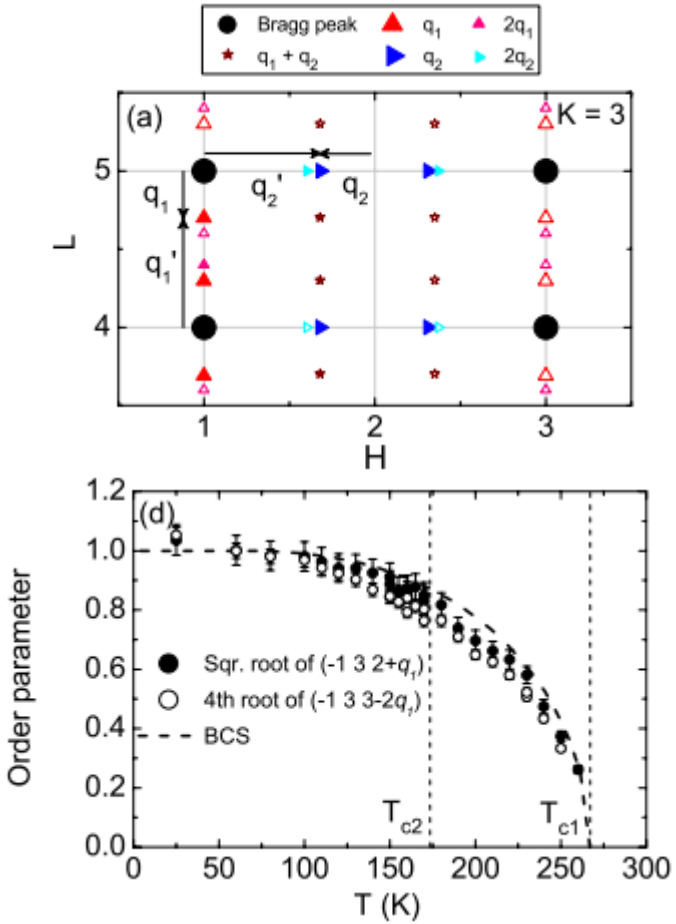
Diffraction measurements which are sensitive to charge (e.g. x-ray, electron) usually confirm CDW

TEM on $SmTe_3$



E. DiMasi *et al, PRB* ***52*** *14516 (1995)*

X-ray diffraction on $ErTe_3$

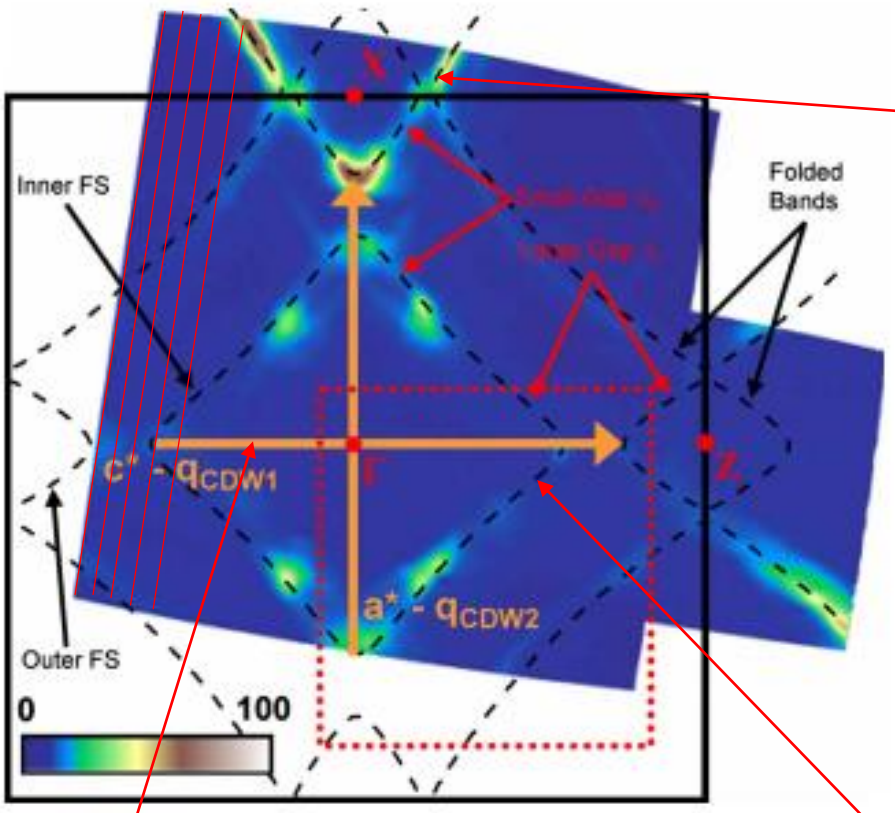


Ru *et al.* PRB **77**, 035114 (2008)

What else is there to learn about CDW?

- What causes it? (structurally or electronically driven?)
- How does it nucleate?
- How much of the Fermi surface is involved?
- How large is the gap?
- What are its collective excitations?

