Phonons in metals - Kohn anomaly

ion background oscillation relative to (fixed) electron

➡ analog to plasma oscillation

$$\Omega_p^2 = \frac{4\pi n_i (Z_i e)^2}{M_i} > 0$$

- M_i ion mass
- n_i ion density
- $Z_i e$ ion charge

screening of Coulomb by (fast) electrons

$$\omega_{\vec{k}}^2 = \frac{\Omega_p^2}{\varepsilon(\vec{k},0)} = \frac{k^2 \Omega_p^2}{k^2 + k_{TF}^2} \approx (c_s k)^2$$

sound velocity

$$c_s^2 \approx \frac{\Omega_p^2}{k_{TF}^2} = \frac{Z m \omega_p^2}{M_i k_{TF}^2} = \frac{1}{3} Z \frac{m}{M_i} v_F^2$$

$$\frac{\Theta_D}{T_F} \sim \frac{c_s}{V_F} = \sqrt{\frac{1}{3} Z \frac{m}{M_i}} \ll 1$$

Kohn anomaly

$$\omega_{\vec{k}}^2 = \frac{\Omega_p^2}{\varepsilon(\vec{k},0)}$$

singular at $2k_F$

$$\left.\frac{\partial \omega_{\vec{k}}}{\partial \vec{k}}\right|_{k \to 2k_F} \to \infty$$

Peierls instability in 1D metal

electrons & elastic ionic background (Jellium model)

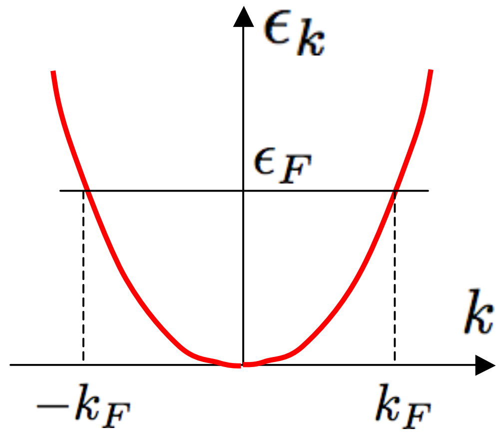
$$\mathcal{H} = \mathcal{H}_{\text{isol}} + \mathcal{H}_{\text{int}}$$

$$\mathcal{H}_{\text{isol}} = \sum_{k,s} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\,s} c_{k\,s} + \frac{\lambda}{2} \int dx \left(\frac{du}{dx}(x) \right)^2$$

electron kinetic energy

elastic energy

$u(x)$ deformation along x



$$k_F = \frac{\pi}{2} n_0$$

electron-phonon coupling

$$\mathcal{H}_{\text{int}} = -n_0 \sum_s \int dx\, dx' \, \underbrace{V(x-x')}_{\text{screened Coulomb}} \underbrace{\frac{d}{dx} u(x)}_{-\delta n(x)/n_0} \underbrace{\hat{\Psi}^\dagger_s(x') \hat{\Psi}_s(x')}_{\hat{\rho}(x')}$$

screened Coulomb (short range) ion-electron

$-\delta n(x)/n_0$ ion density fluctuation

$\hat{\rho}(x')$ electron density

Peierls instability in 1D metal

electrons & elastic ionic background (Jellium model)

$$\mathcal{H} = \mathcal{H}_{\rm isol} + \mathcal{H}_{\rm int}$$

Fourier: $u(x) = \frac{1}{\sqrt{L}} \sum_q u_q e^{-iqx}$ $\quad V(x) = \frac{1}{\sqrt{L}} \sum_q \tilde{V}_q e^{iqx}$

$$\mathcal{H}_{\rm isol} = \sum_{k,s} \frac{\hbar^2 k^2}{2m} c^\dagger_{k\,s} c_{k\,s} + \frac{\Omega \rho_0}{2} \sum_q \omega_q^2 u_q u_{-q}$$

phonon dispersion

$$\omega_q = q\sqrt{\lambda/\rho_0}$$

$$\mathcal{H}_{\rm int} = i \sum_{k,q,s} q \left[\tilde{V}_{-q} u_q \,\widehat{c}^{\,\dagger}_{k+q,s}\, \widehat{c}_{k,s} - \tilde{V}_q u_{-q}\, \widehat{c}^{\,\dagger}_{k,s}\, \widehat{c}_{k+q,s} \right]$$

