

The Kondo Effect Vijay B. Shenoy (shenoy@physics.iisc.ernet.in)

Centre for Condensed Matter Theory Indian Institute of Science



Overview

- What is Kondo effect?
- Motivation Why do this?
- Plan of the Lectures







- This is Jun Kondo…but, whats his effect?
- Something that happens in metals...



Metals, Wonder Materials!

- What is a metal?
- Many electron system with a Fermi Surface
- **Key:** Gapless excitations
 - Linear T specific heat
 - Temperature independent magnetic susceptibility

9 ...

Key: "Protected" from repulsive interactions by Pauli
 Fermi liquid







Almost constant at "low" temperatures...all way to linear at high temperatures



Resistivity in Metals...There's More!



- Increases with impurity content
- Has some "universal" features...



The Kondo Effect!



There is a "resistance minimum" in some cases!



When does this happen?



Impurity susceptibility: Fe in Cu Happens when impurity is "magnetic"!

Whats the big deal? Why bother?





- "Universal" relation between dimensionless "magnetic part" of resistivity and temperature!!
- "Universal" relations observed for other properties (susceptibility etc.)
 The Kondo Effect – 8

SERC School on Magnetism and Superconductivity '06

Not Impressed? How about Quantum Dots?



- Regions that can hold a few hundred electrons!
- Can drive a current through these!
- This is Nano!



Universal Stuff in QDs too!



Universal relation between dimensionless conductance and temperature!





Dimensionless resistivity vs. temperature in "Kondo metals" and dimensionless conductance vs. temperature show the same universal function!!!!



Why Bother?

- **•** These results *cannot* just be happenstance!
- **.**.
- The Kondo problem is a cornerstone in physics...it gave rise to a lot of physics!
- **9** ...
- Two Nobel Prizes!
- **_** ..
- Dynamical Mean Field Theory (DMFT): Revival of interest in quantum impurity problems



Plan of the Lectures

- When is an impurity "magnetic"? Anderson Model
- **•** The *sd* model: "Low energy" physics
- Whence resistivity minimum? ("High" T)
- The Kondo Problem!
- Variational approach to the Kondo ground state ("Low" T)
- "Interpolation" Scaling/RG ideas
- Local Fermi Liquid ideas



Prerequisites

- Must know
 - Band theory of metals (One *e* physics)
 - Essential Stat. Mech.
- No harm if you know
 - Second quantization
 - Greens function
- Great if you know
 - Diagrammatic perturbation theory!

How do we model an impurity in a metal?

Host metal

- A set of Bloch states $|k\sigma\rangle$ (σ spin index)
- Hamiltonian $H_m = \sum_{k\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma}$
- Bandwidth 2D, i. e., $-D \le \varepsilon(k) \le D$
- Density of states $\rho(\varepsilon)$
- Impurity with "d-levels"
 - Impurity "d-level" $|d\sigma\rangle$ with energy ε_d
 - Hamiltonian $H_d = \sum_{\sigma} \varepsilon_d c_{d\sigma}^{\dagger} c_{d\sigma}$
- Most-impurity "Hybridization"
 - Hybridization : $H_h = \sum_{k\sigma} V_k c^{\dagger}_{k\sigma} c_{d\sigma} + V^*_k c^{\dagger}_{d\sigma} c_{k\sigma}$
- Hamiltonian $H = H_m + H_d + H_h$ specified when $\varepsilon(k), \varepsilon_d$ and V_k are given



The Impurity Question

- Siven that we have the host metal at some filling, say the chemical potential is "mid-band" ($\mu = 0$), what "happens" to the impurity *d*-level?
- Is the impurity level occupied?
- Is the impurity "magnetic", i. e., does it retain a "spin"?
- Recap: What happens in a free ion?
- Answer the question in a simple model:
 - Host $\rho(\varepsilon) = \rho_0$ constant..."flat band"
 - $V_k = V$, a constant
 - Now, a three parameter model (ρ_0 , ε_d and V)
 - \checkmark And, μ is given to be zero



The Impure Answer: Physics Arguments

From physics arguments

- Impurity level will be occupied if $\varepsilon_d < \mu$ (Of course!)
- But an electron cannot stay at the impurity for ever...due to hybridization...the impurity state picks up a "lifetime"
- Estimate of lifetime τ $(\hbar = 1)$: $\Delta = \frac{1}{\tau} \sim |V|^2 \rho_0$
- The impurity level behaves like a "virtual state" with "energy eigenvalue" $\mathcal{E}_d = \varepsilon_d \frac{i}{\tau}$
- This implies a "Lorentizan" density of state for the impurity

$$\rho_d(\varepsilon) = \frac{1}{\pi} \frac{\Delta}{(\varepsilon - \varepsilon_d)^2 + \Delta^2}$$



nical Digression: The Resolvent Green's Funct

- **•** Hamiltonian: *H*
- The Green's operator (function)

$$(i\frac{\partial}{\partial t} - H)G(t - t') = \delta(t - t')\mathbf{1}$$

• In frequency language $G^+(\omega) = (\omega^+ - H)^{-1}$

P Recall:
$$\frac{1}{x^+} = \frac{1}{x+i\eta} = \mathsf{P}\left(\frac{1}{x}\right) - i\pi\delta(x)$$

Why bother? Well,

$$\rho(\varepsilon) = -\frac{1}{\pi} \operatorname{Im}(\operatorname{Tr} G(\omega)), \quad \rho_a(\varepsilon) = -\frac{1}{\pi} \operatorname{Im} G_{aa}(\omega)$$

The Greens function: route to calculate density of states!



Back to Impurity Density of States...

