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

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

LECTURES 3 AND 4

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These are preliminary lecture notes, intended only for distribution to participants.

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Kondo effect

EFFET KONDO "CLASSIQUE"

1) Généralités

- Une impureté de spin S – pas de dégénérescence orbitale

$$H = \varepsilon_k C^*_{k\sigma} C_{k\sigma} + \left[V_{kk'} \delta_{\sigma\sigma'} + J_{kk'} \vec{S} \cdot \vec{s}_{\sigma\sigma'} \right] C^*_{k\sigma} C_{k'\sigma'}$$

↳ Matrices (1/2 – 1/2)

Paramètres { densité d'états ρ (un spin) – Coupure D
Couplages V et J (~ $\frac{\text{énergie}}{N}$ N nombre de mailles)

- Si on bloque le spin S, déphasages $\delta_{\parallel}$ et $\delta_{\#}$ pour un électron de conduction. On élimine V en prenant comme base des états de diffusion tels que $\delta^* = \frac{1}{2} [\delta_{\parallel} + \delta_{\#}]$

↳ { $\tilde{V} = 0$, $\tilde{J} = J \cos^2 \delta^*$ ($C^*_{i\sigma} \to \eta_i C_{i-\sigma}$)
Symétrie "électron-trou" : $\tilde{\delta}_{\parallel} = -\tilde{\delta}_{\#}$

On supprime V et on mesure les déphasages depuis δ^*.

- En réalité, $\vec{S}$ fluctue → amplitude de diffusion "spin flip"

$$\tau = J + \rho J^2 \operatorname{Log} \frac{D}{T} + \cdots$$

singularité logarithmique

↳ Minimum de résistance lorsque $J > 0$ (couplage antiferromagnétique)

— Singularités analogues dans toutes les quantités physiques — par exemple la susceptibilité de spin

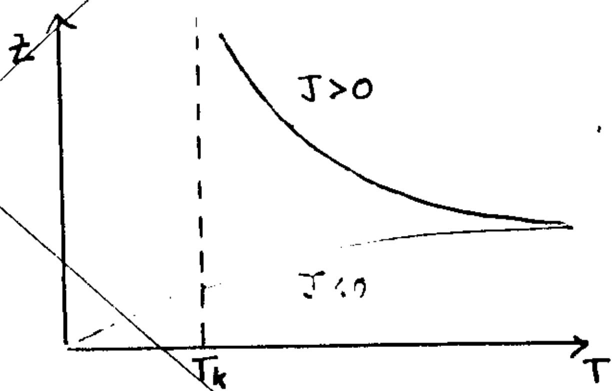
$$\begin{cases}\Delta\chi = \dfrac{\mu^2}{T}\left[1 - \rho J - \rho^2 J^2 \log\dfrac{D}{T} + \dots\right] \\ \mu^2 = (g\beta)^2\, \dfrac{S(S+1)}{3}\end{cases}$$

réduction du moment μ

↳ Température caractéristique $\boxed{T_K = D e^{-1/\rho J}}$

— Un développement de perturbation brutal est du type $(\rho J)^m \left(\log\frac{D}{T}\right)^n$. On sait sommer les termes les plus divergents, $m = n$ (ABRIKOSOV, 1965)

$$z = \rho\tau = \frac{\rho J}{1 - \rho J \log\frac{D}{T}}$$



Pour un couplage antiferro, divergence factice à T_K

↳ Termes suivants nécessaires !

(ii) Perturbation approaches

- originally, summation of the most divergent diagrams
  Abrikosov (1965)

$$(\rho J)^m \left(\log \frac{D}{T}\right)^n \Rightarrow m=n \text{ terms} \qquad J_{eff} = \frac{J}{1-\rho J \log \frac{D}{T}}$$

{ Summation of "parquet diagrams", which can be pushed to next order (PW 1968) : awkward

- Physical Breakthrough of Anderson + Yuval.

$$H = \underbrace{J_\perp \, S_\perp \cdot s_\perp}_{\text{flip}} + \underbrace{J_{\parallel} \, S_z s_z}_{\text{alternating potential } \pm J/4 \text{ on spins } \uparrow \text{ and } \downarrow}.$$

↓

perturbation expansion in $J_\perp$

"history"

(α) For a given history, typical recurrent x-ray edge problems.

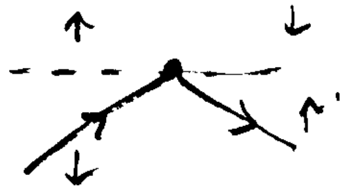
$\boxed{J_z = \text{flipping potential}}$

↑ and ↓ closed loops

↓

$U(t) \sim e^{C_\uparrow + C_\downarrow} L_\uparrow L_\downarrow$

Two open lines at each vertex



It is more convenient to calculate the partition function
Consider for instance the contribution of open lines

n vertices $(\uparrow \downarrow)$ and n vertices $(\downarrow \uparrow)$, alternating
t_i

• $J_z = 0$

- Each line goes from a $\underline{t_i}$ to a $\underline{t'_i}$ (spin conservation)
n lines : contribution $\sim \dfrac{1}{(t)^n}$

- Singularity whenever $t_i = t'_j$
$\hookrightarrow$ Product $\prod_{ij} \left[\dfrac{1}{t_i - t'_j}\right]$ n^2 factors

- Exchange symmetry $\rightarrow$ Vanishing if $t_i = t_j$ or $t'_i = t'_j$
(crossing of lines)

$\hookrightarrow$ $2 \cdot \frac{n(n-1)}{2}$ factors $\prod_{i<j} (t_i - t_j)(t'_i - t'_j)$
Uniqueness

$$\boxed{D_\uparrow = -\frac{\prod_{i<j} (t_i - t_j)(t'_i - t'_j)}{\prod_{ij} (t_i - t'_j)}}$$

poles if $t_i = t'_j$

zeroes if $t_i = t_j$ or $t'_i = t'_j$

- Same contribution for ↓ lines : $D_\uparrow D_\downarrow = D^2$ (3 ter)

••• J_z → multiple scattering of open lines
{ closed loop

$J_\perp$

open lines / closed loop

$1 - \frac{2\delta}{\pi} + \frac{\delta^2}{\pi^2}$

↓

X ray edge problem

$$D^2(t_i, t'_j) \to D^{2\left(1-\frac{\delta}{\pi}\right)^2}$$

↓

Summation for a given history of spins

(β) The next step is summation over histories
↳ far more difficult

↓

- Scaling trick (cut off τ)
  ↳ derive formulation easier

•• Mapping to a soluble case

$$2\left(1-\frac{\delta}{\pi}\right)^2 = 1$$

↳ resonant level problem (see later)

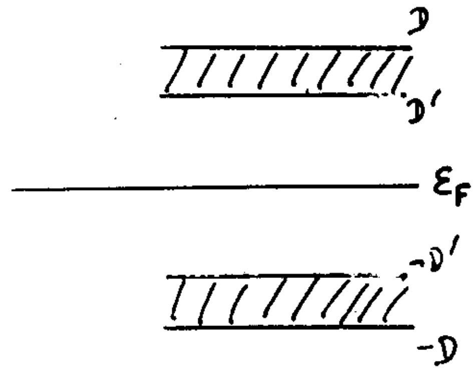
"Toulouse limit" → $\boxed{(100-\varepsilon)\%\ \text{exact solution}}$

Magnificent performance

./.

II Divergence logarithmique → RENORMALISATION

Le comportement asymptotique pour $T \ll D$ est UNIVERSEL, fonction de T/T_K, H/T_K



– Principe de la renormalisation

(i) Reduction de la coupure

$D \to D' \gtrsim T$

$\Downarrow$

Hamiltonien H_{eff} dans espace de Hilbert reduit

(ii) H_{eff} est compliqué $\begin{cases} \text{retardé} \\ \text{couplage multiélectrons} \end{cases}$, mais

piloté par deux variables lentes seulement, V et J.

La symétrie electron trou implique $V \equiv 0$

↳ un seul couplage "lent" : $z = \rho J$

$$\downarrow$$

$$\boxed{\frac{dz}{d\operatorname{Log} D} = \varphi(z)}$$

UNIVERSALITÉ

Si T_K correspond à $z = z_0$

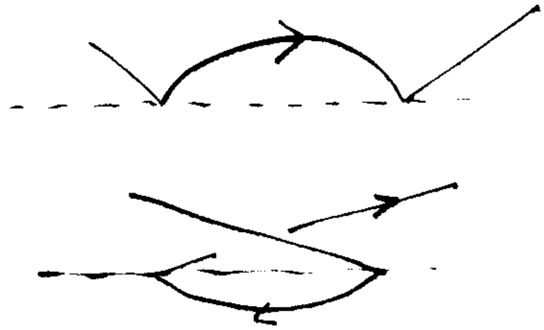
$\Downarrow$

$$\operatorname{Log} \frac{T}{T_K} = \int_{z_0}^{z} \frac{dz}{\varphi(z)}$$

POINT FIXE À $T=0$

z tend vers un zero attractif de $\varphi(z)$

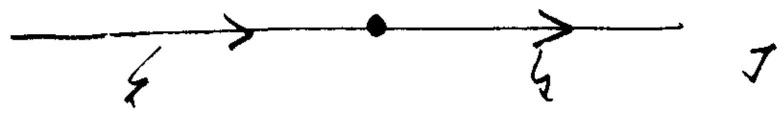
- Weak coupling: poor man's scaling



No compensation due to non commutativity of spins

Amplitude evaluated at Fermi level

$$\frac{dJ}{dD} = -\frac{\nu J^2}{D} \qquad \left(\frac{dg}{dD} = -\frac{g^2}{D} \right)$$



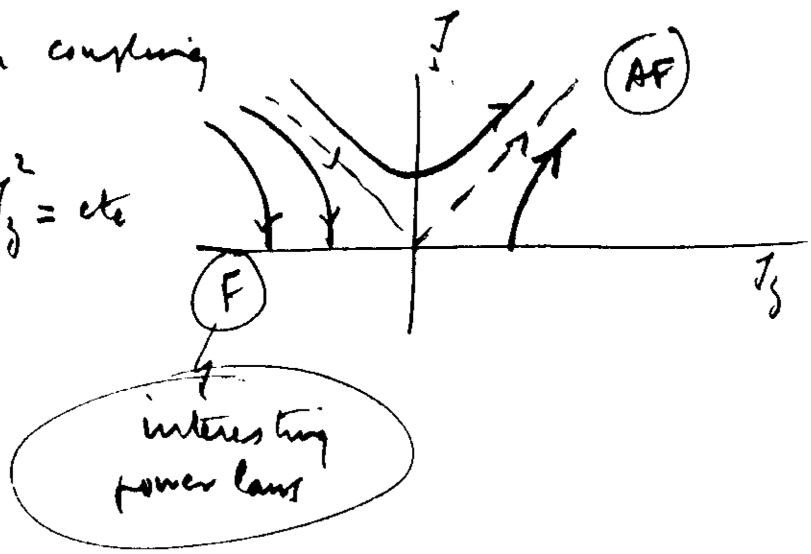
Ferro
↓
decoupled spin
(dangling degree of freedom)

Antiferro
↓
singlet of $S = 1/2$
(Fermi liquid)