electron-phonon coupling as perturbation

Peierls instability in 1D metal

$$\mathcal{H}_{\text{int}} = i \sum_{k,q,s} q[\tilde{V}_{-q} u_q \hat{c}^{\dagger}_{k+q,s} \hat{c}_{k,s} - \tilde{V}_q u_{-q} \hat{c}^{\dagger}_{k,s} \hat{c}_{k+q,s}]$$

screening $\tilde{V}_q$ essentially no q-dependence

2nd-order Rayleigh-Schrödinger perturbation

$$\Delta E^{(2)} = \sum_{k,q,s} q^2 |\tilde{V}_q|^2 u_q u_{-q} \sum_n \frac{|\langle\Psi_0|\hat{c}^{\dagger}_{k,s}\hat{c}_{k+q,s}|n\rangle|^2 + |\langle\Psi_0|\hat{c}^{\dagger}_{k+q,s}\hat{c}_{k,s}|n\rangle|^2}{E_0 - E_n}$$

$$= \sum_q |\tilde{V}_q|^2 q^2 u_q u_{-q} \sum_k \frac{n_{k+q} - n_k}{\epsilon_{k+q} - \epsilon_k}$$

Lindhard function

$$= \Omega \sum_q |\tilde{V}_q|^2 q^2 \chi_0(q,0) u_q u_{-q}$$

correction to phonon dispersion

$$\frac{\Omega\rho_0}{2} \sum_q \omega_q^2 u_q u_{-q}$$

$$\omega_q^{(ren)2} \approx \omega_q^2 + \frac{|\tilde{V}_q|^2 q^2}{\rho_0} \chi_0(q,0)$$

$$= \omega_q^2 - \frac{|\tilde{V}_q|^2 q}{2\pi\rho_0} \ln \left| \frac{q + 2k_F}{q - 2k_F} \right|$$

Peierls instability in 1D metal

$$\omega_q^{(ren)2} \approx \omega_q^2 + \frac{|\tilde{V}_q|^2 q^2}{\rho_0}\chi_0(q,0)$$

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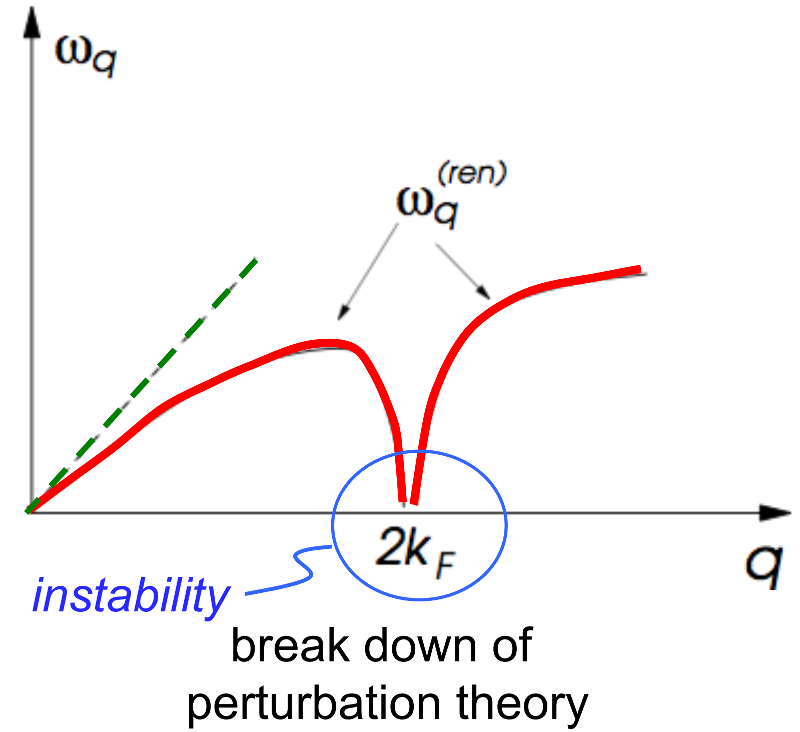


