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SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
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NUMERICAL RENORMALIZATION GROUP STUDIES OF KONDO PROBLEMS

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LECTURE 1

Numerical Renormalization Group Studies of Kondo Problems

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I. A) "M-N-ology": Different kondo impurity numbers and channels – basic results + physics

B) 2-impurity kondo problem.. complete
Issues of particle hole symmetry – 1 vs 2 impurities

II. A) 2-impurity kondo, continued
- Full results in absence of particle-hole symmetry

B) Technique of Wilson's Numerical Renormalization Group

III. Two-impurity, two-channel kondo effect

KONDO M-N-ology

M spin-$\frac{1}{2}$ local moments, impurities

N channels of conduction electrons $J\vec{s}\cdot\vec{S}$ + K.E.

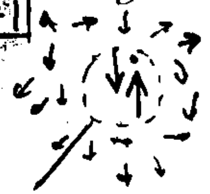
- What is known so far: 1 & 2 impurities multichannel
- Various methods: Numerical Renormalization Grp Bethe Ansatz, conformal field theories, ($\frac{1}{N}$ expansions), ... (Monte Carlo).

Why? General magnetic vs. conduction electron interaction magnetic impurities, heavy fermions, high-Tc(?), ...

- Simple (1+1)-d models can give surprisingly complex results.

N=1
M=1

Single impurity Kondo problem $H = K.E. + J\vec{S}(0)\cdot\vec{S}_0$



resonance
S=0
phase shift $\delta = \frac{\pi}{2}$

Bethe Ansatz (Wiegmann & Tsvelick 1983)
(Andrei & Destri 1985)

Numerical Renormalization Grp (NRG)
Wilson 1975

$J>0$: smooth behavior: crossover $J \to \infty$
singlet g.s. [(archetypal) Fermi liquid]
single E-scale $T_K \sim \sqrt{\rho J}\, e^{-1/\rho J}$

Nozières & Blandin 1979, 1980

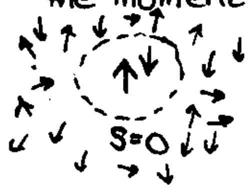
N vs. 2S :
N: total # channels
2S: total impurity spin

$N = 2S$	singlet g.s.
$N < 2S$	undercompensated; net spin, degenerate g.s.
$N > 2S$ (and $S \neq 0$)	overcompensated; net spin=? unusual behavior

Properties of a single Kondo local moment

The Kondo Hamiltonian describes a single spin-$\frac{1}{2}$ magnetic moment (impurity) in a metal.

As $T \to 0$ it experiences the Kondo effect: the moment is quenched.



$$H_K = H_{c.e.} + J\, \vec{s}_c \cdot \vec{S}_0$$

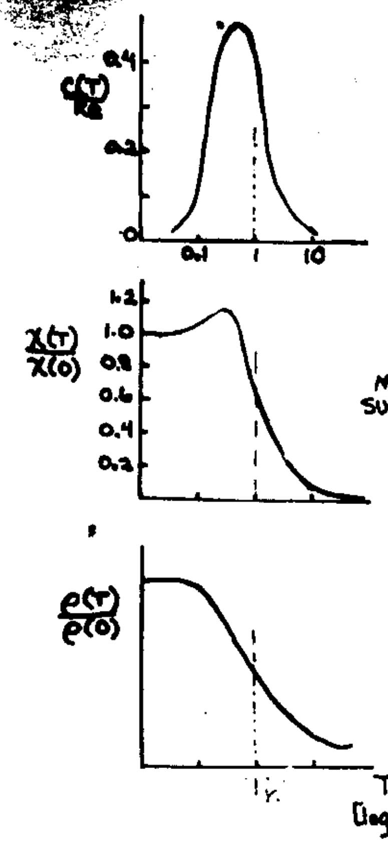
Considered solved after many years. Solution can be interpreted as scaling of coupling J:
- J effectively $\to \infty$ as $T \to 0$
- "J scales to strong coupling"

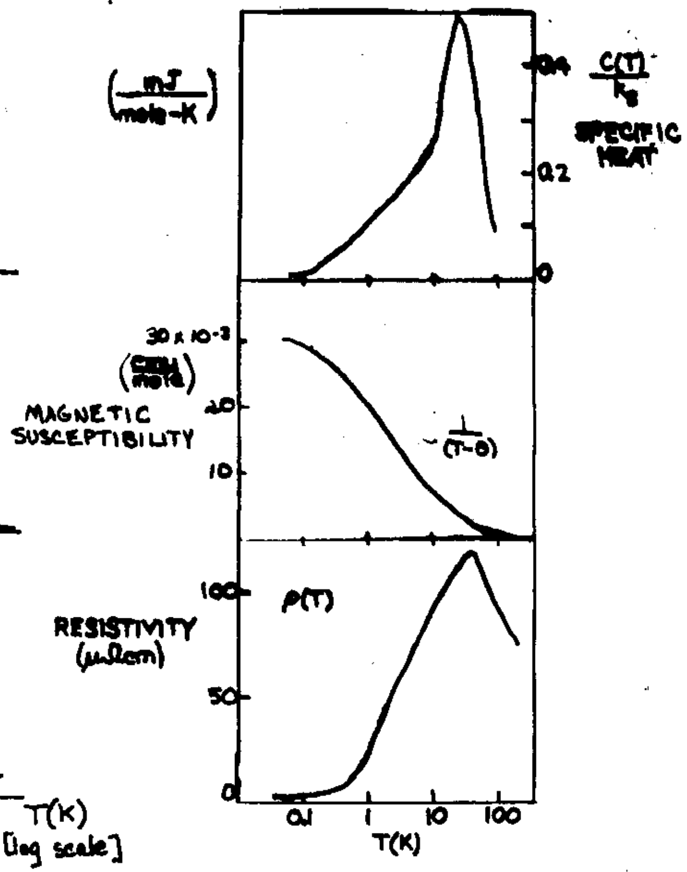
Expts: Dilute magnetic alloys

Universal behavior with a single temperature scale $T_K \sim D\sqrt{|\rho J|}\, e^{-1/|\rho J|}$

DILUTE SYSTEMS

e.g. (La,Ce)B





The Anderson lattice model

$$\boxed{H_A = \sum_{k,\mu} \epsilon_k c^\dagger_{k\mu} c_{k\mu} + \sum_{\mu,i} \epsilon_f f^\dagger_{i\mu} f_{i\mu} + \sum_{k,\mu,i} \left[V_k e^{ik\cdot r_i} c^\dagger_{k\mu} f_{i\mu} + V_k^* e^{-ik\cdot r_i} f^\dagger_{i\mu} c_{k\mu} \right] + U \sum_i (f^\dagger_{i\uparrow} f_{i\uparrow})(f^\dagger_{i\downarrow} f_{i\downarrow})}$$

U: Coulomb repulsion — large + positive

ϵ_f: (bare) f-level — large + negative

$\epsilon_k \mapsto \epsilon_k$

$V_k \mapsto V_k \mapsto V$

The Kondo lattice model

Fix V (above), let $U, -\epsilon_f \to$ large

→ ONLY 1 f per site

→ local moment, Kondo Hamiltonian:

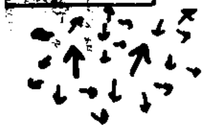
$$\boxed{H_K = \sum_{k\mu} \epsilon_k c^\dagger_{k\mu} c_{k\mu} + J \sum_i \vec{s}_c(r_i) \cdot \vec{S}_i ,}$$

$$\vec{s}_c(r_i) = \sum_{k,k',\mu,\mu'} e^{i(k-k')\cdot r_i} c^\dagger_{k\mu} \frac{\vec{\sigma}}{2} c_{k'\mu'}$$

where $J = 8\frac{V^2}{U}$ $(V \ll U)$ Schrieffer-Wolf formula (1966)

Note that H_A and H_K are both sums of single-site terms.