• Hamiltonian:
$$H = \underbrace{H_m + H_d}_{H_0} + H_h$$
 (Perturbation H_h)

• Notation, $G_0 = (\omega - H_0)^{-1}$, $G_{0d\sigma} = \frac{1}{\omega - \varepsilon_d}$

The impurity Green's function (after a bit of algebra)

$$G_{d\sigma}(\omega) = \frac{G_{0d\sigma}}{1 - G_{0d\sigma} \sum_{k} \frac{|V_{k}|^{2}}{\omega - \varepsilon(k)}} = \frac{1}{\omega - \varepsilon_{d} - \sum_{k} \frac{|V_{k}|^{2}}{\omega - \varepsilon(k)}}$$
$$\approx \frac{1}{\omega - (E_{d} - i\Delta)}, \quad E_{d} = \varepsilon_{d} + \sum_{k} \frac{|V_{k}|^{2}}{\varepsilon_{d} - \varepsilon(k)},$$
$$\Delta = \pi \sum_{k} |V_{k}|^{2} \delta(\varepsilon_{d} - \varepsilon(k))$$

Physics: Impurity level forms a "virtual state"



Impurity Density of States...and...!!

In the simple three parameter model

$$E_d = \varepsilon_d + \rho_0 |V|^2 \ln \left| \frac{\varepsilon_d - D}{\varepsilon_d + D} \right|, \quad \Delta = \pi \rho_0 |V|^2$$

This implies a "Lorentizan" density of state for the impurity

$$\rho_{d\sigma}(\varepsilon) = -\frac{1}{\pi} \operatorname{Im} G_{d\sigma}(\varepsilon) = \frac{1}{\pi} \frac{\Delta}{(\varepsilon - E_d)^2 + \Delta^2}$$

The occupancy of the virtual level

$$\langle n_{d\sigma} \rangle = \int_{-\infty}^{\mu} \mathrm{d}\varepsilon \, n_F(\varepsilon) \, \rho_{d\sigma}(\varepsilon) \underbrace{\approx}_{T=0} \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{E_d - \mu}{\Delta} \right)$$

■ But.. $\langle S_z \rangle \sim \langle n_{d\uparrow} - n_{d\downarrow} \rangle = 0!$ This model says impurity can never have a moment...Whats the missing physics?



The Anderson Model

- Anderson, PR 124, 41 (1961), realized the moment formation has origins in strong correlations! (contribution from Wolff/Fridel)
- Introduced local Coulomb correlations on the impurity

$$H_d = \sum_{\sigma} \varepsilon_d c_{d\sigma}^{\dagger} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow}$$

U is the "*d* orbital" Coulomb repulsion energy **The Anderson Model**

$$H = \sum_{k\sigma} \varepsilon(k) c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{\sigma} \varepsilon_{d} c_{d\sigma}^{\dagger} c_{d\sigma} + U n_{d\uparrow} n_{d\downarrow} + \sum_{k\sigma} V_{k} c_{k\sigma}^{\dagger} c_{d\sigma} + V_{k}^{*} c_{d\sigma}^{\dagger} c_{k\sigma}$$

Can we see that this is likely to produce a moment?



Take a Moment... "See" the Moment

- Impurity spin operator $S = \frac{1}{2} \sum_{\sigma\sigma'} c^{\dagger}_{d\sigma} \vec{\tau}_{\sigma\sigma'} c_{d\sigma'}$
- Now, $\boldsymbol{S} \cdot \boldsymbol{S} = \frac{5}{4}(n_{d\uparrow} + n_{d\downarrow}) \frac{3}{4}n_{d\uparrow}n_{d\downarrow}$
- **•** The impurity Hamiltonian can now be written as

$$H_d = \sum_{\sigma} \underbrace{(\varepsilon_d + \frac{5}{4}U)}_{\varepsilon'_d} c^{\dagger}_{d\sigma} c_{d\sigma} - \frac{3}{4}U \boldsymbol{S} \cdot \boldsymbol{S}$$

- **•** Thus, if *U* is "large enough", and if we can arrange things such that $\langle n_d \rangle \neq 0$, the impurity will maximize $S \cdot S$...will pick up a moment!
- So, what competes with this?...Kinetic energy (hybridization)!



The Hartree-Fock Theory

Hartree-Fock (Mean Field) treatment of Coulomb

$$H_d^{HF} = \sum_{\sigma} \varepsilon_d c_{d\sigma}^{\dagger} c_{d\sigma} + U(\langle n_{d\downarrow} \rangle n_{d\uparrow} + \langle n_{d\uparrow} \rangle n_{d\downarrow} - \langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle)$$

Note: $\langle n_{d\sigma} \rangle$ are unknown (variational) parameters
 HF Anderson Hamiltonian

$$H^{HF} = \sum_{k\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{\sigma} \underbrace{\left(\varepsilon_{d} + U\langle n_{d\bar{\sigma}}\rangle\right)}_{\tilde{\varepsilon}_{d\sigma}} c^{\dagger}_{d\sigma} c_{d\sigma} - U\langle n_{d\uparrow}\rangle \langle n_{d\downarrow}\rangle + \sum_{k\sigma} V_{k} c^{\dagger}_{k\sigma} c_{d\sigma} + V^{*}_{k} c^{\dagger}_{d\sigma} c_{k\sigma}$$

This is a one particle Hamiltonian that we have already solved...apply our results to "each spin channel"...



- Four parameter Anderson model ($\varepsilon_d, \rho_0, V, U$) at chemical potential μ
- Green's function

$$G_{d\sigma}(\omega) = \frac{1}{\omega - (E_{d\sigma} - i\Delta)}$$
$$E_{d\sigma} = \varepsilon_d + \rho_0 |V|^2 \ln \left| \frac{\varepsilon_d - D}{\varepsilon_d + D} \right| + U \langle n_{d\bar{\sigma}} \rangle, \qquad \Delta = \pi \rho_0 |V|^2$$
$$\underbrace{= \varepsilon_d}$$

DOS etc.

$$\rho_{d\sigma}(\varepsilon) = \frac{1}{\pi} \frac{\Delta}{(\varepsilon - E_{d\sigma})^2 + \Delta^2}$$
$$\langle n_{d\sigma} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{E_{d\sigma} - \mu}{\Delta} \right)$$



• The occupancy condition enables us to determine $\langle n_{d\sigma} \rangle$

$$\langle n_{d\uparrow} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{\varepsilon_d + U \langle n_{d\downarrow} \rangle - \mu}{\Delta} \right)$$
$$\langle n_{d\downarrow} \rangle = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left(\frac{\varepsilon_d + U \langle n_{d\uparrow} \rangle - \mu}{\Delta} \right)$$

