Peierls instability and density wave

If the electron dispersion satisfies nesting condition:

$$\varepsilon(k)+\varepsilon(k+Q_N)=0$$

(at least on some finite part of the Fermi surface in metals),

the susceptibility $\chi(Q_N)$ diverges. Then at low temperature any e-e interaction leads to a new many-body state, which is a charge- or spin-density wave (CDW or SDW).

Main features of CDW/SDW:

A gap in electron spectrum appears in CDW or SDW state.
If this gap covers the whole FS, the metal becomes an insulator.

The modulation of charge or spin electron density can be detected by x-ray for CDW and by NMR, neutron or muon scattering for SDW.

Geometrical interpretation of nesting condition

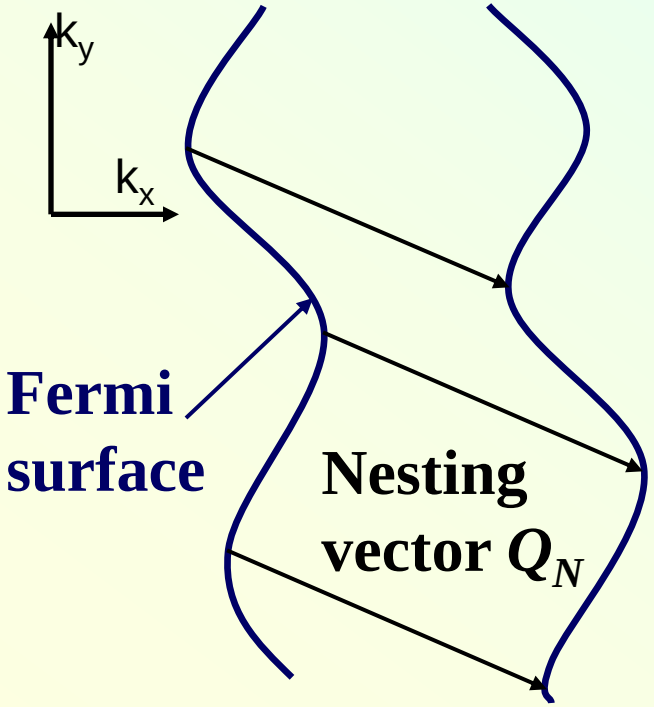
Quasi-1D metals

$$\varepsilon(k) = v_F(|k| - k_F) - 2t_y \cos(k_y b)$$

satisfies nesting condition:

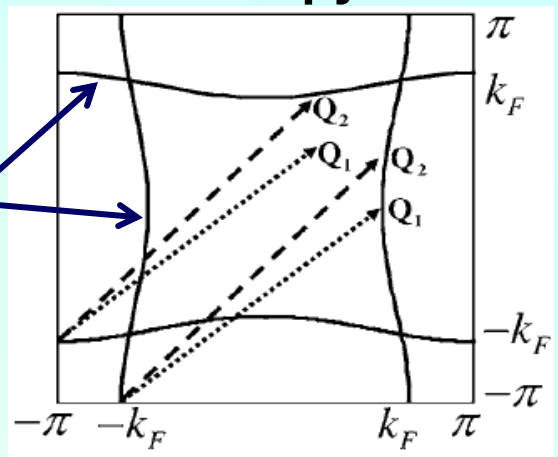
$$\varepsilon(k) + \varepsilon(k + Q_N) = 0$$

with $Q_N = (2k_F, \pi/b)$.



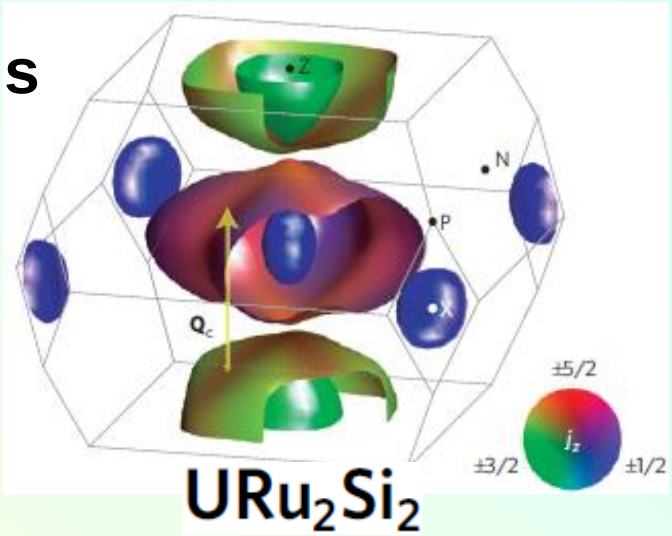
Quasi-2D metals

hidden1D anisotropy



3D metals

partial nesting



URu_2Si_2

Lindhard formula for electron susceptibility χ(Q, T)

The susceptibility of quantity A with respect to quantity B:

$$\chi(\omega) = \frac{i}{\hbar}\int_0^\infty \left\langle \left[\hat{A}(t), \hat{B}(0)\right]\right\rangle e^{i\omega t} dt$$

For the free electron gas in terms of matrix elements it becomes:

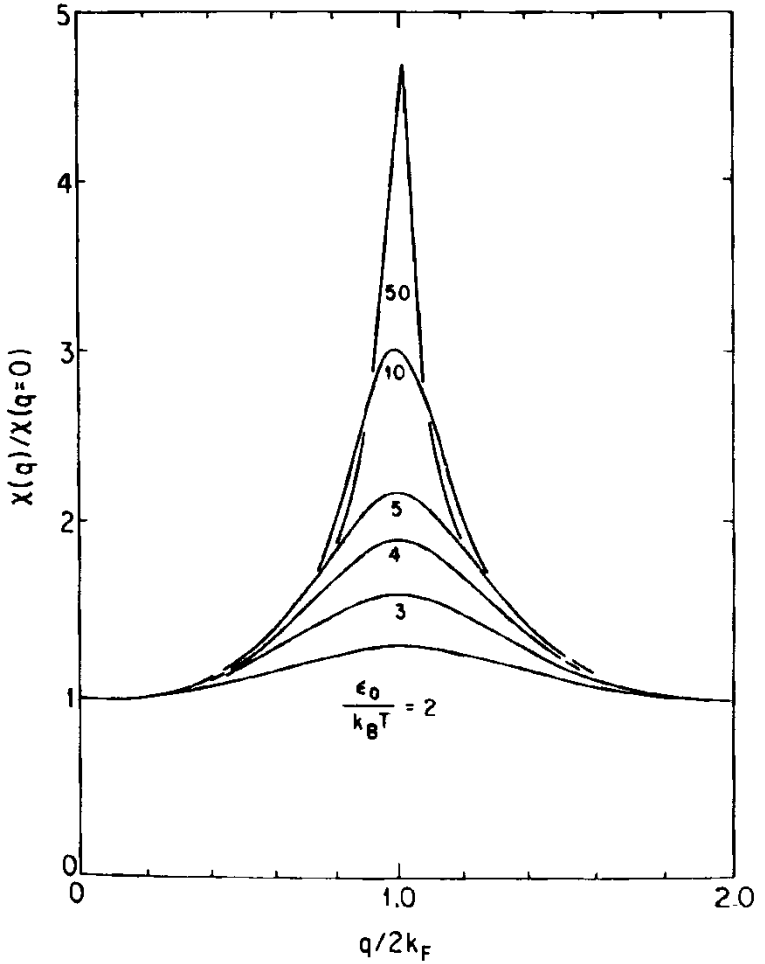
$$\chi(\omega) = \sum_{ml} A_{ml} B_{lm} \frac{n_F(E_m) - n_F(E_l)}{E_l - E_m - \omega - i\delta}$$

