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SMR.627-9

MINIWORKSHOP ON
STRONGLY CORRELATED ELECTRON SYSTEMS

15 JUNE - 10 JULY 1992

"Strongly Correlated Systems in Infinite Dimensions"

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

STRONGLY CORRELATED SYSTEMS IN INFINITE DIMENSIONS

A QUANTITATIVE DESCRIPTION OF THE METAL-INSULATOR TRANSITION IN THE 1-BAND HUBBARD MODEL ($n=1$)

Physical motivations:

- liquid ^3He { - 'incoherent' regime $T \gtrsim T_{S.F}$; - magnetic properties }
- Mott insulators (V_2O_3 etc...)

MAIN MESSAGE:

The $d \to \infty$ limit is the natural generalization to itinerant quantum systems of the concept of 'mean-field' theory in stat. mech.
It retains non-trivial physical ingredients,
While allowing quantitative resolts -

G. KOTLIAR (Rutgers)
W. KRAUTH (ENS)
Q. Si (R)

pioneers:
W. Metzner
D. Vollhardt

DIFFICULTIES :

- Energy scales $kT \ll t \lesssim U$
- Interplay of :

  * 'atomic' (on-site) aspects

  4 states / site $|0\rangle\ |\uparrow\rangle\ |\downarrow\rangle\ |\uparrow\downarrow\rangle \rightarrow$ degeneracies, fluctuations

  * itinerant aspects $\rightarrow$ spatial correlations

$d \to \infty$ describes both on equal footing

long-wavelength $\longrightarrow$ on-site $\quad d$

long-wavelength		on-site
spatial fluctuations (~ spin waves)	- - - - -	temporal ($\tau = it$) fluctuations
~ small $\vec{k}$ expansion		~ instantons (tunnel)

WELL-CONTROLLED LIMITS :

- $d = 1$
- Large degeneracy ('N')
- MEAN FIELD ?!

OUTLINE ...

0\. HOW TO FORMULATE THE $d \to \infty$ limit

1\. THE EXACT 'MEAN-FIELD' PICTURE

2\. CONNECTION W/ 1-IMPURITY KONDO-LIKE PROBLEMS

3\. METHODS OF SOLUTION AND RESULTS :
- phases and phase transitions
- excitation spectrum (1-particle)
- Thermodynamics : C_V vs. T, S vs. T
- Magnetic properties

4 - SOME REMARKS / EXPERIMENTS - (^3He)

5 - PROSPECTS, WORK IN PROGRESS ...

$$\hat{H} = -\sum_{\langle ij\rangle \sigma} t_{ij}\, c^{+}_{i\sigma} c_{j\sigma} + h.c + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

n.n hopping on a lattice of connectivity z

Want to consider $z \to \infty$ limit

HAVE TO SCALE $t_{ij} = \frac{t^*}{\sqrt{2z}}$

ex 1: hypercubic lattice ($z = 2d$) $\to \infty$

$$\varepsilon_k = -2t \sum_{i=1}^{d} \cos k_i \sim t\sqrt{d}$$

More precisely: free ($U=0$) d.o.s

$$D(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_k) \longrightarrow \frac{1}{\sqrt{\pi}} e^{-\varepsilon^2} \qquad (t^* = 1)$$

ex 2: Bethe lattice $z \to \infty$

'like a big matrix'

$$D(\epsilon) \longrightarrow \frac{1}{\pi}\sqrt{2-\epsilon^2} \quad \epsilon \in [-\sqrt{2}, \sqrt{2}]$$

Remarks

- tails in ex. 1
- cf. frustrated spin models
- Exchange $J_{ij} \sim \frac{t_{ij}^2}{U} = O\left(\frac{1}{d}\right) \to 0$ fixed (ij)

  but $J = \sum_{j\ \text{n.n of}\ i} J_{ij} = O(1) \to$ finite T_{Neel}.

It is interesting to compare $N_d(E)$ for different d as shown in Fig. 1.2.

