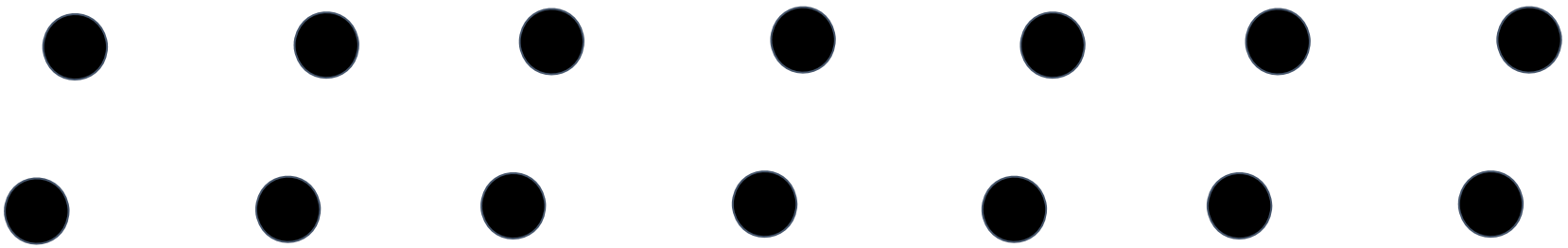
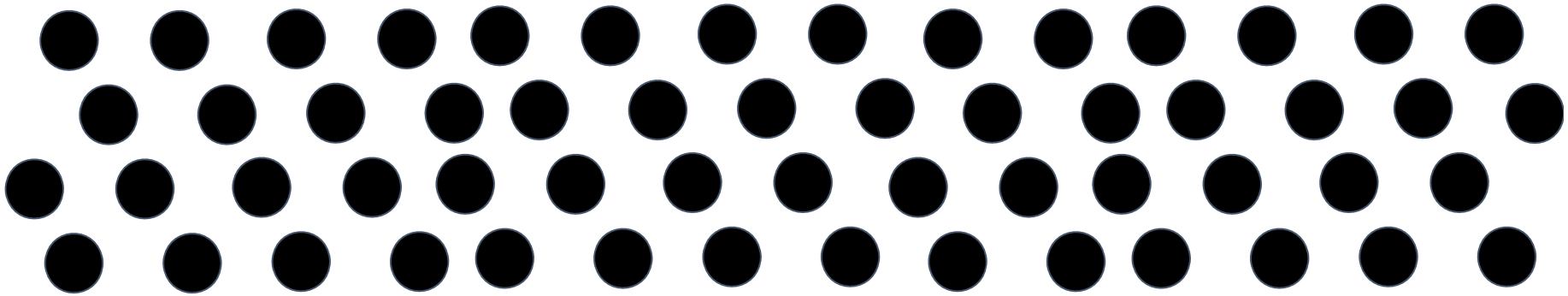
28. Metal - Insulator Transitions

Jan. 28, 2018

Metal-insulator transition



Atoms far apart: insulator



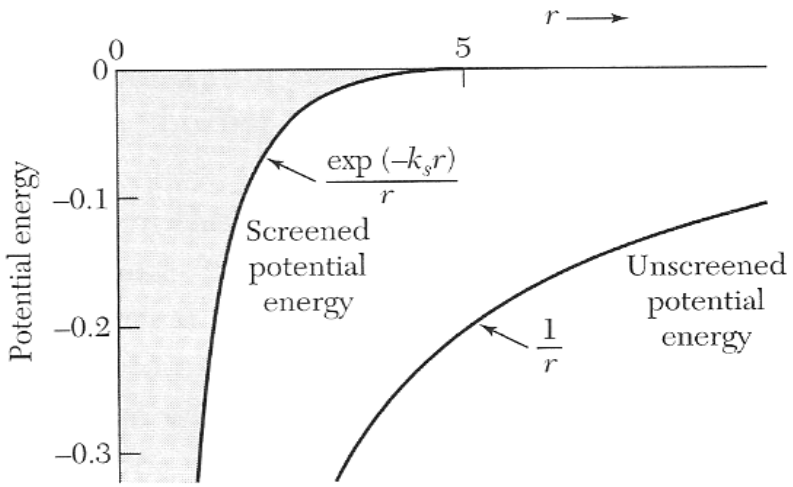
Atoms close together: metal

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



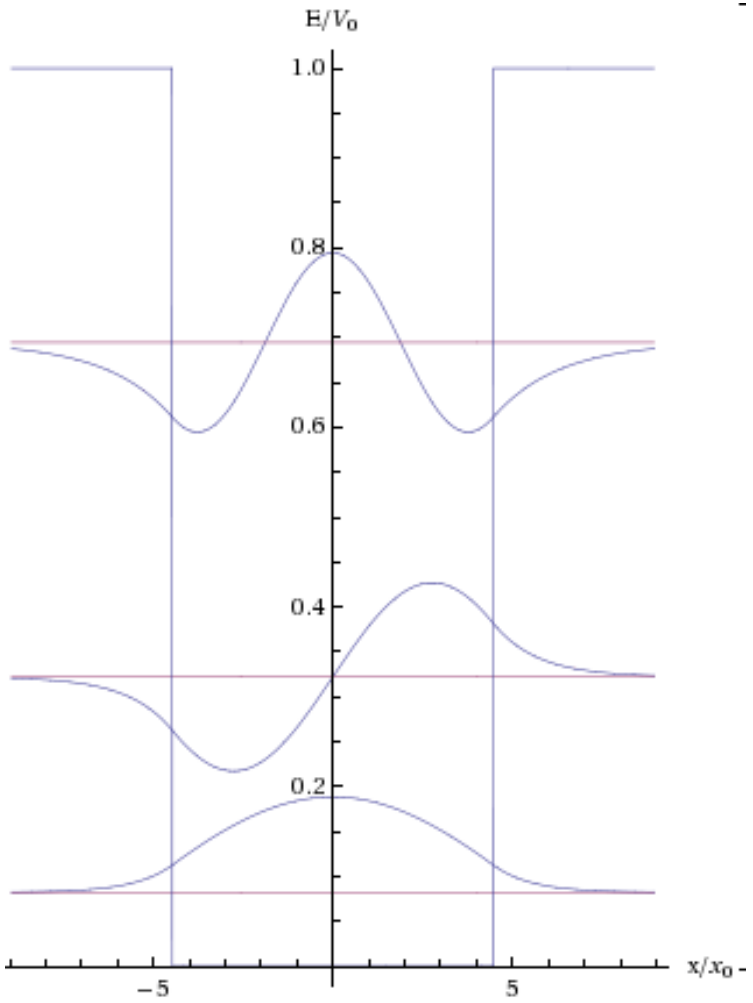
Nevill Francis Mott
Nobel prize 1977

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

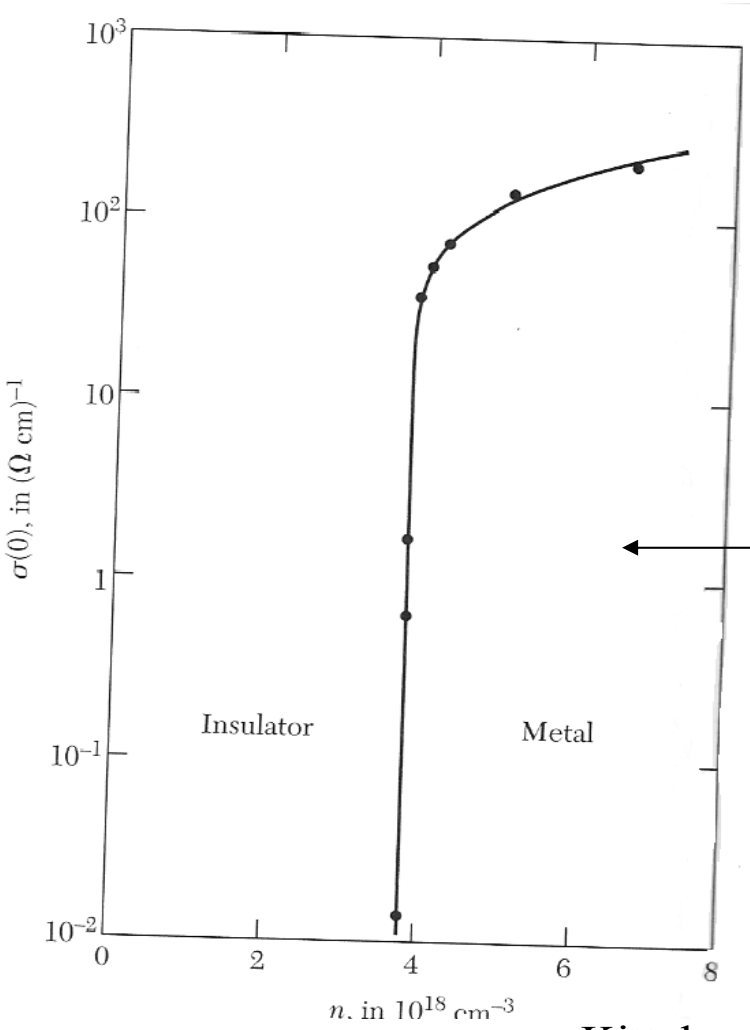
Mott transition



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.