In the CDW response function the quantities A and B are the electron density. One needs the static susceptibility at ω = 0 but at finite wave vector Q:

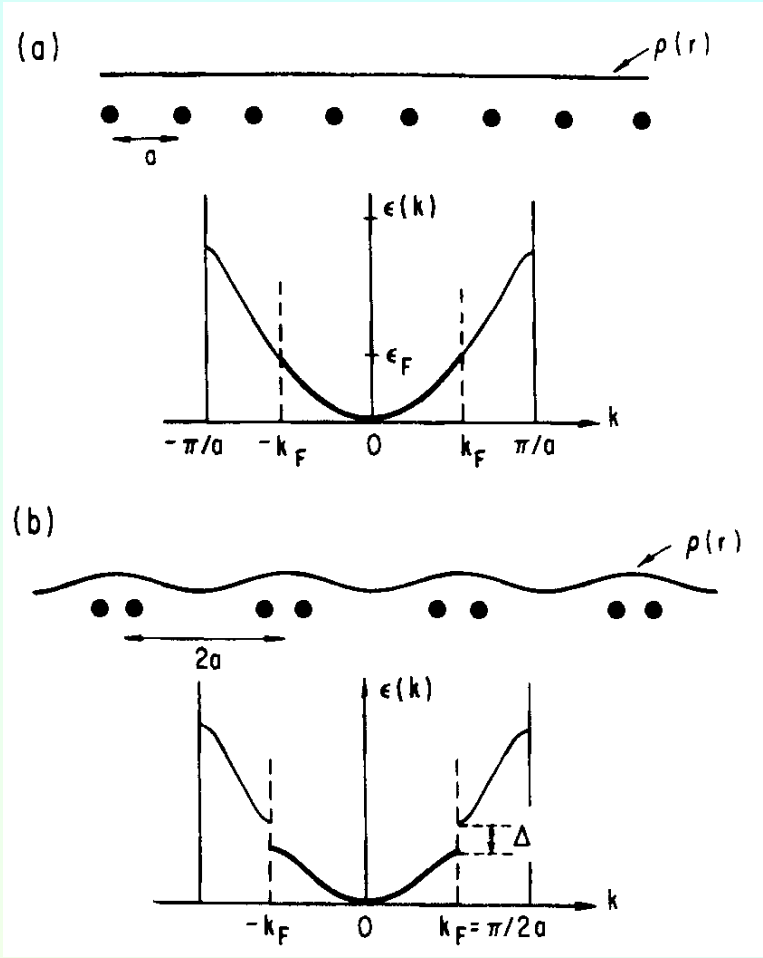
$$\chi(\boldsymbol{Q}) = \sum_{\alpha,\alpha'} \int \frac{4d^d\boldsymbol{k}}{(2\pi)^d} \frac{n_F(E_{\boldsymbol{k},\alpha}) - n_F(E_{\boldsymbol{k}+\boldsymbol{Q},\alpha'})}{E_{\boldsymbol{k}+\boldsymbol{Q},\alpha'} - E_{\boldsymbol{k},\alpha}},$$

The CDW transition temperature T_c is given by the equation: $|U\chi(\boldsymbol{Q}_{max}, T_c)| = 1$

Peierls transition in 1D metals



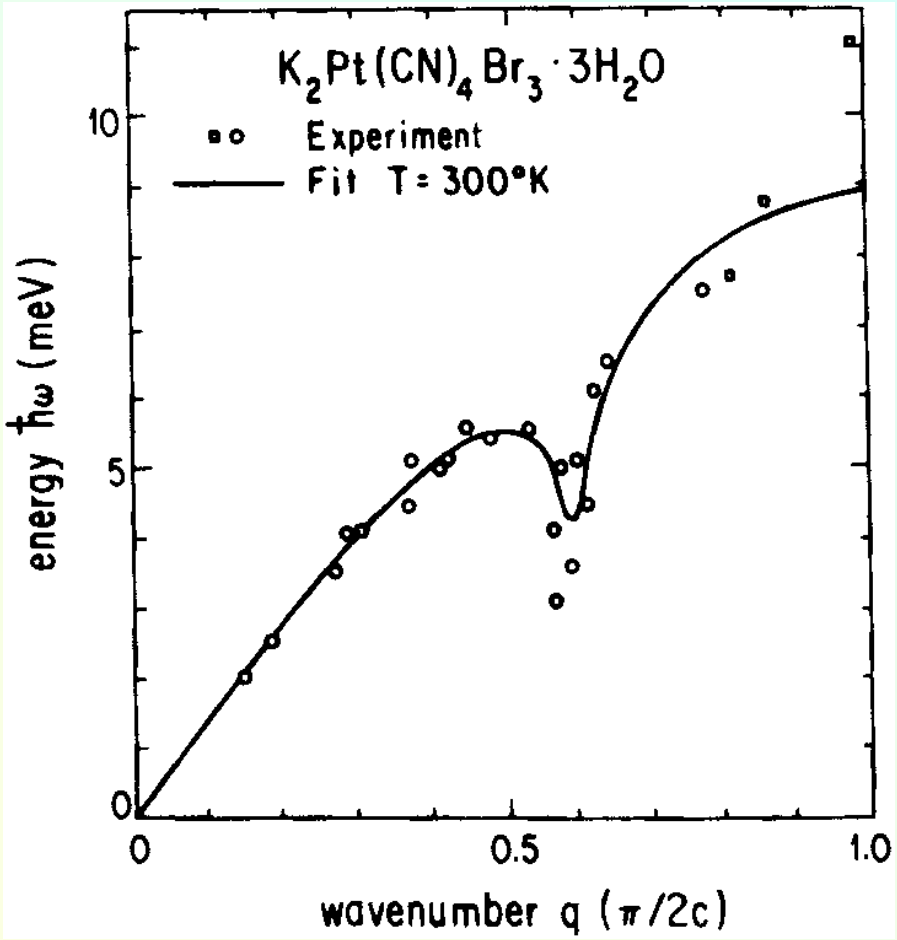
Electronic susceptibility as function wave vector and temperature

