Kondo effect in mesoscopic and nanoscopic systems

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Recap Lecture 1

- Anderson model
- Magnetic moment formation: Stoner criterion
- At second order in the *d* level-electron bath coupling the Anderson model is equivalent to the Kondo model (are the higher order terms important at low energies?)
- Anderson's poor man's scaling:
  - solves problem for ferromagnetic coupling: free impurity at low energies.
  - suggests a singlet ground state for the antiferromagnetic case, but breaks-down at low energy scales $\sim k_B T_K$

Outline of lecture 2

- Numerical renormalization group
  - Numerical solution of the Kondo problem
- Nozières Fermi liquid theory
  - Low energy effective description
- Slave boson mean field theory
  - Variational solution at low energies (Fermi liquid regime)

References

- A. C. Hewson, *The Kondo problem to Heavy Fermions* [book]
- K. G. Wilson , Rev. Mod. Phys. **47** 773 (1975)
- R. Bulla *et al.* Rev. Mod. Phys. **80** 395 (2008)
- P. Nozières J. of Low Temp. Phys. **17** 31 (1974)
- D. Pines and P. Nozières, *The theory of quantum liquids* [book]

Wilson's renormalization group (RG)

- In poor's man scaling approach two couplings are considerered: $\rho_0 J_\perp, \quad \rho_0 J_\parallel$
  - Other couplings that appear in higher order perturbation theory may be important
- Wilson's RG considers **all** couplings.
  - There is no need to guess which couplings to use.
  - Renormalizations are performed until a fixed point is reached where the couplings stop changing.
  - An effective Hamiltonian close to the fixed points

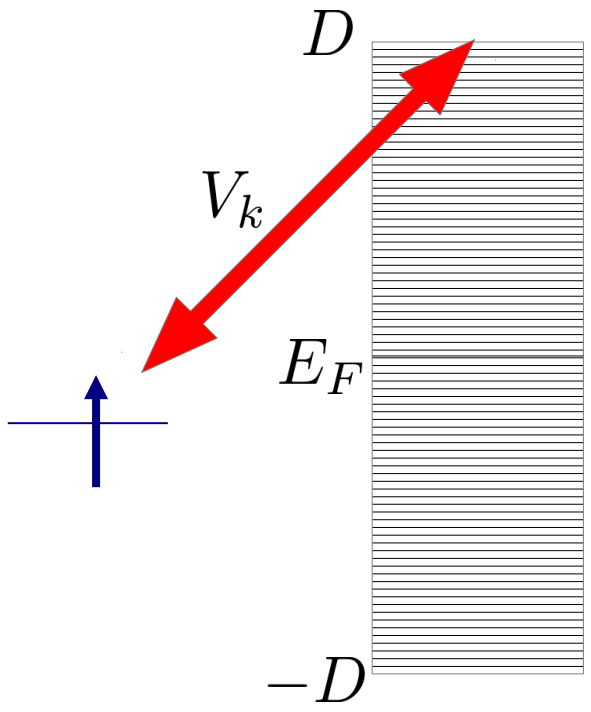
Anderson model

$$H = H_d + H_m + H_V$$

$$H_d = \epsilon_d(\hat{n}_\uparrow + \hat{n}_\downarrow) + U\hat{n}_\uparrow\hat{n}_\downarrow$$

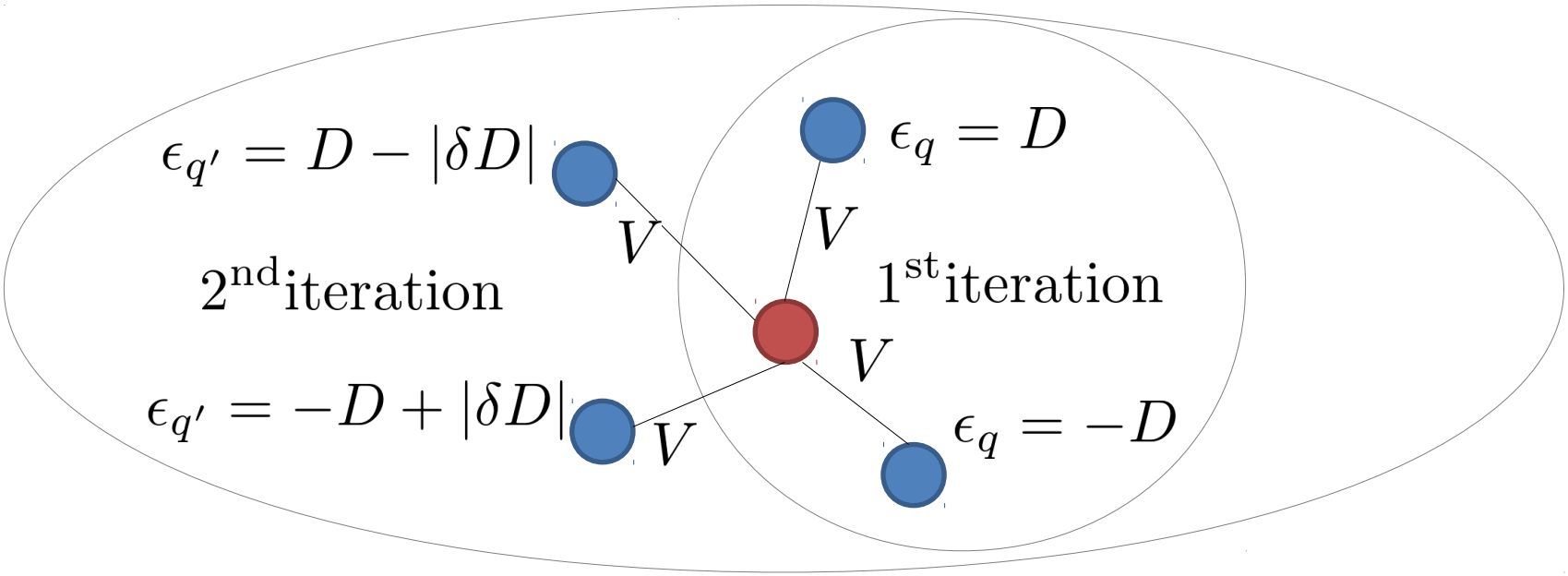
$$H_m = \sum_k \epsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$

$$H_V = \sum_k V_k c^\dagger_{k\sigma} d_\sigma + V^*_k d^\dagger_\sigma c_{k\sigma}$$



renormalization by successive diagonalizations

- Solve exactly by numerical diagonalization the problem of the impurity coupled to a few high energy states.
- At each iteration Include extra conduction band states with decreasing energy.