A tale of two CDWs in $ErTe_3$ (+ more practice reading ARPES data)



Bright regions: remaining Fermi surface

Fermi surface map produced by taking many parallel slices (E vs k), integrating over small energy window near E_F, and interpolating slices together

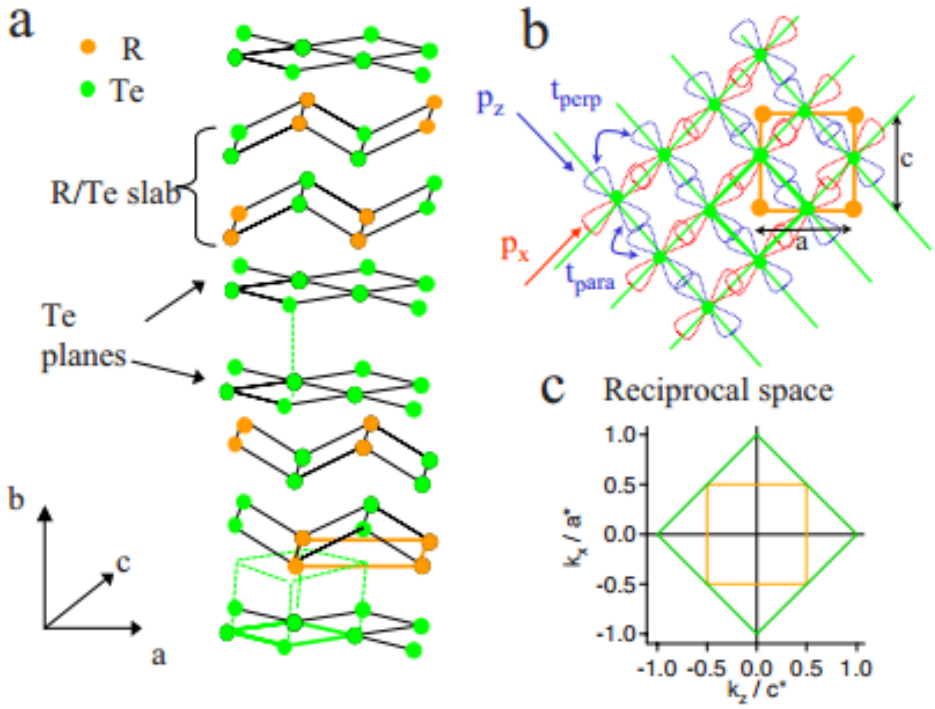
Dark regions formerly occupied by Fermi surface: gapped out by CDW

Nesting wavevector

Moore *et al.* PRB **81**, 073102 (2010)

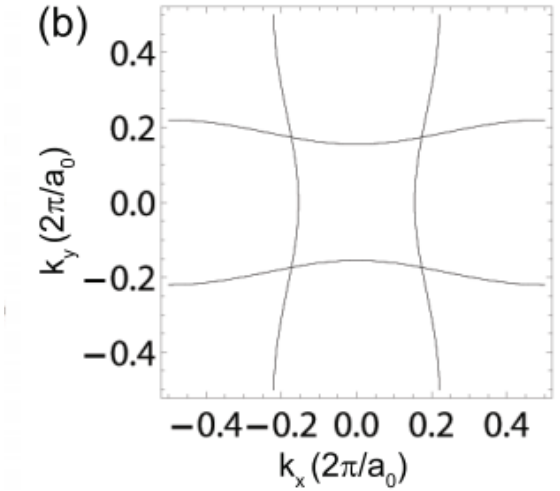
What does the original FS look like?

Good approximation can be achieved via tight-binding model
(Tight binding model: electronic band structure approximated from overlap of atomic orbital on adjacent atoms)



Brouet *et al*. PRB **77**, 235104 (2008)

- Fermi surface originates from Te p-orbitals and is almost 1D (small buckling because $t_\perp \neq 0$



Yao *et al.* PRB **74**, 245126 (2006)

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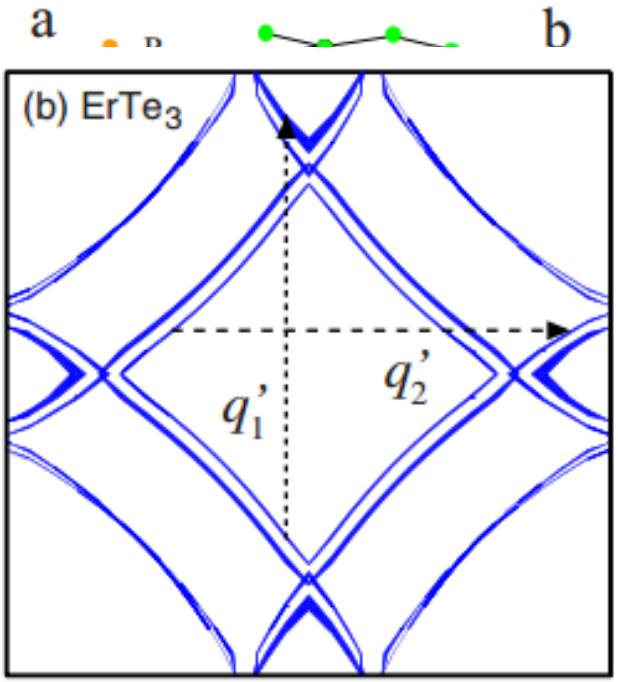
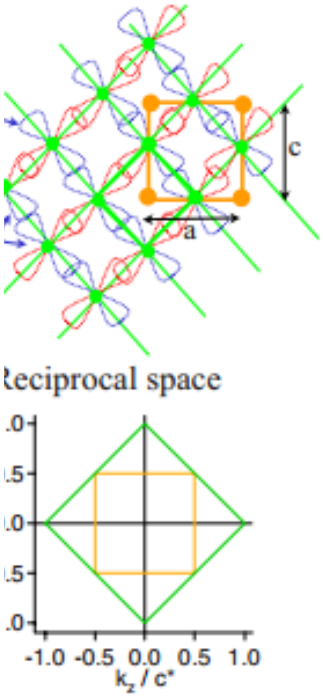
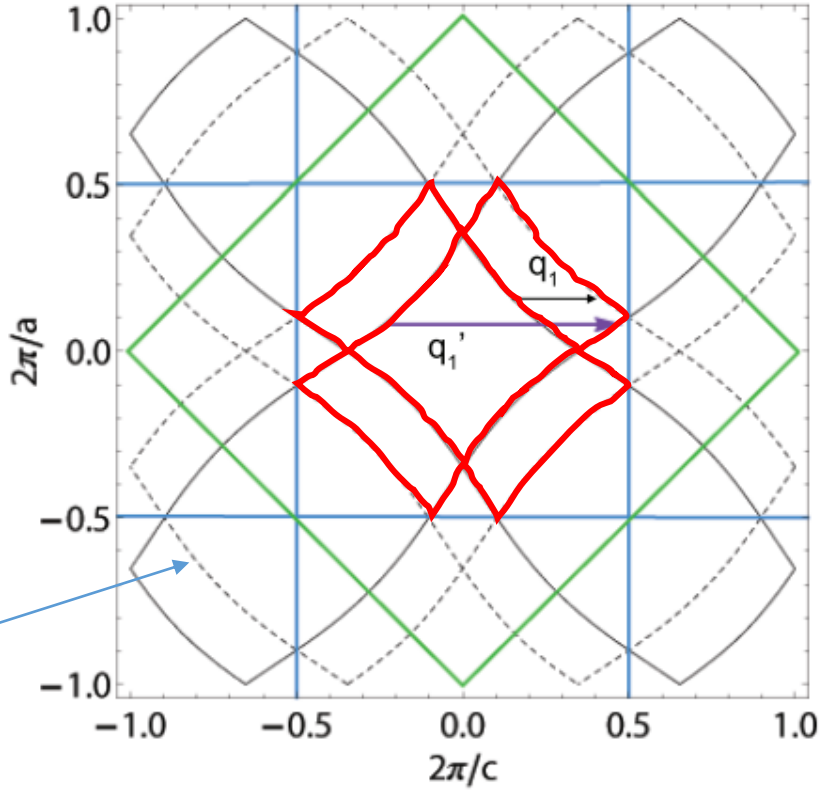




