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SMR. 758 - 9

SPRING COLLEGE IN CONDENSED MATTER
ON QUANTUM PHASES
(3 May - 10 June 1994)

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INFRARED SINGULARITIES:
X-RAY EDGE, KONDO EFFECT, HEAVY PARTICLES etc.

LECTURE 5

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c) A simple example : the Friedel resonant level

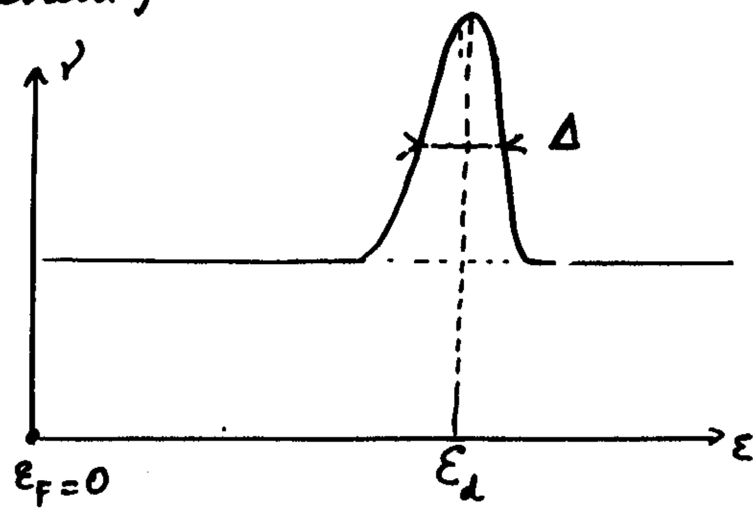
$$H_0 = t_{ij}\, c_i^* c_j + \varepsilon_d\, d^* d + \lambda \left[c_0^* d + d^* c_0 \right]$$

(at this stage, spin is irrelevant)

$\Downarrow$

Lorentzian peak in the density of states

$$\Delta = \pi \nu_0 \lambda^2$$



$\boxed{|\varepsilon_d| \gg \Delta}$

The d-state decouples at low temperature

$\downarrow$

No effect at Fermi level

$\boxed{|\varepsilon_d| \lesssim \Delta}$

Enhanced density of states at Fermi level

Question : does this simple behaviour resist an interaction between s and d electrons?

2) The minimal problem

$$H = H_0 + V\left[d^* d - \tfrac{1}{2}\right]\left[C_0^* C_0 - \tfrac{1}{2}\right]$$

$\frac{1}{2}\left[d^* d + d d^*\right]$

$\bullet\, d$

$\overset{\times}{C_2} \quad \overset{\times}{C_1} \quad \overset{\times}{C_0} \quad \overset{\times}{C_1} \quad \overset{\times}{C_2}$

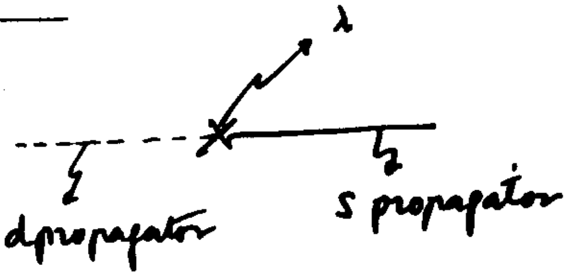
$\downarrow$

Electron hole symmetry if $\varepsilon_d = 0$
(No Fermi level shift)

$\downarrow$

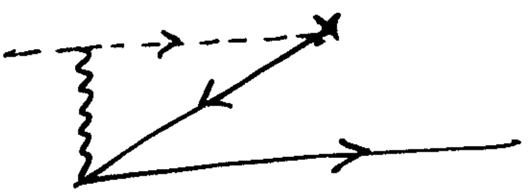
Effect of V ?

a) Perturbative scaling



$\downarrow$

lowest order corrections to λ



If the band width D is reduced by δD

$$\delta\lambda = -\lambda V \frac{\nu\,\delta D}{D}$$

$\Downarrow$

$$\lambda \sim D^{g} \qquad (g = -\nu V)$$

$$\frac{\Delta}{\Delta_0} = \left(\frac{D}{D_0}\right)^{2g}$$

Scaling stops when the resonance is off the band

(i) $D \lesssim |\varepsilon_d|$ Natural crossover energy at which d state decouples

$\Downarrow$

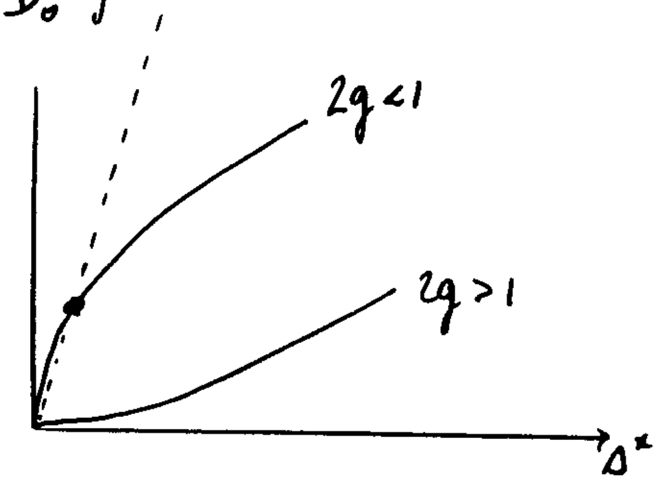
We assume $\varepsilon_d = 0$ (electron-hole symmetry)

(ii) $D \lesssim \Delta$ $\Rightarrow$ self consistency problem !!