N=2
M=2



Two-Impurity Kondo Problem

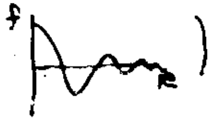
$$H = K.E. + J\left[\vec{s}_c(-\tfrac{R}{2})\cdot\vec{S}_1 + \vec{s}_c(+\tfrac{R}{2})\cdot\vec{S}_2\right]$$

Two energy scales: $T_K \sim \sqrt{\rho J}\, e^{-1/\rho J}$

RKKY $= I(R)$

(Indirectly generated RKKY interaction between impurities: can be FM or AFM

$I(R) = (\rho J)^2 f(R)\, \vec{S}_1\cdot\vec{S}_2$



)

What does one expect? Kondo vs. RKKY

2 limits: 1. I (large) ferromag $\rightarrow$ $S_{imp}=1$, Kondo effect

Expect $S_{TOT}=0$ ↓↑ ↑↓ $S=0$ $\delta_e = \delta_o = \frac{\pi}{2}$ Fermi liquid

2. I large, antiferromag $\rightarrow$ $S_{imp}=0$, no Kondo effect

Expect $S_{TOT}=0$ ↑↓ $S=0$ $\delta_e = \delta_o = 0$ free electrons Fermi liquid

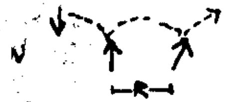
$\Rightarrow$ I intermediate, antiferromag $\rightarrow$??

(we know I=0 gives Kondo effect) $\delta_e = -\delta_o = \frac{\pi}{2}$

Complication when try to go to a lattice: magnetic correlations: the RKKY interaction

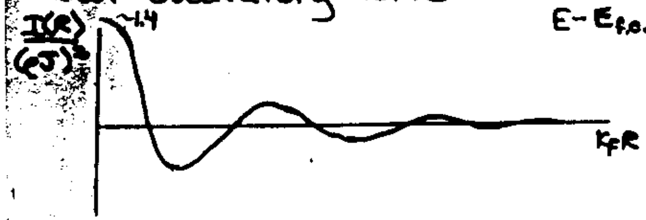
There are no direct interactions between the moments because they are too far apart, tightly bound, etc.

However, there are indirect interactions between the impurities via spin-flip scattering of a conduction electron: a second-order interaction.



If the interaction J between the impurity and conduction electrons is small (compared with the bandwidth), the RKKY interaction, I, can be calculated to give an oscillatory curve:

$$E - E_{F.o.} = \underbrace{f(R)(\rho J)^2 \vec{S}_1\cdot\vec{S}_2}_{I(R)} + O(\rho J)^4$$



Question: What happens in this system as $T\rightarrow 0$?

#moments	"high" temperature	$T\rightarrow 0$
1	$J\vec{S}_c\cdot\vec{S}_o$	$J\rightarrow\infty$ (Kondo effect)
2	$I(R)\propto J^2$ (small) $\longrightarrow$	? (Perturbation th. for I breaks down; contradictory results for I AFM)

$$H = \int d^3k\, \varepsilon_k\, a^\dagger_{k\mu} a_{k\mu} + J \iint d^3k\, d^3k' \left[a^\dagger_{k\mu} \frac{\vec{\sigma}_{\mu\mu'}}{2} a_{k'\mu'} e^{-i(k-k')\cdot \vec{r}_1} \cdot \vec{S}_1 + a^\dagger_{k\mu} \frac{\vec{\sigma}_{\mu\mu'}}{2} a_{k'\mu'} e^{-i(k-k')\cdot \vec{r}_2} \cdot \vec{S}_2 \right]$$

Like the single-impurity problem, by expanding about the center of the 2 impurities, this can be <u>exactly</u> transformed into a 1-D form, w/ $\int d\varepsilon$.

Two channels arise naturally because of reflection symmetry
$\rightarrow$ parity e, o

$$H = \int d\varepsilon\, \varepsilon\, a^\dagger_{\varepsilon\mu} a_{\varepsilon\mu} + J_e \vec{s}_e \cdot (\vec{S}_1 + \vec{S}_2) + J_o \vec{s}_o \cdot (\vec{S}_1 + \vec{S}_2) + J_m \underbrace{(\vec{s}_{eo} + \vec{s}_{oe})}_{\text{flips parity of conduction electrons}} \cdot \underbrace{(\vec{S}_1 - \vec{S}_2)}_{\text{flips impurity spin } S_{TOT}=0 \leftrightarrow S_{TOT}=1 \text{ (odd parity term)}}$$

Schematically written: $J\vec{s}_e \equiv J \int d\varepsilon \int d\varepsilon'\, g_e(\varepsilon) g_e(\varepsilon') a^\dagger_{e\varepsilon\mu} \frac{\vec{\sigma}_{\mu\mu'}}{2} a_{e\varepsilon'\mu'}$

$$g_e(\varepsilon) = \sqrt{1 + \frac{\sin k_\varepsilon R}{k_\varepsilon R}}$$

$$g_o \quad = \quad -$$

<u>**Approximation**</u>: set form factors $g_e(\varepsilon) g_e(\varepsilon')$; $g_e(\varepsilon) g_o(\varepsilon')$ etc. to be indep of ε, <u>as a start</u>, to get a particle-hole symmetric Hamiltonian.

$$\text{RKKY} = (2\ln 2)(\rho J)^2 \left[J_e^2 + J_o^2 - 2 J_m^2 \right]$$

Indep imps: $J_e = J_o = J_m$

<u>Symmetries of H</u> (good quantum numbers)

1. Parity. e, o
2. Total spin $\vec{s}_e + \vec{s}_o + \vec{S}_1 + \vec{S}_2$
3. <u>Vector charge</u> $\vec{J}$

$$J^+ \equiv \sum_{n,p,\text{parity}} (-1)^n f^\dagger_{np\uparrow} f^\dagger_{np\downarrow}$$

$$J^- \equiv (J^+)^*$$

$$J^z \equiv \frac{1}{2} \sum_{n,p} (f^\dagger_{np\uparrow} f_{np\uparrow} + f^\dagger_{np\downarrow} f_{np\downarrow} - 1) = \frac{1}{2} \text{ charge}$$

(more than particle-hole)

$\uparrow\downarrow$	charge $= +1$
$\uparrow, \downarrow$	charge $= 0$
—	charge $= -1$

Note:

i) 2-imp. Hamiltonian is not particle-hole symmetric even with a particle-hole symmetric energy band (unless const-ε g's approx).
(In general case only parity + total S are conserved.)
— see later —

ii) In our previous language,

$$J^+ = \int_{-1} d\varepsilon\, a^\dagger_{\varepsilon\uparrow} a^\dagger_{-\varepsilon\downarrow}$$

$$J^- = \int_{-1} d\varepsilon\, a_{\varepsilon\downarrow} a_{-\varepsilon\uparrow}$$

$$J^z = \frac{1}{2} \int_{-1}^{1} d\varepsilon \left(a^\dagger_{\varepsilon\uparrow} a_{\varepsilon\uparrow} + a^\dagger_{\varepsilon\downarrow} a_{\varepsilon\downarrow} - 1 \right)$$

Results for particle-hole ($\tilde{J}$) symmetry

three regimes of behavior, depending on the ratio I/T_K:

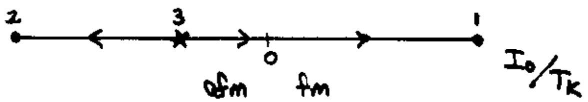
Fermi Liquid states

1. $-2.2\ldots < I/T_K < +\infty$ (FM) Correlated Kondo effect
   $\delta_e = \delta_o = \pi/2$ exactly

2. $-\infty$ (AFM) $< I/T_K < -2.2\ldots$: No Kondo effect
   $\delta_e = 0, \quad \delta_o = \pi$
   Uncompensated singlet with strong afm correlations : RKKY antiferromagnet

