### Charging effects

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



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

## Single electron transistor



#### Coulomb blockade



#### Single electron transistors



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

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http://lamp.tu-graz.ac.at/~hadley/set/ivg/ivg.html



#### Single electron transistor



$$Q = C_1(V - V_1) + C_2(V - V_2) + C_g(V - V_g)$$
$$Q = -ne$$
$$V(n) = \left(-ne + C_1V_1 + C_2V_2 + C_gV_g\right) / C_{\Sigma}$$
$$C_{\Sigma} = C_1 + C_2 + C_g$$

#### Single electron transistor

The potential of the island with *n* electrons on it:

$$V(n) = \left(-ne + C_1 V_1 + C_2 V_2 + C_g\right) / C_{\Sigma}$$

The energy needed to add an infinitesimal charge dq to an island at voltage V(n) is V(n)dq. The energy needed to add a whole electron is:



The energy needed to remove a whole electron is:

$$\Delta E = \int_{0}^{e} V(n) dq = eV(n) + \frac{e^{2}}{2C_{\Sigma}}$$









Jarillo-Herrero, et al., Nature 429, 389 (2004).



# Coulomb blockade suppressed by thermal and quantum fluctuations

Thermal fluctuations

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

2

Quantum fluctuations

 $\Delta E \Delta t > \hbar$ 

Duration of a quantum fluctuation:

$$\Delta t \sim \frac{\hbar 2 C_{\Sigma}}{e^2}$$

 $RC_{\Sigma}$ 

*RC* charging time of the capacitance:

Charging faster than a quantum fluctuation

$$R < \frac{2\hbar}{e^2} \approx 8 \text{ k}\Omega$$
$$\frac{h}{e^2} \approx 25.5 \text{ k}\Omega$$

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

Resistance quantum

#### Metal - insulator transition in 1-d arrays

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

$$\Delta t = \frac{\hbar}{\Delta E} = \frac{2C\hbar}{e^2} > \frac{1}{\Gamma} = RC$$
$$R < \frac{2\hbar}{e^2} \qquad \text{extended state}$$



#### Metal insulator transition

If the tunnel resistances between the crystals is > 25 k $\Omega$ , 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.







Random tunnel barriers, some with resistances above the resistance quantum

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

### 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





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

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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/

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

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

$$\uparrow,\uparrow$$
 or  $\downarrow,\downarrow$ 

They can't hop and the energy is zero.

If the electrons have opposite spin

$$\uparrow,\downarrow$$
 or  $\uparrow,\downarrow$  or  $\uparrow\downarrow,0$  or  $0,\uparrow\downarrow$ 

the states couple together.

$$\begin{split} |\psi\rangle &= a |\uparrow\downarrow,0\rangle + b |\uparrow,\downarrow\rangle + c |\downarrow,\uparrow\rangle + d |0,\uparrow\downarrow\rangle \\ &H |\psi\rangle = E |\psi\rangle \\ H &= -t \sum_{\langle i,j\rangle,\sigma} c_{i,\sigma}^{\dagger} c_{j,\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \\ &\langle\uparrow\downarrow,0|H|\psi\rangle = Ua - tb - tc \\ \begin{bmatrix} U & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & U \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = E \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} \end{split}$$

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

with(LinearAlgebra): U == 1			
t := 1:			
Hubbard := Matrix([[U, -t, -t, 0], [-t, 0, 0])	[-t], [-t, 0, 0, -t], [0, -t, -t, U]]);		
	$\begin{bmatrix} 1 & -1 & -1 & 0 \end{bmatrix}$		
	-1 0 0 -1		
	-1 0 0 -1		
Eigenvectors(Hubbard);			
	4	4	1
	0 (1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1		-1
[ 0 ]	$\left(\frac{1}{2} + \frac{1}{2}\sqrt{17}\right)\left(-\frac{1}{2} + \frac{1}{2}\sqrt{17}\right)$	$\left(\frac{1}{2} - \frac{1}{2}\sqrt{1}\right) \left(-\frac{1}{2} - \frac{1}{2}\sqrt{1}\right)$	
1 1	2	2	
$\frac{1}{2} + \frac{1}{2}\sqrt{17}$	-1 1 1 77	1 1 777	0
1 1	$\frac{1}{2} + \frac{1}{2} \sqrt{17}$	$\frac{1}{2} - \frac{1}{2} \sqrt{17}$	1.1
$\frac{1}{2} - \frac{1}{2}\sqrt{17}$	2	2	
4 4			0
	$\frac{1}{2} + \frac{1}{2}\sqrt{17}$	$\frac{1}{2} - \frac{1}{2} \sqrt{17}$	Ŭ
	0 1		1
		1	1

#### Eigenvectors

$$E = 0 \qquad \begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
$$E = 2.56 \qquad \begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ -0.780776466 \\ -0.780776466 \\ -1.780776466 \\ 1 \end{bmatrix} = \begin{bmatrix} 2.5615529319999997 \\ -2 \\ -2 \\ 2.5615529319999997 \end{bmatrix}$$
$$E = -1.56 \qquad \begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1.2807764064 \\ 1.2807764064 \\ 1 \end{bmatrix} = \begin{bmatrix} -1.5615528128 \\ -2 \\ -2 \\ -1.5615528128 \end{bmatrix}$$
One eigenvalue is less than zero 
$$\begin{bmatrix} 1 & -1 & -1 & 0 \\ -1 & 0 & 0 & -1 \\ 0 & -1 & -1 & 1 \end{bmatrix} \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

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