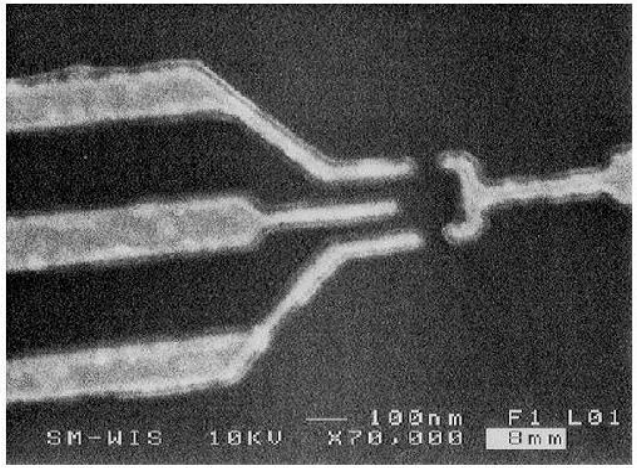
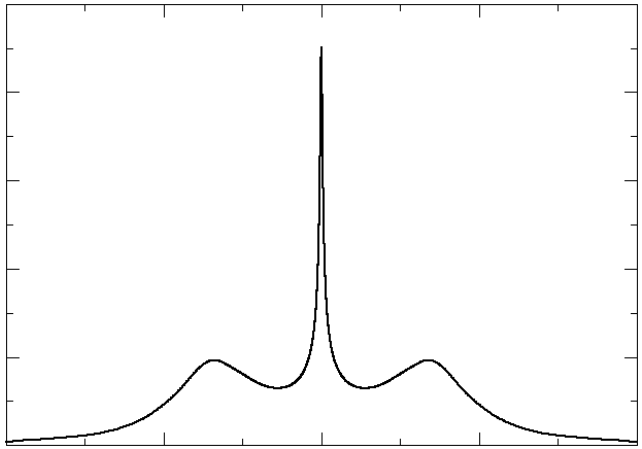
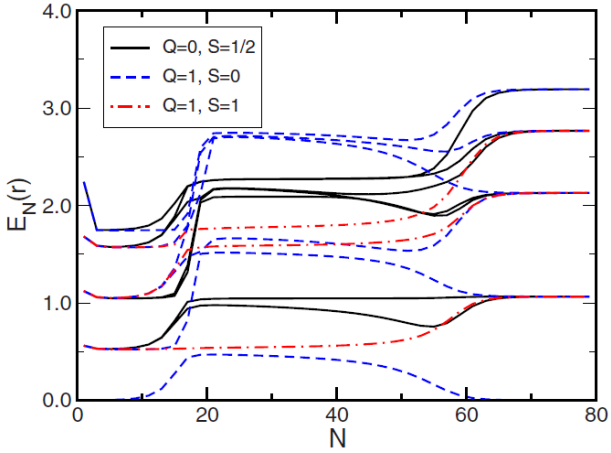
NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS







http://www.staff.science.uu.nl/~mitch003/nrg.html

March 2015

Andrew Mitchell, Utrecht University

Quantum impurity problems

- **Part 1: Quantum impurity problems and theoretical background**
- **Part 2: Kondo effect and RG. 1d chain formulation and iterative diagonalization**
- **Part 3: Logarithmic discretization and truncation. The RG in NRG**
- **Part 4: Physical quantities. Results and discussion.**

General References:

- K. G. Wilson, Rev. Mod. Phys. 47, 773 (1975)
- A. C. Hewson, "*The Kondo problem to Heavy Fermions*" (Cambridge University Press, 1997)
- H. R. Krishnamurthy, J. W. Wilkins and K. G. Wilson, Phys. Rev. B, 21, 1003 (1980); *ibid* 21, 1044 (1980)
- R. Bulla, T. Costi, T. Pruschke, Rev. Mod. Phys. 80, 395 (2008)

NUMERICAL METHODS FOR QUANTUM IMPURITY MODELS

Part 1: Quantum Impurity Problems and theoretical background

March 2015

Andrew Mitchell, Utrecht University

Overview: Part 1

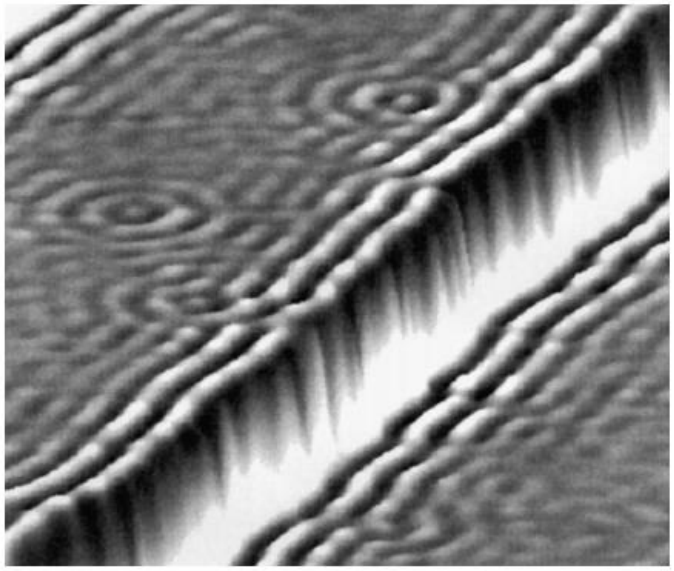
- Impurities in metals
- Quantum dots
- Dynamical Mean Field Theory

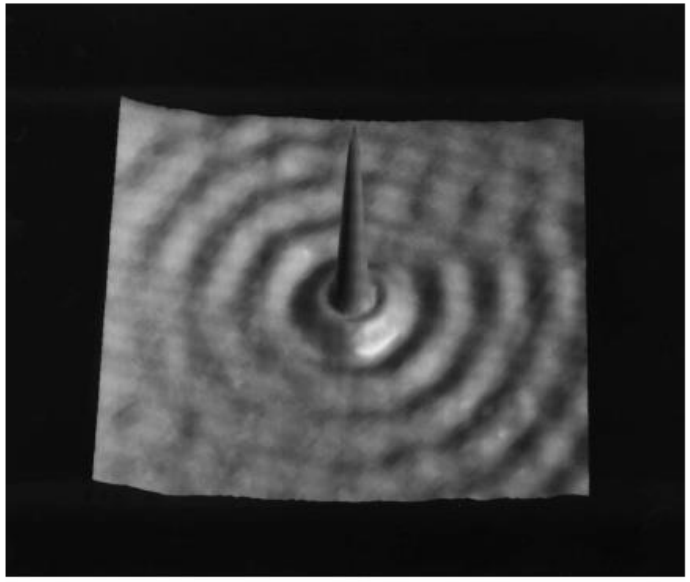
- Non-interacting limit
- Green functions

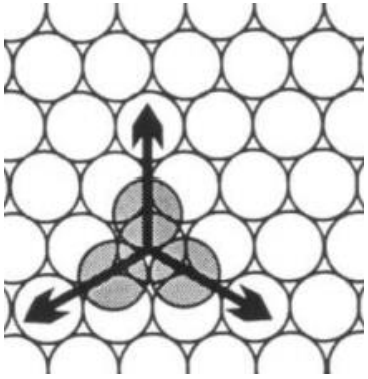
- The problem of interactions

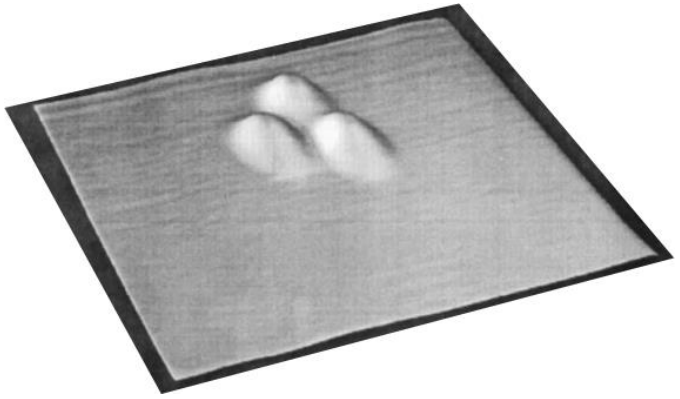
Impurities in metals

- **Defects**
- **Potential scattering centres**
- **Magnetic impurities**



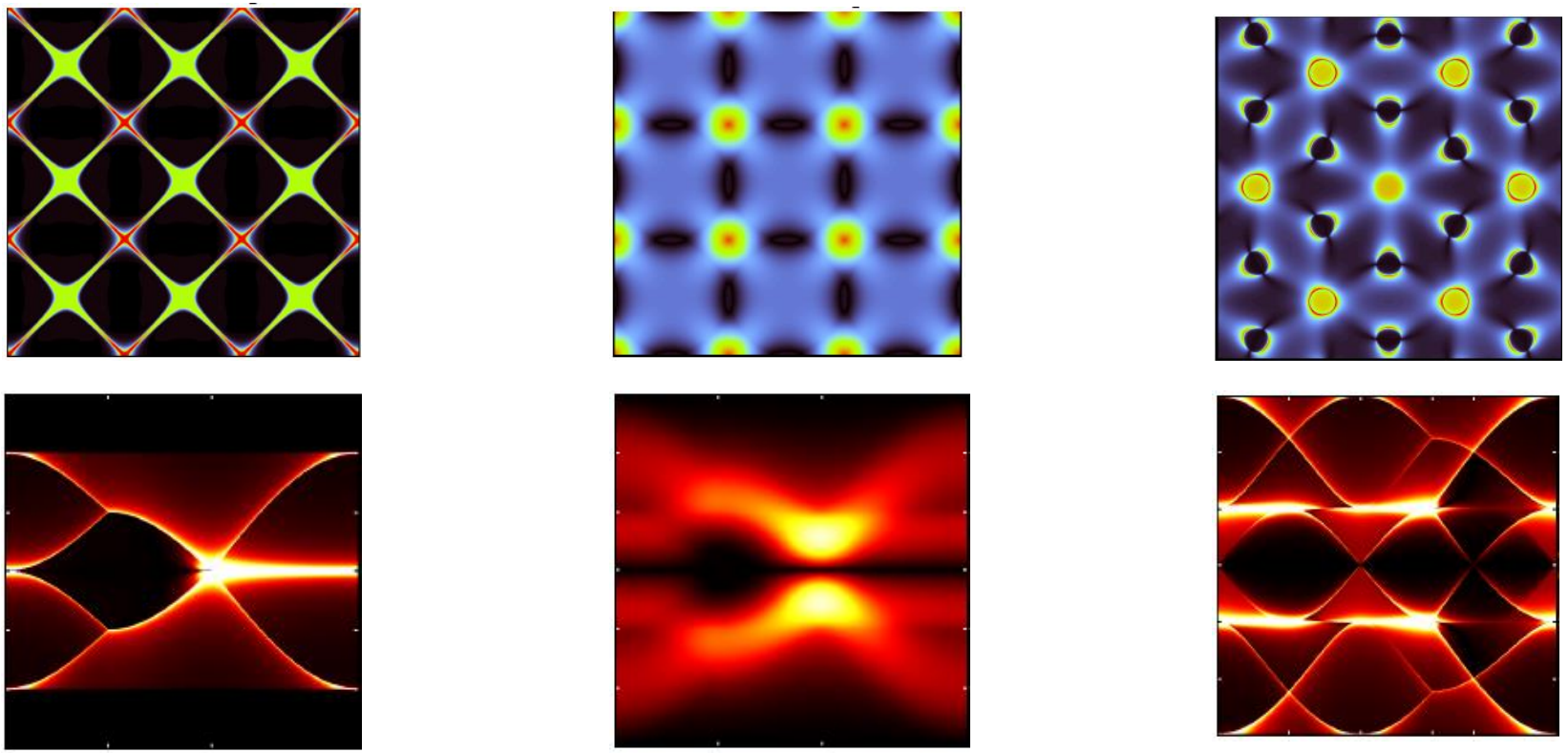






Impurities as probes

- **Break translational symmetry of host**
- **Cause scattering of quasiparticles**
- **FT-STS → quasiparticle interference**



Impurities in metals

- **Quantum impurity problem**
  - **Hamiltonian:**

$$H = H_{host} + H_{imp} + H_{hyb}$$

  - **'Host' consists of non-interacting conduction electrons:**

$$H_{host} = \sum_{k,\sigma} \varepsilon_k \, b^{\dagger}_{k\sigma} b_{k\sigma}$$

('diagonal' or 'k-space' basis)

  - **'Impurity' part: a few local, interacting degrees of freedom**

Impurities in metals

- **Kondo model: a spin-½ impurity, $\vec{S}_{imp}$, coupled by antiferromagnetic exchange to conduction electron spin density of the host at impurity location (0)**

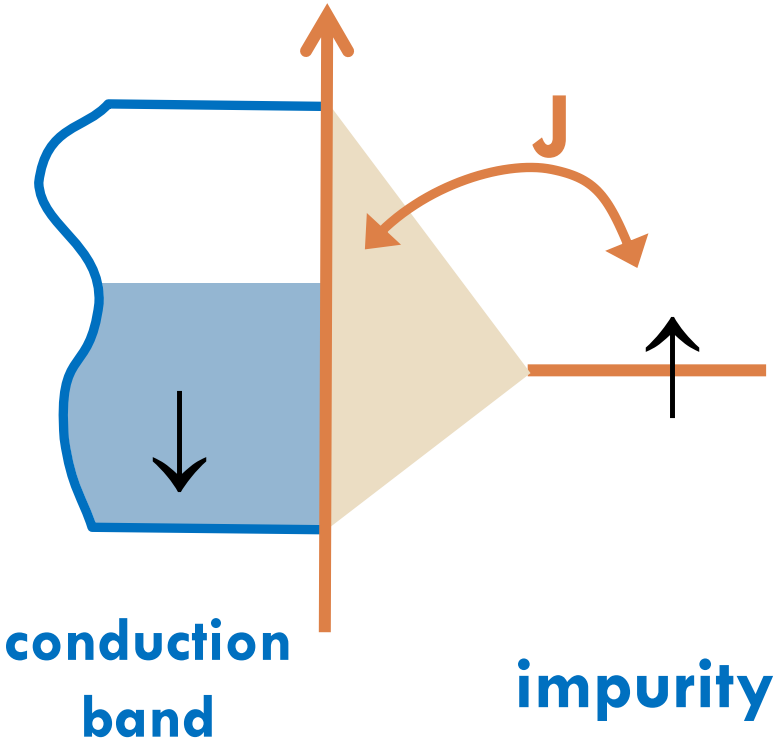
$$H_K = H_{host} + J\ \vec{S}_{imp} \cdot \vec{s}_0$$

$$\sum_{k,\sigma} \varepsilon_k\ b^\dagger_{k\sigma} b_{k\sigma}$$

$$\sum_{k,k'} b^\dagger_{k\,\sigma}\ \frac{\vec{\sigma}_{\sigma\sigma'}}{2}\ b_{k'\,\sigma'}$$

