Electron-electron interactions

Electron-electron interactions

Including electron-electron interactions into the description of solids is very, very difficult.

$$H = -\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_A \frac{\hbar^2}{2m_A}\nabla_A^2 - \sum_{i,A} \frac{Z_A e^2}{4\pi\varepsilon_0 r_{iA}} + \sum_{i<j} \frac{e^2}{4\pi\varepsilon_0 r_{ij}} + \sum_{A<B} \frac{Z_A Z_B e^2}{4\pi\varepsilon_0 r_{AB}}$$

If the electrons do not interact: Pauli exclusion, Fermi function.

$$u = \int_{-\infty}^{\infty} ED(E)f(E)dE$$

Perturbation theory

If fermions are noninteracting, they 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.

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

Landau theory of a Fermi liquid

Landau first considered small displacements of the electrons from the many-electron ground state. The "normal modes" of this 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.

Concepts like the density of states refer to quasiparticles.

Electron screening (Abschirmung)

$$\nabla \cdot \vec{E} = \frac{e\delta(r)}{\varepsilon_0} \qquad \vec{E} = -\nabla V$$

Poisson equation $\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0}$ $\qquad V = \frac{e}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}'\right|}$

If a charge is put in a metal, the other charges will move

$$\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0} - \frac{\rho_{ind}}{\varepsilon_0}$$

If ρ_{ind} is proportional to $-V$,

$$\frac{\rho_{ind}}{\varepsilon_0} = -k_s^2 V$$

The Helmholtz equation in 3-d

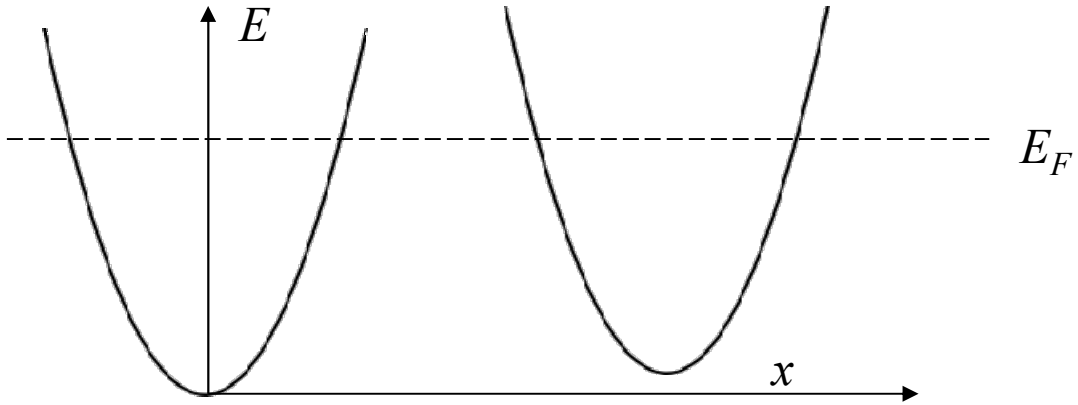
$$\nabla^2 V - k_s^2 V = -\frac{e\delta(r)}{\varepsilon_0}. \qquad V = \frac{e\exp\left(-k_s \left|\vec{r} - \vec{r}'\right|\right)}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}'\right|}$$

Thomas-Fermi screening

$$\Delta n = -D\left(E_F\right)eV$$

$$\rho_{ind} = e\Delta n = -e^2 D\left(E_F\right)V$$

$$D\left(E_F\right) = \frac{3n}{2E_F}$$



$$\nabla^2 V = -\frac{e\delta(r)}{\varepsilon_0} - \frac{\rho_{ind}}{\varepsilon_0} = -\frac{e\delta(r)}{\varepsilon_0} + \frac{3e^2 n}{2\varepsilon_0 E_F} V$$

$$\nabla^2 V - \frac{3e^2 n}{2\varepsilon_0 E_F} V = -\frac{e\delta(r)}{\varepsilon_0}$$

Thomas - Fermi screening length

$$k_s^2 = \frac{3e^2 n}{2\varepsilon_0 E_F} = \frac{3^{1/3} m e^2 n^{1/3}}{\varepsilon_0 \hbar^2 \pi^{4/3}}$$

