Metal-Insulator Transitions

Coulomb blockade suppressed by thermal and quantum fluctuations

Thermal fluctuations $\frac{e^2}{2C_\Sigma} >> k_B T$

Quantum fluctuations $\Delta E \Delta t > \hbar$

Duration of a quantum fluctuation: $\Delta t \sim \frac{\hbar 2C_\Sigma}{e^2}$

RC charging time of the capacitance: RC_Σ

Charging faster than a quantum fluctuation $RC_\Sigma < \frac{\hbar 2C_\Sigma}{e^2}$

$$R < \frac{2\hbar}{e^2} \approx 8\ \mathrm{k}\Omega$$

$$\frac{h}{e^2} \approx 25.5\ \mathrm{k}\Omega$$

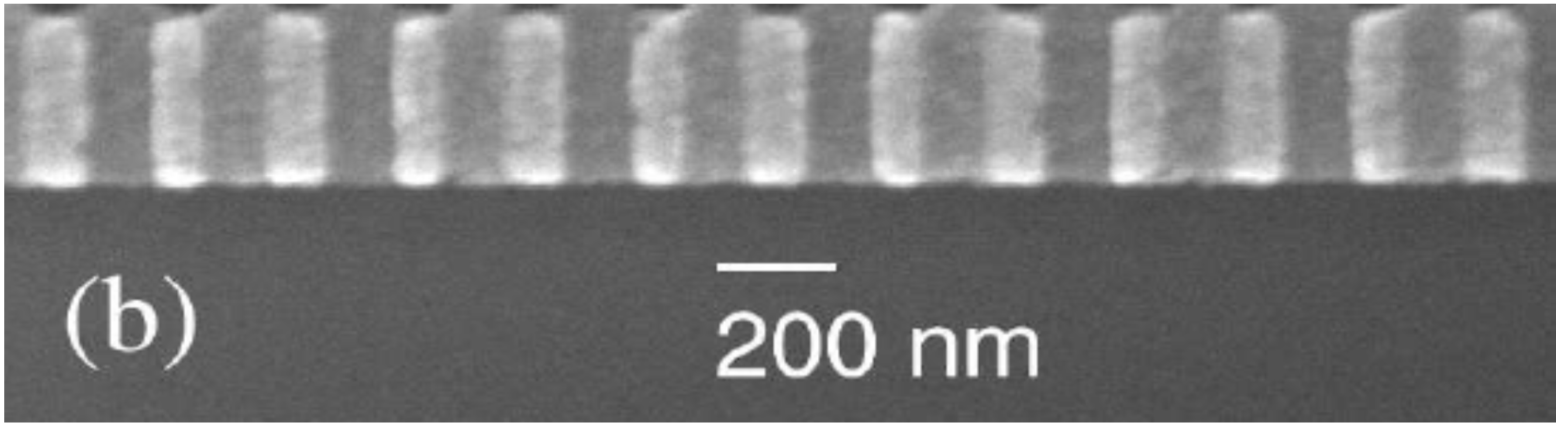
Resistance quantum

Metal - insulator transition in 1-d arrays

Charging energy $\Delta E = e^2/2C$

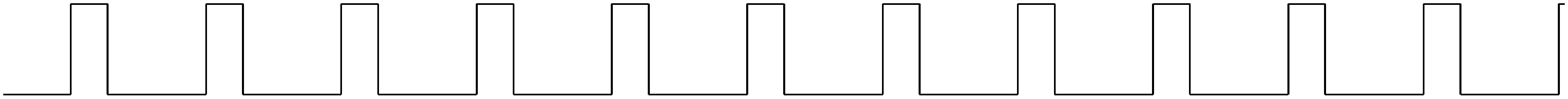
$$\Delta t = \frac{\hbar}{\Delta E} = \frac{2C\hbar}{e^2} > \frac{1}{\Gamma} = RC$$

