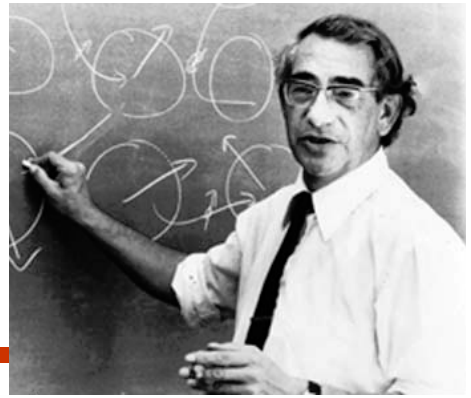
The Hubbard model



John Hubbard

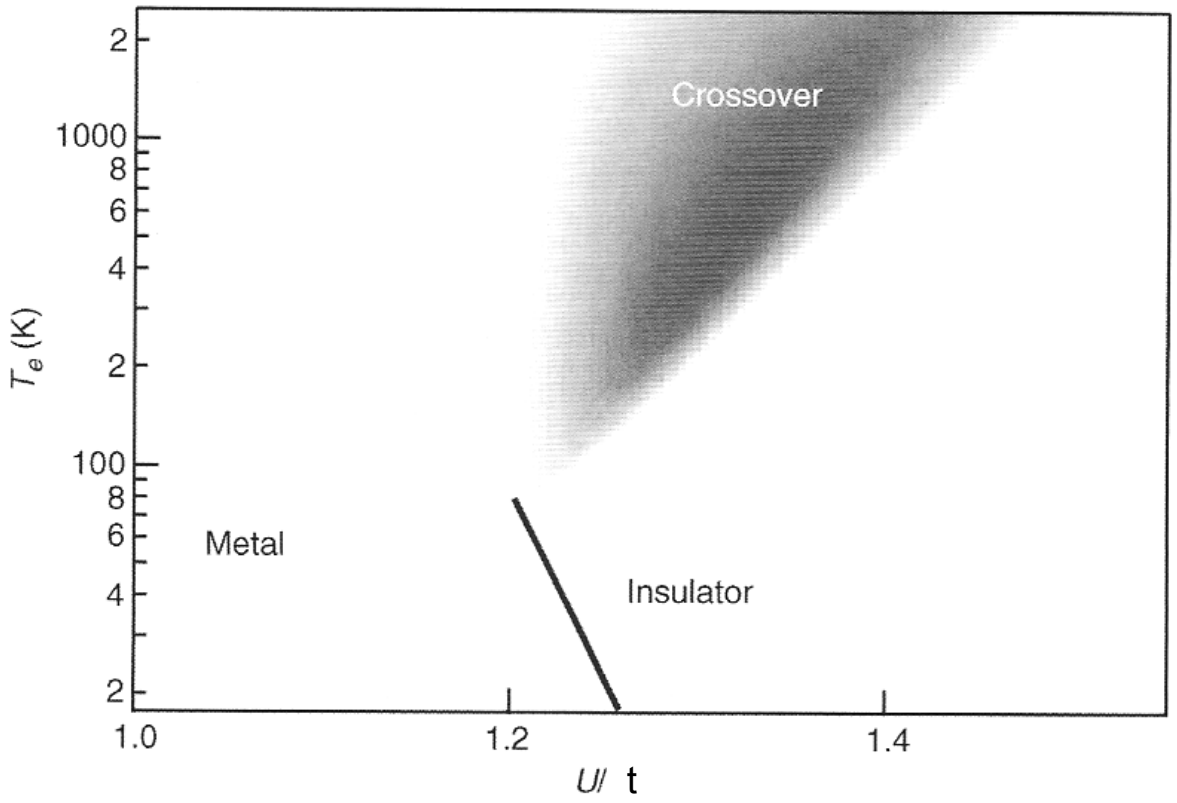
The Hubbard model is an approximate model used, especially in solid state physics, to describe the transition between conducting and insulating systems. -Wikipedia

$$H = -t \sum_{\langle i,j \rangle,\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

It is widely believed to be a good model for correlated electron systems including high temperature superconductors. The Hubbard model is solvable for a few electrons and a few sites but is extremely difficult to solve for many electrons on many sites.

http://nerdwisdom.com/tutorials/the-hubbard-model/

The Hubbard model



Phase diagram of the half-filled one-band Hubbard model.

Dynamics at solid state surfaces and interfaces, Editors: U. Bovensiepen, H. Petek, and M. Wolf

Metal insulator transition (high resistivity)

