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SMR. 758 - 42

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

METAL-INSULATOR TRANSITION IN DISORDERED MATERIALS (THEORY)

PART III

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

(CORRECTED VERSION)

SCALING RESULTS NEAR MI TRANSITION

(Non-interacting case)

$$\sigma(n) = C \frac{e^2}{\hbar \xi^{d-2}} \sim (n-n_c)^{\mu} \qquad \mu = \nu(d-2)$$

$$\text{using} \quad \xi \sim |n-n_c|^{-\nu}$$

Finite frequency:

$$\sigma(\omega, n) = \sigma(0, n)\, f\left(\frac{\omega}{\omega_c}\right) \sim (n-n_c)^{\nu(d-2)}\, f\left[\frac{\omega}{(n-n_c)^{\nu d}}\right]$$

using $\omega_c \sim \frac{1}{N_0 \xi^d}$ N_0 is non-critical (Wegner)

Expect at high ω ($\gg \omega_c$), $\sigma(\omega, n)$ not to depend on $(n-n_c)$ (or ξ), $\Rightarrow f(x) \sim x^{(d-2)/d}$ as $x \to \infty$

$$\text{and} \quad \sigma(\omega, n) \sim \omega^{(d-2)/d} \qquad \omega \gg \omega_c$$

At such high ω, system doesn't know near n_c whether it's a metal or insulator, so in insulator

$$\sigma(\omega, n) \sim \begin{cases} C\, \omega^{(d-2)/d} & \omega \gg \omega_c \\ C'(\xi)\, \omega^2 & \omega \ll \omega_c \end{cases}$$

$\leftarrow$ calc. in insulating phase

$\hookrightarrow$ (logs due to resonant pairs omitted)

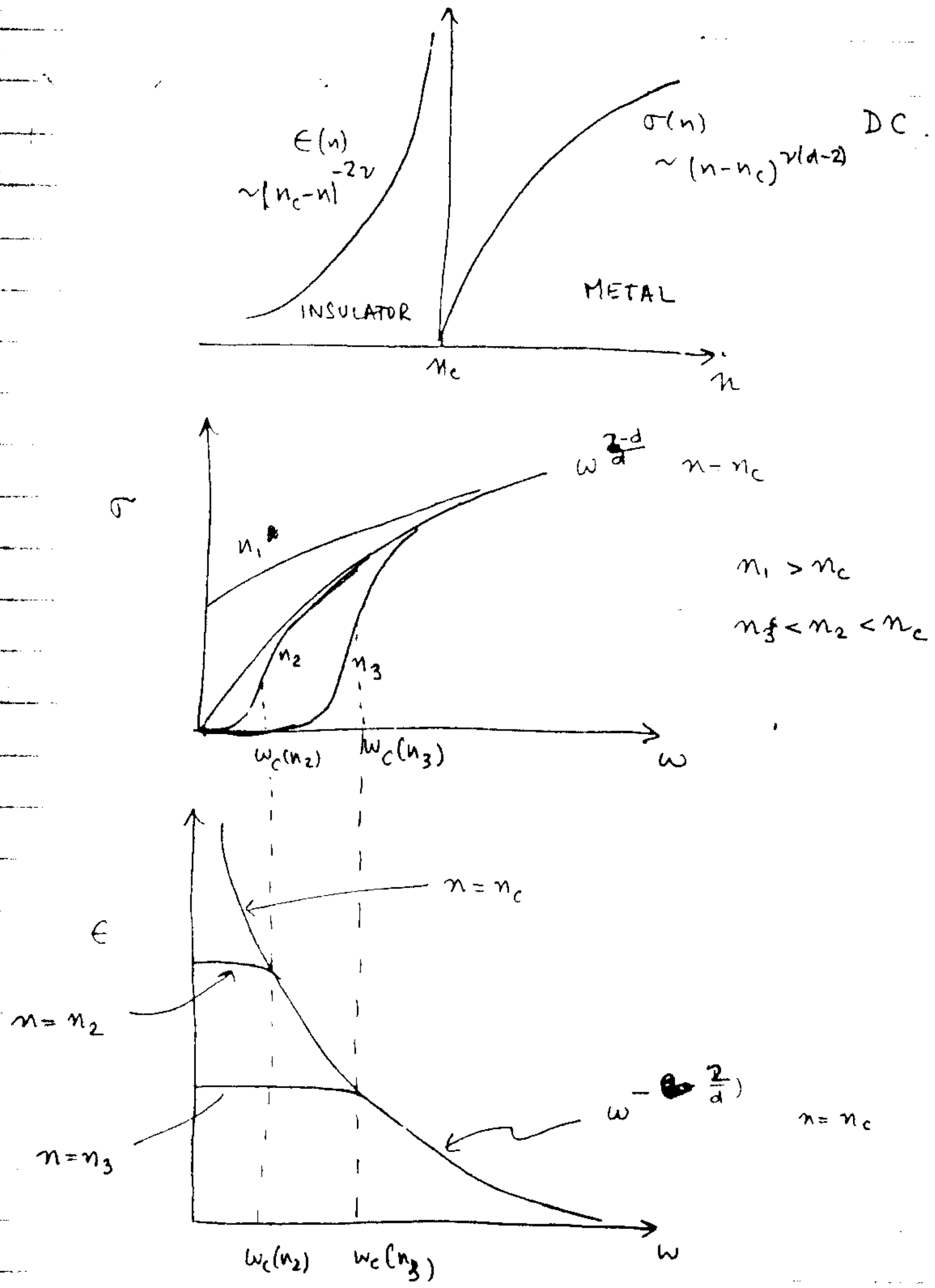
and $C'(\xi) \sim \xi^{d+2}$

by matching at $\omega = \omega_c$.