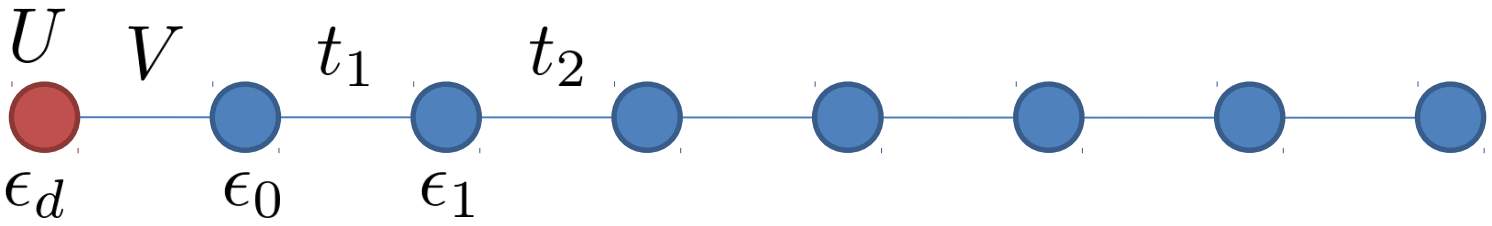


renormalization by successive diagonalizations

- Problems:
  - Too many states to consider at each energy scale in the original Hamiltonian.
  - Exact diagonalization can only be done for a few conduction band states limiting the number of states that can be retained at each iteration.
  - Each extra state increases by a factor 4 the size of the Hilbert space. (Need to discard ¾ of the states at each iteration)
  - In this form the procedure does not converge.

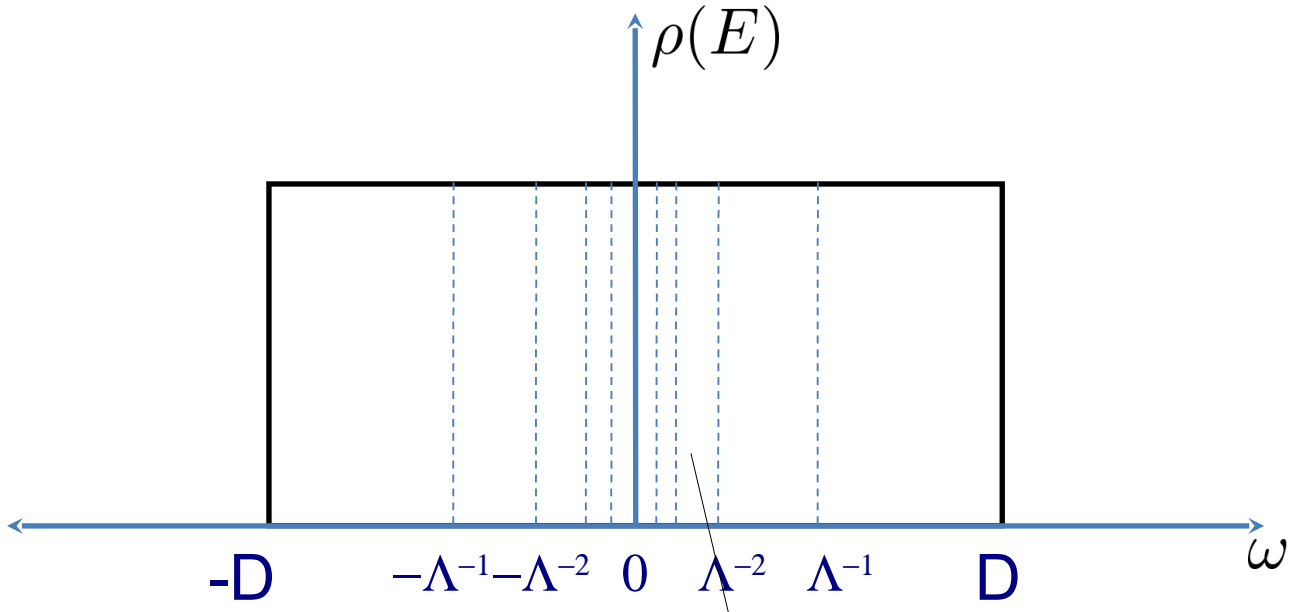
Wilson's numerical renormalization group (NRG)

- Wilson's approach: discretize conduction band in a **logarithmic** way: defines hierarchy of energy scales. Wilson showed that a single electronic state needs to be considered at each energy interval.
- Mapping of the conduction band into a semi-infinite tight-binding chain. Because of the logarithmic discretization, the hopping terms of the chain **decrease exponentially**. The impurity is coupled to the first site of the chain.
- Iterative diagonalization of the impurity problem starting from the impurity and adding sites to the chain. The exponentially growing Hilbert space is truncated keeping a set of low-lying states.



[K. G. Wilson , RMP **47** 773 (1975)]

Logarithmic discretization



$$a_m = \frac{1}{\mathcal{N}_m} \int_{D\Lambda^{-1-m}}^{D\Lambda^{-m}} c_k d\epsilon_k$$

$$\gamma_n^2 = \int_{D\Lambda^{-1-m}}^{D\Lambda^{-m}} \rho(E) dE$$

Lanczos tridiagonalization

- The model can be brought to a one-dimensional tight binding chain using Lanczos tridiagonalization procedure.
- Change of basis states in the metallic host.
  - Define the normalized state:

$$|\phi_0\rangle = f_0^\dagger|0\rangle = \frac{1}{V}\sum_k V_k c_k^\dagger|0\rangle$$

  - where:

$$V = (\sum_k |V_k|^2)^{1/2}$$

$$H_V = \sum_k V_k c_{k\sigma}^\dagger d_\sigma + V_k^* d_\sigma^\dagger c_{k\sigma}$$

Lanczos tridiagonalization

- The *d* level – metal tunneling term simplifies to:

$$H_V = V(f_{0\sigma}^\dagger d_\sigma + d_\sigma^\dagger f_{0\sigma})$$

- Construct an orthonormal basis using:

$$H_m|\phi_0\rangle = \epsilon_0|\phi_0\rangle + t_1|\phi_1\rangle \qquad \langle\phi_0|\phi_1\rangle = 0$$

- with:

$$\epsilon_0 = \langle\phi_0|H_m|\phi_0\rangle, \quad t_1^2 = \langle\phi_0|H_m^2|\phi_0\rangle - \epsilon_0^2$$

- and recursively:

$$t_{n+1}|\phi_{n+1}\rangle = H_m|\phi_n\rangle - \epsilon_n|\phi_n\rangle - t_n|\phi_{n-1}\rangle$$

$$\epsilon_n = \langle\phi_n|H_m|\phi_n\rangle, \quad t_{n+1}^2 = \langle\phi_n|H_m^2|\phi_n\rangle - \epsilon_n^2 - t_n^2$$