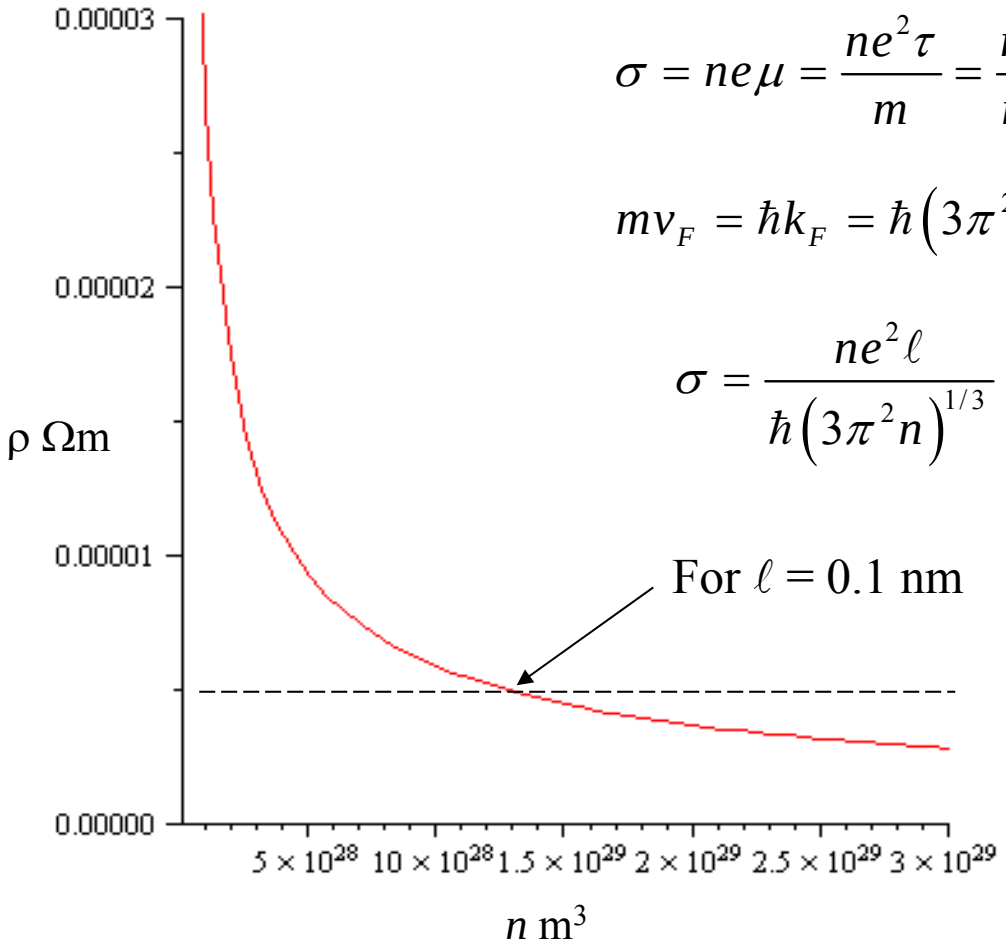
$$R_Q = \frac{h}{e^2} = \frac{\rho \ell}{wt} \approx 25\ \text{k}\Omega$$

For $w = \ell$, $t \approx 0.2$ nm, $\rho = 500\ \mu\Omega$ cm

Materials with resistivities > 1 mΩ cm tend to be insulators (ρ increases as *T* decreases)

High-temperature oxide superconductors / antiferromagnets
Organic semiconductors often have this character.

Metal insulator transition



$$\sigma = ne\mu = \frac{ne^2\tau}{m} = \frac{ne^2\ell}{mv_F}$$

$$mv_F = \hbar k_F = \hbar\left(3\pi^2 n\right)^{1/3}$$

$$\sigma = \frac{ne^2\ell}{\hbar\left(3\pi^2 n\right)^{1/3}}$$

Something is wrong if the mean free path is smaller than an atom

Peierls Transition

A quasi-one dimensional metal will undergo a transition to an insulator at low temperature

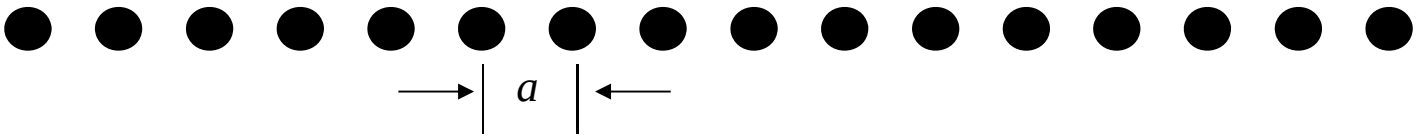
Predicted in the 1930's

Accidentally observed in the 1970's in TTF-TCNQ

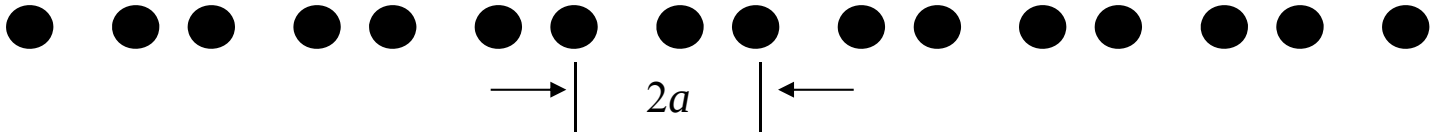
Rudolf Peierls
Quantum Theory of Solids
Surprises in Theoretical Physics
More Surprises in Theoretical Physics

Peierls Transition

Consider a 1-d lattice of atoms with spacing a.

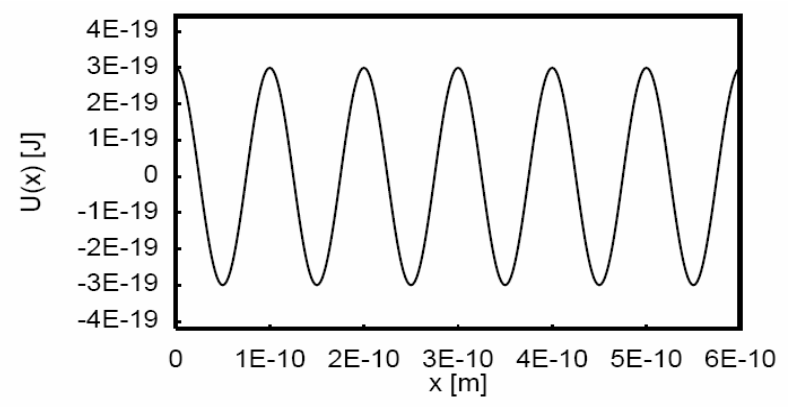


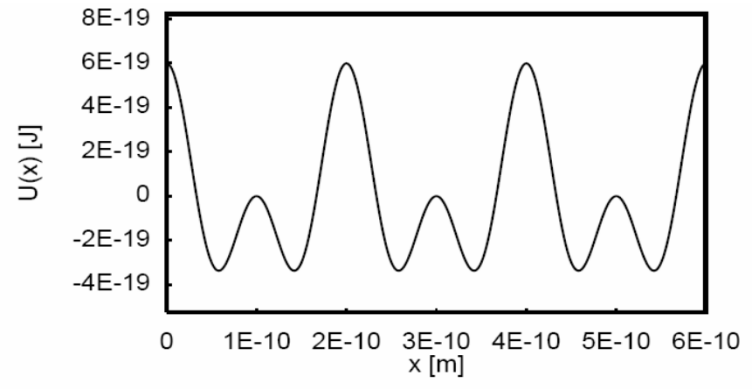
A periodic distortion of a 1-d lattice increases the periodicity to $2a$