Crossover $\frac{\Delta^*}{\Delta_0} = \left(\frac{\Delta^*}{D_0}\right)^{2g}$

$\Downarrow$

$$\Delta^* = \begin{cases} 0 & \text{if } 2g > 1 \\ \Delta_0 \left(\frac{\Delta_0}{D_0}\right)^{\frac{2g}{1-2g}} & \text{if } 2g < 1 \end{cases}$$



$\Downarrow$

Transition depending on the strength of the interaction

Physical interpretation

The resonant width Δ should be compared to the band width

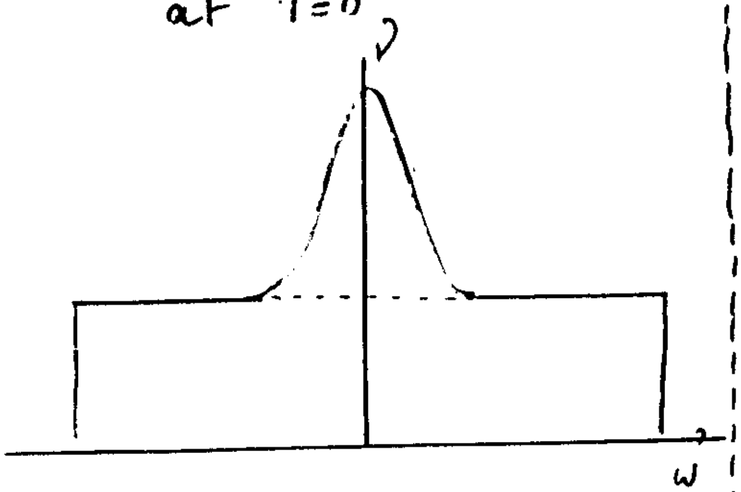
$\boxed{2g<1}$

Δ decreases slower than D

cross over $\Delta \sim D \sim \Delta^*$

Thereafter scaling stops and Δ does not change

Finite density of states at $T=0$



$\boxed{2g>1}$

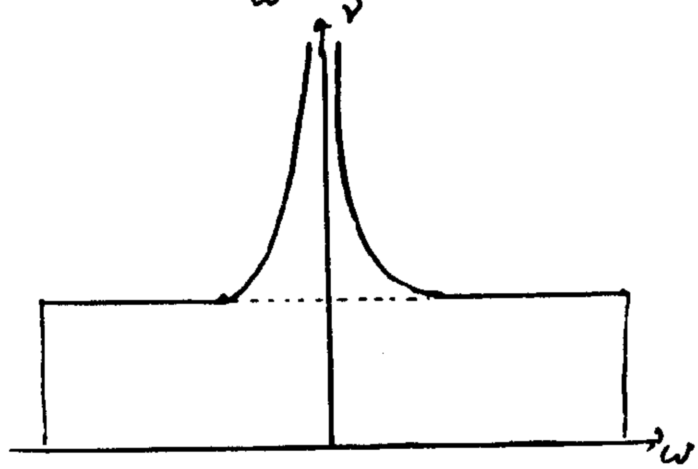
Δ decreases faster than D

It remains $\ll D$: no crossover

Δ scales down to 0

Density of states

$$\nu_I \approx \frac{1}{\pi} \frac{\Delta(\omega)}{\omega^2} \sim \omega^{2g-2}$$

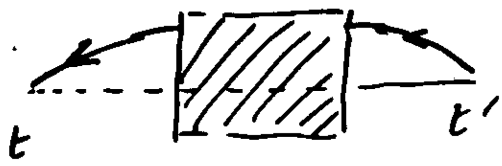


Conclusion: for a strong enough attraction, the Fermi liquid picture breaks down

(analogy to the Caldeira Leggett localization of two level systems)

b) A more exact description : X ray catastrophy

— No hybridization $\lambda = 0$



$\downarrow$

X ray edge problem

ground state with $n_d = 0$

$$G(t-t') = \langle \Psi_0 | d(t') C_0^*(t') \; C_0(t) d^*(t) | \Psi_0 \rangle$$

$$\hookrightarrow \frac{1}{\left[D\,|t-t'|\right]^{\left(\frac{\delta}{\pi}+1\right)^2}}$$

δ is the Fermi level phase shift discontinuity when n_d jumps from 0 to 1

$$\downarrow$$

$$G(\omega) = \frac{1}{D}\left(\frac{\omega}{D}\right)^{2\delta/\pi + \frac{\delta^2}{\pi^2}}$$

multiple scattering of emitted hole

closed loops

$$\begin{cases} G(\omega) \sim \omega^{2g} \\ 2g = \dfrac{2\delta}{\pi} + \dfrac{\delta^2}{\pi^2} \end{cases}$$