Can get $\epsilon(\omega, n) \sim \int \frac{\sigma(\omega', n)}{\omega'^2 - \omega^2}\, d\omega$

$$\epsilon(\omega, n) \sim \begin{cases} \xi^{2} \sim (n_c - n)^{-2\nu} & \omega \ll \omega_c \\ \omega^{-2/d} & \omega \gg \omega_c \end{cases}$$

$\boxed{d > 2}$ Anderson Transition



"BRINKMAN - RICE" Phys. Rev. B $\underline{2}$, 302 (1970)

Based on Gutzwiller Phys Rev A $\underline{134}$, 927 (64);
A 137, 1726 (65)

Gutzwiller's idea for "Hubbard" model: ($\frac{1}{2}$ filled)

$$H = -t \sum c^{+}_{i\sigma} c_{j\sigma} + U \sum n_{i\uparrow} n_{i\downarrow}$$

for $U = 0$ $\quad \underline{\Psi} = \prod_{k<k_F} c^{+}_{k\sigma} |0\rangle$ — Slater det. $\begin{vmatrix} \psi_1(k_1\sigma_1) & \psi_1(k_2\sigma_2) & \dots \\ \psi_2(k_1\sigma_1) & \dots & \\ - & - & - \\ - & - & - \\ - & - & - \end{vmatrix}$

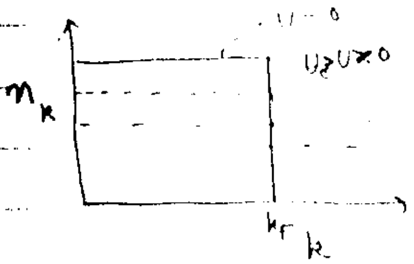
"Gutzwiller assumption"

$$\Psi \longrightarrow \underline{\Psi}_G = \underbrace{(g)}^{\#\text{ Doubly occ. sites}} |\Psi_0\rangle$$

convert to site basis
$|\psi_k\rangle = \sum_i e^{i\vec{k}\cdot\vec{r}_i} |i\rangle$

Minimise w.r.t. g.

"Gutzwiller approx" $\longrightarrow$ evaluating $\langle \Psi_G | H | \Psi_G \rangle$



"$U = U_c$" — $\frac{m^*}{m} \sim \frac{1}{\text{disc}} \sim \frac{1}{(U_c - U)} \longrightarrow \infty$

$$F_0^a \to -3/4$$

$$\boxed{\chi/\gamma \to 4\,\chi_0/\gamma_0}$$

$$\frac{\chi}{\chi_0} \sim \frac{m^*/m}{1+F_0^a} \longrightarrow \infty$$

$$\frac{\gamma}{\gamma_0} \sim m^*/m \longrightarrow \infty$$

$$K \sim \cancel{\frac{m^*/m}{\dots}} \longrightarrow \infty$$

LOCAL MOMENT FORMATION IN THE DISORDERED HUBBARD MODEL*

Milovanovic, Sachdev, Bhatt PRL 63, 82 (89)

$$H = -\sum_{j,\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i} U n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} (\epsilon_i - \mu) c^{+}_{i\sigma} c_{i\sigma}$$

Finite-T Hartree Fock

Positional Randomness $t_{ij} = 2\left(1 + \frac{r_{ij}}{a}\right) e^{-r_{ij}/a}$ $(U=1)$

$$\mathcal{H}_{eff} = -\sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + \sum_{i\sigma} (\tilde{\epsilon}_i - \mu) c^{+}_{i\sigma} c_{i\sigma} + \sum_i \vec{h}_i \cdot \vec{S}_i$$

$$\vec{S}_i \downarrow \frac{1}{2} c^{+}_{i\alpha} \vec{\sigma}_{\alpha\beta} c_{i\beta}$$

Use $F \le \langle H \rangle_{eff} - T S_{eff}$

As in Anderson Local Moment case, get extended one-electron eigenstates but localized susceptibility matrix eigenstates

LOCAL MOMENT DENSITY ~10% near n_c (not 0.1% or 99.9%)

*OPPOSITE TO SCALING APPROACH - Disorder exact, int. in HF

Anderson-Hubbard Model:

$$H = -\sum_{i\neq j,\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow} + \sum_{i\sigma} (\epsilon_i - \mu) c^\dagger_{i\sigma} c_{i\sigma}$$

$$\Big\downarrow \text{ effective field}$$

$$H_{eff}\,[\tilde{\epsilon}_i, \vec{h}_i] = -\sum_{ij\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + \sum (\tilde{\epsilon}_i - \mu)\, c^\dagger_{i\sigma} c_{j\sigma} + \sum_i \vec{h}_i \cdot \vec{s}_i$$

$$\left[\vec{S}_i^{\,\lambda} = c^\dagger_{i\alpha}\, \sigma^\lambda_{\alpha\beta}\, c_{i\beta}/2 \qquad \lambda = x, y, z\right]$$

$$F_{eff} = \langle H \rangle_{eff} - T S_{eff}$$

Minimize:

$$\tilde{\epsilon}_i = \epsilon_i + U \sum |\underbrace{\psi_\alpha(i)}_{\text{wave fn.}}|^2 f(\underbrace{\lambda_\alpha}_{\text{eigenvalues}})$$