Impurities in metals

- **Kondo model**: **spin-flip scattering**



Impurities in metals

- **Anderson model: a single quantum level, with onsite Coulomb repulsion, tunnel-coupled to conduction electrons of host**

$$H_{AIM} = H_{host} + H_{imp} + H_{hyb}$$

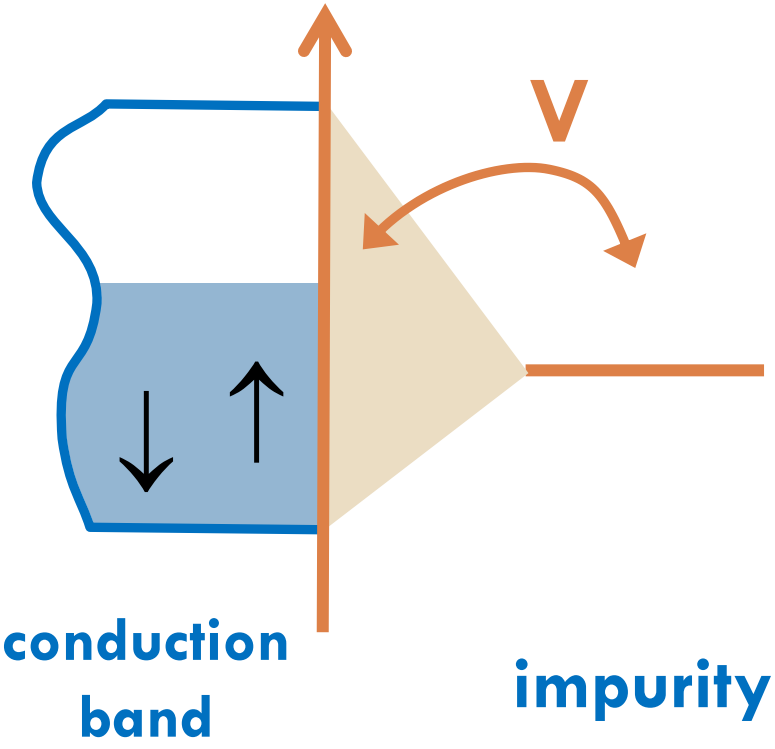
$$H_{host} = \sum_{k,\sigma} \varepsilon_k \, b^\dagger_{k\sigma} b_{k\sigma}$$

$$H_{imp} = \varepsilon_d \left(d^\dagger_\uparrow d_\uparrow + d^\dagger_\downarrow d_\downarrow \right) + U_d \, d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow$$

$$H_{hyb} = \sum_{k,\sigma} \left(V_k \, d^\dagger_\sigma \, b_{k\sigma} + \text{H.c.} \right)$$