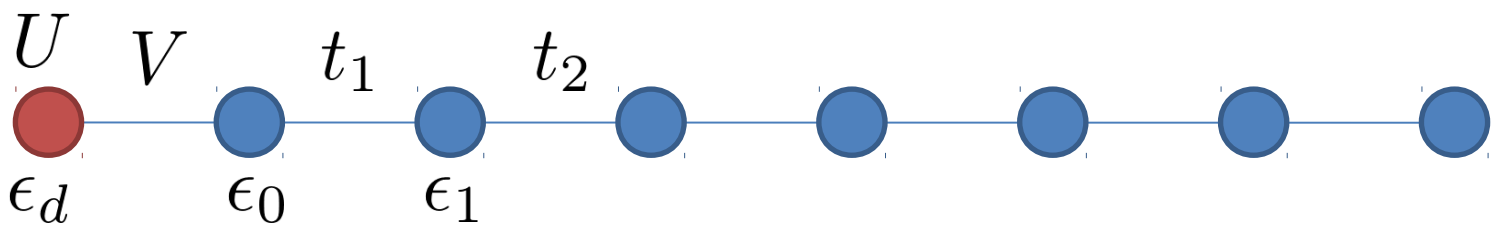
Lanczos tridiagonalization

- We finally have

$$H_d = \epsilon_d(\hat{n}_\uparrow + \hat{n}_\downarrow) + U\hat{n}_\uparrow\hat{n}_\downarrow$$

$$H_V = V(f^\dagger_{0\sigma} d_\sigma + d^\dagger_\sigma f_{0\sigma})$$

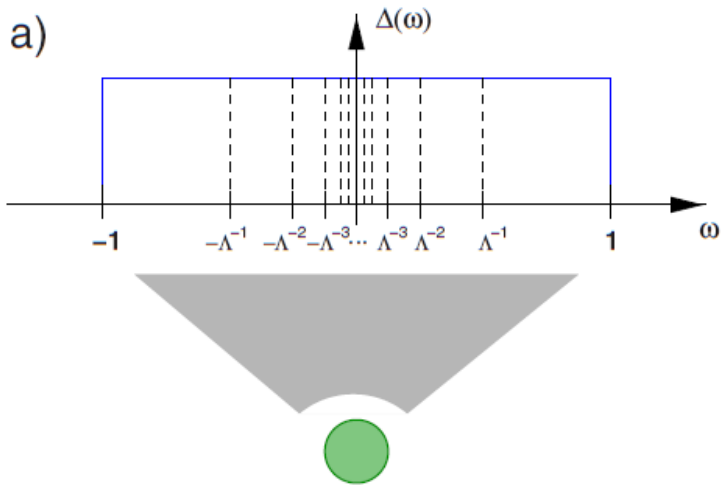
$$H_m = \sum_{n=0} \epsilon_n f^\dagger_n f_n + \sum_{n=0} t_{n+1}(f^\dagger_n f_{n+1} + h.c.)$$



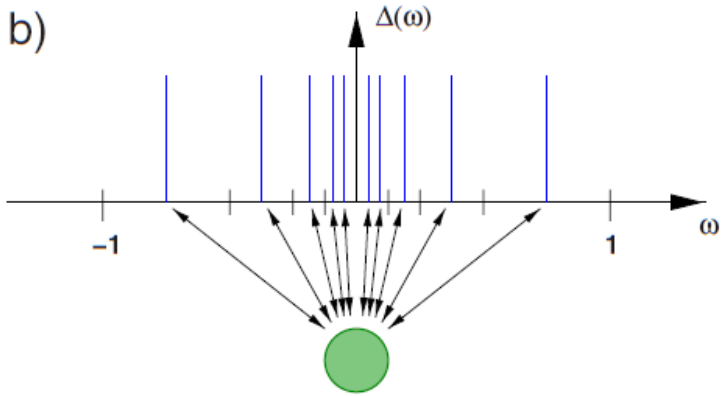
$\Delta(E) = \pi V^2 \rho_0(E)$ ρ_0 is the density of states at site *0*