To $O(h^2)$

$$F_{eff} = F_{eff}(\tilde{\epsilon}_i, \vec{h}_i = 0) + \sum_{ijk} \frac{\chi_{ij}}{4} (\delta_{jk} - U \chi_{jk}) (\vec{h}_i \cdot \vec{h}_k) + O(h^4)$$

$$\leftarrow \quad \chi_{ij} = -\sum_{\alpha\beta} \psi_\alpha(i) \psi^*_\alpha(j) \psi^*_\beta(i) \psi_\beta(j) \frac{f(\lambda_\alpha) - f(\lambda_\beta)}{\lambda_\alpha - \lambda_\beta}$$

SINGLE IMPURITY CASE

(Anderson; Wolff)

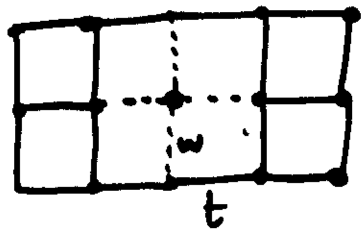
Particle hole symmetry

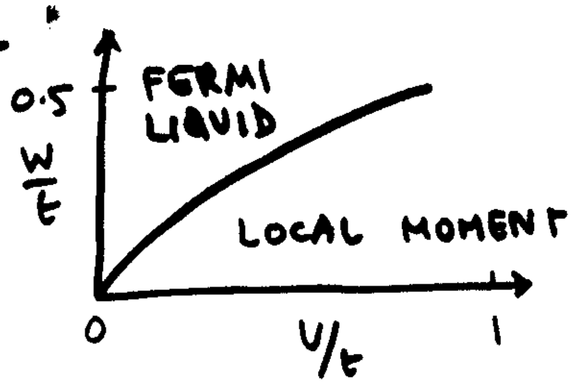
$\mu = \tilde{\epsilon}_i = U/2$

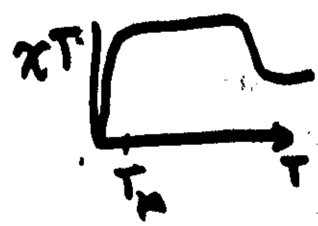
Single ev of χ_{ij}

split off from top of

band $K_\beta = 1/U$ determines phase boundary.