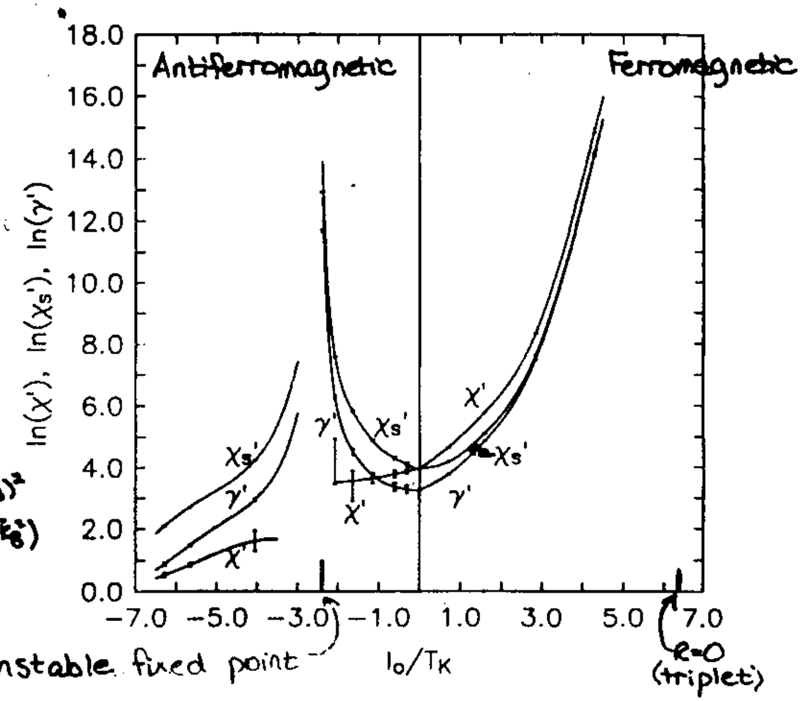
3. $I/T_K \approx -2.2$: Unstable fixed point of complex nature

Critical point: Not Fermi liquid – long range afm order.
- marked by diverging linear coef. of specific heat, and of staggered susceptibility
- normal uniform susceptibility



$\chi' = \chi \frac{D}{(2\mu_B)^2}$

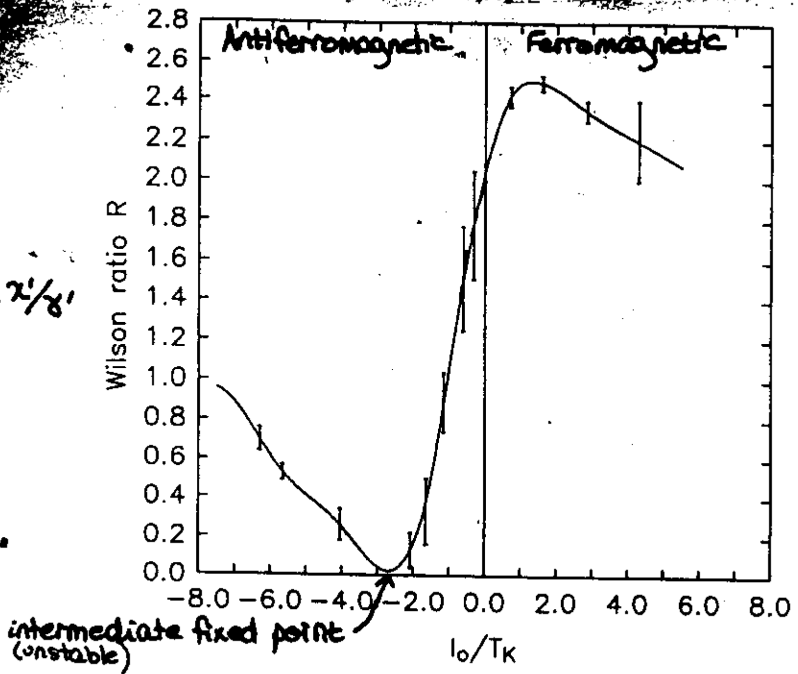
$\gamma' = \gamma \frac{3D}{(\pi^2 k_B^2)}$



Thermodynamic Properties
(particle-hole symmetry)

- χ_{stagg} and γ diverge at unstable fixed point $\sim\left(\frac{I_0}{T_K} - \frac{I_0^*}{T_K}\right)^{-2}$
- Properties are those of free electrons for strong antiferromagnetic intial couplings
- All properties diverge as impurities go to triplet state

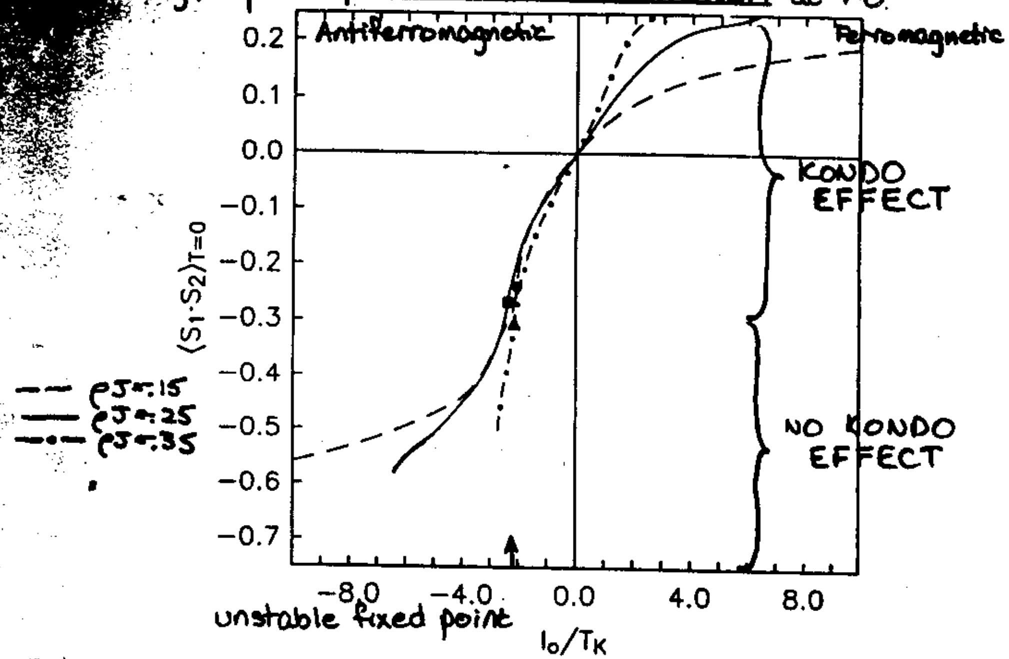
$R = \chi'/\gamma'$



<u>Wilson Ratio</u> $R \equiv \frac{4\pi^2}{3}\frac{k_B^2}{(g\mu_B)^2}\frac{\chi}{\gamma} = \chi'/\gamma'$

- Single-impurity Kondo result is $R = 2$ (universal) (found at $I_0 = 0$).
- Ferromagnetic couplings have R close, but not equal to 2. (May be exactly 2 in limit of zero separation.)
- Antiferromagnetic: R varies widely. (<u>nonuniversal</u>) <u>Zero at intermediate (unstable) fixed point.</u>
- Strong antiferromagnetic couplings: $R \approx 1$, the free-electron result.

(Impurity) <u>Spin-Spin Correlation Function</u> at T=0



$(I_0/T_K)_{transition}$ constant $(-2.2 \pm .2)^*$ through variations in T_K of a factor of 100 (* and fairly large)

$\langle \vec{S}_1 \cdot \vec{S}_2 \rangle$ similar for small aniferromagnetic couplings
$\langle S_1 \cdot S_2 \rangle_{transition} \approx -.25 \pm .05$

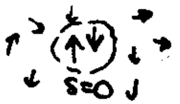
<u>In general,</u>
- $\langle S_1 \cdot S_2 \rangle$ is continuous as a function of coupling consts.
- $\langle S_1 \cdot S_2 \rangle = 0$ only for initially independent impurities. Form is approx. linear at small I_0.

