Lecture 17 – Charge Density Waves

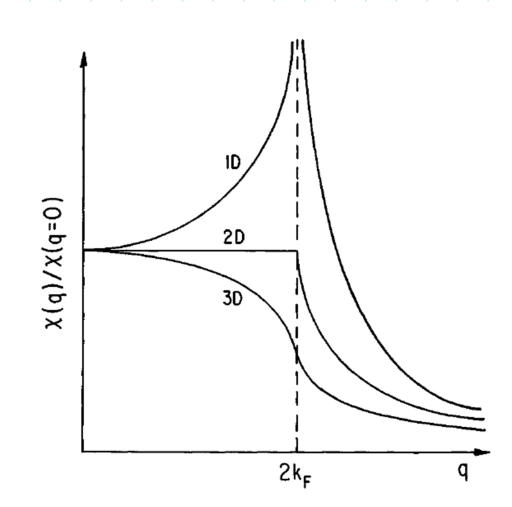
Tuesday, 14. December 2021 09:50

Lindhard response function for different dimensions

$$\chi(\vec{q}) = \int \frac{d\vec{k}}{(2\pi)^d} \frac{f(\vec{k}) - f(\vec{k}+\vec{q})}{E(\vec{k}) - E(\vec{k}+\vec{q})}$$

with $E(\vec{k}) = \frac{\hbar^2 \vec{k}^2}{2m}$

- in 1D: $\chi(\vec{q})$ diverges for $q = 2k_F$

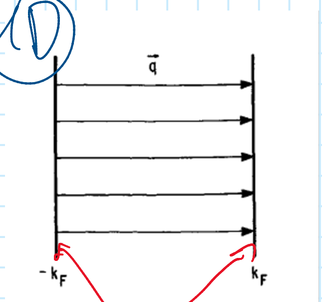


$\Rightarrow$ divergent charge redistribution

$\Rightarrow$ e^- gas is unstable with respect to the formation of a periodically varying charge or spin density period $\lambda = \frac{\pi}{k_F}$

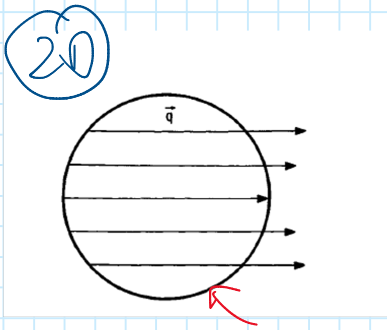
when $q = 2k_F$ $\quad E(k) = E(k + 2k_F)$

1D



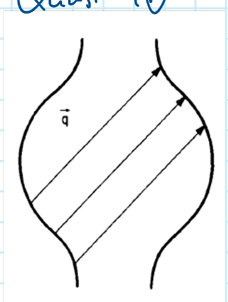
Same Energy

2D



Fermi "circle"

Quasi 1D



- Perfect nesting

Divergence of the response function at $q = 2k_F$ is due to the particular topology/shape of the Fermi surface

↳ sometimes refered to as perfect nesting

"large number of e^- with similar energy"

↳ sometimes refered to as perfect nesting
"large number of e^- with similar energy"

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Three-Dimensional Electron Realm in VSe_2 by Soft-X-Ray Photoelectron Spectroscopy: Origin of Charge-Density Waves

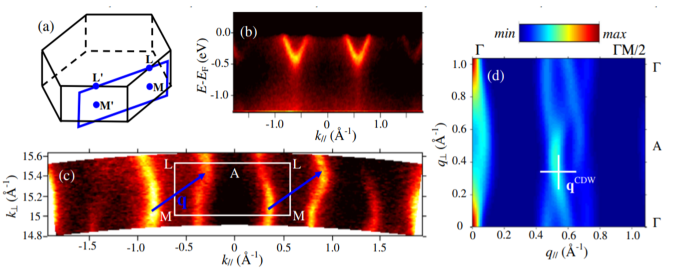
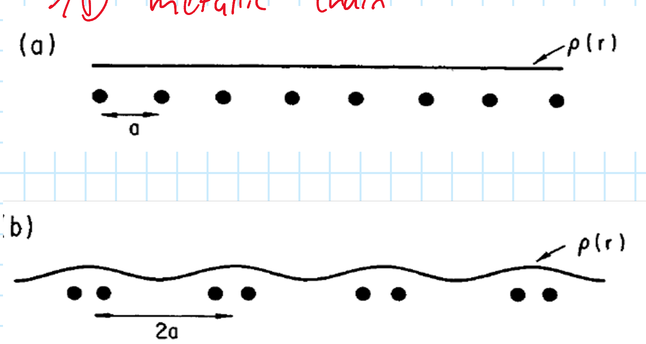


