Metal -Insulator Transitions Electron - Electron Interactions

Electron-electron interactions

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

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

One of the simplest approximation is to say that the electron-electron interactions screen the nuclei-electron interactions.

Screening = Abschirmung

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

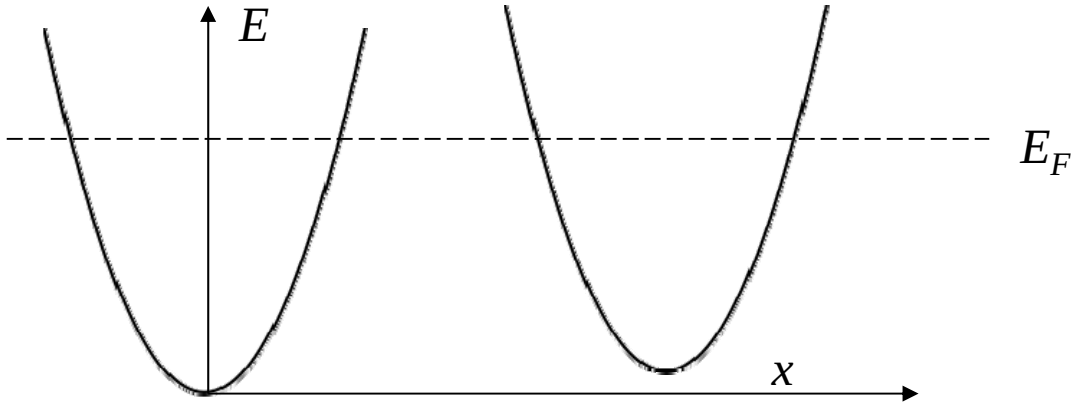
$$\nabla^2 V - k_s^2 V = -\frac{e\delta(r)}{\varepsilon_0}. \qquad V = \frac{e\exp\left(-k_s \left|\vec{r} - \vec{r}'\right|\right)}{4\pi\varepsilon_0 \left|\vec{r} - \vec{r}'\right|}$$

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

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

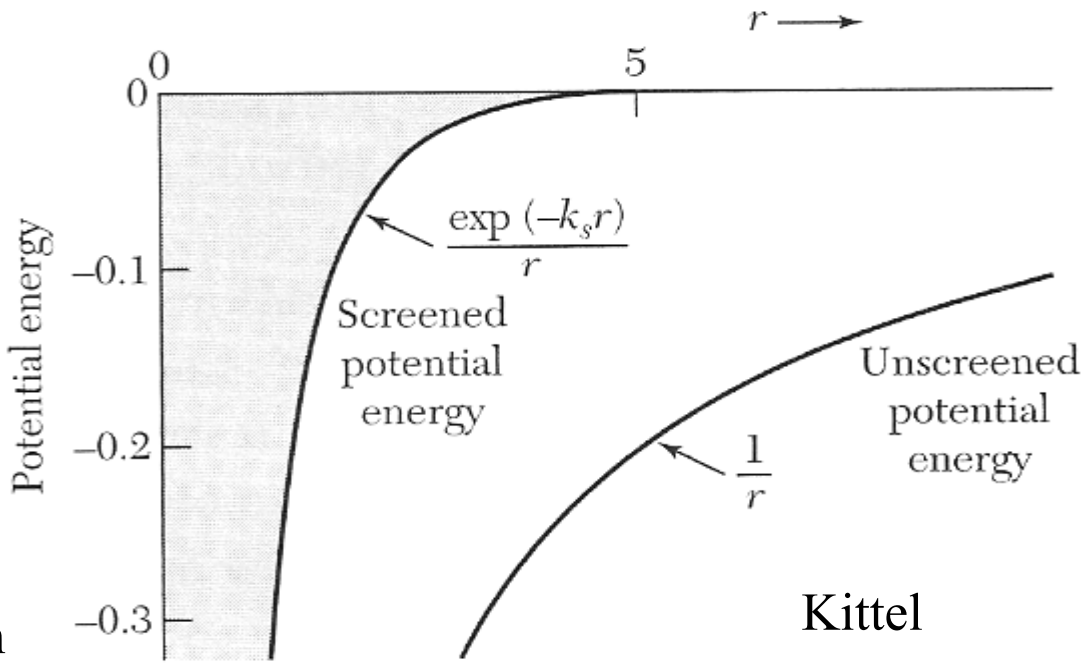
$$V = \frac{-e\exp\left(-k_s\left|\vec{r}-\vec{r}'\right|\right)}{4\pi\varepsilon\left|\vec{r}-\vec{r}'\right|}$$