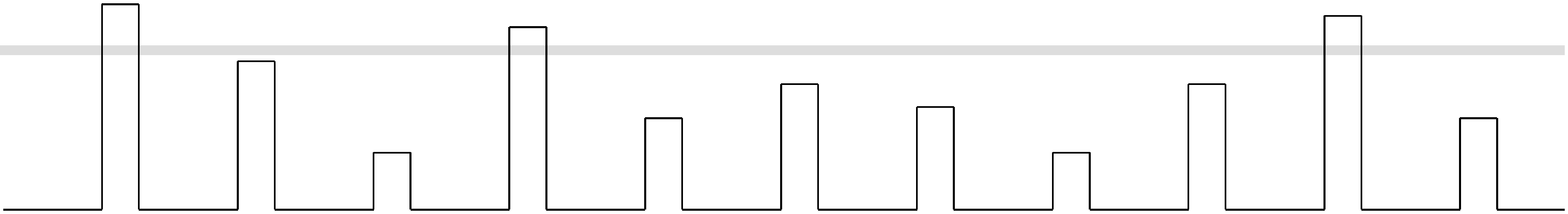
$R < \frac{2\hbar}{e^2}$ extended state



Disorder => Favors insulating state

Uniform tunnel barriers



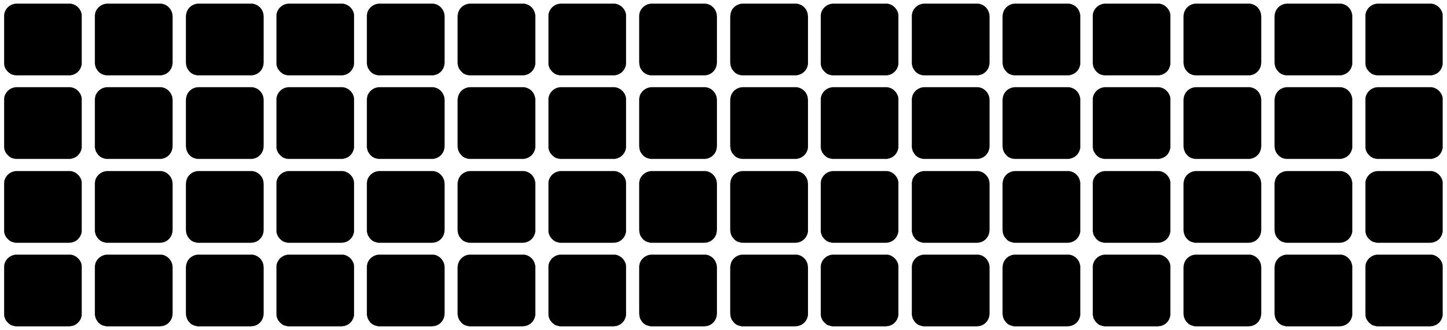


Random tunnel barriers, some with resistances above the resistance quantum

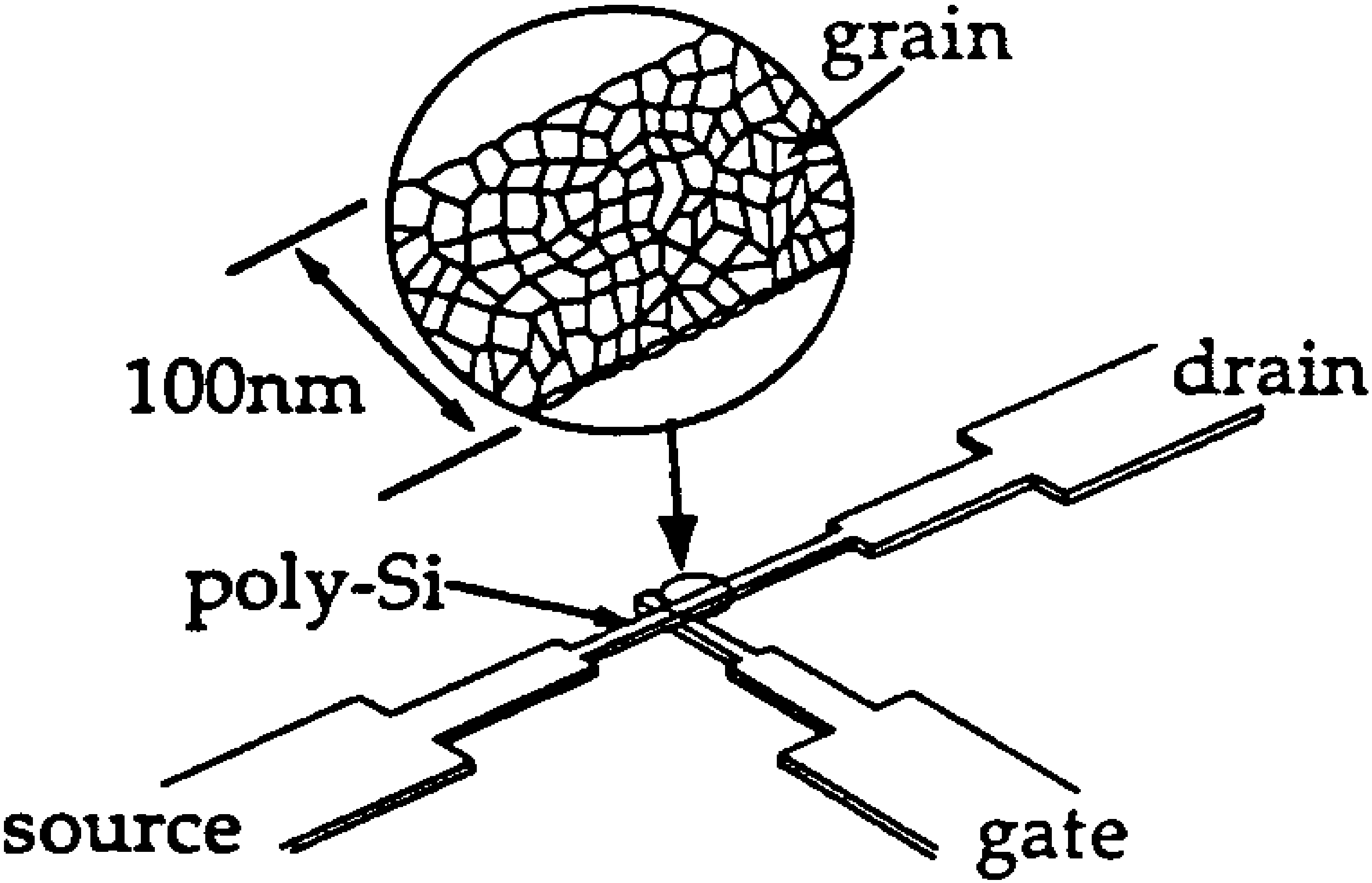
For bigger conducting regions, lower temperatures are needed to see insulating behavior.

Metal insulator transition

If the tunnel resistances between the crystals is > 25 kΩ, the material will be an insulator at low temperature



Strong coupling of metal particles results in a metal.
Weak coupling of metal particle results in an insulator.