Impurities in metals

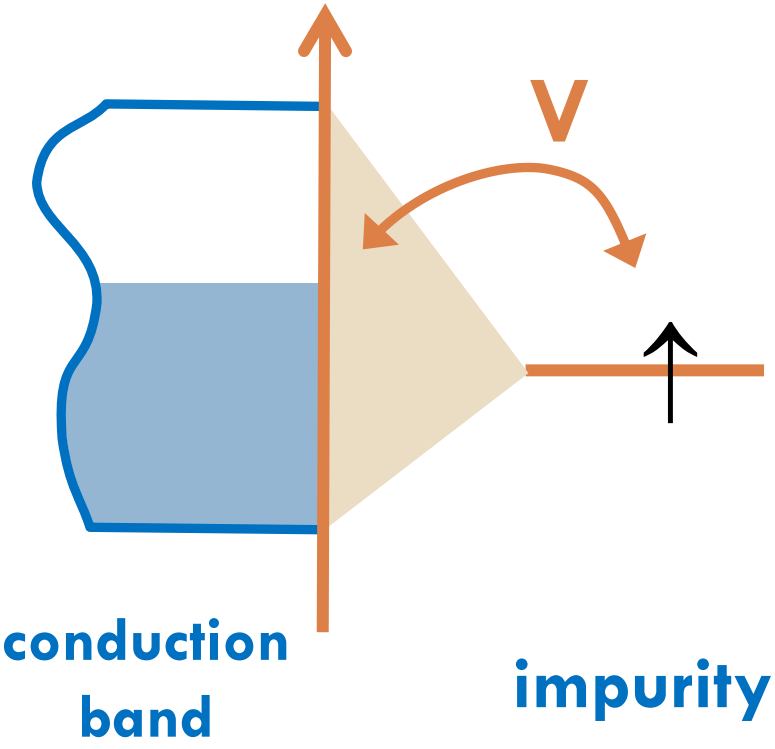
- **Anderson model:**



$$E_{imp} = \varepsilon_d + U_d$$

Impurities in metals

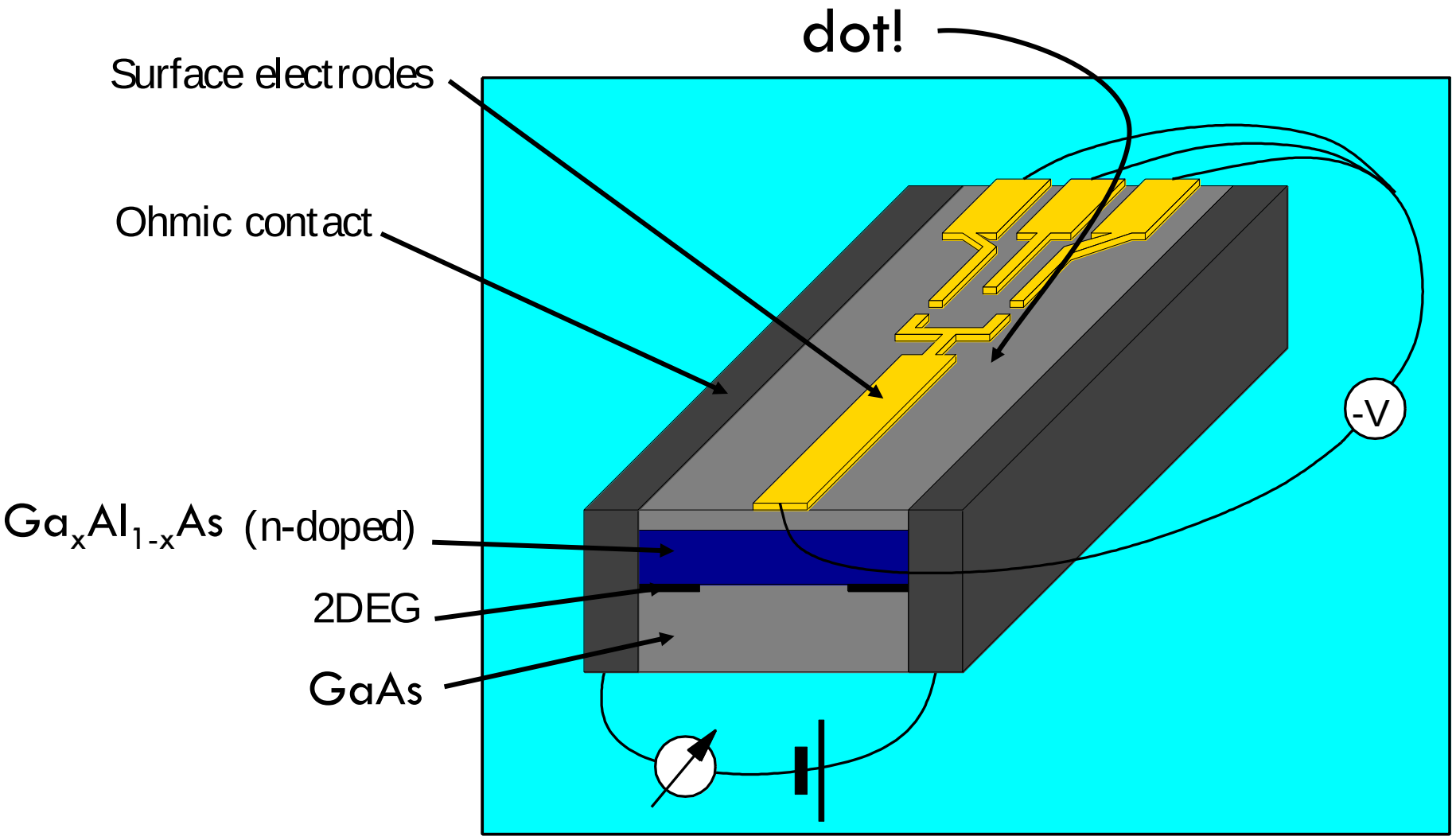
- **Anderson model:**



essentially singly-occupied local moment for

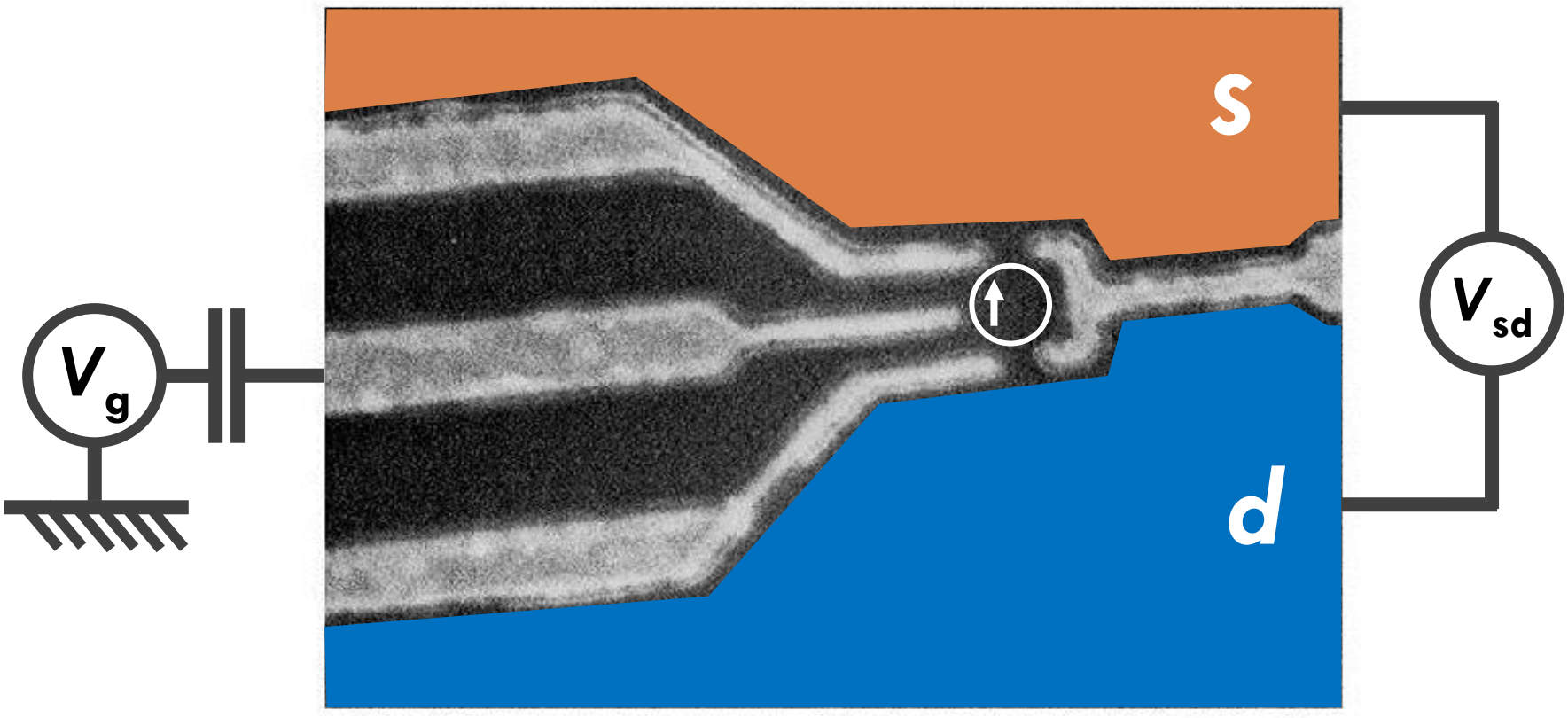
$$-U_d < \varepsilon_d < 0$$

Semiconductor Quantum Dots

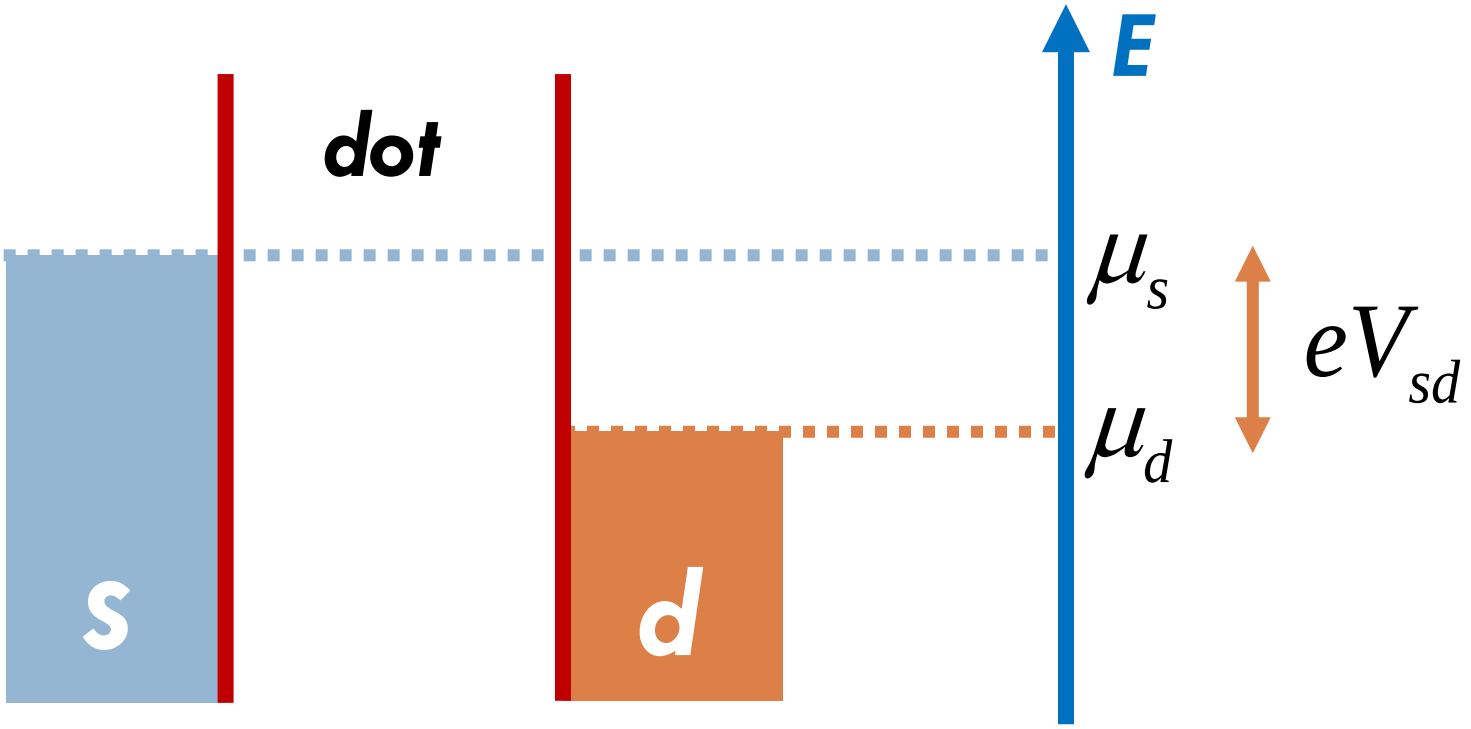


Quantum dots

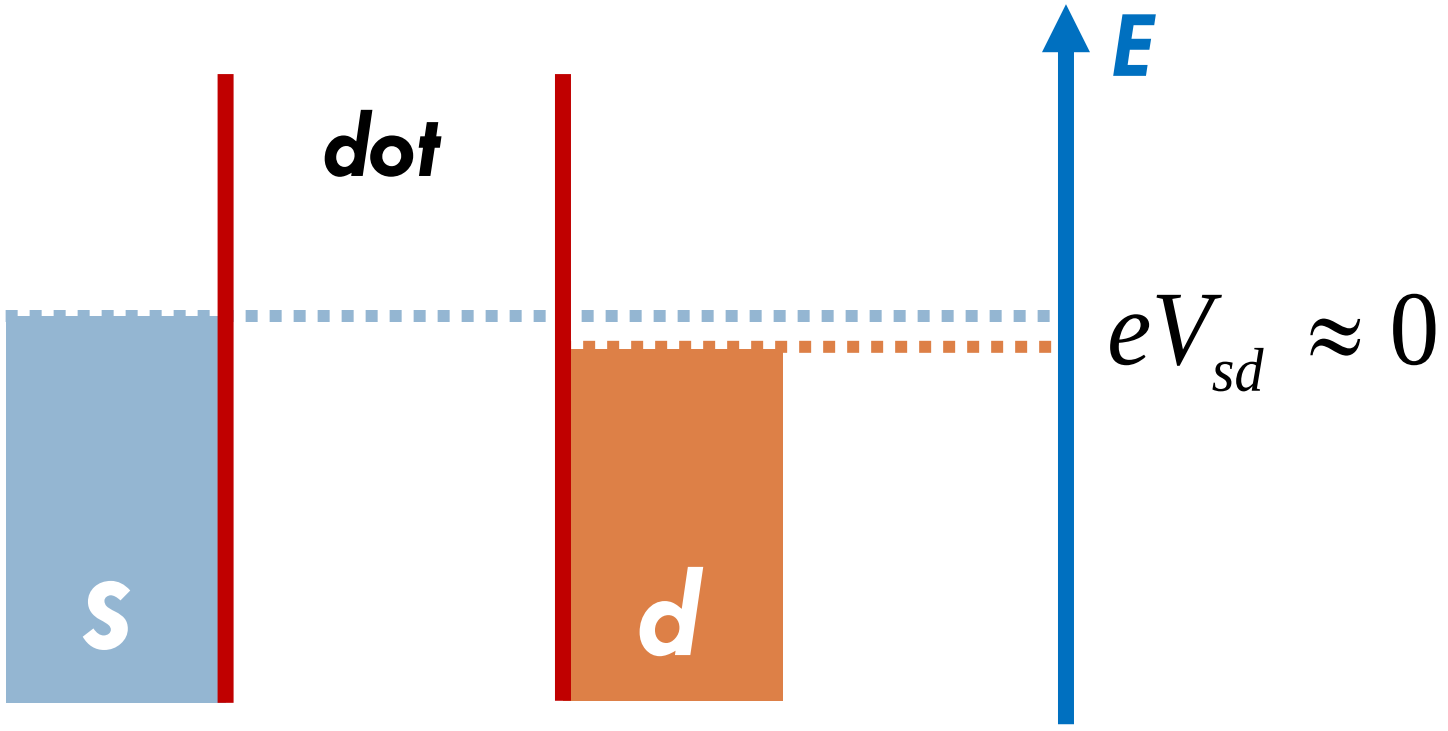
Goldhaber-Gordon *et al.*, Nature 391, 156 (1998)



Coulomb Blockade



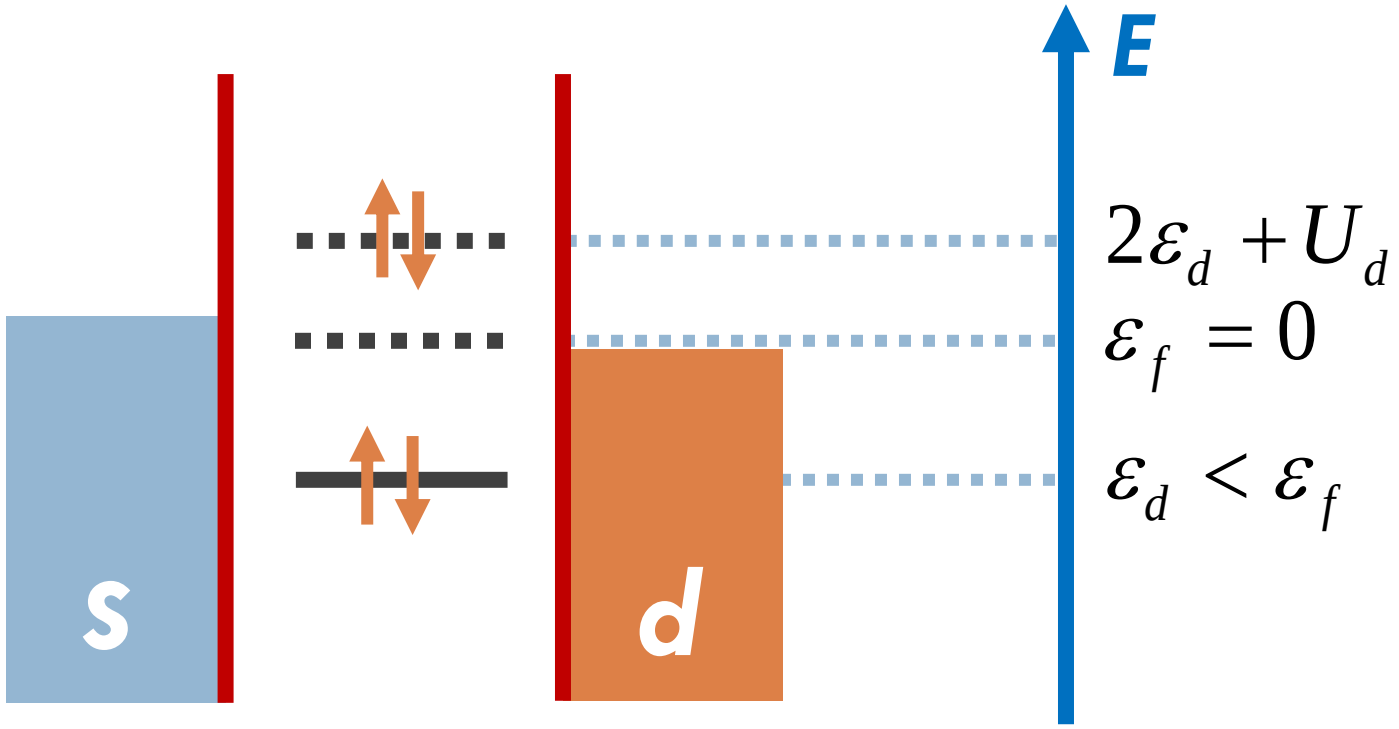
Coulomb Blockade



Coulomb Blockade

Coulomb Blockade

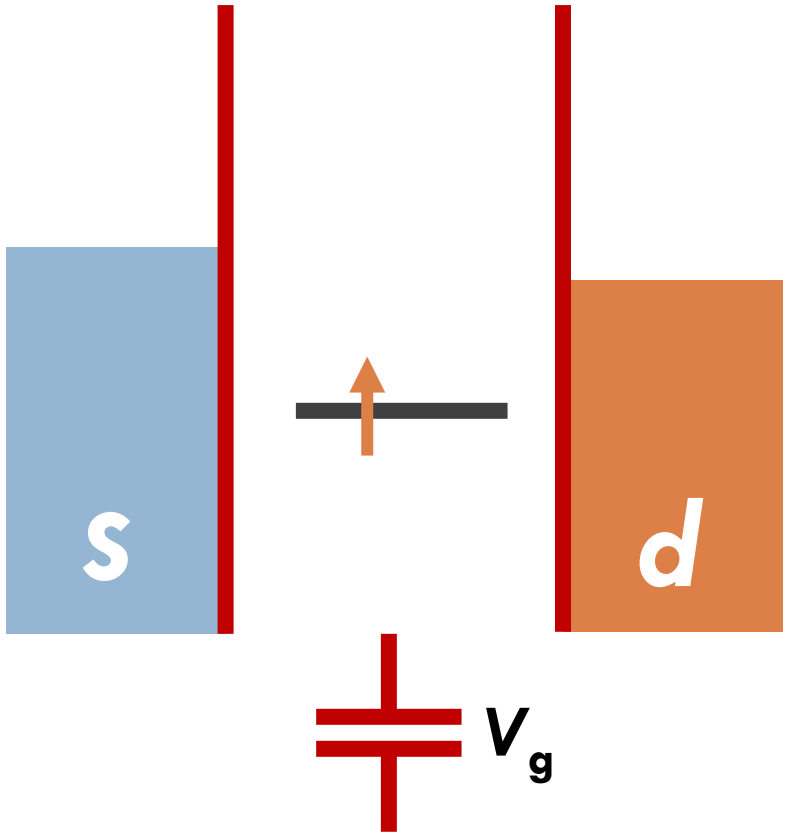
- **Coulomb repulsion blocks sequential tunneling**



- **Active level carries a spin-½ local moment**

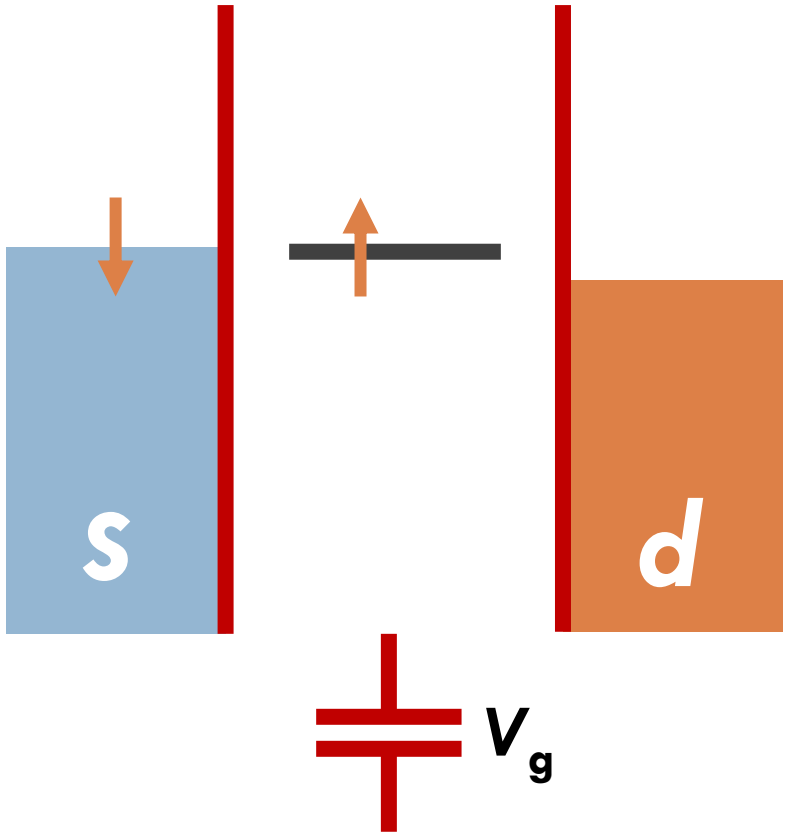
Coulomb Blockade

- **But: gate voltage controls dot occupancy…** $\varepsilon_d \propto V_g$



Coulomb Blockade

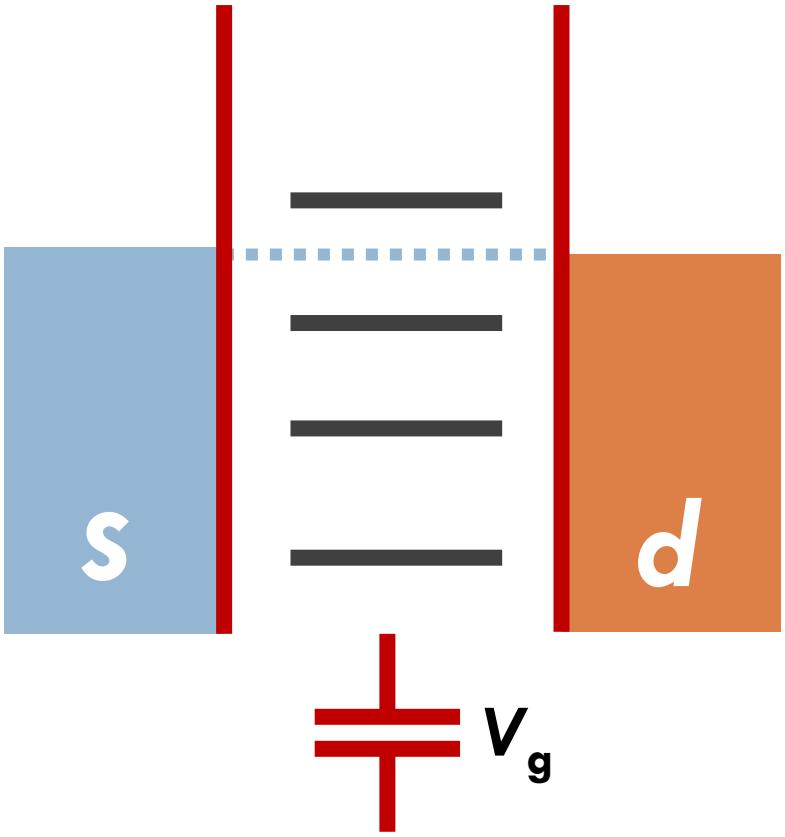
- **But: gate voltage controls dot occupancy…** $\varepsilon_d \propto V_g$