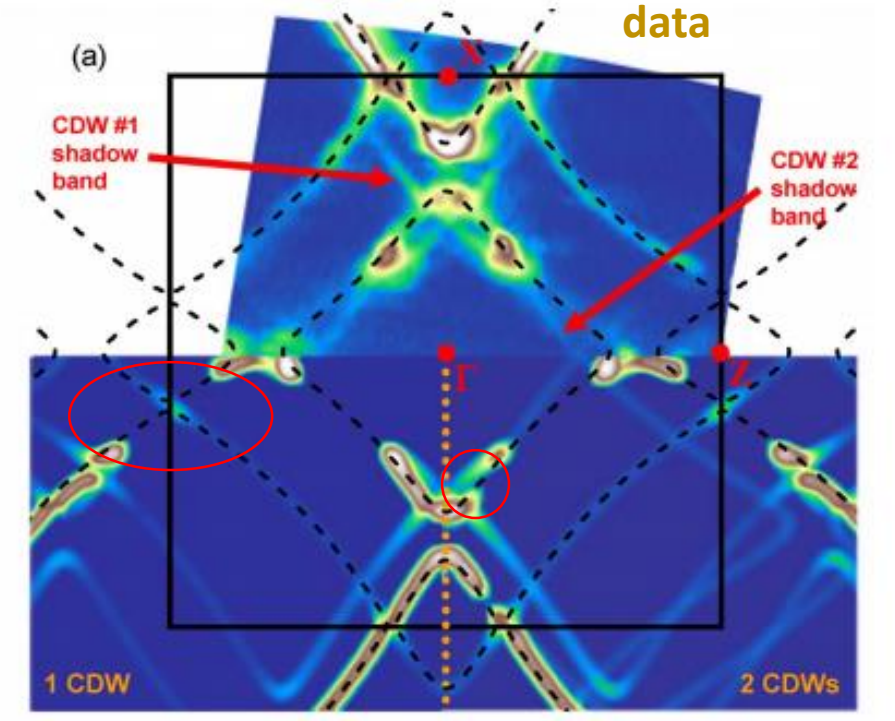
- R/Te slab has lower symmetry than Te layer, making a larger unit cell (smaller Brillouin zone)



LTMO band structure calc
Ru *et al.* PRB **77**, 035114 (2008)

Folded FS

Does data agree with Fermi surface nesting?



Moore *et al.* PRB **81**, 073102 (2010)

Yes!
→Close to a textbook CDW (aside from partial nesting)
→Order is Fermi-surface (electronically) driven

CDW order parameter

Complex order parameter:

$\Psi \sim \Delta e^{i\phi}$

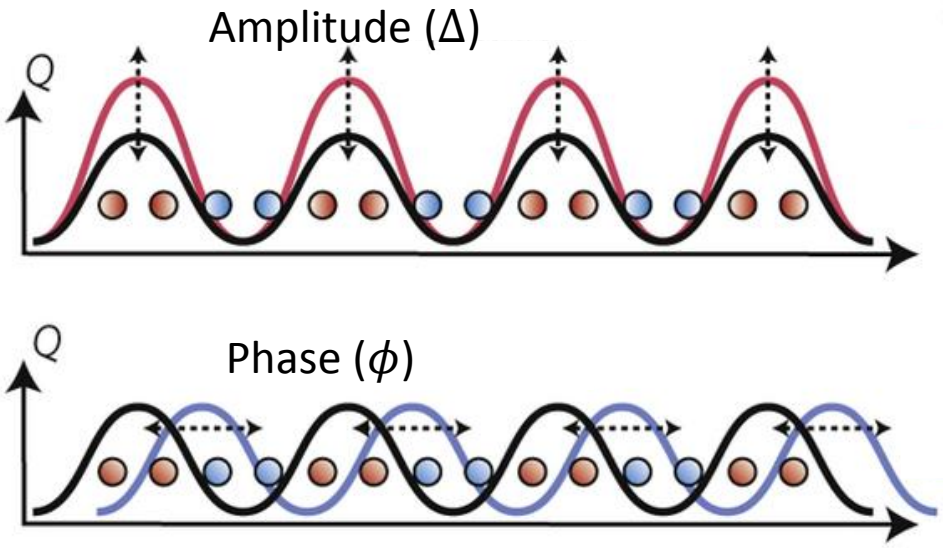


Image source: Torchinsky et al, Nat. Mater. (2013)