Semiconductor conductivity at low temperature

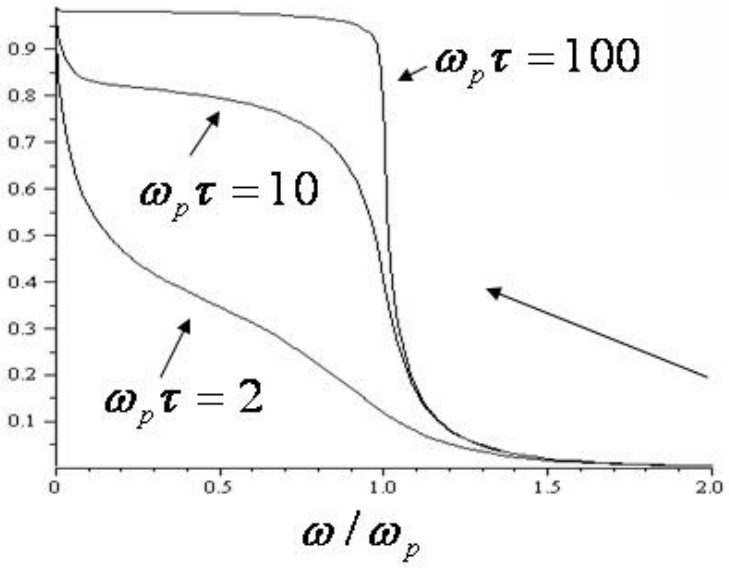
P in Si

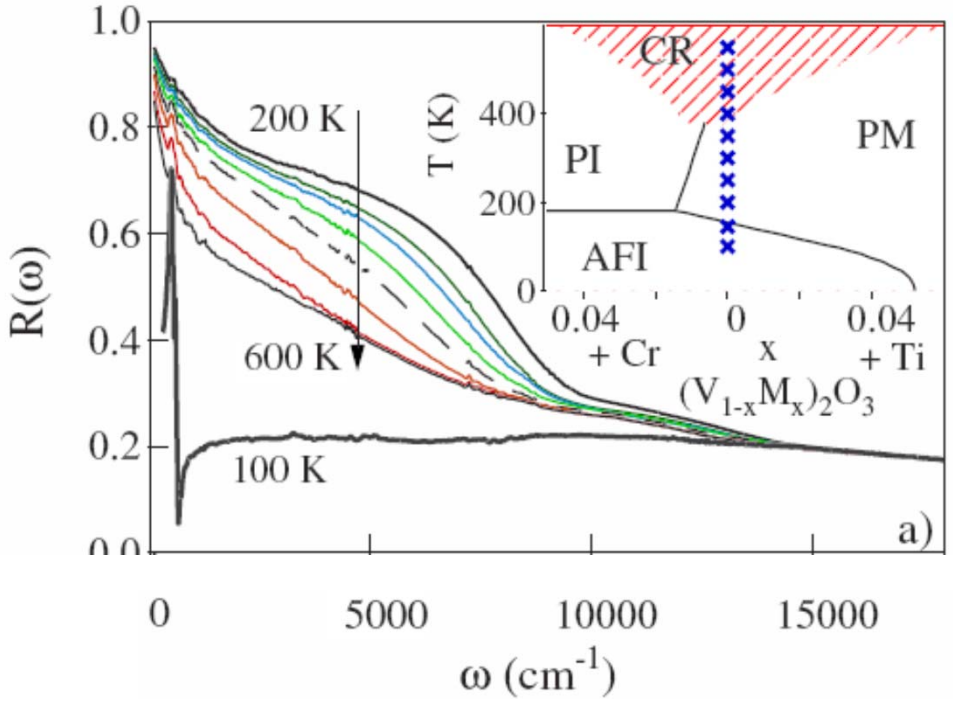


degenerate semiconductor

Kittel

Vanadium sesquioxide V_2O_3



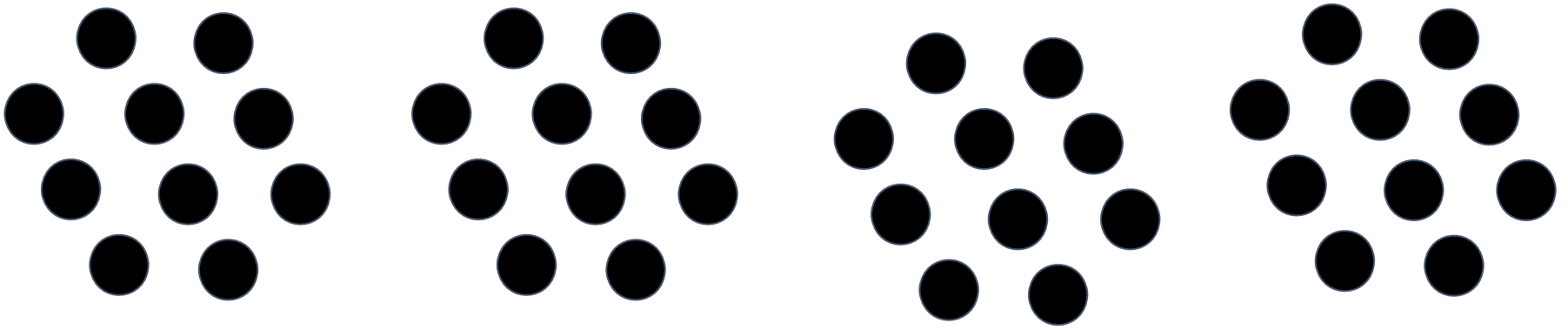


$$R = \frac{(n-1)^2 + K^2}{(n+1)^2 + K^2}$$

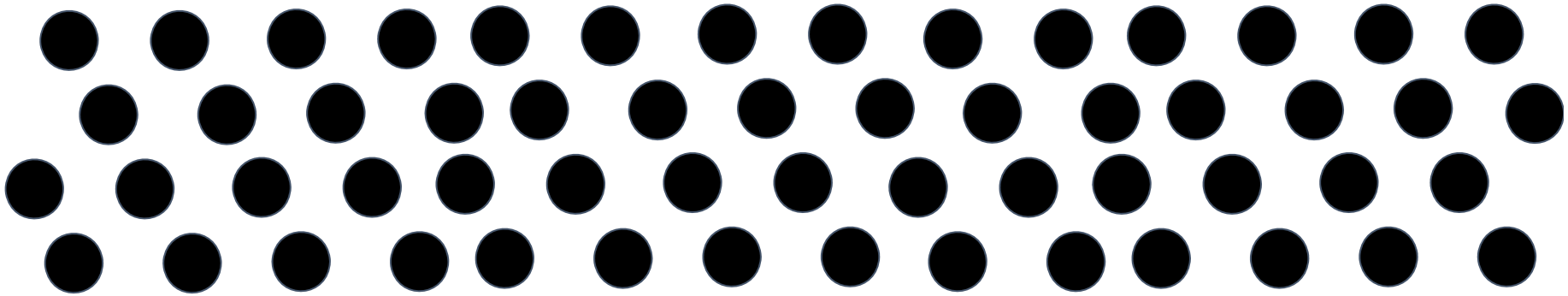
PM paramagnetic metal
PI paramagnetic insulator
AFI Antiferromagnetic insulator
CR crossover regime (poor conductor)