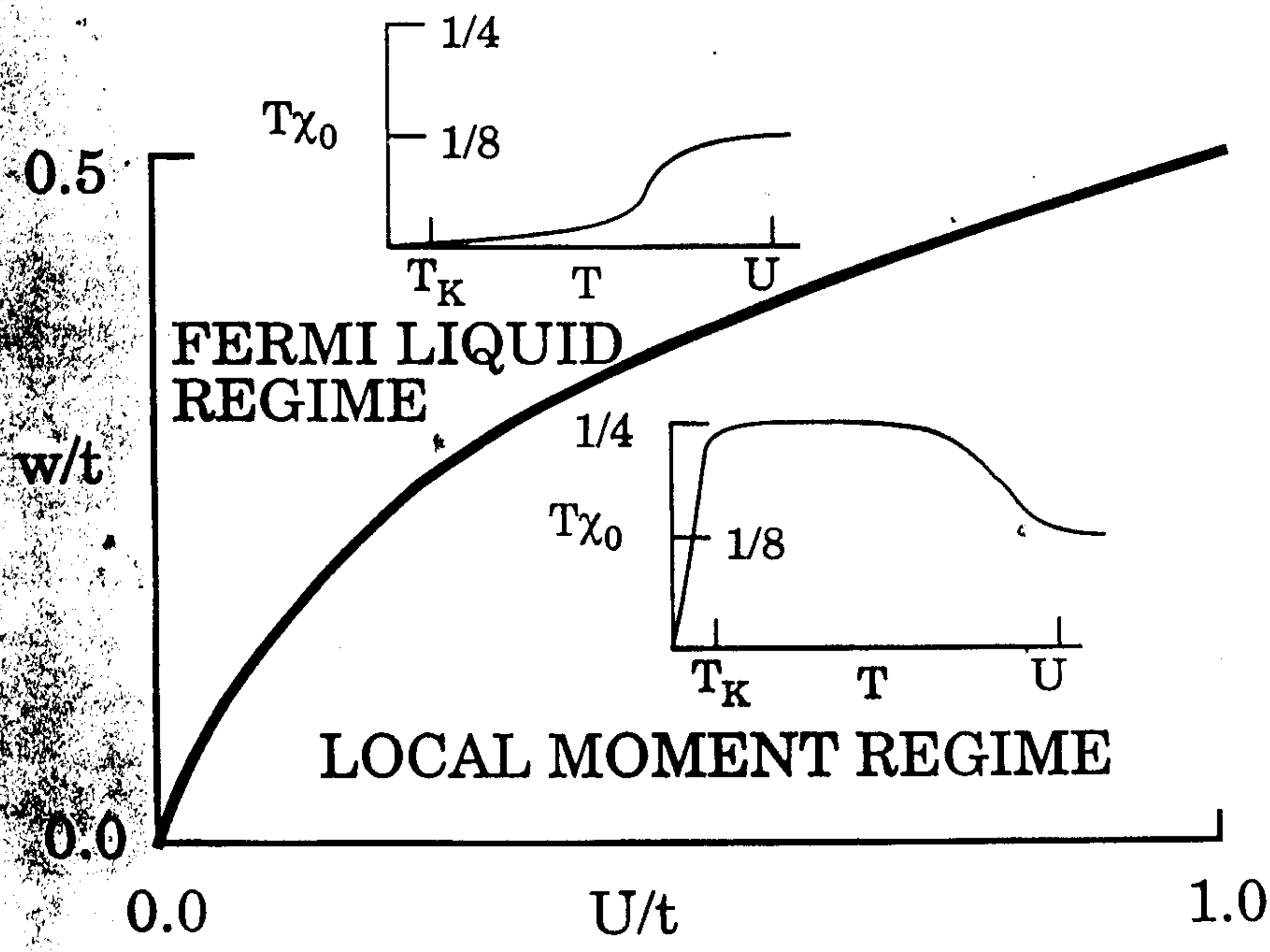
DISORDERED SYSTEM

$$t_{ij} = 2\left(1+\frac{r_{ij}}{a}\right) e^{-r_{ij}/a} \qquad U = 1$$

half filling ~50%   get ~10% local moment instabilities

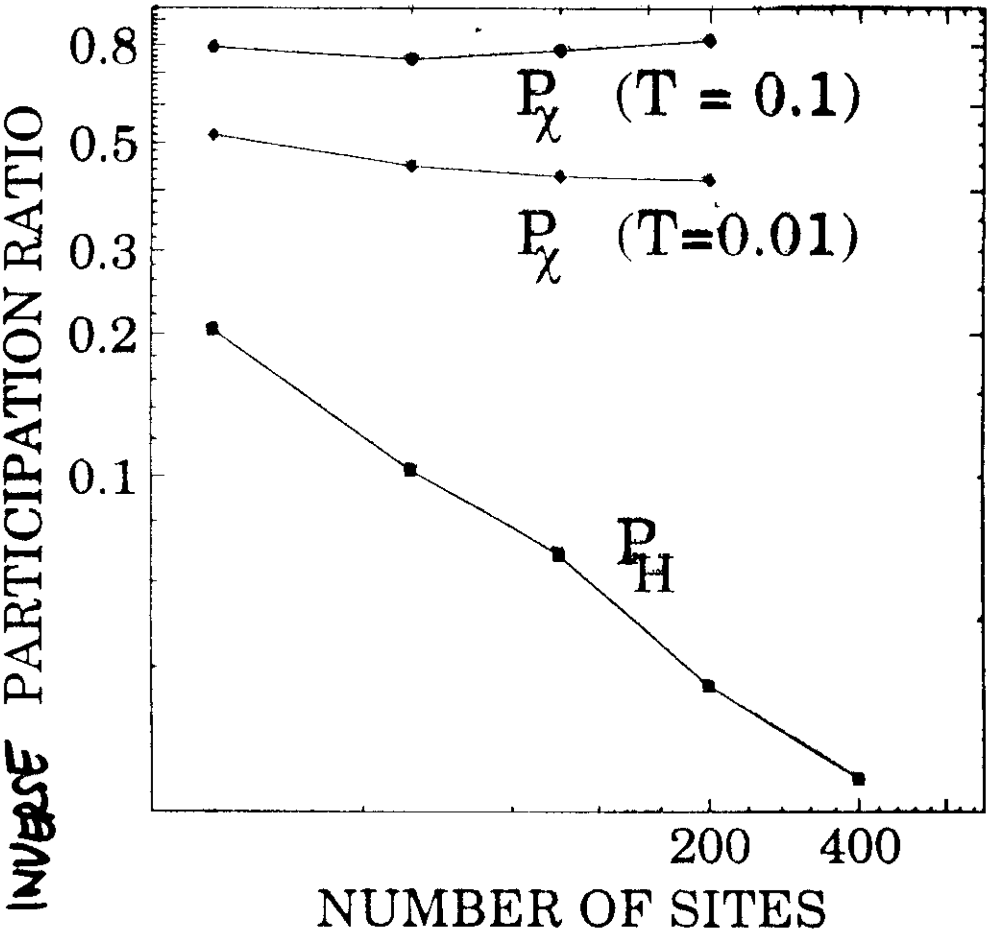
(not 0.1% or 99.9%)

Moments very localized ⇒ independent



1/4
Tχ0
1/8
0.5
T_K
T
U
FERMI LIQUID
REGIME
1/4
w/t
Tχ0
1/8
T_K
T
U
LOCAL MOMENT REGIME
0.0
0.0
U/t
1.0

Milovanovic, Sachdev & Bhatt (89)