Bose-Einstein condensation of coherent phonons

$$u(x) = u_0 \cos(2k_F x)$$

density modulation of ion background

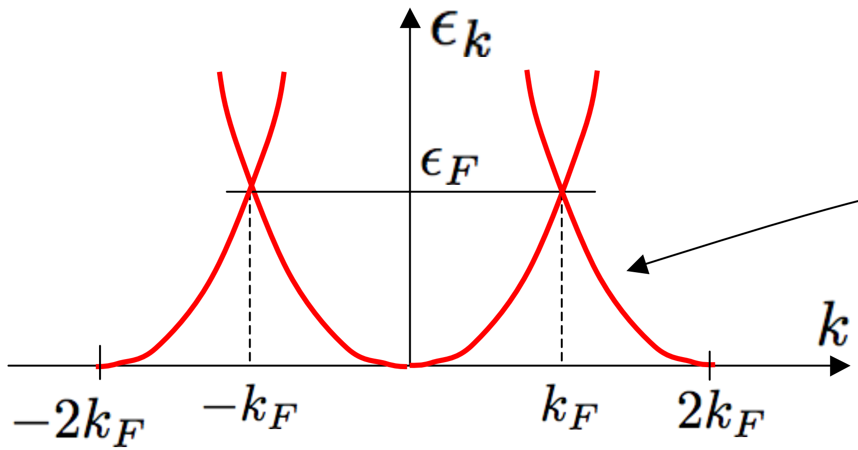
periodically modulated (weak) ion potential

case for
nearly free electron approximation

Peierls instability in 1D metal

nearly free electron approximation

$$u(x) = u_0 \cos(2k_F x)$$

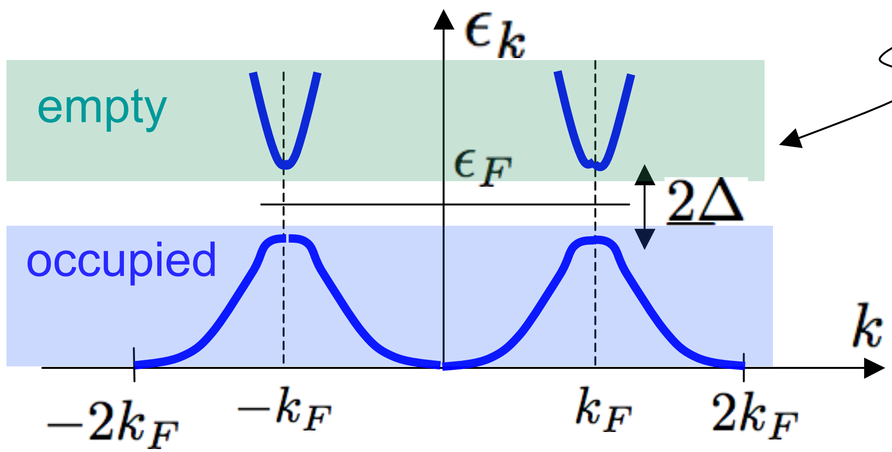


secular equation

$$\det \begin{pmatrix} \frac{\hbar^2 k^2}{2m} - E & \Delta \\ \Delta^* & \frac{\hbar^2 (k-2k_F)^2}{2m} - E \end{pmatrix} = 0$$

$$\Delta = -2ik_F u_0 n_0 \tilde{V}_{2k_F}$$

$$E_k^{\pm} = \frac{\hbar^2}{4m}\left[(k-Q)^2 + k^2 \pm \sqrt{\{(k-Q)^2 - k^2\}^2 + 16m^2|\Delta|^2/\hbar^4}\right]$$



total ground state energy

$$E_{\text{tot}}(u_0) = 2 \sum_{0 \le k < Q} E_k^- + \frac{4k_F^2 \lambda L}{4} u_0^2$$

electronic *gain* — elastic *expense*

Peierls instability in 1D metal

$$E_{\text{tot}}(u_0) = 2\sum_{0\leq k<Q} E_k^- + \frac{4k_F^2\lambda L}{4}u_0^2$$

minimize w.r.t. u_0

$$0 = \frac{1}{L}\frac{dE_{\text{tot}}}{du_0} = -u_0\frac{16k_F mn^2\tilde{V}_{2k_F}^2}{\hbar^2\pi}\text{arsinh}\left(\frac{\hbar^2 k_F}{2mn\tilde{V}_{2k_F}u_0}\right) + \frac{\lambda}{2}(2k_F)^2 u_0$$