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

Metal-insulator transition



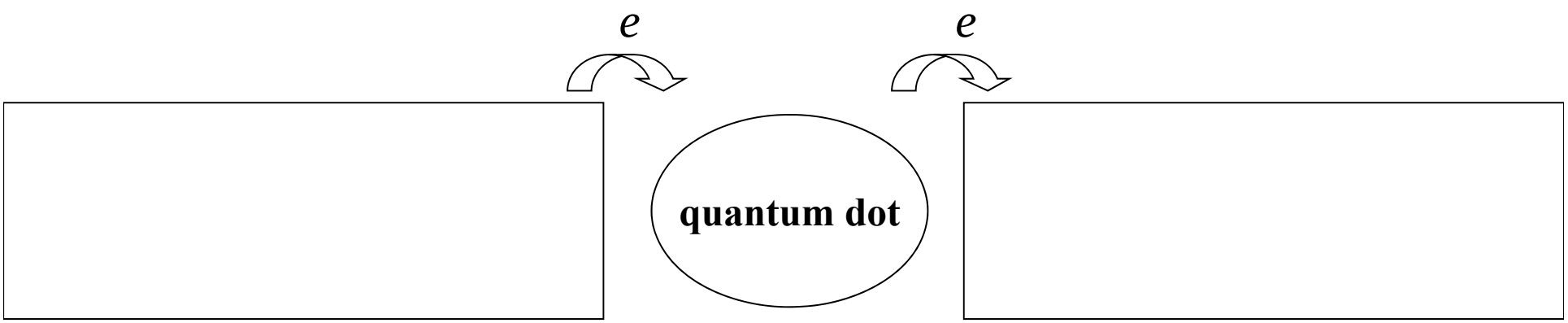
Clusters far apart: insulator



Clusters close together: metal

Charging effects

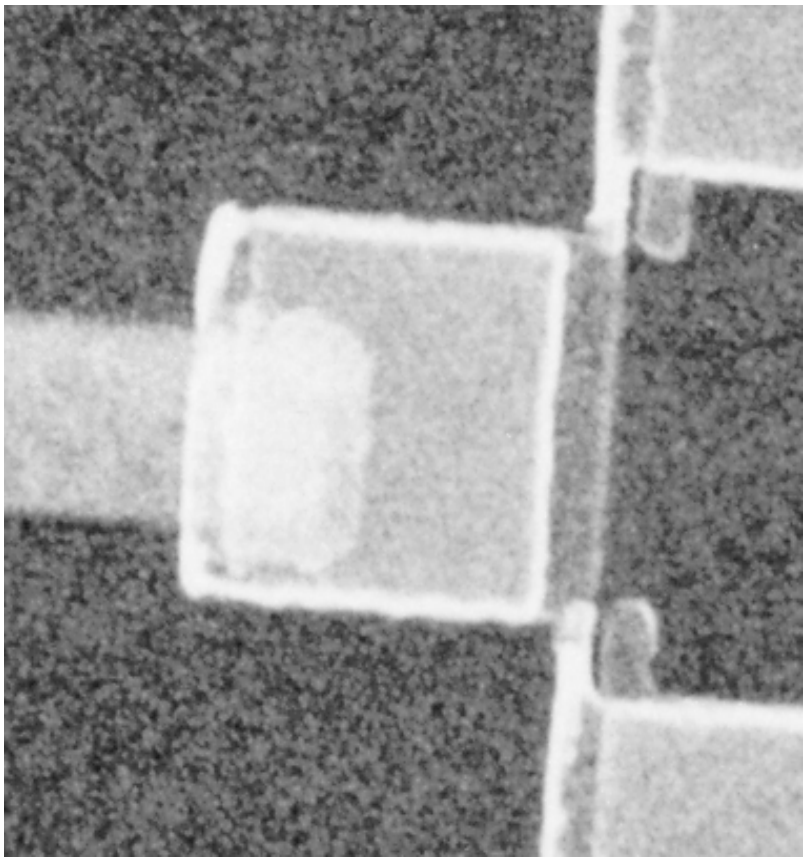
After screening, the next most simple approach to describing electron-electron interactions are charging effects.

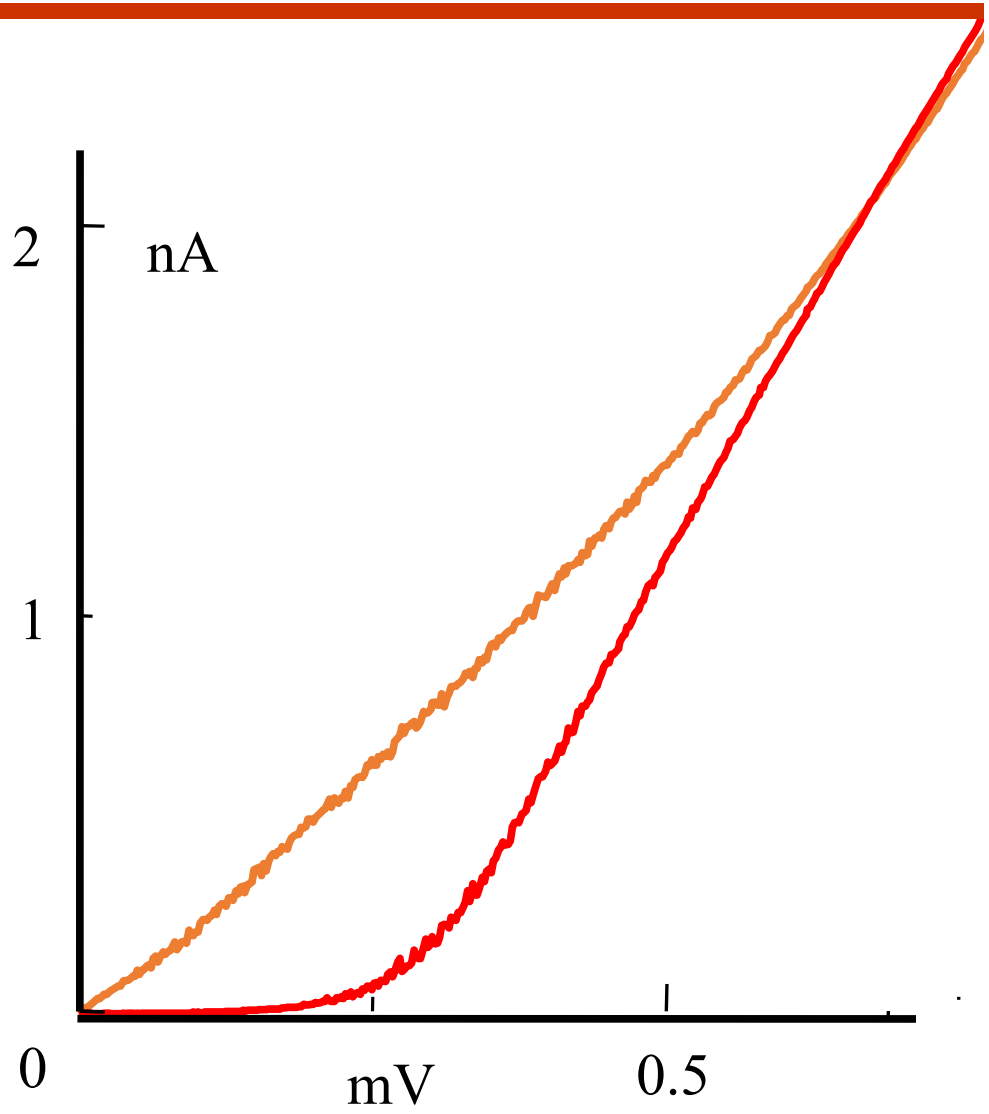


The motion of electrons through a single quantum dot is correlated.

