COLLÈGE DE FRANCE
1530

Chaire de Physique de la Matière Condensée

Des oxydes supraconducteurs aux atomes froids

- la matière à fortes corrélations quantiques -

Antoine Georges

Cycle 2009-2010
Cours 1 - 5 mai 2010

- Une introduction à la physique des systèmes quantiques à fortes corrélations, dans une perspective large.
- Plusieurs types de systèmes physiques seront abordés : *nanostructures de type « points quantiques », atomes froids dans les réseaux optiques, oxydes de métaux de transition.*
- Mettre en lumière les phénomènes et concepts essentiels communs à ces systèmes : *blocage de Coulomb, transition de Mott, descriptions de quasiparticules et leurs limites.*

Programme – Articulation cours/séminaire

- **5 mai** Introduction. Blocage de Coulomb,
  Modèles d'impuretés quantiques, effet Kondo.

  Séminaire : Olivier PARCOLLET (IPhT-CEA-Saclay) *Modèles d'impuretés quantiques: méthodes numériques et applications.*

- **12 mai** Modèles d'impuretés quantiques, effet Kondo (II).

  Séminaire : Serge FLORENS (Institut Néel, Grenoble)

  Effets Kondo exotiques dans les nanostructures.

- **19 mai** Transition de Mott bosonique et atomes froids.

  Séminaire : Matthias TROYER (ETH - Zurich, Suisse)

  Superfluidity near the Mott transition of cold bosonic atom: validating a quantum simulator.

- **26 mai** Liquides de Fermi et quasiparticules.

  Séminaire : Henri GODFRIN (Institut Néel, Grenoble)

  L'Helium 3 liquide bidimensionnel: un liquide de Fermi fait pour intriguer les physiciens !

- **2 juin** Structure et propriétés électroniques des oxydes de métaux de transition : introduction.

  Séminaire : Veronique BROUET (LPS-Orsay) *Les nouveaux supraconducteurs au fer vus par photoémission résolue en angle*

- **9 juin** Transition de Mott et corrélations électroniques dans les oxydes: de Brinkman-Rice à la théorie du champ moyen dynamique.

  Séminaire : Antoine MAIGNAN (CRISMAT, Caen) *Oxydes des métaux de transition : réseaux carrés et triangulaires pour générer de nouvelles fonctionnalités.*

- **16 juin** Supraconducteurs à haute température critique : quelques mystères clés…

  Séminaire : Andrew J. MILLIS (Columbia University, USA)

  Optical conductivity of cuprates and other strongly correlated materials.

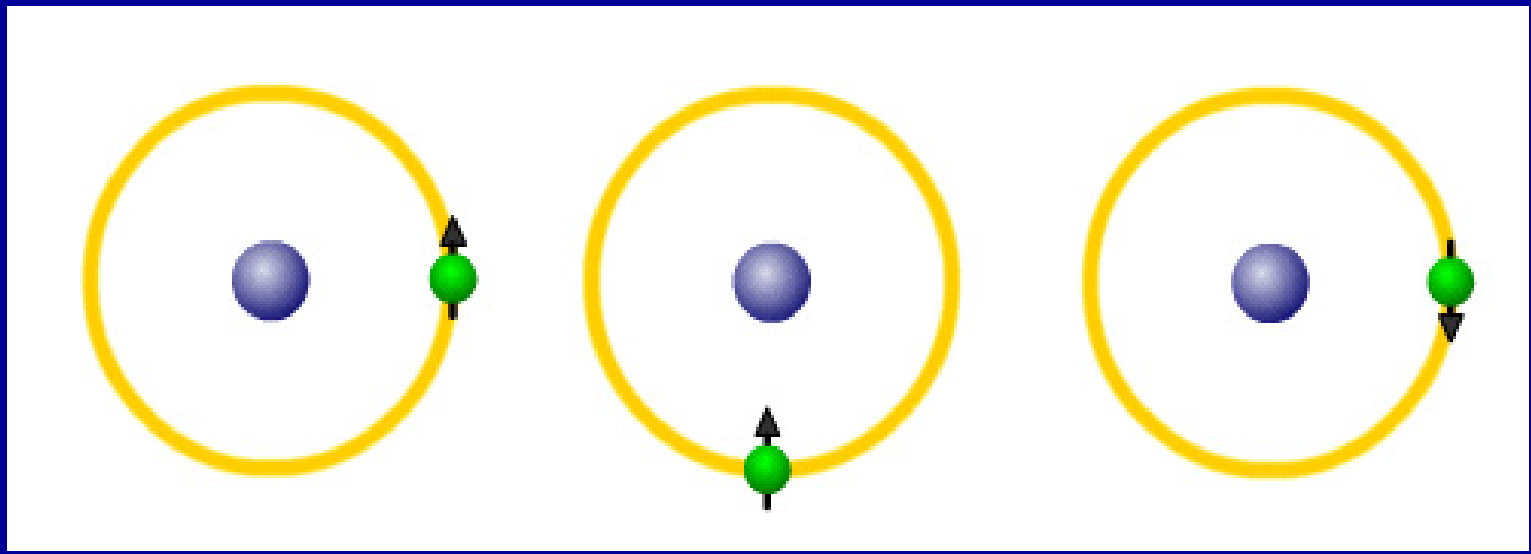
- **23 juin** Corrélations électroniques dans les oxydes: le rôle du couplage de Hund.

  Séminaire : Leon BALENTS (KITP, University of California, Santa Barbara, USA) *Spin-orbit physics in the Mott regime*.

Cycle de cours 2010-2011
(Novembre-Décembre 2010) …

Supraconducteurs
« à haute température critique »
(principalement: cuprates)

A common thread
through this series of lectures:
blocking of electronic motion
(and suppression of density fluctuations)
by repulsive interactions
(« Coulomb blockade »)



The Anderson (et al.) model

- and other `quantum impurity' models - :

Correlation effects « in a nutshell »

"O God! I could be bounded in a nutshell,
and count myself king of infinite space,
were it not that I have bad dreams !"

William Shakespeare (in: Hamlet)

1. The model

$$H = H_{\rm c} + H_{\rm at} + H_{\rm hyb}$$

$$H_{\rm c} = \sum_{{\rm k}\sigma} \varepsilon_{\rm k}\, c^{\dagger}_{{\rm k}\sigma} c_{{\rm k}\sigma}$$

Conduction electron host (``bath'', environment)

$$H_{\rm at} = \varepsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + U\, n^{d}_{\uparrow} n^{d}_{\downarrow}$$

Single-level ``atom''

$$H_{\rm hyb} = \sum_{{\rm k}\sigma} V_{\rm k} (c^{\dagger}_{{\rm k}\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{{\rm k}\sigma})$$

Transfers electrons between bath and atom – Hybridization, tunneling

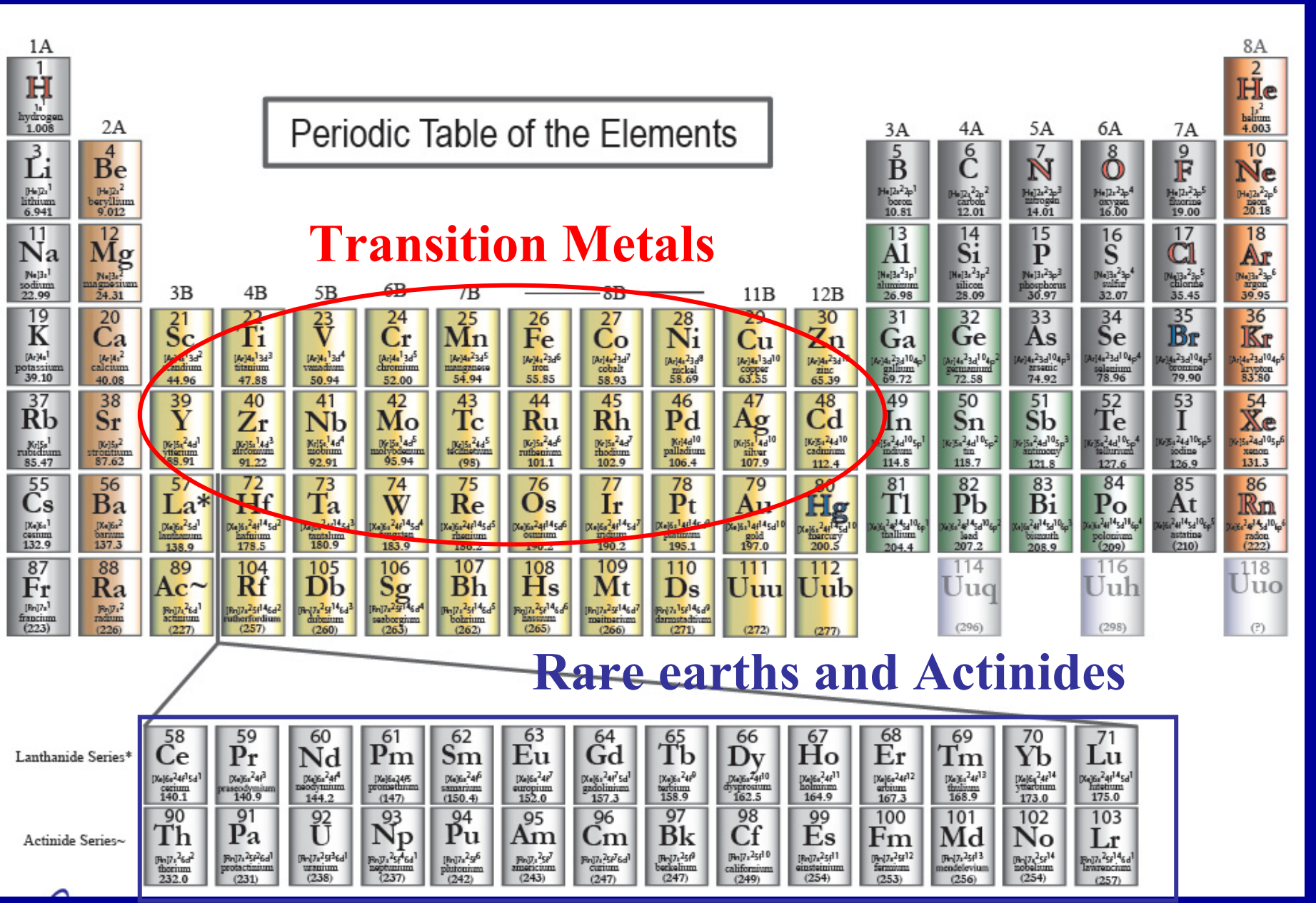
2. Some applications to physical systems
(to be detailed in Lecture 2)