- **Question:** When is it possible to have $\langle n_{d\uparrow} \rangle \neq \langle n_{d\uparrow} \rangle$? Need to find a condition on ε_d , ρ_0 , V, U! This will tell us when an impurity can be magnetic...
- The condition will depend only on two parameters... $(\varepsilon_d \mu)/U$ and Δ/U



If the impurity develops a moment, then the DOS picture will look like



So moment definitely forms when

 $\varepsilon_d < \mu$ with $\Delta \ll |\varepsilon_d - \mu|$, AND $\varepsilon_d + U > \mu$ with $\Delta \ll |\varepsilon_d + U - \mu|$

Physics: (i) Impurity level must be occupied by only "one spin species" (ii) The hybridization should be small enough to "hold this spin species at the impurity"



- Can work out the exact condition for a special case... $|\varepsilon_d \mu| = \frac{U}{2}$...the symmetric Anderson model...
- Here, $\langle n_{d\uparrow} \rangle + \langle n_{d\downarrow} \rangle = 1$ when impurity develops a moment Exercise: Show this.
- If we call $m = \frac{1}{2}(\langle n_{d\uparrow} \rangle \langle n_{d\downarrow} \rangle)$, then from occupancies calculated earlier $2m \approx \frac{1}{\pi} \tan^{-1} \left(\frac{2mU}{\Delta}\right)$ Exercise: Show this.
- **Solution** for moment to exist: $\frac{U}{\pi\Delta} > 1$
- Physics: Coulomb must beat kinetic energy if a moment is to exist!
- $U > \rho_0 \pi^2 |V|^2$...host metals with small density of states at the Fermi level encourage impurities to be magnetic!



VBS

The Hartree-Fock Solution



- \bullet T = 0 phase diagram of the Anderson model
- The shaded region corresponds to the broken symmetry phase...Exercise: The boundary represents a "quantum phase



The Hartree-Fock Extras

- Is in general agreement with available experiments
- Does the impurity "polarize" the conduction electrons? What happens to the conduction electron density of states?....Nothing!! This is called the Anderson compensation theorem. Exercise: Prove this theorem.
- Signatures in specific heat and susceptibility Exercise: First argue, then work out the signatures.
- There is an entirely different (and a more beautiful) way to arrive at this using the Fridel sum rule which states that the number electrons localized on the impurity is equal to the phase shift of the conduction electrons at the chemical potential (modulo factors of π)...you will work this out in the problem set.



The Hartree-Fock Critique

- How good is the Hartree-Fock solution? Sources of discomfort
 - Not a true ground state of the Anderson Hamiltonian!! Quantum fluctuations are important...
 - Phase transition in a finite system!
 - "Correlation time scale" $\frac{1}{U}$ must be much larger than life time of state $\frac{1}{\Delta}$ for HF solution to be good...Thus $\frac{1}{U} \gg \frac{1}{\Delta}$, or $\Delta \gg U$...alas, thus HF solution may not be so good in the magnetic regime!!
 - **9** ...

We now know that there is a lot more to the story WBS than Hartree Fock! The Kondo Effect – 30



Low Energy Physics

- **•** Focus on systems which do show an impurity moment
- Set idea: Large U supresses charge fluctuations on the impurity...the impurity "charge degree of freedom" is "quenched"...
- The only degree of freedom that remains at the impurity is its spin...low energy excitations are only the spin excitations
- What is the effective low energy Hamiltonian for the system? Naturally, such a Hamiltonian should contain only the spin operator of the impurity...
- **Such a Hamiltonian is called the** *sd* **Hamiltonian**...



The *sd* Hamiltonian

The Hamiltonian

$$H = \sum_{k\sigma} \varepsilon(k) c^{\dagger}_{k\sigma} c_{k\sigma} + J \boldsymbol{s} \cdot \boldsymbol{S}$$

 $s = \frac{1}{N} \sum_{k\sigma,k'\sigma'} c_{k\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} c_{k'\sigma'}$ is the conduction electron spin at the impurity site (N is number of sites); J is an exchange term...

$$\frac{J}{2N}\sum_{k,k'}\left[\left(c_{k\uparrow}^{\dagger}c_{k'\uparrow} - c_{k\downarrow}^{\dagger}c_{k'\downarrow}\right)S_{z} + c_{k\uparrow}^{\dagger}c_{k'\downarrow}S_{-} + c_{k\downarrow}^{\dagger}c_{k'\uparrow}S_{+}\right]$$

Notice the spin flip scattering terms...

Whence J? How is this related to the Anderson Hamiltonian?



Whence *sd*? The Physics

- Discuss this in the context of the symmetric Aderson model ($|\varepsilon_d \mu| = U/2$)
- Large U requires that $n_d = 1$ always...
- This is bad for kinetic energy...electron is strongly localized
- So, when "Coulomb is not looking", the impurity...electron hops on to the band, or a band electron hops on to the impurity site to gain kinetic energy...
- This leads to an *antiferromagnetic* exchange interaction between the local impurity spin and the conduction electron spin a the impurity site



Whence *sd*? The Physics



• Thus $J \sim \frac{|V|^2}{U}$, and is *antiferromagnetic* in nature!

- Now for a more detailed calculation to get the
- VBS constant!