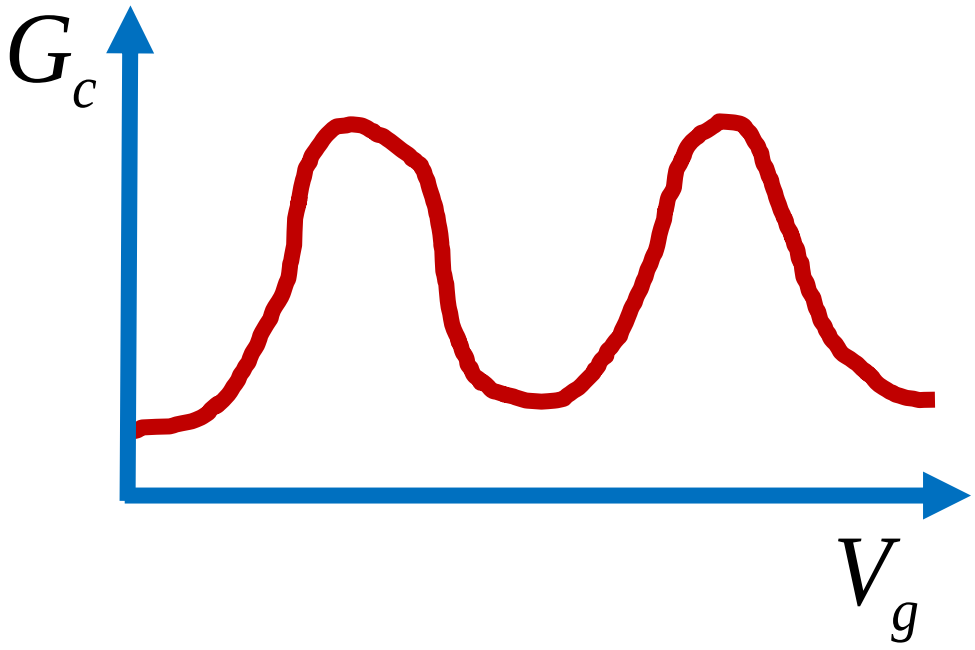


- **Sequential tunneling at points of dot valence fluctuation**
- **Effective level width renormalized by interactions**

Coulomb Blockade

- **Conductance peaks as gate voltage is swept:**

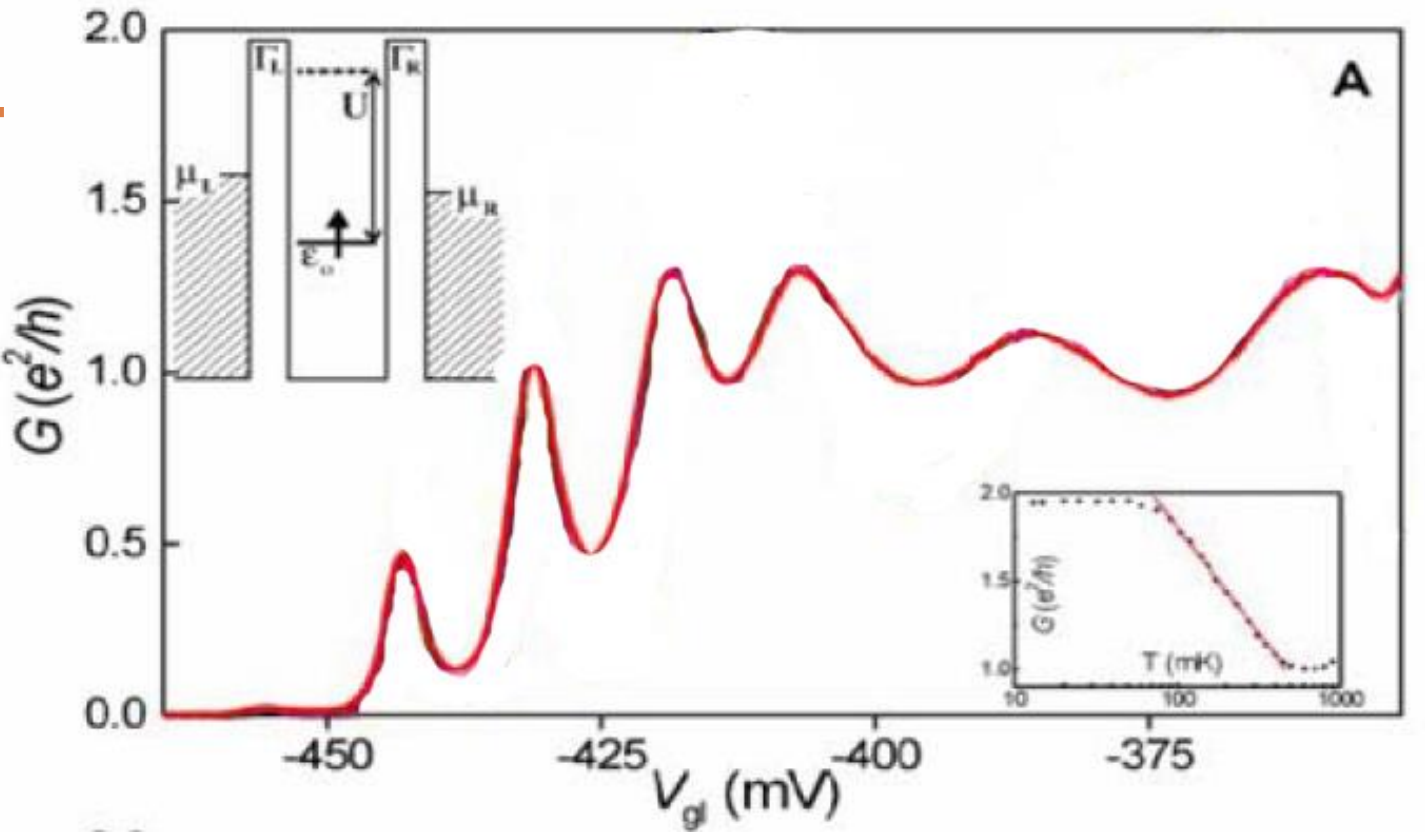




Coulomb Blockade: experiment

- **Conductance peaks as gate voltage is swept:**

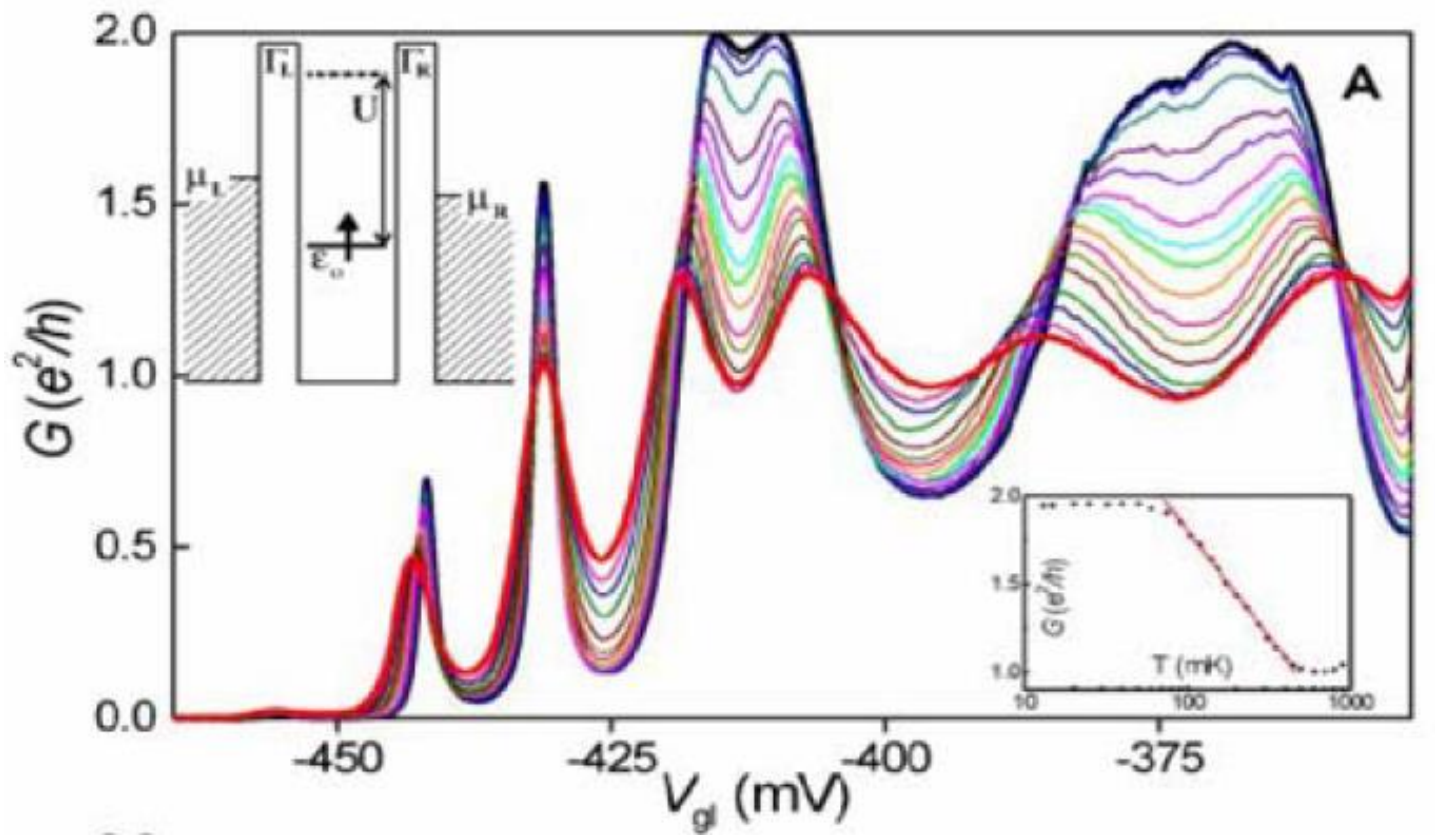
High-T



Van der Wiel et al, Science 289, 2105 (2000)

Kondo Effect

- **Low temperature: quantum many body effects!**



Van der Wiel et al, Science 289, 2105 (2000)

Anderson Impurity Model

- **Real quantum dot devices:**
  - **Model as a single active interacting quantum *level***
  - ***Tunnel-coupled* to source and drain leads**

$$H_{AIM} = H_{leads} + H_{dot} + H_{hyb}$$

$$\sum_{\alpha=s,d} \sum_{k,\sigma} \varepsilon_k b^\dagger_{\alpha k \sigma} b_{\alpha k \sigma}$$

$$\varepsilon_d \left(d^\dagger_\uparrow d_\uparrow + d^\dagger_\downarrow d_\downarrow \right) + U_d \, d^\dagger_\uparrow d_\uparrow d^\dagger_\downarrow d_\downarrow$$

$$\sum_{\alpha,k,\sigma} \left(V_{\alpha k} d^\dagger_\sigma b_{\alpha k \sigma} + \text{H.c.} \right)$$

Anderson Impurity Model

- **Equilibrium (zero bias):**
  - **Combine leads into a single conduction electron channel**

$$H_{hyb} = \sum_{\alpha,k,\sigma} \left(V_{\alpha k}\, d_\sigma^\dagger\, b_{\alpha k \sigma} + \text{H.c.} \right)$$

$$= \sum_{\sigma,k} \left(V_k\, d_\sigma^\dagger\, f_{k\sigma} + \text{H.c.} \right)$$

$$f_{k\sigma} = \frac{1}{V_k} \left(V_{sk}\, b_{sk\sigma} + V_{dk}\, b_{dk\sigma} \right) \qquad V_k^2 = \sum_\alpha V_{\alpha k}^2$$

Anderson Impurity Model

- **Equilibrium (zero bias):**
  - **Combine leads into a single conduction electron channel**