Growth of correlations

Fix T_K, vary I:

$I=0$

- moments uncorrelated; compensating electrons hence also uncorrelated → separate Kondo effects

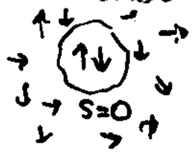


$I=$ large ferromagnetic

- moments in $S=1$ state; compensating electrons also $S=1$

$I=$ large antiferromagnetic

- moments in $S=0$ state → no interactions with conduction electrons; moments disappear from problem, conduction electrons uncorrelated; no Kondo effect



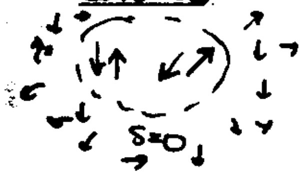
I increases antiferromagnetically from $I=0$

Correlations between the moments grow; hence correlations between Kondo-compensating conduction electrons grows also.

Yet we know correlations between conduction electrons are zero as $I \to$ large antiferromag.

→ Unstable fixed point as a maximum of antiferromagnetic conduction spin correlations.

$I \lesssim I_c$



$I \gtrsim I_c$

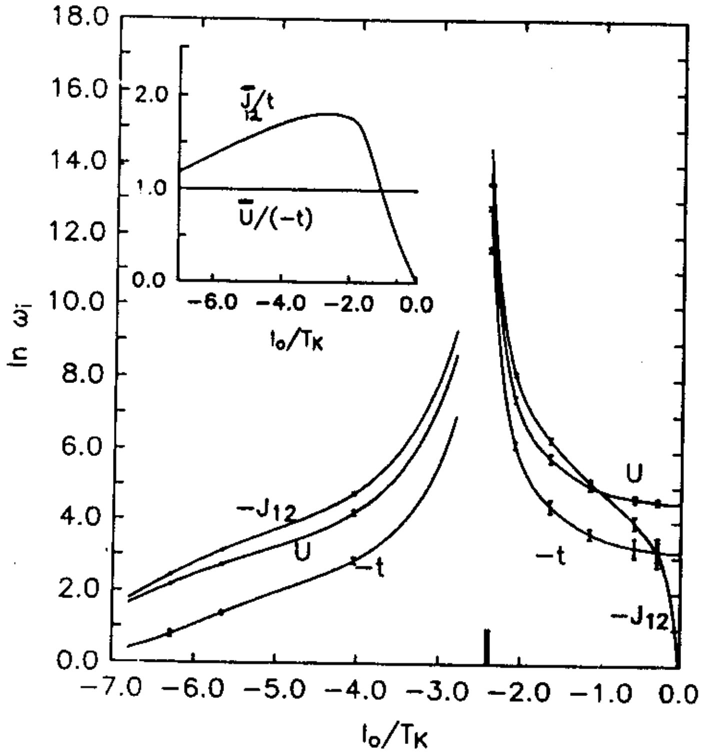
"uncompensated singlet"

(SLIGHT SIMPLIFICATION) FOR ANTIFERROMAGNETIC CASE:

(For no even-odd asymmetry (in coupling constants))

$$\Delta H^{eff} = t\sum_i (f^\dagger_{0i\mu} f_{1i\mu} + h.c.) + U\sum_i q_{0i}^2 - J_{12}\, 4\vec{S}_1\cdot\vec{S}_2$$

$$R = 1 + \left(\frac{U}{|t|} + \frac{J_{12}}{|t|}\right) C(\Lambda) = \text{Wilson Ratio}$$



→ 2-Parameter Fermi Liquid (single-impurity Kondo + spin interactions)

U/t = constant : Nozières' "weak universality"

$U \approx t \approx T_K^{-1}$: <u>single</u> T-scale for 1-impurity problem; universality

LECTURE 2

...ential Scattering: Breaking Particle-Hole ($\mathcal{J}$) Symmetry

Add potential scattering terms in each parity channel to the original Hamiltonian.

$$\Delta H = V_o \iint d\epsilon\, d\epsilon'\, a^{\dagger}_{\epsilon o \mu} a_{\epsilon' o \mu} + V_e \iint d\epsilon\, d\epsilon'\, a^{\dagger}_{\epsilon e \mu} a_{\epsilon' e \mu}$$

(Magnitude of V gives measure of symmetry breaking.)

Results:

1) For general V_e, V_o, critical behavior is washed out.

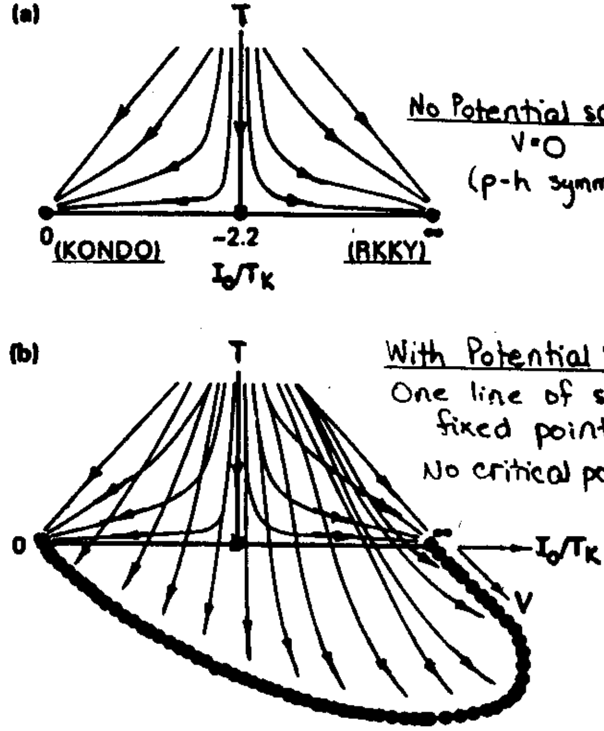
BUT 2) For $V_e = V_o$, critical behavior remains! Line of unstable fixed points, one for every V.
Extent to which away from critical behavior depends only on $|V_e - V_o|$, not on magnitudes separately.

$\vec{J}$ is no longer preserved: what new symmetry is present even for $V_e = V_o$ which causes critical behavior? $[H, n_r] = [H, n_l] = 0$

This new symmetry could be a property of the more general Hamiltonian.

[redacted]

Phase diagrams / Low temp. fixed points for 2 Kondo impurities:

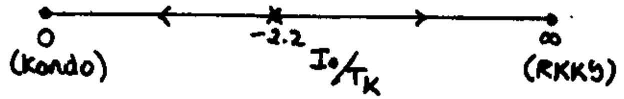


No Potential scattering
$V = 0$
(p-h symmetric)

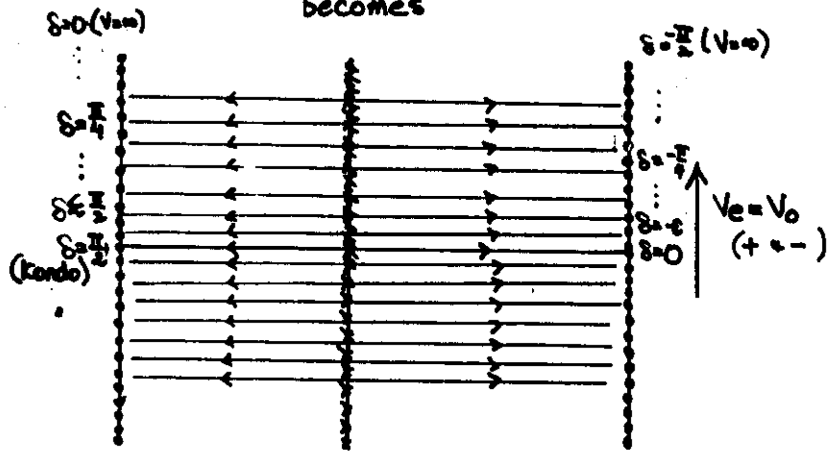
With Potential Scattering
One line of stable fixed points
No critical point for $V \neq 0$

for $V_e = V_o$ and $J_e = J_o$

(number of even and odd electrons separately preserved)