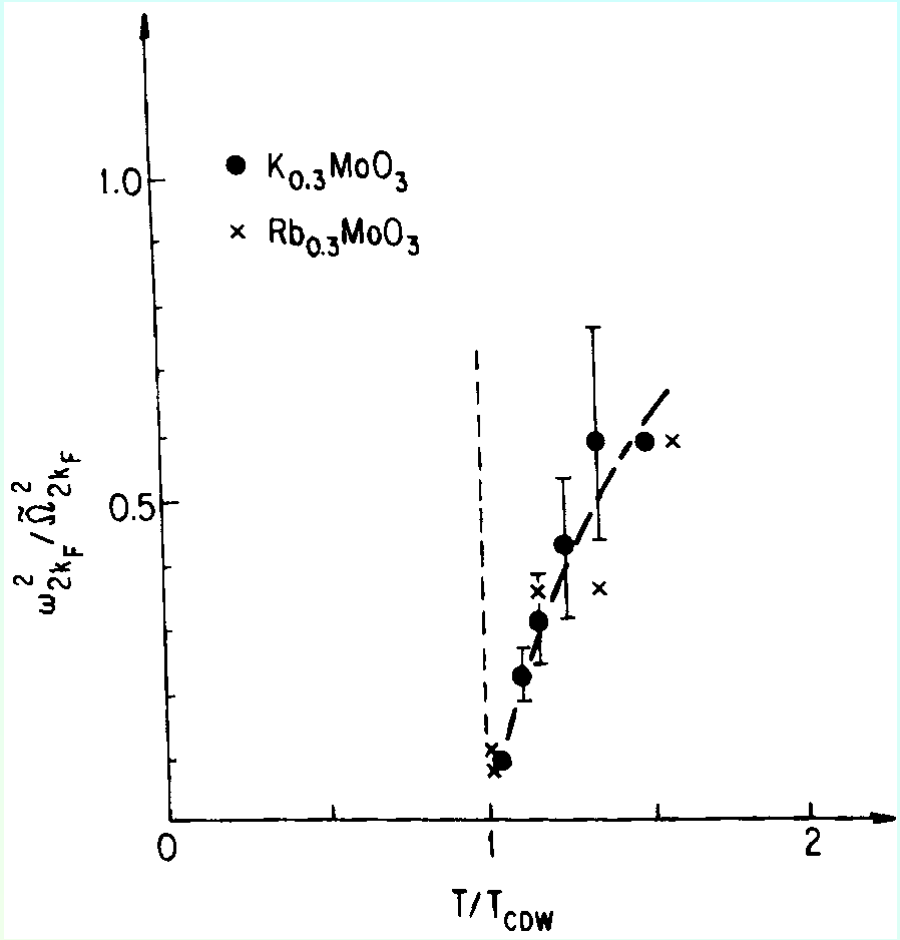


Electron density and lattice distortion for half-filled band

G. Gruener, *Density waves in Solids*, 1994

Phonon mode softening near the CDW transition





Softening of phonon dispersion at CDW wave vector allows independent study of CDW by inelastic neutron scattering.

Charge- and spin-density wave

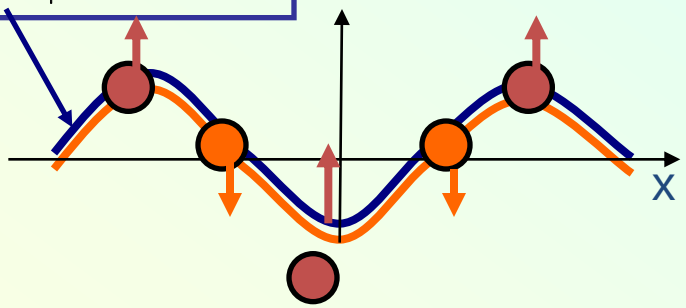
Charge-density wave

Density modulations for two spin components in CDW:

$$\rho_{\uparrow}(x) = \rho_0 + \Delta\cos(Qx) = \rho_{\downarrow}(x)$$

Spin-up electron density $\rho_{\uparrow}(x)$

$\rho_{\uparrow}(x) = \rho_{\downarrow}(x)$



Total charge density is modulated

$$\rho_C(x) = \rho_{\uparrow}(x) + \rho_{\downarrow}(x) = 2\left[\rho_0 + \Delta_0\cos\left(Q\,x\right)\right]$$

Total spin density is constant

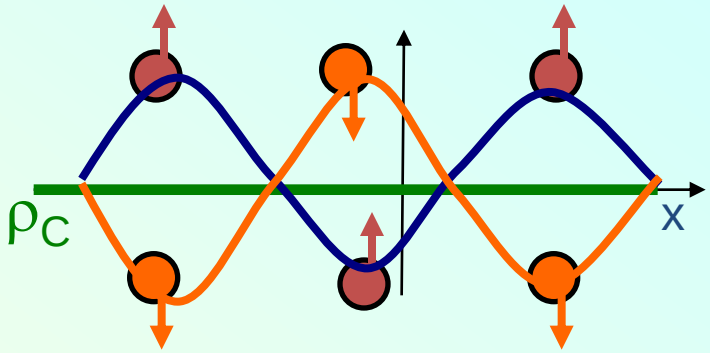
$$\rho_S(x) = \rho_{\uparrow}(x) - \rho_{\downarrow}(x) = 0.$$

Spin-density wave

Density modulations for two spin components in SDW:

$$\rho_{\uparrow}(x) = \rho_0 + \Delta\cos(Qx)$$

$$\rho_{\downarrow}(x) = \rho_0 - \Delta\cos(Qx)$$



Total charge density is constant:

$$\rho_C(x) = \rho_{\uparrow}(x) + \rho_{\downarrow}(x) = const:$$

Total spin density has modulation

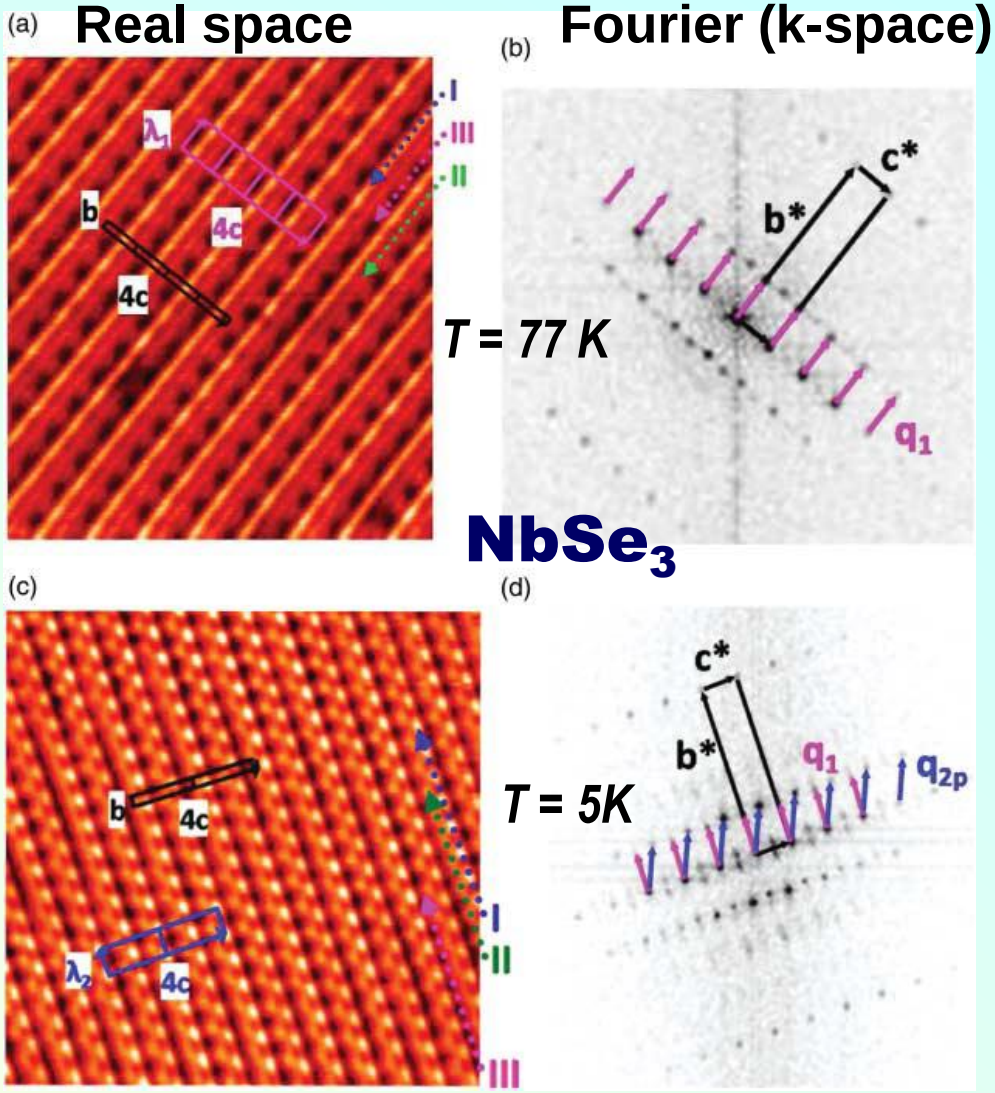
$$\rho_S(x) = \rho_{\uparrow}(x) - \rho_{\downarrow}(x) = 2\Delta_0\cos\left(Q\,x\right).$$