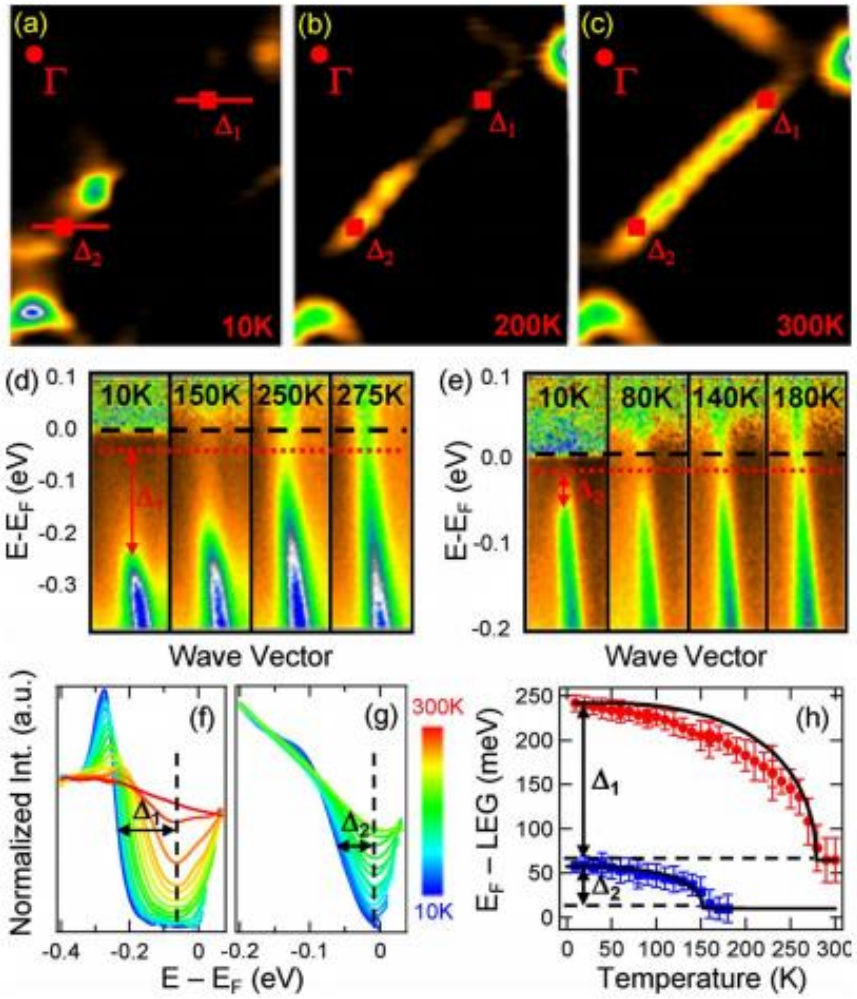
What is an order parameter?

The measure of the degree of order of a given phase. Typically zero above the ordering temperature

What measured/calculated quantities are related to the CDW order parameter?

- Amount of lattice distortion
- Amount of charge involved
- Amplitude of satellite Bragg peak
- Magnitude of gap

Order parameter in ErTe3 (visualizing gaps in ARPES)



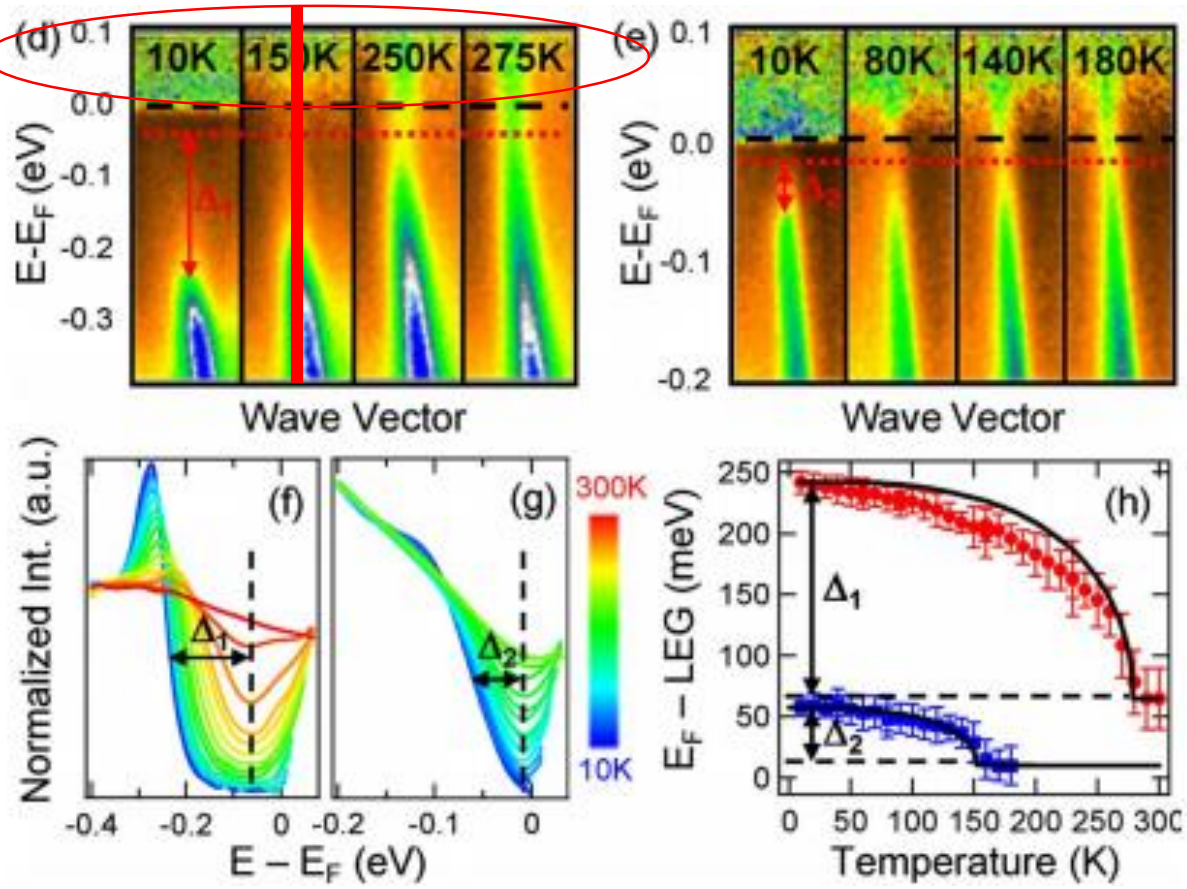
Method 1: Disappearance of intensity in fermi surface map (only works if gap opens at E_F)