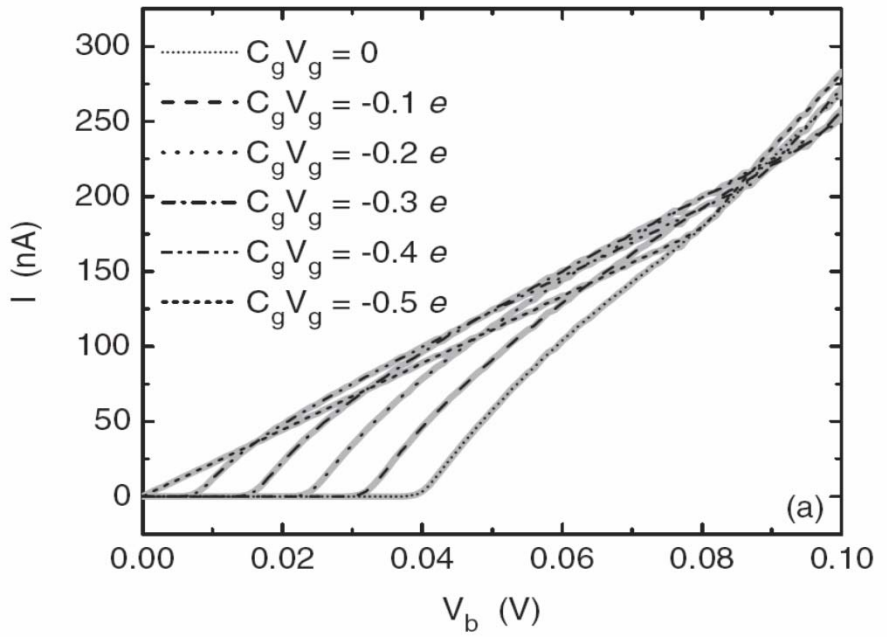
$$Q = CV$$

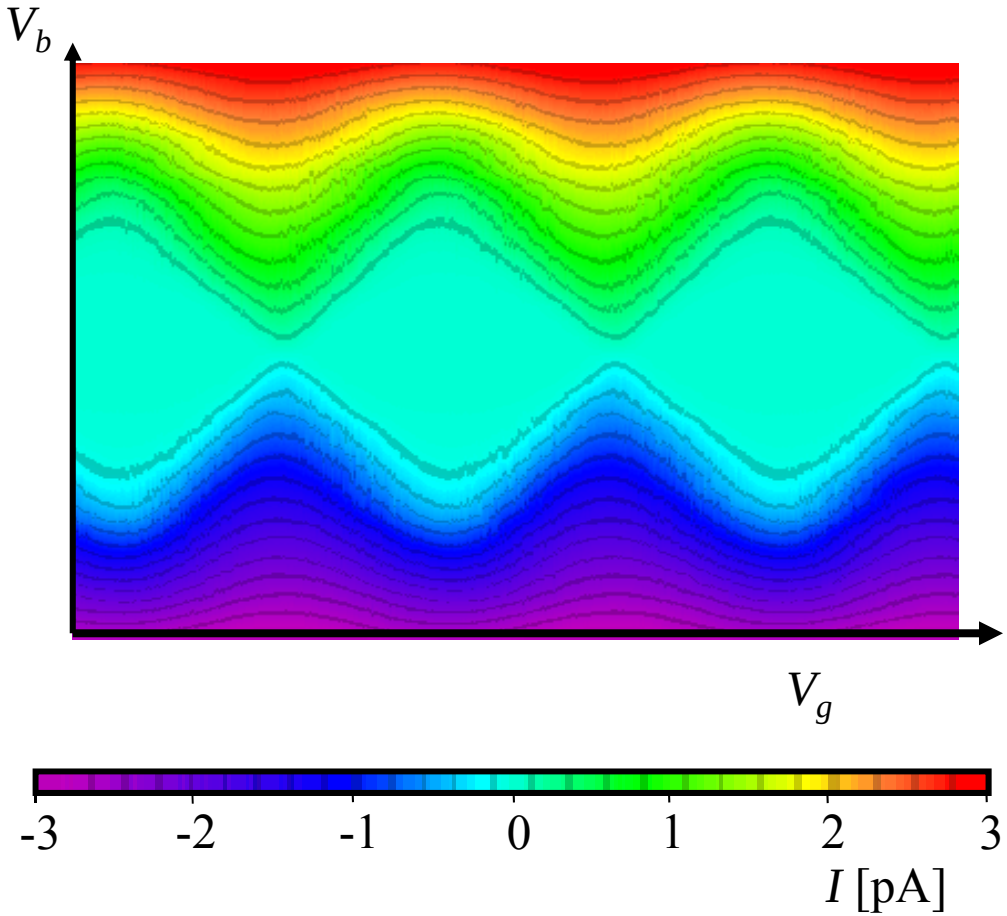
Single electron transistor

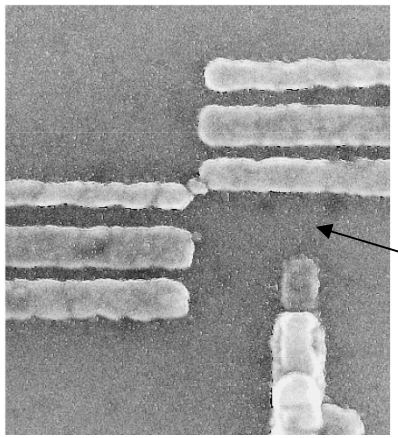




Coulomb blockade

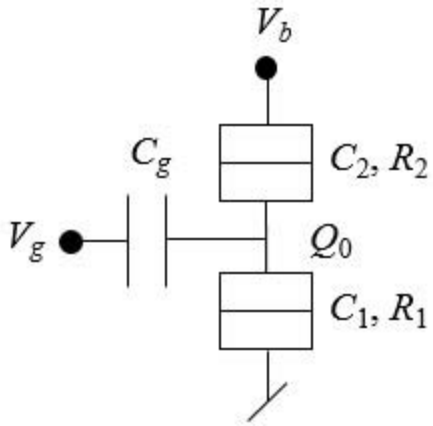


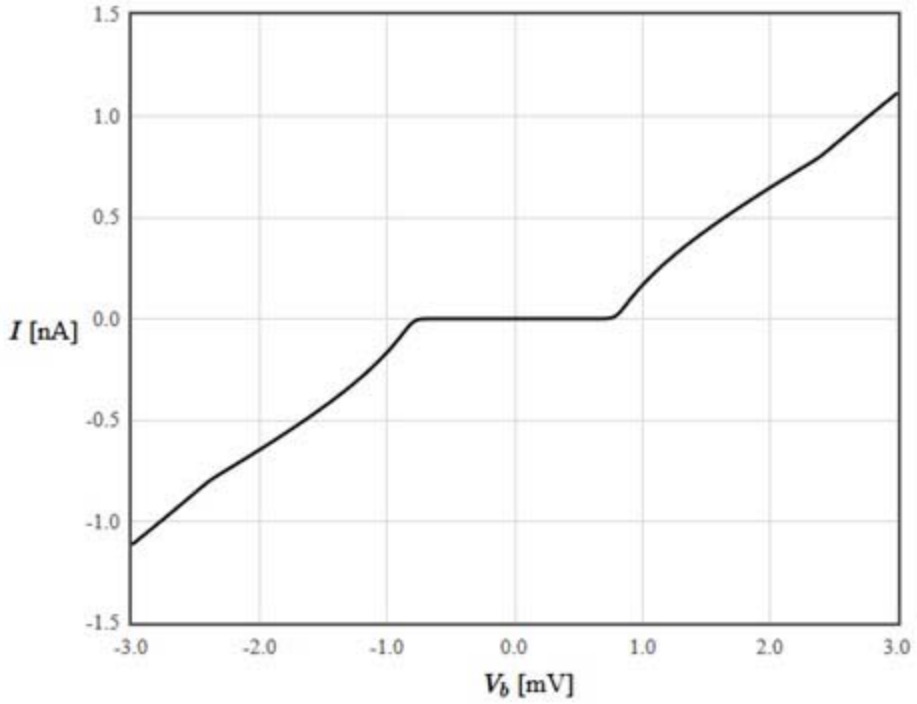




2 nm room temperature SET Pashkin/Tsai NEC

Single electron transistors





C_1 =	1E-16	F
C_2 =	1E-16	F
R_1 =	1E6	Ω
R_2 =	1E6	Ω
C_g =	1E-18	F
V_g =	0	V
Q_0 =	0	e
T =	0.1	K
V_b (start) =	-0.003	V
V_b (stop) =	0.003	V
N =	300	

Replot

http://lamp.tu-graz.ac.at/~hadley/set/asymIV/SETIV.html
http://lamp.tu-graz.ac.at/~hadley/set/symIV/SETIV.html

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 $RC_\Sigma < \frac{\hbar 2C_\Sigma}{e^2}$