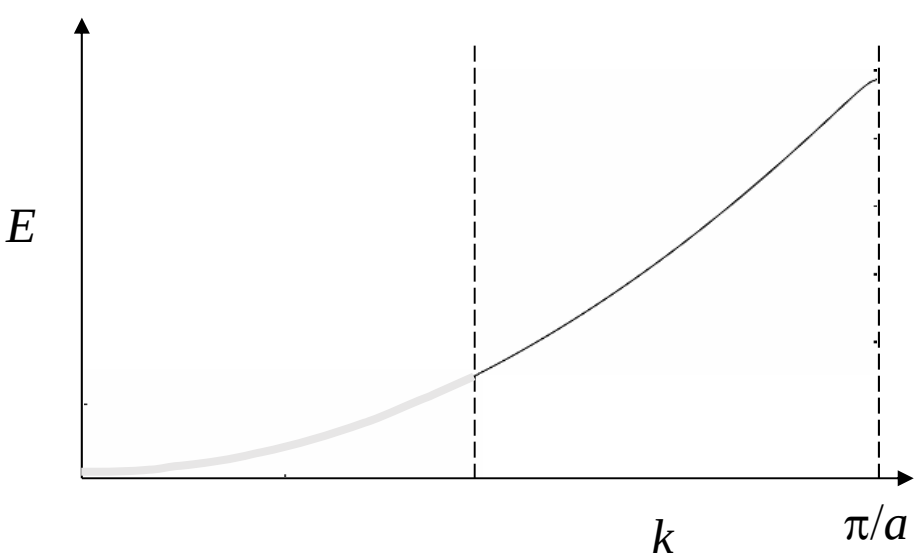


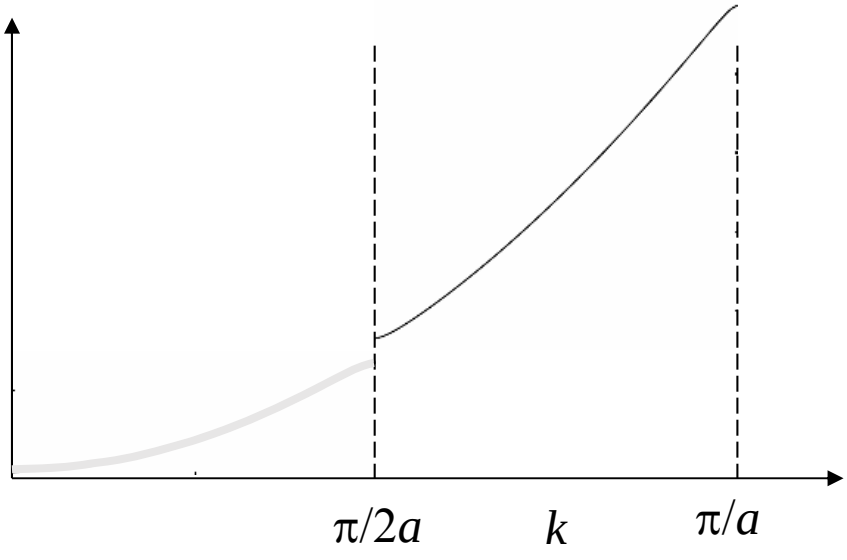
There are $2N$ states in each band. (N is the number of unit cells in the crystal)

Rudolf Peierls, *More Surprises in Theoretical Physics*, Princeton University Press.
G. Grüner, *Density Waves in Solids*, Addison-Wesley Publishing Company, 1994.





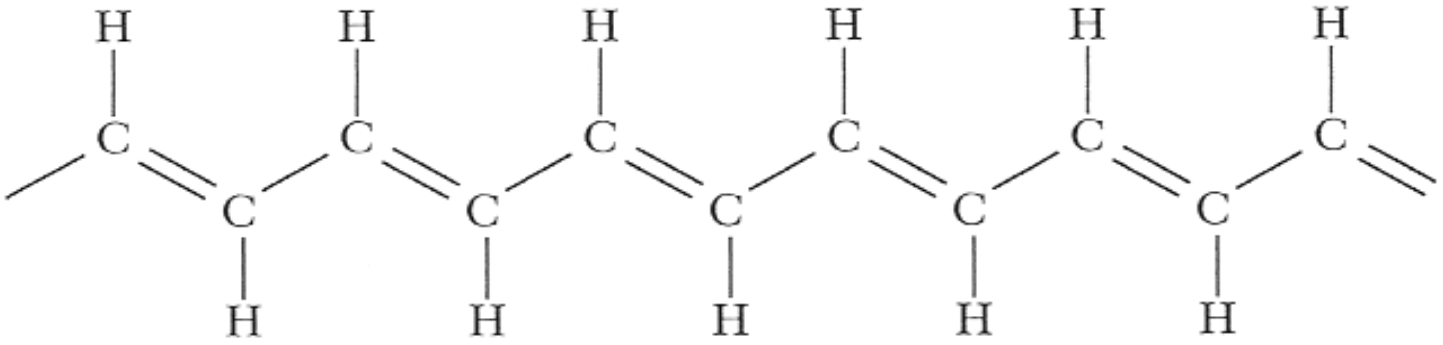




For a distortion of the lattice $\Delta\cos(2k_F x)$, the elastic energy increases like Δ^2 while the electronic energy decreases like Δ.