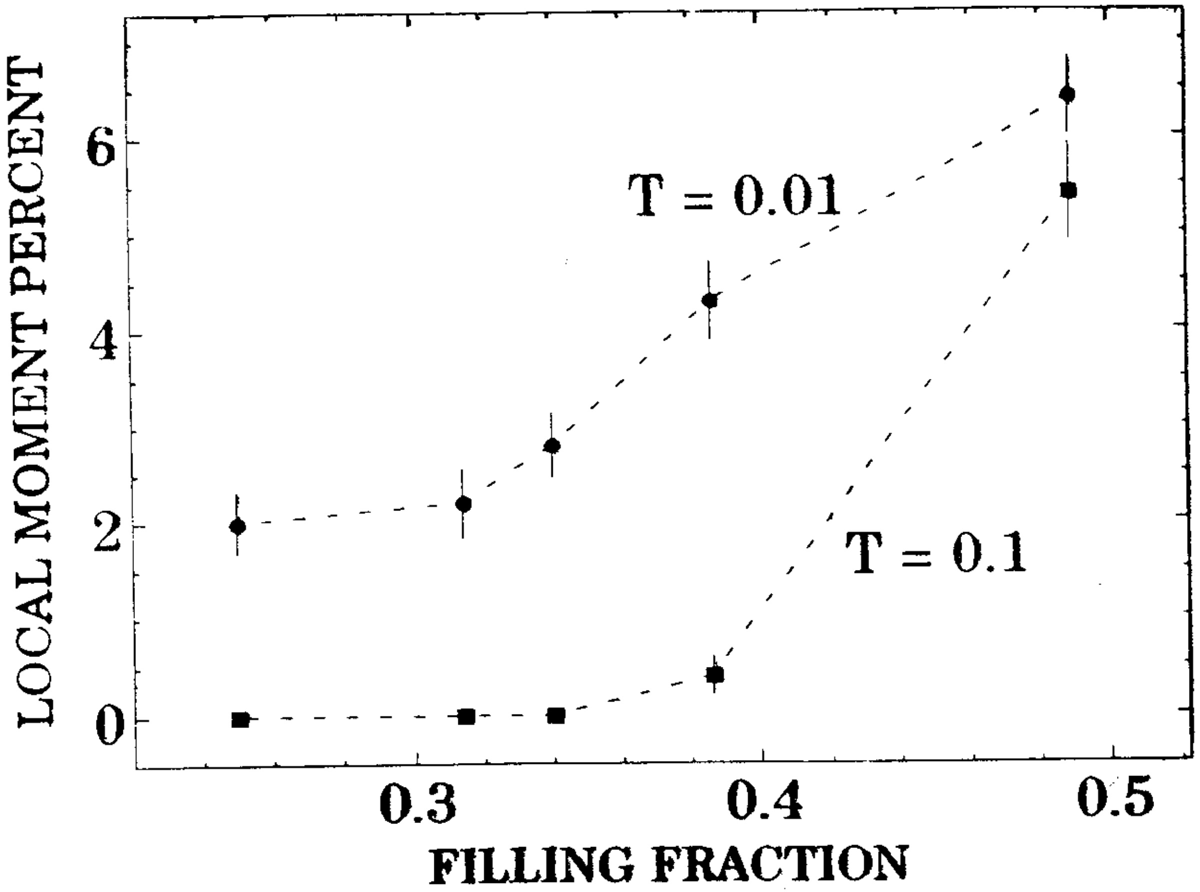


$$\mathrm{IPR} \equiv \frac{\sum_i |\psi_i|^4}{\left(\sum_i |\psi_i|^2\right)^2} - \begin{cases} \sim 1 & \text{localized} \\ \frac{1}{N} & \text{extended} \end{cases}$$

~50% above n_c

Hartree Fock

+ Exact Disorder.

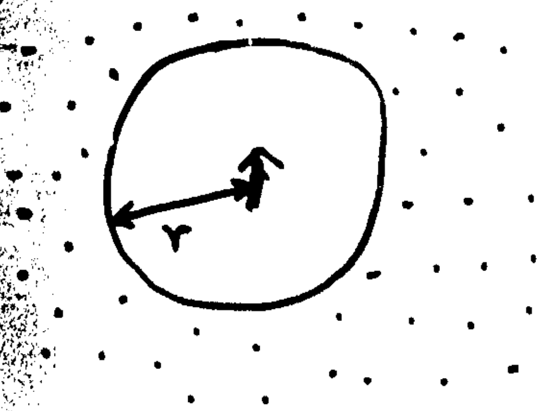


Milovanovic, Sachdev & Bhatt (89)

VG. NO.

KONDO QUENCHING OF RARE SITES/CLUSTERS

[R.N. Bhatt + D.S. Fisher, PRL 68, 3072 (1992)]



Sites with local moments, with an isolation region r gives Curie ($1/T$) susceptibility, provided

$$\boxed{\text{Kondo temp} < T}$$

For Poisson distribution, prob. of isolation region r

$$P(r) = \exp\left[-\frac{4\pi}{3} n r^3\right]$$

$$\therefore \quad \chi(T) = \int_{r_T}^{\infty} \frac{n P(r)\, d^3 r}{T} = \frac{1}{T} \exp\left[-\frac{4\pi}{3} n r_T^3\right]$$

where $T_{\text{kondo}}(r_T) = T$

$$\text{Now,} \quad T_K \sim E_F \exp\left[-\frac{1}{\rho J(r)}\right]$$

$$J(r) \sim \frac{t^2}{u} \sim \exp(-\lambda r)$$

Dobroselvjevic
Kirkpatrick
Kotliar
PRL (1992)

$$\Rightarrow \quad T_K \sim E_F \exp\left[-\frac{e^{\lambda r}}{\rho}\right]$$

$$\therefore \quad r_T \sim \frac{1}{\lambda} \ln\left[\rho \ln\left(\frac{E_F}{T}\right)\right]$$

$$\Rightarrow \quad \chi(T) \sim \frac{1}{T} \exp\left[-\frac{4\pi n}{3\lambda^3} \ln^3\left(\rho \ln \frac{E_F}{T}\right)\right]$$