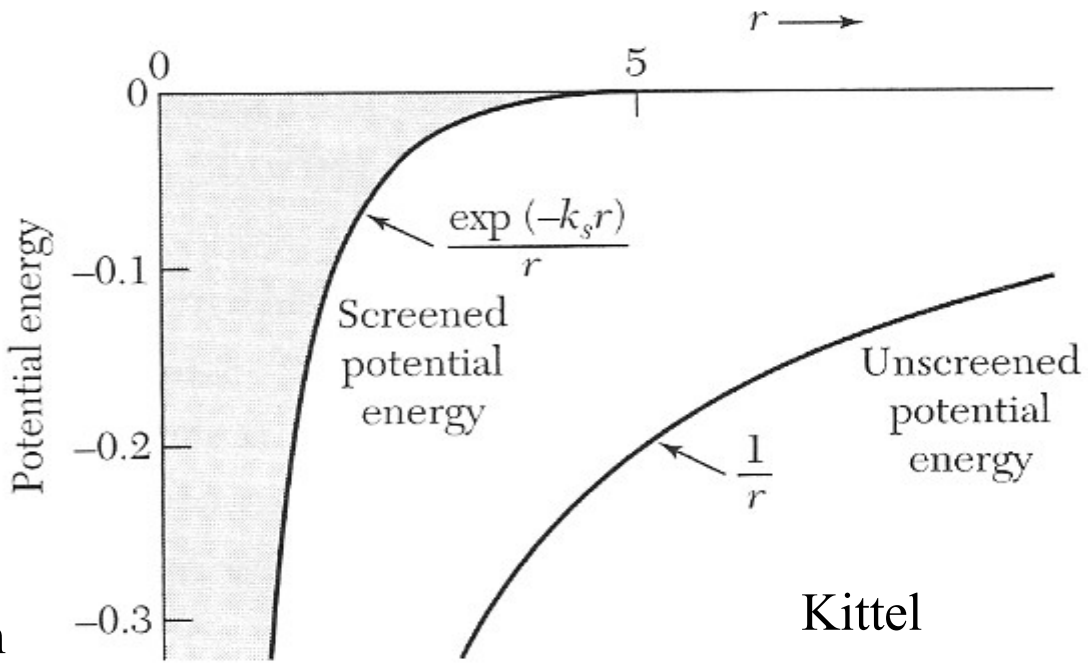
$$V = \frac{-e\exp\left(-k_s\left|\vec{r}-\vec{r}'\right|\right)}{4\pi\varepsilon\left|\vec{r}-\vec{r}'\right|}$$

Electron screening

$$V = \frac{-\exp\left(-k_s \left|\vec{r} - \vec{r}'\right|\right)}{4\pi\varepsilon \left|\vec{r} - \vec{r}'\right|}$$

$$k_s^2 = \frac{3e^2 n}{2\varepsilon_0 E_F} = \frac{3^{1/3} m e^2 n^{1/3}}{\varepsilon_0 \hbar^2 \pi^{4/3}}$$