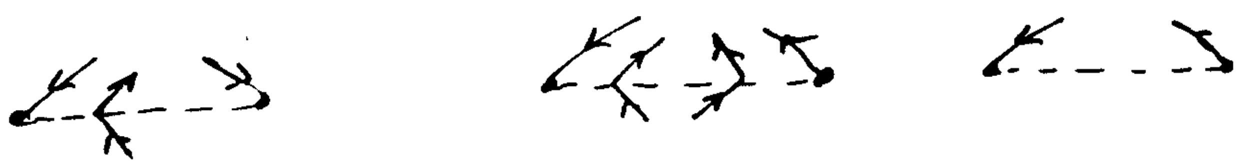
– Half diagram → renormalized λ with any intermediate state $|E_n| > D$

$$\lambda[D] \sim D^{g}$$

g is the same exponent introduced before

↳ $g = -\rho_0 V$ in Born approximation

Rigorous proof "à la Anderson Yuval"



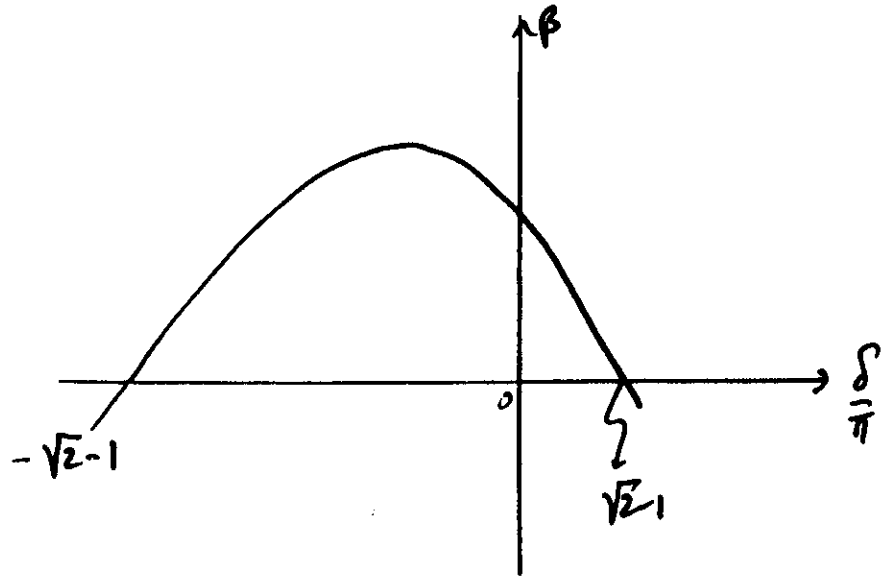
Various contraction → Cauchy determinant in the long time limit

↳ $g = \dfrac{\delta}{\pi} + \dfrac{\delta^2}{2\pi^2}$

~~Other possibility: do the Schlottmann mapping in reverse (VRGA)~~

— Non Fermi liquid behaviour occurs if

$$\beta = 1-2g = 1 - \frac{2\delta}{\pi} - \frac{\delta^2}{\pi^2} < 0$$



δ is the difference of phase shifts for $n_d = 0$ or 1.

In the electron-hole symmetric case, $\delta = 2\delta'$, where δ' is the phase shift for $n_d = 1$

But $\quad \operatorname{tg} \delta' = \dfrac{V \operatorname{Im} G_0}{1 - V \operatorname{Re} G_0}$

↳ zero at Fermi level due to e-h. symmetry

$$\Downarrow$$

$$-\pi/2 < \delta' < \frac{\pi}{2}$$

$$\boxed{-1 < \frac{\delta}{\pi} < +1}$$

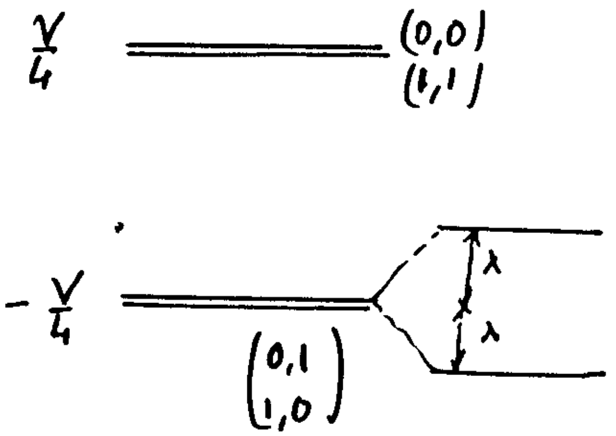
Non Fermi liquid behaviour occurs only for attraction

c) The strong coupling limit

Band width $D \to 0$ $\Longrightarrow$ One site problem

(i) $\varepsilon_d = 0$: resonance at Fermi level

Repulsion



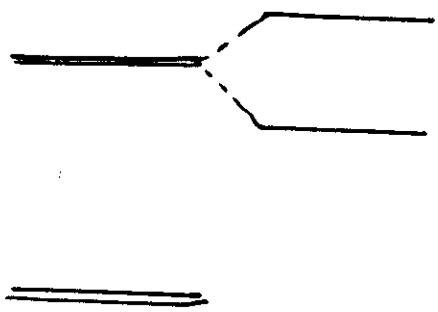
singlet groundstate

$\downarrow$

Fermi liquid

Attraction

$V < -2\lambda$

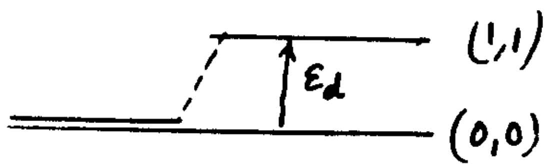


Doublet groundstate (00) (11)