Wilson's transformation of the conduction band

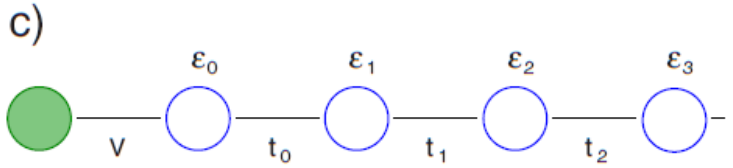
Logarithmic discretization



Single state on each interval

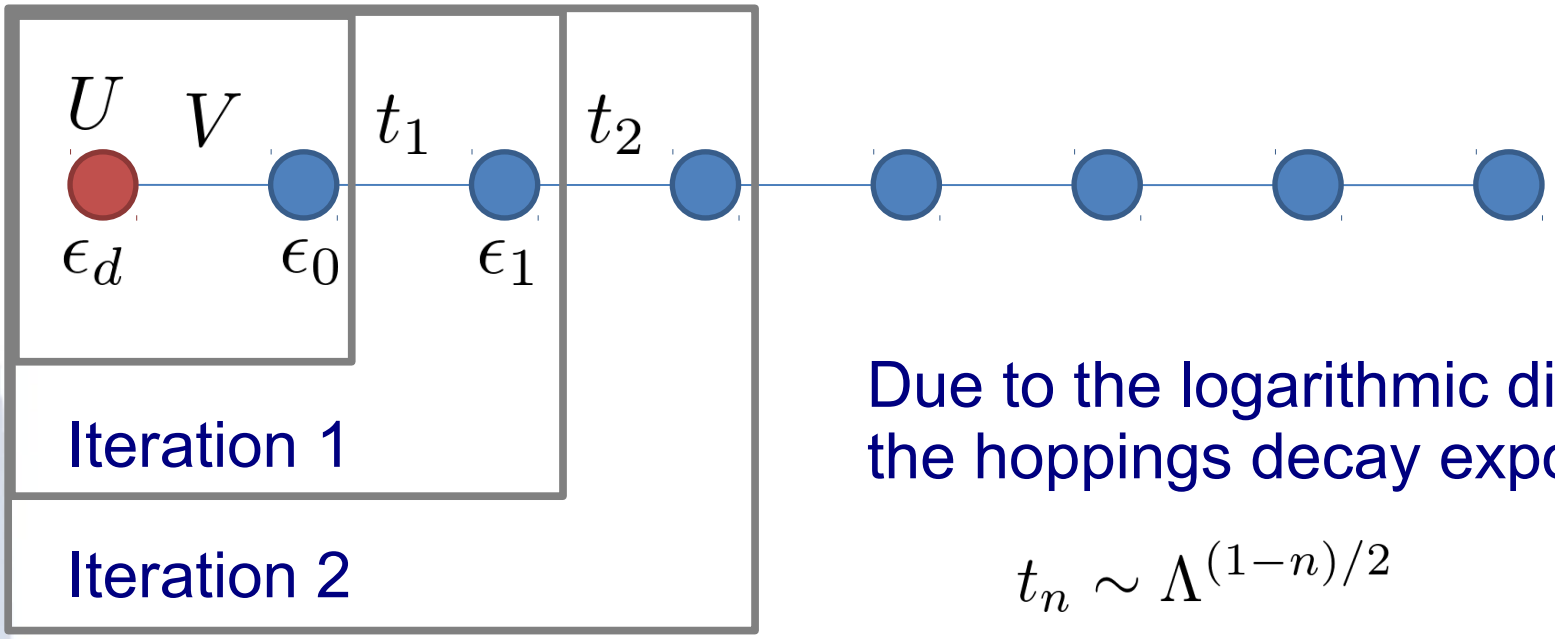


Mapping to a linear chain



R. Bulla *et al.* Rev. Mod. Phys **80** 395 (2008)

Iterative diagonalization

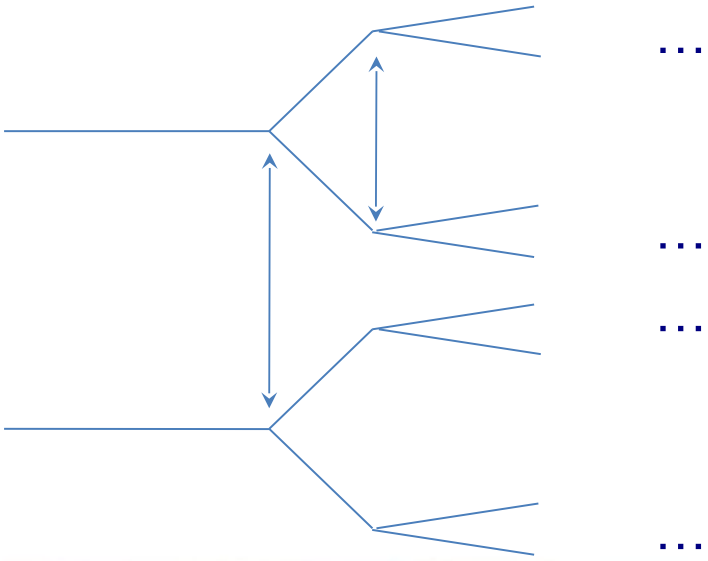


Due to the logarithmic discretization the hoppings decay exponentially

$$t_n \sim \Lambda^{(1-n)/2}$$

Well separated energy scales.

Each RG step produces a perturbation in the spectrum.



Iterative diagonalization

- The size of the Fock space grows exponentially with the number of sites: $N_{st} = 4^{n+1}$
- Discard highest energy states after each iteration.
- In practice converged results for:
  - Λ = 1.5,...,3;
  - retaining N = 400,...,5000 at each iteration
- There are small systematic errors due to the logarithmic discretization. The precision can be much improved averaging over multiple possible discretizations with the same Λ.
  [W Oliveira and L N. Oliveira Phys Rev B 49 11986 (1994)]

Numerical renormalization steps

$$H_{n+1} = \mathcal{R}_\Lambda[H_n]$$

$$H_{n+1} = \sqrt{\Lambda} H_n + \tilde{t}_{n+1}(f^\dagger_{n+1} f_n + f^\dagger_n f_{n+1})$$

$$\tilde{t}_{n+1} = \Lambda^{(n-1)/2} t_{n+1} \sim 1$$

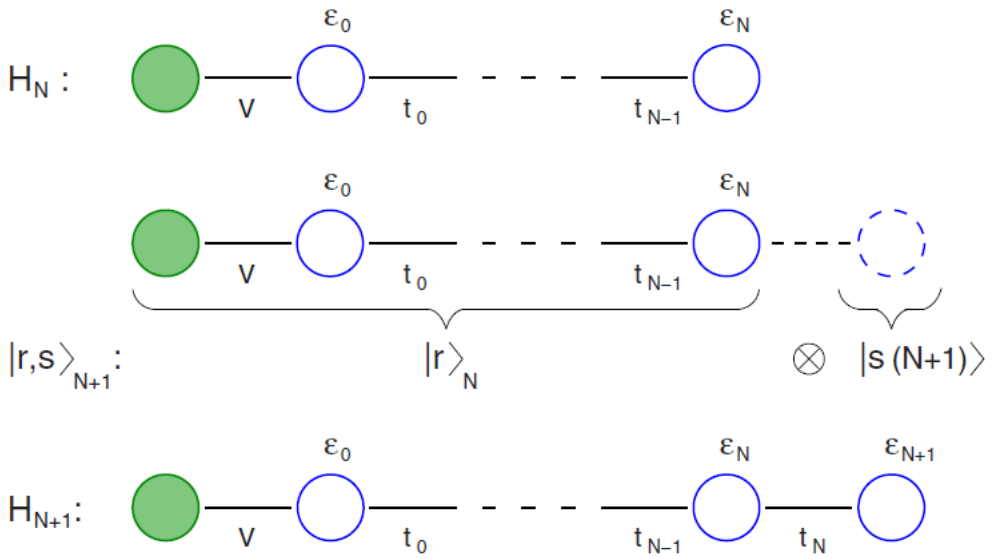
The parity of the number of sites in the chain changes at each NRG step. Two steps are necessary in order to obtain a convergence in the spectrum at a fixed point.