Thomas - Fermi screening length

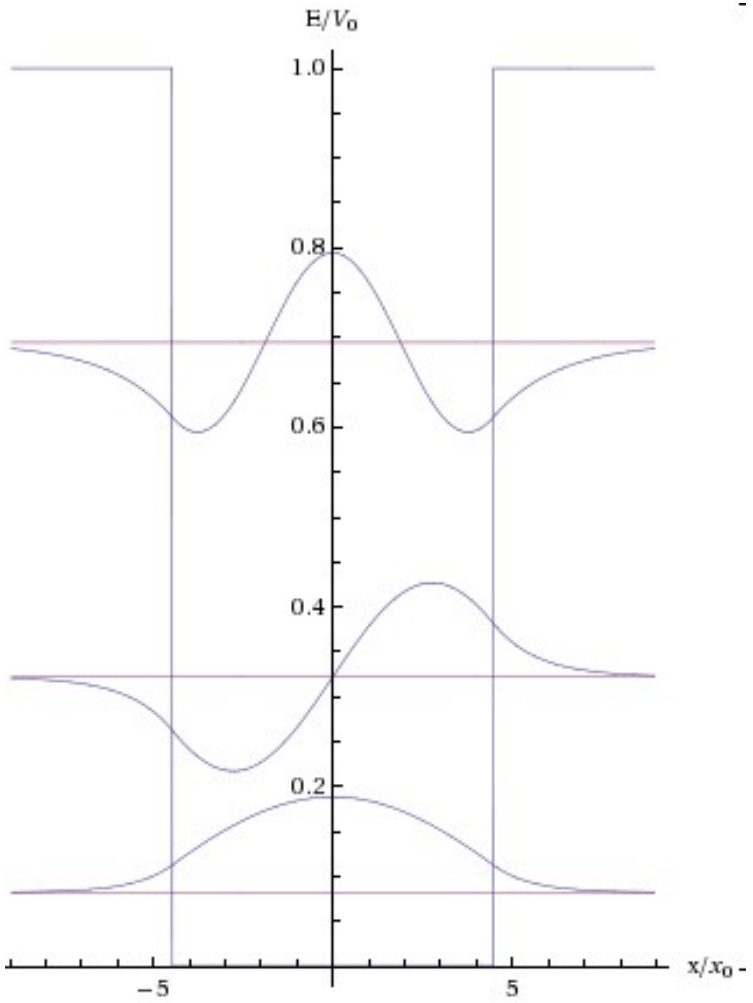


Kittel

$$k_s^2 \propto n^{1/3}$$

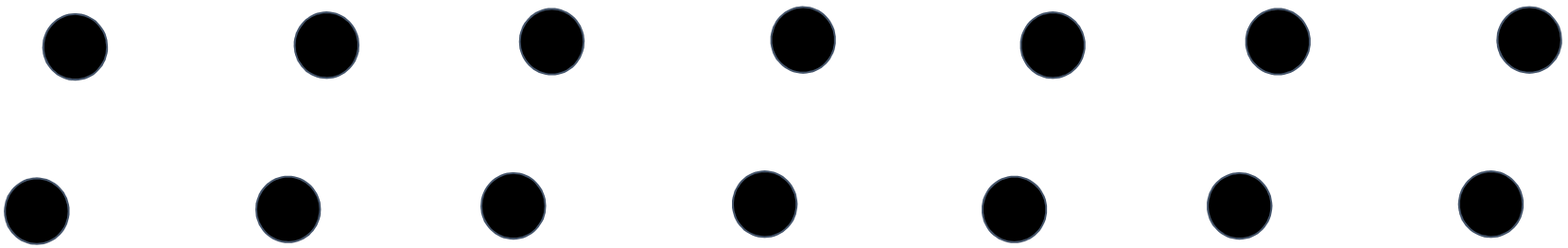
Screening length depends on the electron density

Mott transition

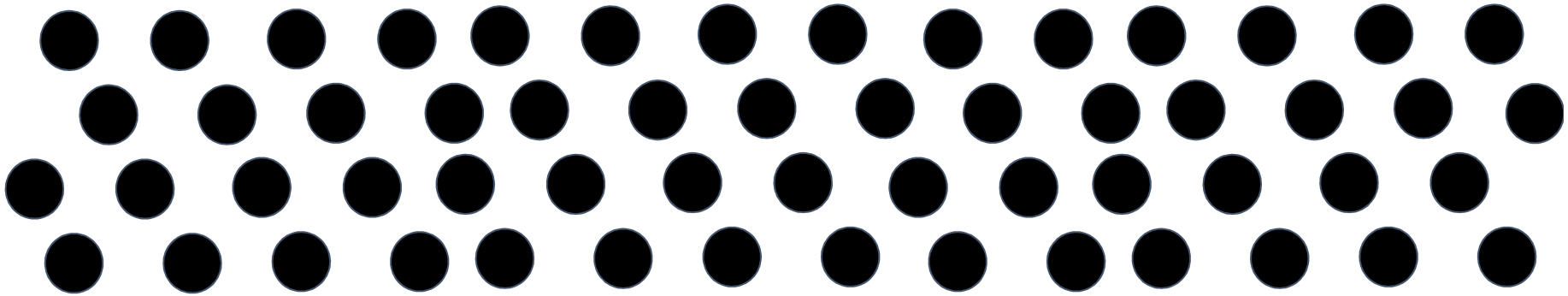


The number of bound states in a finite potential well depends on the width of the well. There is a critical width below which the valence electrons are no longer bound.

