CDWs in ARPES

A momentum space picture of Fermi surface instabilities in crystalline solids

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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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- New periodic potential $\rightarrow$ New Brillouin zone $\rightarrow$ Need identical dispersion in each Brillouin zone
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CDW Review

Peierls Distortion

- Begin with 1D metal
- Introduce new periodicity into lattice with \( q = 2k_F \)
- New periodic potential \( \rightarrow \) New Brillouin zone \( \rightarrow \) Need identical dispersion in each Brillouin zone
- Gaps of magnitude \( 2\Delta \) 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

Implication: 1D systems will spontaneously respond to a potential with $q \approx 2k_F$, but higher dimensions will not.
Nesting: how higher dimensional Fermi surfaces can effectively look 1D

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 ($\phi$) 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 ($\theta$) of photoelectron is simultaneously measured, encoding crystal momentum that electron had inside sample

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

  
  Good for: matrix elements

  
  Good for: short review of formalism

  
  Good for: information about kz and quantifying quasiparticle lifetimes

  
  Good for: Historical overview; formalism; broad review of technique
Case study: $\text{RTe}_3$ ($\text{R}=\text{Tm, Er, Ho, Dy, Tb, Gd}$)

Some members have two CDWs and some become superconducting under pressure

Ru et al. PRB 78, 012410 (2008)

N. Ru thesis
How are CDWs usually discovered?

Often discovered by transport

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

Why is there metallic resistivity at low temperature?

Ru et al. PRB 77, 035114 (2008)

(not the first resistivity measurement on this material)
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$_3$


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

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)

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

Brouet et al. PRB 77, 235104 (2008)

Yao et al. PRB 74, 245126 (2006)
What does the original FS look like?

- 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)
Does data agree with Fermi surface nesting?

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

Moore et al. PRB 81, 073102 (2010)
CDW order parameter

Complex order parameter:
\[ \Psi \sim \Delta e^{i\phi} \]

Amplitude (\(\Delta\))
Phase (\(\phi\))

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 $\rightarrow$ larger gap
- Ratio between ordering temperature and gap can be meaningful
- Concept will come up again in superconductivity topic

Ru et al. PRB 78, 012410 (2008)
Another example: TbTe$_3$

Is there a gap here?


A. Fang et al. PRL 99, 046401 (2007)
Consequences of imperfect nesting

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 $E_F$

The lattice vibrations at $\vec{q}_{\text{CDW}} = 2\vec{k}_F$ 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).

What kind of phonon branch is this?


Image source: https://en.wikipedia.org/wiki/Phonon
Kohn Anomaly in ZrTe$_3$

$T_{\text{CDW}} \sim 63\,\text{K}$

(Different crystal structure from RTe$_3$ discussed thus far)

How to measure acoustic phonon branch?

- Neutron scattering
- Diffuse x-ray scattering


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

Hoesch et al. PRL 102, 086402 (2009)
ARPES on ZrTe3

Crystal structure and Fermi surface map

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

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

EDC divided by Fermi-dirac distribution

Raw EDCs
Resources on CDWs


• Energetic of Peierls instability: Kittel, *Solid State Physics*, Ch14