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

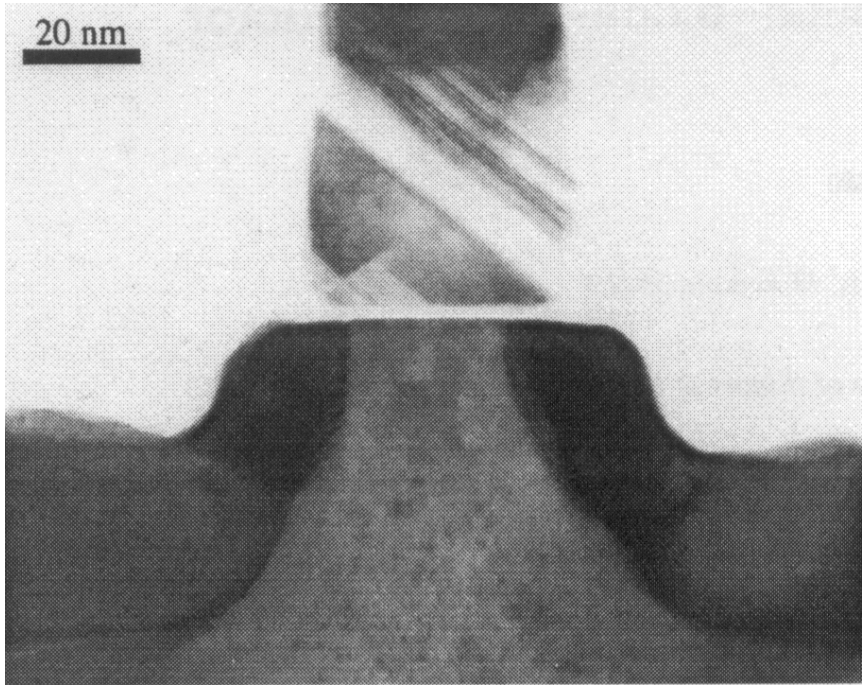
$$\frac{h}{e^2} \approx 25.5\ \mathrm{k\Omega}$$

Resistance quantum

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.

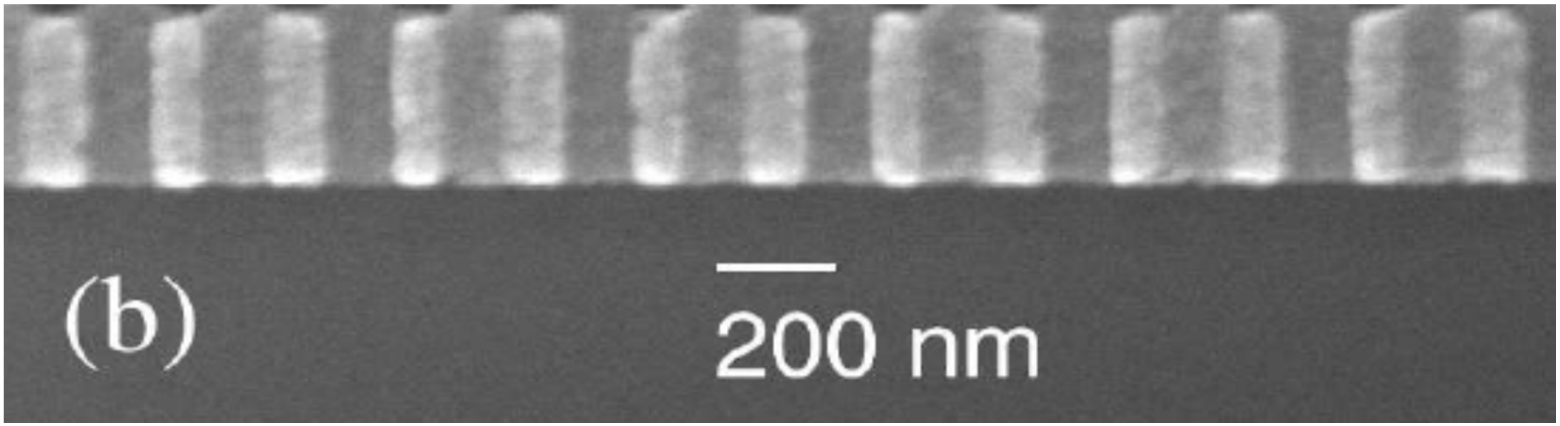


Metal - insulator transition in 1-d arrays

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

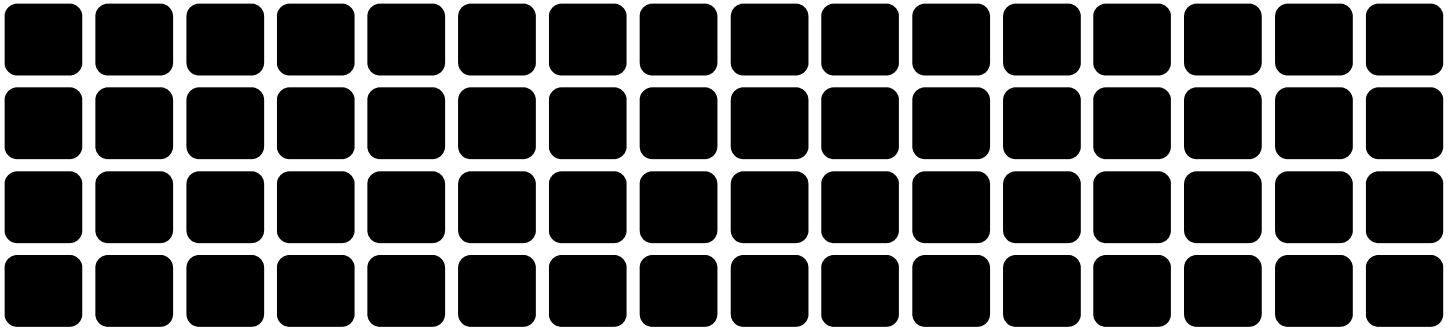
$$\Delta t = \frac{\hbar}{\Delta E} = \frac{2C\hbar}{e^2} > \frac{1}{\Gamma} = RC$$