Metal-insulator transition

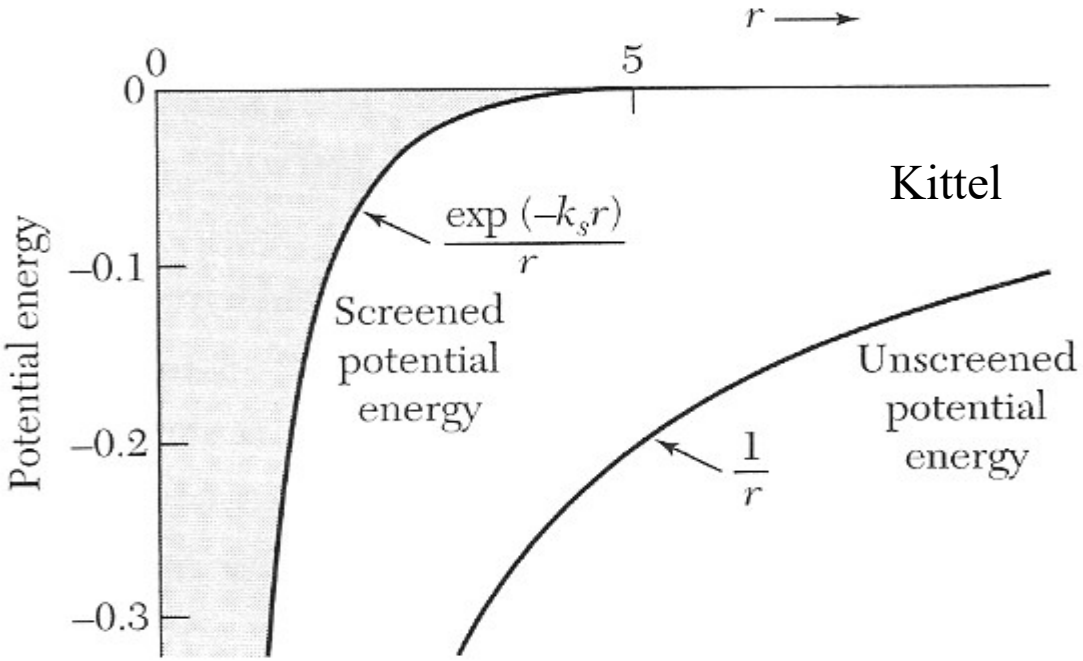


Atoms far apart: insulator



Atoms close together: metal

Mott transition



For low electron densities the screening is weak. The electrons are bound and the material is an insulator.

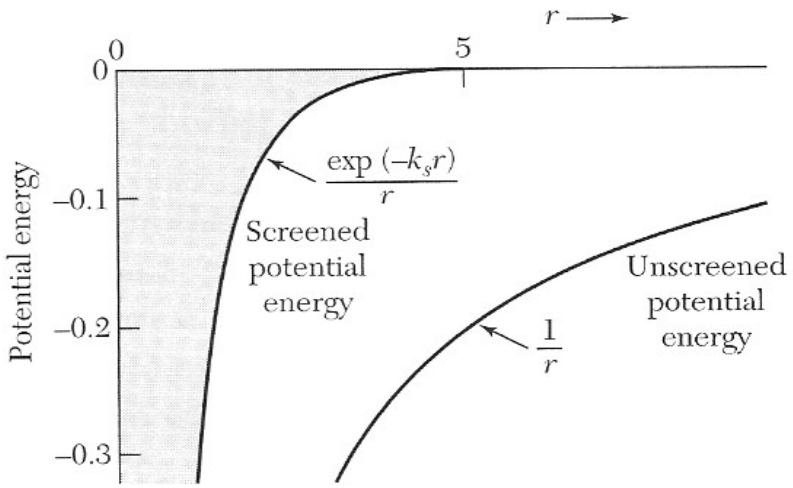
For high electron densities the screening is strong, the valence electrons are not bound and the material is a metal.

Mott transition (low electron density)

There are bound state solutions to the unscreened potential (hydrogen atom)

The 1s state of a screened Coulomb potential becomes unbound at $k_s = 1.19/a_0$.