STM images of CDW

STM images of the (*b, c) plane of NbSe3, scanned area 20 × 20 nm2.*
(a)T = 77 K. Vbias = +100 mV, I = 1 nA.
(b) Fourier transform of the STM image.
(c) *T = 5K, Vbias = +200mV, I = 150 pA*
The Q2 CDW appears
(d) 2D Fourier transform of the STM image shown in (c).

CDW transition temperatures :
T_{P1}= 144K and T_{P2}= 59K

CDW can be visually observed via STM as intensity modulation.



C. Brun *et al.*, PRB 80, 045423 (2009)

also in P. Monceau, Adv. Phys. 61, 325 (2012)

Electron Hamiltonian & anomalous average

The Hamiltonian of electron-phonon system is

$$\mathscr{H} = \sum_k \epsilon_k a_k^\dagger a_k + \sum_q \hbar\omega_q b_q^\dagger b_q + \sum_{k,q} g_q a_{k+q}^\dagger a_k \left(b_{-q}^\dagger + b_q\right)$$

The pure electron Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}}, \quad \text{where} \quad \hat{H}_0 = \sum_{\boldsymbol{k}\sigma} \varepsilon_\sigma(\boldsymbol{k}) a_\sigma^\dagger(\boldsymbol{k}) a_\sigma(\boldsymbol{k})$$

and the electron-electron interaction is given by

$$\hat{H}_{\text{int}} = \frac{1}{2} \sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{Q}\sigma\sigma'} V_{\sigma\,\sigma'}(\boldsymbol{Q}) a_\sigma^\dagger(\boldsymbol{k}+\boldsymbol{Q}) a_\sigma(\boldsymbol{k}) a_{\sigma'}^\dagger(\boldsymbol{k}'-\boldsymbol{Q}) a_{\sigma'}(\boldsymbol{k}')$$

The mean-field approach of CDW assumes a non-zero average $\left(b_{-q}^\dagger + b_q\right)$

or for pure e-e interaction $\Delta_{\boldsymbol{Q}} = U_c(\boldsymbol{Q}) \sum_{\boldsymbol{k}\,\sigma'} \langle a_{\sigma'}^\dagger(\boldsymbol{k}+\boldsymbol{Q}) a_{\sigma'}(\boldsymbol{k}) \rangle$

CDW / SDW band structure

Electron Hamiltonian in the mean field approximation:

$$\hat{H}_Q = \sum_{k\sigma} \varepsilon_\sigma(k) a_\sigma^+(k) a_\sigma(k) + \sum_{k\sigma} \hat{\Delta}_Q \, a_\sigma^+(k+Q) a_\sigma(k).$$

The order parameter $\hat{\Delta} \equiv g \sum_{k'\sigma'} a_{\sigma'}^+(k'-Q) a_{\sigma'}(k')$

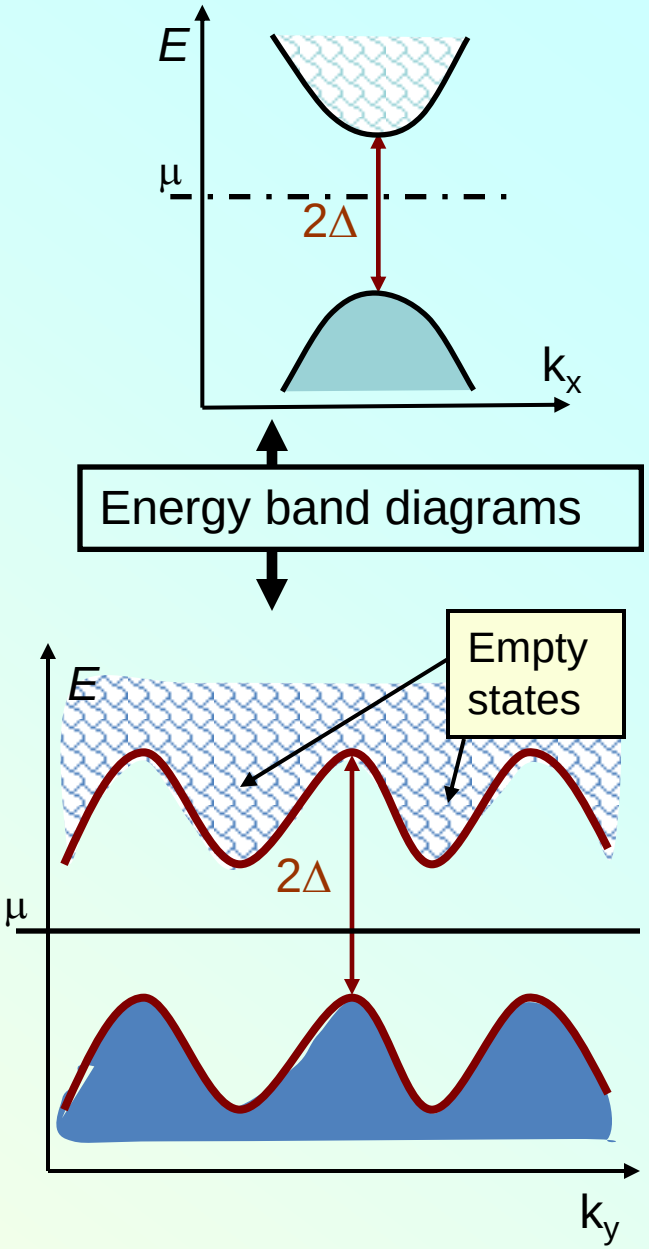
is a number for CDW, and a spin operator

for SDW: $\hat{\Delta}_Q = \Delta_0 (\hat{\sigma} \cdot l).$

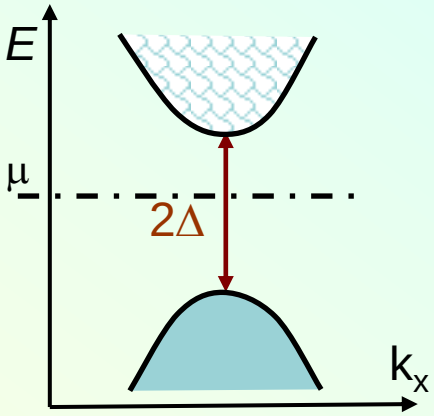
Energy spectrum in the CDW /SDW state

$$E(k) = \frac{\varepsilon(k) + \varepsilon(k+Q_N)}{2} + \sqrt{\left(\frac{\varepsilon(k) - \varepsilon(k+Q_N)}{2}\right)^2 + \Delta^2}.$$