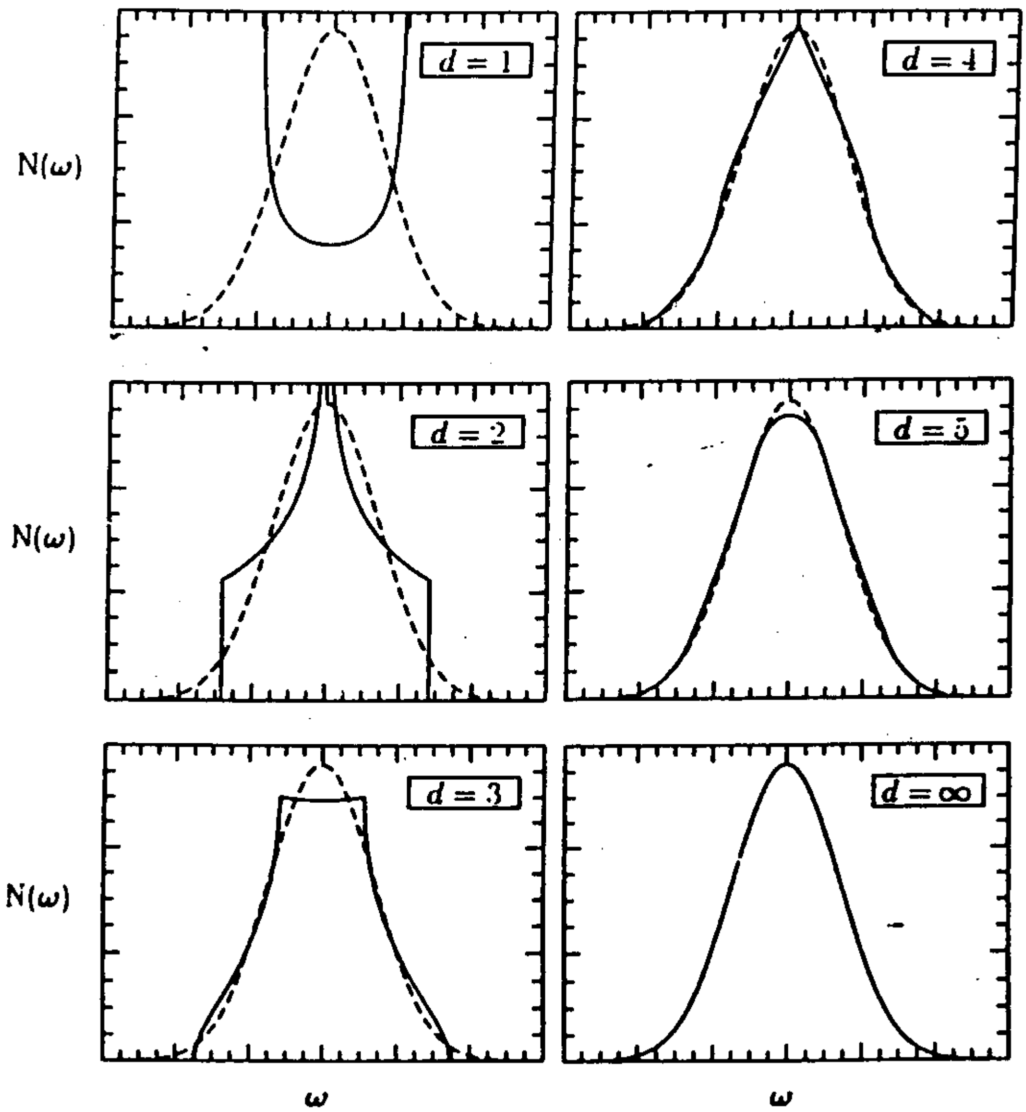


Fig. 1.2 Tight-binding density of states in $d = 1, 2, 3, 4, 5$ as compared with the result for $d = \infty$. (from D. Vollhardt's review).

EARLIER WORKS :

Metzner & Vollhardt '88

→ Variational wave functions (Gutzwiller...)
Metzner, Vollhardt, Gebhardt, Van Dongen, ...

→ Weak-coupling studies
Müller-Hartmann, Menge, Schweitzer, Czycholl, ...

→ Exact solutions, G.F techniques
* Brandt & Mielsch, Van Dongen

FACTS AND FANCY REGARDING $d=\infty$

- Hartree-Fock does NOT become exact
- Gutzwiller approximation becomes exact for the evaluation of averages with the G. wave function
- G.W.F is NOT the exact g.s w.f
- Weak-coupling expansions simplify remarkably: all propagators can be taken to be local in a skeleton diagram.