Bohr radius



Nevill Francis Mott
Nobel prize 1977

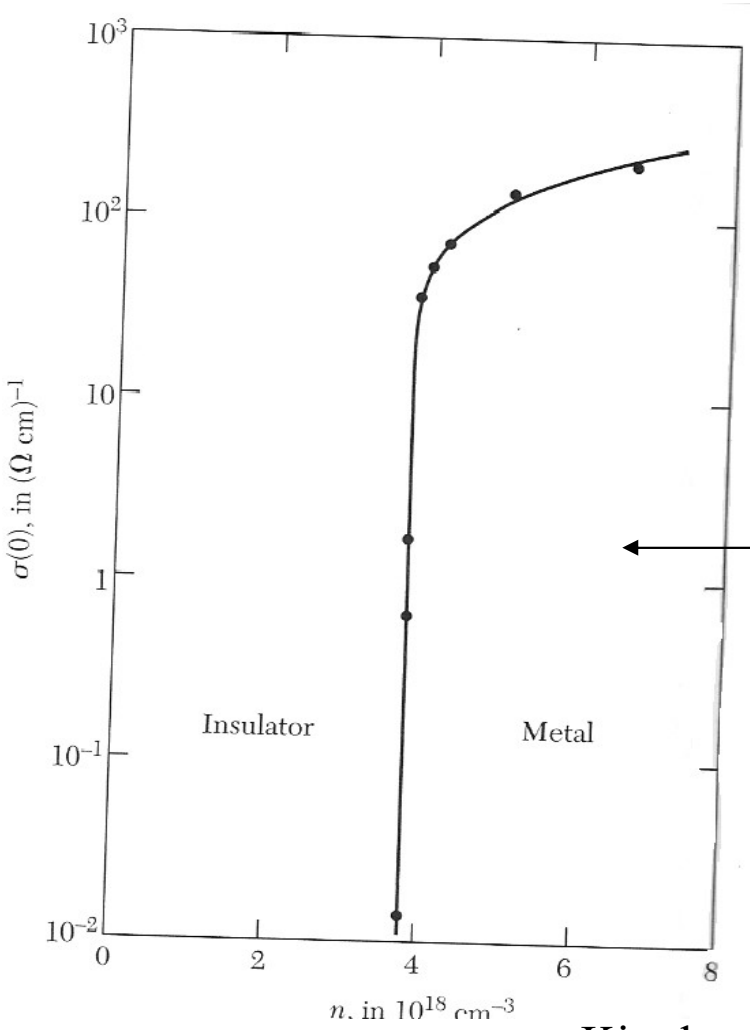
Mott argued that the transition should be sharp.