$\Downarrow$

Non Fermi liquid

(ii) If $\varepsilon_d \neq 0$, the degeneracy of (0,0) and (1,1) is lifted



$\Downarrow$

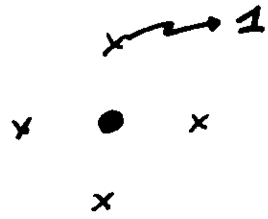
Crossover to singlet behaviour when $T < \varepsilon_d$

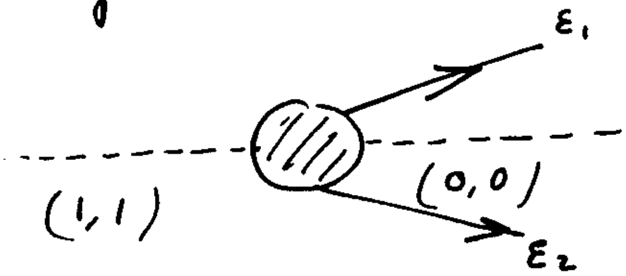
(iii) The central site is frozen

$\downarrow$

Flip operator $|1,1\rangle = A^* |0,0\rangle$

The low temperature relevant operators involve only the $\ell = 0$ first layer of neighbours





Problem: mapping to ferromagnetic Kondo effect?

$\Longrightarrow$ Vertex $\gamma(\varepsilon_1, \varepsilon_2)\, A^*\, c_1\, c_1$

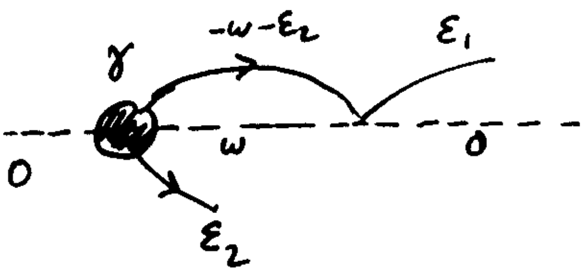
Exclusion principle $\rightarrow$ $\gamma(\varepsilon_1, \varepsilon_2) = -\gamma(\varepsilon_2, \varepsilon_1)$

$$\Downarrow$$

$$\gamma \sim (\varepsilon_1 - \varepsilon_2)$$

The vertex is retarded : no equivalent hamiltonian

(iv) As $D \to 0$, γ scales to zero



(+ symmetric diagram)

$\rightarrow$ $\dfrac{d\gamma}{dD} \sim - \dfrac{\gamma^\nu}{D}$

$\downarrow$

power law decay

$\downarrow$

Non Fermi liquid

d) Coupling to other channels

- Potential V with a finite range

$\Downarrow$

Phase shifts δ_ℓ' in other channels

The hybridization produces a discontinuity

$\delta_\ell = 2\delta_\ell'$ in the phase shift

- Infrared catastrophe in the $\ell \neq$ channels without injection of a carrier

$\downarrow$

$$2g = \left(1 + \frac{\delta_0}{\pi}\right)^2 + \sum_\ell (2\ell+1)\frac{\delta_\ell^2}{\pi^2} - 1$$

$\downarrow$

$$\beta = 1 - \frac{2\delta_0}{\pi} - \frac{\delta_0^2}{\pi^2} - \sum_\ell (2\ell+1)\frac{\delta_\ell^2}{\pi^2}$$

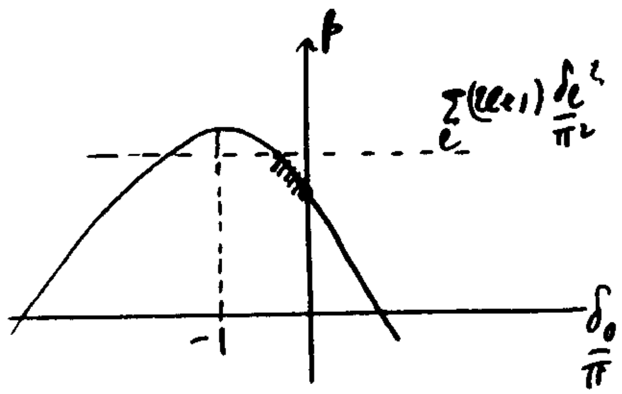
Other channels enhance non Fermi liquid behaviour

$\Downarrow$

It can occur even for a repulsion

$\Downarrow$

Unlikely!