$$\longrightarrow \infty \quad \text{as } T \to 0$$

Can show $\gamma = \frac{C_V}{T} \to \infty$ as $T \to 0$ Similarly

[in $d > 1$ $\quad \chi(T) \sim \dfrac{\exp -[\ln\ln\frac{1}{T}]^d}{T}$

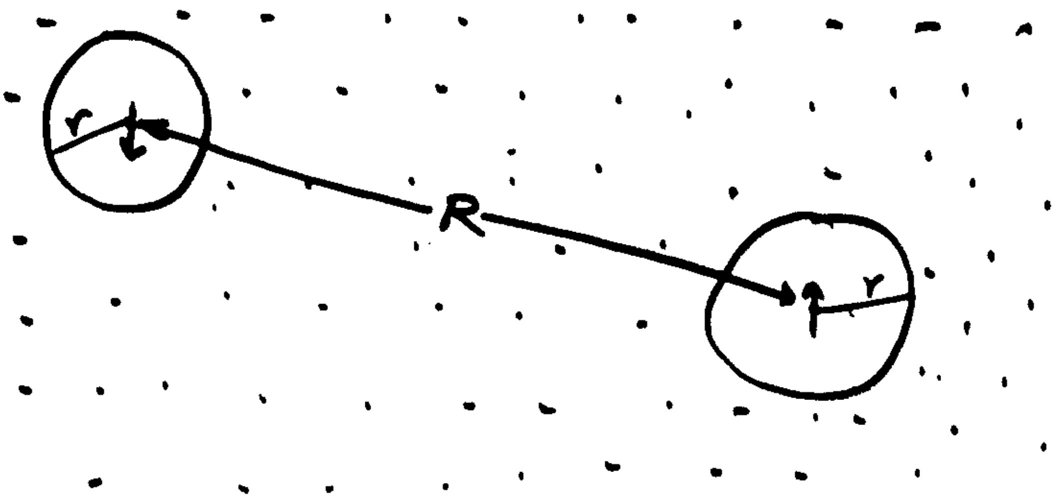
$d = 1$ $\quad \chi(T) \sim T^{-x}$

$x < 1$]

$\Rightarrow$ THESE RARE SITES ARE SO WEAKLY COUPLED TO ITINERANT FLUID THAT A KONDO-TYPE QUENCHING IS NOT EFFECTIVE ENOUGH TO KILL THE DIVERGENCE IN $\chi(T)$ as $T \to 0$.

(χ is product of $\frac{1}{T}$ and # of sites, and sites get quenched as a slower fn. of T)

RKKY INTERACTIONS



· Typical distance R to an "r-isolated" site

$$\frac{4\pi n}{3} R^3 \; P(r) \sim 1$$

$$\Rightarrow \quad R^3 \sim \frac{3}{4\pi n} \, e^{\frac{4\pi}{3} n r^3}$$

RKKY interaction between pair

$$J_{RKKY}(R) = \frac{J^2(r)}{R^3} \quad \text{(oscillatory fn.)}$$

Assume <u>all</u> RKKY are antiferromagnetic <u>and</u> whenever a pair has $J_{RKKY} \sim T$, they form singlet.

This should <u>underestimate</u> susceptibility

So $$\chi(T) \sim \frac{1}{T} \exp\left[-\frac{4\pi}{3} n \tilde{r}_T^{\,3}\right]$$

where $\tilde{r}_T$ is such that the corresponding

$J_{RKKY}(R_T) \sim T$.

i.e. $$T = \frac{J^2(\tilde{r}_T)}{R_T^{\,3}}$$

also $$\frac{4\pi}{3} n R_T^3 = \exp\left[+\frac{4\pi}{3} n \tilde{r}_T^{\,3}\right]$$

$$\therefore \chi(T) \sim \frac{3}{4\pi n\, R_T^3 T} \sim \frac{3}{4\pi n\, J^2(\tilde{r}_T)}$$

$$\sim \exp\left[\ln \frac{1}{T}\right]^{1/d}$$

(for d-dimen.)

$$\rightarrow \infty \text{ as } T \rightarrow 0$$

but <u>slower</u> than power law.

Actual χ may be higher.

Thus even in the "metallic" phase

non-Fermi liquid behavior

i.e. $\chi(T) \xrightarrow[T\to 0]{} \infty$

$$\gamma(T) \equiv \frac{C_v}{T} \xrightarrow[\text{as } T\to 0]{} \infty$$

Analogous to Griffiths Singularities in random magnets (eg. spin glass) where long time dynamics dominated by rare clusters. (in principle)

How strong effects are will depend on systems ~~-~~ Poisson distributed sites particularly good because of "maximal randomness" at microscopic level. But in Principle should apply to all systems undergoing MI Transition to an Insulating phase with local moments.