All limits must be studied separately

- Generalization to anisotropic coupling

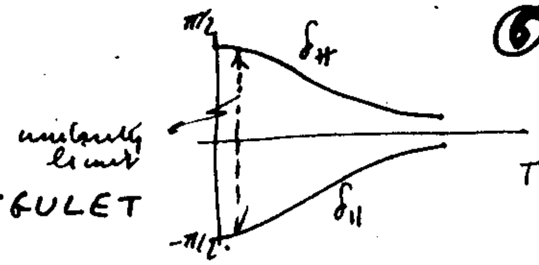
$$\left.\begin{aligned} \frac{dJ_\perp}{d\log D} &= -\nu J_\perp J_z \\ \frac{dJ_z}{\partial \log D} &= -\nu J_\perp^2 \end{aligned}\right\} \qquad J_\perp^2 - J_z^2 = cte$$



Antiferromagnetic case

III La limite du couplage fort

[redacted]



(i) Impureté + <u>un</u> électron $\longrightarrow$ SINGULET

Energie de liaison $\quad \mathcal{E}_s \sim J\cdot\rho D = \underset{(\to\infty)}{Z}\,\underset{(\to 0)}{D} \sim T_K$

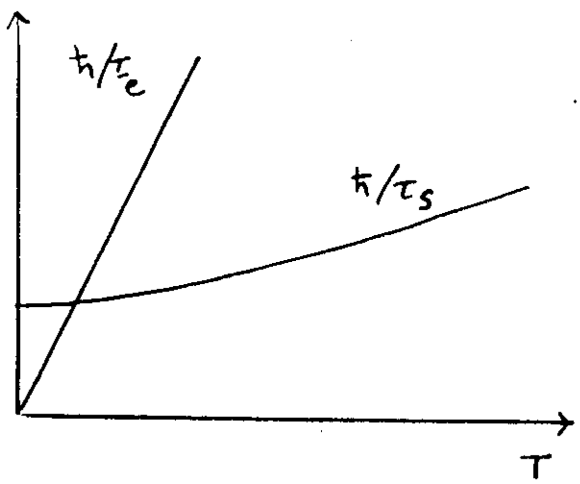
(ii) Singulet = diffuseur <u>non magnétique</u> et <u>impénétrable</u> pour les autres électrons

(iii) Mais singulet <u>polarisable</u> $\Rightarrow$ INTERACTION LOCALISÉE ENTRE ELECTRONS DE CONDUCTION

— Interprétation physique

Temps de fluctuation du spin $\quad \tau_s = \begin{cases} \dfrac{\hbar}{\mathcal{E}_s} & \text{pour } T \ll T_K \\[2ex] \dfrac{\hbar}{T(\rho J)^2} & \text{pour } T \gg T_K \text{ (KORRINGA)} \end{cases}$

Temps de passage d'un paquet d'ondes thermique sur l'impureté $\quad \tau_e = \dfrac{\hbar}{T}$



$T \gg T_K$, $\tau_e \ll \tau_s$

L'électron <u>voit</u> un spin instantané bien défini

$\left.\begin{array}{l} T \ll T_K \\ \tau_e \gg \tau_s \end{array}\right\}$ L'électron <u>voit</u> un spin moyen nul

— Description phénoménologique "liquide de Fermi" (4)

Déphasage δ_σ fonction $\begin{cases} \text{de l'énergie } \varepsilon \\ \text{de la distribution } n_{\sigma'}(\varepsilon') \end{cases}$ via local interaction

$$\underbrace{\delta_\sigma}_{} = \underbrace{\delta_0}_{\text{point fixe}} + \underbrace{\alpha\varepsilon + \varphi_{\sigma\sigma'}\,\delta n_{\sigma'}(\varepsilon')}_{\text{approche du point fixe}} \qquad (\delta n = n - n_0)$$

(i) La charge déplacée est $\Delta n = \dfrac{\delta_\uparrow + \delta_\downarrow}{\pi} \Rightarrow \underbrace{1}_{\text{singulet}} + \underbrace{2\dfrac{\delta_\uparrow}{\pi}}_{\text{Interaction résiduelle}}$

Donc $\delta_0 = \lim_{T\to 0} \delta_\uparrow = \delta^* - \frac{\pi}{2}$

(ii) $\begin{cases} \varphi_{\uparrow\uparrow} = 0 \quad \text{(principe d'exclusion)} \\ \varphi_{\uparrow\downarrow} = \varphi \text{ est fixé par l'UNIVERSALITÉ lorsque } T_K \ll D \end{cases}$

Singularité liée à $\varepsilon_F \implies \alpha + \rho_0\phi = 0$

↳ un seul paramètre $\alpha \sim \frac{1}{T_K}$ (échelle d'énergie)

⇓

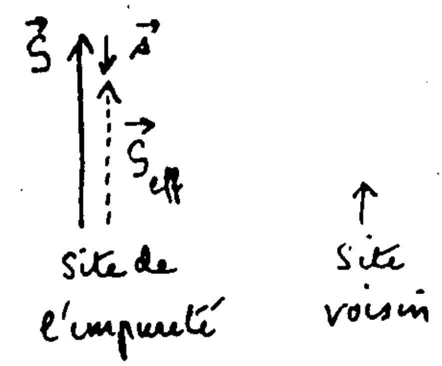
$$\begin{cases} \dfrac{\Delta C_V}{C_V} = \dfrac{\alpha}{\pi\rho} \quad , \quad \dfrac{\Delta\chi}{\chi} = \dfrac{1}{\pi}\left[\dfrac{\alpha}{\rho_0} - \phi\right] = 2\,\dfrac{\Delta C_V}{C_V} \\ \text{Résistivité contrôlée par processus élastiques et inélastiques} \quad \dfrac{R(T)}{R_0} = 1 - \pi^2\alpha^2T^2 \text{ si } \delta^* = 0 \end{cases}$$

CONCLUSION : le comportement à $T \ll T_K$ résulte de $\begin{cases} \text{SYMETRIE} \\ \text{UNIVERSALITÉ} \end{cases}$

⇓

Problème de raccordement $\qquad \boxed{\alpha = \dfrac{0{,}323}{T_K}}$ Solution numérique de WILSON

7) [redacted]ite du couplage fort : $S \neq \frac{1}{2}$



Un seul canal orbital

$\Downarrow$

Un seul électron piégé sur l'impureté

$\Downarrow$

Impureté habillée de spin $S_{eff} = S - \frac{1}{2}$

Le saut virtuel sur le site d'impureté donne un couplage résiduel $\vec{S}_{eff} \cdot \vec{s}$ ferromagnétique $J_{eff} = \frac{t^2}{J}$

Couplage AF fort avec $\vec{S}$ $\Longrightarrow$ Couplage F faible avec $\vec{S}_{eff}$

— La transition se fait pour $D \sim T \sim T_K$. On a alors

$$\rho D \, J_{eff} \sim -\frac{D^2}{\varepsilon_s} \sim -T_K$$

$\longrightarrow \rho J_{eff} \sim 1$ pour $D \sim T_K$

— Pour $T \ll T_K$, $J_{eff} = -0$ est un point fixe stable

~~$\rightarrow$ comportement logarithmique en $\log \frac{T}{T_K}$ (ici < 0)~~

~~Impureté $\vec{S}_{eff}$ découplée à $T=0$~~

~~$\rightarrow$ dégénérescence 2S~~

~~susceptibilité de Curie~~

~~— Ici encore, comportement simple pour $T \gg T_K$, $T \ll T_K$~~

· Seul problème : raccorder les définitions "haute" et "basse" de T_K.

(IV) Ferromagnetic Kondo effect:

less studied – but actually it is far more interesting

non Fermi liquid behaviour

- Isotropic case ($J_0 < 0$)

$$\frac{d\,J}{d\log D} = -\nu J^2 \quad \rightarrow \quad J = \frac{J_0}{1 - \nu J_0 \log \frac{D}{D_0}}$$

Same cross over temperature $T_K \sim D_0 \exp\left[-\frac{1}{\nu |J_0|}\right]$

At $T \ll T_K$, $\nu J \sim -\frac{1}{\log \frac{D}{D_0}}$ with $D = \max(T, H)$

(i) Susceptibility

$$\Delta\chi = \frac{\mu^2}{T}\left[1 - \nu J_{eff}\right] \rightarrow \boxed{\Delta\chi = \frac{\mu^2}{T}\left[1 + \frac{1}{\log \frac{T}{T_K}}\right]}$$

if $H \ll T \ll T_K$

In high field

$$\boxed{\frac{M}{\mu} = 1 + \frac{1}{2\log \frac{H}{T_K}}}$$

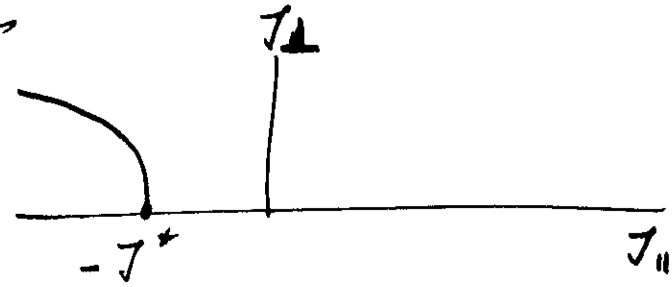
$$\chi \sim \frac{\mu_{eff}^2}{T}$$

(ii) <u>Specific heat</u> : more complicated (Kondo)

$$S = \log(2S+1) - \frac{cte}{\log(T/T_K)^3}$$

$\downarrow$

$\left\{ \begin{array}{l} \text{decoupled magnetic impurity} \\ \text{logarithmic corrections} \end{array} \right.$



• <u>Anisotropic case</u> :

$J_\parallel$ remains finite

• $J_\perp^2 = J_\parallel^2 - J^{*2} \Longrightarrow \left\{ \begin{array}{l} J_\perp = J^* \,\mathrm{sh}\, y. \\ J_\parallel = - J^* \,\mathrm{ch}\, y. \end{array} \right.$

$x = \log \frac{D_0}{D}$

$$\left. \begin{array}{l} \dfrac{dJ_\perp}{d\log D} = -\nu J_\perp J_\parallel \\[2ex] \dfrac{dJ_\parallel}{d\log D} = -\nu J_\perp^2 \end{array} \right\} \Rightarrow \boxed{\frac{dy}{dx} = -\nu J^* \,\mathrm{sh}\, y.}$$

$\downarrow$

straightforward integration

$\downarrow$

$$\mathrm{th}\,\frac{y}{2} = e^{-\nu J^* x}$$

$\downarrow$

$$\boxed{\begin{array}{l} J_\parallel = - J^* \coth \nu J^* x. \\ J_\perp = J^* / \mathrm{sh}\, \nu J^* x. \end{array}}$$

(13)

At these lower temperatures

$$J_\perp \simeq 2J^2 e^{-\nu J^2 x} = \boxed{2J^* \left(\frac{D}{D_0}\right)^{\nu J^*} = J_\perp}$$

We recover power laws with exponents that depend on the coupling

---

(V) Treatments of the crossover region for antiferromagnetism

Main difficulty → successively simpler formulations

↳ complete description of $T \sim T_K$

matching of low and high T expansions

$$\underset{\text{Fermi liquid}}{\alpha} = \underset{(?)}{cte} / \underset{\text{from perturbation expansion}}{T_K}$$