FIG. 3 (color online). 3D warping of the FS in the nesting region as the 3D CDWs precursor. (a) $MLL'M'$ plane of the BZ going through the nesting region; (b) experimental $I(E, k_{\parallel})$ image along the MM' line ($h\nu$ = 890 eV); (c) experimental out-of-plane FS cut in the $MLL'M'$ plane ($h\nu$ = 880 to 960 eV) normalized similar to Fig. 1(c). The $k_\perp$ dispersions are asymmetric due to the threefold symmetry of the BZ interior. 3D warping of the FS contours results in nesting with the indicated **q** close to $\mathbf{q}^{CDW}$ of the 3D CDWs; (d) corresponding $R(\mathbf{q})$ autocorrelation map showing an arclike maximum near $\mathbf{q}^{CDW}$.

↳ In the 1D system, it becomes unstable against the formation of a charge modulation (Peierls transition)

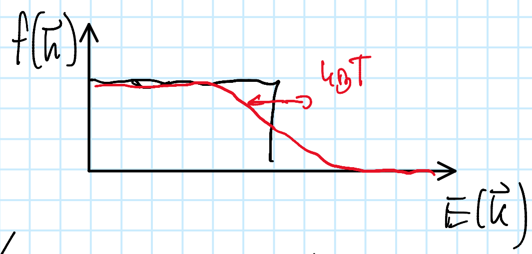
1D metallic chain

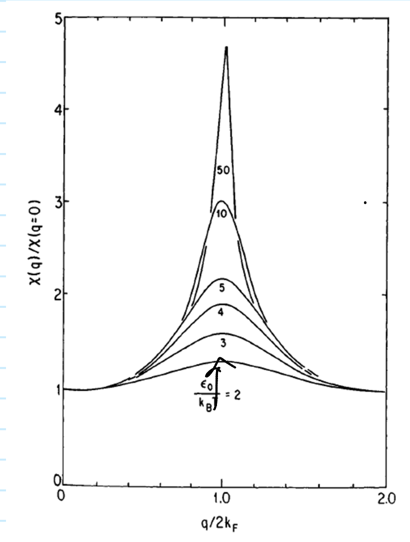


Structural transition
new periodicity of the lattice

for a "charge density wave" this transition will be driven via the electron-phonon-interaction

- Effect of temperature





↳ smoothens out the divergence

- One can show

$$\chi(2k_F, T) = -e^2\, n(\varepsilon_F) \cdot \ln\left(\frac{1.14\, \varepsilon_0}{k_B T}\right)$$

Peierls Instability

Peierls' idea was to couple the unstable e^- gas to the underlying ionic lattice to show that this drives a structural phase transition

- Fröhlich – Hamiltonian

$$H = \underbrace{\sum_k \overset{\frac{\hbar^2 k^2}{2m}}{\varepsilon_k}\, a_k^\dagger a_k}_{\text{1D } e^- \text{ gas}} + \overbrace{\sum_q \hbar \omega_q\, b_q^\dagger b_q}^{\text{lattic vibrations}} + \underbrace{\sum_{k,q} g_q\, a_{k+q}^\dagger a_k \left(b_{-q} + b_q\right)}_{e^- \text{-phonon-coupling}}$$

ω_q: normal mode frequency

g_q: coupling parameter

Rudolf Peierls (1907 – 1995)
Herbert Fröhlich (1905 - 1991) } no Noby

- Effect of the e^--ph-coupling on the lattice vibrations
  $\Rightarrow$ renormalized phonon frequencies

$$\omega_{ren,q}^2 = \omega_q^2 + \frac{2 \cdot g^2 \cdot \omega_q}{\hbar} \chi(q,T) \quad \leftarrow @\, q$$

now independent of q

$$\omega_{ren,2k_F}^2 = \omega_{2k_F}^2 - \frac{2 \cdot g^2 \cdot n(\varepsilon_F)}{\hbar\, \omega_{2k_F}} \cdot \ln\left(\frac{1.14\, \varepsilon_0}{k_B T}\right) \quad \leftarrow @\, 2k_F$$

$$= \omega_{2k_F}^2 \left[1 - \underbrace{\frac{2 \cdot g^2\, n(\varepsilon_F)}{\hbar\, \omega_{2k_F}}}_{\to 2\lambda} \cdot \ln\left(\frac{1.14\, \varepsilon_0}{k_B\, T}\right)\right]$$

for 1D case: $\chi(q,T)$ has a maximum @ $q = 2k_F$
↳ Softening of the Phonon frequencies will be most significant here

with decreasing $T \rightarrow \omega_{ren,2k_F}$ goes to 0

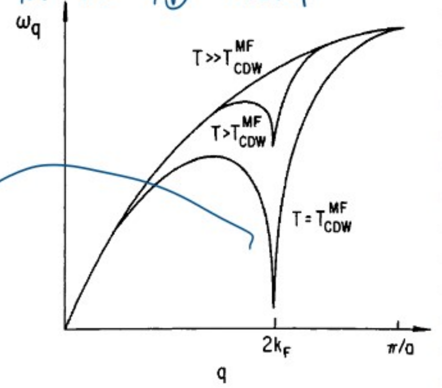
→ Transition temperature with a „frozen-in" lattice distortion (macroscipically occupied phonon mode) lattice distortion (macroscopically occupied phonon mode)