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



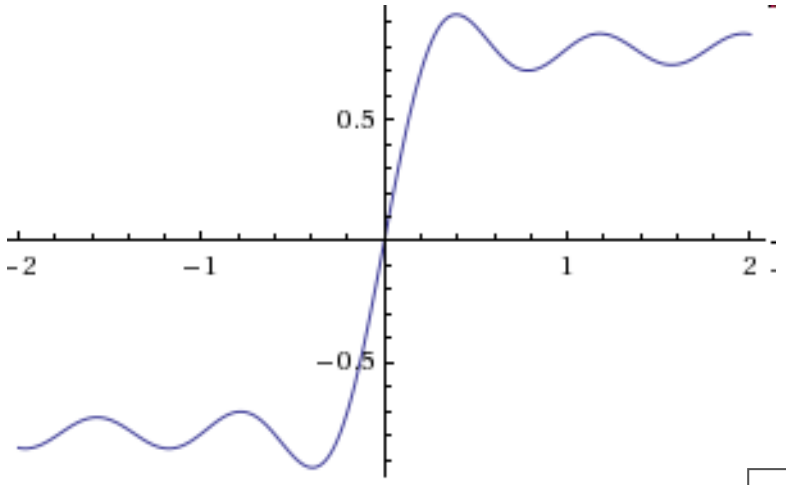
Kittel

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

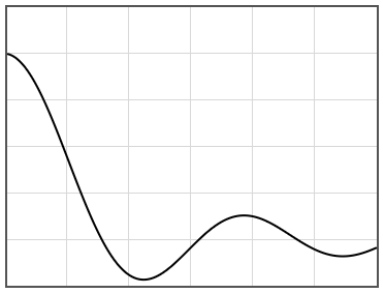
Screening length depends on the electron density