~~[illegible]~~ Numerical approach of Wilson

- Construction of infinite system as an "onion"

↳ iteration scheme for lowest eigenstates

↳ numerical coefficients

Powerful, but elaborate. Has been extended to many other systems (2 impurities, resonant level, etc.....)
Not very enlightening

~~(i)~~ Ansatz de Bethe → brief outline

- Problem basically 1d

$$k \to \begin{cases} l = 0 \\ \text{energy } |k| \end{cases}$$: two, outgoing and ingoing, modes for each energy

$$H = \sum_{\substack{k \\ \downarrow \\ \text{modulus}}} \varepsilon_k \, c^{*}_{k0\sigma} c_{k0\sigma} + \sum_{kk'} J \vec{S}.\vec{s}_{\sigma\sigma'} \, c^{*}_{k0\sigma} c_{k'0\sigma'} \, \frac{\nu}{\nu_0}$$

ν = total density of states
ν_0 = s-wave density of states } preserves normalization

- May replace ingoing and outgoing waves for $r > 0$ by right moving waves for $x > 0$ (outgoing) or < 0 (ingoing)

↓

$\boxed{\text{Reflection = phase shift at origin}}$

↓

really 1d problem with one side of Fermi surface

- The spectrum is linear, with a Fermi velocity v_F

$$\varepsilon_k - \mu = v_F (k - k_F)$$

↓

$$\frac{H}{v_F} = \int dx \left[\psi^{*}_{\sigma}(x) \left(-i\frac{\partial}{\partial x}\right) \psi_{\sigma}(x) + \rho J S.s_{\sigma\sigma'} \psi^{*}_{\sigma}(x) \psi_{\sigma'}(x) \delta(x) \right]$$

The Schrödinger eq. is first order → trivial phase shifts

- Then construct a wave function with given wave vectors, and careful combination of phase shift and spin index permutations at the origin, preserving antisymmetrization

↳ Trivial for 2 electrons
Not obvious for N electrons
(factorization condition)

↓

Elaborate formulation for professionals

Important issue: particles follow each other at velocity v_F: they only interact indirectly via the spin at origin
↳ "memory mechanism"

↓

- Analytical results at $T = 0$, $\forall H$
- Numerical results at finite T
- Expansions for $T \gg T_K$ or $T \ll T_K$

Useful, but not very enlightening

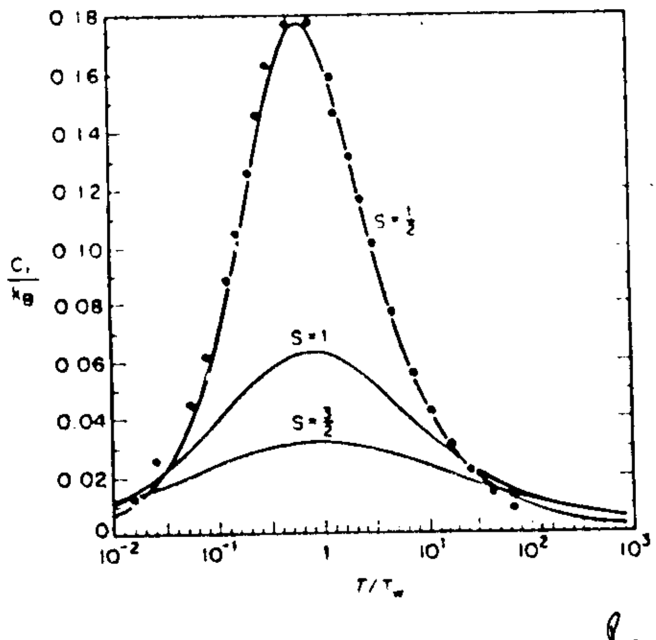
Résultats : ils confirment entièrement l'analyse qualitative

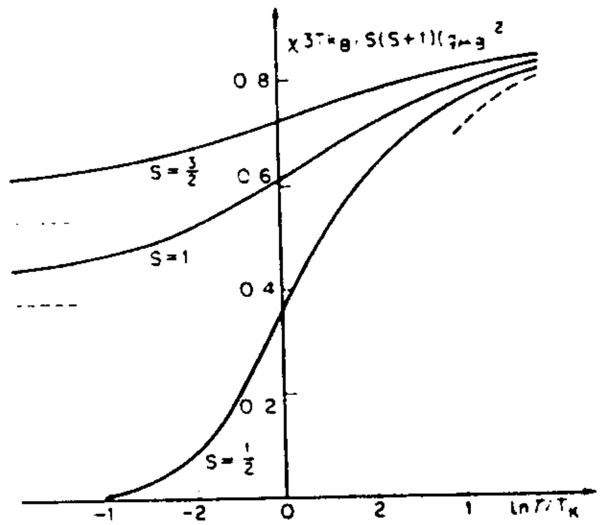
$\boxed{T \gg T_K}$ Développement pour un spin S en $\varepsilon = \left[\text{Log}\,\frac{T}{T_K}\right]^{-1} > 0$

$\boxed{T \ll T_K}$ $\begin{cases} \text{Résultat analytique en } T \text{ si } S = \frac{1}{2} \quad (\text{SINGULET}) \\ \text{Développement en } \varepsilon = \left[\text{Log}\,\frac{T}{T_K}\right]^{-1} < 0 \text{ pour un spin } (S-\frac{1}{2}) \\ \quad \text{si } S \geq 1 \end{cases}$

- Ils fournissent la valeur de α : accord avec WILSON

- Ils décrivent la région de transition





Beware : Log scales !!

Les points sont les résultats numériques du calcul à la WILSON (WILKINS et al)

L'asymptote correspond à $3\chi T = (S-\frac{1}{2})(S+\frac{1}{2}) = S^2 - \frac{1}{4}$

spin $S=1/2$

~~(iii) Bosonization~~ Very popular nowadays, as it is compact and easy to use (once again, copied on 1d systems, equivalent to Tomonaga-Luttinger liquids).

P. SCHLOTTMANN J. de Phys. C6 1486 (1978).

(a) Start from 1d equivalent system

↓

Fermion fluctuations = density fluctuation with boson operator

$$b^*_{q\sigma} = \sqrt{\frac{2\pi}{q}} \sum_k c^*_{k\sigma} c_{k-q\sigma}$$

↓

$$\varphi^*_\sigma(x) = -i \sum_q \sqrt{\frac{2\pi}{q}}\, b^*_q\, e^{iqx}$$ Bose field in x space.

⇓

$$\boxed{\psi_\sigma(x) = e^{-i\varphi^*_\sigma(x)}\, e^{i\varphi_\sigma(x)} \times \text{const}}$$

(Describes the excitation of density fluctuations when a particle is created)

~~↓ C of $\varphi_\sigma(x)$~~

~~Decomposition into charge density fluctuations → completely decoupled~~

~~spin density fluctuations → coupled to impurity~~

In this way, the exchange coupling is expressed in terms of Boson fields

$J_\parallel$ (no spin flip) couples linearly to $\frac{\partial \varphi}{\partial x}$ at $x = 0$

$J_\perp$ couples S_+ and S_- to $\cos[\varphi(0)]$ and $\sin[\varphi(0)]$

From then on, one can play the game of unitary transformations

$\boxed{\text{Emery, Kivelson}}$

(b) Qualitatively, one decomposes $\varphi_\sigma(x)$ in a charge and a spin

$$\varphi_c = \varphi_\uparrow + \varphi_\downarrow \quad , \quad \varphi_s = \varphi_\uparrow - \varphi_\downarrow$$

φ_c decouples entirely from the problem.

Problem with φ_s only

One may then play the bosonization game in reverse

one field $\varphi_s \rightarrow$ fictitious spinless fermions γ^*

Effective Hamiltonian

$$H = k v_F \gamma_k^* \gamma_k + A\left(S^+ \underset{\text{(site 0)}}{\gamma_0} + S^- \gamma_0^*\right) + \frac{B S_z}{2}\left[\gamma_0^* \gamma_0 + \gamma_0 \gamma_0^*\right]$$

A and B are constants that are related to $J_\perp$ and $J_\parallel$ in a non trivial way (shift → $J_\perp = J_\parallel = 0$ is not $A = B = 0$)

Route followed by Schlottmann in 1978 : ahead of its time

(c) If now $S^- = d$, $S^+ = d^*$, $S_z = d^*d - 1/2$,

then the Hamiltonian becomes.

$$\boxed{H = \hbar v_F \, \gamma_k^\dagger \gamma_k + A\left(d^* \gamma_0 + \gamma_0^\dagger d\right) + B\left(d^* d - \tfrac{1}{2}\right)\left(\gamma_0^* \gamma - \tfrac{1}{2}\right)}$$

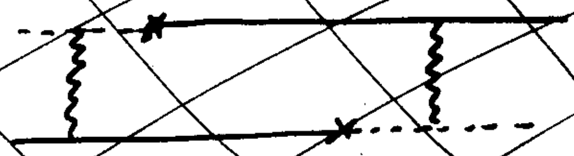
. The Kondo problem has been transformed into a spinless resonant impurity level with interactions between the d orbital and the local band orbital

Spin fluctuations ⟷ charge fluctuations

The isomorphism is approximate, but physically faithful. (Bethe Ansatz is exact)

(d) In the framework, the isomorphism is better understood in another language, which explains the shift of origin

~~3) Renormalization of V ?~~



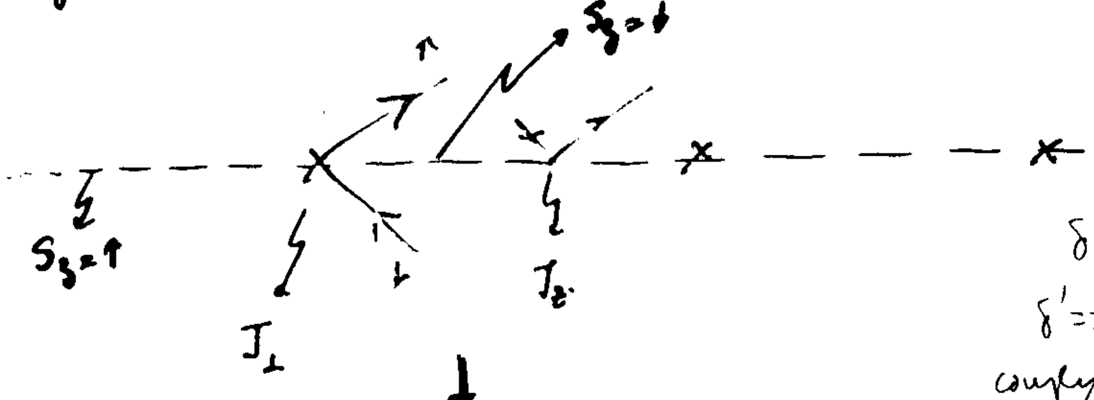
~~does it affect the transition ?~~

Mapping to a ~~[illegible]~~ Resonant level problem:

(SCHLOTTMANN, WIEGMANN + FINKELSTEIN)

$$H = t_{ij}\, c^{+}_{i\sigma} c_{j\sigma} + J_z\, S_z\, (\sigma_z)_{\sigma\sigma'}\, c^{+}_{0\sigma} c_{0\sigma'}$$
$$+ \frac{J_\perp}{2} \left\{ S_+ (\sigma_-)_{\sigma\sigma'} + S_- (\sigma_+)_{\sigma\sigma'} \right\} c^{+}_{0\sigma} c_{0\sigma'}$$

Long time approximation → ANDERSON + YUVAL



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

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

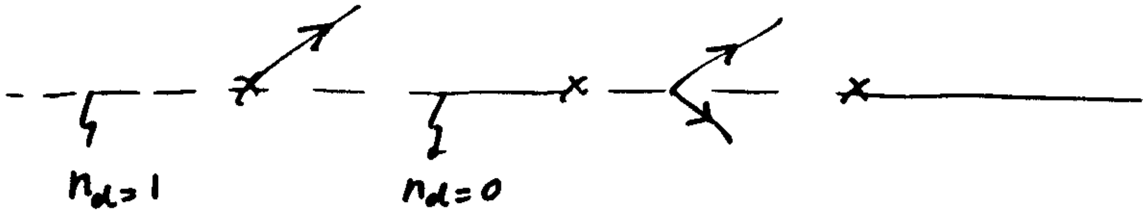
for spin

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

$\delta = \pi$ means $\delta' = \pi/2$: infinite coupling J_z

singlet formation no more scattering : OK

To be compared to the spinless resonant level problem



$$\Downarrow$$

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

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

$$\downarrow$$

Same problem

(i) Alternate flip between two 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 $\quad 2\left[-1 + \frac{\delta_K}{\pi}\right]^2 = \left[-1 + \frac{\delta_R}{\pi}\right]^2$

$$\Downarrow$$

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

* Approximate Solution of Anderson

$\delta_R = 0$ corresponds to the "Toulouse limit" in the Kondo problem

$\Downarrow$

Soluble model

$\delta_K = 0$ corresponds to the transition between Fermi and non Fermi liquid in resonant level

BEWARE : The isomorphism is approximate

e) The Schlottmann formulation

(Equivalent to a Born approximation to δ_R, δ_K)

~~Kondo : bosonization of charge and spin fluctuations~~

~~$\downarrow$~~

~~S couples only to spin fluctuations~~

~~$\downarrow$~~

~~Two level system coupled to a single field~~

~~$\downarrow$~~

~~Resonant level model~~

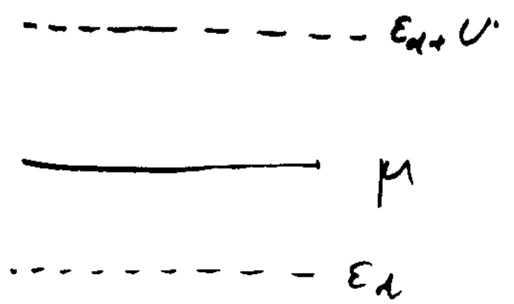
~~$\Downarrow$~~

~~Precise mapping of coefficients~~

(iv) Mean field slave boson approaches

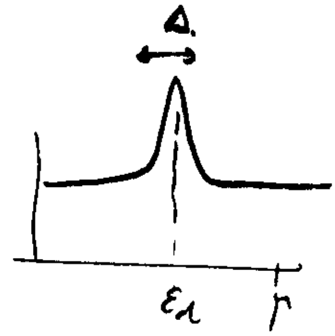
• Return to the underlying Anderson Model

$$H = \underbrace{H_0}_{\text{conduction band kinetic energy}} + \lambda \left[c^\dagger_{k\sigma} d_\sigma + d^\dagger_\sigma c_{k\sigma} \right] + U n_{d\uparrow} n_{d\downarrow} + E_d n_{d\sigma}$$



local atomic problem.

(All particle energies are measured from μ).



(i) $\left\{ \begin{array}{l} \text{resonance width } \Delta = \rho \lambda^2 \\ \text{For } U = 0\text{, Lorentzian density of states} \end{array} \right.$

(ii) If $\Delta \ll |E_d|, |E_d + U|$, the low temperature configuration has one d electron with arbitrary spin

↳ Kondo model ("Schrieffer-Wolff transf.)

$$\boxed{H = H_0 + \frac{J}{2} d^\dagger_\sigma d_{\sigma'} c^\dagger_{k\sigma'} c_{k\sigma}} \qquad (1)$$

$$\frac{J}{2} = \lambda^2 \left[\frac{1}{E_d + U} - \frac{1}{E_d} \right]$$

The form (1) is equivalent to the s-d hamiltonian, more amenable to approximations

- Old formulation of Cyrot-Lacroix:

(i) Decomposition of interaction term via a Hubbard Stratonovitch trick for the partition function

$$\exp\left[\beta \frac{J}{2} \quad d_\sigma^* C_{k\sigma} \quad C_{k'\sigma'}^* d_{\sigma'}\right]$$

$$= \int d\phi \ \exp\left[\phi \, d_\sigma^* C_{k\sigma}\right] \qquad \exp\left[-\frac{\phi^2}{2\beta J}\right]$$

- Exact representation if one sums over all histories $\phi(t)$

(ii) Static approximation: ϕ = constant
Saddle point approximation $\phi = \phi^*$

$\Downarrow$

Amounts to using an effective hybridization

$$H_{eff} = \frac{\phi^*}{\beta}\left(d_\sigma^* C_{k\sigma} + c.c.\right)$$

where ϕ^* is obtained from the saddle point condition

$\Downarrow$

Approximate treatment of the crossover
Decent estimate of T_K Very compact.

5

- The slave boson formulation of Coleman:

(i) Assume $U = \infty$: no double occupancy

$\boxed{\Delta \ll \varepsilon_d}$	$\boxed{\Delta \sim \varepsilon_d}$
Kondo model	Valence fluctuations
$n_d = 1$	$n_d = 0$ or 1
$\frac{J}{2} = \frac{\lambda^2}{\lvert\varepsilon_d\rvert}$	

- Question: how to implement the condition $n_{d\uparrow} n_{d\downarrow} = 0$?

(ii) $d_\sigma^* = f_\sigma^* b$

f_σ^*: fermion operator that carries information of σ

b: boson operator that follows the presence of a hole irrespective of its spin

$\downarrow$

Constraint $Q = f_\sigma^* f_\sigma + b^* b = 1$

$f_\sigma^* f_\sigma$: electron with spin σ

$b^* b$: hole: $n_d = 0$

Can discard the $U n_\uparrow n_\downarrow$ (cared for by constraint)

$\downarrow$

$$\boxed{H = H_0 + \varepsilon_d f_\sigma^* f_\sigma + \lambda \left[f_\sigma^* b\, c_{k\sigma} + c_{k\sigma}^* f_\sigma b^* \right]}$$

The complexity is now in the hybridization term

$\Downarrow$

Exact formulation if constraint is enforced at all times

(iii) Mean field approximation: constraint obeyed on average

$\downarrow$

- Lagrange multiplier

$$-\eta\,[f_\sigma^+ f_\sigma + b^+ b]$$

- b replaced by a C number ("Bose condensation of slave boson)

Effective resonant level model

$\Downarrow$

Two parameters b, η $\rightarrow$ Two conditions: constraint, number of particles

$\Downarrow$

Elegant treatment that covers both Kondo and valence fluctuations

(iv) In the Kondo limit $E_d \ll -\Delta$, equivalent to the Cyrot Lavagna approach

Detailed algebra straightforward (cf. book of Henson)

↓

$\left\{ \begin{array}{l} T_k \\ \text{Physical quantities } S(T),\ \chi(T) \end{array} \right.$

Qualitatively OK in the two limits $\left\{ \begin{array}{l} T \gg T_k \\ T \ll T_k \end{array} \right.$

Sensible interpolation in between, but not very good (error ~ 30%). Misses all log structure

Spurious discontinuity at a temperature $T_c \sim T_k$ ⇒ Curie if $T > T_c$

- Improvements : include fluctuations of b (difficult and not very reliable).

↓

Fluctuations are small if the number of spin states n goes to ∞

↳ 1/n expansion (here n = 2 !!)

Such theories are fundamentally unreliable : justified a posteriori !

Conclusions

- High T and low T well understood

Most of the physics can be understood with perturbation arguments in the two limits

- Stability of the fixed point
- Relevant operators → local phenomenology
- Symmetry and universality of Th + D

Missing link = matching of low T and high T expansions

- ↳ numerical for the $\boxed{\alpha \sim 1}$

- Interpolation → α and behaviour for $T = T_K$

- Exact theory (Bethe Ansatz), with partial answers (Nothing on correlations) - $\boxed{\text{Delicate}}$

- Approximate theories (e.g. Bosonization) ↳ phenomenology, useful matched to exact results (cf. 1d systems)

- Naive "mean field" descriptions

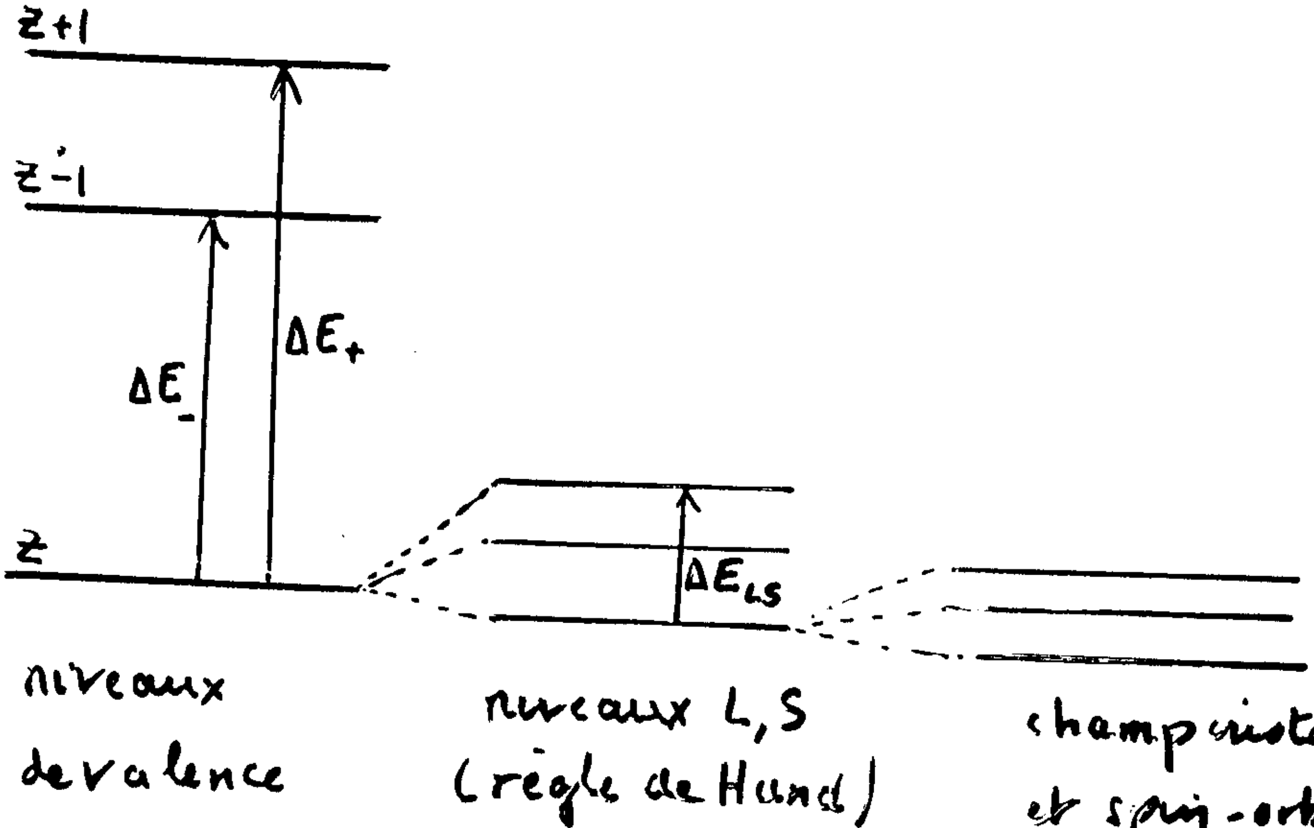
But the first thing to do is low T and large T