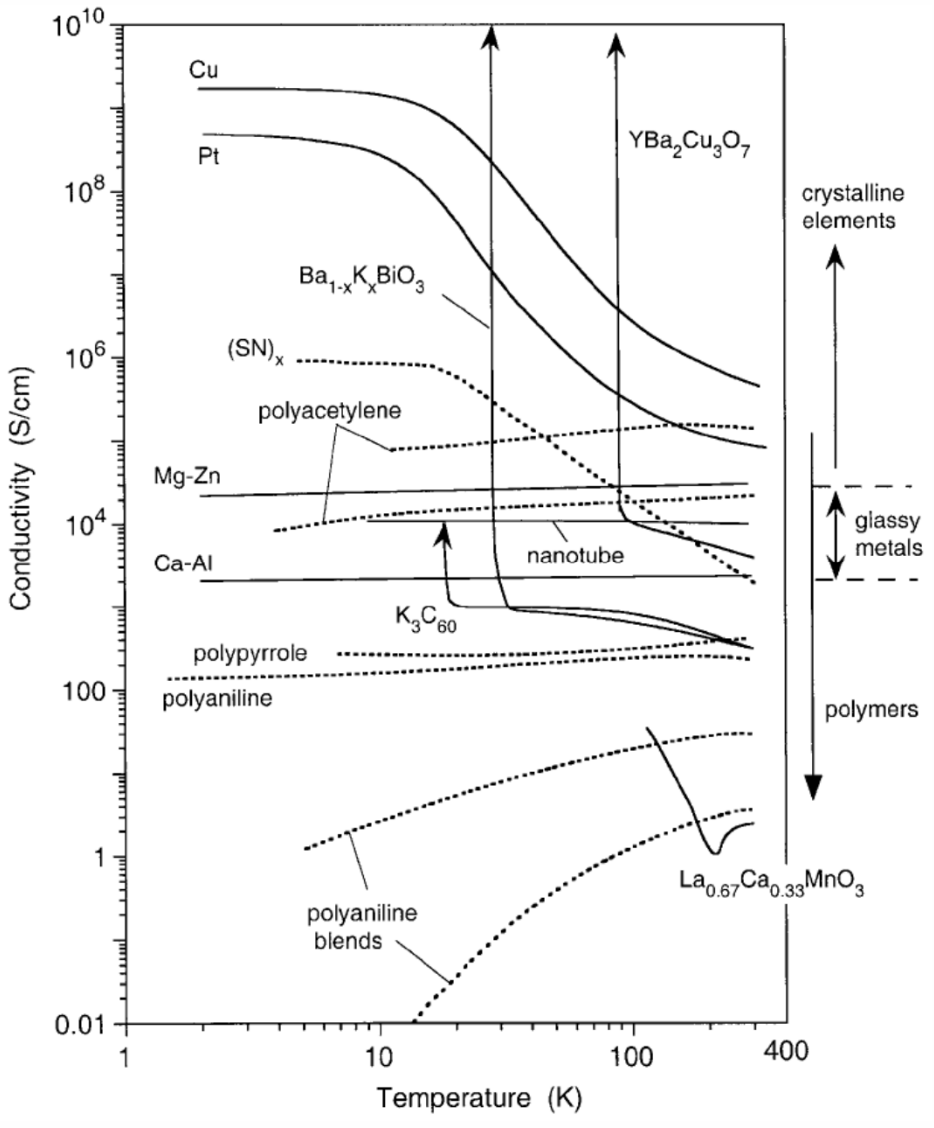
http://lamp.tu-graz.ac.at/~hadley/ss1/bloch/bloch.php

Peierls transition in polyacetylene



e **12** Structure of polyacetylene. Due to the Peierls distortion, the lattice is dimerized, atoms joined by double bonds in the diagram closer together than those linked by s The Peierls distortion opens a semiconducting gap of approximately 1.5 eV.

Temperature dependence of the conductivity

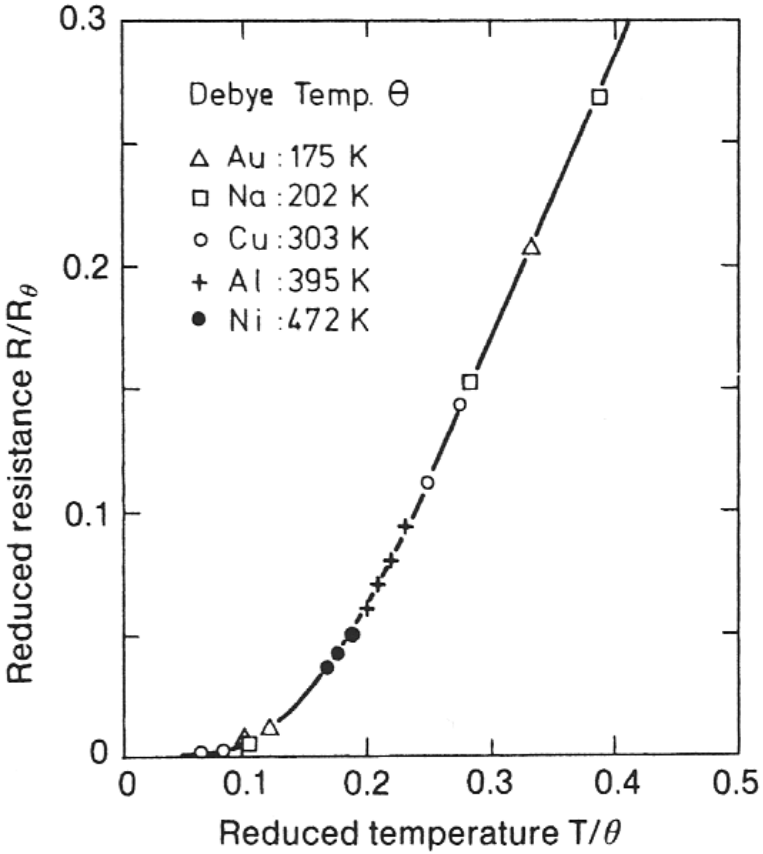


σ vs *T* tells us about the electron - electron and electron phonon interactions

A B Kaiser 2001 *Rep. Prog. Phys.* **64** 1

Temperature dependence of conductivity

Grueneisen model $\rho_{phonons} = A\left(\frac{T}{\Theta_D}\right)^5 \int_0^{\Theta_D/T} \frac{x^5}{\left(e^x - 1\right)\left(1 - e^{-x}\right)} dx$