- 2.1 Magnetic impurities in metals

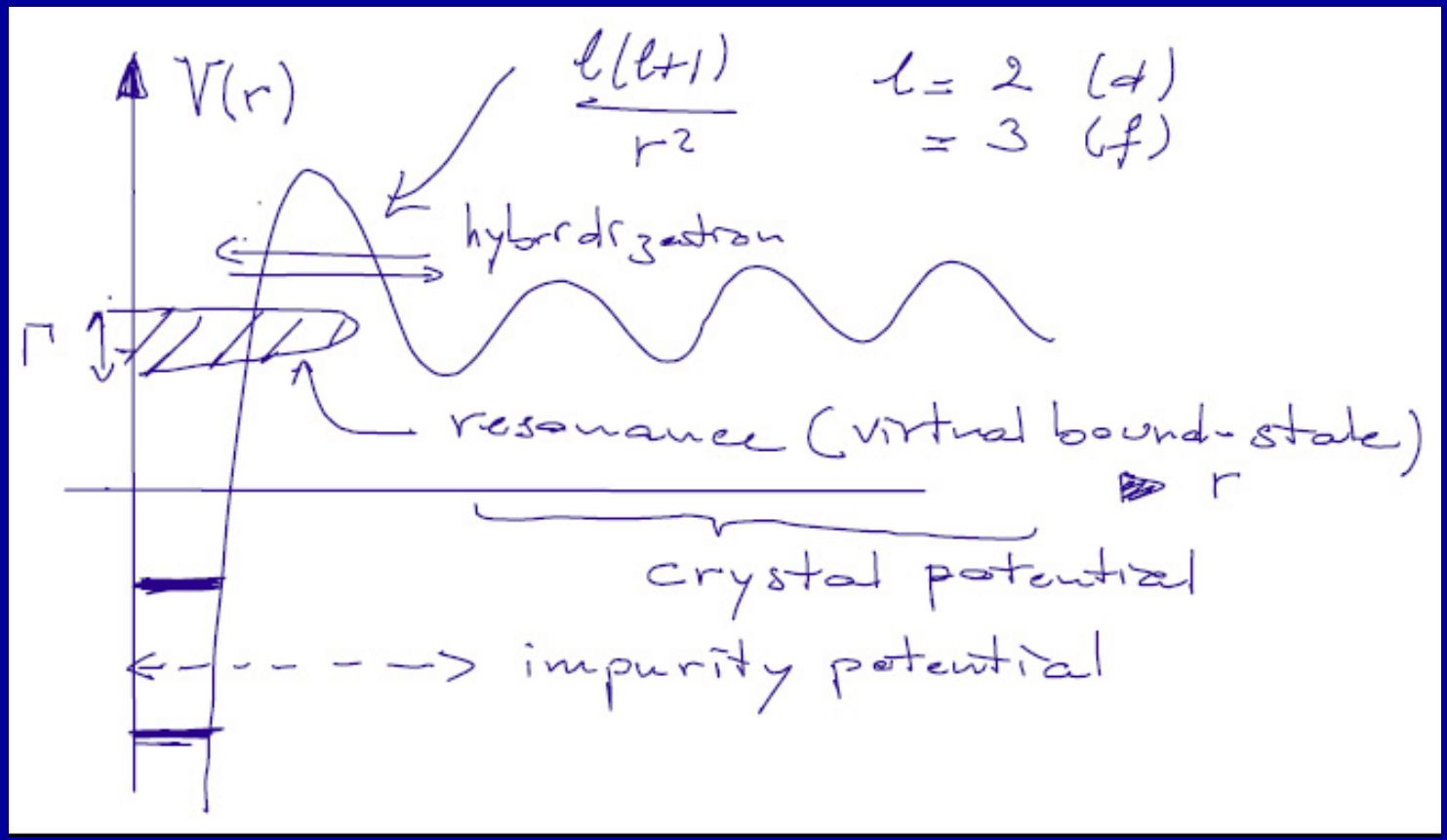
- Low concentration of magnetic atoms, with quite localized orbitals, into metallic host

- e.g. 3d transition metals (Mn, Cr, Fe) into Au or Cu or Al
  4f dilute rare-earth compounds e.g. $Ce_xLa_{1-x}Cu_6$ ($x << 1$)

In some cases, all range of solid solution can be studied,
from dilute to dense system (Kondo alloy to Heavy-Fermion regime)


Periodic Table of the Elements
Transition Metals
Rare earths and Actinides
1A
2A
3A
4A
5A
6A
7A
8A
3B
4B
5B
6B
7B
8B
11B
12B
Lanthanide Series*
Actinide Series~

Friedel's virtual bound-state concept



Cf. Jacques Friedel Can.J.Phys 34, p. 1190 (1956)
Nuov Cim Supp 7, p.287 (1958)
Varenna school XXXVII, 1966

Single-orbital Anderson model ignores many realistic aspects - especially: orbital degeneracy

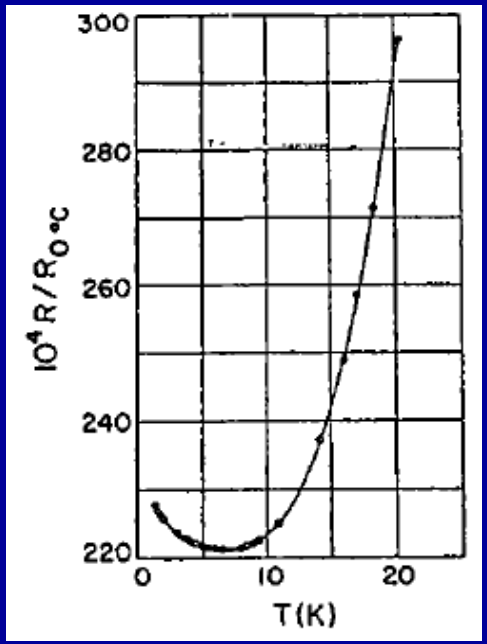
$$H = \sum_{k,\sigma} \epsilon_k \, a^+_{k\sigma} \, a_{k\sigma} + \sum_{\sigma,m} \epsilon_{\mathrm{d}} \, n_{m\sigma} + \sum_{k,m,\sigma} (V_{km} \, a^+_{k\sigma} \, a_{m\sigma} + \mathrm{cc})$$
$$+ \tfrac{1}{2} U \sum_{m,m'} n_{m\sigma} \, n_{m'-\sigma} + \tfrac{1}{2}(U-J) \sum_{m \neq m',\sigma} n_{m\sigma} \, n_{m'\sigma}$$
$$- \tfrac{1}{2} J \sum_{m \neq m',\sigma} a^+_{m\sigma} \, a_{m-\sigma} \, a^+_{m'-\sigma} \, a_{m'\sigma} + \tfrac{1}{2} J \sum_{m,\sigma} n_{m\sigma} \, n_{m-\sigma} + (\text{crystal field})$$