"ECONOMY"

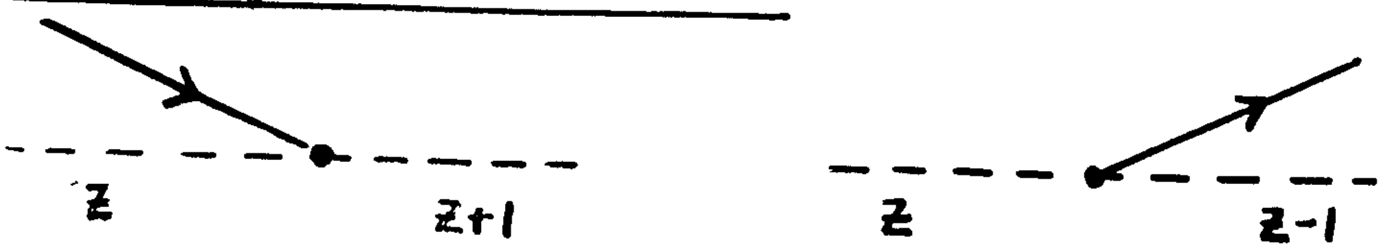
• Hamiltonien d'Anderson

$$H = \varepsilon_k c^*_{k\sigma} c_{k\sigma} + H_{at}$$
$$+ V_k \left[d^*_{lm\sigma} c_{k\sigma} Y_{lm}(\hat{k}) + c.c. \right]$$

Hiérarchie des niveaux atomiques



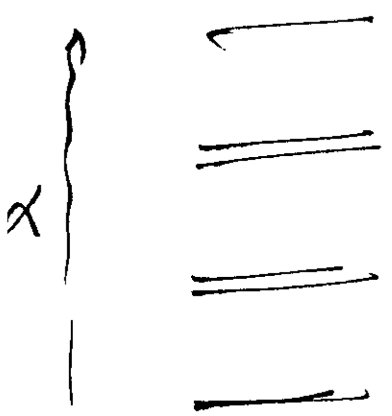
Couplages élémentaires



• <u>Schrieffer Wolff transformation</u>

(i) Effective hamiltonian on the subspace with valency z.

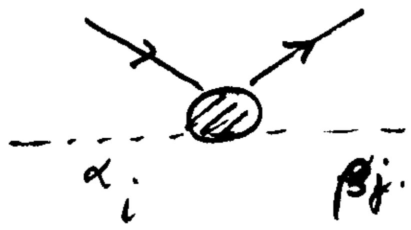
↓



Atomic eigenstates α (degenerate)

↓

$H = t_{\alpha\beta}$



"impurity operator"
via structure $t_{\alpha_i \alpha_j}^{\beta_i \beta_j}$

conduction
electron operator

(ii) Successive crossovers as D spans the various splitting $E_\alpha - E_0$

$D \gg E_\alpha - E_0$.

Level splitting is negligible
(H spans all components α)

$D \ll E_\alpha - E_0$

level α is decoupled
↓
virtual fluctuations
may cause the ground
state physics

(iii) In between, logarithmic crossovers → T_K^{α}

The crossovers are well separated if the $(E_\alpha - E_0)$ form a sequence of distinct energy scales limite $T \to 0$: on travaille sur le fondamental de H_{at}

↳ Hamiltonien effectif réduit

- Exemples (i) Etat L, S sans spin orbite ni champ cristallin

$$H = J_{pq} \{\vec{L} . \vec{\ell}\}^{p}_{mm'} \{\vec{S} . \vec{s}\}^{q}_{\sigma\sigma'} \, c^{*}_{km\sigma} c_{k'm'\sigma'}$$

avec $q = 0, 1$, $p = 0, 1 \ldots \mathrm{Min}(L, \ell)$

(ii) Découplage spin orbite sans champ cristallin (état de $\vec{J} = \vec{L} + \vec{S}$ donné)

$$H = J_{pq} (\vec{J} . \vec{\ell})^{p}_{mm'} (\vec{J} . \vec{s})^{q}_{\sigma\sigma'} \, c^{*}_{km\sigma} c_{k'm'\sigma'}$$

(iii) Découplage en états propres du champ cristallin

- Etapes de l'analyse

(I) Renormalisation à haute température (en général, une combinaison des J_{pq} l'emporte)

(II) Identification du point fixe $T = 0$ (en général couplage fort, mais il faut choisir parmi les états piégés en fonction des rapports des J_{pq})

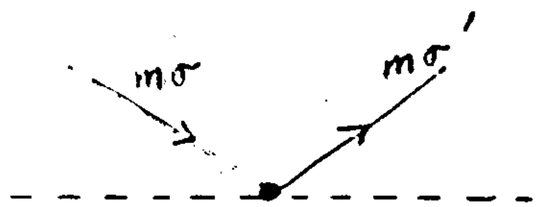
(III) Analyse phénoménologique à $T = 0$ (exploitation des symétries et de l'universalité)

⇓

Description presque complète sans aucun calcul

2) Exemple :
$\begin{cases} \text{Singulet orbital} \\ \text{Pas de champ cristallin} \end{cases}$

$$H = J \sum_{\substack{kk' \\ m}} \vec{S}.\vec{s}_{\sigma\sigma'}\, C^*_{km\sigma} C_{k'm\sigma'}$$



le vertex élémentaire conserve m (symétrie de rotation orbitale)

— le problème a deux paramètres

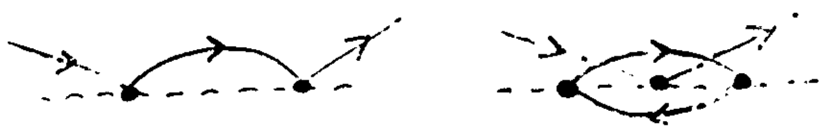
$\begin{cases} \text{spin } S \\ \text{nombre de canaux } n = 2\ell+1 \end{cases}$

En général, la règle de Hund → $\boxed{S = \frac{n}{2}}$ (Mn dans Cu)

le cas $n \neq 2S$ peut résulter du champ cristallin, ou mieux du couplage hyperfin A : si $T_K \ll A$, $\vec{J}$ se couple à $\vec{F} = \vec{I} + \vec{S}$.

Selon le signe de A, n est $\gtrless 2F$

— Renormalisation haute température



$$\frac{dz}{d\operatorname{Log} D} = -z^2 + n z^3 + \cdots$$

n n'intervient pas à l'ordre le plus bas (canaux découplés)

↳ début du scaling inchangé $\boxed{T_K \sim D e^{-1/\mathcal{J}J}}$

~~(ρ est la densité d'états par canal)~~

Mais l'évolution ultérieure dépend de n !

(4)

— <u>Comportement pour $J \to +\infty$</u>

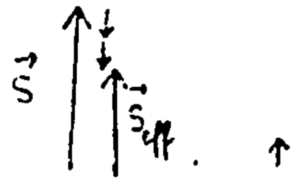
On piège un électron par canal sur le site d'impureté

↳ centre habillé de spin $S_{eff} = \left| S - \frac{n}{2} \right|$

(i) $\boxed{n = 2S}$ Point fixe <u>non magnétique</u>

↳ description à la Landau (diffuseur scalaire polarisable)

(ii) $\boxed{n < 2S}$ Ecran incomplet



⬇

couplage résiduel ferromagnétique

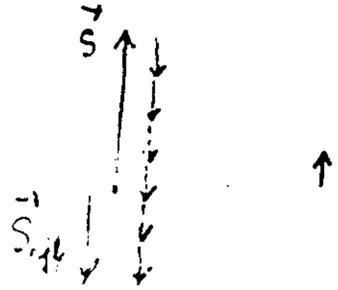
⬇

point fixe attractif $\begin{cases} J \to +\infty \\ J_{eff} \sim \frac{1}{J} \to 0^- \end{cases}$

⬇

Découplage de $\vec{S}_{eff}$ à $T=0$ (dégénérescence, $\chi \sim \frac{1}{T}$)

(iii) $\boxed{n > 2S}$ Surcompensation de $\vec{S}$

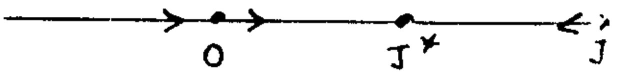


⬇

couplage résiduel antiferro

⬇

point fixe répulsif $J_{eff} \to 0^-$ ↘ Le point fixe <u>stable</u> est à J^* fini (lorsque $n \gg 1$, les perturbations donnent $\rho J^* = z^* = \frac{1}{n} \ll 1$)



⇓

$\boxed{\text{COMPORTEMENT CRITIQUE}}$

$$\frac{dz}{d\log T} = \varphi(z) \simeq \beta(z - z^*) \Rightarrow (z - z^*) \sim \left(\frac{T}{T_K}\right)^{\beta}$$

$$\frac{d\log S}{d\log T} = f(z) \Rightarrow S \sim \left(\frac{T}{T_K}\right)^{f(z^*)}$$

Les quantités physiques F, S, M, etc... sont d'ordre T^{α}, H^{α}

↓

EXPOSANTS CRITIQUES

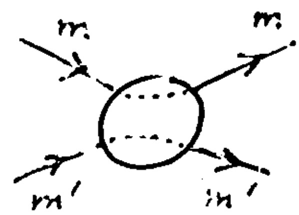
Description phénoménologique du cas $n = 2S$

– Déphasage $\delta_{m\sigma}(\varepsilon)$ fonction de $n_{m'\sigma'}(\varepsilon')$

$$\delta_{m\sigma}(\varepsilon) = \delta_0 + \alpha\varepsilon + \phi_{m\sigma}^{m'\sigma'}\, \delta n_{m'\sigma'}(\varepsilon') + \dots$$

A priori, $(2l+1)$ paramètres ϕ (interaction de deux électrons l dans la même bande)

– Argument de symétrie



la renormalisation préserve

la conservation de m

L'interaction $\frac{1}{2}\left\{a\, \rho_m \rho_{m'} + b\, \vec{S}_m \cdot \vec{S}_{m'}\right\}$