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



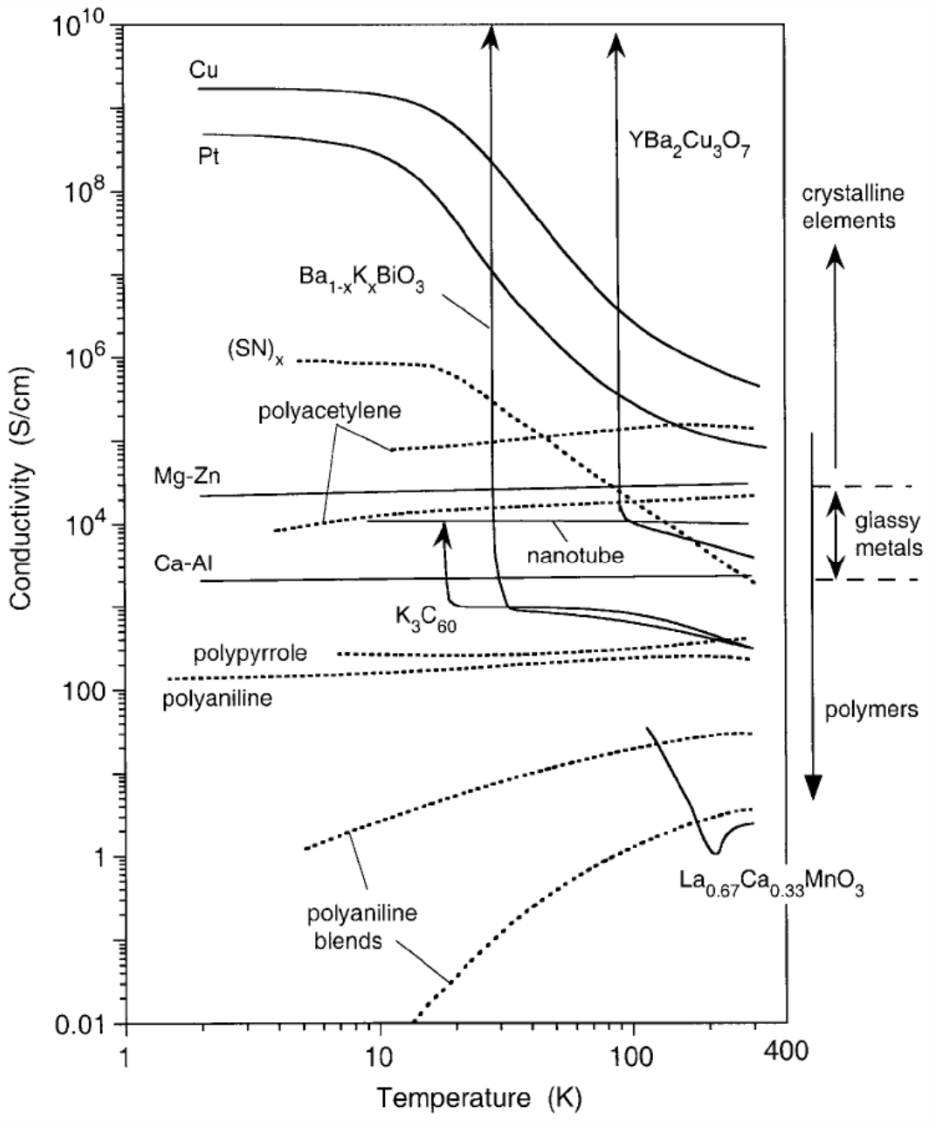
Metal insulator transition

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.

Temperature dependence of the conductivity

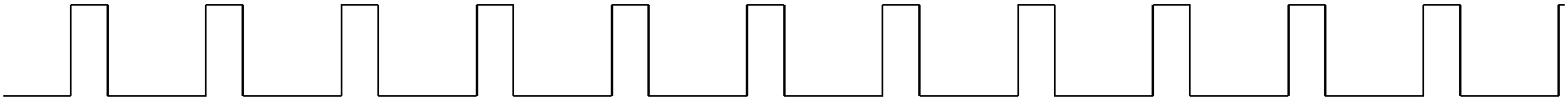


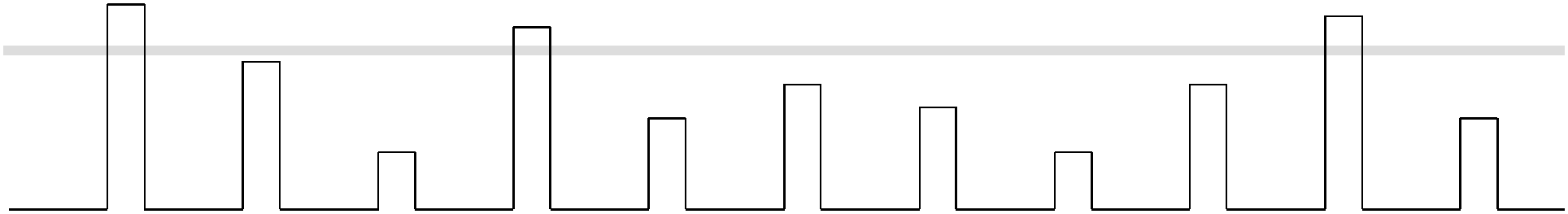
σ vs *T* tells us about the electron - electron and electron phonon interactions

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

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 (high resistivity)

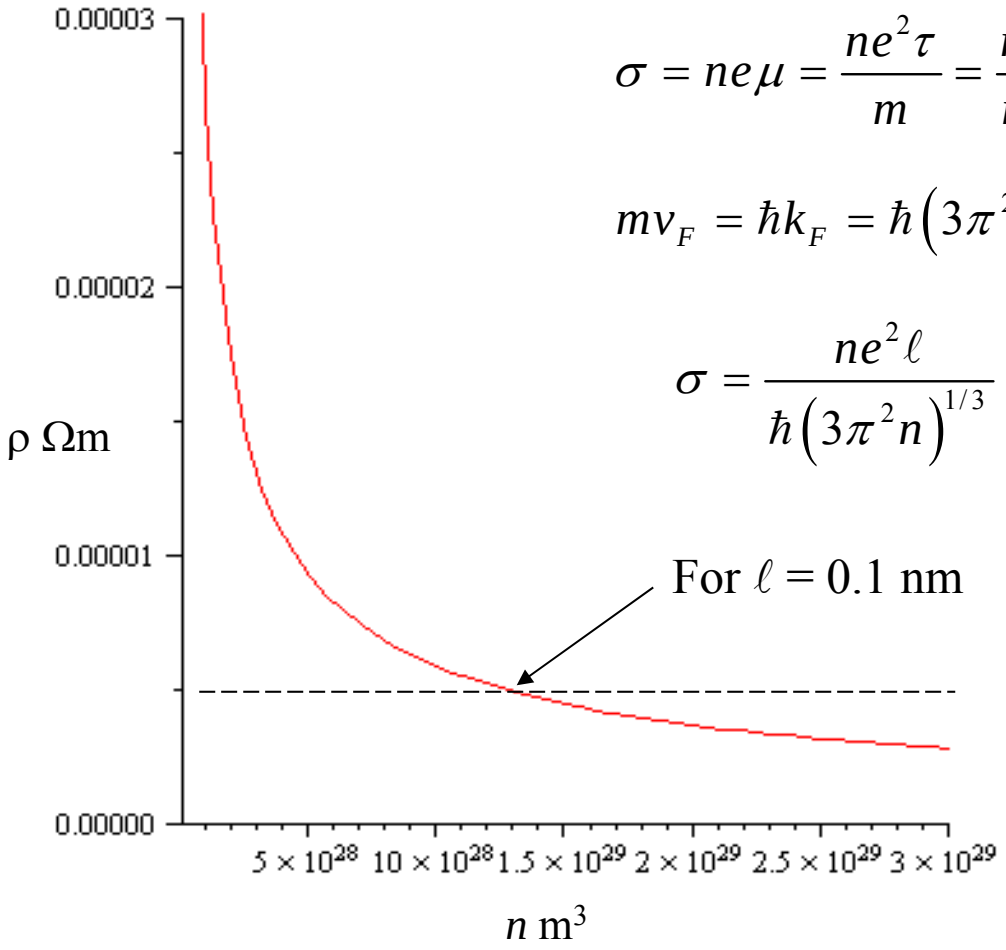
$$R_Q = \frac{h}{e^2} = \frac{\rho \ell}{wt} \approx 25\ \text{k}\Omega$$

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

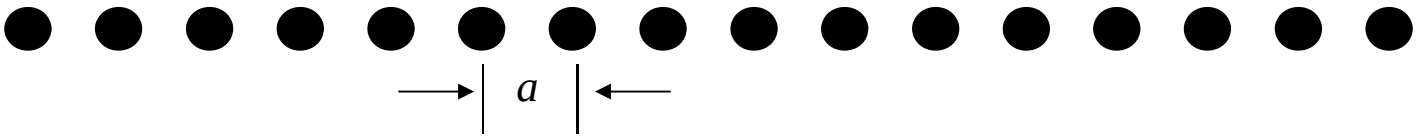
Predicted in the 1930's

Accidentally observed in the 1970's in TTF-TCNQ

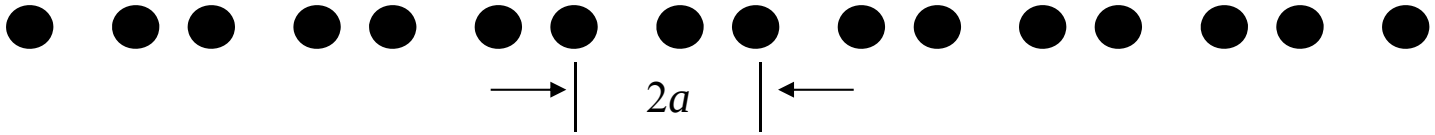
Rudolf Peierls
Quantum Theory of Solids
Surprises in Theoretical Physics
More Surprises in Theoretical Physics