Friedel oscillations

Only wave vectors $k < k_F$ can contribute to the screening

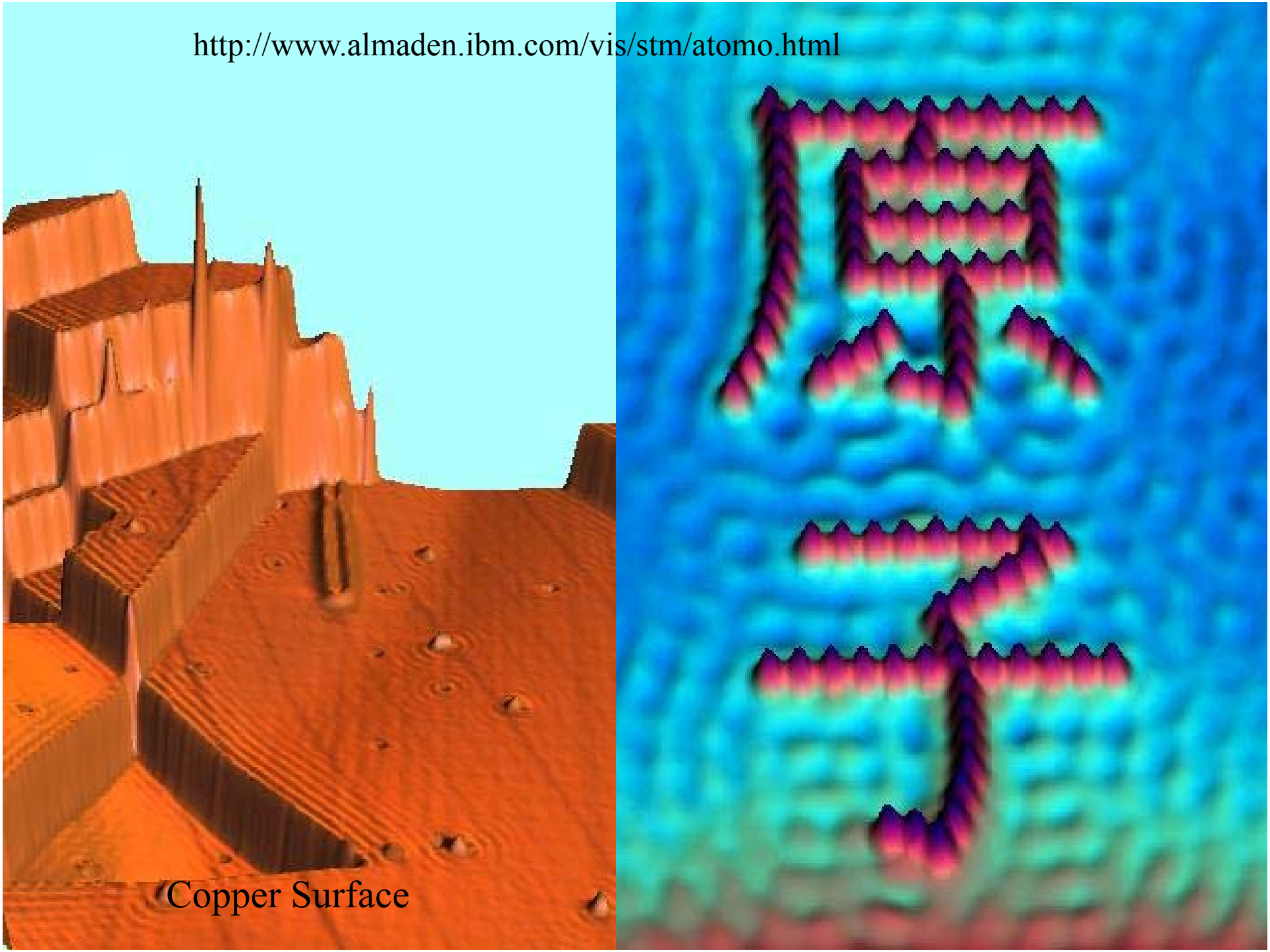


Around a point defect $\dfrac{\sin(k_F r)}{r}$



Friedel oscillations or Rudermann-Kittel oscillations

http://www.almaden.ibm.com/vis/stm/atomo.html



Copper Surface

Direct Observation of Friedel Oscillations around Incorporated Si_{Ga} Dopants in GaAs by Low-Temperature Scanning Tunneling Microscopy