$$k_s^2 = \frac{4}{a_0}\left(\frac{3n}{\pi}\right)^{1/3}$$

High-temperature oxide superconductors / antiferromagnets

Semiconductor conductivity at low temperature

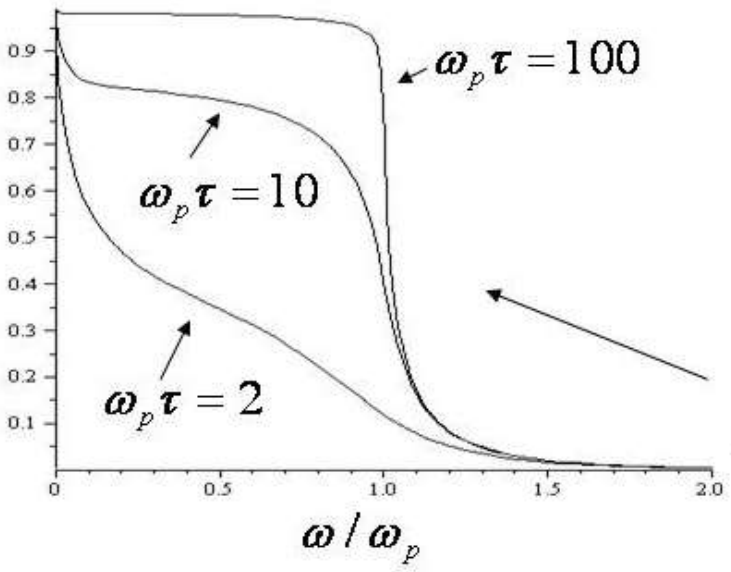
P in Si

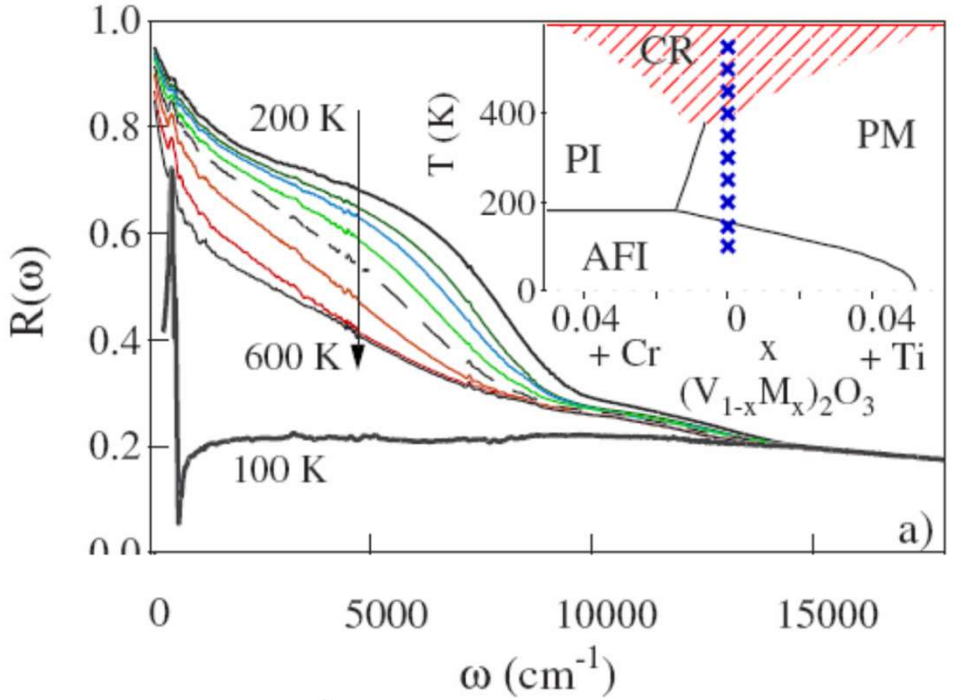


degenerate semiconductor

Kittel

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)

Wigner crystal

At low electron densities, electrons moving in a uniform positive background should form a crystal.

The kinetic energy can be minimized by allowing the electron states to spread out over the whole system giving them the lowest values of k and p. This leads to a higher potential energy.

The potential energy is lowest if the electrons are at fixed positions as far apart as possible.

For low electron densities, the total energy is lowest for a crystal of electrons.

Eugene Wigner

Peierls Transition

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

Rudolf Peierls

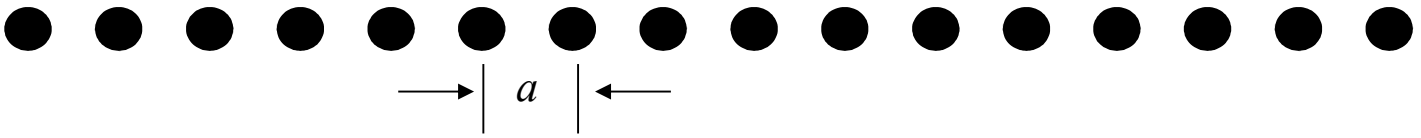
Predicted in the 1930's

Accidentally observed in the 1970's in TTF-TCNQ

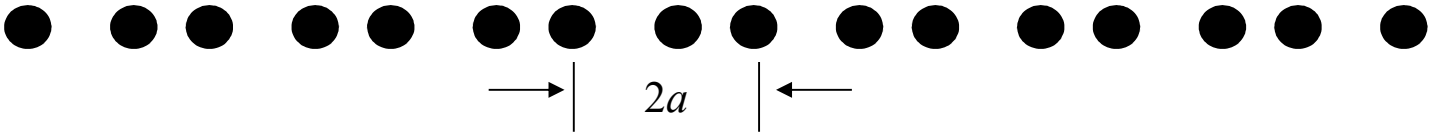
Rudolf Peierls, *More Surprises in Theoretical Physics*, Princeton University Press.
G. Grüner, *Density Waves in Solids*, Addison-Wesley Publishing Company, 1994.