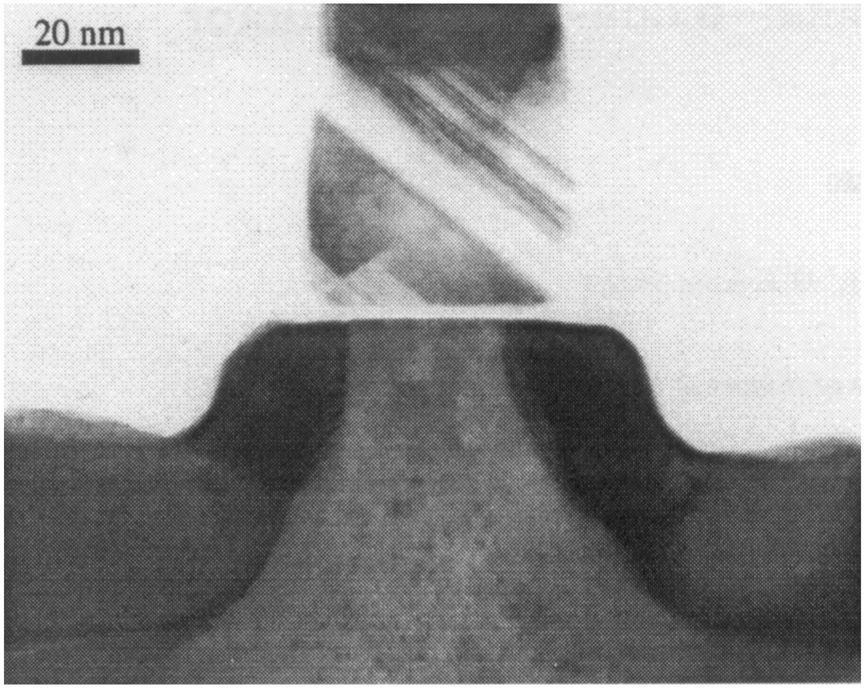


Yano

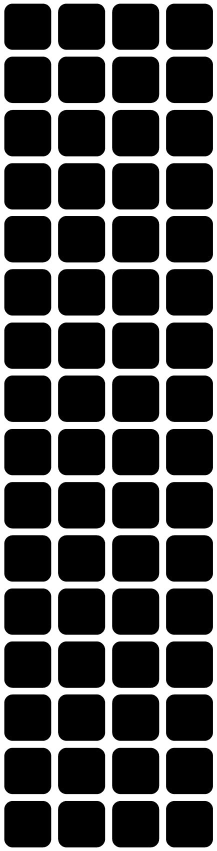
Single electron effects

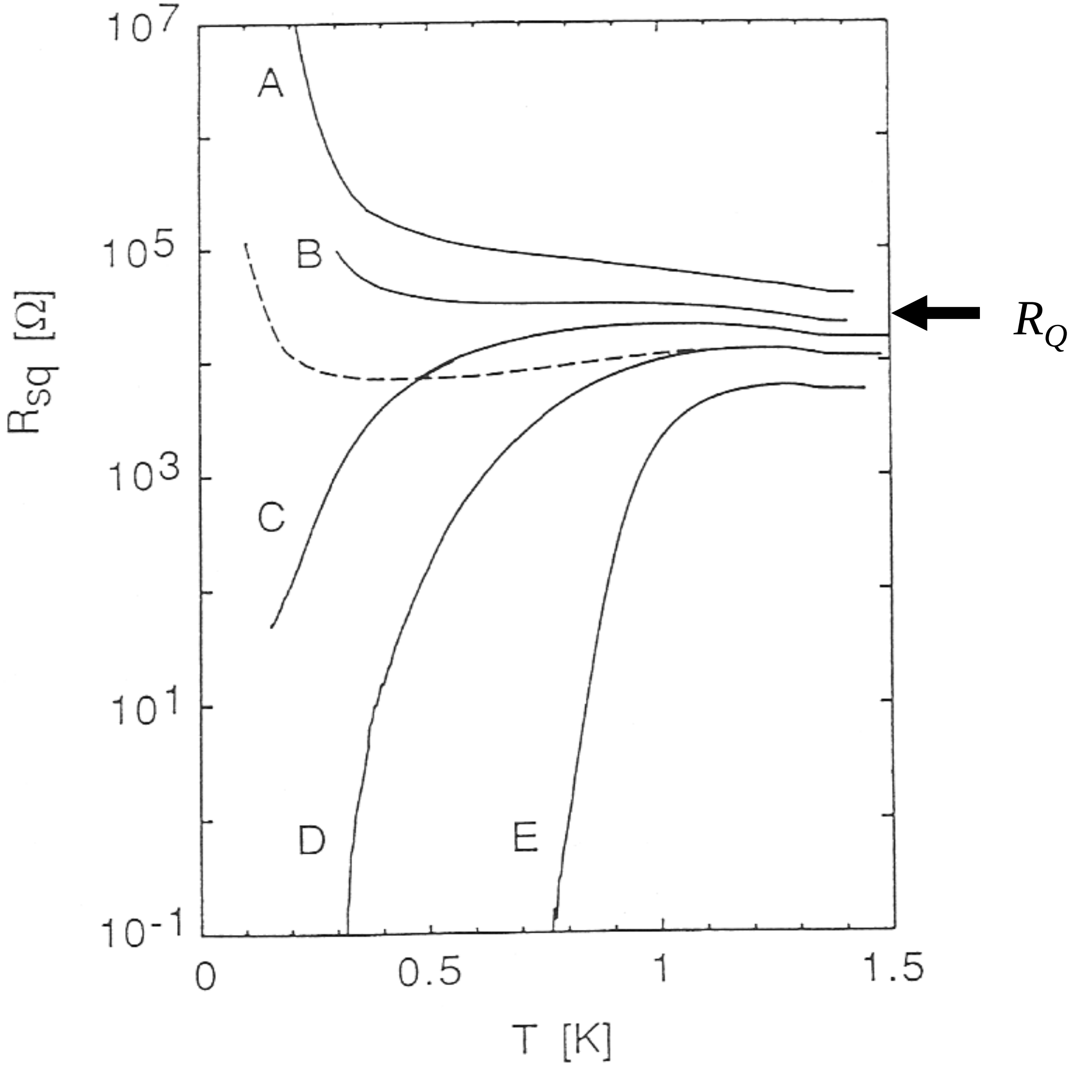
Single-electron effects will be present in any molecular scale circuit