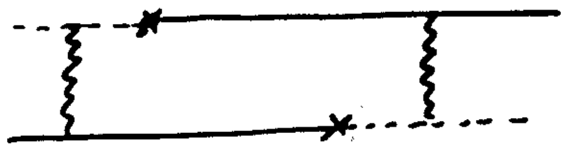


Note: Spin may be a channel index if there is no $V n_{d\uparrow} n_{d\downarrow}$ on the d impurity

3) Renormalization of V ?

↓

does it affect the transition ?



↓

Mapping to a Kondo problem:

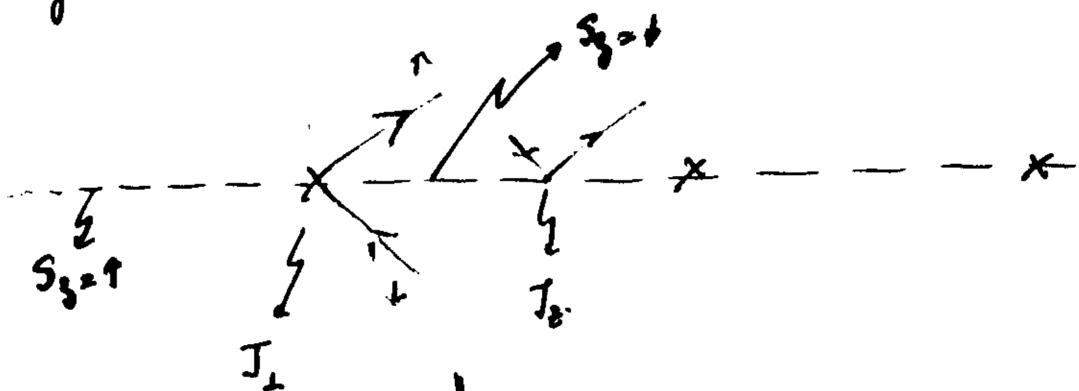
(SCHLOTTMANN, WIEGMANN + FINKELSTEIN)

in reverse

$$H = t_{ij}\, c^{+}_{i\sigma} c_{j\sigma} + J_z S_z (\sigma_z)_{\sigma\sigma}\, c^{+}_{0\sigma} c_{0\sigma}$$

$$+ \frac{J_\perp}{2} \left\{ S_+ (\sigma_-)_{\sigma\sigma'} + S_- (\sigma_+)_{\sigma\sigma'} \right\} c^{+}_{0\sigma} c_{0\sigma'}$$

Long time approximation → ANDERSON + YUVAL



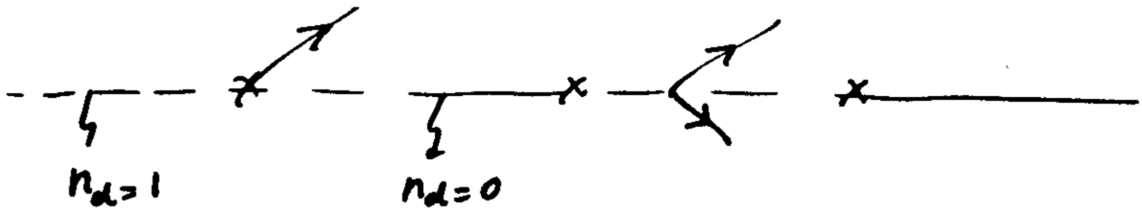
↓

$$\left[\text{Cauchy determinant} \right]^{n}$$

$$n = \underbrace{2}_{\text{for spin}} \left[1 + \frac{\delta}{\pi} \right]^{2}$$

$\delta = 2\delta'$ is the phase shift discontinuity upon spin flip

To be compared to the resonant level problem



$$\downarrow$$

$$\left[\text{Cauchy determinant}\right]^n$$

$$n = \left[1 + \frac{\delta}{\pi}\right]^2$$

$$\downarrow$$

<u>Same problem</u>

(i) Alternate flip between <u>two</u> states

$S_z = \uparrow, \downarrow$ in Kondo	$n_d = 0, 1$ in resonant level

(ii) Discontinuity of phase shift at each flip

δ_K	δ_R.

$$\Downarrow$$

Isomorphism if $2\left[1 + \frac{\delta_K}{\pi}\right]^2 = \left[1 + \frac{\delta_R}{\pi}\right]^2$

$$\Downarrow$$

$$\frac{\delta_R}{\pi} = \sqrt{2} - 1 + \frac{\delta_K}{\pi}\sqrt{2}.$$

$\delta_R = 0$ corresponds to the "Toulouse limit" in the Kondo problem ⇓ Soluble model	$\delta_K = 0$ corresponds to the transition between Fermi and non Fermi liquid in resonant level

BEWARE : The isomorphism is approximate

a) The Schlottmann formulation
(Equivalent to a Born approximation to δ_R, δ_K)

Kondo : bosonization of charge and spin fluctuations
↓
S couples only to spin fluctuations
↓
Two level system coupled to a single field
↓
Resonant level model

⇓

Precise mapping of coefficients

spin density at site 0

$$\cancel{H_K = \varepsilon_k C^*_{k\sigma} C_{k\sigma} + \frac{J_{\perp 0}}{2}\left[S^+ s_0^- + S^- s_0^+\right] + \sum_\ell J_{z\ell}\, S_z\, s_{z\ell}}$$