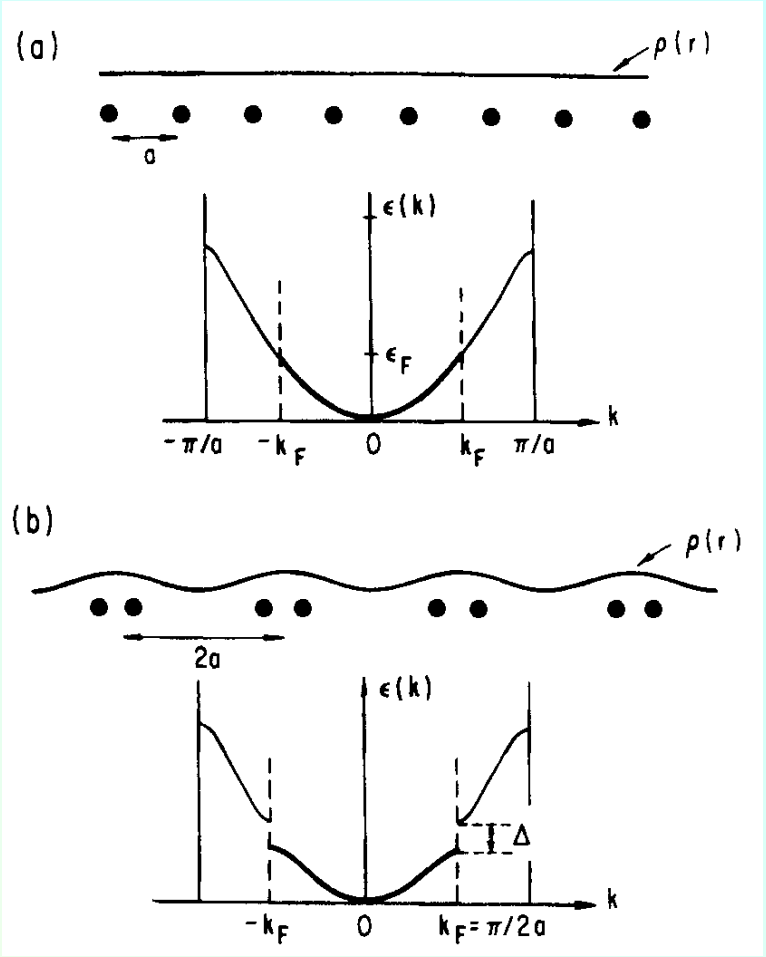
Perfect nesting condition: $\varepsilon(k) + \varepsilon(k+Q_N) = 0.$



Energy gain in CDW (qualitative picture)



The formation of an energy gap on the Fermi level decreases the total energy, because the energy of filled electron states decreases, while energy of empty electron states increases.



Electron density and lattice distortion for half-filled band

Energy gain in CDW (electron energy)

After diagonalization of electron states the Hamiltonian becomes

$$\mathcal{H} = \sum_k E_k\left(\gamma^\dagger_{1,k}\gamma_{1,k} + \gamma^\dagger_{2,k}\gamma_{2k}\right) + \frac{\hbar\omega_{2k_f}\Delta^2}{2g^2}$$

where the energy of electron states $E_k = \epsilon_f + \mathrm{sign}(k-k_f)\left[\hbar^2 v_F^2 (k-k_f)^2 + \Delta^2\right]^{1/2}$

Due to the gap opening the electron energy is lowered by

$$E_{el} = \sum_k \left(-E_k + v_F k\right) = n(\epsilon_F)\int_0^{\epsilon_f}\left(\epsilon - \left(\epsilon^2+\Delta^2\right)^{1/2}\right)d\epsilon$$

which after some algebra becomes

$$E_{el} = \frac{n(\epsilon_F)}{2}\left\{\epsilon_F^2 - \left[\epsilon_f\left(\epsilon_F^2+\Delta^2\right)^{1/2} + \Delta^2 \log\frac{\epsilon_F + \left(\epsilon_F^2+\Delta^2\right)^{1/2}}{\Delta}\right]\right\}$$

In the weak coupling limit ($\epsilon_F \gg \Delta$) the expansion of the log term gives

$$E_{el} = n(\epsilon_F)\left[-\frac{\Delta^2}{2} - \Delta^2\log\left(\frac{2\epsilon_F}{\Delta}\right)\right] + O\left(\frac{\Delta}{\epsilon_f}\right)$$

Pure electron energy has an ultraviolet logarithmic divergence!

Energy gain in CDW (total energy)

The lattice distortion leads to an increase in the elastic energy

$$E_{\text{latt}} = \frac{N}{2} M\omega_{2k_f}^2 \langle u(x)\rangle^2 = \frac{\hbar\omega_{2k_f}\Delta^2}{2g^2} = \frac{\Delta^2 n(\epsilon_F)}{\lambda}$$

where the average lattice distortion is

$$\langle u(x)\rangle = \left(\frac{\hbar}{2NM\omega_{2k_f}}\right)^{1/2} \left\{ i\left(\langle b_{2k_f}\rangle + \langle b^{+}_{2k_f}\rangle\right) e^{i2k_f x} + c.c. \right\}$$

$$= \left(\frac{\hbar}{2NM\omega_{2k_f}}\right)^{1/2} \frac{2|\Delta|}{g} \cos(2k_f x + \phi) \qquad (3.23)$$

The total energy change is given by the two terms

$$E_{\text{tot}} = E_{\text{el}} + E_{\text{latt}} = n(\epsilon_f)\left[-\frac{\Delta^2}{2} - \Delta^2 \log\left(\frac{2\epsilon_f}{\Delta}\right) + \frac{\Delta^2}{2\lambda} \right]$$