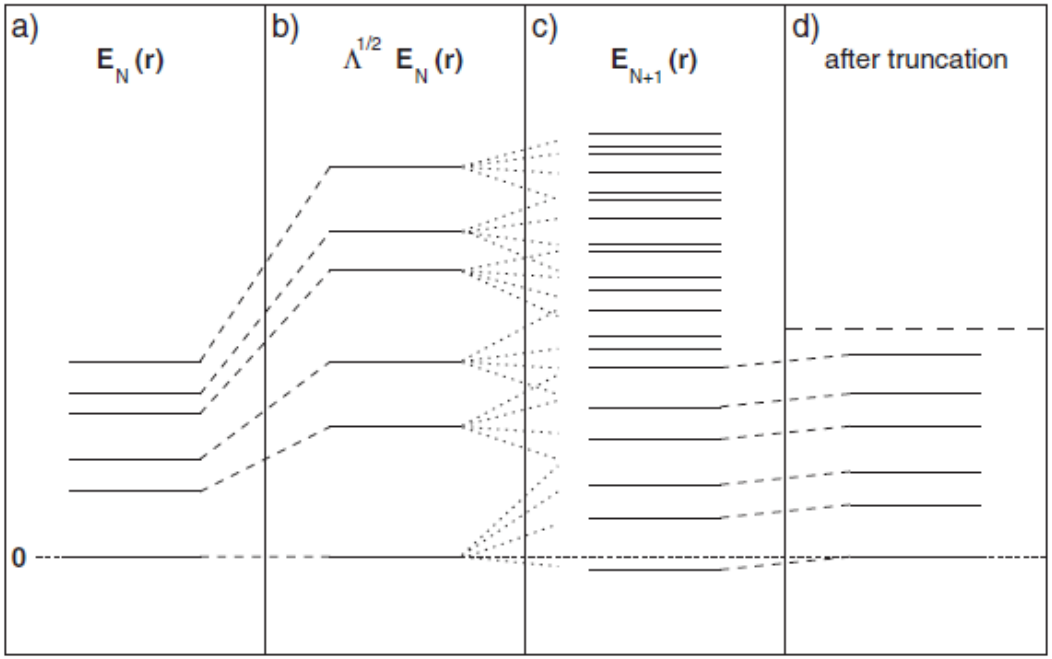
Numerical renormalization steps

The Hamiltonian is diagonalized to obtain the eigenenergies and eigenfunctions.

The high energy states are truncated.

A new site is coupled to the chain.





NRG flow for the Anderson model

Three different regimes:

-Free orbital

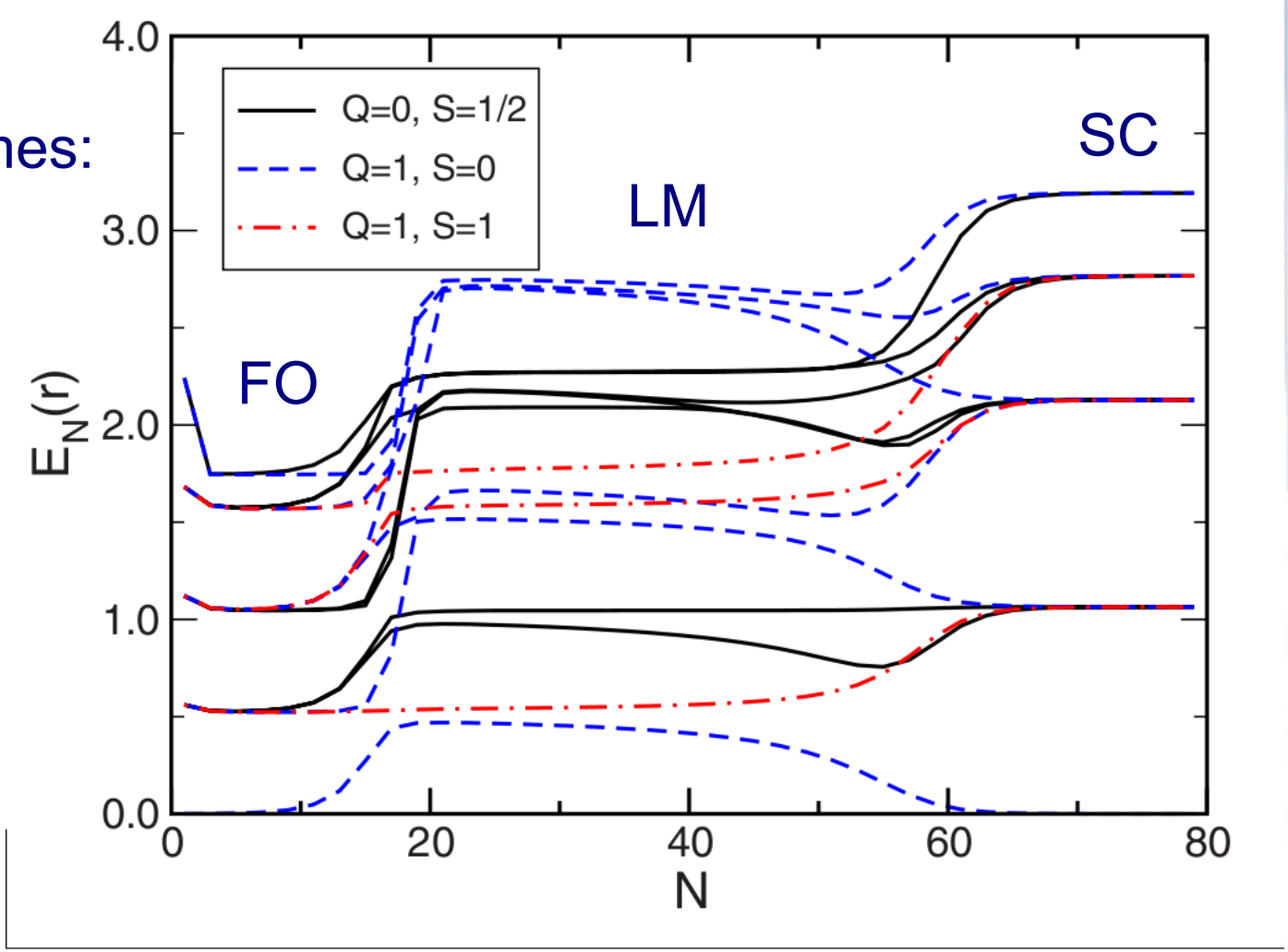
$U = V = 0$

-Local moment

$J = 0$

-Strong coupling.