Usually considered undesirable and are avoided by keeping the resistance below the resistance quantum.

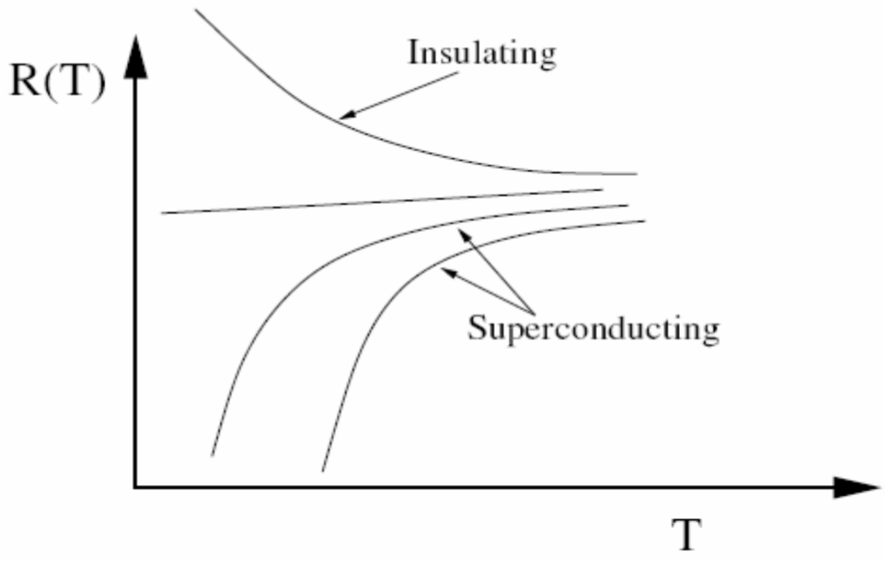


Josephson junction array





Geerligs PRL 63, p. 326 (1989).



The Bose-Hubbard Model:
From Josephson Junction Arrays to Optical Lattices

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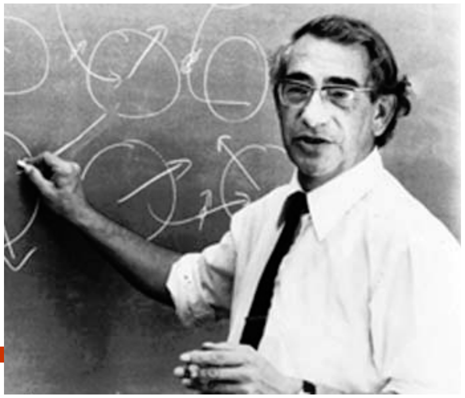
The Hubbard model



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

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

Consider 2 electrons and two sites. If the electrons have the same spin:

$$\uparrow,\uparrow \quad \text{or} \quad \downarrow,\downarrow$$

They can't hop and the energy is zero.

If the electrons have opposite spin

$$\uparrow,\downarrow \quad \text{or} \quad \uparrow,\downarrow \quad \text{or} \quad \uparrow\downarrow,0 \quad \text{or} \quad 0,\uparrow\downarrow$$

the states couple together.