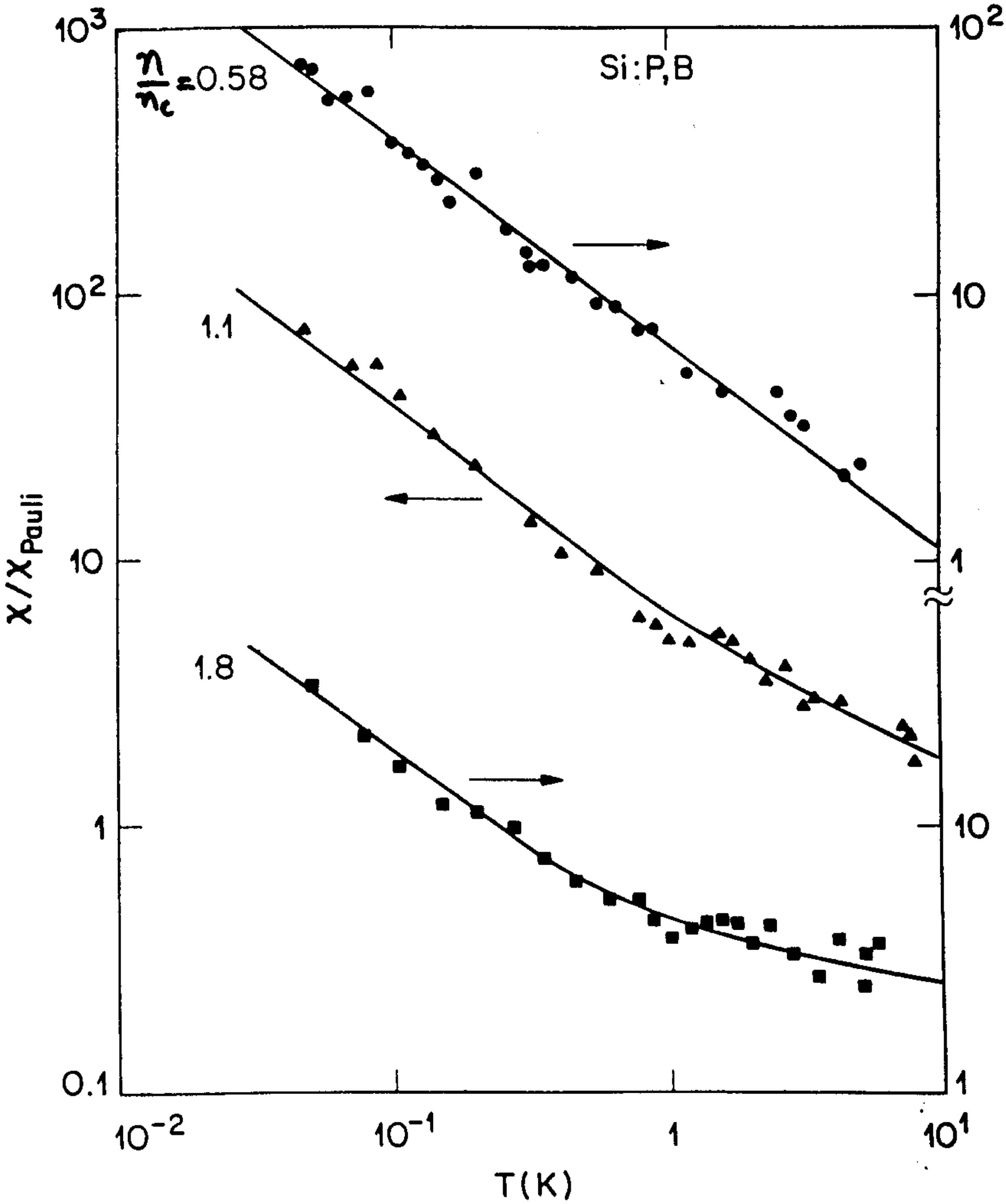
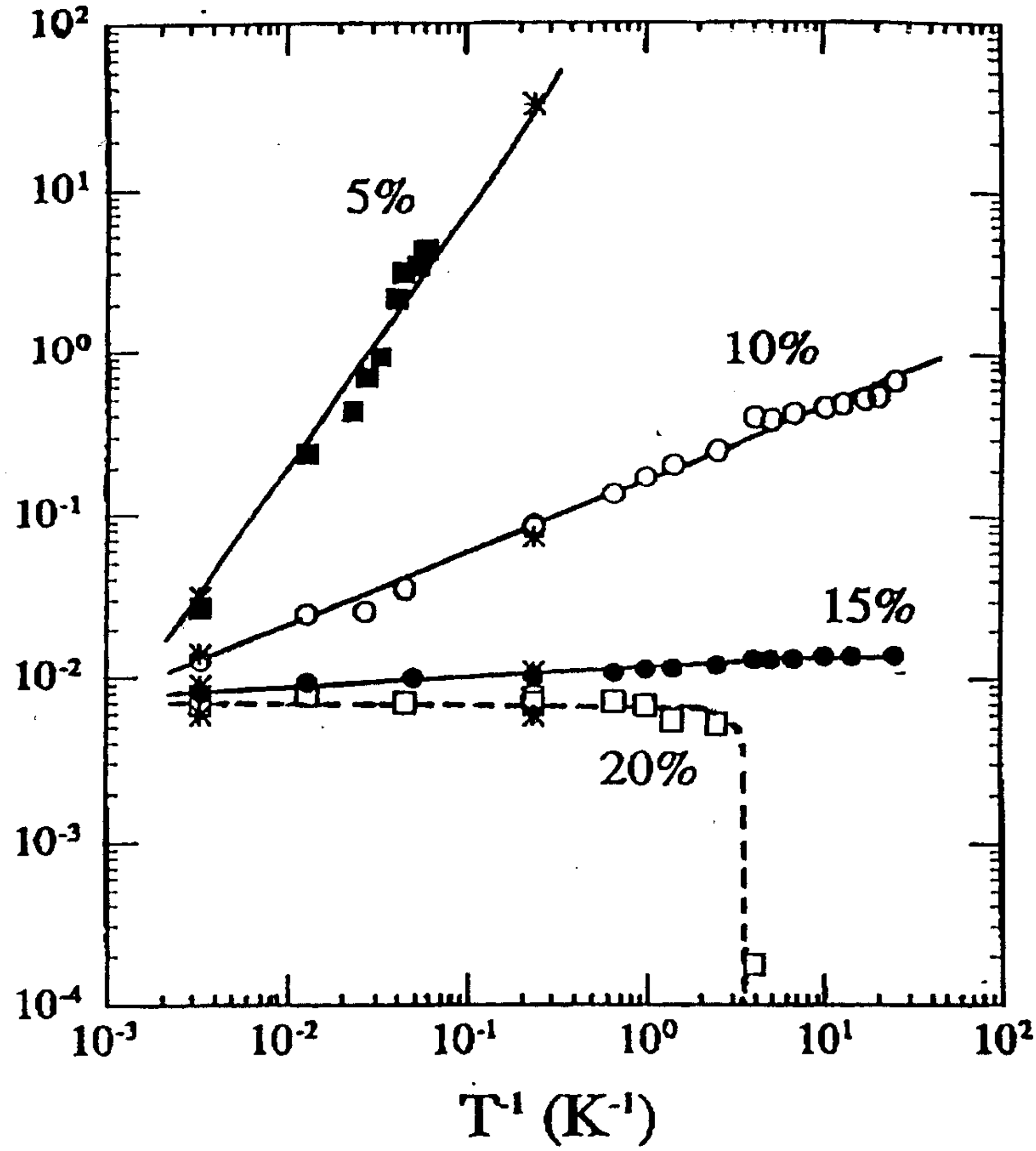