$J \to \infty$



R. Bulla *et al.* Rev. Mod. Phys **80** 395 (2008)

Fixed points

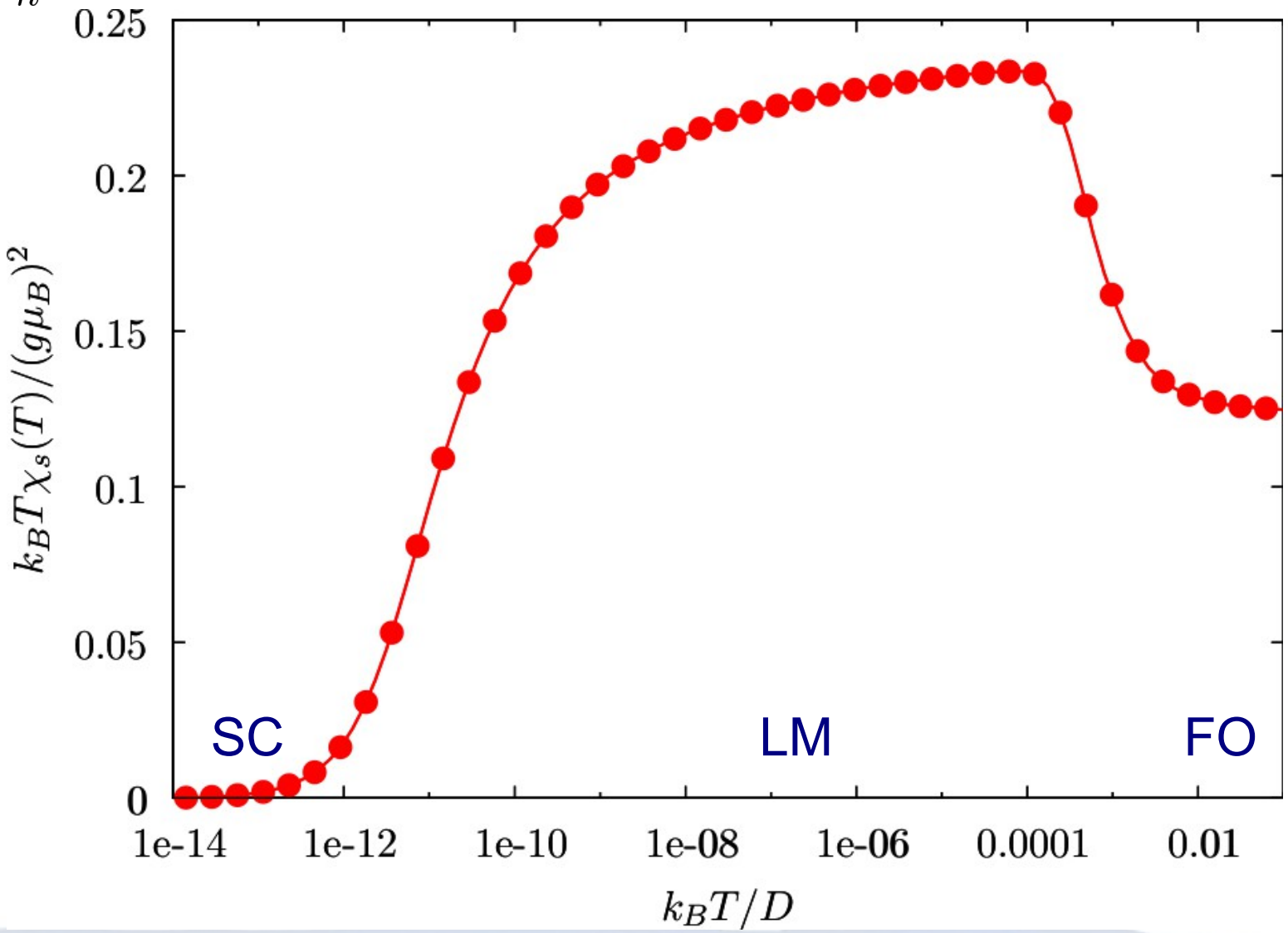
- Free orbital: $k_B T > U, V$
  - The orbital is effectively decoupled
- Local moment $k_B T_K \ll k_B T < U, V$
  - Free spin
- Strong coupling: $k_B T \ll k_B T_K$
  - Screened spin: no remaining magnetic moment.
  - Energy spectrum identical to that of a system with: $J = \infty$
  - Additive spectrum: Fermi liquid behavior.

At iteration *n*

- Set of eigenfunctions with given quantum numbers:
  - charge, spin and energy: $|Q, S, S_z, E, i\rangle_n$
- The energies span a range of roughly an order of magnitude and allow the calculation of thermodynamic properties at a temperature: $T_n \sim D\Lambda^{-(n-1)/2}$
- For dynamic properties, a broadening of the levels is required due to the discrete spectrum: bad resolution at high energies.
  - Many developments in recent years to improve resolution: some using Oliveira's trick.

Thermodynamic properties

At a given iteration, thermodynamic properties can be calculated at a temperature $T_n \sim D\Lambda^{-(n-1)/2}$



Thermodynamic properties

At low temperatures Fermi liquid like behavior

Compensated spin (no divergence) $\chi(T \to 0) \propto \frac{1}{k_B T_K}$

$$C(T \to 0) = \gamma_{\rm imp} T \propto \frac{T}{T_K}$$

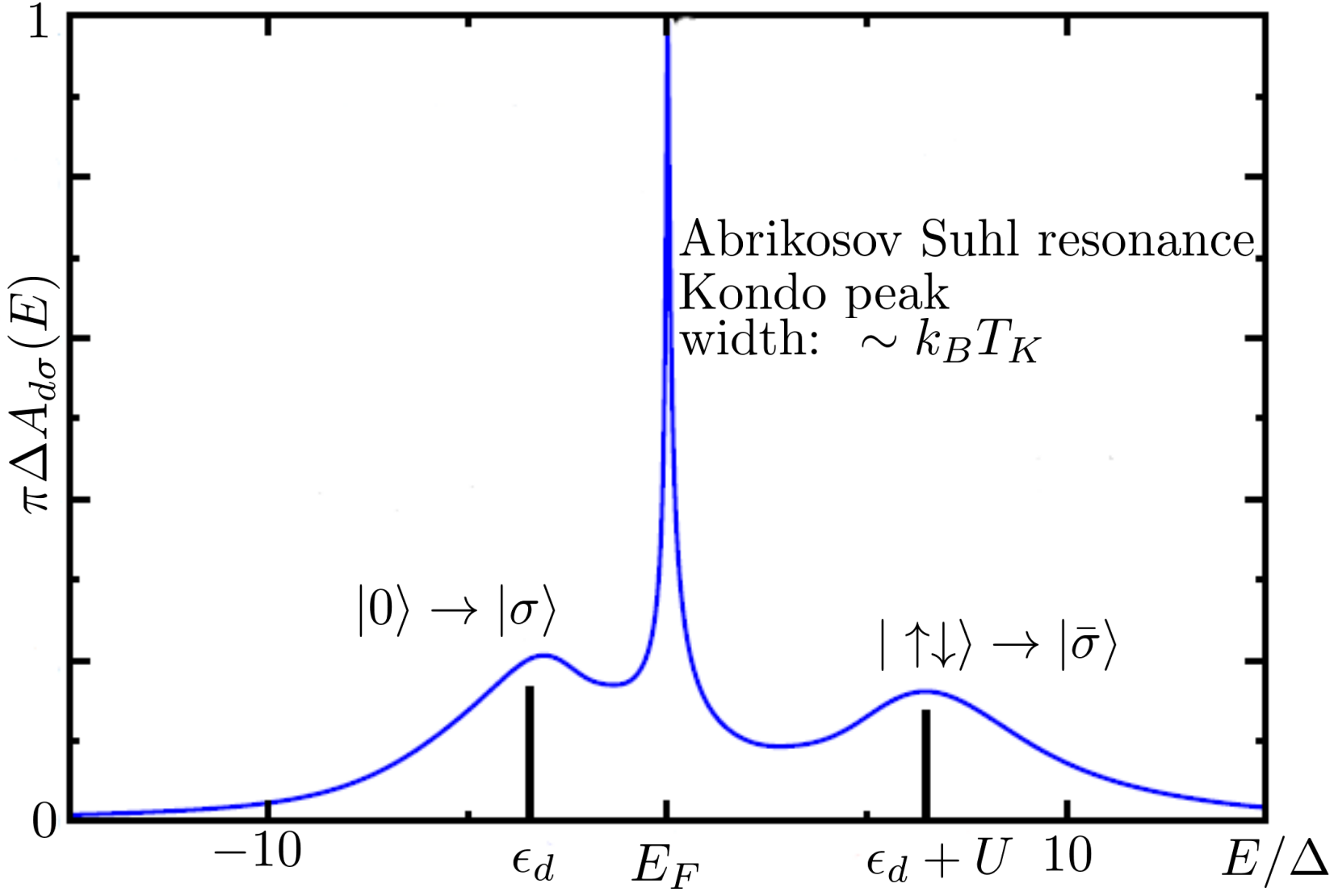
In the Kondo regime there is a single relevant energy scale: $k_B T_K$