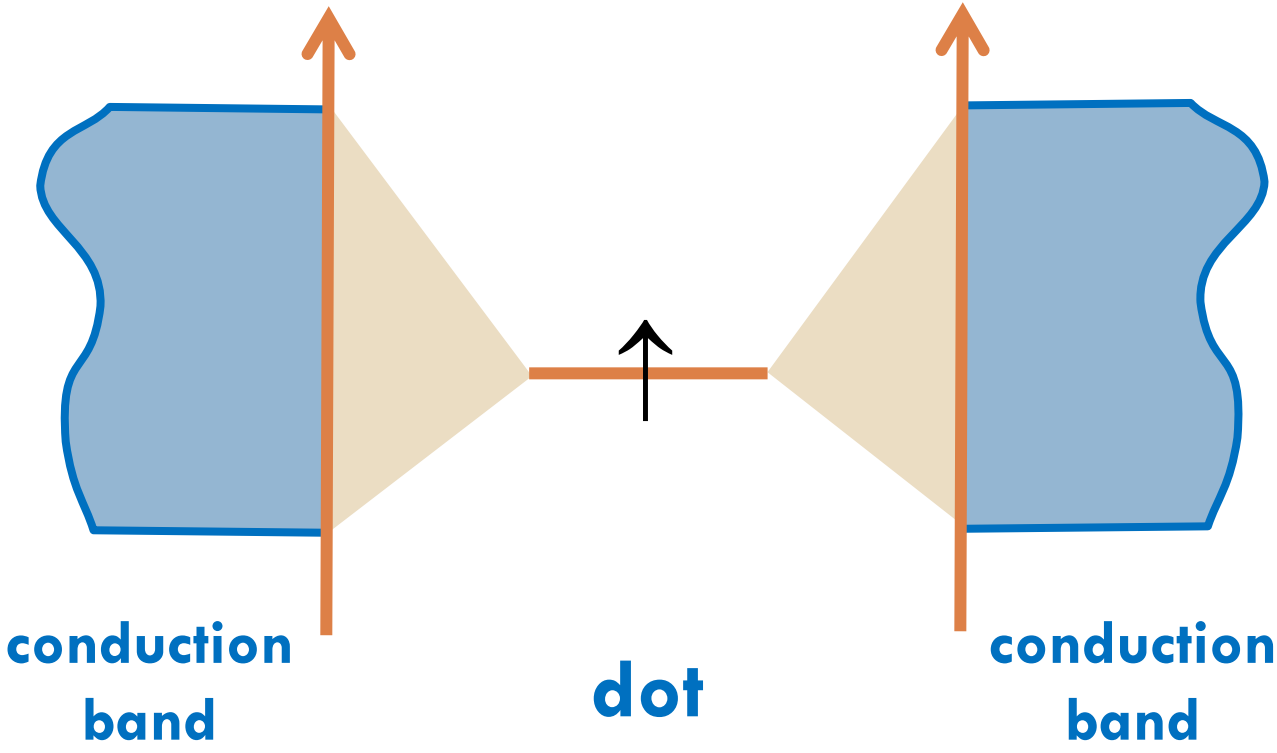
$$H_{leads} = \sum_{\alpha=s,d} \sum_{k,\sigma} \varepsilon_k b^{\dagger}_{\alpha k \sigma} b_{\alpha k \sigma}$$

$$= \sum_{\sigma,k} \varepsilon_k f^{\dagger}_{k\sigma} f_{k\sigma}$$

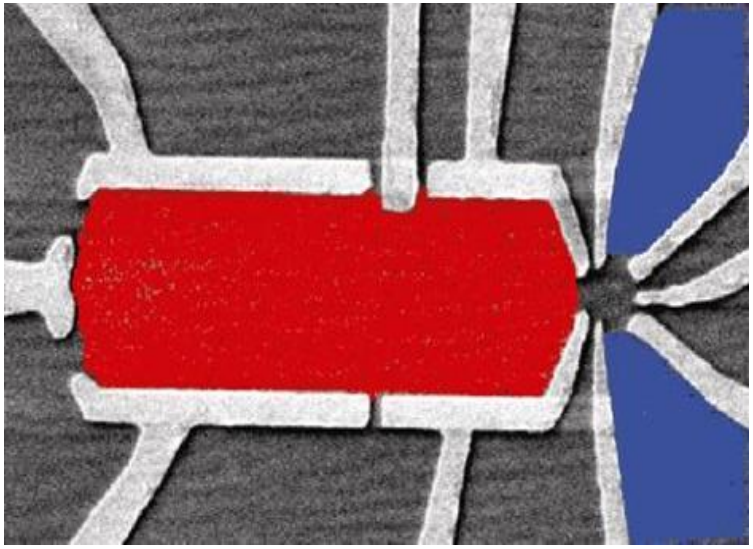
  - **Other bath degrees of freedom decouple**

$$g_{k\sigma} = \frac{1}{V_k}\left(V_d\, b_{sk\sigma} - V_s\, b_{dk\sigma}\right)$$

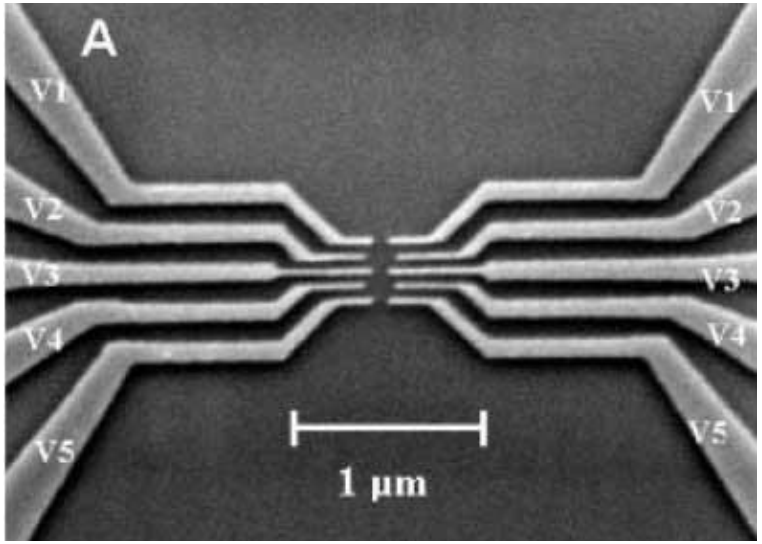
Two-lead device: single channel



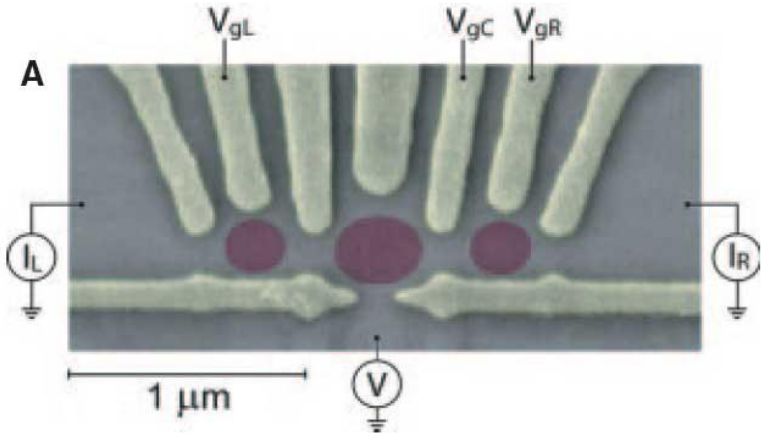
Coupled Quantum Dots



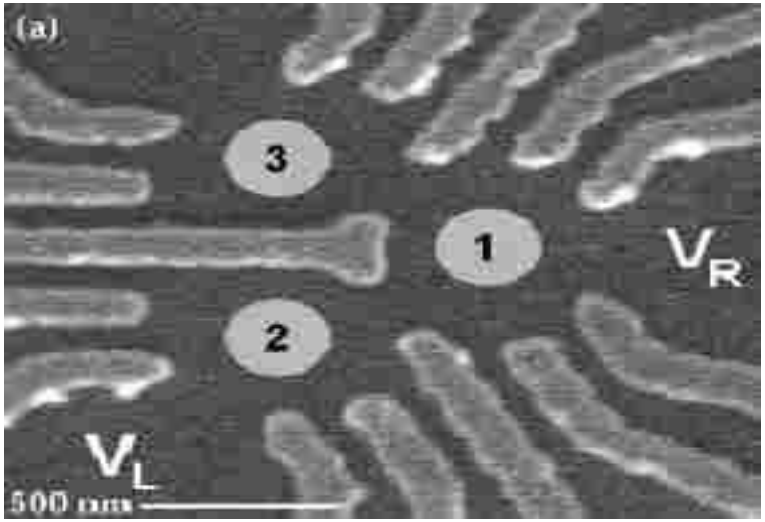
R. Potok *et al.*, Nature 446, 167 (2007)



H. Jeong *et al.*, Science 293, 2221 (2001)

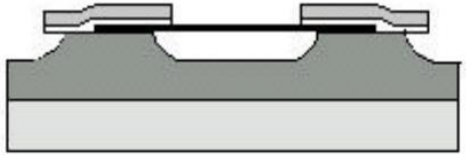


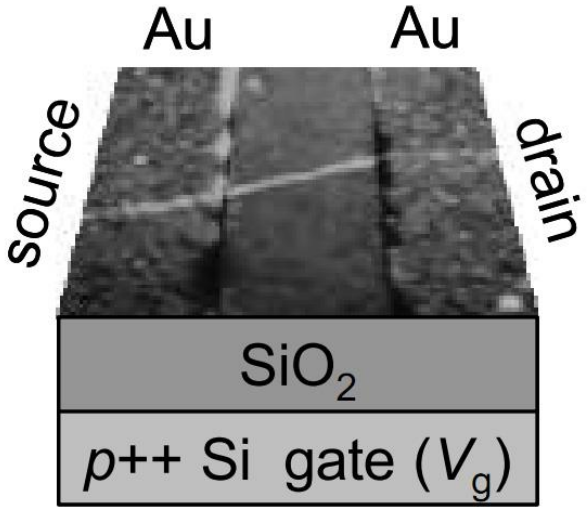
N. Craig *et al.*, Science 304, 565 (2004)



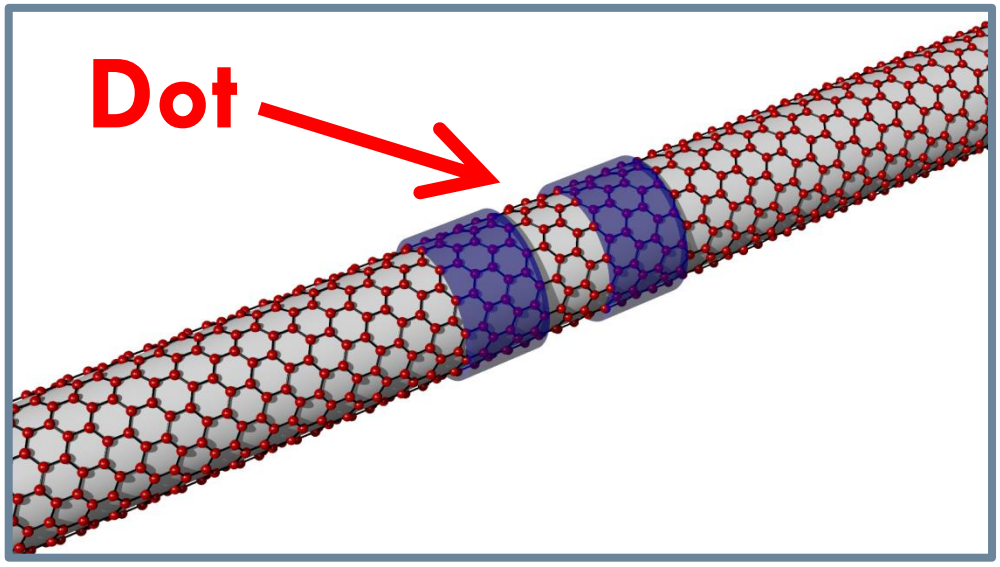
A. Vidan *et al.*, App. Phys. Lett. 85, 3602 (2004)

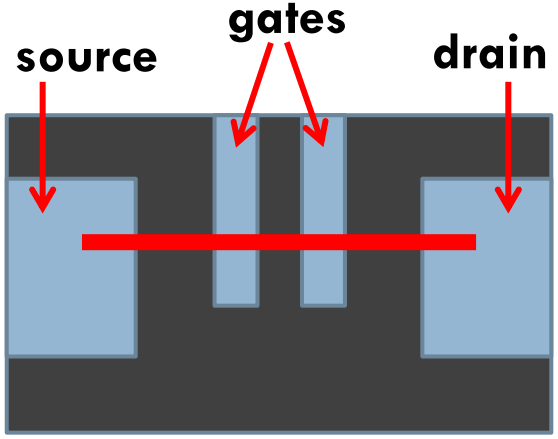
Nanotube Quantum Dots





Nygard et al, Nature 408, 342 (2000)