Peierls Transition

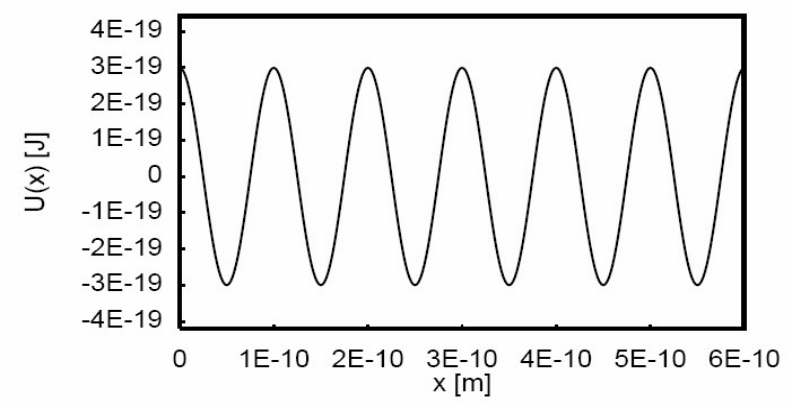
Consider a 1-d lattice of atoms with spacing a.

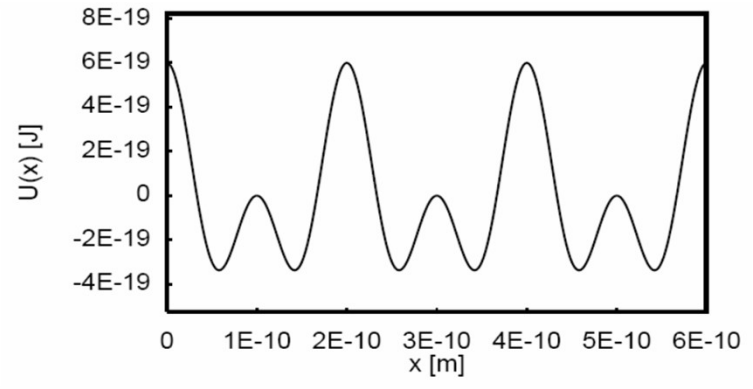


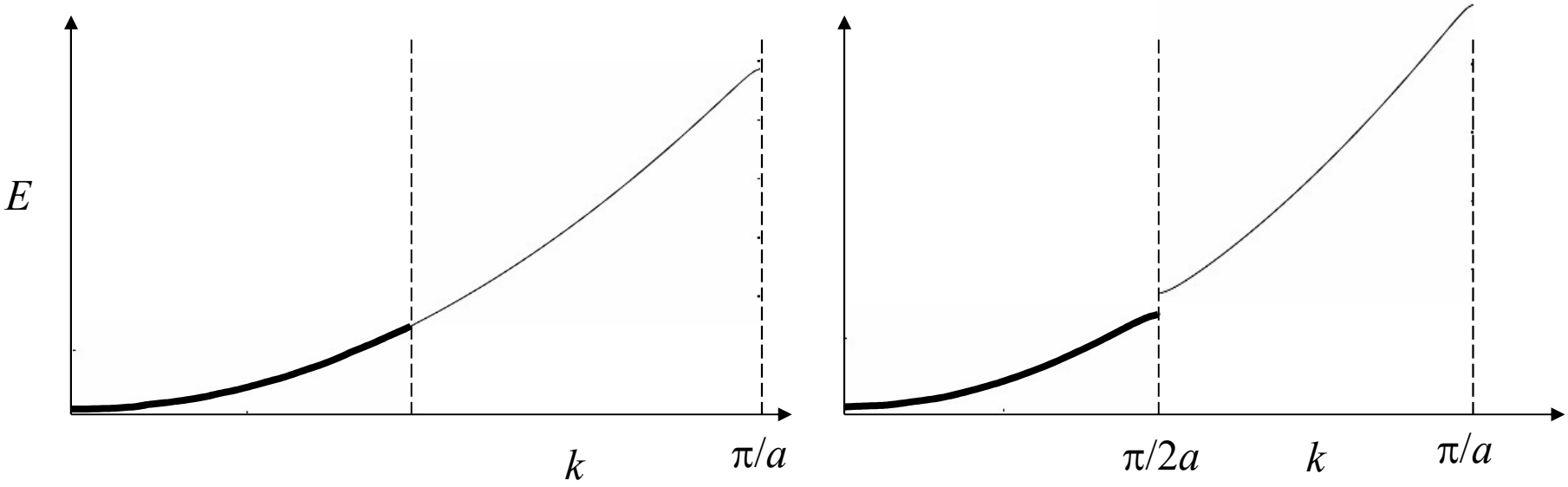
A periodic distortion of a 1-d lattice increases the periodicity to $2a$



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







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