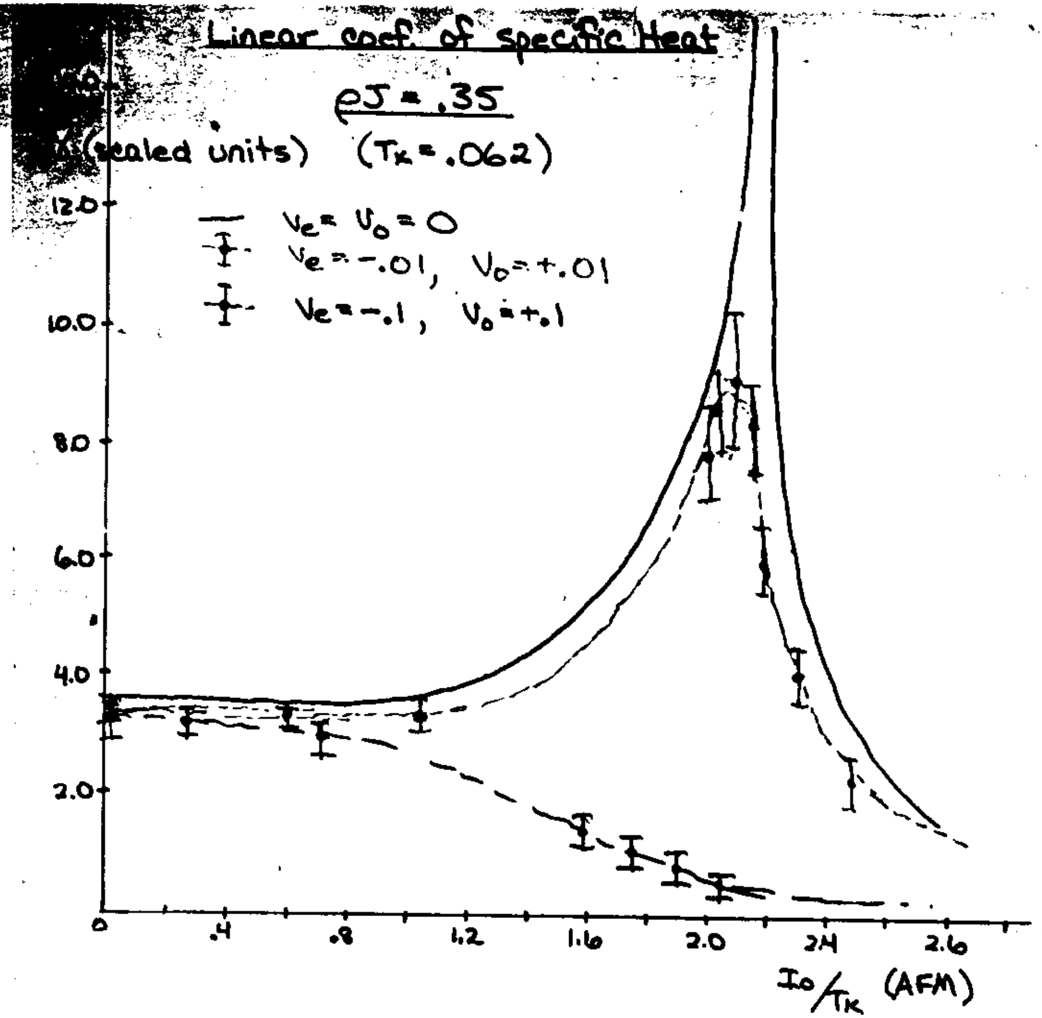


becomes



Lines of Fermi-liquid and non-Fermi-liquid fixed points, parameterized by a phase shift

- Analogous to effect of potential scattering for single-impurity problem (irrelevant operator).
- Non-Fermi liquid fixed points washed out only if $V_e \neq V_o$ OR $V_e = V_o \neq 0$ but $J_e \neq J_o$



Work in progress: crossover exponents

Unstable non-Fermi liquid state of 2-impurity problem:

What do we know?

γ, $\chi_{staggered} \to \infty$

$\chi_{uniform}$ normal

- maximum of $\vec{S}_r \cdot \vec{S}_l$ quasiparticle interactions
- $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = -\frac{1}{4}$ (notation: $1 \equiv r$, $2 \equiv l$)
  impurity spins
- Symmetry develops: $\vec{S}_e$, $\vec{S}_o$ separate quantum numbers
  (quasiparticle spins)

- Washed out by potential scattering?

	$V=0$	$V_e = V_o$	$V_e \neq V_o$
$J_e = J_o$	no	no	yes
$J_e \neq J_o$	no	yes	yes

What is the physical nature of this state??

Summary, Conclusions & Quandries

[illegible]y coupling and Kondo effect determine low-temp behavior even for $I_0 << T_K$; $I_0 \geq T_K$

Effects are mixed far more than naive theory would predict.

2) Ground state (for $K \neq 0$) is always* a singlet, Fermi liquid.
(*except at unstable pt.)

Separated impurities are correlated even though both may experience Kondo effect; compensation is collective, not individual.
($e \neq 0$)

3) For antiferromagnetic correlations behavior can be very complex, including new unstable fixed point at fixed ratio of I_0/T_K (and certain symmetry).

4) Uneven potential scattering washes out the critical behavior. However, depending on the crossover exponents, remnants of the critical behavior can persist (Divergence in γ, χ_s changes to peak.)

→ Single particle result (i.e, Kondo effect) is strongly modified by two-spin results.

Pair interaction effects must be included in theories for a lattice.
. . .

• Lattice as sum of pair-wise H's, with physics as above?

• How robust is the instability to changes in the model?

⇒ How likely are we to find such two-impurity effects in real materials?

Intriguing current experimental situation:

i) Most H.F. are on verge of magnetic state (pressure, doping), but with very small moments

ii) Neutron scattering finds AFM correlations in at least 10 H.F. compounds

- strange magnetic states, odd ordering

• And how do we do the lattice?

— current work: 1/N expansion —

• How do magnetism and superconductivity interact?

H.F.: simultaneous SC + magnetic states:

UPt_3, U_2Zn_{17}, ...

AND?

Method: Numerical Renormalization Group

Computationally intensive, but not a black box

Analytically intensive

Powerful: gives exact ground states

[Can only be used on a subset of problems]

Wilson's method, specifically, restricts type of problem

Exact calcutions of: ground state(s)

leading irrelevant and marginal operators (Fermi liquid f.p.)

correlation functions

low-T thermodynamics

low-T effective Hamiltonians

<u>Much</u> more physical insight than Bethe Ansatz (and than conformal field theories)

Provides a check for other methods, particularly those intended for a lattice

Numerical Renormalization Group

Example (historical): single-impurity Kondo problem

$$H = K.E. + J\vec{s}_c(0)\cdot\vec{S}_0$$

$$= \int d^3k\, \varepsilon_k\, a^\dagger_{k\mu} a_{k\mu} + J \iint d^3k\, d^3k'\, \underbrace{e^{-i(k-k')\cdot\vec{r}_0}}_{1}\, a^\dagger_{k\mu} \frac{\vec{\sigma}_{\mu\nu}}{2} a_{k'\nu}\cdot\vec{S}_0$$

3 steps:

1. Change of bases — analytic — DO ONCE
2. numerical iterative calculation
3. analytic analysis of fixed points, relevant operators

} REPEAT TO FILL PARAMETER SPACE

Step 1: Changes of bases (Conversion of Hamiltonian to iterative form) — Basic techique

Exact A) Convert H to 1-D ε (rather than 3-D $\vec{k}$) form.