$\downarrow$

<u>Identification</u>

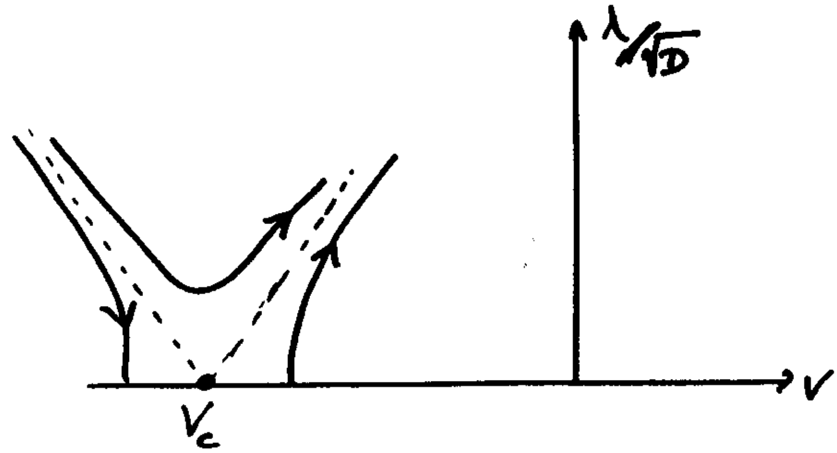
$$\begin{cases} S^+ \to d^* \quad , \quad S_z \to \left[d^* d - 1/2\right] \\ J_{\perp 0} \to \lambda \quad , \quad J_{z0} \to V_0 \sqrt{2} + 2\pi v_F \left(\sqrt{2} - 1\right) \\ J_{z\ell} \to V_\ell \sqrt{2} \end{cases}$$

(Note the shift in V_0)

(i) <u>Second order scaling</u>

$$\begin{cases} \dfrac{\partial J_{\perp 0}}{\partial \log D} = - J_{z0} J_{\perp 0} \\[2ex] \dfrac{\partial J_{z0}}{\partial \log D} = - J_{\perp 0}^{\,2} \\[2ex] \dfrac{\partial J_{z\ell}}{\partial \log D} = 0 \end{cases}$$

(Valid only near V critical)



Remarks

(i) The simple calculation corresponds to $\lambda \to 0$

(ii) The mapping holds near V_c

$$\frac{d\lambda}{d\log D} \sim -\lambda V \qquad \underline{\text{OK}}$$

$$\frac{dV}{d\log D} \sim -\lambda^2 \qquad \underline{\text{No}} \qquad \left(-\lambda^2 V \to -\lambda^2 V_c\right)$$

(iii) E_d acts as a magnetic field on the equivalent Kondo problem $\rightarrow$ stopped renormalization

(iv) The other channels do not affect the line of fixed points $J_\perp \sim \lambda = 0$

Question: is the strong coupling limit an attractive fixed point in the multi channel case ? (?)

Higher order scaling

- The expansion in J_{z0}, $J_{z\ell}$ generates the phase shifts δ_ℓ and the δ_ℓ^2 terms

- The expansion in $J_{\perp 0}^2$ is uncontrolled

  ↳ strong coupling fixed point

  ↳ Fermi liquid

- The influence of the other channels is unclear

  - limit of V_ℓ ?

  - Stability of the strong coupling fixed point ?

    ↳ anomalous fixed point at finite J as in multichannel Kondo effect ?

↓

currently studied

conclusion : { the one channel case is fairly clear

the multichannel case is still open

?

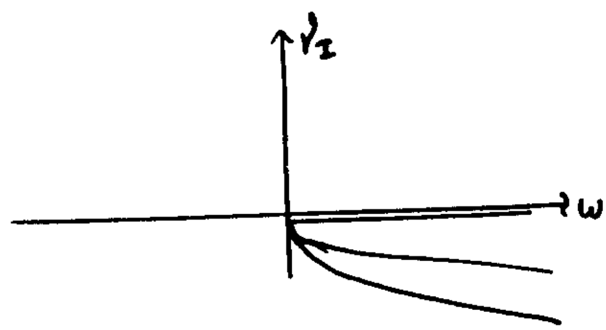
4) Physical implications in non Fermi liquid case

a) Residual entropy at $T=0$: $S_0 = \log 2$

b) Total impurity density of states
(on "d" and on "s" orbital)

$$\begin{cases} \delta(\omega) = -\operatorname{Arctg}\left[\frac{\Delta(\omega)}{\omega}\right] \approx -\frac{\Delta(\omega)}{\omega} \\ \nu_I = \frac{1}{\pi}\frac{\partial \delta}{\partial \omega} = \frac{\Delta - \omega\Delta'}{\omega^2} \end{cases}$$

Assume $\Delta \approx \omega^{2g} \Rightarrow \nu_I = (1-2g)\,\omega^{2g-2}$



$\downarrow$

$C_{vI} \sim -T^{2g-1}$

?

c) Resistivity

Conduction electron self energy $\Sigma = \lambda^2 G_d = \frac{\lambda^2}{\omega - i\Delta} \approx \omega^{2g-1}$