Peierls Transition

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

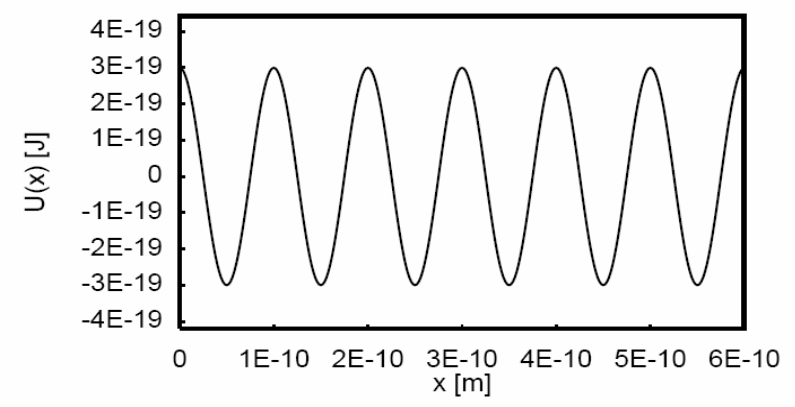


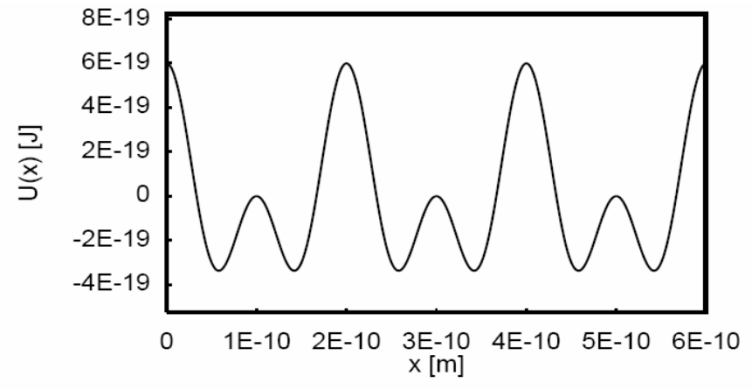
A periodic distortion of a 1-d lattice increases the periodicity to $2a$

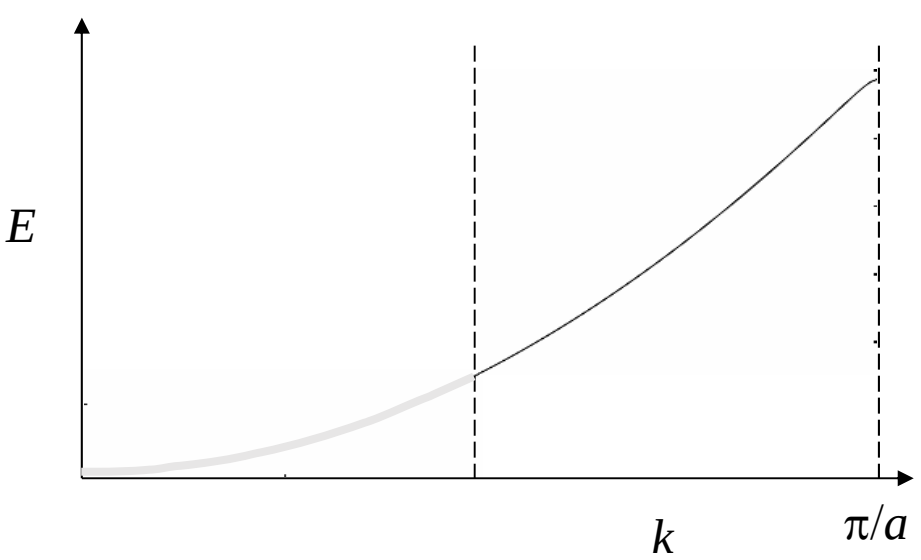


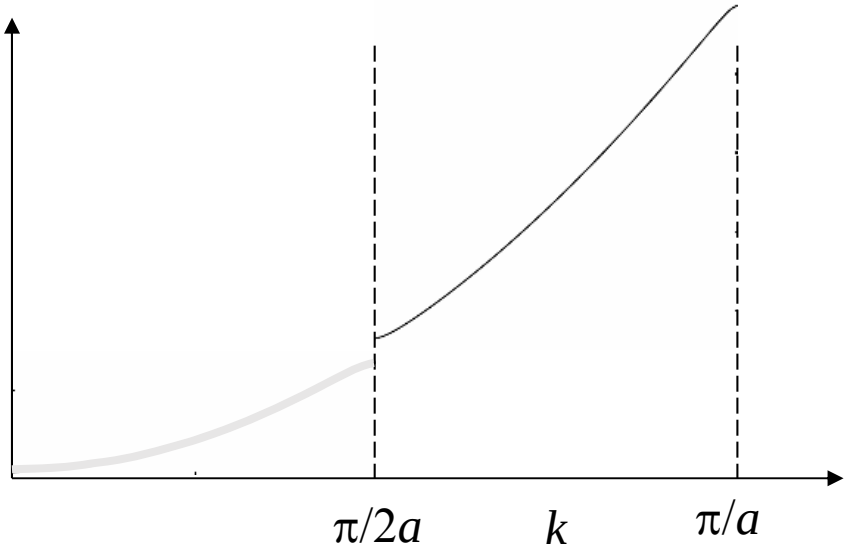
There are $2N$ states in each band. (N is the number of unit cells in the crystal)

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





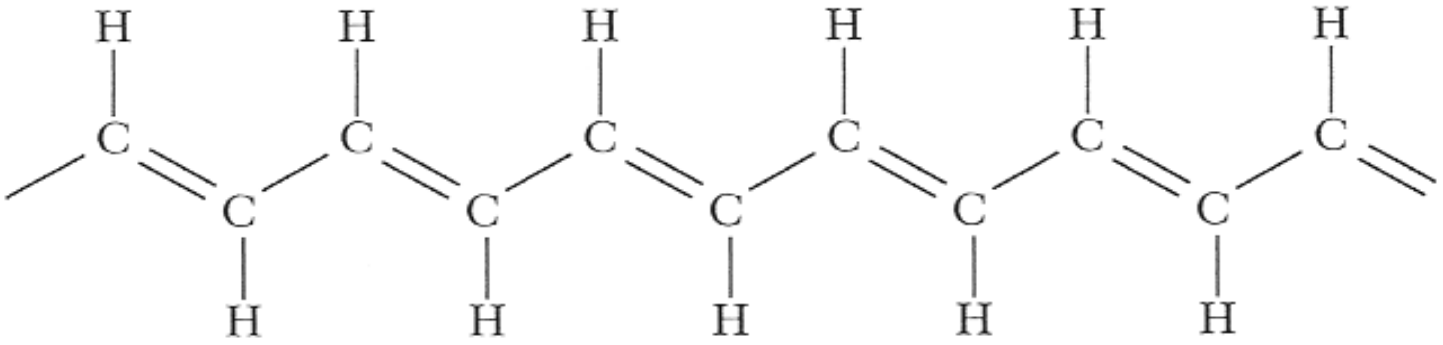




For a distortion of the lattice $\Delta\cos(2k_F x)$, the elastic energy increases like Δ^2 while the electronic energy decreases like Δ.

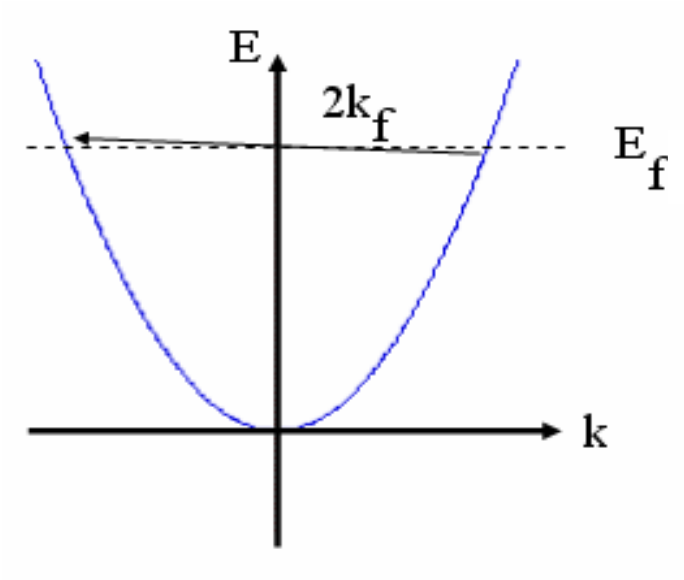
http://lamp.tu-graz.ac.at/~hadley/ss1/bloch/bloch.php

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.