electronic *gain*

elastic *expense*

$$u_0 \approx= \frac{\hbar^2 k_F}{mn\tilde{V}_{2k_F}}\exp\left[-\frac{\hbar^2 kF\pi\lambda}{8mn^2\tilde{V}_{2k_F}^2}\right] = \frac{2}{k_F}\frac{\epsilon_F}{n\tilde{V}_{2k_F}}e^{-1/N(0)g}$$

density of states at Fermi energy

$$N(0) = \frac{2m}{\pi\hbar^2 k_F}$$

electron-phonon coupling constant

$$g = \frac{4n_0^2\tilde{V}_{2k_F}^2}{\lambda}$$

$$\Delta = 4\epsilon_F\exp\left(-\frac{1}{N(0)g}\right)$$

energy gap of insulating phase

Peierls instability

⬇

instability of Fermi surface

Peierls instability in 1D metal

charge modulation of electrons and ions

electron wave function (NFEA)

$$\psi'_k(x) = \frac{1}{\sqrt{\Omega}} \frac{\Delta e^{ikx} + (E_k - \epsilon_k) e^{i(k-2k_F)x}}{\sqrt{(E_k - \epsilon_k)^2 + |\Delta|^2}}$$

$$\delta\rho_e(x) = \frac{e n_0 |\Delta|}{16 \epsilon_F} \ln \left| \frac{2\epsilon_F}{|\Delta|} \right| \sin(2k_F x)$$

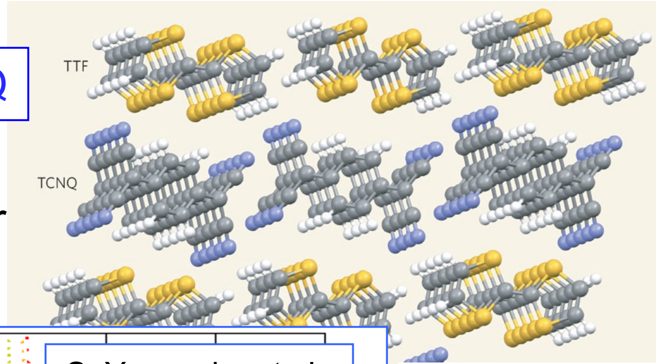
$2k_F$

Charge Density Wave

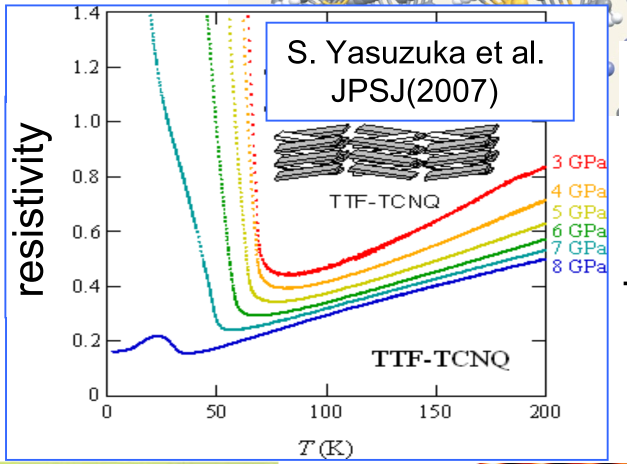
experimental systems

TTF-TCNQ

organic conductor

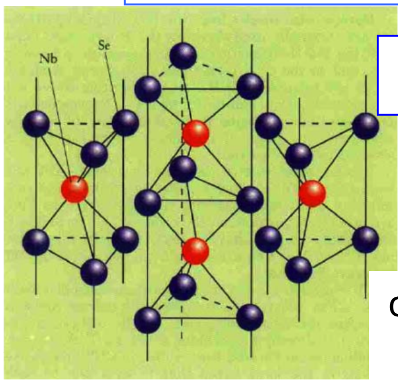


H. Alves et al.
Nature Materials



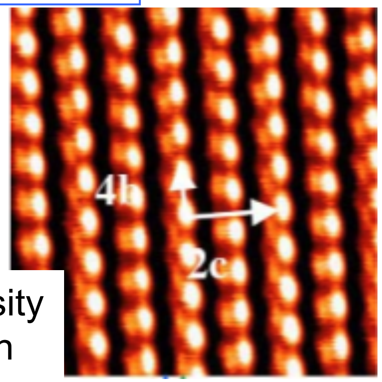
S. Yasuzuka et al.
JPSJ(2007)

metal-insulator transition



$NbSe_3$

STM →



charge density modulation