- Expand $a^\dagger_{k\mu}$ in spherical harmonics about the origen
  - m=0 doesn't couple to impurit(ies) (typically)
  - # of ℓ = # of scattering channels = # impurities
    $\ell=0$ for 1 impurity
    specific sums of even and odd ℓ for 2 imps, etc.

so $a^\dagger_{k\mu} \rightarrow \underbrace{f(\varepsilon,R)}_{\text{form factors}}\, a^\dagger_{\varepsilon\mu}$ =1 for 1 impurity

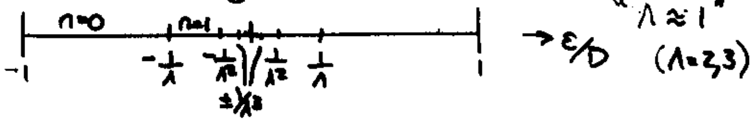
$$H = \int_{-1}^{1} d\varepsilon\, a^\dagger_{\varepsilon\mu} a_{\varepsilon\mu}\, \varepsilon + J \iint d\varepsilon\, d\varepsilon'\, a^\dagger_{\varepsilon\mu} \frac{\vec{\sigma}_{\mu\nu}}{2} a_{\varepsilon'\nu}\cdot\vec{S}_0$$

$f(\varepsilon,R)f(\varepsilon',R)$

Logarithmic Discretization (Wilson, 1975)

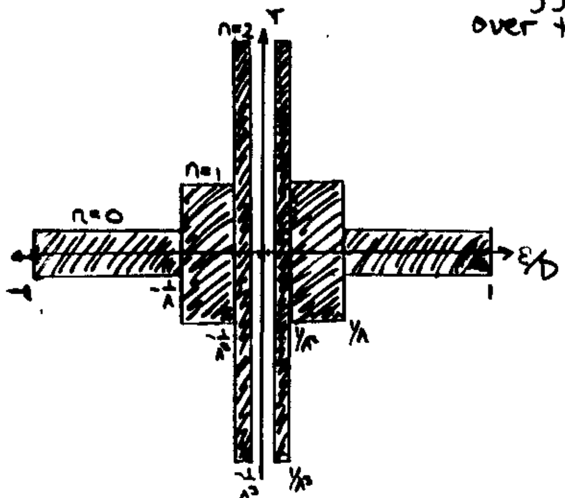
Parameter Λ chosen, $\Lambda = 2$–3 (or larger)

Divide up ε-space — logarithmic set of ε-scales



- expand operators a_ε in Fourier series in each interval
- Approximation: include only 0^{th} Fourier component
  (Throw away states not peaked at the impurity site.)
  Confirmed by numerical tests.

So now there is one operator corresponding to each interval n.: the average of each energy operator over the interval



At this point,
Kinetic Energy is diagonal in n, J-interaction connects each n with every other.

1) Conversion to "Wannier" states

• Define new operators $\{f_n\}$ such that only f_0 interacts directly with the impurity(ies).

f_n $\{n=1,2,3,\ldots\}$ chosen to be orthogonal to f_0.

AND

to couple at most n to $n\pm1$ in the kinetic energy.

$$H = \underbrace{\sum_{\substack{n=0\\ \rho,\mu}}^{\infty} \xi_n \Lambda^{-n/2} \left[f^{\dagger}_{n\rho\mu} f_{(n+1)\rho\mu} + f^{\dagger}_{(n+1)\rho\mu} f_{n\rho\mu} \right]}_{H_{KE}} + H_{int}$$

H_{int} involves only f_0 and the impurity (localized) operators.

f_n's have specific localization in both ε and r space.

• $|f_n\rangle$ has spread in $\varepsilon \sim \Lambda^{-n/2}$
extent about origin $\sim \Lambda^{n/2}$

$|f_0\rangle$ most localized, biggest ε-spread (~ 1)

Same picture in (inverse) ε-space:

ONIONSKINS

$$H = H_{K.E.} + J f^{\dagger}_{0\mu} \frac{\vec{\sigma}_{\mu\mu'}}{2} f_{0\mu'} \cdot \vec{S}_0$$

2) Re-express in iterative form

$$H \propto \lim_{N\to\infty} \Lambda^{-(N-1)/2} H_N$$

$$H_N = H_0 + \sum_{n=0}^{N} \xi_n \Lambda^{-n/2} \left(f_n^{\dagger} f_{n+1} + h.c. \right)$$

$$H_{N+1} = \Lambda^{1/2} H_N + \xi_N \left(f^{\dagger}_{N\mu(\rho)} f_{N+1\,\mu(\rho)} + f^{\dagger}_{N+1\,\mu(\rho)} f_{N\mu(\rho)} \right)$$

• Diagonalize H_0 (J-term) by hand

H_1, H_2, etc. diagonalized by computer

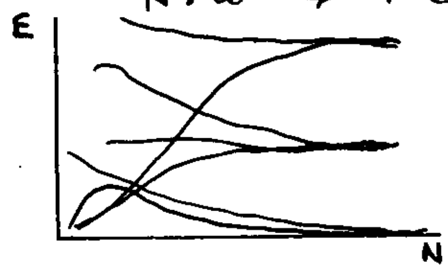
Step 2: Computer formations of matrices corr. to H_N, diagonalization

Output of each iteration is a set of eigenvalues (energies) and eigenvectors (states)

Approx: Keep only the lowest-energy 1000-1500 or so states (good for low-T properties)

Iterate until energies stabilize ($\rightarrow$ stable fixed point)

$N \to \infty \;\Rightarrow\; T \to 0$ as $\Lambda^{-N/2}$



CAN STOP AT FINITE N AS SOON AS CAN IDENTIFY STABLE FIXED POINT

3. • Analysis of fixed-point eigenlevels (degeneracies and energies) to identify fixed point

• Analysis of flow to fixed point to obtain low-T effective Hamiltonian

- expansion in irrelevant operators
- calculation of low-T thermodynamics

EXAMPLE: 1-imp Kondo problem

Set $J=0$

$$H_{N\,\text{free elects}} = \sum_{n}^{N} \xi_n \Lambda^{-n/2} (f_n^\dagger f_{n+1} + \text{h.c.})$$

Exactly diagonalizable.

One set of levels for N even, one for N odd

Wilson found $N \to \infty$ f.p. of Kondo problem corresponded to N-1 free electrons:

one electron is frozen with impurity, making a total spin=0 (as if impurity were not there):

Kondo effect

$$H_{\text{free elects}} = \sum_n \epsilon_n (g_{n\mu}^\dagger g_{n\mu} + h_{n\mu}^\dagger h_{n\mu})$$ ← holes

For a Fermi liquid fixed point, can express H as sum of (single) particle and hole operators

$g_n^\dagger$ + $h_n^\dagger$ are linear combs of original $f_n^\dagger$

Non-Fermi liquid fixed points

How to tell a fixed point is not a Fermi liquid:

Fermi liquid ground state (energies, g.s.'s) characterized by the filling of a set of single-particle levels,

plus perhaps a phase shift,

plus perhaps a finite set of extra degrees of freedom, such as a free spin

It is straight forward to tell if fixed-point degeneracies can not be derived in this way

(e.g. degeneracy 17, or any odd number if no extra spin, ...)

Example:

	degeneracy:	
⋮		
———	7	← ??!
———	8	← ok so far {e↑, e↓, o↑, o↓ particles + holes
———	1	← no free spin

• How to study a non-Fermi liquid point:

Example:

Can calculate thermo, correlation functs etc.

- up to the border of a finite-size region
- arbitrarily close for a line

At finite Temperature: (finite N)

fixed-pt energy levels ← T=0 ground state

flow to fixed pt levels as function of N
gives finite-T props

Expand $H_{f.p.}$ in leading irrelevant operators

$$H = H_{\substack{\text{free}\\ \text{elects}\\ N}} + \Lambda^{-N/2}\Big[t\,(f^{+}_{1\mu}f_{0\mu} + f^{+}_{0\mu}f_{1\mu}) + U(n_0-1)^2 + \dots\Big] = H_{\text{free elects}} + \delta H$$

- ops must preserve symmetries of orig. Hamiltonian
  → limits their number

Use δH a. perturbation on $H_{\text{free.elect}}$: calculate
C, χ

Applications of the NRG

$S = S = \frac{1}{2}$

1975 Wilson Single-impurity Kondo

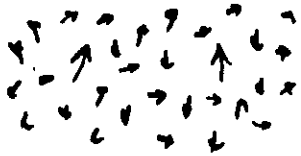
1978-1980 Cragg & Lloyd
- Potential Scattering for 1 Kondo
- S=1 impurity with 1 channel, 2, etc.
- 1980 Spin $\frac{1}{2}$ + 2 channels

1980 Krishnamurthy Single-impurity Anderson

1986 Oliveira
- Extension of Wilson technique to finite frequency $\Lambda^{-z}, \Lambda^{-z-1}, \Lambda^{-z-2}, \dots$
  $0 \le z \le 1$

1990 Spectral Density for Fermion Tunneling Between Two Centers in a Metallic Environment

1987, 1988, ... Jones & Varma 2 Kondo Impurities



+ Cox + Pang, etc. (Shiba, more Oliveira, ...)