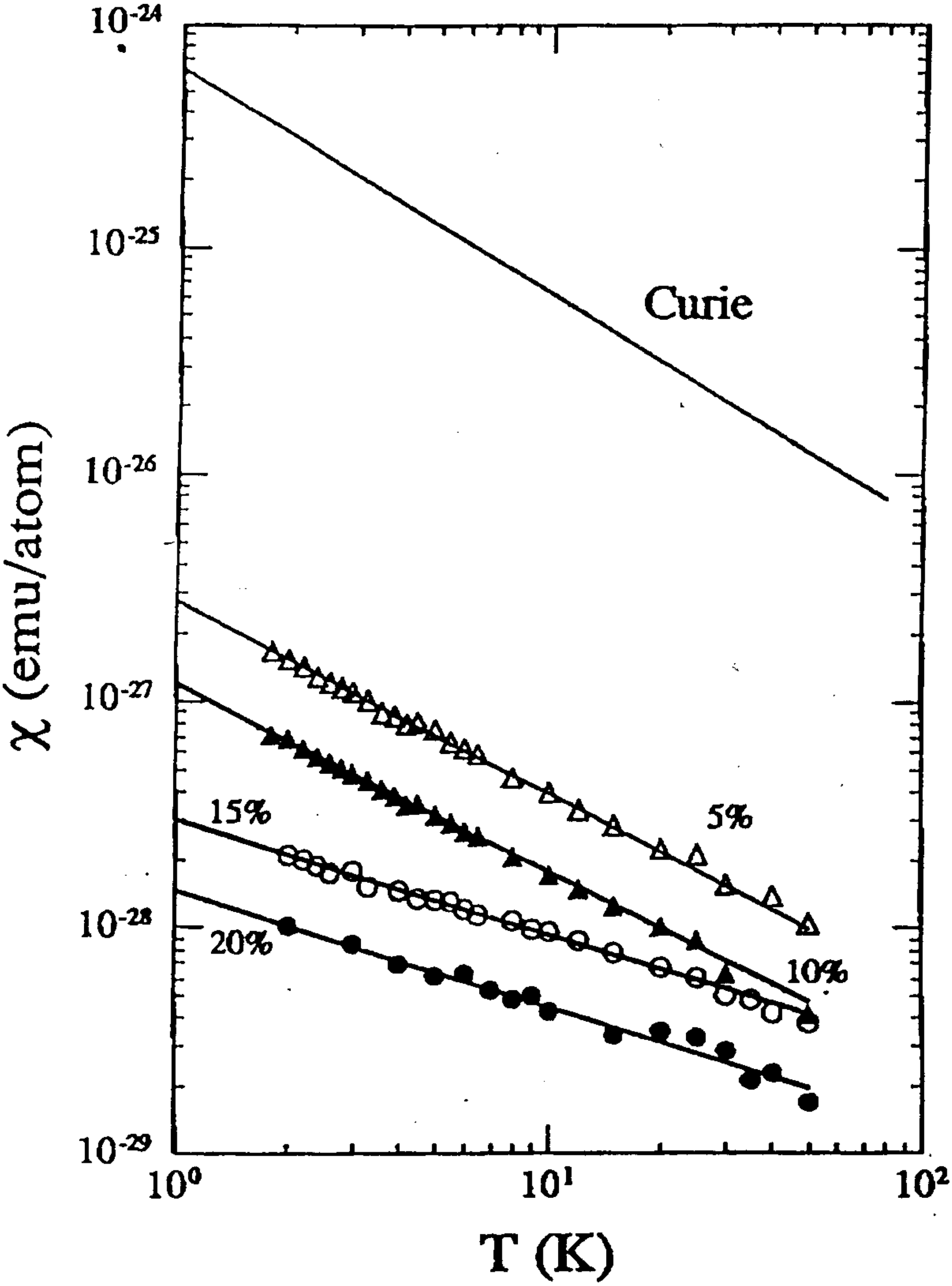
FIG. 1

Hirsch, Holcomb, Bhatt + Paalanen
PRL 68, 1418 (1992)



10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
ρ (Ωcm)
5%
10%
15%
20%
10^{-3}
10^{-2}
10^{-1}
10^0
10^1
10^2
T^{-1} (K^{-1})

Nb-Si ($n_c \approx 11.5\%$)



Allen, Paalanen & Bhatt ([redacted])
Europhys. Lett (1993)

CONCLUDING REMARKS / FUTURE DIRECTIONS

1. DISORDERED METAL $\neq$ FERMI LIQUID ($\chi \to$ const; $\frac{C}{T} \to$ const as $T \to 0$)

   Instead $\sigma \to$ const
   but χ, $\frac{C}{T} \to \infty$ } as $T \to 0$

2. OTHER SYSTEMS:
   (a) Nb-Si
   (b) Larger value in (compensated) Si: P, B
   χ
   Y. Huo & R.N.B. (in preparation)
   $\Rightarrow$ more local moments ?
   or more ferromagnetic interactions?

3 INTERESTING EXTENSIONS -
   Disordered (Amorphous) Heavy Fermions
   Low dimensional analogs (eg. δ-doped semicond, - 2D)
   Magnetic ions in systems near MI Transition

4. Here DISORDER essential; other cases
   - Quadrupolar Kondo
   - high T_c cuprates (?)