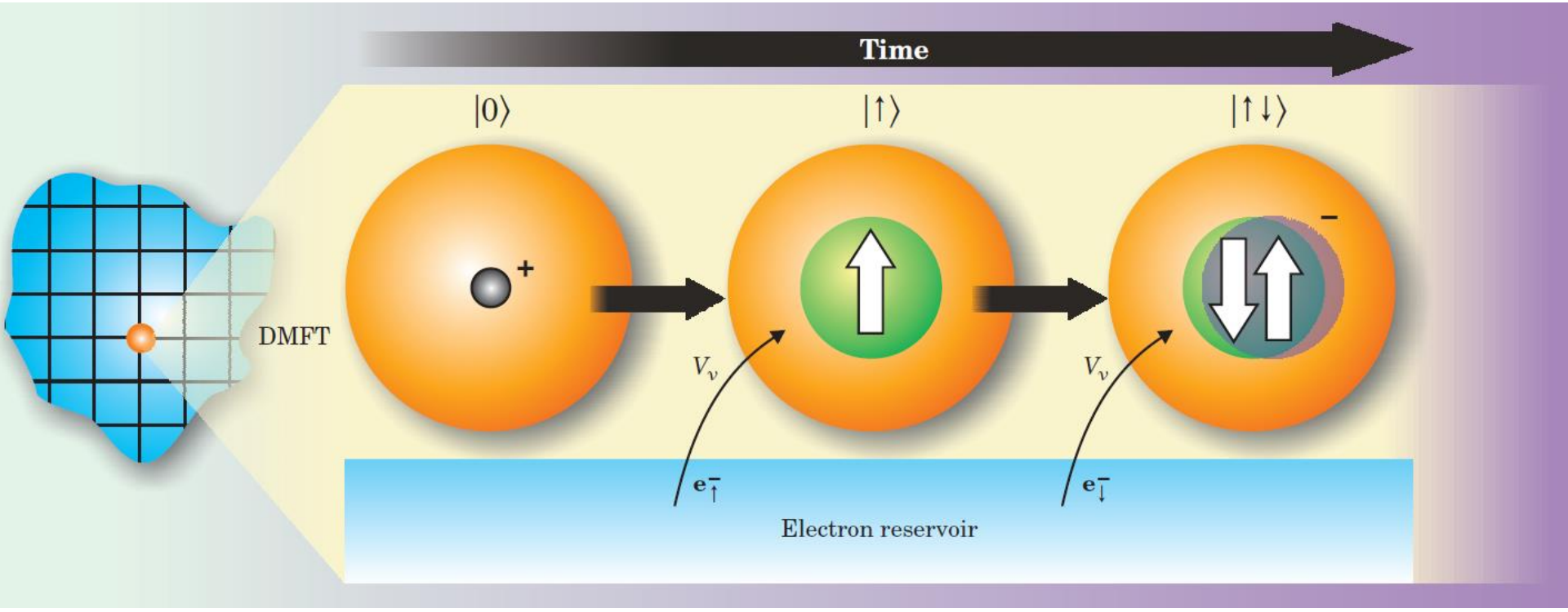
Dynamical Mean Field Theory

- **'DMFT'**

  A. Georges, G. Kotliar, W. Krauth, M. Rozenberg
  Rev. Mod. Phys. 68, 13 (1996)

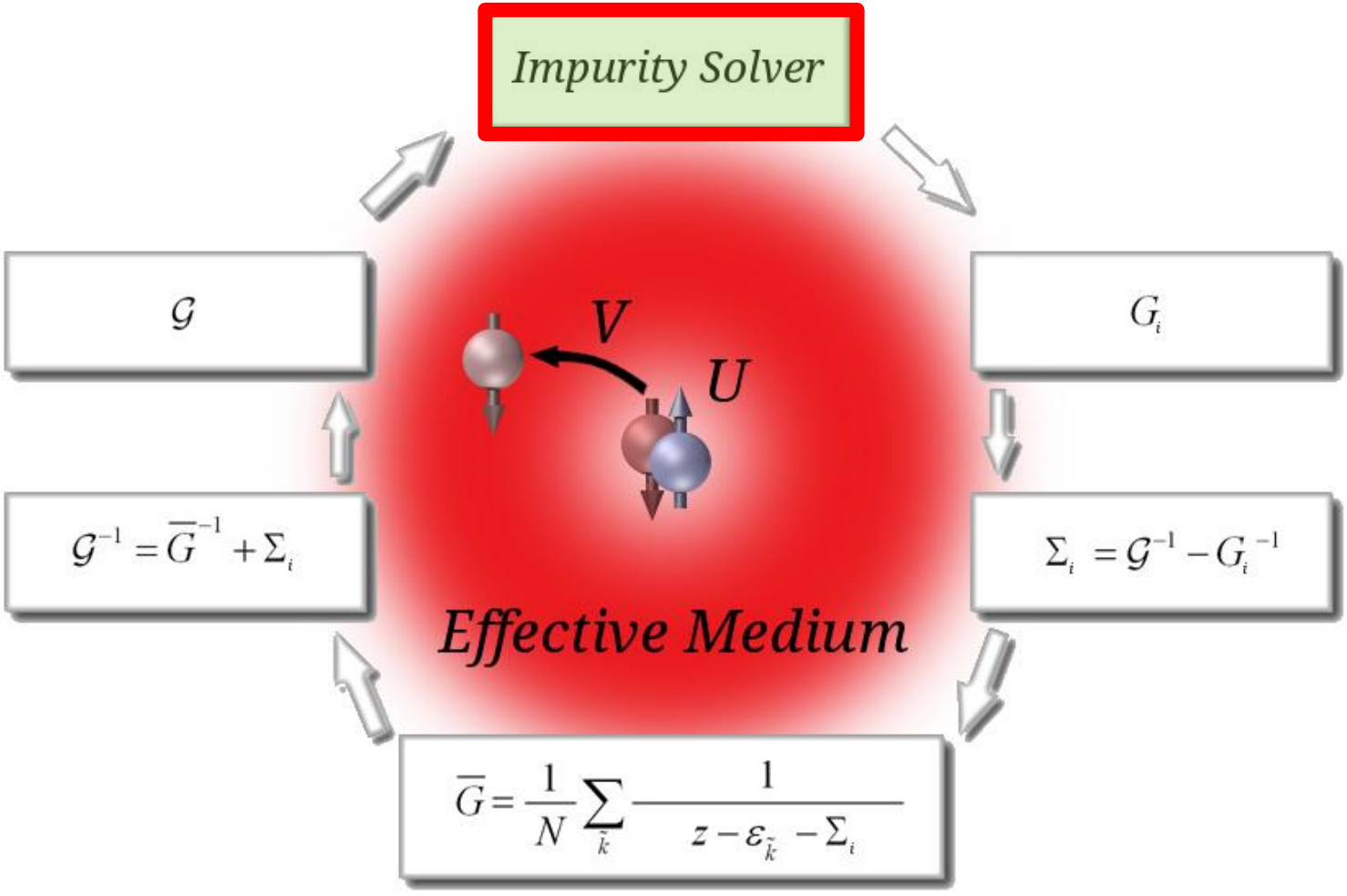
  - **For correlated lattice problems (Hubbard model etc)**
  - **Local self-energy approximation (exact in the limit of infinite dimensions)**
  - **Map onto a single-impurity Anderson impurity model in a bath that must be determined self-consistently**

Dynamical Mean Field Theory



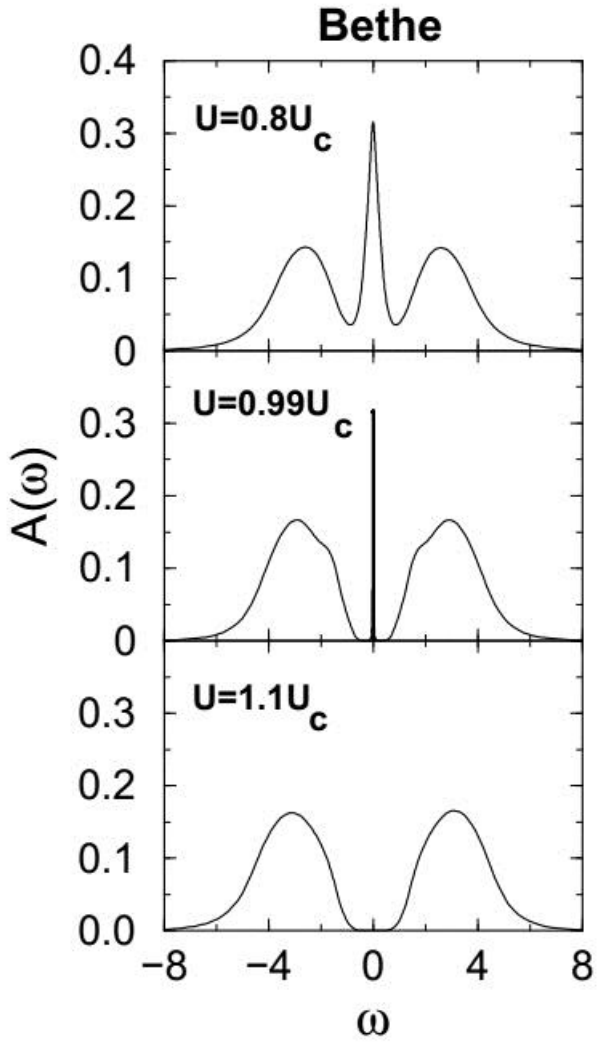
Kotliar & Vollhardt, Physics Today (2004)

Dynamical Mean Field Theory



Dynamical Mean Field Theory

- Hubbard Model in d = ∞
- R. Bulla, PRL **83**, 136 (1999)
- Mott Metal-Insulator transition at *T=0*



Quantum impurity problems

- **Why are quantum impurity problems hard to solve?**

  → strong electron correlations

- **Before we try to solve the impurity problem…**

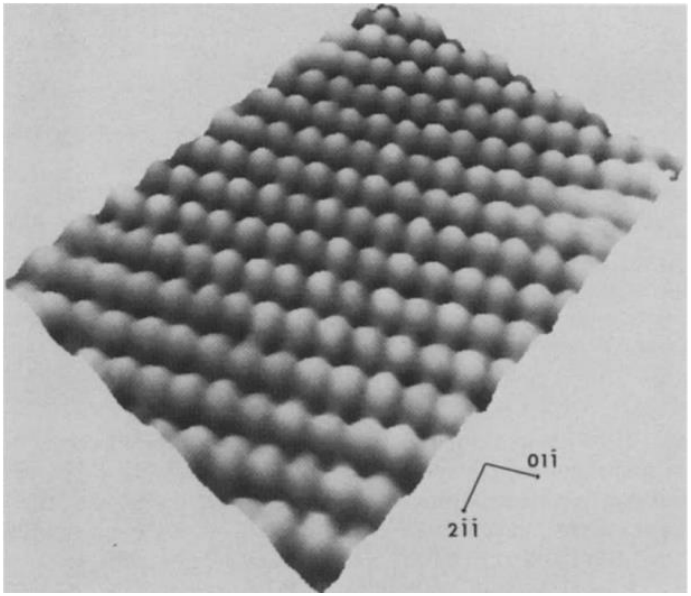
  …let's look again at the 'easy' bit:

  representations of the non-interacting host

  that we will need later

Bulk metal:

- **Host metal: real-space representation**



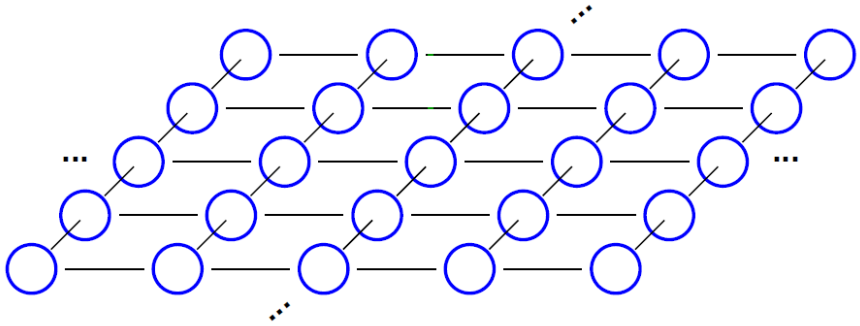
STM image

Bulk metal:

- **Host metal: real-space representation**
  - **Non-interacting tight-binding model**

$$H_{host} = \sum_{\sigma} \sum_{<i,j>} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma}$$

$$\equiv \sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma}\, \underline{\underline{T}}\, \vec{c}_{\sigma}$$



$$\vec{c}^{\,\dagger}_{\sigma} = \left(c^{\dagger}_{1\sigma},\ c^{\dagger}_{2\sigma},\ c^{\dagger}_{3\sigma},\ \ldots \right) \quad ; \quad \underline{\underline{T}} = \begin{bmatrix} t_{11} & t_{12} & \cdots \\ t^{*}_{12} & t_{22} & \\ \vdots & & \ddots \end{bmatrix}$$

Bulk metal:

- **Host metal: diagonal representation**

$$H_{host} = \sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma} \underline{\underline{T}}\, \vec{c}_{\sigma} = \sum_{\sigma} \vec{b}^{\,\dagger}_{\sigma} \underline{\underline{D}}\, \vec{b}_{\sigma}$$

$$= \sum_{\sigma} \sum_{k} \varepsilon_k \, b^{\dagger}_{k\sigma} b_{k\sigma}$$

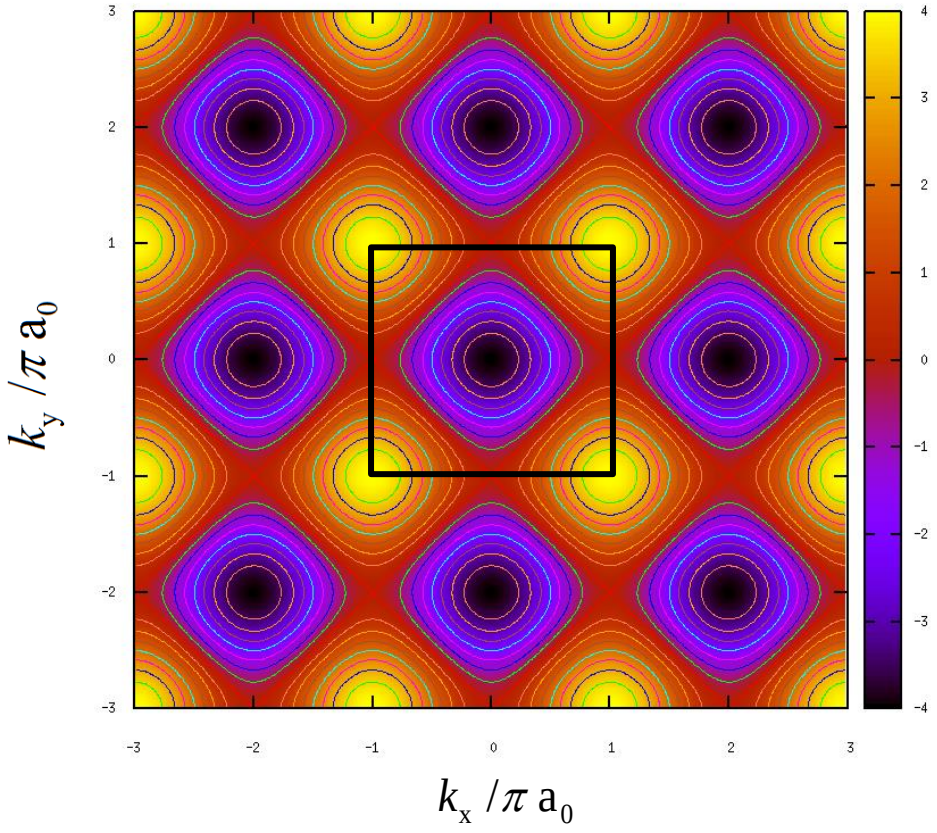
where,

$$\vec{b}_{\sigma} = \underline{\underline{A}}\, \vec{c}_{\sigma}$$

$$\left[\underline{\underline{D}} \right]_{k,k'} = \left[\underline{\underline{A}}^{\dagger}\, \underline{\underline{T}}\, \underline{\underline{A}} \right]_{k,k'} = \varepsilon_k \, \delta_{k,k'}$$