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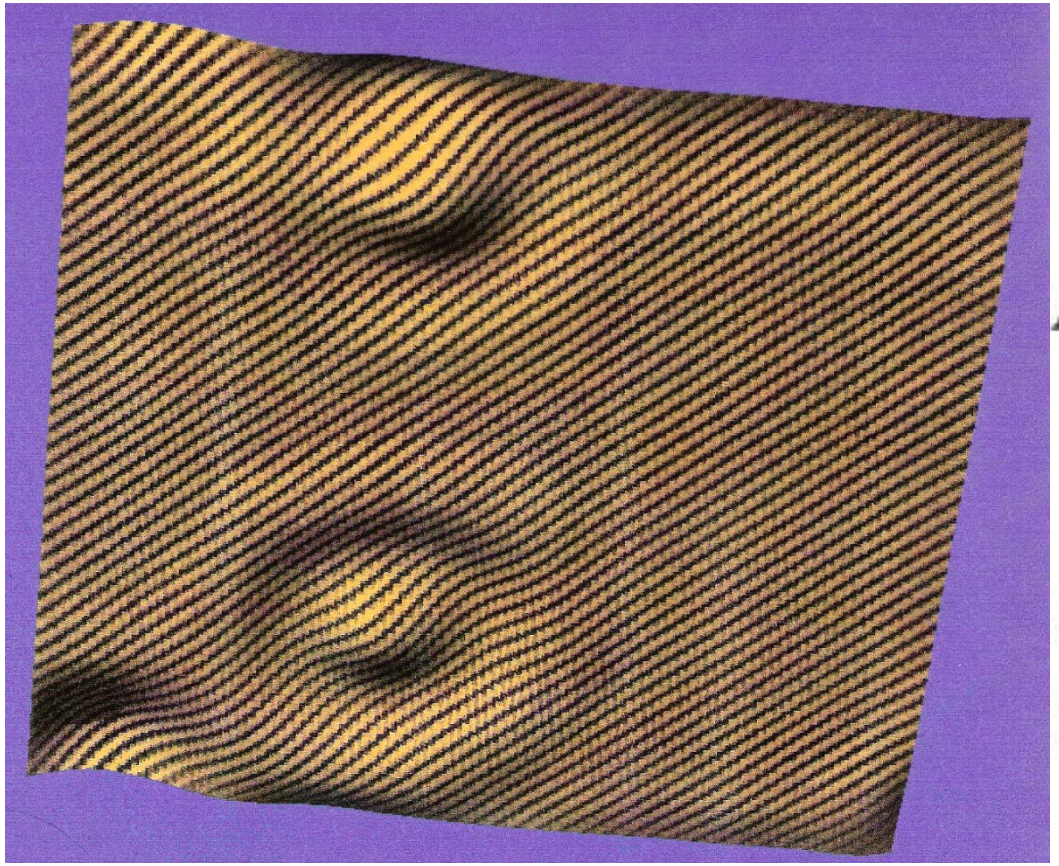
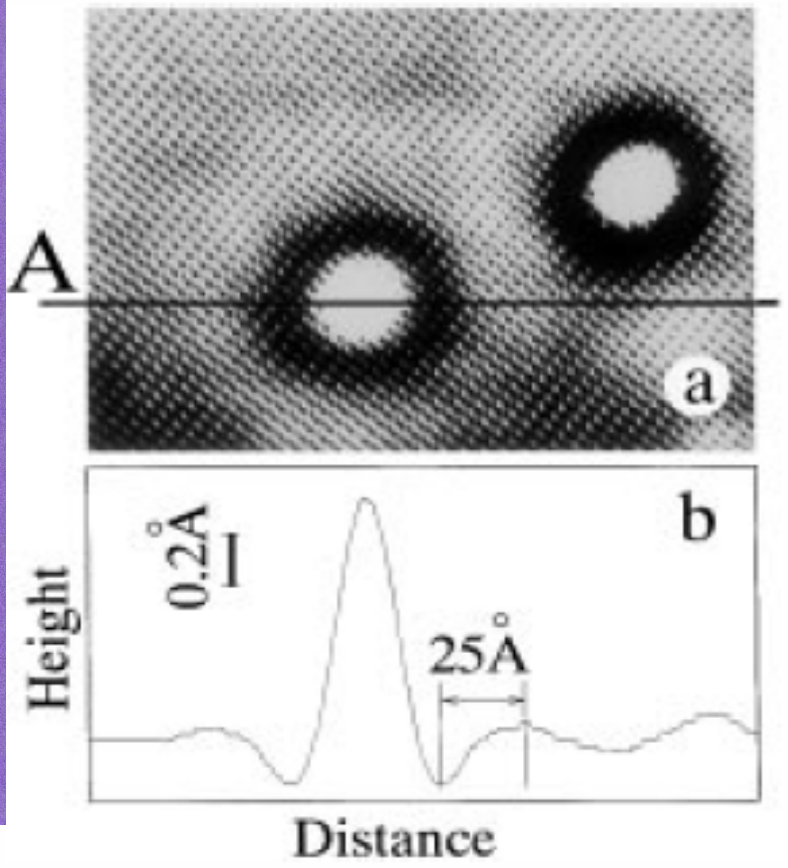
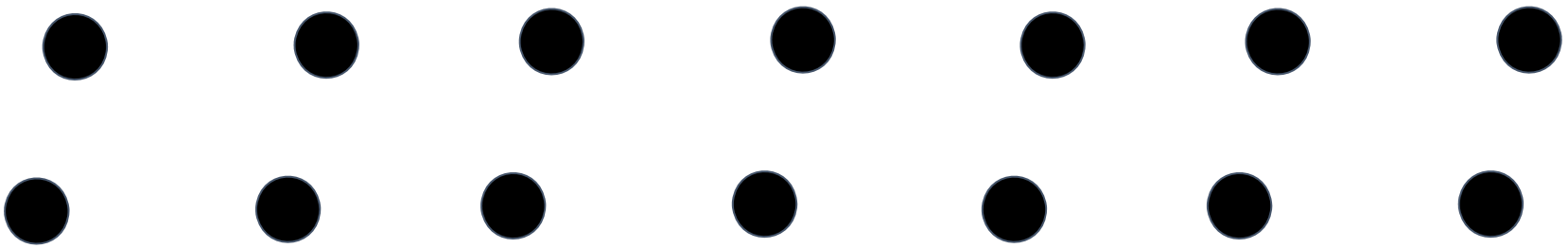
(Received 25 July 1995)