J: Hund's coupling

Rotational invariance in spin and orbital space:

Cf. Caroli, Caroli and Fredkin Phys Rev 178 (1969) 599

Dworin and Narath Phys Rev Lett 25 (1970) 1287

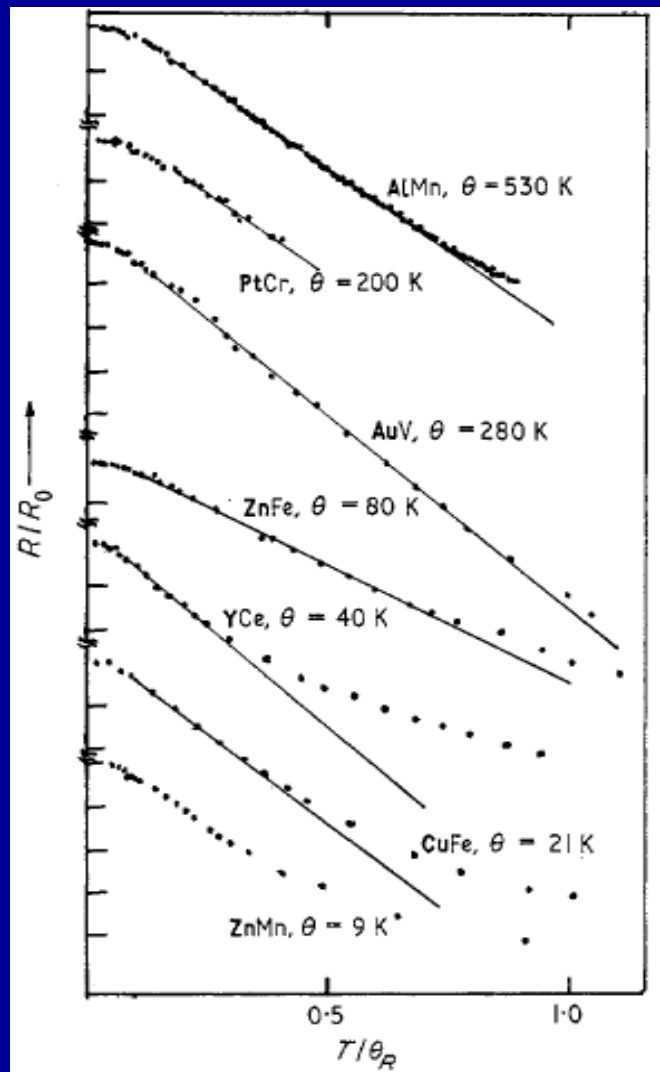


The Kondo effect :

contribution of magnetic impurities to resistivity increases as T is lowered !

De Haas, de Boer
and van den Berg,
Physica 1 (1934) 1115

``*The resistivity of the gold wires Measured (not very pure) has a Minimum.*''



Impurity contribution to resistivity of different alloys, plotted against reduced temperature scale.

[After Rizzuto et al. J. Phys F 3, p.825 (1973)]

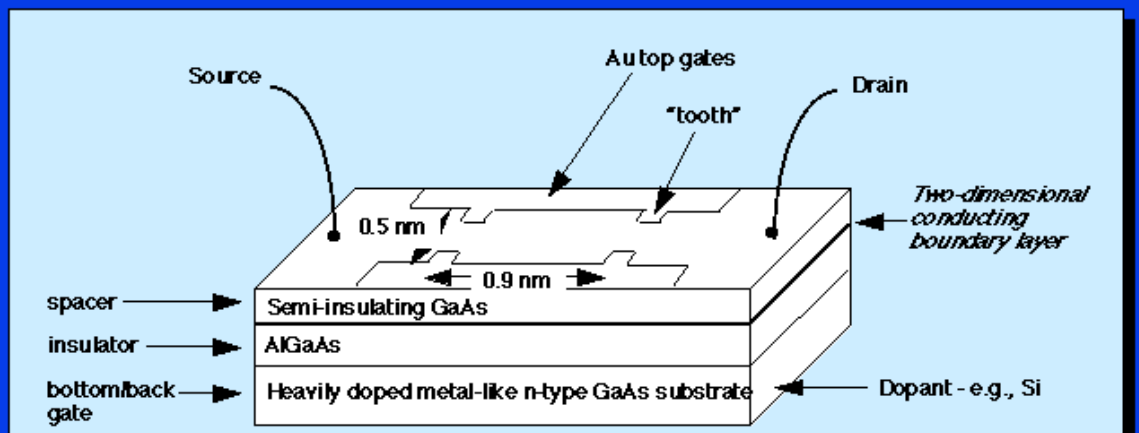
Note wide range of θ, defined from low-T:

$$\rho/\rho_0 = 1 - (T/\theta)^2 + \cdots$$

- 2.2 Nanostructures: Many-Body effects on the Coulomb blockade

20 September 1995

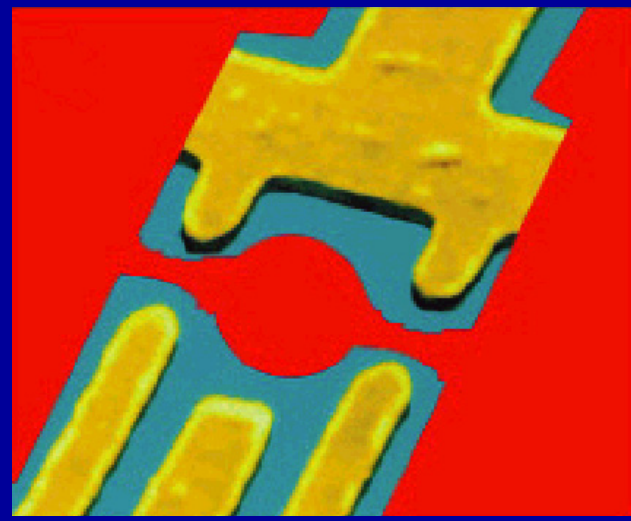
Schematic of a Quantum Dot: Single-electron transistor



- Negative bias on gold electrodes confines electrons to narrow channel
- Electrons traveling between source and drain in boundary layer must tunnel through barrier created by gold "teeth"
- Creates field-effect transistor (FET)

Figure adapted from Meirav, Kastner, and Wind, Phys. Rev. Lett. (1990)

MITRE



$$U \approx e^2/C$$

Coulomb repulsion on the dot increases as the size (capacitance) decreases

Extremely simplified model: a slight modification of the Anderson single-impurity model (w/ 2 baths)

$$H = H_{\text{dot}}[d_\sigma, d_\sigma^\dagger] + \sum_{p=L,R} \sum_\sigma \left[V_p \, d_\sigma^\dagger a_{p\sigma} + h.c + E_p \, a_{p\sigma}^\dagger a_{p\sigma} \right]$$

Hybridization to the leads

Leads

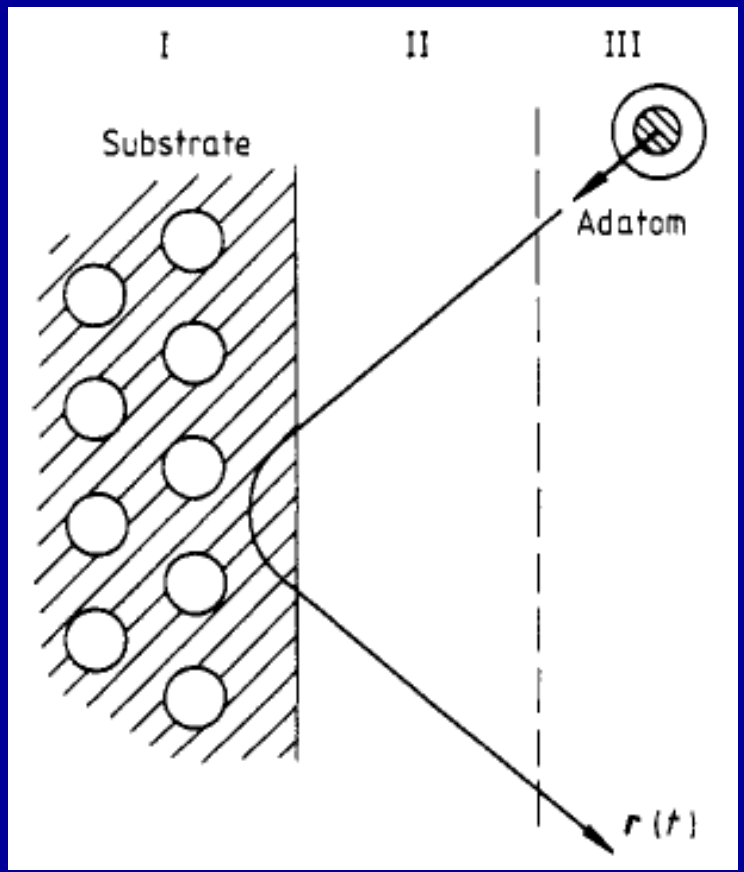
$$H_{\text{dot}} = \varepsilon_d \sum_\sigma n_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

Coulomb blockade on the dot

Valid for widely separated energy levels on the dot, considering a single level (NOT correct for a metallic island, OK for 2DEG dots).