I.C. Limitations

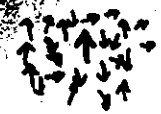
* PROBLEM MUST HAVE A CENTER OF SYMMETRY

NOT TOO USEFUL IN PRESENT FORM FOR THE LATTICE / OR PURELY ITINERANT STATES.

LECTURE 3

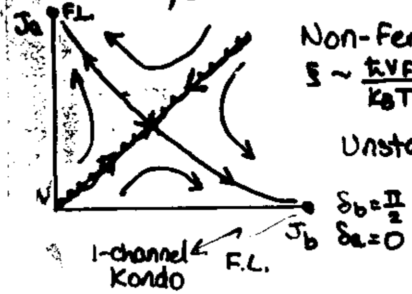
Two-Channel Kondo = Quadrupolar Kondo effect

Cragg + Lloyd; Nozières 1979-80
D. Cox + H. Pang 1987



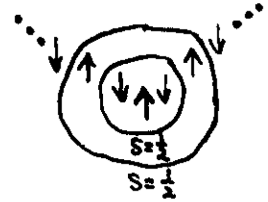
$$H = K.E. + J_a\, \vec{s}_a \cdot \vec{S}_0 + J_b\, \vec{s}_b \cdot \vec{S}_0$$

"Overcompensated": each Kondo effect gives $S_{net} = \frac{1}{2}$ when $J_a = J_b$



Non-Fermi liquid state
$\xi \sim \frac{\hbar v_F}{k_B T}$, nonuniversal exponents,

Unstable to $J_a \neq J_b$



Quadrupolar Kondo effect:

- quadrupolar split ground state doublet on impurity ion
- local quartet of conduction partial waves –
  orbital 2-fold degenerate ⊗ channel "spin"
  (spin) (time-reversed)

(Apparently some quadrupolar Kondo is ubiquitous: nonmagnetic low-degeneracy ground states interact w/ higher-E orbitals.
(spin orbit + crystal field split)

When symmetries are right, get 2-channel coupling.)

Tunneling expts (Ralph + Buhrman, etc.)
2-level systems

"Two"-channel, Two-Impurity Kondo Effect

BAJ with K. Ingersent (Ohio State)

$H = \text{K.E.} + J_a\left[s_a(-\tfrac{R}{2})\cdot\vec{S}_1 + s_a(+\tfrac{R}{2})\cdot\vec{S}_2\right] + J_b\left[s_b(-\tfrac{R}{2})\cdot\vec{S}_1 + s_b(\tfrac{R}{2})\cdot\vec{S}_2\right]$

As with previous 2-impurity case, symmetry induces two (parity) channels, even and odd.

Now we also have two flavor/orbital channels → 4 total. ⇒ overcompensated

NRG treatment: set $J_a = J_b$ for simplicity.

Results depend on 3 parameters: T_K, RKKY ≡ I, and a third: $\underline{J_e - J_o} \propto J_{RL}$, coef. of $c_R^\dagger c_L$

roughly analogous to $J_a - J_b$ asymmetry

- "Quadrupolar" Kondo point unstable to any RKKY, fm or afm.
- Regions of finite volume in parameter space of non-Fermi liquid ground state. (multiple new fixed points)

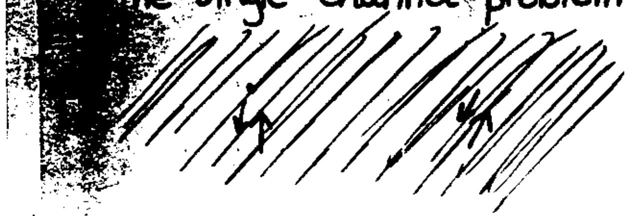
Given reflection symmetry, $J \cdot \sum_{j=1}^{2} \vec{s}_i(\vec{r}_j)\cdot\vec{S}_j$ can be expanded as

$$\underline{J_e^{(R)}} s_{e,i}\cdot(\vec{S}_1+\vec{S}_2) + \underline{J_o^{(R)}} s_{o,i}\cdot(\vec{S}_1+\vec{S}_2) + \underline{J_m^{(R)}}(s_{oe,i} + s_{eo,i})\cdot(\vec{S}_1-\vec{S}_2)$$

J_e, J_o, + J_m depend on impurity spacing R.

$J_e = J_o$ only at certain impurity distances.

the single-channel problem,



Also has these two interactions $\underbrace{(\text{RKKY}, J_e - J_o)}_{}$, produced by having two impurities

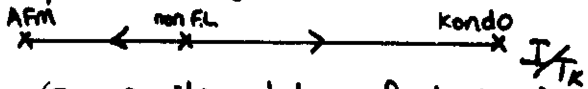
but for $\underline{\text{one channel}}$ (in the particle-hole symmetric limit we will be discussing),

$\underline{J_e - J_o}$ $\underline{\text{is}}$ an $\underline{\text{irrelevant}}$ operator:

$J_e - J_o \to 0.$

(We will bring up J_m again later)

...And the phase diagram is one-dimensional:



(2 impurities, 1 type of electron)

For $\underline{\text{two channels}}$ of electrons, $J_e - J_o$ turns out to be a $\underline{\text{relevant operator}}$:

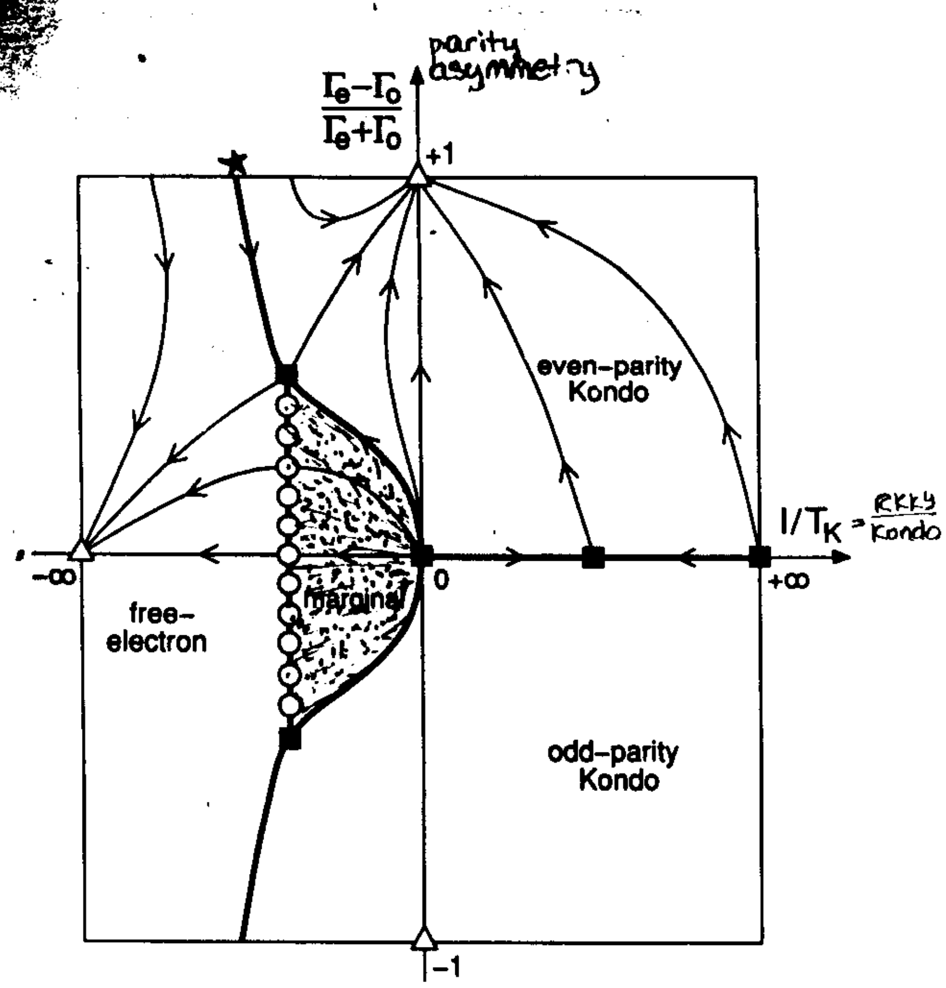


Figure 1

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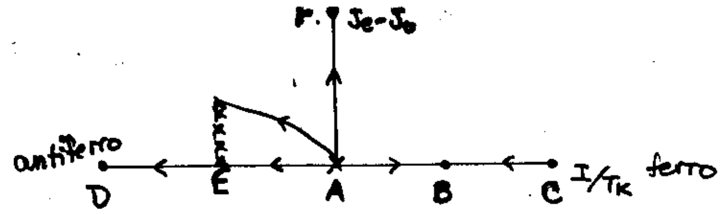
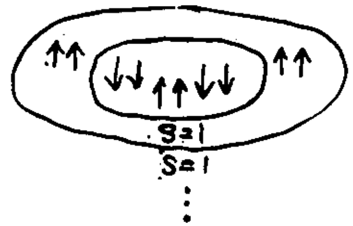