for $T > \theta_D$, the number of phonons is proportional to T

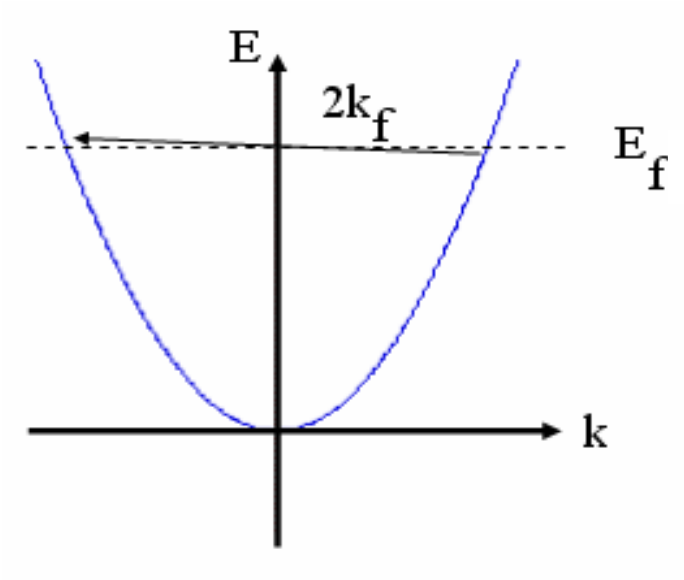
$$\rho_{phonons} \propto T$$

Low T: Only phonons with small q -> small angle scattering

$$\rho_{phonons} \propto T^5$$

$$k + q = k' + q' + G$$

Suppression of backscattering in 1-D

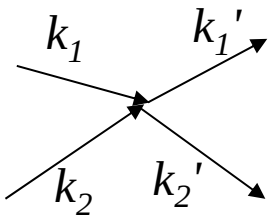


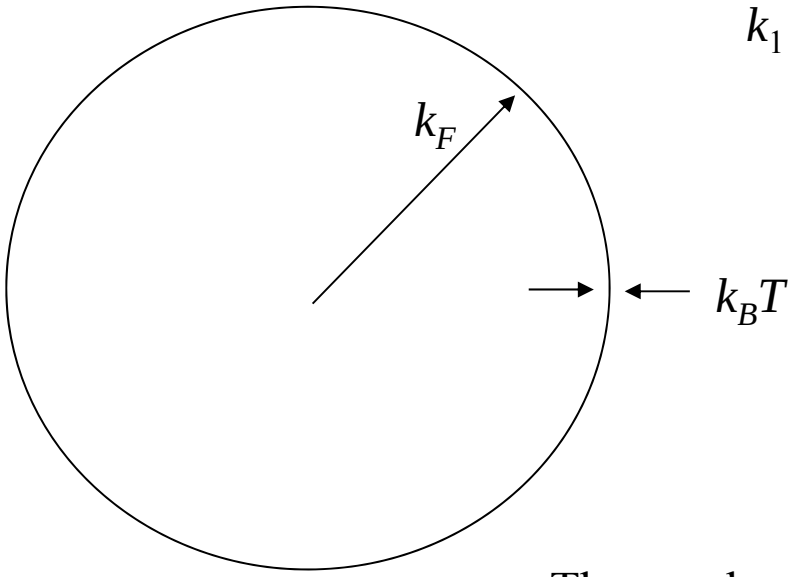
There are no phonons with momentum $2k_f$ at low T

H. Sakaki, Jpn. J. Appl. Phys. Vol. 19 (1980) L735-L738

$\rho \sim T^2$ for electron-electron scattering

$$\Gamma = \frac{2\pi}{\hbar}\left|\left\langle \psi_{k_1}\psi_{k_2}\left|H\right|\psi_{k_1'}\psi_{k_2'}\right\rangle\right|^2 \delta\left(E_{k_1}+E_{k_2}-E_{k_1'}-E_{k_2'}\right)$$