Applications (cont'd)

- 2.3 Adsorption and Scattering of atoms on surfaces



As-atom trajectory classical r(t)

→ Time dependence of V(t), $\varepsilon_d(t)$

Questions, e.g:

- Probability of finding scattered atom into given charge state

- Particle-hole excitations excited in the Substrate, etc…

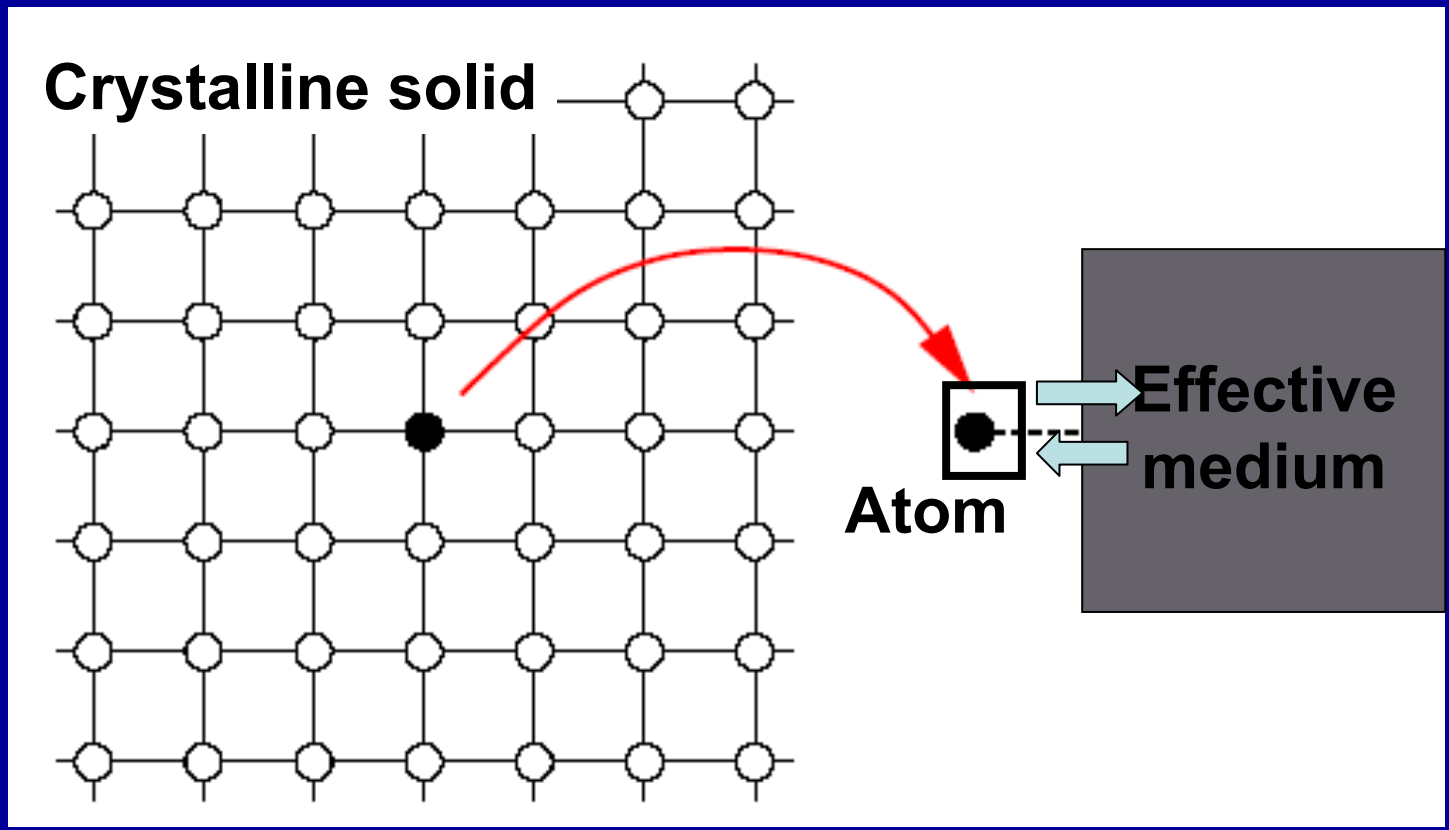
A non-equilibrium problem which could be reconsidered with more modern tools ?

Review: Brako and Newns, Rep Prog Phys 52 (1989) 655

Applications (cont'd)

- 2.4 Dynamical Mean-Field Theory and `self-consistent' quantum impurity models

(cf. Lecture 6)



Organisation des cours 1-2 :

- Cours 1: Méthodes et principaux outils théoriques
- Cours 2: Retour sur les applications à différents systèmes physiques, et effets Kondo `exotiques'

3. A simple limit: the isolated `atom'

$$H_{\rm at} = \varepsilon_d \sum_\sigma d^\dagger_\sigma d_\sigma + U\, n^d_\uparrow n^d_\downarrow$$

Eigenstates:

- $|0\rangle \;\;,\;\; E = 0$
- $|\uparrow\rangle$ and $|\downarrow\rangle$, $E = \varepsilon_d$, *doubly degenerate* (in zero-field).
- $|\uparrow\downarrow\rangle$, $E = 2\varepsilon_d + U$

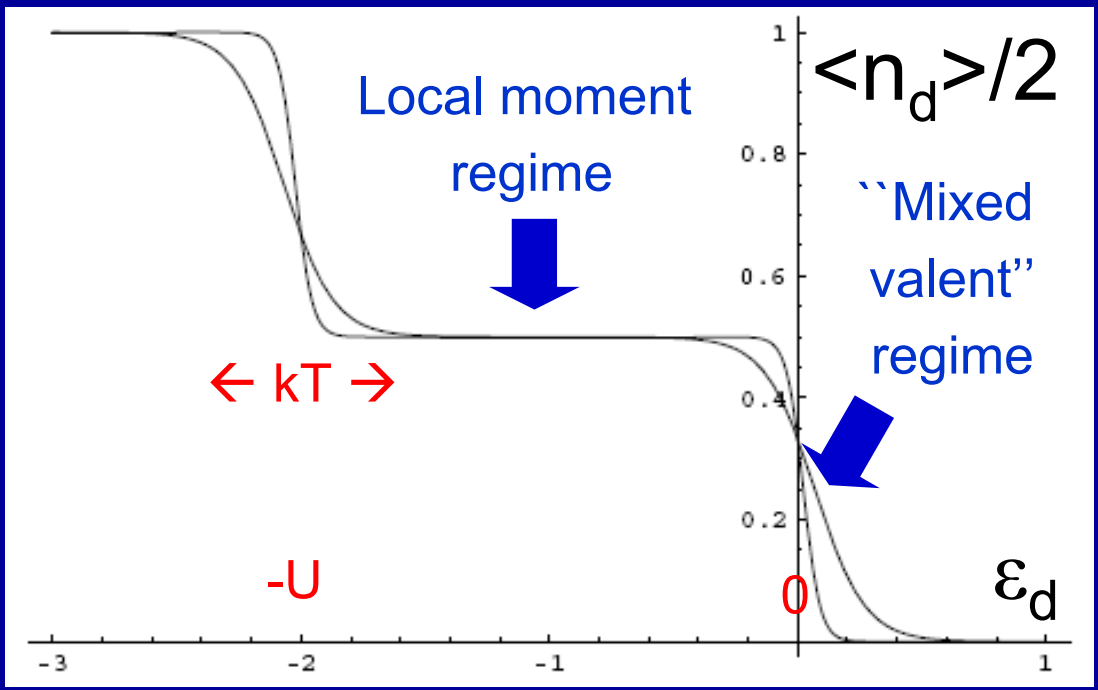
Level crossings:

- Between |n=0> and |n=1> at $\varepsilon = 0$
- Between |n=1> and |n=2> at $\varepsilon = -U$

Occupancy of the isolated atom :

$$n_{d\sigma} \equiv \langle d_\sigma^\dagger d_\sigma \rangle = \frac{n_d}{2} = \frac{1}{Z}\left(1 \times e^{-\beta\varepsilon_d} + 1 \times e^{-\beta(2\varepsilon_d+U)}\right)$$

$$Z = 1 + 2e^{-\beta\varepsilon_d} + e^{-\beta(2\varepsilon_d+U)}$$



Plot of $n_d/2$ vs. ε_d for $U = 2$ at $\beta = 30$ and $\beta = 10$.