Method 2: Energy vs k dispersion

Method 2.5: Energy distribution curve (EDC) + reasonable definition of gap edge

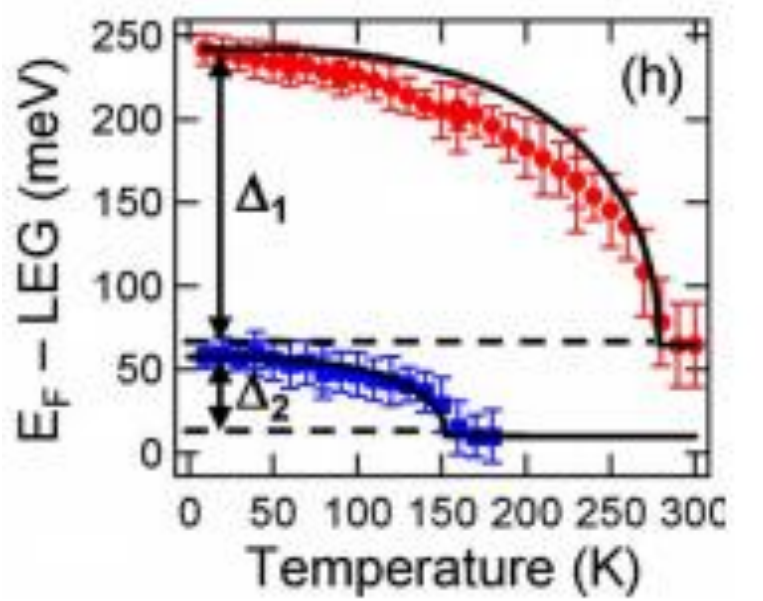
Moore *et al.* PRB **81**, 073102 (2010)

Extracting spectral gaps



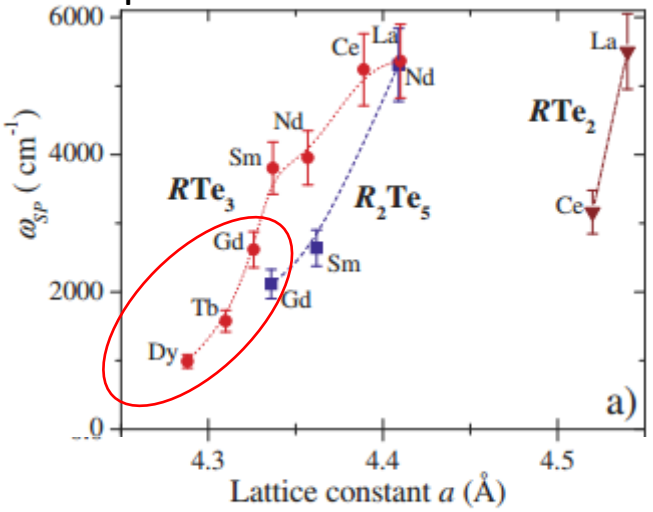
1. Get rid of Fermi-Dirac cutoff by dividing by Fermi-Dirac distribution or symmetrizing (only if there is e-h symmetry)
2. Plot energy distribution curves (EDCs): intensity vs energy at fixed momentum
3. Quantify gap in reasonable way
   - Peak-to EF
   - Leading edge gap (LEG)
   - Fit to model

Comments on CDW gap

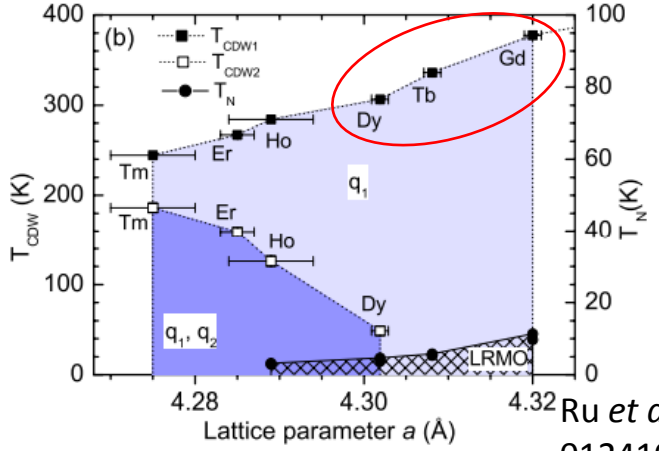


- Larger ordering temperature → larger gap
- Ratio between ordering temperature and gap can be meaningful
- Concept will come up again in superconductivity topic