Straightforward minimization of the total energy leads, for $\lambda << 1$, to

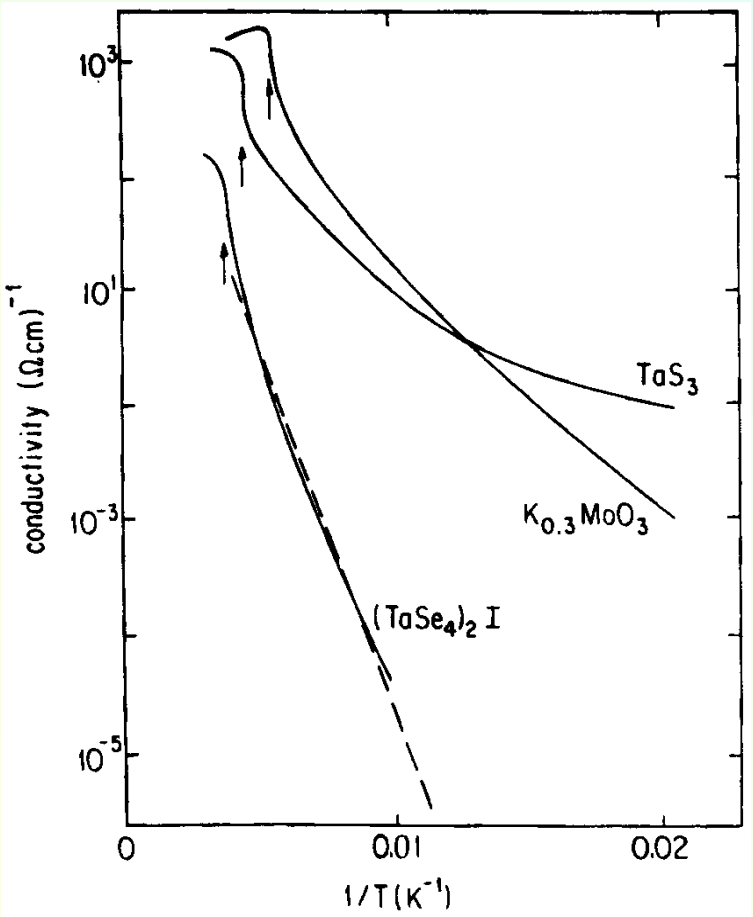
$$\Delta = 2\epsilon_F e^{-1/\lambda}$$

and to CDW energy gain

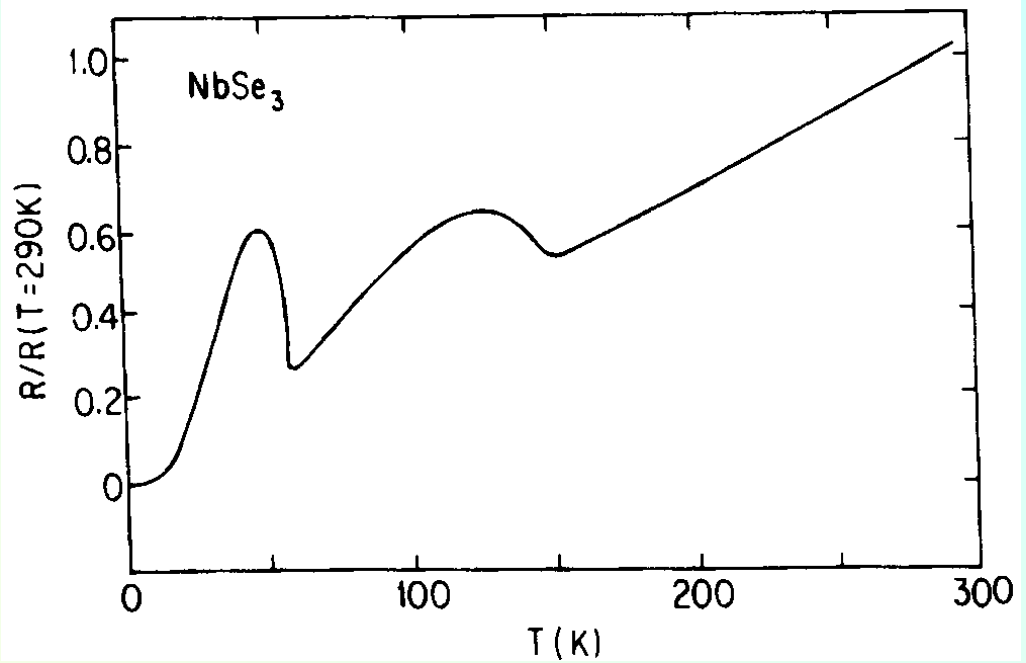
$$E_{\text{con}} = E_{\text{normal}} - E_{\text{CDW}} = \frac{n(\epsilon_F)}{2}\Delta^2.$$