``Coulomb staircase'': Blocking of charge by Repulsive interactions, Except at points of level-crossing (charge degeneracy)

Spectroscopy of the isolated atom

One-particle spectral function, at T=0:

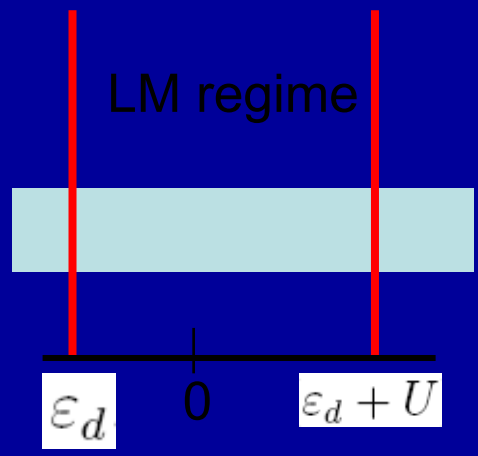
$$\begin{aligned} A_d(\omega) &\equiv \sum_A |\langle \Psi_A | d_\sigma^\dagger | \Psi_0 \rangle|^2 \, \delta(\omega + E_0 - E_A) \quad (\omega > 0) \\ &\equiv \sum_B |\langle \Psi_B | d_\sigma | \Psi_0 \rangle|^2 \, \delta(\omega + E_B - E_0) \quad (\omega < 0) \end{aligned}$$

and, at finite temperature:

$$A_d(\omega) \equiv \frac{1}{Z} \sum_{A,B} |\langle \Psi_A | d_\sigma^\dagger | \Psi_B \rangle|^2 \, \left(e^{-\beta E_A} + e^{-\beta E_B} \right) \delta(\omega + E_B - E_A)$$

$$\begin{aligned} A_d(\omega) &= \frac{e^{-\beta\varepsilon_d} + e^{-\beta(2\varepsilon_d + U)}}{Z} \delta(\omega - \varepsilon_d - U) + \frac{1 + e^{-\beta\varepsilon_d}}{Z} \delta(\omega - \varepsilon_d) \\ &= \frac{n_d}{2} \delta(\omega - \varepsilon_d - U) + (1 - \frac{n_d}{2}) \, \delta(\omega - \varepsilon_d) \end{aligned}$$

$[|\sigma\rangle \leftrightarrow |\uparrow\downarrow\rangle \text{ transition}] + [|\sigma\rangle \leftrightarrow |0\rangle \text{ transition}]$



4. Is the atomic limit singular ?

- 4.1 Exact solution for a single site in the bath

$$H = H_{\rm at} + V \sum_{\sigma} \left(c^{\dagger}_{\sigma} d_{\sigma} + d^{\dagger}_{s} c_{\sigma} \right)$$

Conserved quantum numbers:
N, S, S^z

1+4+6+4+1=16 states

- $N = 0$: one state $|0\rangle$ $(S = S^z = 0)$
- $N = 1$: 4 states, $S = 1/2, S^z = \pm 1/2$
- $N = 2$: $S = 1$ a triplet of states
- $N = 2$: $S = 0$ three singlet states
- $N = 3$: 4 states
- $N = 4$: one states: $|\uparrow\downarrow, \uparrow\downarrow\rangle$

Focus on N=2 (ground-state) sector in LM regime:

- The $N = 2, S = 1$ triplet sector has eigenstates: $|\uparrow,\uparrow\rangle$, $|\downarrow,\downarrow\rangle$ and $\frac{1}{\sqrt{2}}[|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle]$. These states are insensitive to the hybridization V because the Pauli principle does not allow for hopping an electron through. Hence their energy is ε_d.

The $N = 2, S = 0$ sector is more interesting.

Basis set: $|\uparrow\downarrow, 0\rangle$, $\frac{1}{\sqrt{2}}[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle]$ $|0,\uparrow\downarrow\rangle$.

The matrix reads:
$$\begin{pmatrix} 2\varepsilon_d + U & \sqrt{2}V & 0 \\ \sqrt{2}V & \varepsilon_d & \sqrt{2}V \\ 0 & \sqrt{2}V & 0 \end{pmatrix}$$

Symmetric case ε_d=-U/2

$$E = 0 \ , \ E_\pm = -\frac{U}{4} \pm \frac{1}{2}\sqrt{\frac{U^2}{4} + 16V^2}$$

The *ground-state* has energy E_-. For $V \ll U$, this reads:

$$E_0 = E_- \simeq -\frac{U}{2} - \frac{8V^2}{U} + \cdots$$

Energy in SINGLET SECTOR is lowered by virtual hops

Double occupancy → energy denominator ~ U

Ground-state wave-function:

$$|\Psi_0\rangle = \sqrt{1-\eta^2}\,|\mathcal{S}\rangle + \eta\,|\mathcal{D}\rangle$$

$$|\mathcal{S}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right]$$

$$|\mathcal{D}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow,0\rangle + |0,\uparrow\downarrow\rangle\right]$$

with $\eta \sim \frac{V}{U} \ll 1$.

Key points:

- Because of virtual hopping and the Pauli principle, a spin-singlet ground-state has been stabilized, in which the impurity spin is screened out by a conduction electron.
- Virtual hopping has induced a (small) admixture of states with $n_d = 0$ and $n_d = 2$ in the wave-function, hence allowing for charge fluctuations on the atom.

- The atomic limit V=0 is SINGULAR in the LM regime
- A non-zero V lifts the ground-state degeneracy
- The ground-state becomes a singlet: the impurity moment is ``screened'' by binding w/ a conduction electron

4.2 Effective Hamiltonian: the Kondo model

1-site: low-energy Hilbert space ={ground-state + triplet S=1}

$$H_{\rm eff} = J_K \, \vec{S}_d \cdot \vec{S}_c \;\; , \;\; J_K = \frac{8V^2}{U}$$

Sd, Sc: spin operators

Can be generalized to a full conduction electron band:

(Schrieffer-Wolff transformation –eliminating states w/ nd=0,2) -1966-

$$H_{\rm eff} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}} \, c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \vec{S}_d \cdot \sum_{\mathbf{k}\mathbf{k}'\alpha\alpha'} J_{\mathbf{k}\mathbf{k}'} \frac{1}{2} c^\dagger_{\mathbf{k}'\alpha'} \vec{\sigma}_{\alpha\alpha'} c_{\mathbf{k}\alpha} + \sum_{\mathbf{k}\mathbf{k}'\alpha} V^{\rm pot}_{\mathbf{k}\mathbf{k}'} c^\dagger_{\mathbf{k}'\alpha} c_{\mathbf{k}\alpha}$$

$$J_{\mathbf{k}\mathbf{k}'} = 2V_{\mathbf{k}} V_{\mathbf{k}'} \left[\frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_d} + \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}} \right] \rightarrow 2V_{\mathbf{k}} V_{\mathbf{k}'} \frac{U}{|\varepsilon_d(\varepsilon_d + U)|}$$

$$V^{\rm pot}_{\mathbf{k}\mathbf{k}'} = \frac{1}{2} V_{\mathbf{k}} V_{\mathbf{k}'} \left[\frac{1}{\varepsilon_{\mathbf{k}'} - \varepsilon_d} - \frac{1}{\varepsilon_d + U - \varepsilon_{\mathbf{k}}} \right]$$

→ 0 in symmetric case

Jun Kondo

5. Expansion in the Kondo coupling: singularities

Not surprisingly in view of the above, the perturbative expansion in J is plagued w/ singularities (when the conduction electron bath is metallic - gapless)

The original calculation by Kondo deals w/ the resistivity, in which the log's appear at 3rd order:

$$R_{\rm imp} \propto (J_K\rho)^2 \left[1 - 2J_K\rho \ln\frac{T}{D} + \cdots\right]$$

- Hints at an explanation of the `resistance minimum (R increases as T is lowered)
- Perturbation theory FAILS BELOW a characteristic scale : $T_K \sim De^{-1/(J_K\rho)}$

``Kondo temperature''

Similarly, in magnetic and thermo. properties:

Impurity susceptibility:

$$\chi_{\rm imp} \equiv \frac{\partial \langle S^z \rangle}{\partial h_{\rm imp}} = \int_0^\beta d\tau \, \langle S^z(0) S^z(\tau) \rangle$$

$$\chi_{\rm imp} = \frac{(g\mu_B)^2 S(S+1)}{3T} \left[1 - J_K\rho + (J_K\rho)^2 \, \ln \frac{T}{D} + c(J_K\rho)^2 + \cdots \right]$$