Optics measurements of CDW gap

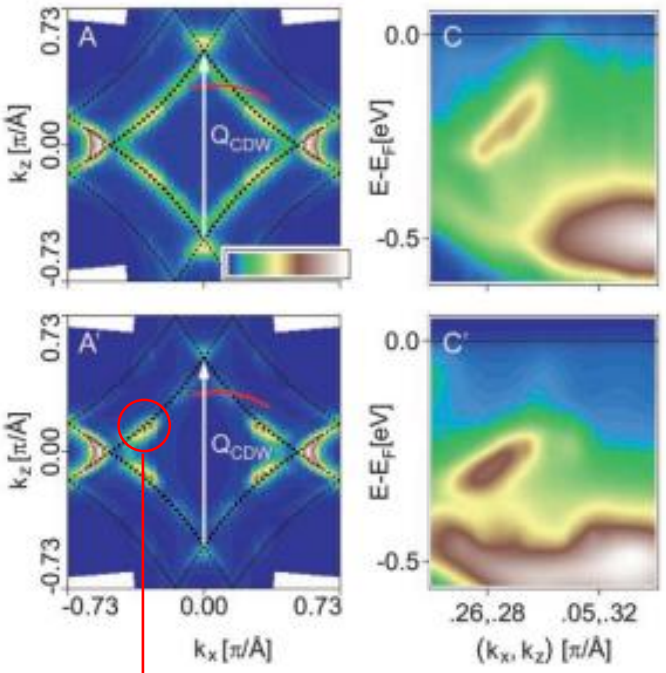


Pfuner *et al.* Eur. Phys. J. B 63, 11–16 (2008)



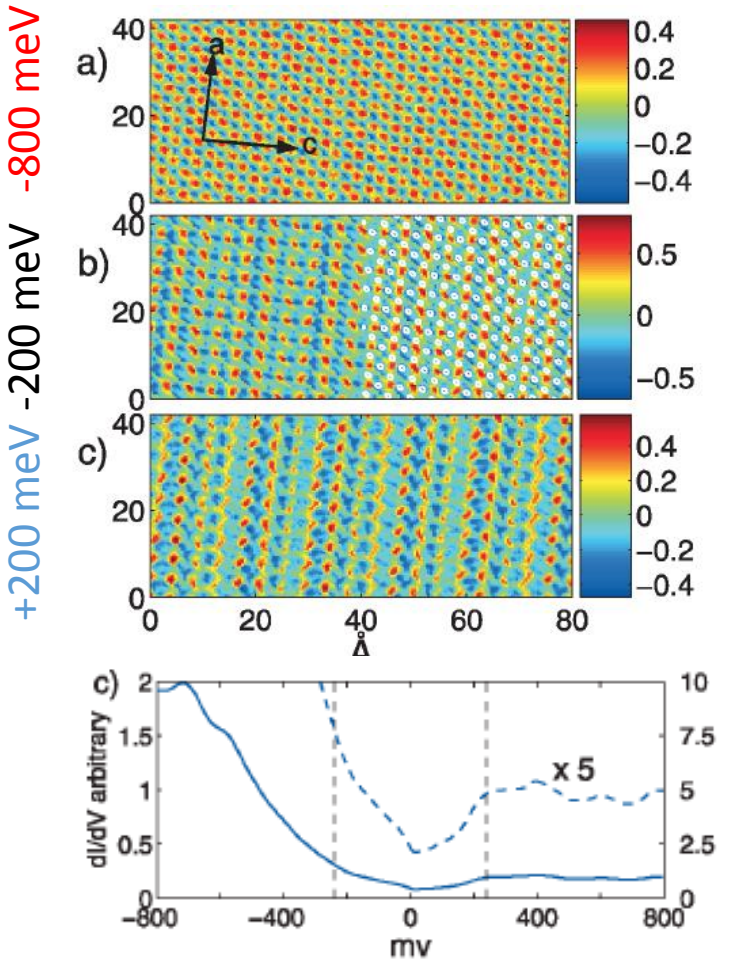
Ru *et al.* PRB **78**, 012410 (2008)

Another example: $TbTe_3$



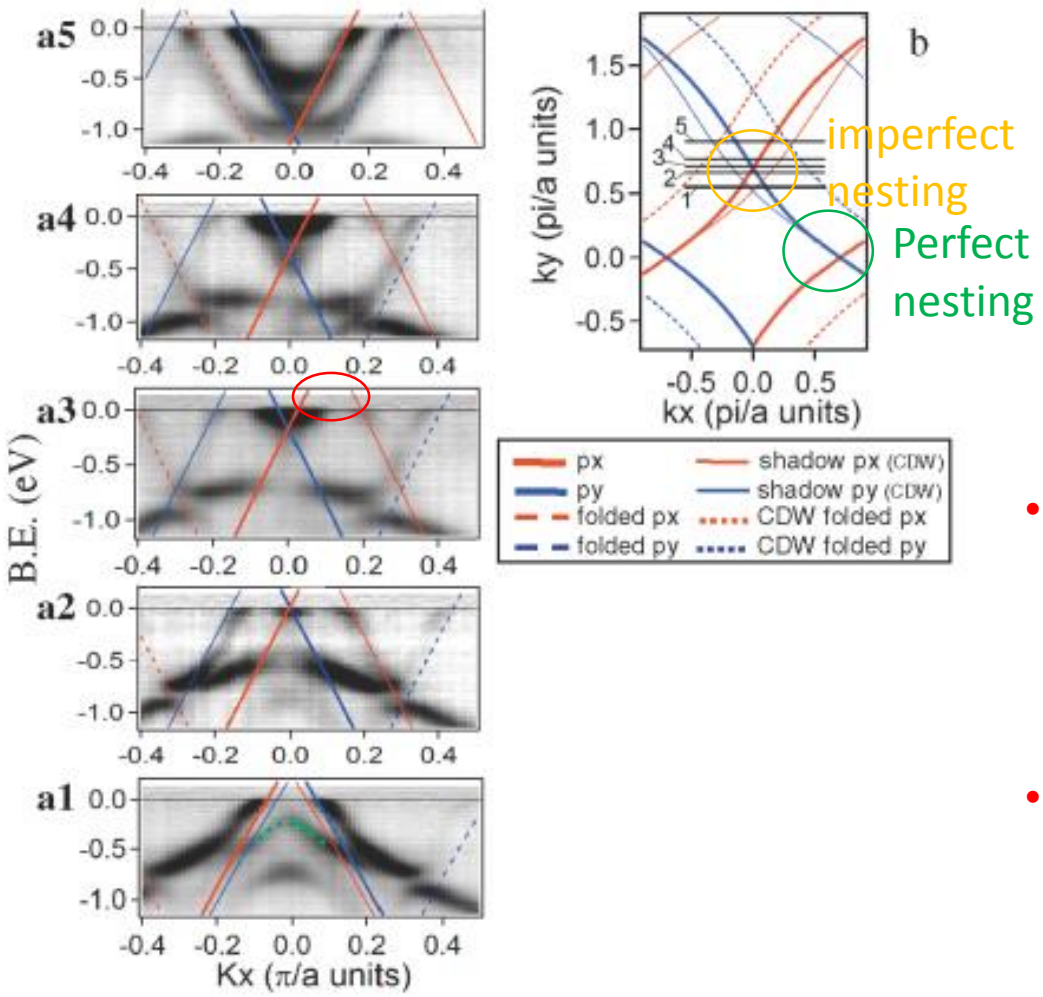
Is there a gap here?