Whence *sd*? The Formal Stuff

- Several ways: Projection, Canonical Trans. etc..
- Projection Technique: "Break up" the Hilbert space into three subspaces... corresponding to $n_d = 0$, $n_d = 1$ and $n_d = 2$...we are looking to develop an effective Hamiltonian in the $n_d = 1$ subspace..
- State $|\Psi\rangle = |\Psi_0\rangle + |\Psi_1\rangle + |\Psi_2\rangle$
- The eigenvalue problem $H|\Psi\rangle = E|\Psi\rangle$ can now be cast as

$$\begin{pmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ 0 & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} |\Psi_0\rangle \\ |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix} = E \begin{pmatrix} |\Psi_0\rangle \\ |\Psi_1\rangle \\ |\Psi_2\rangle \end{pmatrix}$$

 H_{00}, H_{11}, H_{22} are Hamiltonians in the 0, 1, 2 subspaces, H_{01} etc are "hopping operators" from one subspace to another; obviously $H_{10} = H_{01}^{\dagger}$


Whence *sd*? The Formal Stuff

A bit of algebra gives

$$\underbrace{\left(H_{11} + H_{10}(E - H_{00})^{-1}H_{01} + H_{12}(E - H_{22})^{-1}H_{21}\right)}_{H_{11}^{eff}}|\Psi_1\rangle = E|\Psi_1\rangle$$

A bit of thought gives

$$H_{01} = \sum_{k\sigma} V_k c^{\dagger}_{k\sigma} c_{d\sigma} (1 - n_{d\bar{\sigma}}), \quad H_{21} = \sum_{k\sigma} V^*_k c^{\dagger}_{d\sigma} c_{k\sigma} n_{d\bar{\sigma}}$$

And, after a few ten sheets of paper, some lost sleep and hair...we may get..



Whence sd? The Formal Stuff

• ...the additional part to H_{11} in H_{11}^{eff} ; two terms

 $\sum_{k,k'} J_{kk'} \left[\left(c_{k\uparrow}^{\dagger} c_{k'\uparrow} - c_{k\downarrow}^{\dagger} c_{k'\downarrow} \right) S_z + c_{k\uparrow}^{\dagger} c_{k'\downarrow} S_- + c_{k\downarrow}^{\dagger} c_{k'\uparrow} S_+ \right] + \sum_{k\sigma,k'\sigma'} \mathcal{V}_{kk'} c_{k\sigma}^{\dagger} c_{k'\sigma}$

sd like interaction

Potential scattering

$$J_{kk'} = V_k^* V_{k'} \left(\frac{1}{\varepsilon_d + U - \varepsilon(k')} + \frac{1}{\varepsilon(k) - \varepsilon_d} \right)$$
$$\mathcal{V}_{kk'} = \frac{V_k^* V_{k'}}{2} \left(\frac{1}{\varepsilon(k) - \varepsilon_d} - \frac{1}{\varepsilon_d + U - \varepsilon(k')} \right)$$

- **•** Note $J_{kk'}$ is antiferromagnetic for states near the chemical potential..
- Approximation, set $J_{kk'} = \frac{J}{2N}$, and $V_{kk'} = 0$...get the sd model...
- Can we now explain the Kondo effect...i.e., the
- VBS resistivity minimum? There are only two parametersedin- 37



Electrical Transport: Recap

- The famous formula $\sigma = \frac{ne^2\tau}{m}$
- Image the "transport life time"...all transport physics is in τ ..
- **9** au is obtained from the T matrix t

$$\frac{1}{\tau} = 2\pi \int \mathrm{d}^3 k' |T_{k',k}|^2 (1 - \cos \theta_{kk'}) \delta(\varepsilon(k') - \varepsilon(k)), \qquad k \sim k_f$$

- Strategy: Treat sd as perturbation, and obtain $\frac{1}{\tau}$ as a series in J
- **•** But, before that, what is the T matrix?



The T Matrix

- Consider $H = H_0 + \mathcal{V}$ where \mathcal{V} is an "external potential" (like the *sd* interaction term)
- Roughly, the T matrix represents an "effective" potential seen by the "bare states"
- $\blacksquare \quad \mathbf{Recall,} \ G = (\omega H)^{-1} \Longrightarrow G = G_0 + G_0 \mathcal{V}G$
- **Definition** $TG_0 = \mathcal{V}G$, implies

 $\langle a|S|b\rangle = \delta_{ab} - 2\pi \langle a|T|b\rangle \delta(\varepsilon_a - \varepsilon_b)$

$$T = \mathcal{V} + \mathcal{V}G_0\mathcal{V} + \mathcal{V}G_0\mathcal{V}G_0\mathcal{V} + \dots = \mathcal{V}(1 - G_0\mathcal{V})^{-1}$$

Think of the connection to the path integral...

● Physics: The rate of transition from $|a\rangle$ to $|b\rangle$ induced by \mathcal{V} is given by $2\pi |\langle a|T|b\rangle|^2 \delta(\varepsilon_a - \varepsilon_b)$...generalization of the Fermi golden rule!

The T matrix is connected to the S matrix, for any two states $|a\rangle, |b\rangle$,

VBS

The Kondo Effect - 39



Resistivity in the sd model

- In the sd model, we expect lifetimes to be spin dependent, i. e., we need to calculate τ_{\uparrow} and τ_{\downarrow}
- There is an added technical complication: if we set out to calculate $T_{k\sigma,k'\sigma'}$, we have to *trace over* the impurity spin states...we will adopt a notation that $T_{k\sigma,k'\sigma'}$ is a " 2×2 " matrix,...we calculate such matrices and in the final step take the trace of the impurity states...this will naturally handle the intermediate impurity states
- We shall use diagram techniques for this calculation, useful to rewrite sd interaction as

$$\frac{J}{2N}\sum_{k,k'}\left[\left(c_{k\uparrow}^{\dagger}c_{k'\uparrow}-c_{k\downarrow}^{\dagger}c_{k'\downarrow}\right)S_{z}+c_{k\uparrow}^{\dagger}c_{k'\downarrow}S_{-}+c_{k\downarrow}^{\dagger}c_{k'\uparrow}S_{+}\right]$$

SERC School on Magnetism and Superconductivity '06

T matrix elements to $\mathbf{1^{st}}$ order in J



Diagrams for the first order process

- **P** Thus, if we stop at 1^{st} order in J for T, we get

$$\frac{1}{\tau} = \frac{1}{\tau_{\uparrow}} + \frac{1}{\tau_{\downarrow}} \sim J^2 \langle 2S_z^2 + S_-S_+ + S_+S_- \rangle \sim J^2$$

independent of temperature!! Bad news!!