Wilson's ratio measures residual interaction between quasiparticles

$$R = \frac{4(\pi k_B)^2}{3(g\mu_B)^2} \frac{\chi_{\rm imp}}{\gamma_{\rm imp}} = 2$$ (strong coupling $U \to \infty$)

$R = 1$ For non-interacting quasiparticles

Dynamic properties



Dynamic properties

- Kondo peak of width: $\propto k_B T_K$
- And height: $A_{d\sigma}(E=0,T=0) = \dfrac{\sin^2(\pi n_{d\sigma})}{\pi\Delta}$ (sum rule)
- Charge fluctuation peaks of reduced height compared to non-interacting results.
- No spin symmetry breaking: $A_{d\uparrow}(E,B=0) = A_{d\downarrow}(E,B=0)$

Appplications

- Interacting impurity in a superconductor, ferromagnetic or pseudogapped host.
  - [Satori *et al.* 1992], [Martinek *et al.* 2003], [Ingersent 1996]
- Anderson-Holstein model (coupling to local phonons).
  - [Hewson and Meyer 2002]
- Coupling to a boson bath.
  - [Bulla 2003]
- Coupling to phonon and fermion baths.
  - [Glossop and Ingersent 2008]
- Impurity solver for DMFT (currently limited to at most two conduction bands)
  - [Bulla 1999]

Nozières local Fermi liquid

- Close to the strong coupling fixed point the local moment captures a spin from the conduction band to form a singlet. No spin-flip scattering remains and the energy spectrum can be fitted assuming weakly interacting quasiparticles.
- Based on Anderson's and Wilson's results Nozières constructed a Fermi liquid theory to describe the quasiparticles in terms of the scattering phase shifts.
- The Fermi liquid is described by a set of Landau parameters. Nozières inferred the value of the parameters. e. g. effective mass $\propto 1/T_K$ and scattering phase shift $\delta_0 = \pi/2$

$$A_{d\sigma}(E=0,T=0) = \frac{\sin^2(\pi n_{d\sigma})}{\pi\Delta}$$

[P. Nozières J. of Low Temp. Phys. **17** 31 (1974)]

Slave boson mean field theory

- Variational approach, exact in large N limit: SU(N) symmetry (N=2 for the spin ½ Kondo model).
- Construct a representation of the impurity states extending the Fock space to include auxiliary boson: b

$$[b, b^\dagger]_- = 1$$

$$[f_\sigma, f_\sigma^\dagger]_+ = 1$$

$$d_\sigma \to b^\dagger f_\sigma$$

$$U = \infty$$

constraint: $b^\dagger b + \sum_\sigma f_\sigma^\dagger f_\sigma = 1$

$$|0\rangle \to b^\dagger |vac\rangle |0\rangle$$

$$|\uparrow\rangle \to f_\uparrow^\dagger |vac\rangle |0\rangle$$

$$|\downarrow\rangle \to f_\downarrow^\dagger |vac\rangle |0\rangle$$

[P. Coleman 1984, Kotliar and Ruckenstein 1986]

Slave bosons U=infinity

$$H_{U=\infty} = \epsilon_d(\hat{n}_\uparrow + \hat{n}_\downarrow) + \sum_k \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_k V_k c^\dagger_{k\sigma} d_\sigma + V_k^* d^\dagger_\sigma c_{k\sigma}$$

$$d_\sigma \to b^\dagger f_\sigma$$

$$H = \epsilon_d \sum f^\dagger_\sigma f_\sigma + \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} + \sum_{k,\sigma} V_k c^\dagger_{k\sigma} b^\dagger f_\sigma + V_k^* b f^\dagger_\sigma c_{k\sigma}$$

Impose the constraint in the partition function using the representation of the Kronecker delta function:

$$\delta_{n,0} = \frac{\beta}{2\pi} \int_{-\pi/\beta}^{\pi/\beta} e^{-i\lambda\beta n} d\lambda \qquad \beta = \frac{1}{k_B T}$$

$$Z = \mathrm{Tr} \frac{\beta}{2\pi} \int_{-\pi/\beta}^{\pi/\beta} e^{-\beta H - i\lambda\beta(b^\dagger b + \sum_\sigma f^\dagger_\sigma f_\sigma)} d\lambda$$

Calculate Z in the mean field approximation replacing the Bose operators by their expectation values:

$$r = \langle b \rangle, \quad r = \langle b^\dagger \rangle$$

The effective mean field Hamiltonian has the form:

$$H_{mf} = (\epsilon_d - i\lambda) \sum f_\sigma^\dagger f_\sigma + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} r V_k c_{k\sigma}^\dagger f_\sigma + r V_k^* f_\sigma^\dagger c_{k\sigma}$$

$$H_{mf} = \tilde{\epsilon}_d \sum f_\sigma^\dagger f_\sigma + \sum_{k,\sigma} \epsilon_k c_{k\sigma}^\dagger c_{k\sigma} + \sum_{k,\sigma} \tilde{V}_k c_{k\sigma}^\dagger f_\sigma + \tilde{V}_k^* f_\sigma^\dagger c_{k\sigma}$$

Non interacting model with renormalized parameters

Slave bosons U=infinity

The Free energy can be calculated and minimized using $\tilde{\epsilon}_d$ and r as variational parameters.