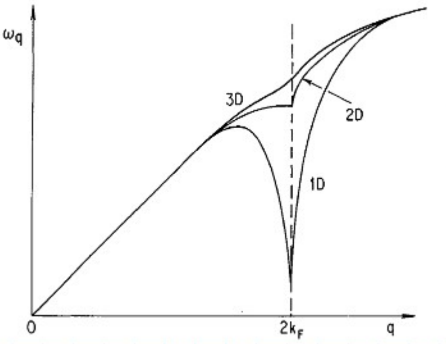
$$k_B T_{CDW}^{MF} = 1.14\, \varepsilon_0 \cdot e^{-1/\lambda}$$

$$\lambda = \frac{g^2\, n(E_F)}{\hbar \omega_{k_F}}$$

dimensionless e^--ph-coupling

Acoustic phonon dispersion in a 1D metal





Kohn anomaly

Walter Kohn (1923 – 2016) Noby 1998

Observation of Giant Kohn Anomaly in the One-Dimensional Conductor $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$

B. Renker, H. Rietschel, L. Pintschovius, and W. Gläser
Institut für Angewandte Kernphysik, Kernforschungszentrum Karlsruhe, 75 Karlsruhe, Germany

and

P. Brüesch, D. Kuse, and M. J. Rice
Brown Boveri Research Center, CH-5401 Baden, Switzerland

(Received 19 March 1973)

Longitudinal acoustic phonons have been measured by coherent inelastic neutron scattering in the direction of the platinum chains of a single crystal of the one-dimensional conductor $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$ at room temperature. The phonon dispersion curve shows a pronounced anomaly at the phonon wave number $q_0 = 0.32$ Å^{-1} and is interpreted as the logarithmic Kohn anomaly characteristic of a one-dimensional metal.

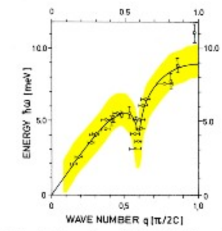


FIG. 2. LA phonon branch of $K_2Pt(CN)_4Br_{0.3} \cdot 3H_2O$ in [001] direction at room temperature. Solid line, fit of the simple free-electron model discussed in the text.

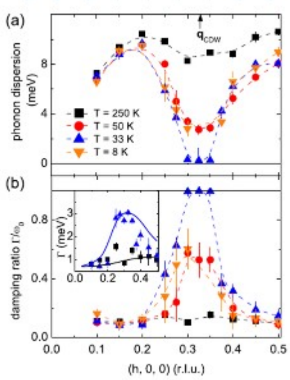


FIG. 3 (color online). Experimentally obtained dispersion and damping ratio of the soft-phonon branch in $2H$-$NbSe_2$ at four temperatures 8 K ≤ T ≤ 250 K. Plotted are (a) the frequency of the damped harmonic oscillator $\omega_q = \sqrt{\tilde{\omega}_q^2 - \Gamma^2}$ and (b) the damping ratio $\Gamma/\tilde{\omega}_q$. Lines are guides to the eye. Note that phonons at $h = 0.325, 0.35$ and $T = 8$ K were not detectable due to strong elastic intensities. The inset in (b) shows the experimentally observed damping Γ of the damped harmonic oscillator (symbols) and scaled DFPT calculations (see Fig. 4) of 2γ (lines, offset 0.7 meV) with $\sigma = 0.1$ eV (black) and 1 eV (red).