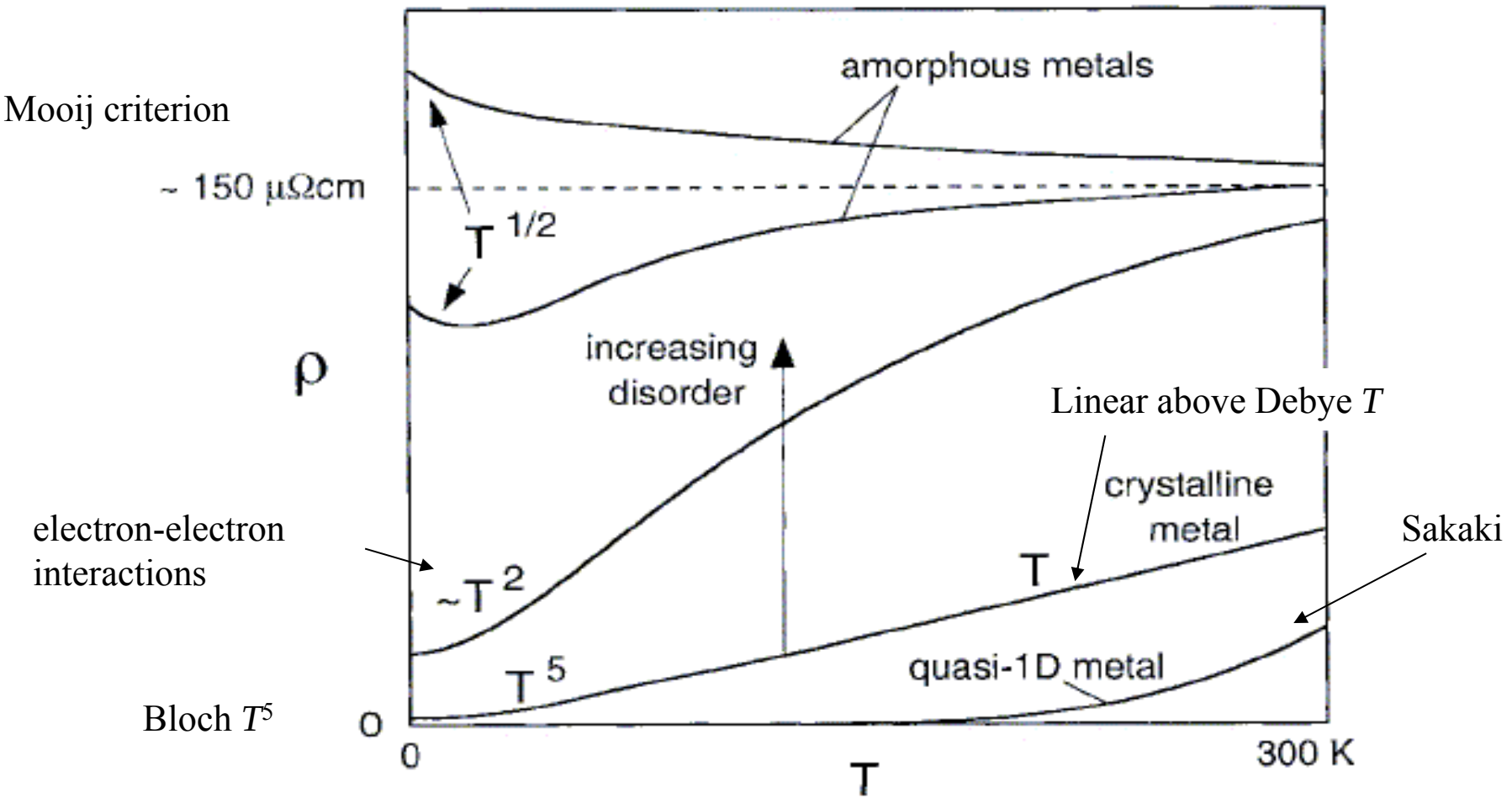


$$k_1 + k_2 = k_1' + k_2' + G$$

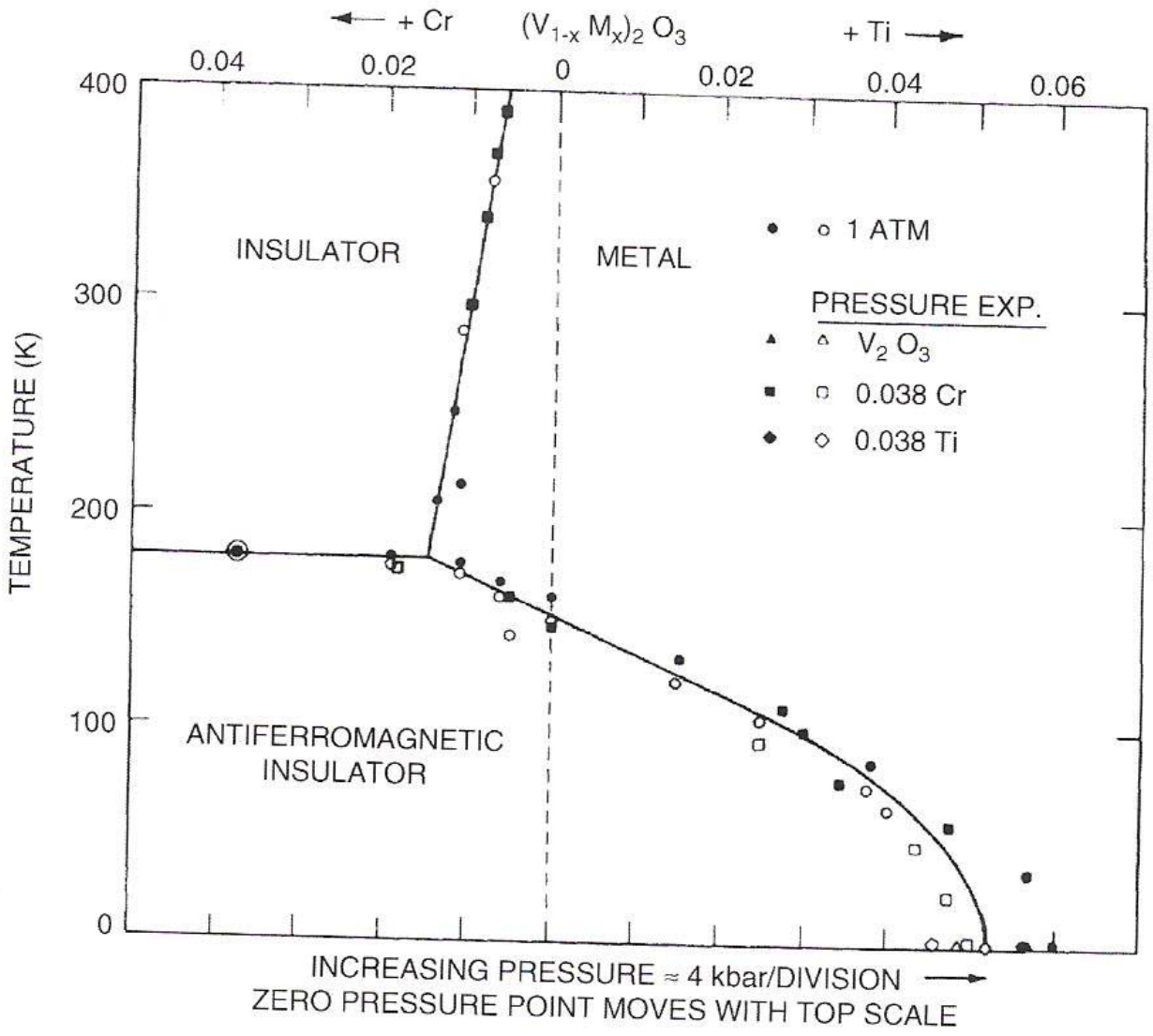
The number of available states depends on the temperature