Schmitt *et al,* Science **321** (2008)



A. Fang et al. PRL 99, 046401 (2007)

Consequences of imperfect nesting



Brouet *et al.* PRL **93** (2004)

Terminology:

- Folded = extra bands from larger 3D unit cell
- Shadow = band from new periodicity introduced by CDW (often called folded band in literature)

- If a portion of the FS is poorly nested, original band and 'shadow' band will intersect away from E_F
- Gap will open at band crossing, but it will not be centered at E_F

Density wave without nesting: gap not centered at E_F

Electron-phonon coupling

- The lattice vibrations at $\vec{q}_{CDW} = 2\vec{k}_F$ *freeze in (also called softening)*
- This type of distortion is called a Kohn anomaly
- Electron-phonon coupling is important to charge order if the lattice is involved in any way (leading, following, simultaneous)

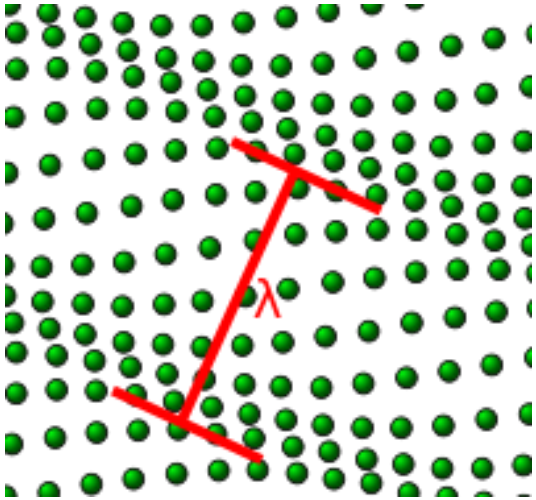
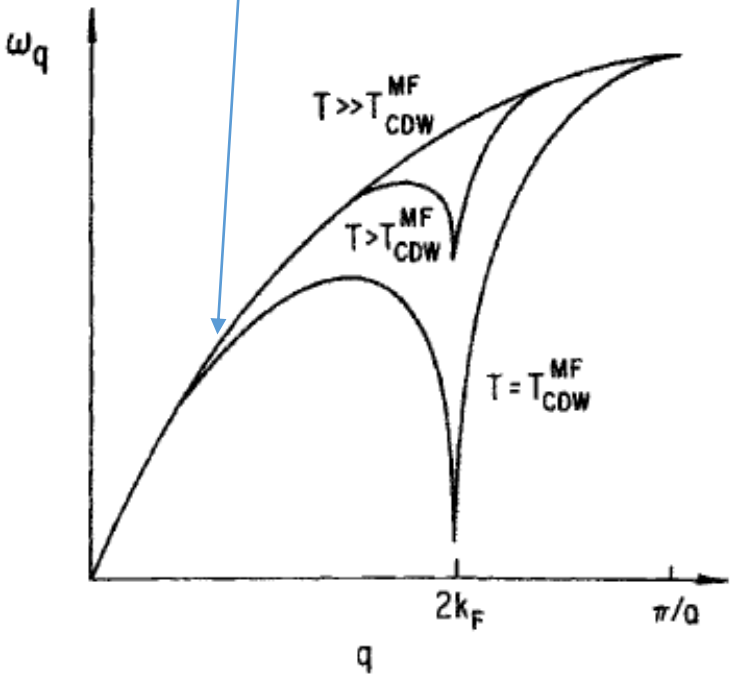


Image source: https://en.wikipedia.org/wiki/Phonon

What kind of phonon branch is this?

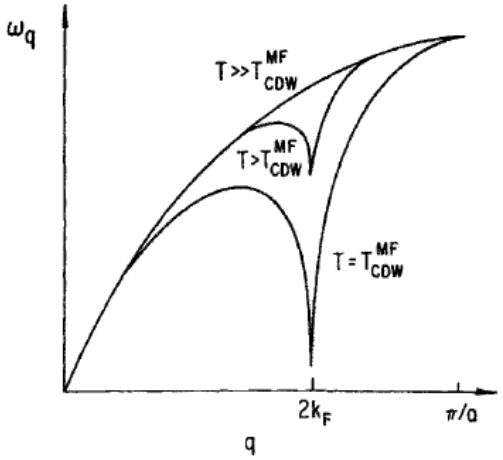


From "Density Waves in Solids" by George Gruner - 1994.