T matrix elements 2nd order in J - "Direct terms"





T matrix elements $\mathbf{2^{nd}}$ order in J - "Flip terms"







T matrix elements 2nd order in J

• Matrix elements up to 2nd order in J

$$T_{k'\uparrow k\uparrow}^{(2)} = \frac{J}{N}S_z + \frac{J^2}{N^2} \left[S_z^2 (P(\varepsilon(k) + H(\varepsilon(k))) + S_-S_+P(\varepsilon(k)) + S_+S_-H(\varepsilon(k))) \right]$$
$$T_{k'\downarrow k\uparrow}^{(2)} = \frac{J}{N}S_+ + \frac{J^2}{N^2} \left[(S_zS_+ + S_+S_z)(P(\varepsilon(k)) + H(\varepsilon(k))) \right]$$

What are P and H

$$P(\omega) = \sum_{q} \frac{(1 - n_F(\varepsilon(q)))}{\omega - \varepsilon(q)} \quad H(\omega) = \sum_{q} \frac{n_F(\varepsilon(q))}{\omega - \varepsilon(q)}$$

Note that for our simple two $P(\omega) + H(\omega) \approx 0$ for $\omega \approx \mu$!! Even otherwise, $P(\omega) + H(\omega) \approx 0$ is independent of temperature!



T matrix elements 2^{nd} order in J

• Thus, using some spin algebra $S_{\pm}S_{\mp} = \frac{3}{4} - S_z^2 \pm S_z$

$$T_{k'\uparrow k\uparrow}^{(2)} = \frac{J}{N}(1 - 2Jh(\omega)) \quad h(\omega) = \frac{1}{N}\sum_{q}\frac{n_F(\varepsilon(q))}{\varepsilon(q) - \omega}$$

In our case

$$h(\omega) \sim \rho_0 \int_{-D}^{D} \mathrm{d}\varepsilon \frac{n_F(\varepsilon)}{\varepsilon - \omega}, \quad \text{For } T > 0 \quad h(\mu = 0) \sim \rho_0 \int_{-D}^{-k_B T} \mathrm{d}\varepsilon \frac{1}{\varepsilon} = \rho_0 \ln\left(\frac{k_B T}{D}\right)$$

Note that $h(\omega)$ is logarithmically divergent as $\omega \to \mu$ and $T \to 0$...the key to this divergence is the intermediate spin flip scattering in the direct process! It is the quantum nature of the spin that rears its head!

Physics: Spin flip scattering leads to a logarithmically divergent inverse lifetime!



And, the Kondo Result for Resistivity

From the T matrix elements, obtain the lifetime $\tau(\varepsilon)$, and use it in the formula for conductivity

$$\sigma(T) \sim \int \mathrm{d}\varepsilon \rho(\varepsilon) \epsilon \tau(\epsilon) \frac{\mathrm{d}n_F(\varepsilon)}{\mathrm{d}\varepsilon}$$

• We get resistivity R

$$R_{sd}(T) = c \left[R_0 - R_1 \ln \left(\frac{k_B T}{D} \right) \right]$$

c- concentration

- **•** Total resistivity $R = AT^5 + R_{sd}(T)$
- Minimum occurs at $T_M = Bc^{\frac{1}{5}}$

This one-fifth power law has been experimentally
VBS verified!
The Kondo Effect – 46



And Experiments



In a certain temperature regime near the resistivity minimum, the 2nd order T matrix theory works quite well!

VBS Are there signatures in other properties? The Kondo Effect – 47



Magnetic Susceptibility

- We know that the susceptibility drops (compared to the Curie behaviour as temperature is decreased...)
- **•** How to we understand this from the *sd* Hamiltonian?
- Imagine an applied magnetic field...if there were no sd interaction, then the spin will point in the direction of the field...
- **Now turn on the** *sd* **interaction...what happens?**
- The spin flip scattering from the conduction electrons acts to "reduce the" moment pointing along the direction of the magnetic filed...we expect susceptibility to fall with reducing temperature...



Magnetic Susceptibility

In fact, a little thought will tell you that the spin flip process (which was the key in giving raise to the upturn of resistivity) is also the key player here, and contributes to a logarithmic correction to the susceptibility

$$\chi(T) \sim \frac{1}{k_B T} \left[C_0 + (2J\rho_0)^2 \ln\left(\frac{k_B T}{D}\right) \right]$$

Note that the above result includes the conduction band polarization..

The logarithm is rearing its head again...this is in general agreement with experiments in a certain temperature range...but there *is* a problem is going to lower temperatures...



What have we learnt?

We learnt the following from low order perturbative calculations

- Spin flip scattering is the key to much of the physics seen
- Becomes increasingly effective at lower temperatures...this is due to the fact that the thermal kicks that the impurity and the conduction electrons experience destroy the coherent spin flip scattering at higher temperatures...
- In the temperature regime where the spin flip process just begins to rear its head, we notice that all properties show logarithmic temperatures corrections...
- The simple low order perturbative calculation leave us clueless vis-a-vis low temperature experiments... S
 S



How do we "chill-out"?

- The "obvious" thing to do is to extend the perturbation theory to all orders and hope for the best…
- The "obvious" is technically a bit tight! Abrikosov was a key player in working out the techniques required to sum the most singular spin flip diagrams...it has now been done for various responses...
- **P** Results for "all orders in J"

$$R(T) \sim \frac{J^2}{1 - 2J\rho_0 \ln\left(\frac{k_B T}{D}\right)}$$
$$\chi(T) \sim \frac{1}{k_B T} \left(1 + \frac{(2J\rho_0)^2 \ln\left(\frac{k_B T}{D}\right)}{1 - 2J\rho_0 \ln\left(\frac{k_B T}{D}\right)}\right)$$

Groat



Chill! The Kondo Problem!

…everything blows up on our face at

$$k_B T_K = D e^{-\frac{1}{2J\rho_0}}$$

the Kondo scale

- This *is* TROUBLE! Things are blowing up at a FINITE temperature T_K ...
- Interestingly, ALL calculated properties blow up at T_K ...
- This is therefore the key energy scale in the problem...but what could such an energy scale be associated with? Note the nonanalyticity in J...
- How to get around this? May be start from T = 0...