Entropy:

$$S_{\rm imp} = \ln(2S+1) - \frac{\pi^2}{3} S(S+1)(J_K\rho)^3 \left[1 - 3J_K\rho \, \ln \frac{T}{D} + \cdots \right]$$

Hints at a gradual quenching of the moment:

``effective Curie constant'', and moment entropy, decrease

Some more details on these calculations…

Kondo interaction:

$$J_\perp \left[S_c^+ f_\downarrow^+ f_\uparrow + S_c^- f_\uparrow^+ f_\downarrow \right] + J_z S_c^z \left(f_\uparrow^+ f_\uparrow - f_\downarrow^+ f_\downarrow \right)$$

obviously $[\hat{H}, \hat{Q}] = 0$

We are interested in $Z_1 = \mathrm{tr}\, e^{-\beta \hat{H}}\big|_{Q=1}$

Introduce λ s.t.

$$H = H_c + H_J - \lambda \sum_\sigma f_\sigma^+ f_\sigma .$$

$$Z = \mathrm{tr}\, e^{-\beta \hat{H}} = Z_0 + Z_1 e^{\beta\lambda} + Z_2 e^{2\beta\lambda} \qquad [H, Q] = 0$$

$$= Z_c^0 \left[1 + e^{2\beta\lambda} \right] + Z_1 e^{\beta\lambda}$$

because f term $\to$ only $Q = 0, 2$

choose $1 + e^{2\beta\lambda} = 0$

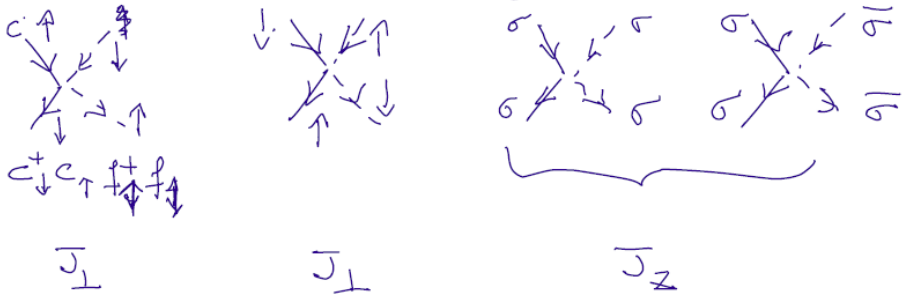
$$\boxed{\beta\lambda = i\frac{\pi}{2}}$$

Abrikosov trick.

$$\langle f^+ f \rangle : \quad G_f(\tau) \sim e^{i\frac{\pi}{2}\frac{\tau}{\beta}} g_g(\tau)$$

$$\frac{1}{i\omega_n + \lambda} = \frac{1}{i\omega_n + i\frac{\pi}{2\beta}}$$

Vertices:



$$G_0(i\omega_n) = \sum_k \frac{1}{i\omega_n - \varepsilon_k} \to \frac{1}{2D}\int_{-D}^{D} \frac{d\varepsilon}{i\omega - \varepsilon}$$

$$G_0(\tau) \sim \frac{g_0}{\tau} \quad @ \text{ large } \tau$$

Look e.g. at χ_{imp}:

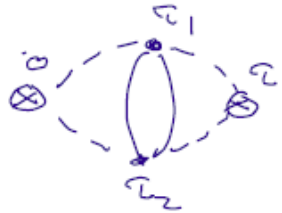
0th order 

$G_f(\tau) G_f(-\tau) \sim$ const.

$\chi_{imp} = \int_0^\beta d\tau \to \beta$.

1st order 

regular corrections $G_0(0)$.

2nd order 

$$\int d\tau_1 \int d\tau_2 \, G_{c0}(\tau_1 - \tau_2)\, G_{c0}(\tau_2 - \tau_1) \; sg(\tau_1) sg(\tau_2) \; sg(\tau - \tau_1) sg(\tau - \tau_2)$$

$$\sim \int d\tau_1 \int d\tau_2 \frac{1}{(\tau_1 - \tau_2)^2} \to \text{log div !}$$

6. Scaling and the Renormalization Group

RG approach: integrate out (recursively) only over high-energy conduction electron states, and reformulate the result as a new Hamiltonian with a scale-dependent coupling.

Integrate only over shell: $\varepsilon_{\mathbf{k}} \in [D - \delta D, D]$

Calculate corresponding change in interactions (2-particle vertex):

$$\delta J_z = J_\perp^2 \frac{\delta D}{D} \ , \ \delta J_\perp = J_z J_\perp \frac{\delta D}{D}$$

Define scale parameter:

$$D(l) = De^{-l}$$

Flow to Lowest order:

$$\frac{dJ_z}{dl} = J_\perp^2$$

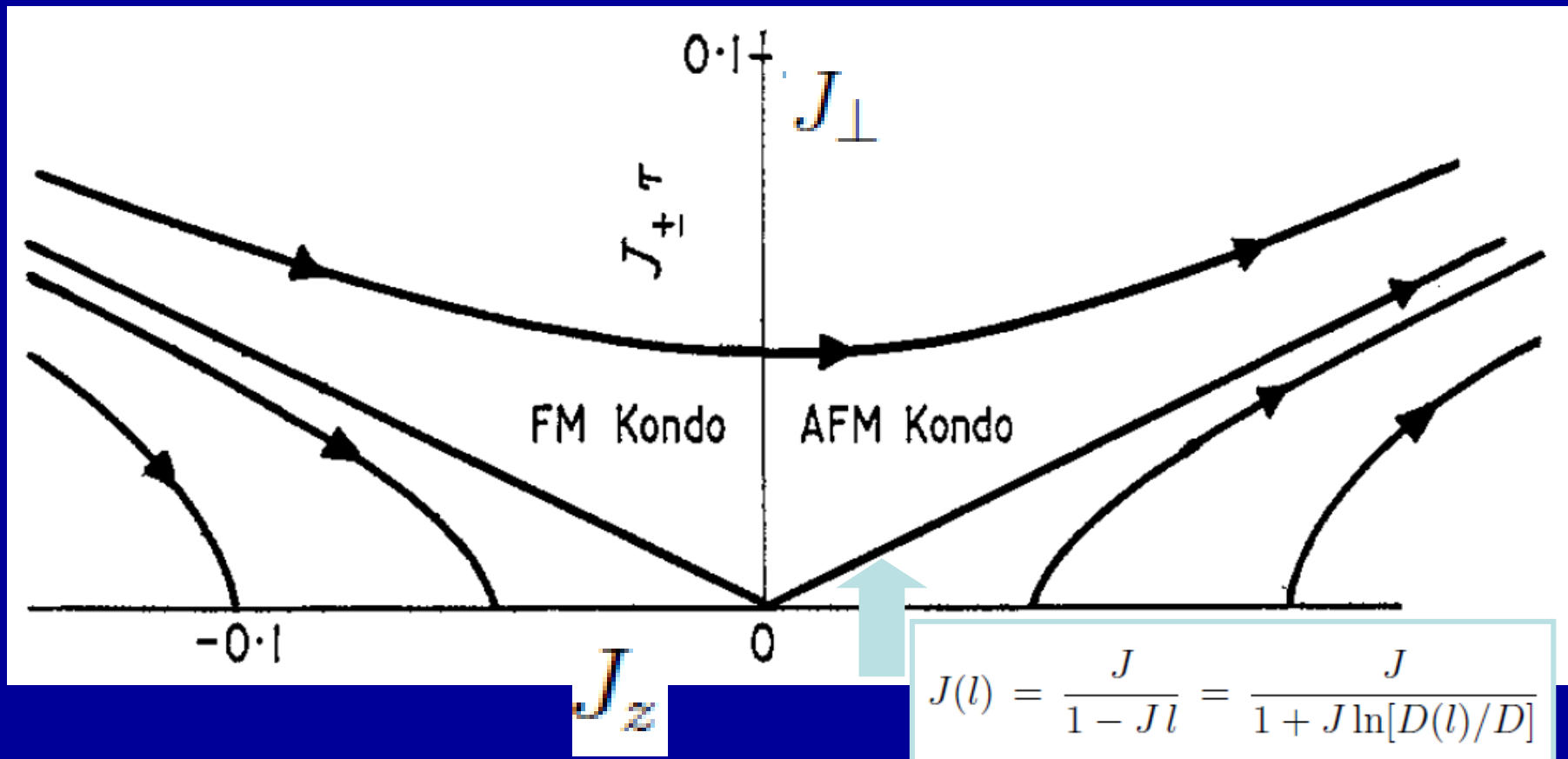
$$\frac{dJ_\perp}{dl} = J_z J_\perp$$

RG flow: AF model flows to strong coupling

$$\frac{dJ_z}{dl} = J_\perp^2$$
$$\frac{dJ_\perp}{dl} = J_z\, J_\perp$$

→ $J_z^2 - J_\perp^2 = \text{const.}$

Coupling becomes large at $D(l_K) \sim T_K$



$$J(l) = \frac{J}{1 - J\,l} = \frac{J}{1 + J \ln[D(l)/D]}$$

Flow of the coupling (all orders): $\frac{dJ}{dl} = \beta(J)$ → $\int_J^{J(l)} \frac{dx}{\beta(x)} = l$

$$\chi\left[T, D; J\right] = \chi\left[T, D(l); J(l)\right] = \frac{1}{D(l)}\tilde{\chi}\left[\frac{T}{D(l)}; J(l)\right]$$