The Hubbard model

$$\left|\psi\right\rangle = a\left|\uparrow\downarrow,0\right\rangle + b\left|\uparrow,\downarrow\right\rangle + c\left|\downarrow,\uparrow\right\rangle + d\left|0,\uparrow\downarrow\right\rangle$$

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle$$

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

$$\begin{aligned}\left\langle\uparrow\downarrow,0\right|H\left|\psi\right\rangle &= a\left\langle\uparrow\downarrow,0\right|H\left|\uparrow\downarrow,0\right\rangle + b\left\langle\uparrow\downarrow,0\right|H\left|\uparrow,\downarrow\right\rangle + c\left\langle\uparrow\downarrow,0\right|H\left|\downarrow,\uparrow\right\rangle + d\left\langle\uparrow\downarrow,0\right|H\left|0,\uparrow\downarrow\right\rangle \\ &= Ua - tb - tc\end{aligned}$$

$$\begin{bmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{bmatrix}\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = E\begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

States where electrons have opposite spin have lower energy (antiferromagnetic).

Eigenvectors

$E = 0$

$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$E = 2.56$

$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -0.780776466 \\ -0.780776466 \\ 1 \end{bmatrix} = \begin{bmatrix} 2.5615529319999997 \\ -2 \\ -2 \\ 2.5615529319999997 \end{bmatrix}$$

$E = \text{-}1.56$

$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1.2807764064 \\ 1.2807764064 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.5615528128 \\ -2 \\ -2 \\ -1.5615528128 \end{bmatrix}$$