Typical resistivity behavior during the CDW/SDW phase transition

1. Total FS is gapped => exponential (insulating) temperature dependence

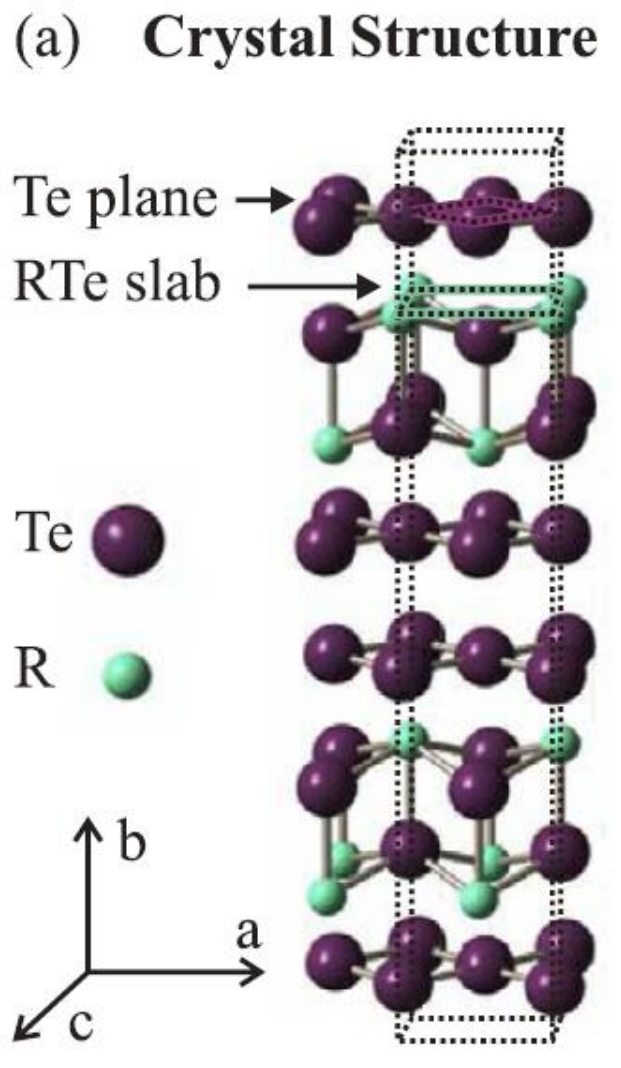


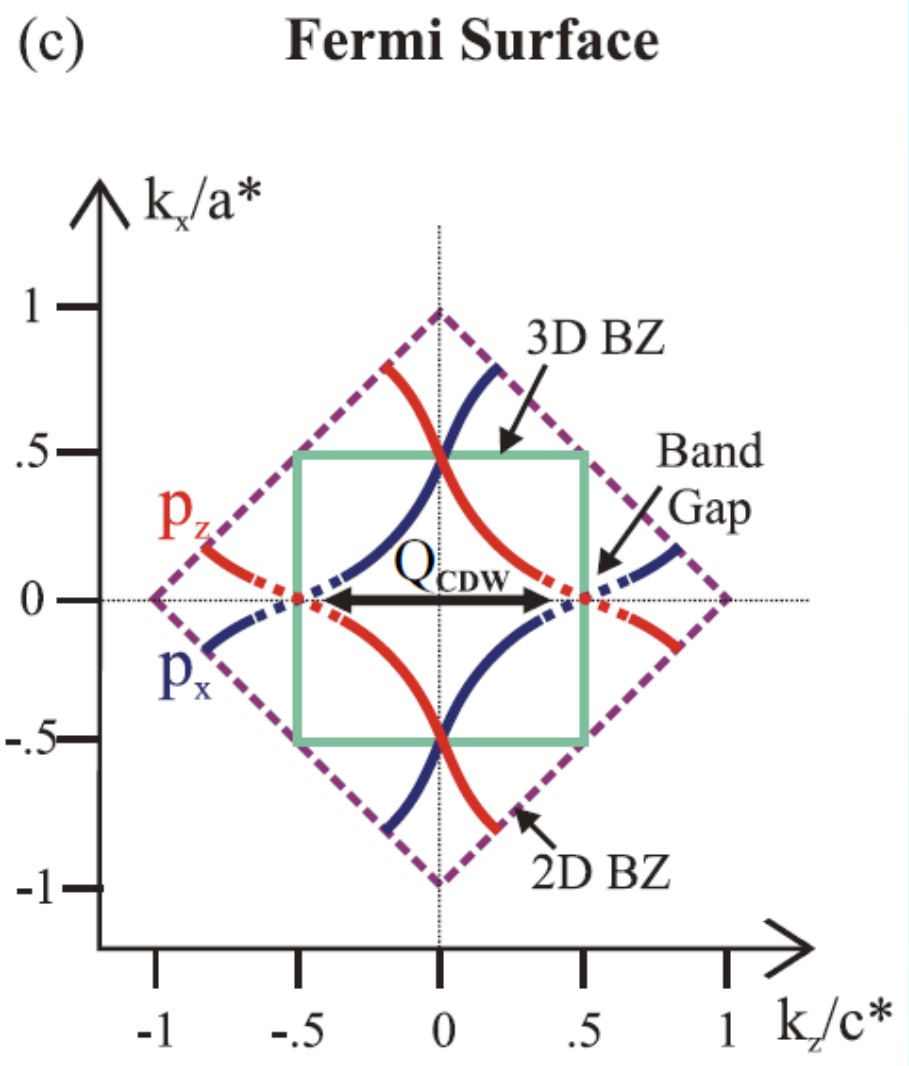
2. FS is partially gapped => temperature dependence of R is metallic with jump at T_p and different slope in a CDW state.



G. Gruener, *Density waves in Solids*, 1994

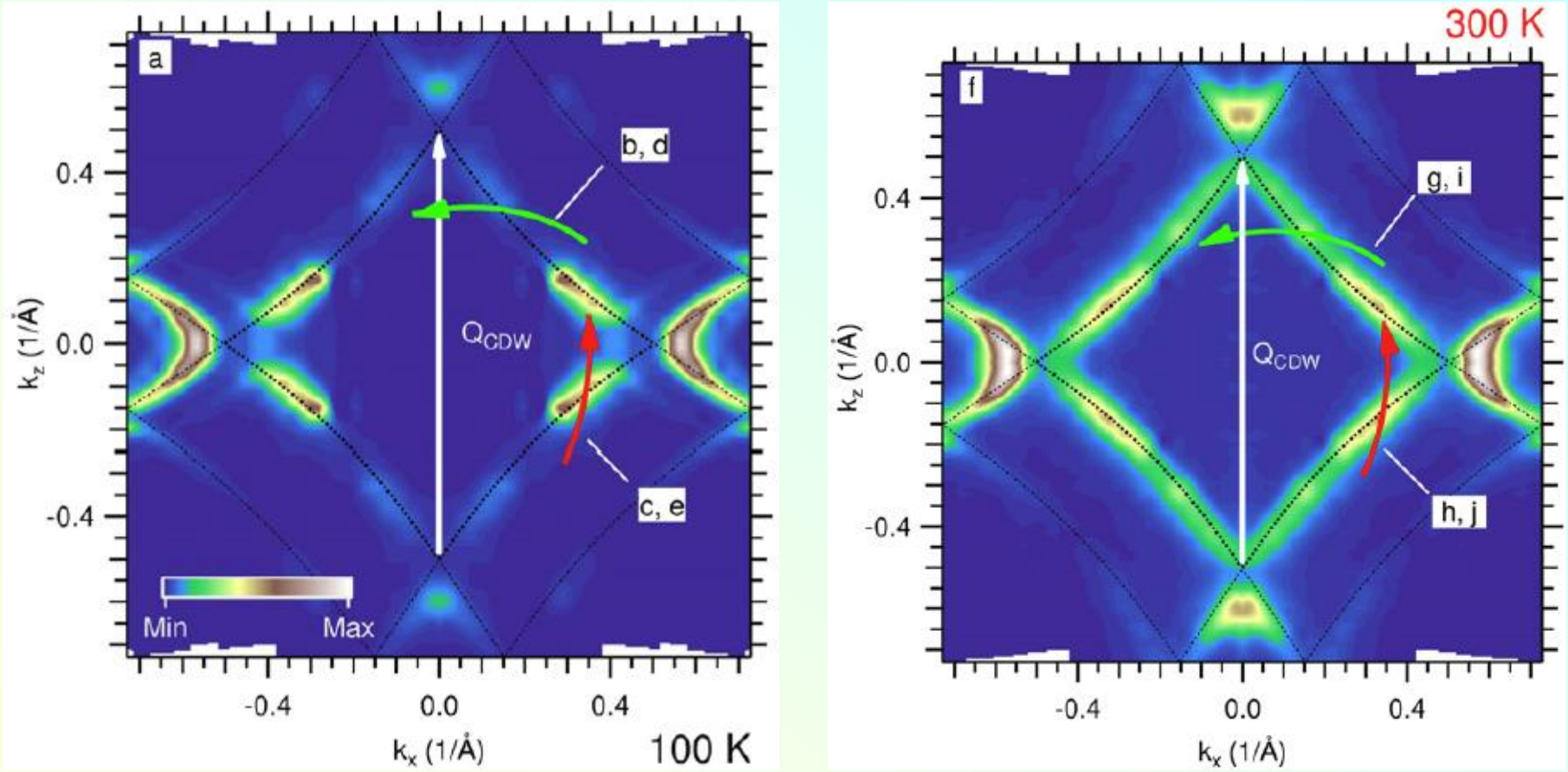
Crystal structure of rare-earth tritellurides RTe_3