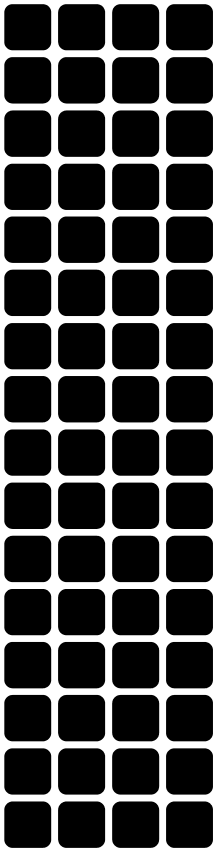
Suppression of backscattering in 1-D

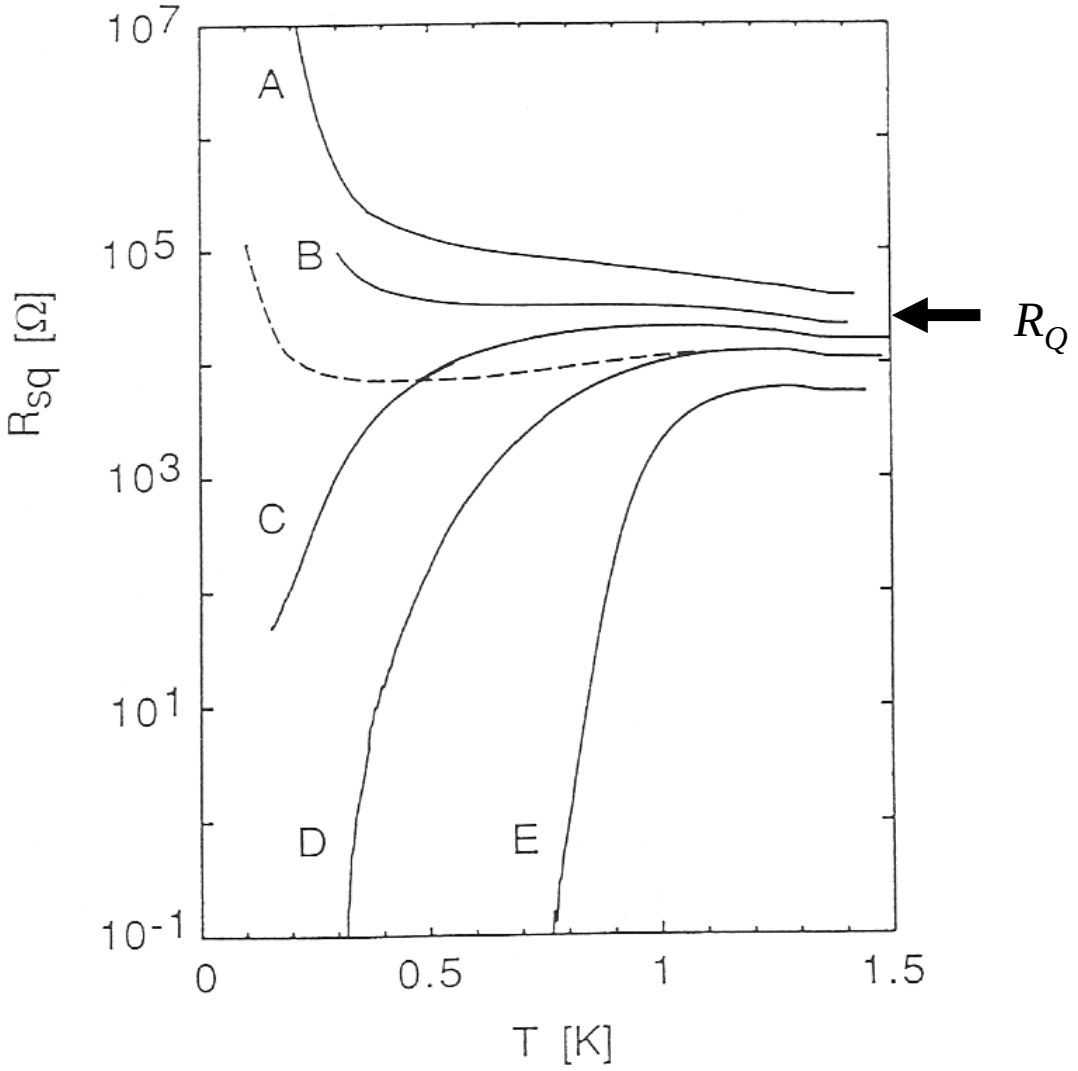


There are no phonons with momentum $2k_f$ at low T

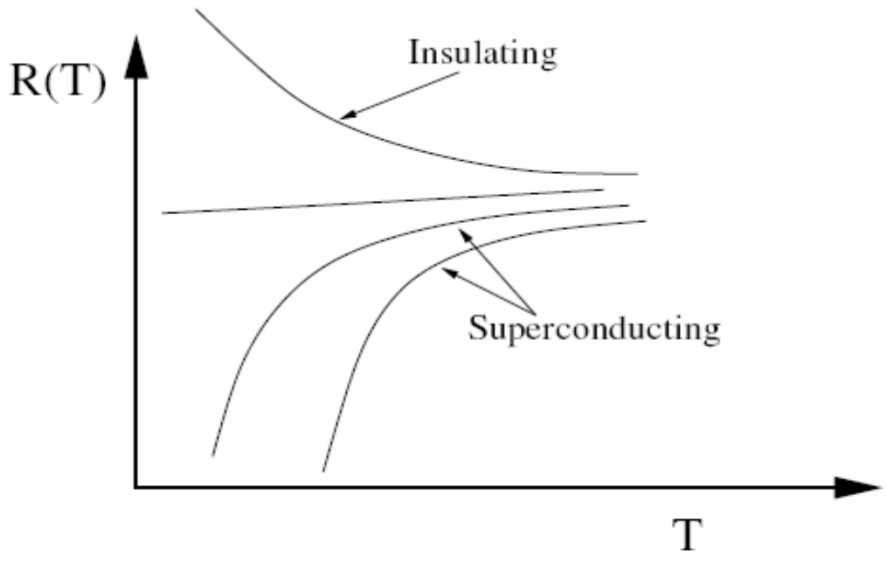
H. Sakaki, Jpn. J. Appl. Phys. Vol. 19 (1980) L735-L738

Josephson junction array





Geerligs PRL 63, p. 326 (1989).



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

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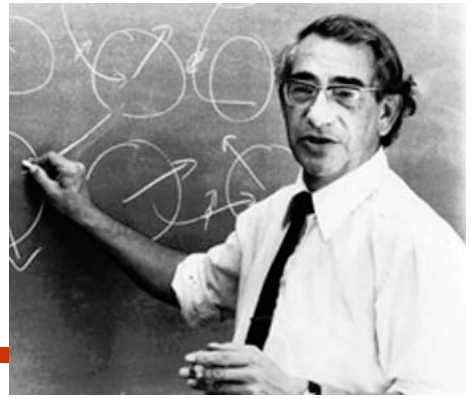
[2] NEST-INFM & Scuola Normale Superiore, Piazza dei Cavalieri 7, 56126 Pisa, Italy

[3] Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

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

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

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

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

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

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

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

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

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

Eigenvectors

$E = 0$

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

$E = 2.56$

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

$E = -1.56$

One eigenvalue is less than zero

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

$E = 1$

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

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

Ground state for various U/t

Table 7: Ground state energy and coefficients for $N = 2$, $N_+ = 1$ and different values of U/t; The ground state is $|\psi_0\rangle^{2,2}_{m_S=1}(U,t) = c_1|+-,0\rangle + c_2|+,-\rangle + c_3|-,+\rangle + c_4|0,+-\rangle$.

U	t	E_0	$\vec{c}$ (not normalized to)
0	1	-2.0000	1.0000 1.0000 1.0000 1.0000
0.1	1	-1.9506	1.0000 1.0253 1.0253 1.0000
0.5	1	-1.7656	1.0000 1.1328 1.1328 1.0000
1	1	-1.5616	1.0000 1.2808 1.2808 1.0000
1.5	1	-1.3860	1.0000 1.4430 1.4430 1.0000
2	1	-1.2361	1.0000 1.6180 1.6180 1.0000
3	1	-1.0000	1.0000 2.0000 2.0000 1.0000
5	1	-0.7016	1.0000 2.8508 2.8508 1.0000

The antiferromagnetic states become more occupied for larger U/t

R. Messner, A. Postl