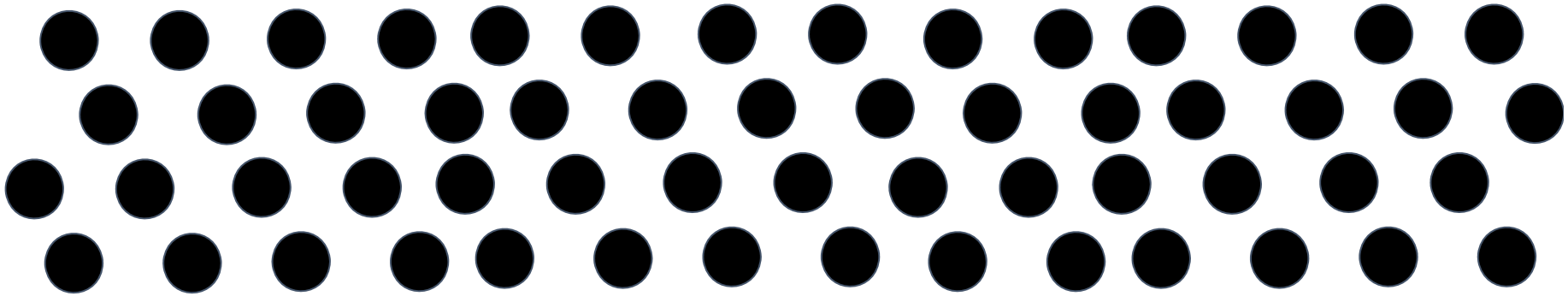




Metal-insulator transition

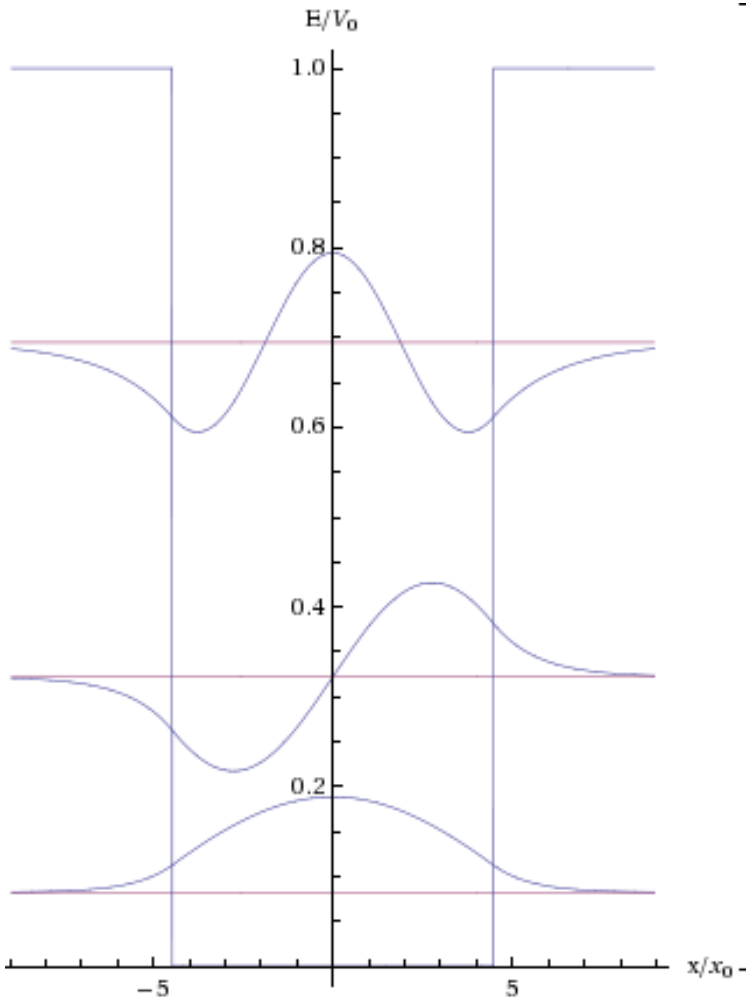


Atoms far apart: insulator



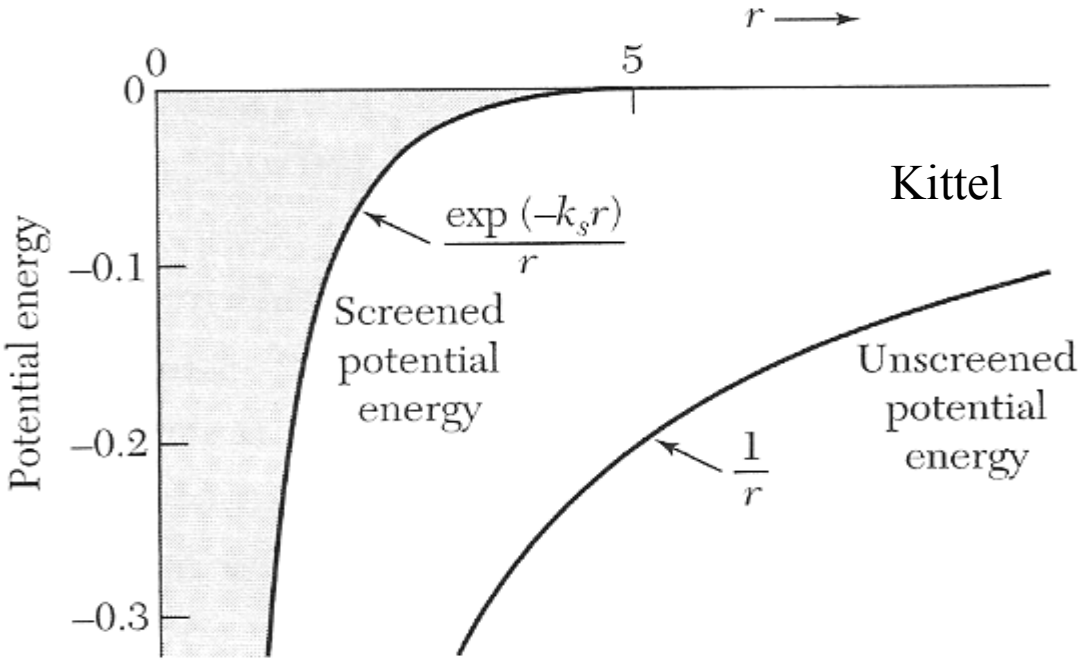
Atoms close together: metal

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.