Kondo scale: $T_K = D(l_K)\ ,\ l_K = \ln\frac{D}{T_K}$

$$\chi = \frac{1}{T_K}\tilde{\chi}\left[\frac{T}{T_K}; J(l_K)\right] = \frac{1}{T_K}\tilde{\chi}\left[\frac{T}{T_K}; J^*\right]$$

+ small corrections

Universal scaling function associated with strong-coupling fixed point

Refined estimate to next order: $T_K = D\sqrt{J}e^{-1/J}$

Nature of the strong-coupling fixed point and its vicinity:

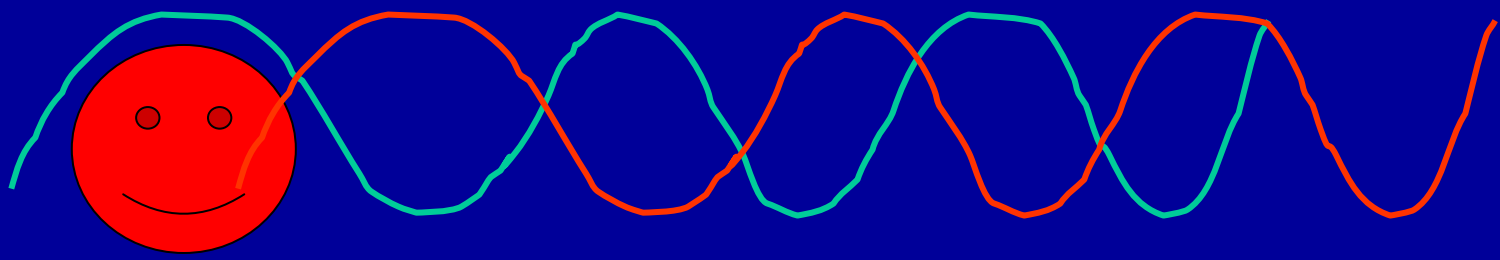
singlet formation and local Fermi liquid

Nozières, Anderson, Wilson

- Singlet ground-state formed between impurity spins and conduction electrons (cf. one conduction orbital calculation)

- Seen from the conduction electron viewpoint:

N sites → N-1 sites (impurity site inaccessible) → **$\pi/2$ "phase shift"**



Low-T physics: fixed point+leading irrelevant operator = Fermi liquid

This is best described using a one-dimensional description of fermions, associated with s-wave (I=0) channel. Cf. Affleck, arXiv:0809.3474

Kondo Hamiltonian: R- and L-movers on r>0 half-axis

$$H = \frac{v_F}{2\pi} i \int_0^\infty dr \left(\psi_L^\dagger \frac{d}{dr} \psi_L - \psi_R^\dagger \frac{d}{dr} \psi_R \right) + v_F \lambda \psi_L^\dagger(0) \frac{\vec{\sigma}}{2} \psi_L(0) \cdot \vec{S}$$

Folded to full axis, L-movers only, with boundary condition:

$$\psi_R(r) = \psi_L(-r), \quad (r > 0)$$

$$H = \frac{v_F}{2\pi} i \int_{-\infty}^\infty dr \psi_L^\dagger \frac{d}{dr} \psi_L + v_F \lambda \psi_L^\dagger(0) \frac{\vec{\sigma}}{2} \psi_L(0) \cdot \vec{S}.$$

Hamiltonian close to fixed point:

- Impurity degree of freedom is GONE !
- Fermions have undergone a $\pi/2$ phase-shift, i.e a change of b.c
- Operators at fixed point:
- 1) A marginal one $\psi^{\dagger\alpha}(0)\psi_\alpha(0)$ → Potential scattering, forbidden by p-h stry in stric case
- 2) Two leading irrelevant ones of dimension 2, i.e. $\langle O(0)O(t)\rangle \sim 1/t^4$

$J(0)^2$ and $\vec{J}(0)^2$ with: $J \equiv \psi^{\dagger\alpha}\psi_\alpha, \quad \vec{J} \equiv \psi^{\dagger\alpha}\frac{\vec{\sigma}_\alpha^\beta}{2}\psi_\beta.$

Only second one has a sizeable coeff ($\sim 1/T_K$, not 1/D)

Effective hamiltonian at s.c. fixed point:

$$H = \frac{v_F}{2\pi} i \int_{-\infty}^{\infty} dr \psi_L^\dagger \frac{d}{dr}\psi_L - \frac{1}{6T_K}\vec{J}_L(0)^2.$$

with modified b.c (phase shift)

$$\psi_R(r) = -\psi_L(-r), \quad (r > 0).$$

Note: coefficient in front of 2nd term specifies a convention for defining T_K

Physical quantities at low-T:

Characteristic behavior of Fermi-liquid

2nd term (LIO) is small and can be treated in perturbation theory, as a weak scattering term:

$$\chi_{\rm imp} = \frac{1}{4T_K}\left[1 - c(\frac{T}{T_K})^2 + \cdots\right]$$

$$S_{imp} \to \frac{\pi^2 T}{6T_K}.$$

Wilson ratio:

$$R_W \equiv \frac{\chi_{\rm imp}/\chi_{c0}}{\gamma_{\rm imp}/\gamma_{c0}} = \frac{4\pi^2}{3}\frac{\chi_{\rm imp}}{\gamma_{\rm imp}} = 2$$

Resistivity:

$$\rho = \rho_u\left[1 - \frac{\pi^4}{16}\left(\frac{T}{T_K}\right)^2 + \cdots\right]$$

In which rho_u is the maximal possible resistivity induced by an impurity (unitary limit):

$$\rho_u = \frac{3n_i}{(ev_F\nu)^2}.$$

7.The non-interacting case (U=0)

- A different point of view, offered by the Anderson model (not available for Kondo model)
- In contrast to the V-expansion, small U and large U are smoothly connected.

$$H_{U=0} = \sum_{\mathbf{k}\sigma} \varepsilon_{\mathbf{k}}\, c^{\dagger}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \varepsilon_d \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + \sum_{\mathbf{k}\sigma} V_{\mathbf{k}} (c^{\dagger}_{\mathbf{k}\sigma} d_{\sigma} + d^{\dagger}_{\sigma} c_{\mathbf{k}\sigma})$$

$$G^{-1}_{d0}(i\omega_n) = i\omega_n - \varepsilon_d - \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

``Integrating out'' c-electrons, or simple diagrammatics, or eqs of motion

Key quantity: hybridization function

$$\Delta(i\omega_n) \equiv \sum_{\mathbf{k}} \frac{|V_{\mathbf{k}}|^2}{i\omega_n - \varepsilon_{\mathbf{k}}}$$

$$\Gamma(\varepsilon) \equiv \pi \sum_{\mathbf{k}} |V_{\mathbf{k}}|^2\, \delta(\varepsilon - \varepsilon_{\mathbf{k}}) = -\operatorname{Im} \Delta(\varepsilon + i0^{+}) = \pi \Delta(\varepsilon)$$

Case of a broad band w/ structureless d.o.s:

(Note: the integrable case, by Bethe ansatz, for arbitrary U)

$$\Gamma(\varepsilon) = \Gamma = \pi\Delta(0) \quad , \quad \text{for}\, \varepsilon \in [-\mathrm{D}, +\mathrm{D}]$$

$$\Delta(i\omega_n) = -\frac{\Gamma}{\pi} \ln \frac{D - i\omega_n}{-D - i\omega_n} \rightarrow -i\Gamma \mathrm{sign}(\omega_n)$$

(D→ infinity)

$$\Delta(\omega + i0^+) = \frac{\Gamma}{\pi} \ln \left| \frac{\omega + D}{\omega - D} \right| - i\Gamma \rightarrow -i\Gamma$$

$$\Gamma = \pi V^2 \rho_c$$

`Virtual bound-state' resonance

Width given by Fermi's Golden rule

In this limit:

$$A_d^0(\omega) = \frac{1}{\pi} \frac{\Gamma}{(\omega - \varepsilon_d)^2 + \Gamma^2}$$

$$\frac{n_d}{2} = \int_{-\infty}^{+\infty} d\omega\, A_d^0(\omega) = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\varepsilon_d}{\Gamma}$$

No Coulomb blockade. of course

Goes smoothly from n=0 to n=2

Key issue:

- How does one interpolate from $U/\Gamma=0$ limit

(1 broadened atomic level centered at ε_d)

to atomic limit $\Gamma/U=0$?