$\downarrow$

Energie Hartree Fock $\varepsilon_{m\sigma} = (a + b\sigma\sigma')\,\bar{n}_{m'\sigma'} - \frac{2b}{4}\,\bar{n}_{m,-\sigma}$

le déphasage ne dépend que de $\underline{2}$ paramètres ϕ :

$$\delta_{m\sigma}(\varepsilon) = \delta_0 + \alpha\varepsilon + \sum_{m'\neq m}\left[\varphi + \sigma\sigma'\psi\right]\delta n_{m'\sigma'} + \left(\varphi - \frac{3\psi}{4}\right)\delta n_{m,-\sigma}$$

(lorsque $m' = m$, le principe d'exclusion force les deux électrons dans un état singulet $\Rightarrow$ combinaison $\left(\varphi - \frac{3\psi}{4}\right)$)

- Arguments d'universalité

(i) Universalité faible : δ invariant par translation simultanée de ε et de tous les μ_m (singularité attachée au niveau de Fermi)

$$\hookrightarrow \quad \alpha + \rho_0 \left[(2n-1)\varphi - \frac{3}{4}\psi \right] = 0$$

(ii) Universalité forte : un électron de conduction ne change jamais de canal m

$\hookrightarrow$ δ_m est indépendant de $\mu_{m' \neq m}$

$\hookrightarrow$ $\varphi = 0$

• L'interaction résiduelle est complètement fixée

$\hookrightarrow$ un seul paramètre $\alpha \sim 1/T_K$

- L'analyse à la Landau donne

$$\begin{cases} \dfrac{\Delta C_v}{C_v} = \dfrac{n\alpha}{\pi\rho} \\[2ex] \dfrac{\Delta \chi}{\chi} = \dfrac{2}{3}(n+2)\,\dfrac{\Delta C_v}{C_v} \end{cases}$$

(χ = susceptibilité de spin seulement)

. Résultat confirmé par la solution exacte – obtenu ici sans aucun calcul •

Chaleur spécifique

~~Vassas~~ $\rho_0 =$ densité d'états par canal $m\sigma$

$$\delta C_v = \frac{2\pi^2}{3} n \delta\rho_0 = \frac{2n\pi\alpha}{3}$$

$$\downarrow$$

$$\delta\rho_0 = \frac{\alpha}{\pi} \longrightarrow \frac{\delta C_v}{C_v} = \frac{n\,\delta\rho_0}{\rho} = \frac{n\alpha}{\pi\rho}$$

Susceptibilité

$$\bar{\mathcal{E}}_{m\sigma} = \varepsilon - \sigma g\beta H - \frac{\alpha\varepsilon}{\pi\rho_0} + \frac{3\psi}{4\pi\rho_0}\delta n_{m,-\sigma} - \frac{\psi_{\sigma\sigma'}}{\pi\rho_0}\delta n_{m'\neq m,\sigma'}$$

$$\downarrow$$

canal $m\sigma$ $\quad \varepsilon = \sigma g\beta H \left[1 + \frac{\alpha}{\pi\rho_0} + \frac{2\psi}{4\pi\rho_0}(n-1)\rho_0 + \frac{3\psi}{4\pi\rho_0}\rho_0\right]$

$$= \sigma g\beta H\left[1 + \frac{\alpha}{\pi\rho_0} + \frac{\psi}{4\pi}(2n+1)\right]$$

$$\delta M = \left(\frac{g\beta}{2}\right) n\rho_0(\mu_\uparrow - \mu_\downarrow)$$

$$\delta\chi = 2n\rho_0\left(\frac{g\beta}{2}\right)^2\left[\frac{\alpha}{\pi\rho_0} + \frac{\psi}{4\pi}(2n+1)\right]$$

$$= \frac{2n\alpha}{\pi}\left(\frac{g\beta}{2}\right)^2\left[1 + \rho_0\psi\frac{(2n+1)}{4\alpha}\right] \qquad \text{Mais } \frac{3\psi}{4}\rho_0 = \alpha.$$

$$\delta\chi = \frac{2n\alpha}{\pi}\left(\frac{g\beta}{2}\right)^2\left[1 + \frac{2n+1}{3}\right] = \frac{2n\alpha}{\pi}\left(\frac{g\beta}{2}\right)^2\frac{2}{3}(n+2)$$

A comparer avec

$$\chi = 2\rho\left(\frac{g\beta}{2}\right)^2 \qquad \boxed{\frac{\Delta\chi}{\chi} = \frac{n\alpha}{\pi\rho}\,\frac{2}{3}(n+2)} = \frac{2}{3}(n+2)\frac{\Delta C_v}{C_v}.$$

$$\frac{T\delta\chi}{\delta C_v} = \frac{2(n+2)}{\pi^2}\left(\frac{g\beta}{2}\right)^2 = \frac{3}{\pi^2}\left(\frac{g\beta}{2}\right)^2\frac{2}{3}(n+2) \quad \text{ok}$$

Le Modèle de Coqblin Schrieffer

Impureté de valence $z_d = 1$

$$\left.\begin{array}{l} L = \ell \\ S = 1/2 \end{array}\right\} \rightarrow \text{moment total } J \quad \text{si fort spin orbite}$$

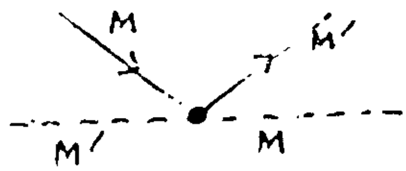
↳ Hamiltonien effectif

$$H = \left[a\,\delta_{MM'} + b \right] C^*_{kM}\, C_{k'M'}\, d^*_{M'}\, d_M$$

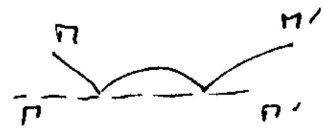
(exact si excitation vers $z_d = 0$, approché si excitation vers $z_d = 2$)

↓

Nouvelle symétrie : conservation de M



(i) Renormalisation haute température



$$\begin{cases} \dfrac{\partial b}{\partial \log D} = -\dfrac{2J+1}{2}\, \rho b^2 \\[2ex] \dfrac{\partial a}{\partial \log D} = +\rho b^2 \end{cases}$$

Schrieffer Wolff → $b_0 > 0$

$b \to +\infty$, $a \to -\infty$

⇓

$$T_K \sim D_0 \exp\left\{ -\frac{2}{\rho b_0 (2J+1)} \right\}$$

La dégénérescence augmente T_K

En l'absence de spin orbite, $2[2\ell+1]$ canaux indépendants

$(z_d = 1)$ $\quad \hookrightarrow T_K \sim D_0 \exp\left[-\frac{1}{(2\ell+1)\rho b_0}\right]$

Résultat à comparer au même hamiltonien avec

$z_d = 2\ell+1$ ($\Rightarrow L=0$ par la règle de Hund)

$$b \langle L=0; S, \tau | d^*_{m\sigma} d_{m'\sigma'} | L=0; S\tau' \rangle = \delta_{mm'} \vec{S}_{\tau\tau'} \cdot \vec{s}_{\sigma\sigma'} J$$

$$\Downarrow J = \frac{b}{2\ell+1} \longrightarrow T_K \sim D_0 \exp\left[-\frac{2\ell+1}{\rho b_0}\right]$$

T_K est élevé pour $z_d = 1$, très faible pour $z_d = 2\ell+1$

(ii) Nature du point fixe $b = +\infty$, $a = -\infty$.

– Résonance entre $\begin{cases} \text{un électron } d \\ p \text{ électrons } s \end{cases}$ dans des canaux différents

$\hookrightarrow \begin{cases} p \text{ états d'énergie } pa + b \\ \text{un état d'énergie } pa - pb \end{cases}$

le fondamental correspond à p maximum : $p = 2J$

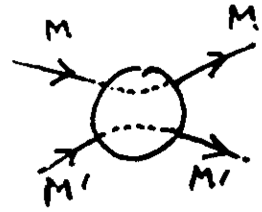
$\hookrightarrow$ état symétrique et non dégénéré

(iii) Phénoménologie à basse température

– SYMETRIE Conservation de M

$\downarrow$

Interaction effective $\sum_{M' \neq M} C^*_{K_1 M} C^*_{K_2 M'} C_{K_3 M'} C_{K_4 M}$



$\downarrow$

Déphasage

$$\delta_M(\varepsilon) = \delta_0 + \alpha\varepsilon + \varphi \sum_{M' \neq M} \delta n_{M'}$$ Un seul paramètre φ

– **UNIVERSALITÉ**

δ invariant par translation de ε et μ :

$\hookrightarrow \alpha + 2J\rho_0\varphi = 0$ (ρ_0 = densité d'états par canal)

(Un électron s peut changer de canal
$\hookrightarrow$ pas d'universalité forte)

– **THERMODYNAMIQUE**

Energie Zeeman $-g\beta\vec{J}.\vec{H}$ (seul compte le g de l'impureté.

$\downarrow$

Quasiparticules d'énergie $\bar{\varepsilon}_M = \varepsilon\left[1 - \frac{\alpha}{\pi\rho_0}\right] - \frac{\phi}{\pi\rho_0}\sum_{M'\neq M}\delta n_{M'} - Mg\beta H$

Chaleur spécifique $\delta\rho_0 = \frac{\alpha}{\pi} \Longrightarrow \frac{\delta C_v}{C_v} = \frac{2J+1}{2}\,\frac{\alpha}{\pi\rho}$

Susceptibilité totale : Niveau de Fermi $\bar{\varepsilon}_M = 0$

$\downarrow$

$$\left.\begin{array}{l} \delta n_M = \rho_0 Mg\beta H\left[1 + \frac{\alpha}{\pi\rho_0} - \frac{\phi}{\pi}\right] \\ \text{Aimantation} = \sum_M Mg\beta H\,\delta n_M \end{array}\right\} \rightarrow \frac{\delta\chi}{\chi} = \frac{\delta C_v}{C_v}\,\frac{2(J+1)(2J+1)}{3}$$

En l'absence de spin orbite, $n = 2l+1$ canaux orbitaux

$$\delta_{m\sigma} = \delta_0 + \alpha\varepsilon + \varphi\sum_{\substack{m\sigma \\ \neq m'\sigma'}}\delta n_{m'\sigma'} \Longrightarrow \alpha + (2n-1)\rho_0\varphi = 0$$

$\Downarrow$

$$\frac{\delta C_v}{C_v} = \frac{n\alpha}{\pi\rho} \quad , \quad \frac{\delta\chi^s}{\chi^s} = \frac{\delta C_v}{C_v}\,\frac{2n}{2n-1}$$

(où χ_s est la susceptibilité de spin seule)

3) The overscreened situation $n > 2S$

(The underscreened case is equivalent to the usual case $n = 1$, $S > 1/2$ $\Rightarrow$ residual ferromagnetic coupling)

- Stability argument indicates the existence of a finite J fixed point

Must have power law singularities with non trivial exponents (cf critical phenomena)

$\downarrow$

Universal behaviour independent of J (exponents depend on n and S)

$\downarrow$

Outside reach of perturbation expansion

- Perturbation theory works if $n \to \infty$

$$\frac{dz}{d\log D} = -z^2 + n z^3 \qquad z^* = \frac{1}{n}$$

Predicted by Blandin many years ago - confirmed by more elaborate theories

$\downarrow$

not very useful if $n = 2$!!