- Since the coupling is antiferromagnetic, it is reasonable to assume that the ground state is a singlet...total spin zero state!
- Mattis *proved* that the ground state *is* a singlet...but did not find the ground state wavefunction...
- Given that we know the ground state is a singlet, can we guess the wavefunction?
- We make one such guess, and learn something!



- The true singlet ground state might be complicated...we ask a different question analogous to Cooper's question in the superconductivity context...
- Given a filled Fermi sphere $|FS\rangle$ and an impurity spin, what happens if I add *one more electron* ?
- We may imagine the ground state of the system to be the *undisturbed* Fermi sphere and a singlet that forms between the added electron and the impurity...This will be consistent with Mattis...
- The wavefunction is

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \sum_{k>k_f} a_k \left(c_{k\uparrow}^{\dagger} | FS; \Downarrow\rangle - c_{k\downarrow}^{\dagger} | FS; \Uparrow\rangle \right)$$

with $\sum_{k>k_f} |a_k|^2 = 1$ Note that the added electron lives outside the Fermi



- **•** We need to determine a_k ...how?
- The "optimal" a_ks are the ones that minimize the ground stated energy
- Need to calculated $E_g(\{a_k\}) = \langle \Psi | H | \Psi \rangle$...a bit of calculation shows (μ is set to zero)

$$E_g(\{a_k\}) = \sum_{k>k_f} \varepsilon(k) |a_k|^2 + \frac{3J}{2N} \sum_{k,k'>k_f} a_k^* a_{k'}$$

• Minimizing subject to the condition $\sum_{k>k_f} |a_k|^2 = 1$ using a Lagrange multiplier *E*, gives

$$(\varepsilon(k) - E)a_k - \frac{3J}{4N}\sum_{k'>k_f}a_k = 0$$



Resulting secular equation

$$\frac{4}{3J} = \frac{1}{N} \sum_{k>k_f} \frac{1}{\varepsilon(k) - E} = \rho_0 \int_0^D \mathrm{d}\varepsilon \frac{1}{E - \varepsilon} \Longrightarrow E = -De^{-\frac{4}{3J\rho_0}}$$

- **•** The gain in energy does look like the Kondo scale, but it is *larger* than k_BT_K ...
- Physics: The added electron has "localized" around the impurity and formed a singlet with it...There is, of course, increase of kinetic energy due to localization, but gain in exchange energy...all of it eventually results in a non analytical gain of $De^{-\frac{4}{3J\rho_0}}$...Note that for any antiferromagnetic J no matter how small, the singlet we have assumed will be lower in energy...



Electron localized around the impurity ("Kondo cloud")



- Length scale of the cloud $\frac{v_f}{De^{-\frac{4}{3J\rho_0}}}$...
- But is this the real story?



Better Variations...

- **•** Energy gain $De^{-\frac{4}{3J\rho_0}}$ is less than k_BT_K
- Variational state is not an eigenstate of the sd Hamiltonian! sd interaction can create particle-hole excitations...
- Solution State A state of the state of the
- It contains a "Kondo cloud" that screens the impurity spin by forming a singlet...it is true many-body state...
- The "dressed Kondo impurity" scatters any electronic excitations with the maximum possible phase shift $(\pi/2)$ and the T = 0 resistivity is the maximum possible resistivity permitted by unitarity...

arming up from T = 0...Finding the connection

- Moving the ground state is good...but knowing the nature of excitations above the ground state is key...
- **•** There has been a lot of effort to calculate properties, but most will work only for $T \ll T_K$...
- On one hand we have a theory that works well for $T \gg T_K$, and on the other hand another theory for $T \ll T_K$...
- What about a "smooth connection" between the two?
- Anderson provided a key insight as to why it is difficult to obtain a smooth connection by usual techniques...This work contained in it certain ideas that were later key to the complete solution of the Kondo problem by Wilson...



- Anderson asked the following question: What are the most important degrees of freedom in the Kondo problem? Can one write out an effective Hamiltonian just for these degrees of freedom?
- Clearly the key degrees of freedom at low temperatures are the states near the chemical potential... They can undergo scattering from the impurity that may be direct or spin-flip...
- He considered the Hamiltonian of the form

$$\sum_{k} \varepsilon(k) c_{k\sigma}^{\dagger} c_{k\sigma} + \sum_{k,k'} J_{z} \left(c_{k\uparrow}^{\dagger} c_{k'\uparrow} - c_{k\downarrow}^{\dagger} c_{k'\downarrow} \right) S_{z} + J_{\perp} c_{k\uparrow}^{\dagger} c_{k'\downarrow} S_{-} + J_{\perp} c_{k\downarrow}^{\dagger} c_{k'\uparrow} S_{+}$$

This is an "anisotropic sd Hamiltonain" with J_z , J_{\perp} ...



What is the effective Hamiltonian in the band reduced by δD as shown? $\neg |\delta D|$ \leftarrow $|\delta D|$ \leftarrow

- We expect to get a Hamiltonian with the same form as the sd but with new "renormalized" values of the Js...
- Bow can we find the new Js? Let us say that J_z goes to \tilde{J}_z Interpret J_z : it is the amplitude for scattering from $|k \uparrow \rangle$ to $|k' \uparrow \rangle$...
- Now if k, k' belong to the reduced band, the amplitude of this scatteringy will be a sum of direct scattering in the band (J_z) , and scattering from k to k' via all intermediate states which lie in the *shaded part of the band* (call this δJ_z)...
- Clearly we need only to worry about spin flip scattering..