$\downarrow$

$\rho(T) \sim T^{2g-1} + \text{const}$

5) Extension to spin ½ fermions

- Numerical work (VARMA, RUCKENSTEIN, PERAKIS)

Electron hole Symmetry

$\varepsilon_d = 0$

$\Downarrow$

Similar Behaviour past V_c

No electron hole symmetry

$\varepsilon_d \neq 0$

$\Downarrow$

Two stable Fermi liquid fixed points, with a quantum transition in between (in the mixed valence region)

$$H = \varepsilon_k C^*_{k\sigma} C_{k\sigma} + \varepsilon_d n_d + U[n_{d\uparrow} - ½][n_{d\downarrow} - ½]$$

$$+ \lambda \left[d^*_\sigma C_{o\sigma} + C^*_{o\sigma} d_\sigma \right] + V[n_d - 1][n_o - 1]$$

(If $U=0$, spin is a channel index!)

- Classification by looking at strong coupling limit

$D = 0 \Rightarrow$ One site problem.

$\hookrightarrow$ 16 states, $E_n[\varepsilon_d, U, V, \lambda]$

Ground state singlet : Fermi liquid

Ground state multiplet : anomalous behaviour if attractive fixed point

Conclusion : In order to identify eligible

low temperature fixed points :

look at strong coupling
one site limit

(i) Choice of ground states

(ii) Relevant operators in its vicinity

(iii) Stability of these operators

$\hookrightarrow$ systematic classification

(cf Kondo !)

Motion of heavy particles in a metal

(e.g., muons in Cu)

$$H = \lambda\, d_i^* d_j + \underbrace{H_0}_{\text{conduction electrons}} + V$$

interaction ∼ un corps.

$$d_i^* d_i \; V_q \; C_k^* C_{k+q}\, e^{iqR_i}$$

$$= \sum_n V(R_i - r_n)$$

(As if new, no spin)

λ makes the particle hop

↳ inelastic scattering, edge singularity

1) Elastic scattering

$|\Psi_0(i)\rangle$ = ground state of electron gas when particle is at i

↓

renormalized "Mössbauer" amplitude

$$\lambda \langle \Psi_0(i) | \Psi_0(j) \rangle$$

Discontinuity of potential

↳ electron hole pair excitations

&

orthogonality catastrophe

$$\langle \Psi_0(i) | \Psi_1(j) \rangle = \frac{1}{N^{K}}$$

exponent depending on V and on separation $|R_i - R_j| = a$

K may be obtained { perturbatively

↳ log N singularities : KONDO, 1978.

exactly (with errors!) YAMADA et al

~~[illegible]~~

2) K may be obtained exactly calculating a determinant (à-la Anderson)

↳ It is simpler to calculate the ~~[illegible]~~ transition probability for hopping

$$\nu = 2\pi \sum_f \lambda^2 |\langle \Psi_0(i) | \Psi_f(j) \rangle|^2 \delta[E_f - E_0]$$

final state with particle at j

2nd order perturbation theory

We may write

$$\nu = 2\lambda^2 \mathrm{Re} \int_0^\infty dt \; |\langle \Psi_0(i) | \Psi_f(1) \rangle|^2 e^{i(\mathcal{E}_f - \mathcal{E}_0)t}$$

$$\downarrow$$

$$\boxed{\begin{aligned} \nu &= 2\lambda^2 \mathrm{Re} \int_0^\infty dt \; \mathcal{G}(t) \\ \mathcal{G}(t) &= \langle \Psi_0(i) | e^{i(H_f - H_i)t} | \Psi_0(i) \rangle \end{aligned}}$$

Note the resemblance with the X-ray edge problem.

Remarks : if $V = 0$, $H_f = H_i = H_0$

$$\downarrow$$

$$\mathcal{G} = 1$$

ν is infinite : the states at i and f are degenerate

It is inelastic processes that provide a finite mobility

- When calculating $\mathcal{G}(t)$, transient potential $\overline{V} = V_f - V_i$ between times 0 and t

  ↳ structureless perturbation : EXPONENTIATION closed loop

$\longleftarrow - - - (14) - - - \longrightarrow \qquad \mathcal{G}(t) = e^{C}$

In lowest order, and for a constant potential

$V_i - V_j \qquad V_i - V_j$

$$C = \int_0^t d\tau\, d\tau' \left(g_{ii} + g_{jj} - g_{ij} - g_{ji}\right)^2$$

C involves non local propagators

$$\downarrow$$

$$\mathcal{G} \sim \frac{1}{(Dt)^{2K}} \qquad \text{(squared matrix element)}$$

- At temperature T, the time integral will be cut at

$t \sim \frac{1}{T}$

$$\boxed{\nu \sim \frac{\lambda^2}{D}\left[\frac{T}{D}\right]^{2K-1}}$$

upper cut off.

Result first obtained by Kondo

$\downarrow$

Precise coefficients of Yamada (irrelevant: D is qualitative)

3) Calculation of K (spinless electrons).