Mott transition



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

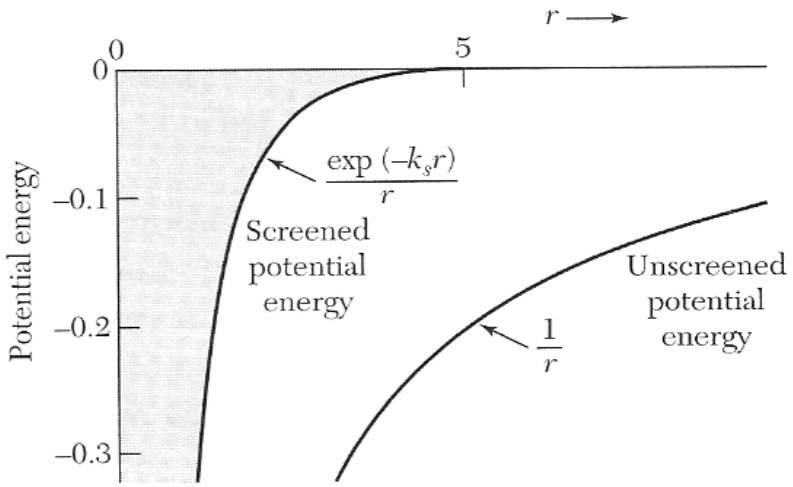
For high electron densities the screening is strong, the valence electrons are not bound and the material is a metal. The 1s state of a screened Coulomb potential becomes unbound at $k_s = 1.19a_0$.

Mott transition (low electron density)

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

There are bound state solutions to the screened potential for $k_s < 1.19/a_0$

Bohr radius



Nevill Francis Mott
Nobel prize 1977

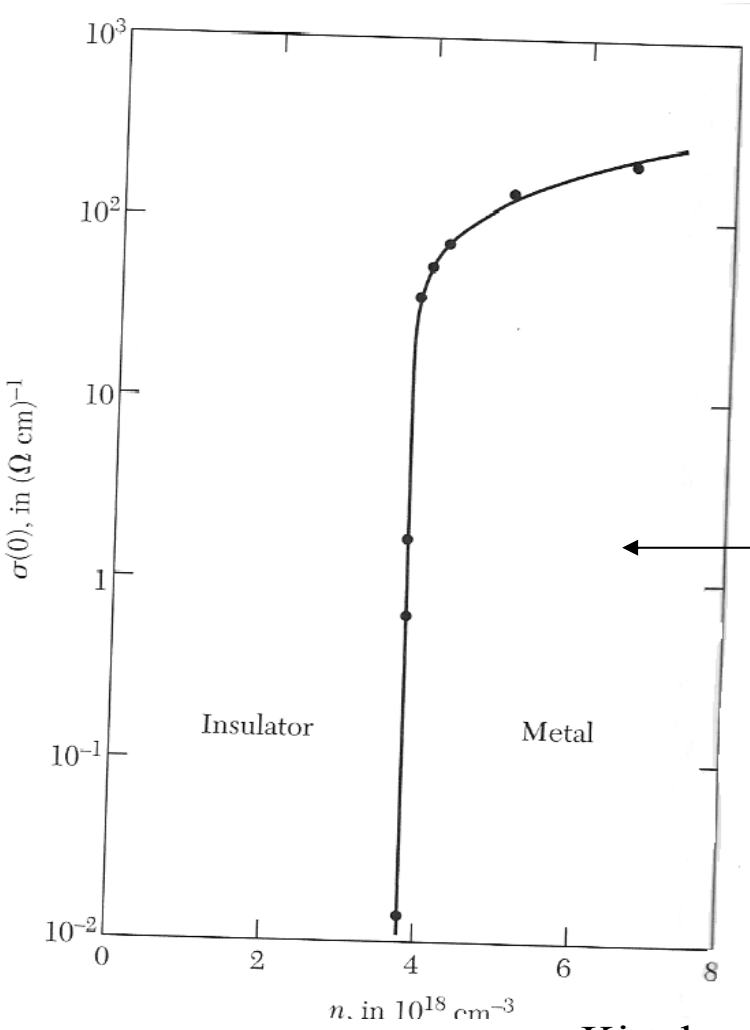
Mott argued that the transition should be sharp.