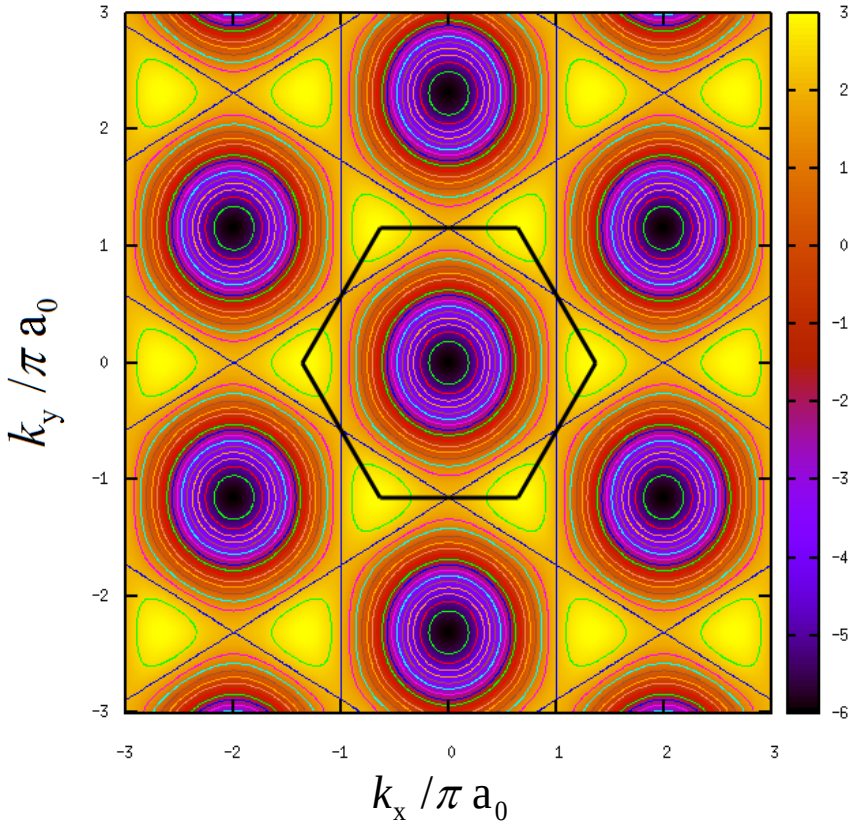
Bulk metal:

- ε_k **is the dispersion:**
  - **For example, 2d square lattice:**



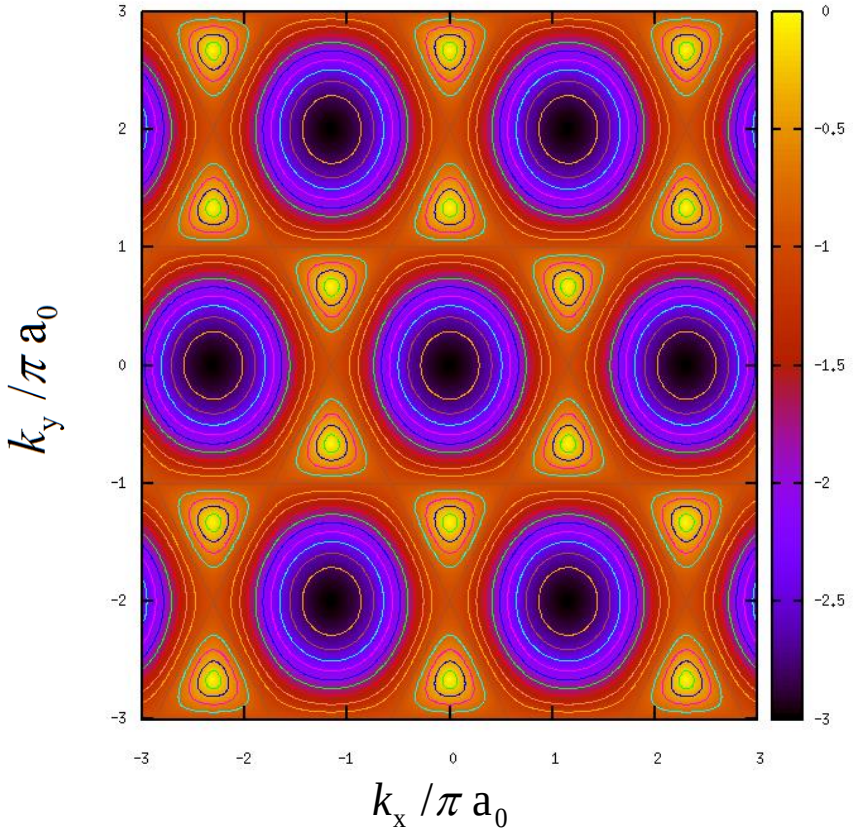
Bulk metal:

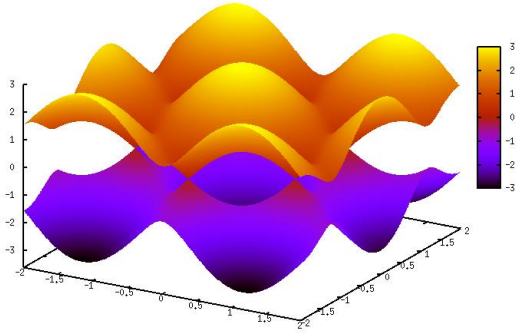
- ε_k **is the dispersion:**
  - **For example, triangular lattice:**



Bulk metal:

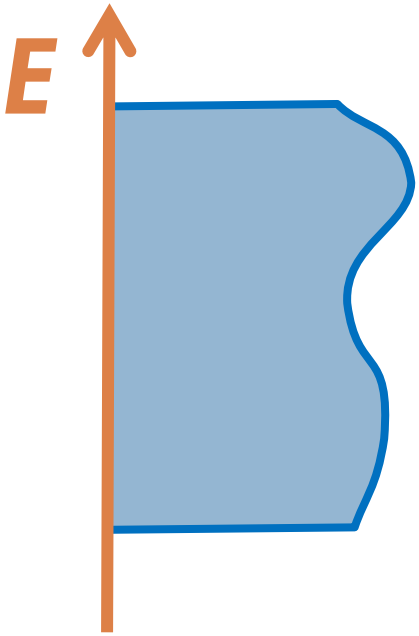
- ε_k **is the dispersion:**
  - **For example, honeycomb (graphene) lattice:**





Density of states:

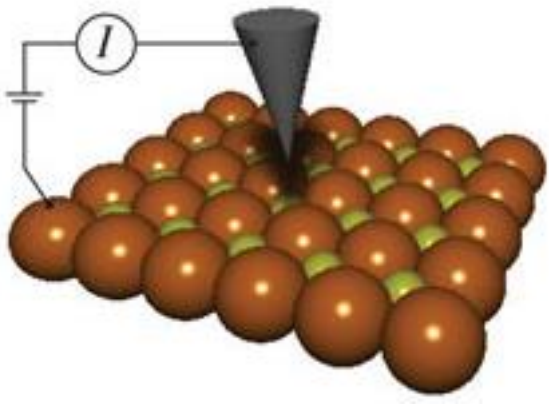
- **Total density of states:**



$$\rho_{tot}(E) = \sum_k \delta(E - \varepsilon_k)$$

Density of states:

- **Local density of states (LDOS):**
  - **As measured locally at a given point in real space**
  - **Obtained experimentally by STM**



$$\rho_{i,\sigma}(E) = \sum_k |a_{i,k}|^2 \, \delta(E - \varepsilon_k)$$

Expansion coefficients of real-space site *i* in terms of *k*-space orbitals

$$\left[\underline{\underline{A}}\right]_{i,k} = a_{i,k}$$

Density of states:

- **Local density of states (LDOS):**
  - **Related to local (real-space) Green function…**

$$\rho_{i,\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left[G_{ii,\sigma}(\omega)\right]$$

$$G_{ii,\sigma}(\omega) = \left\langle\!\left\langle\, c_{i\sigma}\,;\, c_{i\sigma}^{\dagger}\,\right\rangle\!\right\rangle_{\omega}$$

$$\overset{FT}{\Leftrightarrow}\quad G_{ii,\sigma}(t) = -i\theta(t)\left\langle\, \left\{ c_{i\sigma}(t), c_{i\sigma}^{\dagger}(0) \right\}_{+} \,\right\rangle$$

Free host Green functions

- **But what is the local host Green function?**

$$G_{i\,i,\sigma}(\omega) = \left\langle\!\left\langle\, c_{i\sigma}\,;\, c_{i\sigma}^{\dagger}\,\right\rangle\!\right\rangle_{\omega}$$

$$= \sum_{k,k'} (a_{ik})(a_{ik'})^{*} \left\langle\!\left\langle\, b_{k\sigma}\,;\, b_{k'\sigma}^{\dagger}\,\right\rangle\!\right\rangle_{\omega}$$

$$= \sum_{k,k'} (a_{ik})(a_{ik'})^{*}\, G_{k\,k',\sigma}(\omega)$$

Diagonal representation!

$$G_{k\,k',\sigma}\left(\omega + i0^{+}\right) = \frac{\delta_{k,k'}}{\omega + i0^{+} - \varepsilon_{k}}$$

Free host Green functions

- **But what is the local host Green function?**

$$G_{i\,i,\sigma}(\omega) = \sum_{k,k'} \frac{|\,a_{ik}\,|^2}{\omega + i0^+ - \varepsilon_k}$$

$$\Rightarrow \quad \rho_{i,\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\left[G_{i\,i,\sigma}(\omega)\right]$$

$$= \sum_{k} |\,a_{ik}\,|^2\ \delta(\omega - \varepsilon_k)$$

Free host Green functions

- **Dyson representation:**

$$\left[G_{d\,d,\sigma}(\omega) \right]^{-1} = \left[\tilde{G}_{d\,d,\sigma}(\omega) \right]^{-1} - \Delta(\omega)$$

isolated d-level Green function:

$$\frac{1}{\omega + i0^{+} - \varepsilon_d}$$

hybridization with rest of system

$$\Rightarrow \quad G_{d\,d,\sigma}(\omega) = \frac{1}{\omega + i0^{+} - \varepsilon_d - \Delta(\omega)}$$

Potential scatterer

- **Potential scattering 'impurity'**

$$H_{host} = \sum_{\sigma} \sum_{<i,j>} t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} \; + g_d \sum_{\sigma} c^{\dagger}_{d\sigma} c_{d\sigma}$$

- **Modified LDOS:**

defined without impurity

$$\left[G^{ps}_{d\,d,\sigma}(\omega) \right]^{-1} = \left[G^{(0)}_{d\,d,\sigma}(\omega) \right]^{-1} - g_d$$

T matrix

- **T matrix describes scattering between diagonal eigenstates of the free system, induced by the impurity:**

$$G_{k\,k',\sigma}(\omega) = \delta_{k,k'}\, G^{(0)}_{k\,k,\sigma}(\omega) + G^{(0)}_{k\,k,\sigma}(\omega)\,\mathrm{T}_{k,k'}(\omega)\,G^{(0)}_{k'\,k',\sigma}(\omega)$$

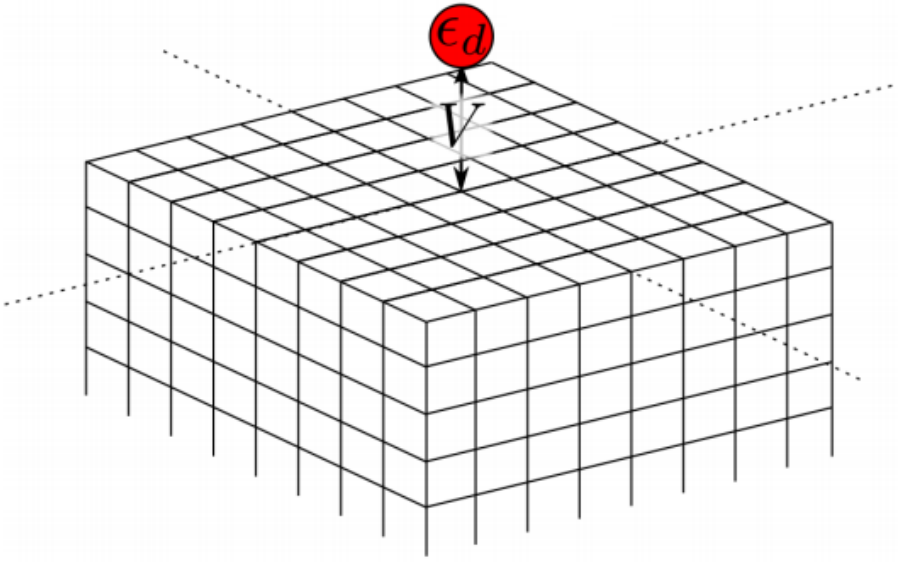
$$\Rightarrow \quad \mathrm{T}_{k,k'}(\omega) = \left(a_{d,k}\right)^{*}\left(a_{d,k'}\right)\left[\frac{g_d}{1 - g_d\, G^{(0)}_{d\,d,\sigma}(\omega)}\right]$$

Born approx: $\mathrm{T}_{k,k'}(\omega) \approx \left(a_{d,k}\right)^{*}\left(a_{d,k'}\right)\, g_d$

Resonant level

- **'Resonant level' impurity:**
  (non-interacting U=0 Anderson model)

$$H_{RL} = \sum_{\sigma} \sum_{<i,j>} \left(t_{ij}\, c^{\dagger}_{i\sigma} c_{j\sigma} \right) + \varepsilon_d d^{\dagger}_{\sigma} d_{\sigma} + V \left(d^{\dagger}_{\sigma} c_{0\sigma} + \text{H.c.} \right)$$