- Exact Solution via Bethe Ansatz

(i) (For $n = 2S$ and $n < 2S$, confirmation of previous results)

$$\Delta F = -T \log \frac{\sin\left[\pi \frac{2S+1}{n+2}\right]}{\sin \frac{\pi}{n+2}} + \overline{\Delta F}$$

residual entropy at $T = 0$

$$\begin{cases} S = \log g \\ g = \dfrac{\sin\left[\pi \frac{2S+1}{n+2}\right]}{\sin\left[\frac{\pi}{n+2}\right]} \end{cases}$$

Noninteger (limits $T \to 0$ and $\Omega \to \infty$)

Spectacular signature of anomalous behaviour.

(ii) $\overline{\Delta F} \to \begin{cases} \overline{S} = -\dfrac{\partial \overline{\Delta F}}{\partial T} & \to \quad C_v = \Omega \dfrac{\partial S}{\partial T} \\ \Pi = \dfrac{\partial \overline{\Delta F}}{\partial H} & \to \quad \chi = \dfrac{\partial \Pi}{\partial H} \end{cases}$

The limits $T \ll H$ and $H \ll T$ are very different

$\boxed{H \ll T}$

$$\bar{S} \sim \left[\frac{T}{T_k}\right]^{\frac{4}{n+2}} \to C_m \bar{S}$$

$$M \sim \frac{H}{T}\,\bar{S} \sim \frac{H}{T_k}\left(\frac{T}{T_k}\right)^{\frac{2-n}{2+n}}$$

$\boxed{T \ll H}$

$$M \sim \left(\frac{H}{T_k}\right)^{\frac{2}{n}}$$

$$\bar{S} \sim \frac{T}{H}\,M \sim \frac{T}{T_k}\left[\frac{H}{T_k}\right]^{\frac{2-n}{n}}$$

Note the presence of two distinct anomalous dimensions for T and H

$\downarrow$

<u>Cross over</u> when the two expressions are comparable

$$\left(\frac{T}{T_k}\right)^{\frac{2-n}{n+2}} = \left(\frac{H}{T_k}\right)^{\frac{2}{n}-1}$$

$\Downarrow$

$$\boxed{\frac{H}{T_k} = \left(\frac{T}{T_k}\right)^{\Delta} \quad \text{with } \Delta = \frac{n}{n+2}}$$

Hence the universal cross over function

$$S = f\left[\frac{H\,T_k^{\Delta-1}}{T^{\Delta}}\right]\left(\frac{T}{T_k}\right)^{\frac{4}{n+2}}$$

$$f(0) \sim 1 \qquad\qquad f(x\to\infty) \sim x^{\frac{2-n}{n}}$$

(iii) The case $\begin{cases} S = 1/2 \\ n = 2 \end{cases}$ is marginal

↳ critical exponents $\dfrac{4}{n+2} = \dfrac{2}{n} = 1$

(Unfortunate for C. L. N who made numerical Wilson analysis of the anomalous fixed point
↳ unspectacular results

$\Downarrow$

logarithmic corrections

$$\begin{cases} S \sim T \log T & \text{if } H \ll T \\ M \sim H \log H & \text{if } T \ll H \end{cases}$$

(Note the weak divergence of the Sommerfeld constant
↳ "marginal Fermi liquid behaviour")

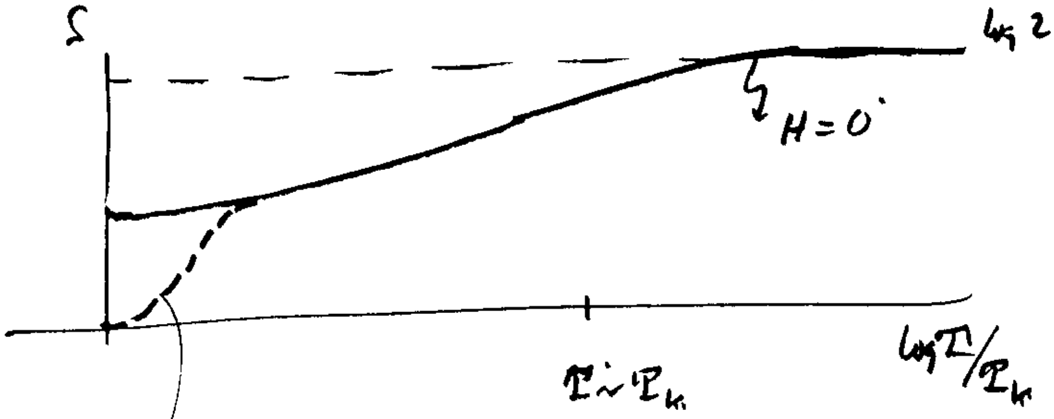
The residual entropy is

$$\boxed{S^* = \log \frac{\sin \pi/2}{\sin \pi/4} = \frac{1}{2} \log 2}$$

__Half__ the spin entropy is quenched at $T = 0$?

Numerical calculation of Sacramento & Schlottmann

Phys Rev B 43, 13294 (1991)



Logarithmic crossover
↓
several decades!

H ≠ 0
↓
second crossover

if $T \sim T^*(H) = T_K \left(\frac{H}{T_K}\right)^{1/\Delta}$

(If $H \ll T_K$, two peak structure in $C_V(T)$)

CONCLUSION

- Complete thermodynamical description
- Marginal behaviour if $n=2$, $S=1/2$.
- Physics not very clear

4) Physical realizations

• Orbital degeneracy in transition metals

(i) d electrons → 5 orbital channels

↓

Hund's rule: $\boxed{\text{align spins first.}}$

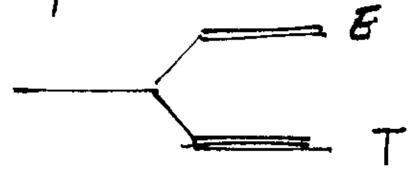
5 electrons → $S = 5/2$, orbital singlet (all once occupied)

↳ Mn in Cu.

In the absence of crystal field effects, Hund's rule implies $n = 2S$ for an orbital singlet

(ii) Many involve crystal field splitting

Cubic environment →



⇓

Hund's rule → orbital singlet

$n_d = 3$, $S = 3/2$

$n_d = 8$, $S = 1$.

If $J_E = J_T$, overscreened situation:

5 channels, $2S = 2$ or 3. (?)

But in practice, such a mechanism produces extreme anisotropy $J_E \neq J_T$.

Example, $n_d = 3$

• Impurity   × Conduction band

- A T electron in the conduction band may hop on the d level, and screen the local spin
  $\downarrow$
  large J_T

- An E electron can hop in, but it does not screen the spin S, except via configurational splittings in excited states
  $\hookrightarrow$ higher order effects: small J_E.

Hence $J_E \ll J_T$ (The same holds if $n_d = 2$)

(iii) Unfortunately, such a channel anisotropy makes the 1^* fixed point unstable $\rightarrow$ lowest order calculation

$$
\begin{cases}
\dfrac{d z_T}{d \log D} = - z_T^2 + z_T \left[3 z_T^2 + 2 z_E^2 \right] \\[2ex]
\dfrac{\partial z_E}{\partial \log D} = - z_E^2 + z_E \left[3 z_T^2 + 2 z_E^2 \right]
\end{cases}
$$

Log.

The nontrivial fixed point corresponds to

$$z_E = z_T = \frac{1}{5}$$

$$\downarrow$$

linear stability analysis

$$z_\alpha = \frac{1}{5} + J_\alpha.$$

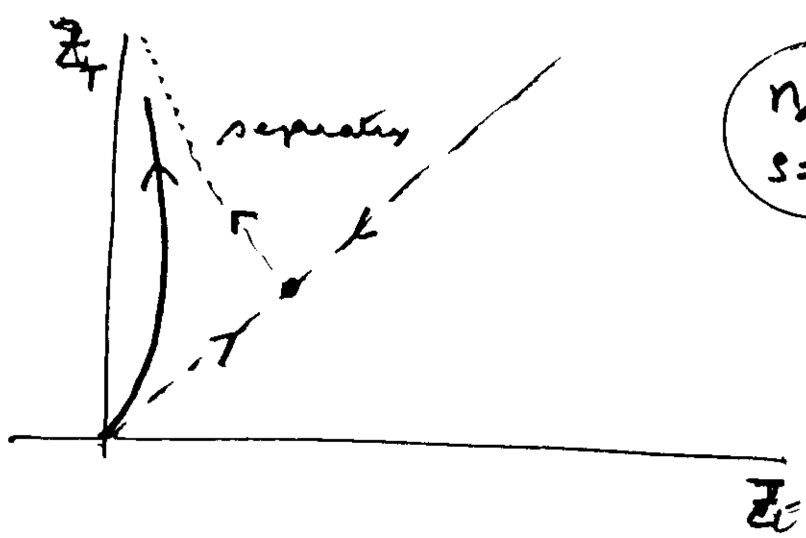
$$\downarrow$$

$$\begin{cases} \dfrac{\partial J_E}{\partial \log D} = -\dfrac{J_E}{25} + \dfrac{6 J_T}{25} \\[2ex] \dfrac{\partial J_T}{\partial \log D} = \dfrac{4 J_E}{25} + \dfrac{J_T}{25} \end{cases}$$

Hence the eigenvectors and eigenvalues

$J_E = J_T$, $\lambda = \frac{1}{5}$ stable

$J_E = -\frac{3}{2} J_T$, $\lambda = -1/5$ unstable

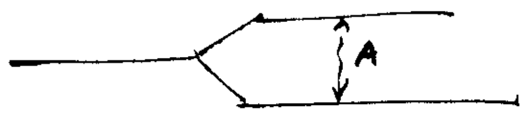


$n_d = 3$
$s = 3/2$

Physically, we are driven back to the Fermi liquid limit

$$n = 2S = 3.$$

- Another possibility is to invoke <u>hyperfine</u> coupling with a nuclear spin I $\qquad F = I + S$

S 

Depending on the sign of A, F can be $>$ or $<$ S.

If it is $< S$, then $n = 2S > F$

↓

$\boxed{\text{Anomalous behaviour if } T_K \ll A}$

Seems rather far fetched!!

- The most interesting possibility is that of Cox.

↓

The crucial feature is <u>channel degeneracy</u>

↓

$\boxed{\text{Interchange of spin and orbit}}$

Ground state = orbital spinless doublet

↓

"Fictitious spin"

The real spin index plays the role of channel index

↓

<u>strict</u> Kramers degeneracy

(i) In practice, Uranium in UBe_{13}.

↳ configuration $5f^2$

↓

Ground multiplet $J = 4$

$S = 1$ (spins aligned)
$L = 5$ (L maximum)
$J = 4$ spin orbit

Hund's rule

Crystal field splitting → ground state doublet Γ_3 (spin less)

= quadrupolar degeneracy

A Schrieffer Wolff transformation → Quadrupolar Kondo effect

Spin 1/2 conduction electrons → 2 channels

⇓

$\boxed{\text{Finally, } S = 1/2 \text{ (orbit)}, \; n = 2 \text{ (spin)}}$

(ii) Indeed, evidence for residual entropy $\frac{1}{2} \log 2$.

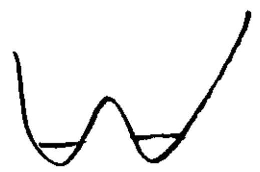
for a $T \log T$ specific heat

But data on concentrated samples (a few % of U ions).
↳ single impurity calculation very doubtful

?