Some general remarks about the solution:

In the Kondo regime $\langle f_\sigma^\dagger f_\sigma \rangle \lesssim 1/2$

Taking averages on the constraint we get: $r^2 = 1 - \sum_\sigma \langle f_\sigma^\dagger f_\sigma \rangle \ll 1$

Resonance at the Fermi level $\langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle = \dfrac{1}{E - \tilde{\epsilon}_d + i\tilde{\Delta}}$

$\tilde{\epsilon}_d \lesssim E_F \quad \tilde{\Delta} = \pi r^2 V^2 \rho_0$

$\langle\langle d_\sigma, d_\sigma^\dagger \rangle\rangle = r^2 \langle\langle f_\sigma, f_\sigma^\dagger \rangle\rangle$

Kondo peak of width $\tilde{\Delta}$ and height $\sim \dfrac{1}{\pi\Delta}$ $\qquad k_B T_K \propto \tilde{\Delta}$

Slave bosons U=infinity

The effective Hamiltonian is quadratic in the fermion operators: It is a Fermi gas with renormalized parameters.

The Free energy can be calculated and minimized for the parameters: λ and r

The approach can be formulated in terms of a variational in terms of a Fermi gas: it can only be valid if the ground state is a Fermi liquid. In the Kondo problem it provides a description at low temperatures.

Slave bosons Kondo model

$$H_K = J(S^+ f^\dagger_{0\downarrow} f_{0\uparrow} + S^- f^\dagger_{0\uparrow} f_{0\downarrow} + S_z(f^\dagger_{0\uparrow} f_{0\uparrow} - f^\dagger_{0\downarrow} f_{0\downarrow}))$$

$$H_K = J(d^\dagger_\uparrow d_\downarrow f^\dagger_{0\downarrow} f_{0\uparrow} + d^\dagger_\downarrow d_\uparrow f^\dagger_{0\uparrow} f_{0\downarrow} + \frac{1}{2}(d^\dagger_\uparrow d_\uparrow - d^\dagger_\downarrow d_\downarrow)(f^\dagger_{0\uparrow} f_{0\uparrow} - f^\dagger_{0\downarrow} f_{0\downarrow}))$$

Mean field decoupling:

$$d^\dagger_\uparrow d_\downarrow f^\dagger_{0\downarrow} f_{0\uparrow} \to d^\dagger_\uparrow \langle d_\downarrow f^\dagger_{0\downarrow}\rangle f_{0\uparrow} + f^\dagger_{0\downarrow}\langle f_{0\uparrow} d^\dagger_\uparrow\rangle d_\downarrow - \langle f^\dagger_{0\downarrow} d_\downarrow\rangle\langle f_{0\uparrow} d^\dagger_\uparrow\rangle$$

The Kondo coupling to the band turns into a hopping term:

$$\tilde{H}_K = \tilde{J}\sum_\sigma (d^\dagger_\sigma f_{0\sigma} + h.c.)$$

$$\tilde{J} = J\langle d_\downarrow f^\dagger_{0\downarrow}\rangle = J\langle d_\uparrow f^\dagger_{0\uparrow}\rangle$$

Slave bosons Kondo model

Using the equation of motion we can write the correlation function:

$$\langle\langle f_{0\sigma}, d_\sigma^\dagger \rangle\rangle = i\pi\rho_0 \tilde{J} G_\sigma(E)$$

In terms of the d-level Green's function and we obtain an ecuation for $\langle f_0, d_\sigma^\dagger \rangle$

$$\langle f_{0\sigma}, d_\sigma^\dagger \rangle = -\frac{1}{\pi}\int_{-D}^{D} dE f(E)\pi\tilde{J}\rho_0 Re[G_\sigma(E)]$$

$$G_\sigma(E) = \frac{1}{E + i\tilde{\Delta}} \qquad \tilde{\Delta} = \pi\langle d_\downarrow f_{0\downarrow}^\dagger \rangle^2 J^2 \rho_0$$

Slave bosons

$$\langle f_{0\sigma}, d_\sigma^\dagger \rangle = -\frac{1}{\pi}\int_{-D}^{D} dE f(E)\pi\tilde{J}\rho_0 Re[G_\sigma(E)]$$

$$\frac{1}{\rho_0 J} = -\int_{-D}^{D} dE f(E)\frac{E}{E^2+\tilde{\Delta}^2}$$

$$T = 0$$

$$\frac{1}{\rho_0 J} = -\int_{-D}^{0} dE \frac{E}{E^2+\tilde{\Delta}^2} = \ln\sqrt{1+(D/\tilde{\Delta})^2}$$

Width of the T=0 the resonance $\tilde{\Delta} \sim De^{-1/\rho_0 J} = k_B T_K$

Slave bosons

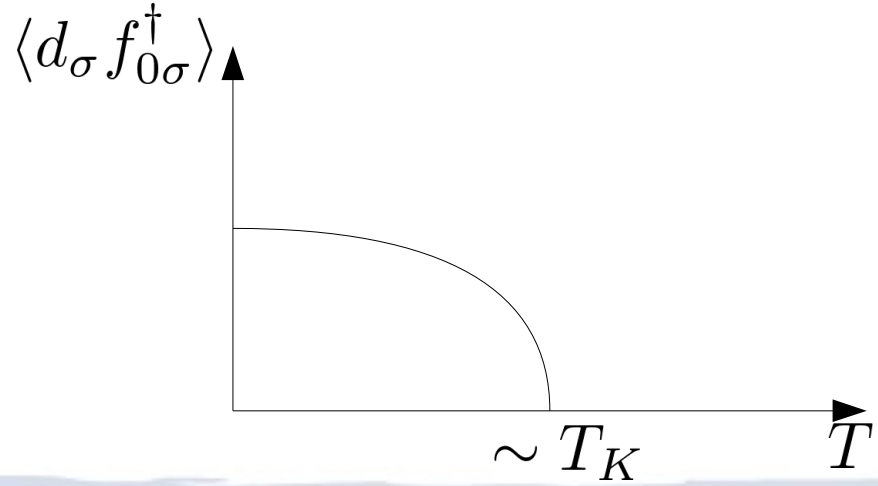
Finite temperatures:

$$\frac{1}{\rho_0 J} = \int_0^D dE \tanh[\beta E/2] Re[G_\sigma(E)]$$

$$\frac{1}{\rho_0 J} \simeq \int_0^{2T} dE \frac{\beta E}{2} Re[G_\sigma(E)] + \int_{2T}^D dE Re[G_\sigma(E)]$$

This method gives a spurious transition at $T \sim T_K$ where the impurity decouples $\tilde{\Delta}(\sim T_K) = 0$

At high temperatures the local spin is free.



Conclusions Lecture 2

- Numerical Renormalization Group gives a complete solution of the Kondo problem and can be used to study other related model systems.
- At low temperatures, when the ground state is a Fermi liquid, a simple mean field approach can give a semi-quantitative description of the low energy physics.
- The slave boson description can also be extended to study more complex systems [Lechermann 2007]
- Next lecture:
  - Electronic Transport in nanostructures.
  - Molecular transistors: molecular vibrations an the Kondo effect