Resonant level

- **Resonant level Green function:**

$$G_{d\,d,\sigma}(\omega) = \frac{1}{\omega + i0^{+} - \varepsilon_d - \Delta(\omega)}$$

local host Green function

Hybridization with rest of system

$$\Delta(\omega) = V^2\, G^{(0)}_{0\,0,\sigma}(\omega)$$

Hybridization function

$$\Delta(\omega) = V^2 \, G^{(0)}_{00,\sigma}(\omega)$$

$$\Rightarrow \quad -\mathrm{Im}\ \Delta(\omega) = -V^2 \, \mathrm{Im}\, G^{(0)}_{00,\sigma}(\omega)$$

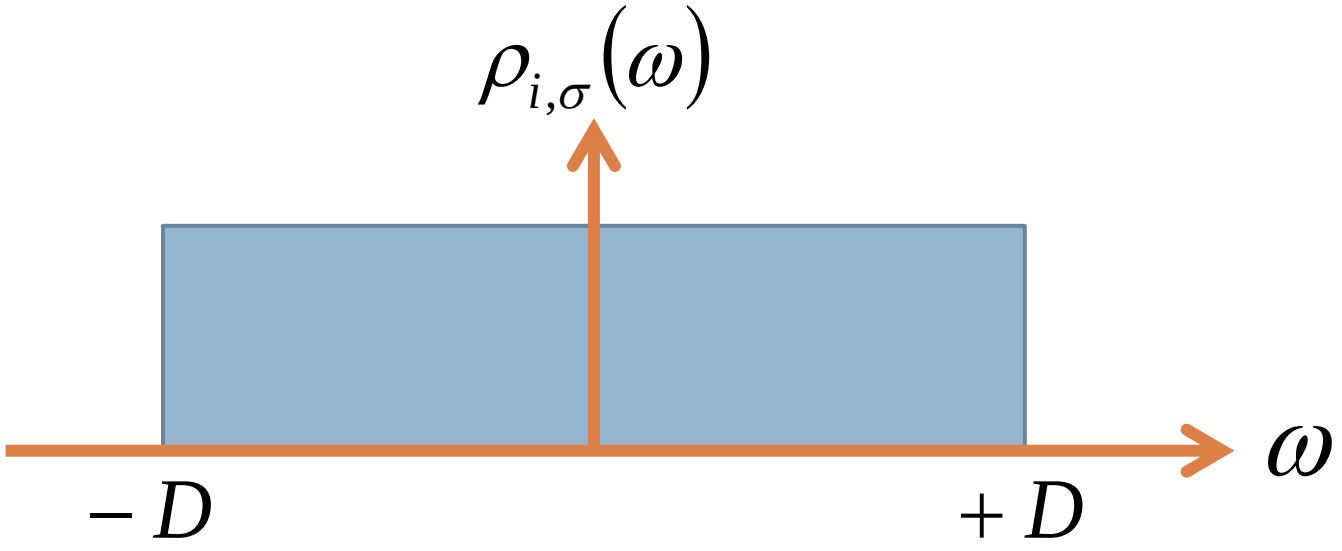
$$= \pi V^2 \rho_{i,\sigma}(\omega)$$

Local Density of States (LDOS) of host site to which impurity is coupled

Hybridization function

- **Consider wide flat conduction band:**

$$\rho_{i,\sigma}(\omega) = \left(\frac{1}{2D}\right)\theta(D - |\omega|)$$



Hybridization function

- **Hybridization function by Kramers-Kronig:**

$$\Delta(\omega) = V^2\, G^{(0)}_{0\,0,\sigma}(\omega)$$

$$= V^2\left[P\int d\varepsilon \left(\frac{\rho_{i,\sigma}(\varepsilon)}{\omega - \varepsilon} \right) - i\pi\, \rho_{i,\sigma}(\omega) \right]$$

- **For wide flat band:** $\Delta(\omega) \cong -i\,\Gamma_0 = -i\pi V^2 \rho_0$

$$\left[\rho(\omega) \equiv \rho_0\right]$$

Impurity spectral function

- **Flat conduction band:**

$$G_{d\,d,\sigma}(\omega) = \frac{1}{\omega + i0^{+} - \varepsilon_d + i\,\Gamma_0}$$

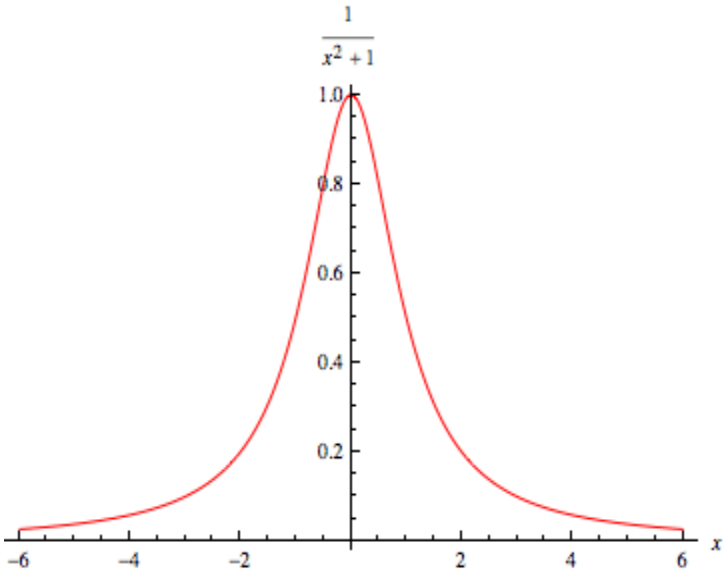
- **Spectrum:**

$$A_{d,\sigma}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\;G_{d\,d,\sigma}(\omega)$$

$$= \frac{\Gamma_0/\pi}{(\omega - \varepsilon_d)^2 + (\Gamma_0)^2}$$

Impurity spectral function

- **Spectrum:** $$\pi \Gamma_0 A_{d,\sigma}(\omega) = \frac{1}{\left[(\omega - \varepsilon_d)/\Gamma_0\right]^2 + 1}$$
- **Lorentzian, centred on** ε_d
- **Effective level width** Γ_0
- **Peak height pinned to** $1/\pi\Gamma_0$



- **Quadratic approach to maximum value**

T matrix

- **T matrix for resonant level:**

$$G_{k\,k',\sigma}(\omega) = \delta_{k,k'}\, G^{(0)}_{k\,k,\sigma}(\omega) + G^{(0)}_{k\,k,\sigma}(\omega)\,\mathrm{T}_{k,k'}(\omega)\,G^{(0)}_{k'\,k',\sigma}(\omega)$$

$$\Rightarrow \quad \mathrm{T}_{k,k'}(\omega) = \left(a_{d,k}\right)^{*}\left(a_{d,k'}\right)\left[V^{2}\, G_{d\,d,\sigma}(\omega)\right]$$

Impurity Green function

Interacting problem:

- **The Anderson impurity model with strong interactions U>0 is MUCH more difficult!**

Why?!

Interacting problem:

- In the non-interacting case, the Hamiltonian can be brought into diagonal form by performing a canonical transformation of *operators*:

$$\sum_{\sigma} \vec{c}^{\,\dagger}_{\sigma} \underline{\underline{T}} \vec{c}_{\sigma} \;\; = \;\; = \sum_{\sigma} \sum_{k} \varepsilon_k \, b^{\dagger}_{k\sigma} b_{k\sigma}$$

with $\vec{b}_{\sigma} = \underline{\underline{A}} \, \vec{c}_{\sigma}$

- Achieved by simply diagonalizing the hopping matrix $\underline{\underline{T}}$ which is of dimension *N* x *N* for an *N*-particle system

Interacting problem:

- For an **interacting** problem, containing terms like

  $$U_d \left(c^\dagger_{d\uparrow} c_{d\uparrow} c^\dagger_{d\downarrow} c_{d\downarrow} \right)$$

  (not quadratic in electronic operators), the Hamiltonian itself cannot be brought to diagonal form by transformation of operators.

- **Must construct the Hamiltonian matrix with elements** $\langle \psi_a | \hat{H} | \psi_b \rangle$ **in the many-particle basis.**

- **Fermions: matrix is of dimension** $4^N \times 4^N$

Interacting problem:

- **So: we cannot do exact diagonalization (except for very small systems, and at high T)**

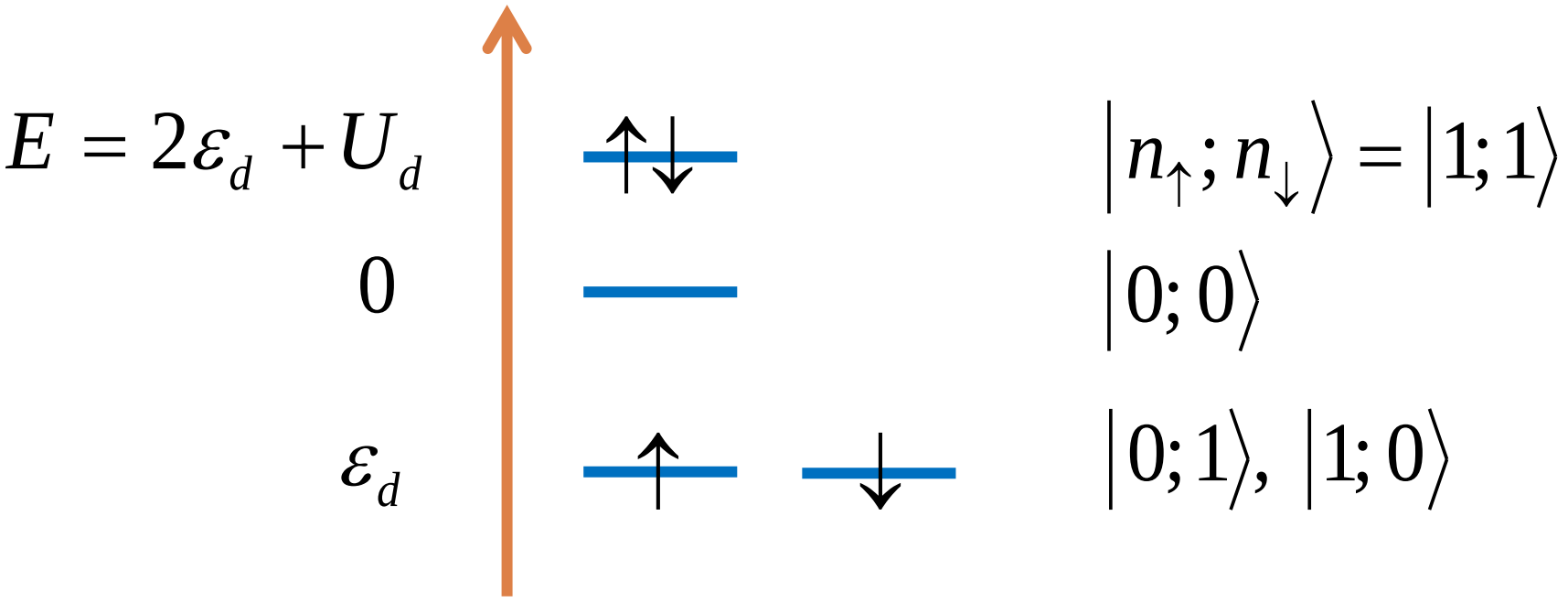
- **Perturbation theory in the interaction *U* does not give information about the strongly correlated regime. Plagued by divergences!**

- **Mean field approaches completely fail to capture the physics**

Aside: many-particle levels

- **Consider a single interacting quantum level:**

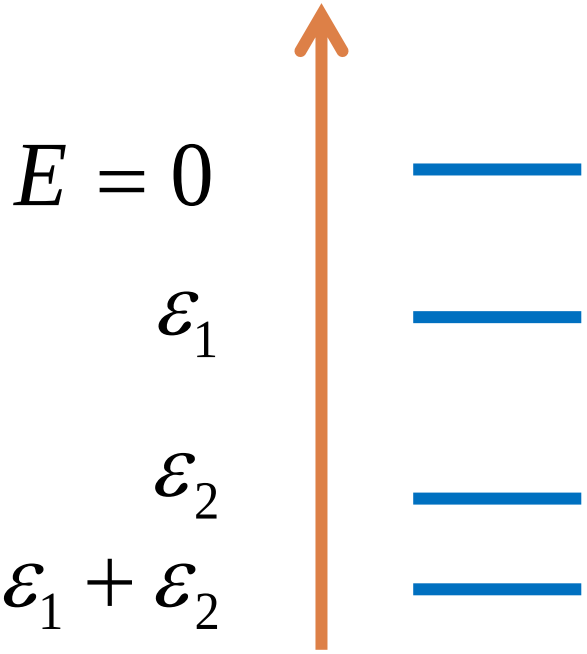
$$H_{imp} = \varepsilon_d \left(c^\dagger_{d\uparrow} c_{d\uparrow} + c^\dagger_{d\downarrow} c_{d\downarrow} \right) + U_d \left(c^\dagger_{d\uparrow} c_{d\uparrow} c^\dagger_{d\downarrow} c_{d\downarrow} \right)$$



Aside: many-particle levels

- **NOT possible to reproduce these many-particle energies just using single-particle levels:**

$$H_{non-\text{int}} = \varepsilon_1 \left(c_{1\uparrow}^{\dagger} c_{1\uparrow} \right) + \varepsilon_2 \left(c_{2\downarrow}^{\dagger} c_{2\downarrow} \right)$$



… unless *U=0*

Interacting problem:

- **Large U: Schrieffer-Wolff transformation:**
  - **Project into singly-occupied (spin) manifold of dot**
  - **Perturbatively eliminate virtual excitations to empty or doubly-occupied dot states to second order in** H_{hyb}

$$H_{eff} = \hat{1} H_{hyb} \left[E_0 - H_{imp} \right]^{-1} H_{hyb} \hat{1}$$

projector: $\hat{1} = |\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|$

Interacting problem:

- **Large U: Schrieffer-Wolff transformation:**
  - **Low-energy effective model is the Kondo model**

$$H_{eff} = H_{host} + J\,\vec{S}_{\mathrm{imp}} \cdot \vec{s}_0$$

$$\sim + \frac{V^2}{U_d}$$

AF exchange

impurity spin-½

conduction electron spin density at impurity

$$c^{\dagger}_{0\sigma}\,\frac{\vec{\sigma}_{\sigma\sigma'}}{2}\,c_{0\sigma'}$$

The Kondo problem

- **But what is the physics of the Kondo model?!**

First full solution obtained by the

Numerical Renormalization Group…

… see part 2!