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

High-temperature oxide superconductors / antiferromagnets

Semiconductor conductivity at low temperature

P in Si



degenerate semiconductor

Kittel

Wigner crystal

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

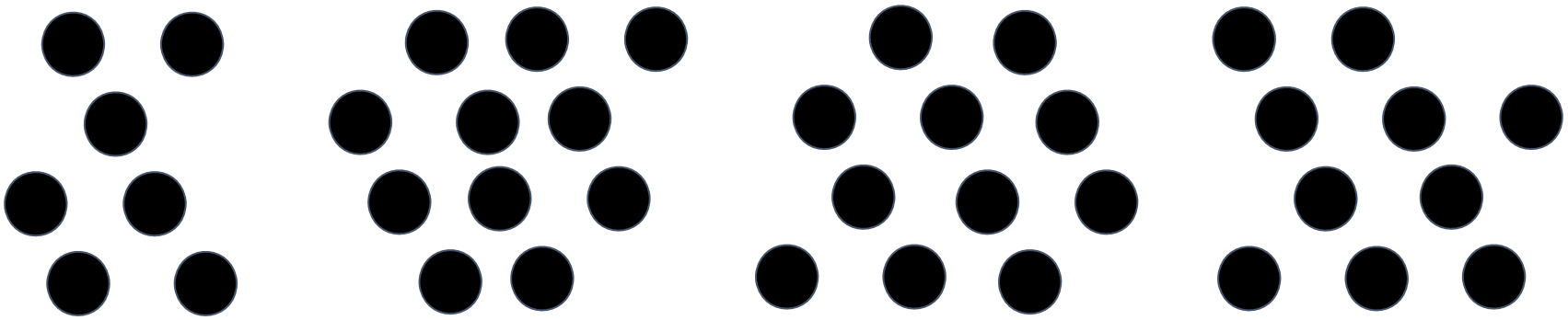
The kinetic energy can be minimized by allowing the electron states to spread out over the whole system giving them the lowest values of k and p. This leads to a higher potential energy.

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

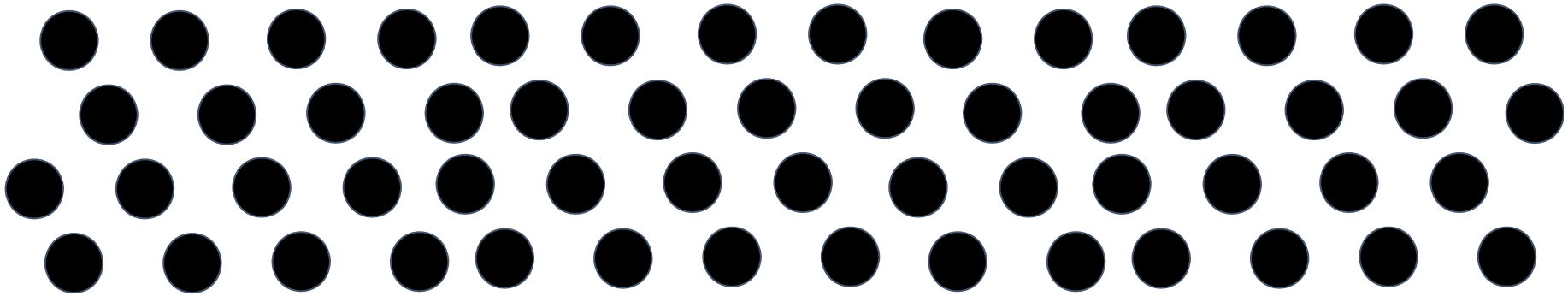
For low electron densities, the total energy is lowest for a crystal of electrons.