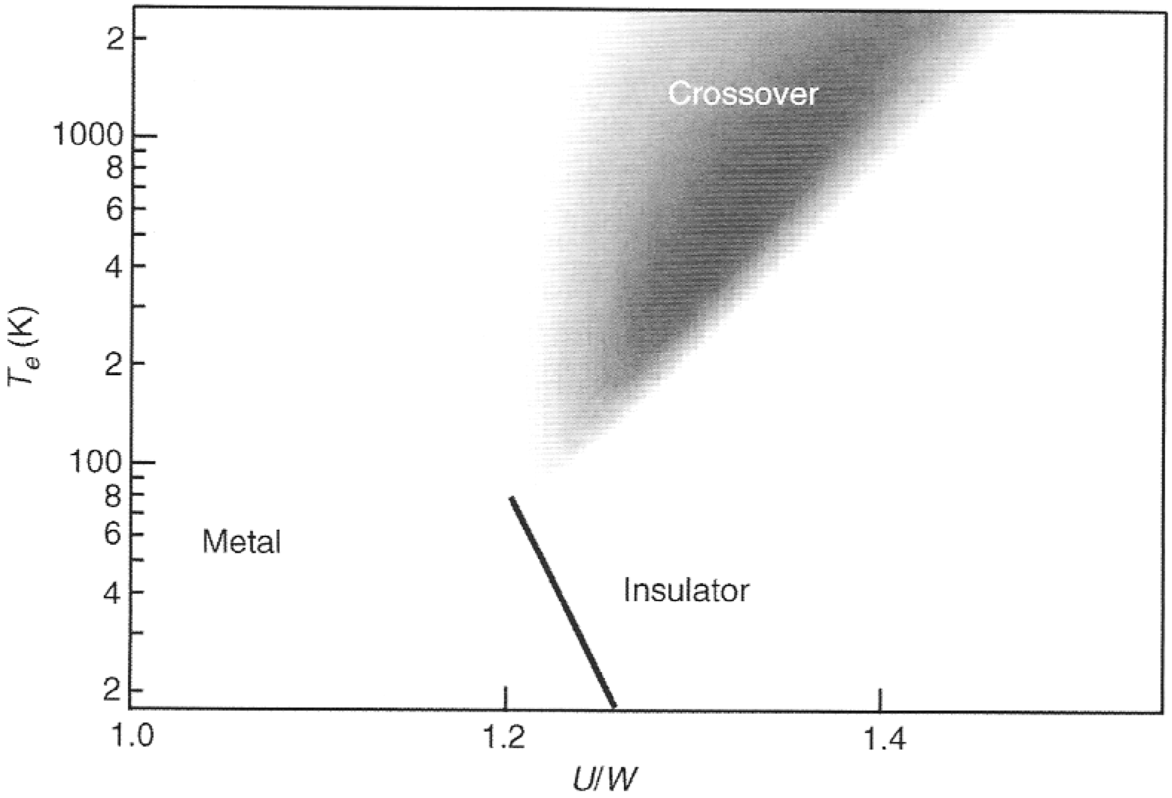
One eigenvalue
is less than zero

$E = 1$

$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

The ground state of a half-filled band is antiferromagnetic.
The Hubbard model rapidly becomes intractable for more sites.

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)

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

For $w = \ell, \qquad t \approx 0.2\ \mathrm{nm}, \quad \rho = 500\ \mu\Omega\ \mathrm{cm}$

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

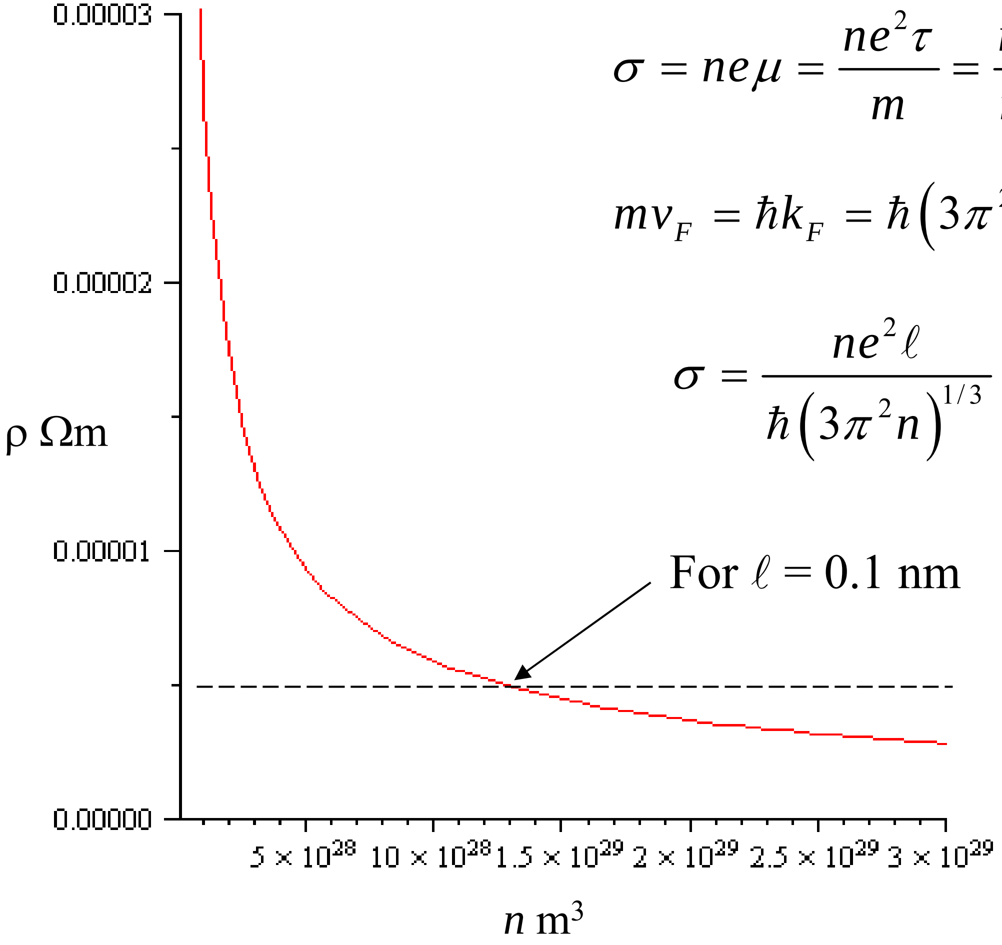
High-temperature oxide superconductors / antiferromagnets
Organic semiconductors often have this character.

Metal insulator transition

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

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

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



For $\ell = 0.1$ nm

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