(2 sharp peaks ~ atomic transitions,

doubly deg. ground-state)

8. General many-body theory and (local) Fermi-liquid considerations

Focus on dynamics of impurity orbital: integrate out conduction electrons

→ Effective action for impurity orbital:

$$S = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^\dagger(\tau') G_{d0}^{-1}(\tau-\tau') d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow$$

also reads:

$$\begin{aligned} S &= S_{\rm at} + S_{\rm hyb} \\ S_{\rm at} &= \int_0^\beta d\tau \sum_\sigma d_\sigma^\dagger(\tau) \left(-\frac{\partial}{\partial\tau} + \varepsilon_d\right) d_\sigma(\tau) + U \int_0^\beta d\tau n_\uparrow n_\downarrow \\ S_{\rm hyb} &= \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d_\sigma^\dagger(\tau') \Delta(\tau-\tau') d_\sigma(\tau) \end{aligned}$$

Feynman rules associated with this action (involving only time):

- A vertex U (local in time)
- A `bare' propagator (retarded): $G_{d0}(\tau - \tau') \sim \rho_c/(\tau - \tau') + \cdots$

The interaction leads to a self-energy for the d-orbital:

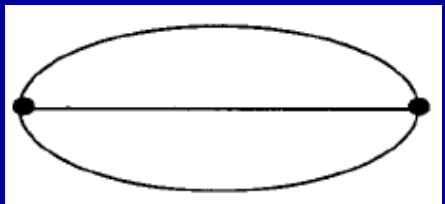
$$G_d(i\omega_n)^{-1} = G_{d0}(i\omega_n)^{-1} - \Sigma(i\omega_n)$$

(Local) Fermi-liquid form of self-energy, at T=0:

$$\Sigma'(\omega) = \Sigma(0) + \left(1 - \frac{1}{Z}\right)\omega + \cdots$$

$$\Sigma''(\omega) = -A\,\omega^2 + \cdots$$

First non-trivial diagram $O(U^2)$:



$$\sim U^2 \frac{1}{\tau^3} \rightarrow \Sigma'' \propto \omega^2$$

d-level spectral function, wide bandwidth limit:

$$A_d(\omega) = \frac{1}{\pi} \frac{\Gamma - \Sigma''(\omega)}{\left[\omega - \varepsilon_d - \Sigma'(\omega)\right]^2 + \left[\Gamma(\omega) - \Sigma''(\omega)\right]^2}$$

Hence, at low-frequency:

$$A_d(\omega \simeq 0) = \frac{Z}{\pi} \frac{\widetilde{\Gamma}}{(\omega - \widetilde{\varepsilon}_d)^2 + \widetilde{\Gamma}^2}$$

Resonance with renormalized level position and width, overall spectral weight Z:

$$\widetilde{\varepsilon}_d = Z\left[\varepsilon_d + \Sigma(0)\right] \quad , \quad \widetilde{\Gamma} = Z\,\Gamma$$

In particular, in particle-hole symmetric case (LM regime) $\varepsilon_d = -\frac{U}{2}$

$$A_d(\omega \simeq 0) = \frac{Z}{\pi} \frac{Z\Gamma}{\omega^2 + (Z\Gamma)^2} \qquad A_d(\omega = 0) = \frac{1}{\pi\Gamma}$$

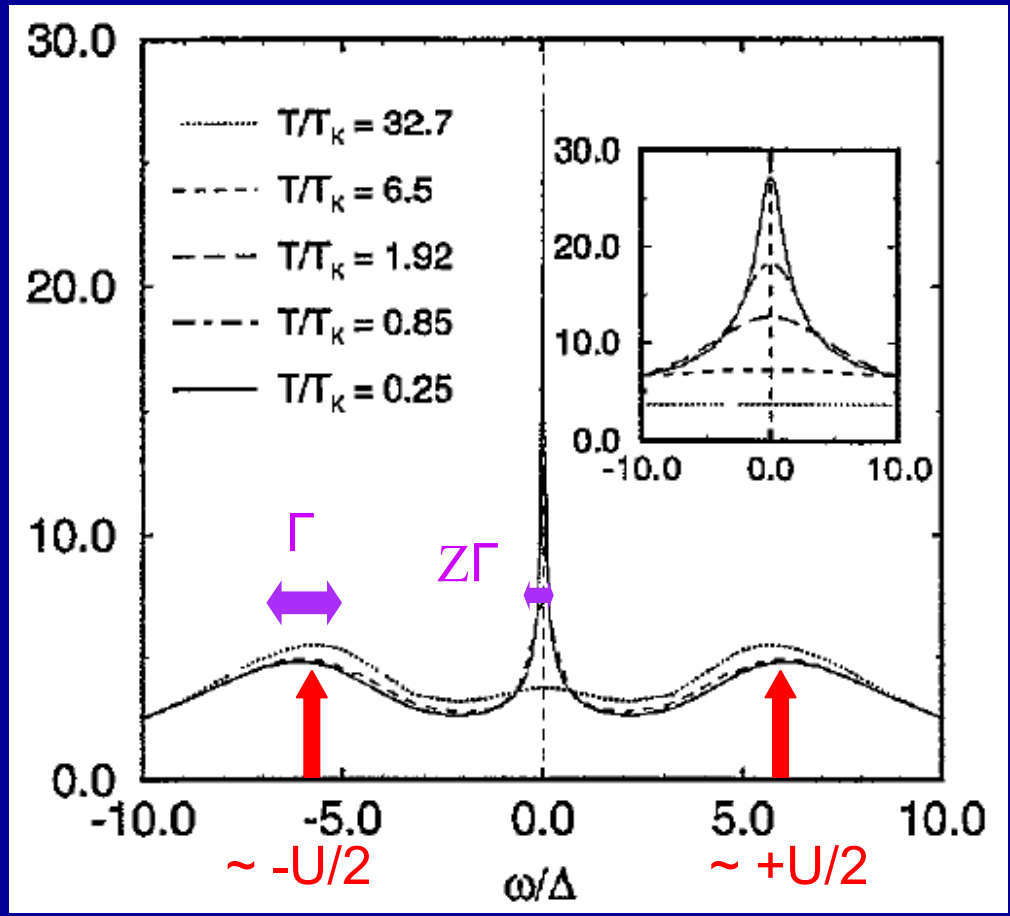
Width, Weight ~ Z

Height unchanged !

Numerical Renormalization Group (NRG) calculation

T.Costi and A.Hewson, J. Phys Cond Mat 6 (1994) 2519

Cf. seminar by Olivier Parcollet



$$Z \sim T_K/\Gamma$$

$$T_K \sim \Lambda\, e^{-1/J_K \rho_c} \sim \Lambda \exp -\frac{\pi U}{8\Gamma}$$

The conduction electron viewpoint:

$$G_{\mathbf{k}\mathbf{k}'}(i\omega_n) = \frac{1}{i\omega_n - \varepsilon_{\mathbf{k}}}\delta_{\mathbf{k}\mathbf{k}'} + \frac{V_{\mathbf{k}}^*}{i\omega_n - \varepsilon_{\mathbf{k}}} G_d(i\omega_n) \frac{V_{\mathbf{k}'}}{i\omega_n - \varepsilon_{\mathbf{k}'}}$$

→ $T_{\mathbf{k}\mathbf{k}'}(i\omega_n) = V_{\mathbf{k}}^* G_d(i\omega_n) V_{\mathbf{k}'}$ T-matrix

Phase-shift: $T_{\mathbf{k}\mathbf{k}'}(\omega + i0^+) = -|T_{\mathbf{k}\mathbf{k}'}| e^{i\delta_{\mathbf{k}\mathbf{k}'}(\omega)}$

Particle-hole symmetry: T is purely imaginary → $\delta = \pi/2$

→ Unitary-limit scattering

From $G_c = G_{c0} + [G_{c0}]^2 V^2 G_d$

We get: Im Gc(0) = 0

Conduction electron d.o.s vanishes at impurity site !

Bibliography – Lecture 1

- Kondo and Anderson models:
- I.Affleck *Quantum impurity problems in condensed matter physics Lecture notes at Les Houches, arXiv:0809.3474*
- A.Hewson *The Kondo problem to heavy fermions, Cambridge UP*
- G.Grüner and A.Zawadowski *Rep Prog Phys 37 (1974) 1497*
- D. Cox Lectures at Boulder school, 2003 http://sexton.ucdavis.edu/CondMatt/cox/
- D. Cox and A. Zawadovski Adv. Phys. **47**, 599 (1998)
- + Many other references…