A: Decoupled impurities: 2 independent 2-channel Kondo

2 independent $S=\frac{1}{2}$'s: $\underbrace{\uparrow\downarrow\uparrow\downarrow}_{S=\frac{1}{2}}$ $\quad \underbrace{\rightleftarrows}_{S=\frac{1}{2}}$ non-Fermi liquids

B: Above "super"-$\frac{1}{2}$'s lock in triplet $\uparrow \quad \uparrow$

C: S=1 overcompensated Kondo



Kondo and ferromagnetic RKKY not competing: Kondo does not shield RKKY, RKKY does not quench Kondo

D: Impurity singlet: simplest Fermi liquid ↑↓ $S=0$ $\quad s=0$

E: Super-$\frac{1}{2}$'s lock into singlet? ↑ ?? ↓ non-Fermi liquid finite volume of f.p.!

F: $J_e \neq J_o$: larger of $\{J_e, J_o\}$ scales to ∞ fastest: Kondo effect in that parity channel only

Fermi liquid $\delta_{e,a} = \frac{\pi}{2} = \delta_{e,b}$, $\delta_{o,a} = 0 = \delta_{o,b}$ $\quad$ ↓↑ ↓↑ $S=0$ } even parity elects. of both "orbital" channels

For ferromagnetic RKKY, any $J_e \neq J_o$ destabilizes all the "exotic" fixed points, and flow is to a normal '2-impurity' Kondo effect in the larger of J_e or J_o.

$J_e \neq J_o$ equiv. to $J_a \neq J_b$

Parity channels play same role as "orbital" channels

For antiferromagnetic RKKY, RKKY does inhibit Kondo: for large enough I, system behaves as free electrons, spins self-quench.

$J_e - J_o$ does not completely destabilize interesting non-Fermi liquid states (continuum) until $\frac{J_e - J_o}{J} \sim 0.7$

- Parity $\longleftrightarrow$ orbital analogy not complete

Old friend the unstable fixed pt of the normal 2-imp problem appears (★) - related somehow to the other non-Fermi liqu. phases?

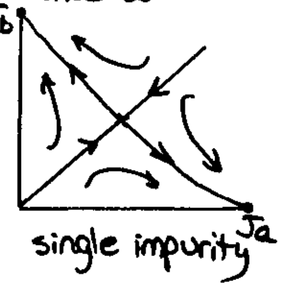
Increase RKKY from zero at single-(isolated) impurity limit:

Why differences between fm and afm sides of phase diagram? (Why single imp fixed pt. unstable?)

Ferromagnetic RKKY: $J_e \neq J_o$ behaves like a channel inequality

$\begin{Bmatrix} e \\ o \end{Bmatrix} \longleftrightarrow \begin{Bmatrix} a \\ b \end{Bmatrix}$

even and odd act as independent channels – no mixing "$J_m \to 0$"

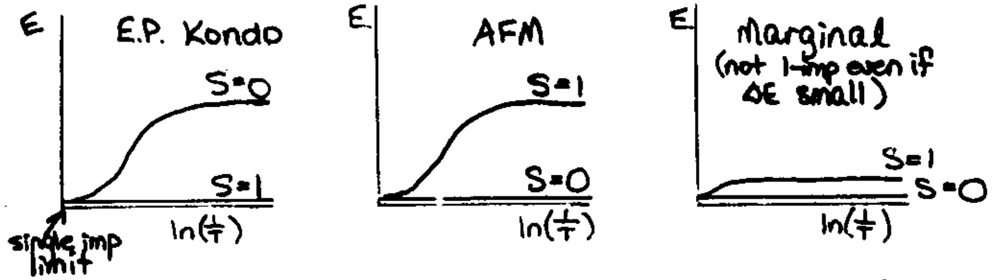


Antiferro RKKY: independent e,o analogy
- does not hold, until $J_e - J_o$ becomes large.

J_m initially large for afm case → e,o mixing persists

mix e,o $\Longleftrightarrow$ mix S=0, S=1 of impurities (neither Kondo nor afm)

schematic



Multichannel (1-imp) ground state v. degenerate (4x); likely to be broken by a perturbation. RKKY drives singlet and triplet apart: exactly what we see in lowest states. Break degeneracy ⟺ new fixed point. (contrast 1-channel)

Low-Energy Excitations

About each Fermi-liquid fixed point, one may expand into a finite number of leading (irrelevant) operators.

These operators describe the low-energy quasiparticle excitations.

[→ thermodynamics]

11 terms

4 are Hubbard-like : t_e, t_o ; U_e, U_o

$$\begin{cases} \vec{S}_{e,g} \cdot \vec{S}_{o,g} + h \\ \vec{S}_{e,g} \cdot \vec{S}_{e,h} \\ \vec{S}_{o,g} \cdot \vec{S}_{o,h} \\ \vec{S}_{e,g} \cdot \vec{S}_{o,h} + \vec{S}_{e,h} \cdot \vec{S}_{o,g} \end{cases}$$

$\rightarrow (\vec{S}_{eo,g} + \vec{S}_{oe,g}) \cdot (\vec{S}_{eo,h} + \vec{S}_{oe,h})$ (hopping as spin flip)

$\vec{Q}_{e,g} \cdot \vec{Q}_{o,g} + h$ $\vec{Q}$ = axial charge

$\rightarrow (n_{eo,g} - n_{oe,g})(n_{eo,h} - n_{oe,h})$

All diverge at the same rate near the non-FL points ... except the last.

Effect of potential scattering

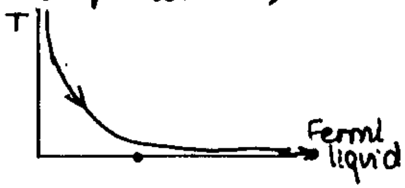
Given finite volume of non-Fermi liquid points,

might expect that more resistant to effects of p.h. symmetry breaking.

Expectations incorrect: potential scattering appears to wash out non-Fermi liquid pts.

Fermi liquid behavior is the, apparently, natural ground state for many (most) Kondo impurity problems.

Exotic non-Fermi liquid states will affect behavior at low temperatures, but not ground state.



crossover exponents will determine how much effect non-Fermi liquid phases have.

Summary of 2-impurity multichannel Kondo

- Isolated-impurities ground state is intrinsically unstable to RKKY because of its highly spin-degenerate ground state (4-fold: easily split into S=0 and S=1 states)
- Even and odd parity asymmetry can act analogously to channel asymmetry.
- No region of stability can be found around single-impurity fixed point. Flows are either to one-parity Kondo (Fermi liquid) or to "marginal" state. (non-Fermi liquid)

Remaining questions:

- Precise nature of region of non-Fermi liquid states? 2 channel, 2 impurity unstable point still not understood, new f.p. even less so.
- Superconducting pairing? Of what symmetry?
- Thermodynamics, correlation functs, etc.
- What is the physical nature of the effects of potential scattering? Why does it act as a marginal operator in some cases, others as a relevant operator?