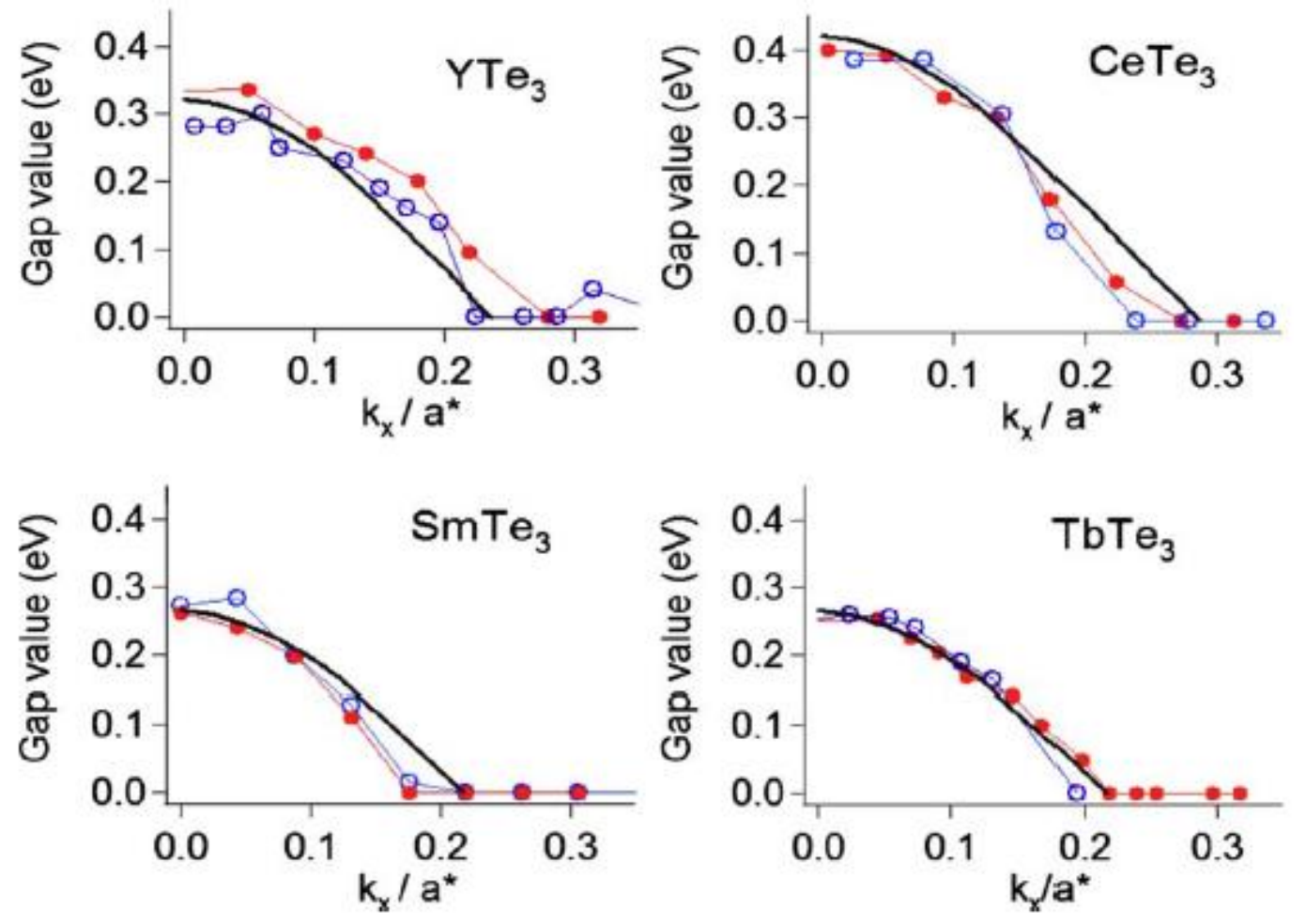
F. Schmitt et al., New Journal of Physics 13, 063022 (2011)

ARPES data on momentum dependence of CDW energy gap in $TbTe_3$



F. Schmitt et al., New Journal of Physics 13, 063022 (2011)

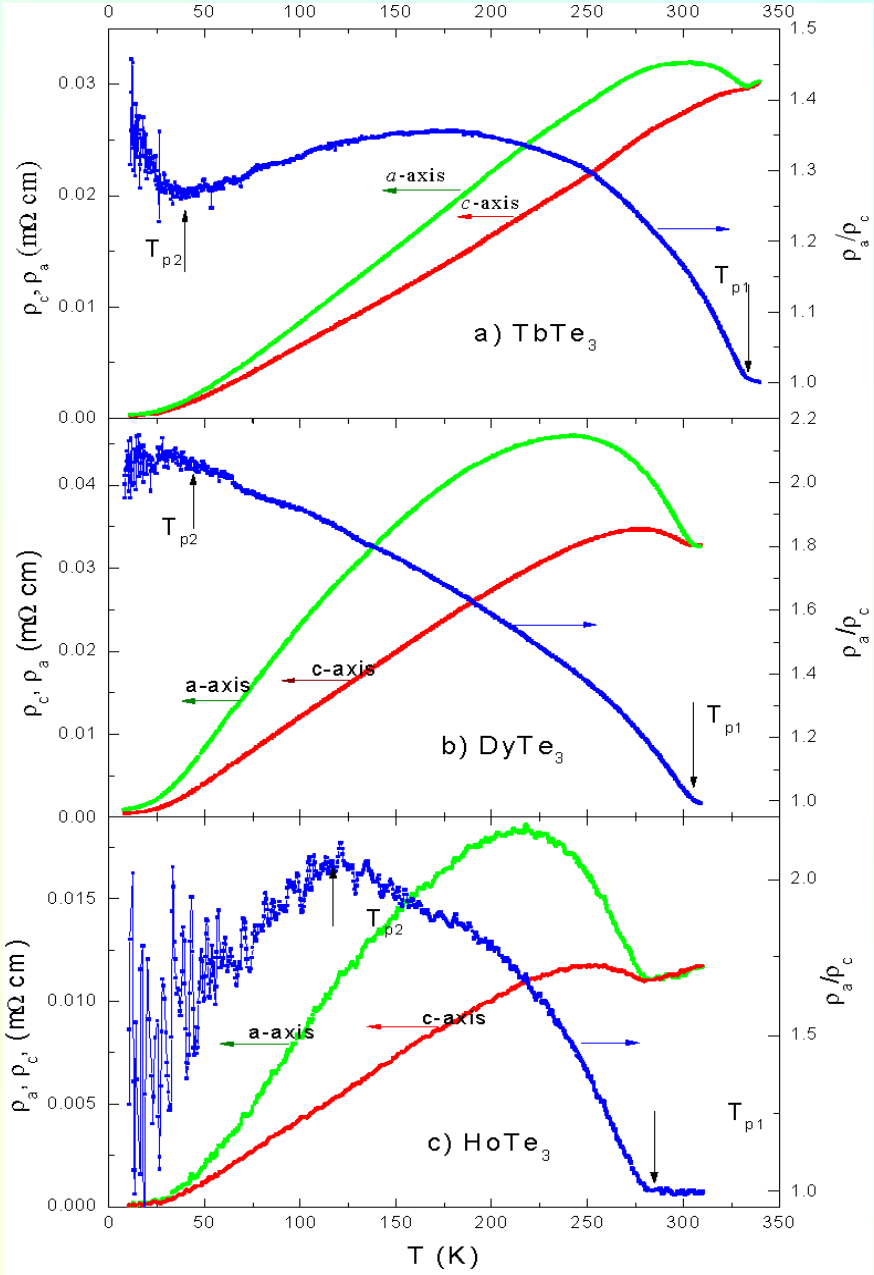
Momentum dependence of CDW energy gap (determined from ARPES)



V. Brouet et al., Phys. Rev. B 77, 235104 (2008)

Experimental data:

Anisotropy of in-plane conductivity in RTe_3



Experimental observations:

Above CDW transition temperature T_{p1} (=336K for $TbTe_3$) the in-plane conductivity is isotropic: $\rho_c = \rho_a$

Below T_{p1} the in-plane conductivity is anisotropic: $\rho_a > \rho_c$

Resistivity increases stronger in the direction $a \perp Q_N \parallel c$, which expels domain-wall CDW scenario

Notations:

a **and** ***c*** **along conducting layers**