Flow equation for Js best seen by diagrams



$$\delta J = J_{\perp}^2 S_{-} S_{+} \left(-\rho_0 \frac{\delta D}{D} \right) + J_{\perp}^2 S_{+} S_{-} \left(\rho_0 \frac{\delta D}{D} \right) = -2\rho_0 J_{\perp}^2 \left(\frac{\delta D}{D} \right) \Longrightarrow \frac{\mathrm{d} J_z}{\mathrm{d} \ln D} = -2\rho_0 J_{\perp}^2 \left(\frac{\delta D}{D} \right)$$

With a similar equation for J_{\perp} , we have

$$\frac{\mathrm{d}J_z}{\mathrm{d}\ln D} = -2\rho_0 J_\perp^2$$
$$\frac{\mathrm{d}J_\perp}{\mathrm{d}\ln D} = -2\rho_0 J_\perp J_z$$





Solution Key point: Suppose we start with $J_z = J_{\perp} = J > 0$ (antiferromagnetic), then the coupling constant Jflows to infinity...cannot do any pertubation theory



- Note that for our sd-model, De^{-1/2Jρ0} = De^{-1/2Jρ0}!! Thus the Kondo temperature is preserved along the trajectory!! Thus the key energy scale remains "invariant"
- Changing *D* is like changing *T*, and hence we expect all properties to be "universal functions" of $\frac{T}{T_{K}}$
- In many ways, this *is* the solution of the Kondo problem! But the full solution by Wilson is a treat in itself...



- Key observation: The problems are caused by a logarithmic divergence...consider $\int_a^b \frac{d\varepsilon}{\varepsilon} = \ln\left(\frac{b}{a}\right)$
- We ask "why" is $\int_0^1 \frac{d\varepsilon}{\varepsilon} = \infty$? To see this, break up [0,1] into intervals $[\Lambda^{-(n+1)}, \Lambda^{-n}]$ with $\Lambda > 1$...Thus

$$[0,1] = \bigcup_{n=0}^{\infty} [\Lambda^{-(n+1)}, \Lambda^{-n}] \implies \int_{0}^{1} \frac{\mathrm{d}\varepsilon}{\varepsilon} = \sum_{n=0}^{\infty} \int_{\Lambda^{-(n+1)}}^{\Lambda^{-n}} \frac{\mathrm{d}\varepsilon}{\varepsilon} = \sum_{n=0}^{\infty} \ln \Lambda = \infty !!$$

The divergence occurs because all the "logarithmic intervals" contribute *equally*...

To study the Kondo model, Wilson considered a simplified Hamiltonian

$$H = \int_{-1}^{1} \mathrm{d}k \; k c_{k\sigma}^{\dagger} c_{k\sigma} + J \boldsymbol{s} \cdot \boldsymbol{S}$$



Starting from $H = \int_{-1}^{1} dk \ k c_{k\sigma}^{\dagger} c_{k\sigma} + J s \cdot S$, and using log descretization

$$-1 \qquad -\frac{1}{\Lambda} \qquad -\frac{1}{\Lambda^2} \qquad -\frac{1}{\Lambda^3} \qquad 0 \qquad \frac{1}{\Lambda^3} \qquad \frac{1}{\Lambda^2} \qquad \frac{1}{\Lambda} \qquad 1$$

reduced to

$$H = \frac{1}{2} (1 + \Lambda^{-1}) \sum_{n=0}^{\infty} \Lambda^{-n} (c^{\dagger}_{+n\sigma} c_{+n\sigma} - c^{\dagger}_{-n\sigma} c_{-n\sigma}) + J \boldsymbol{s} \cdot \boldsymbol{S}$$

 $c_{\pm n\sigma}$ are electron operators to the right (left) of $\mu(k=0)$

Now

$$\boldsymbol{s} = \frac{1}{2} f_{0\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} f_{0\sigma'} \quad f_{0\sigma} = \frac{1}{\sqrt{2}} \int_{-1}^{1} \mathrm{d}k \ c_{k\sigma}$$
$$f_{0\sigma} \approx \left(\frac{1}{2} (1 - \Lambda^{-1})\right)^{1/2} \sum_{n=0}^{\infty} \Lambda^{-n/2} (c_{+n\sigma} + c_{-n\sigma})$$

Thus, the impurity couples equally to states of *all energies*! This *is* <u>the</u> problem!



By sheer genius (bordering on subterfuge!) Wilson mapped this Hamiltonian to

$$H = \sum_{n=0}^{\infty} \Lambda^{-n} (f_{n\sigma}^{\dagger} f_{n+1\sigma}^{\dagger} + f_{n+1\sigma}^{\dagger} f_{n\sigma}) + J \frac{1}{2} f_{0\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} f_{0\sigma'} \cdot \boldsymbol{S}$$

This is a "1-D" semi-infinite chain with the first site interacting with the impurity, and an exponentially falling hopping between neighbours!



Solution We know what $f_{0\sigma}^{\dagger}$ does...what do the operators $f_{n\sigma}^{\dagger}$





- $f_{0\sigma}^{\dagger}$ corresponds to a "spherical wave packet" localized around the impuritiy... $f_{1\sigma}^{\dagger}$ is a wave packet which peaks at a larger distance from the impurity... and so on!
- Electrons can "hop" from one wavepacket state to the "neighbouring" wave packet states...
- **•** The states $f_{n\sigma}^{\dagger}$ can be obtained from $c_{\pm n\sigma}^{\dagger}$...via Lanczos tridiagonalization of the kinetic energy!

Why all this? Impurity now couples only to one state!



- Wilson then used a numerical renormalization group technique to diagnolize the Hamiltonian which involves the following step
- Define

$$H_N = \Lambda^{(N-1)/2} \left(\sum_{n=0}^{N-1} \Lambda^{-n} (f_{n\sigma}^{\dagger} f_{n+1\sigma}^{\dagger} + f_{n+1\sigma}^{\dagger} f_{n\sigma}) + J \frac{1}{2} f_{0\sigma}^{\dagger} \vec{\tau}_{\sigma\sigma'} f_{0\sigma'} \cdot \boldsymbol{S} \right)$$

- Why do this?: $N \to \infty$ is like taking $T \to 0$, note that $\Lambda^{(N-1)/2}J$ which is the effective exchange coupling at N (temperature T) goes to infinity as $N \to \infty$ $(T \to 0)....$
- Define a transformation $H_{N+1} = \Lambda^{1/2} H_N + f_{N\sigma}^{\dagger} f_{N+1\sigma} + f_{N+1\sigma}^{\dagger} f_{N\sigma}$



- **•** Take J = 0 to start with, and ask what happens for large N?
- You will see with a bit of thought that you will get two types of spectrum depending on if N is even or odd..
- **•** For $\Lambda = 2$ Wilson showed that the eigenvalues are

even N : $0, \pm 1.297, \pm 2.827, \pm 4\sqrt{2}... \pm 2^{\ell-1}\sqrt{2}...$ odd N : $\pm 0.6555, \pm 1.976, \pm 4, \pm 8, ..., \pm 2^{\ell}$

• Thus RG transformation $H_{N+2} = R[H_N]$ has two "fixed points" – one corresponding to even number N and another odd number N...