Kohn Anomaly in ZrTe3

T_{CDW}~63K

(Different crystal structure from RTe3 discussed thus far)

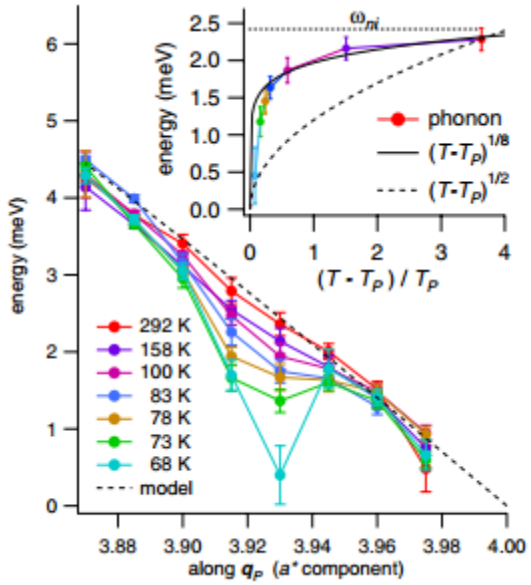


From "Density Waves in Solids" by George Gruner - 1994.

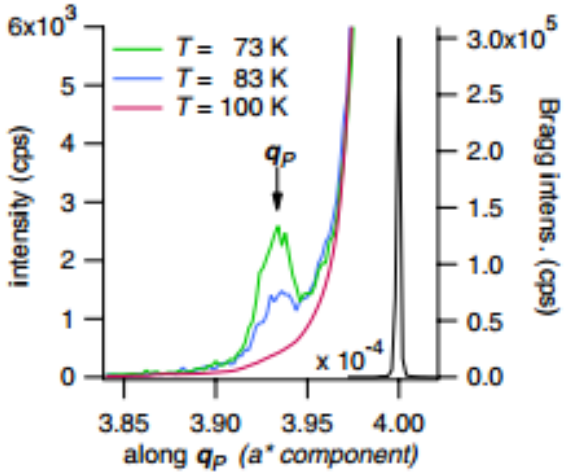
How to measure acoustic phonon branch?

- Neutron scattering
- Diffuse x-ray scattering

phonons



electrons

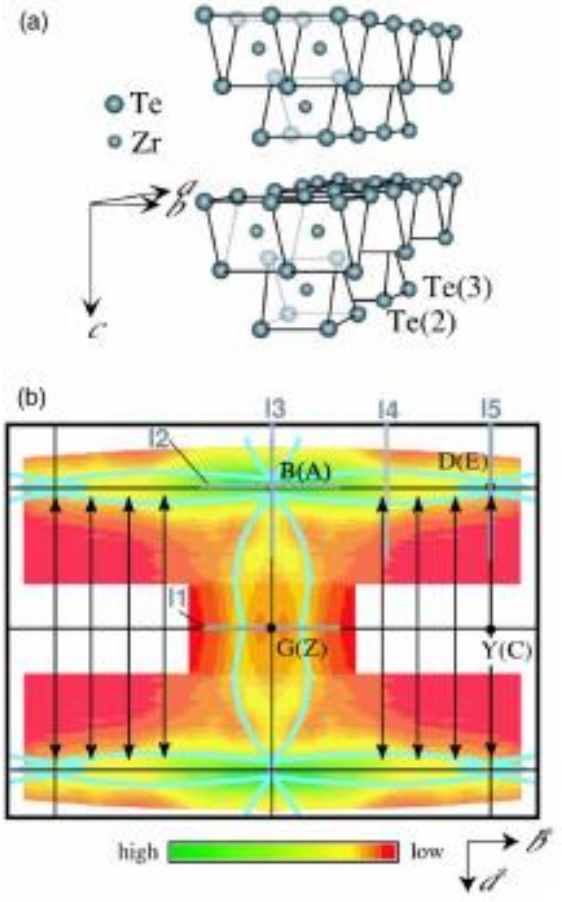


- Phonon softening at q_{CDW} begins $T \gg T_{CDW}$
- Intensity of satellite Bragg peak begins to increase at the same q a bit above T_{CDW}

Hoesch *et al.* PRL 102, 086402 (2009)

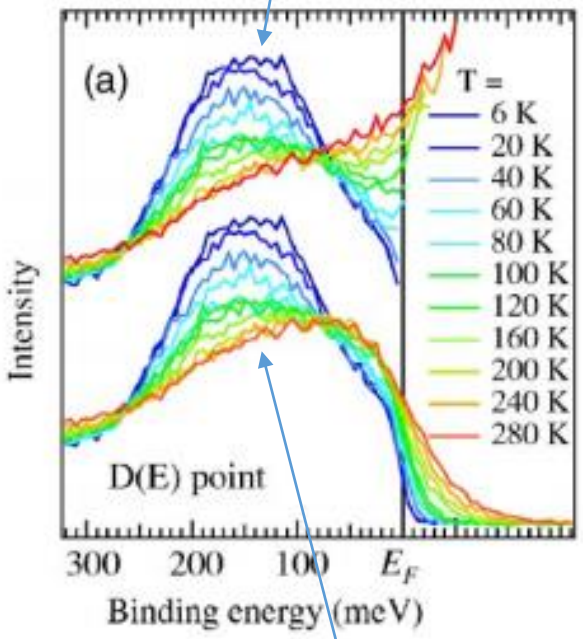
ARPES on ZrTe3

Crystal structure and
Fermi surface map



Yokoya *et al*. PRB B 71, 140504sRd (2005)

EDC divided by Fermi-dirac distribution



Raw EDCs

- Gap opens <120K>T_{CDW}
- Why?
- Importance of good match between material and experiment

Resources on CDWs

- General overview of everything: Gruner, *Density waves in solids* (1994)
- Energetic of Peierls instability: Kittel, *Solid State Physics*, Ch14
- Recent review: P. Monceau, https://arxiv.org/pdf/1307.0929.pdf