$NbSe_2$ - Prototype CDW material

$T_{CDW} = 33K$

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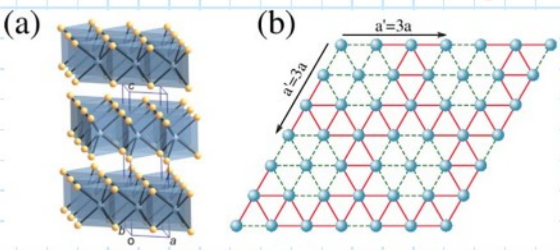
inelastic X-Ray Scattering



- now let's switch to the electronic side

transition is connected to a lowering of the total energy

↳ opening of a gap at $\pm k_F$

↳ Metal-insulator transition (Peierls transition)

↳ depending on the band filling: periodicity of CDW changes: commensurate or incommensurate

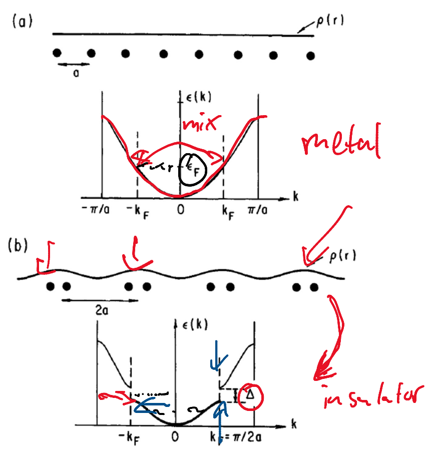
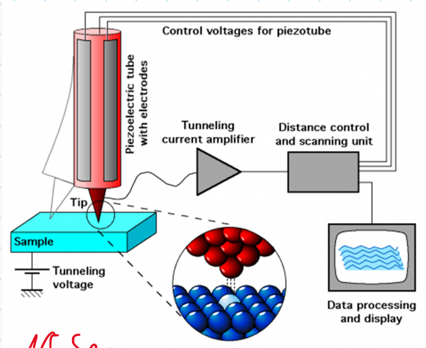


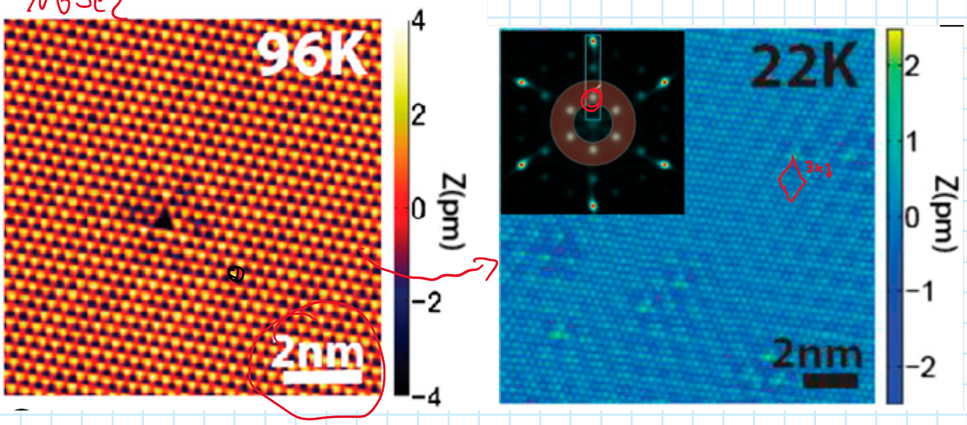
Figure 3.5. The single particle band, electron density, and lattice distortion in the metallic state above T_{CDW} and in the charge density wave state at $T = 0$. The figure is appropriate for a half-filled band.

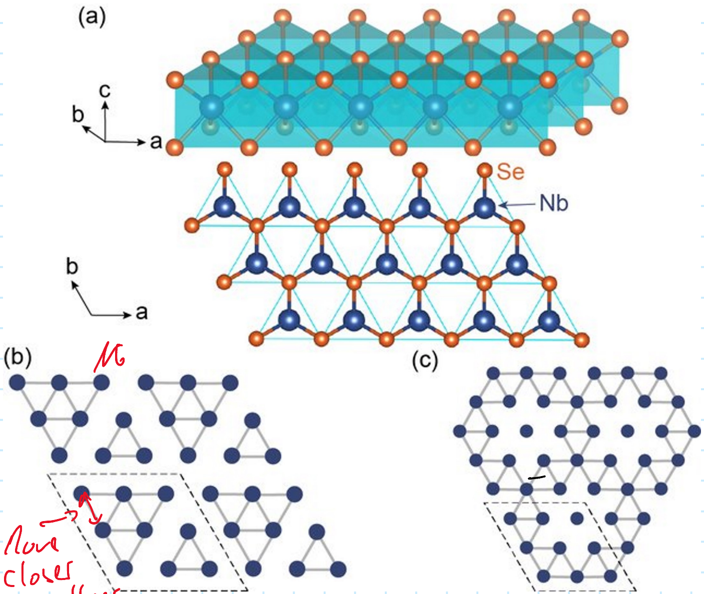
Scanning tunneling microscope (STM)



- Measures the quantum mechanical tunneling current between tip + sample
- local density of states

$NbSe_2$





Nb

move closer together

last note

- in a real system, things are more complicated...
- Nesting might not drive phase transition (see literature)

↳ Ilias