Eugene Wigner

Metal-insulator transition



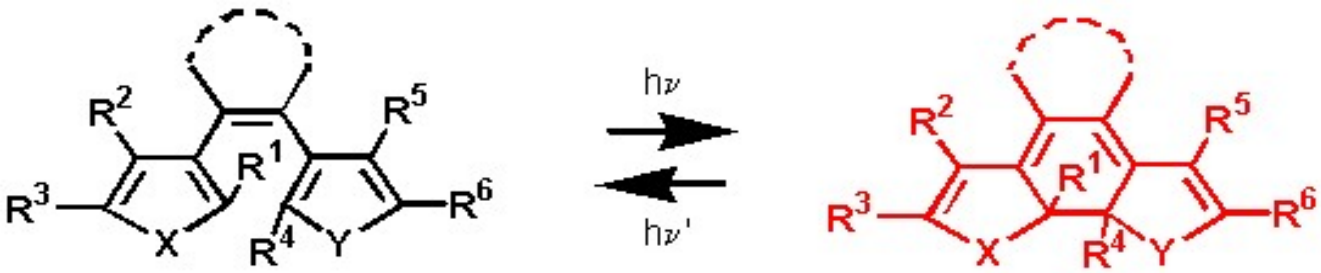
Clusters far apart: insulator

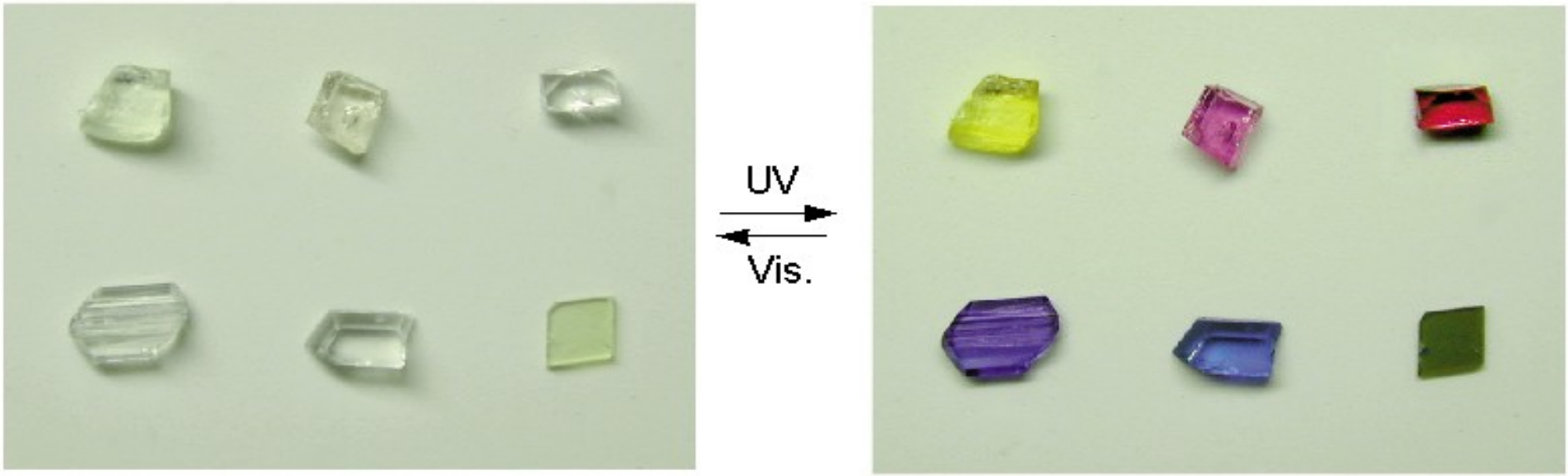


Clusters close together: metal

Quantum dots

Consider a solid formed by weakly coupling quantum dots together

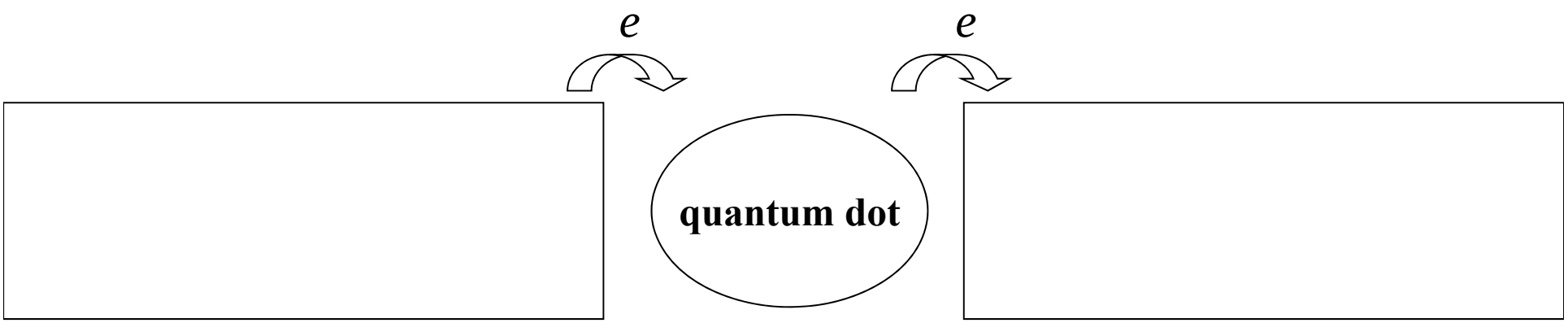




The molecules are weakly coupled in the crystals and act like quantum dots.

Charging effects

After screening, the next most simple approach to describing electron-electron interactions are charging effects.



The motion of electrons through a single quantum dot is correlated.

Single electron transistor