$\rho \sim T^2$

ρ vs. T

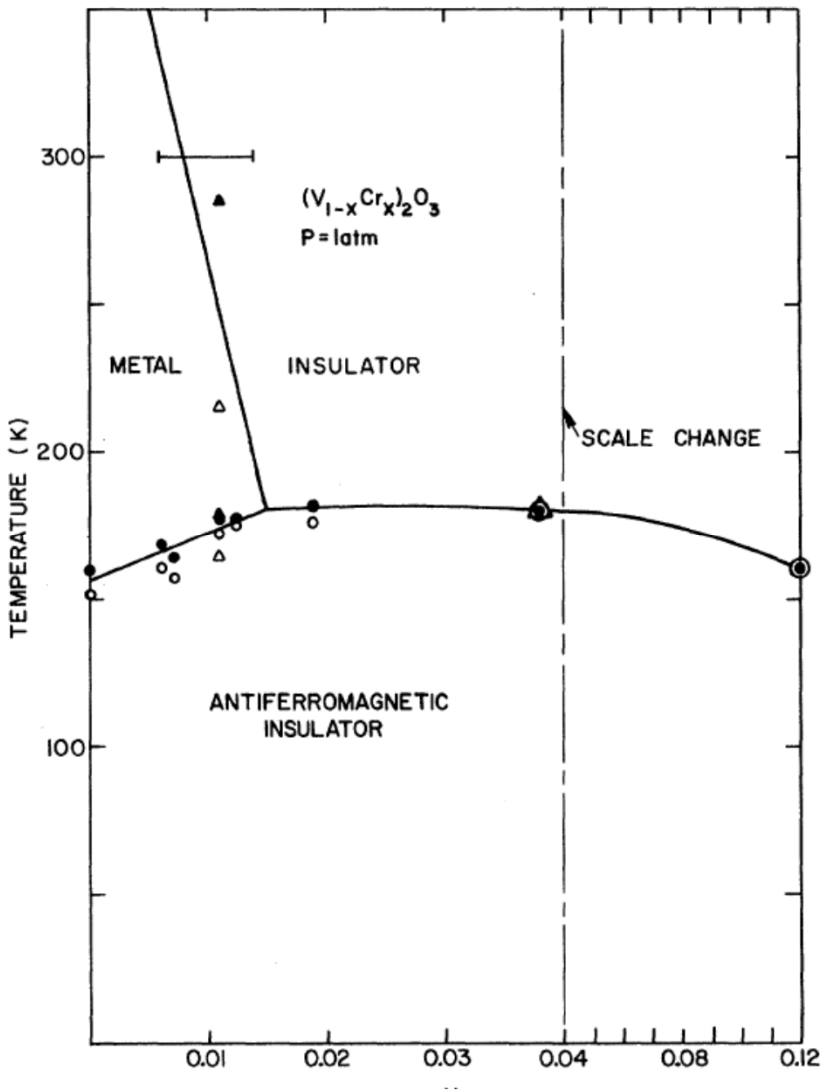


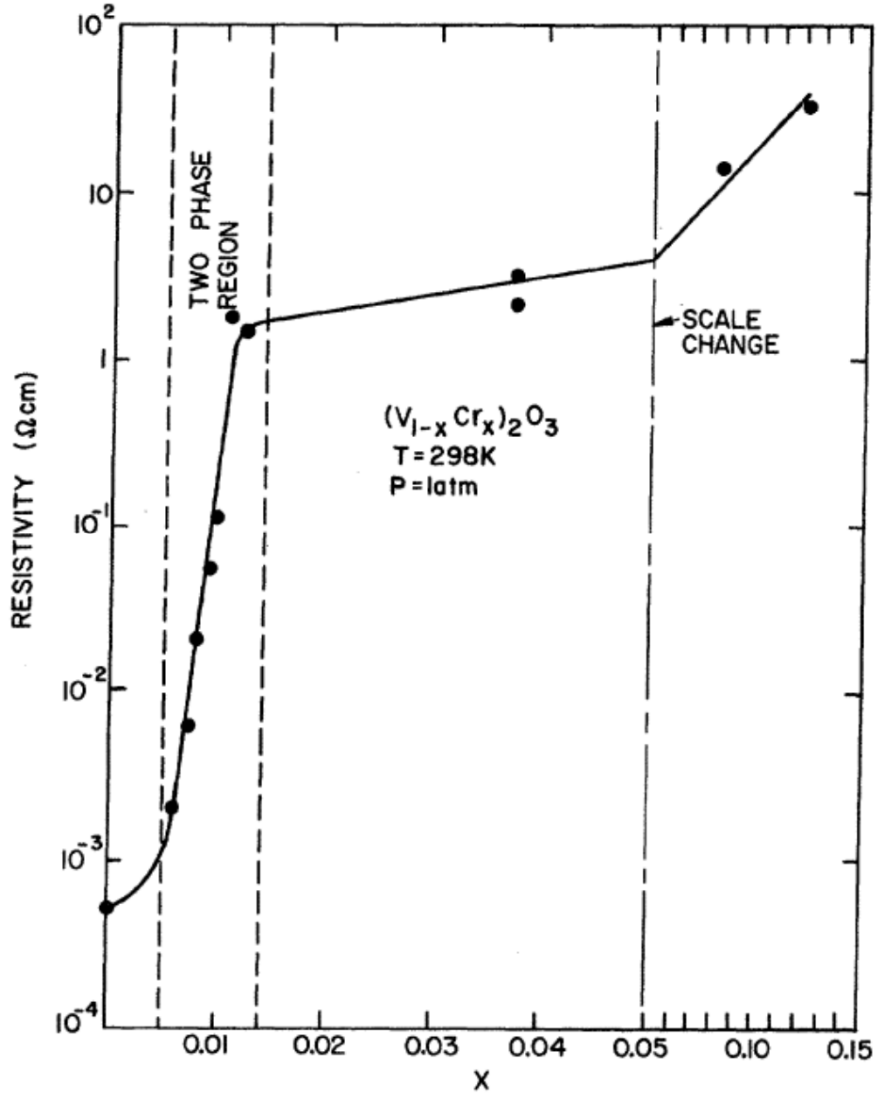
A B Kaiser 2001 *Rep. Prog. Phys.* **64** 1