- **•** Now start with a very small $J \neq 0$...and focus on N even...
- **●** Until N becomes large enough so that $J_{eff} = \Lambda^{(N-1)/2} J \le 1$, the eigenvalues will look like those of even N...
- For even larger N the $J_{eff} \rightarrow \infty$...what does this mean...the site 0 will from a singlet with the impurity and completely drop out of the Hamiltonian...i. e., the site 0 will decouple from the chain since it fully couples with the impurity!! This means although there are N is even, the spectrum of H_N will be similar to that of odd N!
- Solution When you start with a tiny J, there is a range of N (high T) where the behaviour is same as that of the J = 0 fixed point (this is where perturbation theory works)... and as N is increased it flows to the $J \to \infty$ fixed point (the Kondo singlet)!


Wilson's RG Appoach to The Kondo Problem



RG flow in the Kondo problem...all well and good..what about quantitative things?



Wilson's RG Appoach to The Kondo Problem

• Using the fact that $T \sim \Lambda^{-N}$, and using an iterative scheme that correctly calculates the *low* energy excitations of the Hamiltonians at large N, Wilson obtained the universal function for susceptibility...





Wilson's RG Appoach to The Kondo Problem

- So what determines the flow towards the strong coupling fixed point?
- Wilson argued that the flow is governed by the *leading* irrelevant operators...
- Based on "symmetry arguments" Wilson proposed that the leading irrelevant operators are of the form

$$H_N = H_{\infty}^* + \Lambda^{-N/2} \left(a (f_{1\sigma}^{\dagger} f_{2\sigma} + f_{2\sigma}^{\dagger} f_{1\sigma}) + b (f_{1\sigma}^{\dagger} f_{1\sigma} - 1)^2 \right)$$

Leading Irrelevant Operators

Note that the second irrelevant operator looks like an onsite interaction at site 1!!

Now using a combination of perturbation theory and numerics, Wilson showed that

$$W = \frac{R_{imp}}{R_{free \ electron}} = 2 \quad \text{where} \quad R = \frac{T\chi}{C_v} \quad \text{W is the "Wilson ratio"}$$



Noziéres Local Fermi Liquid Picture

- Noziéres made very a insightful observation that near the fixed point Hamiltonian H_{∞}^* is that of a non interacting Hamiltonian, and near the fixed point $T \ge 0$, there is just a "local" interaction on the site 1...
- Noticing that $(f_{1\sigma}^{\dagger}f_{1\sigma}-1)^2 = 2n_{1\uparrow}n_{1\downarrow} (n_{1\uparrow} + n_{1\downarrow} 1)$, he realized that the system would behave like a *Fermi liquid*...
- He now used Fermi liquid arguments; the scattering phase shift of a quasiparticles of energy ε is a functional of the number density of all quasi-particles n_{σ}

$$\delta_{\sigma}[\varepsilon, n_{\sigma}] = \delta_{0}(\epsilon) + \sum_{\varepsilon', \sigma'} f_{\sigma, \sigma'}(\varepsilon, \varepsilon') \delta n_{\sigma'}(\varepsilon)$$

0 corresponds to "equilibrium" $(n_0(\varepsilon) = n_F(\varepsilon))$



Noziéres Local Fermi Liquid Picture

• Expanding about the chemical potential (= 0)

 $\delta_0(\varepsilon) = \delta_0 + \alpha \epsilon$

and taking $f_{\sigma,\bar{\sigma}} = f$ as energy independent, and that the quasiparticle scatters off only "an opposite spin" quasiprticle, the second term can be written as

$$\sum_{\varepsilon',\sigma'} f_{\sigma,\sigma'}(\varepsilon,\varepsilon') \delta n_{\sigma'}(\varepsilon) = f \sum_{\varepsilon'} \delta n_{\bar{\sigma}}$$



$$\delta_{\sigma}(\varepsilon) = \delta_0 + \alpha\varepsilon + f \sum_{\varepsilon'} \delta n_{\bar{\sigma}}$$

Note that $\delta_0 = \pi/2$, and that there are two parameters α and f...



Noziéres Local Fermi Liquid Picture

Noziéres argued that the phase shift will not be affected by small changes in the chemical potential...gives the condition

$$\alpha + f\rho_0 = 0$$

This leaves only one parameter!

- Noting that the impurity density of states is given by $\rho_d(\varepsilon) = \frac{1}{\pi} \frac{\partial \delta}{\partial \epsilon}$, we get (accounting from spins), $\rho_d(\mu) = \frac{2\alpha}{\pi}$, thus $\frac{C_{imp}}{C_{FE}} = \frac{2\alpha}{\pi}$...
- Now by the Fridel sum rule magnetization
 m = ¹/_π(δ_↑ − δ_↓) in presence of a magnetic field
 B...m ~ ^(2α-2fρ₀)/_πB i.e., ^{χ_{imp}}/_{χ_{FE}} = ^{4α}/_π

 This simple argument gives W = 2!!



What about the Anderson Model?

The Anderson model was solved by NRG techniques by Krishnamurthy et al.





An Important Piece in AM...

• The impurity develops a "resonance" at the chemical potential for $T < T_K$...the Abrikosov-Shul resonance aka Kondo resonance



VBS This is consistent with increase of resistivity Exercise: Why?



To Conclude...

Kondo problem is solved, but it taught us...

- Correlation physics
- Mean field theory
- Projection technique (Low energy physics)
- Transport calculations
- Perturbative (Diagram) calculations
- RG ideas

Future...

- Mondo lattice etc..
- Correlations at the nanoscale..