(Via orthogonality exponent or via $G(t)$: (OK))

↓

- Transient Muskhelishvili problem with a 2×2 structure

$$\begin{pmatrix} G^{11} & G^{12} \\ G^{21} & G^{22} \end{pmatrix}$$

Same difficulties as for Raman scattering: the G-matrices do not necessarily commute

↳ standard method fails

- But here, the 2×2 matrix is diagonalized by a time independent transformation

↳ two decoupled contributions to C

Detailed algebra painful.

- The calculation is carried in a very simple case

↓

$\boxed{\text{Swave scattering only} \rightarrow \text{phase shift } \delta}$

(Extension to several channels non trivial, as they are coupled by the breakdown of rotational invariance.)

The new ingredient is $g_{12}(t) = \sum_k e^{i\vec{k}.\vec{a}}\, e^{-i\varepsilon_k t}$

free propagator

For long times, only k near the Fermi surface matter

$\downarrow$

angular average on $\vec{k}_F$

$\downarrow$

$$\boxed{g_{12}(t) = \underbrace{J_0(k_F a)}_{=\,x}\, g_{11}(t).}$$

x is a constant independent on t

- The rest of the algebra is messy, but straightforward.

$$\boxed{K(x,\delta) = \left\{\frac{1}{\pi}\,\mathrm{Arctg}\left[\frac{\sqrt{1-x}\ \mathrm{tg}\,\delta}{\sqrt{1+x\,\mathrm{tg}^2\delta}}\right]\right\}^2}$$

Result valid if $|\delta| < \pi/2$ (convergent series)

Outside this range, proceed by continuity

$\frac{\pi}{2} < \delta < \pi$?

$$K(x,\delta) = \left\{\frac{2}{\pi}\,\mathrm{Arctg}\sqrt{\frac{1-x}{x}} - \frac{1}{\pi}\,\mathrm{Arctg}\left[\frac{\sqrt{1-x}\ |\mathrm{tg}\,\delta|}{\sqrt{1+x\,\mathrm{tg}^2\delta}}\right]\right\}^2$$

Only results for $|\delta| < \frac{\pi}{2}$ are really to be trusted

4) Discussion of results

- $\boxed{x=1}$ (i.e. $a=0$).

  ↳ $\boxed{K=0}$: no discontinuity of potential and no edge singularity

- $\boxed{x=0}$ (remote impurities).

  $$\boxed{K=\frac{\delta^2}{\pi^2}}$$

  - The suppression of the potential at site i
    ↳ contribution $K_i=\frac{\delta^2}{2\pi^2}$
    (see first lecture)
  - Same contribution for the creation of a potential at site j
  - No interference

- If one restores spins, K is doubled (two spin channels)

  ↳ $K_{max}=\frac{1}{2}$ for $\delta=\pi/2$.

Extension to higher phase shifts implies the presence of bound states

↳ possibility to have $K>1$?

5) Low temperature cut off and localization

- Poor man's scaling

↓

Reduction of hopping amplitude

$$\lambda \to \lambda \left(\frac{D'}{D}\right)^{K} = \lambda'$$

All right if new cut off D' remains $> \lambda'$

(otherwise, blurring of singularity due to recoil)

↓

- Two regimes (as in the resonant level case)

$K < 1$

λ decreases less fast than D ($\sim T$)

↓

Natural cut off when

$$\lambda' \sim D' \sim T^*$$

$$\frac{T^*}{\lambda_0} = \left(\frac{T^*}{D_0}\right)^{K}$$

$$T^* = \left[\frac{\lambda_0}{D_0^{K}}\right]^{1/1-K}$$

$K > 1$

λ decreases faster than D

↓

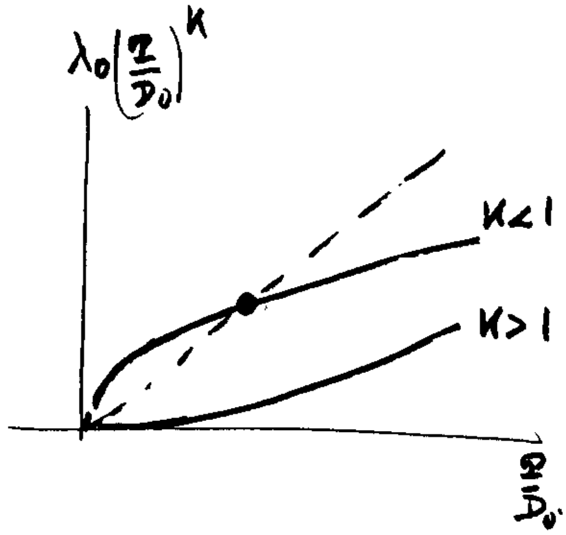
Scaling down to $T = 0$

↓

Hopping stops at $T = 0$

$\boxed{\text{LOCALIZATION}}$

Geometrical representation



For an s wave scatterer with no bound states, $K < 1/2$

↓

Apparently no localization
But strange power laws.

• Actual discussion of hopping rate
↓
Much more delicate than the simple 2^{nd} order calculation

⇓

Phase coherence problems
Transition between band conduction and incoherent hopping

⇓

Density matrix formulation (Yu. KAGAN)
Many different regimes
Outside the scope of these lectures

Note the analogy with the resonant level problem

(Here, degeneracy ($E_d = 0$) is ensured by <u>translational invariance</u>)