Dynamics at solid state surfaces and interfaces, Editors: U. Bovensiepen, H. Petek, and M. Wolf

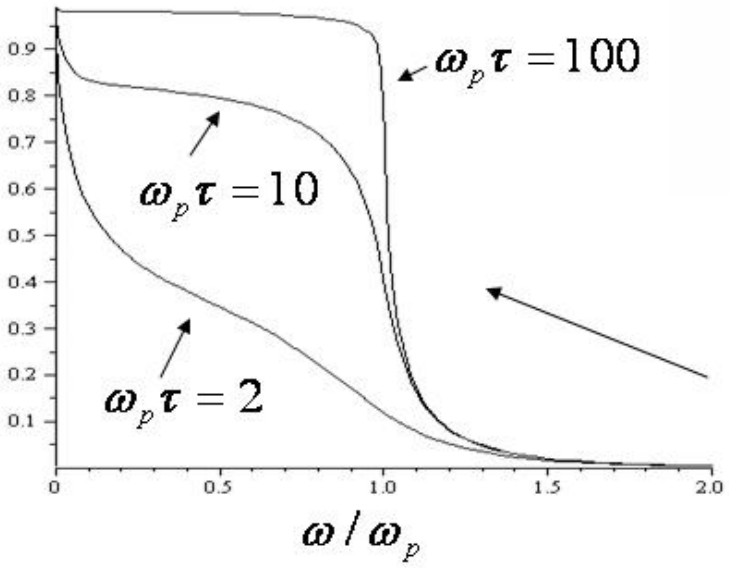
$(V_{1-x}Cr_x)_2O_3$

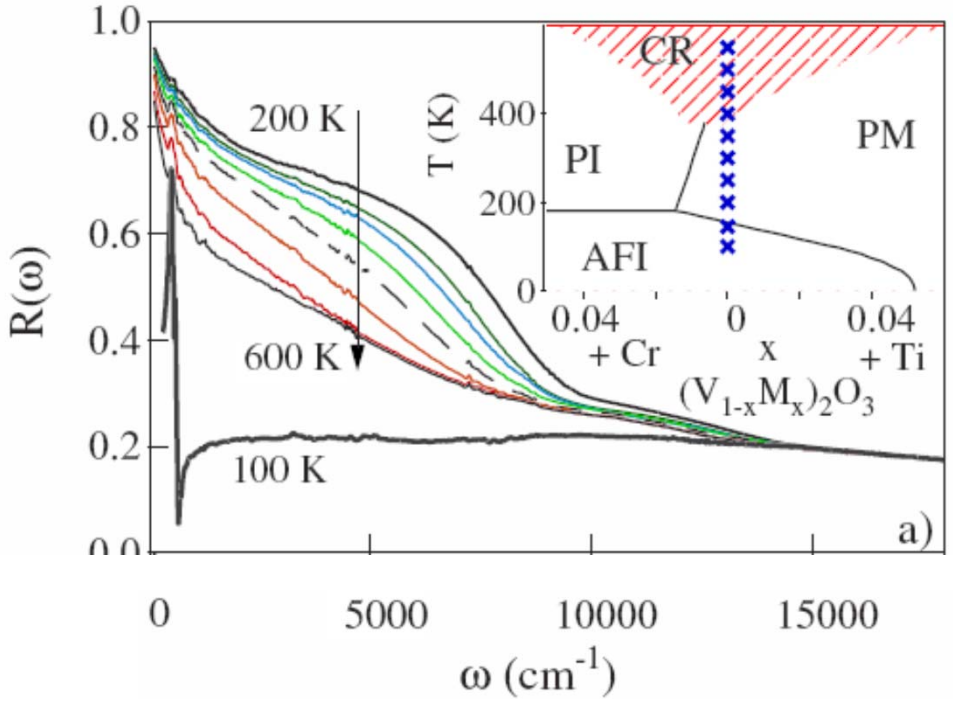




D. B. McWhan and J. P. Remeika, PRB 3 p. 3734 (1970)

Vanadium sesquioxide V_2O_3





$$R = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}$$

PM paramagnetic metal
PI paramagnetic insulator
AFI Antiferromagnetic insulator
CR crossover regime (poor conductor)

L. Baldassarre, et al., Phys. Rev. B 77, 113107 (2008)

Landau theory of a Fermi liquid

The free electron model = 'Fermi gas' is very successful at describing metals but it is not clear why this is so since electron-electron interactions are completely ignored.

Landau first considered the "normal modes" of an interacting electron system. The low lying excitations he called quasiparticles.

The quasiparticles have as many degrees of freedom as the electrons. They can be labeled by k.

Quasiparticles can be have the same spin, charge, and k vectors as the electrons.

It is not easy to calculate $E(k)$.

Concepts like the density of states refer to quasiparticles.

Landau theory of a Fermi liquid

If there are no electron-electron interactions, electrons have an infinite lifetime and the probability that a state is occupied is given by the Fermi function.

If there are interactions, quasiparticles have a finite lifetime. The lifetime can be calculated by Fermi's golden rule.

The occupation probability of a state depends on the occupation the other states. You solve for the probability distribution by solving a master equation. The occupation probability is not given by the Fermi function.

$$\Gamma_{k\to k'} = \frac{2\pi}{\hbar}\left|\langle \psi_k | H | \psi_{k'} \rangle\right|^2 \delta\left(E_k - E_{k'}\right)$$