— ~ —

(iii) Extension to other 2-level systems coupled to conduction electrons (metallic glasses)



↓

Same behaviour!

5) The Emery Kivelson approach

- Very elegant work based on bosonisation (Same as Schlottmann + flavour !)

$$H = H_0 + J_\lambda \, S_{\lambda\cdot} (\sigma_\lambda)_{\sigma\sigma'} \, c^\dagger_{\sigma\alpha} c_{\sigma'\alpha}$$

J_λ: spin index, $J_\parallel \neq J_\perp$

α: channel index 1, 2 (= flavour)

(i) Bosonisation of $c_{i\sigma\alpha}$

→ Boson fields $\phi_{\sigma\alpha}$

↓

diagonalization

$$\begin{cases} \phi_c = \sum_{\sigma\alpha} \phi_{\sigma\alpha} \\ \phi_s = \sum_{\sigma\alpha} \sigma \, \phi_{\sigma\alpha} \\ \phi_f = \sum_{\sigma\alpha} \alpha \, \phi_{\sigma\alpha} \\ \phi_{sf} = \sum_{\sigma\alpha} \sigma\alpha \, \phi_{\sigma\alpha} \end{cases}$$

ϕ_c and ϕ_f drop out (charge and flavour are irrelevant if spin does not enter)

$$H = H_0 - \frac{J_z}{2\pi} S_z \left.\frac{\partial \phi_s}{\partial r}\right|_{r=0}$$

$$+ \underbrace{\frac{J_\perp}{\pi a}}_{\text{cutoff}} \left\{ S_x \cos\phi_s(0) + S_y \sin\phi_s(0) \right\} \underbrace{\cos\phi_{sf}(0)}_{\text{new feature}}$$

(ii) Rotation around the z-axis in order to eliminate S_y.

↓

Shift of the S_z term

$$J_z \to J_z - 2\pi v_F = \overline{J_z}$$

For a specific value of J_z, $\overline{J_z}$ vanishes: "Toulouse limit"

↓

$$H = H_0 + \frac{J_\perp}{\pi} S_x \cos\phi_{sf}(0)$$

~~In the one channel case, $\cos\phi_{sf}(0)$ is ~~[illegible]~~ replaced by $\cos\phi_s$~~

~~↓~~

~~resonant level~~

Question: Si "unsend canal"

$\cos\phi_s(0)\,\cos\phi_{sf}(0) \Longrightarrow \cos\sqrt{2}\,\phi_s(0)$

Scaling back to $\cos\phi_s(0)$

↓

Schlottmann

$2\cdot\left[1-\frac{\delta}{\pi}\right]^2 = 1$

Scaling to 1

↓

decoupled spin for another J_z.

$H = \tau_x$??

$\boxed{\delta = \pi}$

$\boxed{\delta' = \pi/2}$ (strong coupling)

(iii) Refermionization of $\phi_{sf} \rightarrow \psi_{sf}(x)$

↓

Effective Hamiltonian

$$H = H_0 + J_\perp S_x\left[\psi_{sf}(0) + \psi_{sf}^*(0)\right]\sqrt{\frac{2}{\pi a}}$$

One then represents S_x by fictitious fermions d, d^*

$$\boxed{H = H_0 + \frac{J_\perp}{\sqrt{2\pi a}}\left[\psi_{sf}(0) + \psi_{sf}^*(0)\right]\left[d^* - d\right]}$$

(The d and the ψ_{sf} anti commute $\rightarrow$ H hermitian)

(iv) Note that one may write the spin operators as

$$d^* = \frac{a + i \cdot b}{\sqrt{2}}$$

$$d = \frac{a - i b}{\sqrt{2}}$$

Real fermion operators ("Majorana")

$\downarrow$

The conduction band couples only to b ("Half the impurity")

<u>Conclusion</u> : Hamiltonian bilinear in ψ and d

$\downarrow$

Exact solution

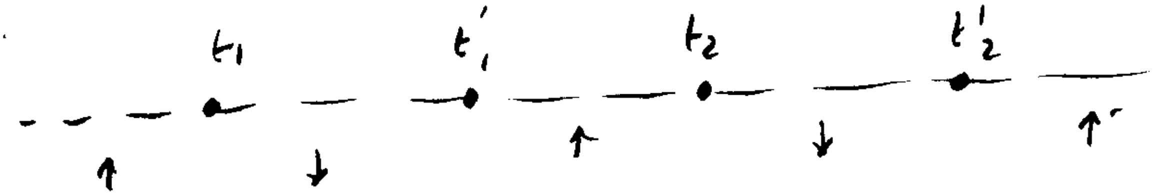
Note the difference with the <u>one channel case</u>

$$H = H_0 + J_\perp \left[\psi_s^* \, d + d^* \psi_s \right]$$

First look at formal origin of this result.

• <u>Perturbation expansion</u>

(i) A priori, result of E.K very surprising



The propagators are the same for every vertex, whether $(\uparrow \downarrow)$ or $(\downarrow \uparrow)$

$t_i \quad \downarrow \quad t_i'$

Contribution $\sim \dfrac{1}{(t_i - t_j')\,(t_i - t_j)\,(t_i' - t_j')}$

To be compared with the Cauchy determinants

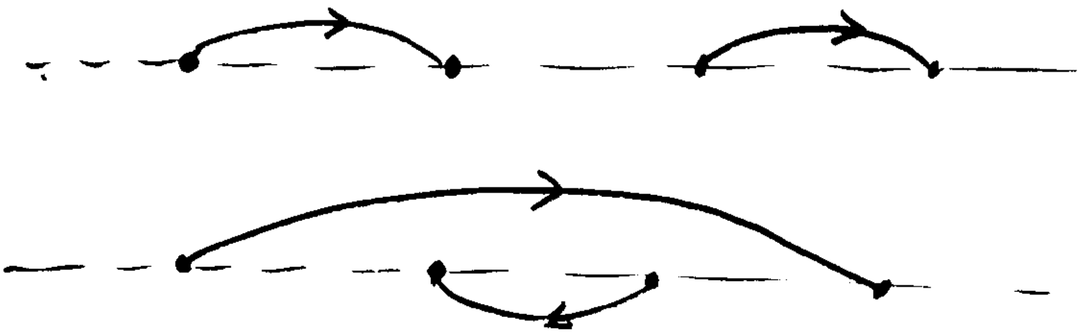
(?) of Anderson Yuval

$$\frac{(t_i - t_j)\,(t_i' - t_j')}{(t_i - t_j')}$$

The answer should lie in the reshuffling of terms

(ii) Original perturbation expansion

(α) $J_z = 0$, fourth order



Two contributions for lines originating from ↑↓

Same for lines from ↓↑

One channel

↓

factorisation

$L_\uparrow L_\downarrow$

↓

Δ^2

↳ Cauchy determinant

Two channels

Factor 2 for each closed loop

↓

No factorisation

↓

Contribution F which remains finite when $t_i = t_j$ or $t'_i = t'_j$

(Crossing symmetry disrupts the number of closed loops)

28

(β) $J_z \neq 0$

δ = phase shift discontinuity
$= 2\,\delta'$ due to J_z

Multiple scattering of open line unchanged (→ flavour is conserved)

factor $\Delta^{-2 \cdot \frac{2\delta}{\pi}}$

spin

Closed loop contribution multiplied by 2

$$e^{+2 \cdot 2 \cdot \left(\frac{\delta}{\pi}\right)^2}$$

spin flavour

Hence an overall contribution

$$\boxed{\Delta^{4\frac{\delta^2}{\pi^2} - 4\frac{\delta}{\pi}} \cdot F}$$

(for a specific history of $J_\perp$)

(to be compared to $\Delta^{2\left[1-\frac{\delta}{\pi}\right]^2}$ in the one channel case)

~~(iii) Assume that $\delta = \pi/2$~~

(iii) One can rewrite the perturbation result as

$$\frac{F}{\Delta} \quad \Delta^{\left(\frac{2\delta}{\pi}-1\right)^2}.$$

If $\delta = \pi/2$, it reduces to F/Δ, which is the E.K result.

F | has double poles at $t_i = t'_j$.
| is finite at $t_i = t_j$. (On)

$\frac{F}{\Delta}$ has single poles at $t_i = t'_j$ and $t_i = t_j$.

Questions :- Detailed proof of equivalence ?
(Counting)

- $\delta = \pi/2$ means finite J_z. ($\delta' = \pi/4$)

~~↳ can one formulate the soluble limit directly starting from that assumption?~~

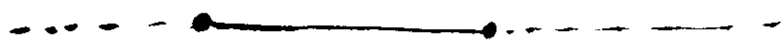
- Physical consequences

(i) Particle number is not conserved

↳ 2×2 "Nambu" Green's function

$$\Delta = \begin{pmatrix} d \\ d^* \end{pmatrix} \quad , \quad \underset{\sim}{G} = -i \langle T \left[\Delta(t)\, \Delta^{+}(0) \right] \rangle$$

Hybridization provides a "self energy" for d particles



$$\begin{cases} \psi_{cf} + \psi_{cf}^* = \eta \\ \langle \eta(0)\, \eta(t) \rangle \to \text{Fourier transform} \cdot g(\omega) \sim \frac{i}{v_F}. \end{cases}$$

density of states

$$\begin{cases} \underset{\sim}{G}^{-1} = \omega\, \underset{\sim}{1} - i \cdot \frac{\Gamma}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \omega\, \underset{\sim}{1} - \frac{i\Gamma}{2}\left[1 - 2\tau_x\right] \\ \Gamma = \frac{J_\perp^2}{\pi v_F a} \quad \text{: resonance width} \end{cases}$$

(ii) From $\underset{\sim}{G}$ one infers the spectral density

$$A(\omega) = \mathrm{Tr}\left[\mathrm{Im}\, \underset{\sim}{G}\right]$$

The trace is invariant under rotation $\tau_x \to \tau_z$.

$$A = \mathrm{Tr} \cdot \begin{bmatrix} \frac{1}{\omega - i\cdot\Gamma} & 0 \\ 0 & \frac{1}{\omega} \end{bmatrix}$$

$$\Downarrow$$

$$\boxed{A = \pi\,\delta(\omega) + \frac{\Gamma}{\omega^2 + \Gamma^2}}$$

Half the spectral density is a δ-function

$\downarrow$

Decoupled spin

Residual entropy $\frac{1}{2}\log 2$ at $T=0$

The other half is a resonant level of ordinary type

At this level of approximation, there is no singularity magnetic susceptibility (Φ_s is decoupled)

Similarly, the specific heat is regular (NO $T \log T$ term)

(iii) Singularities in C_v as well as χ_s appear away from the solvable limit

$\downarrow$

2nd order treatment of Sengupta + Georges

$\downarrow$

Expected results

$$\boxed{\frac{\chi T}{C_v} = \frac{8}{3}}$$

Conclusion

Formally satisfactory treatment

But underlying physics still somewhat mysterious

Pending questions in the perturbation approach (exactly solvable case $\delta' = \pi/4$, more accurate than propagation which implies a Born approximation)

$\Downarrow$

Physical meaning ?