  In particular: $\Sigma = \Sigma(i\omega_n)$
- Magnetic exchange & correlations are not suppressed in the $d \to \infty$ limit

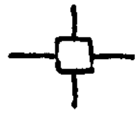
  Note : $J_{ij} \sim \frac{t_{ij}^2}{U} \sim \frac{1}{d} \to$ finite magnetic energy.

$$G(\vec{k}, i\omega_n) = \left[i\omega_n + \mu - \varepsilon_{\vec{k}} - \Sigma\right]^{-1} \quad \text{(no LRO)}$$

THE [EXACT] "MEAN-FIELD" PICTURE -

G + G. Kotliar
ndt + Mielsch
Janis.

= (a) A single-site (quantum) problem


: $|0\rangle \quad |\uparrow\rangle \quad |\downarrow\rangle \quad |\uparrow\downarrow\rangle$

(b) A self-consistency condition.


site <-> environment

N.B: Ising model (a) $H_{site} = \sum_i h_i^{eff} S_i$

$(m_i = \tanh(\beta h_i))$.

(b) $h_i^{eff} = \sum_{j(i)} J_{ij} m_j$

Here:

(a) $c_\sigma(\tau)$ obeying the quantum dynamics:

$$\boxed{S = U\int_0^\beta d\tau\, n_\uparrow(\tau) n_\downarrow(\tau) + \sum_\sigma \int_0^\beta d\tau \int_0^\beta d\tau'\, c_\sigma^+(\tau)\, G_0^{-1}(\tau-\tau')\, c_\sigma(\tau')}$$

$\rightarrow$ solve for $G_{imp}^{-1}[G_0; i\omega_n] = G_0^{-1}(i\omega_n) - \Sigma_{imp}[G_0; i\omega_n]$

(b) $\Sigma_{imp} = \Sigma$, provided G_0 is chosen such that:

$\sum_{\vec{k}} G(\vec{k}, i\omega_n) = G_{imp}(i\omega_n)$, i.e:

$$\boxed{G_{imp}(i\omega_n) = \int_{-\infty}^{+\infty} \frac{d\epsilon\, D(\epsilon)}{i\omega_n + \mu - \Sigma_{imp}(i\omega_n) - \epsilon}}$$

REMARKS

* $U = 0$: (a) $\to \begin{cases} G = G_0 \\ \Sigma = 0 \end{cases}$ (b) $\to G = G_{free}$
* $t_{ij} = 0$: $D(\epsilon) = \delta(\epsilon)$

  (b) $\to G = (i\omega_n + \mu - \Sigma)^{-1} \Rightarrow G_0^{-1} = i\omega_n + \mu$

  (a) $\to G = G_{atomic}$ (S = hamiltonian pb.)
* $\Sigma(\omega)$ is only frequency-dependent.
* free energy, response functions ? $\sim \Gamma_{imp}(\tau_1 \cdots \tau_4)$
* Phases w/ magnetic LRO

(a) $S = \int_0^\beta U n_\uparrow n_\downarrow \, d\tau - \sum_\sigma \int d\tau \int d\tau' \, c_\sigma^+(\tau) G_{0\sigma}^{-1}(\tau - \tau') c_\sigma(\tau')$

(b) F : $G_\sigma(i\omega_n) = \tilde{D}(i\omega_n + \mu - \Sigma_\sigma)$

AF : $G_\sigma(i\omega_n) = \sqrt{\frac{\zeta_{\bar\sigma}}{\zeta_\sigma}} \, \tilde{D}\left(\sqrt{\zeta_\sigma \zeta_{\bar\sigma}}\right)$ $\quad \zeta_\sigma \equiv i\omega_n + \mu - \Sigma_\sigma$

* "FALICOV-KIMBALL" model

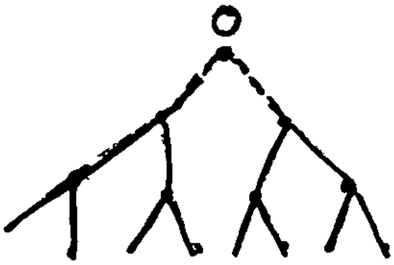
  $t_\uparrow \neq t_\downarrow = 0 \longrightarrow$ exact solution in $d = \infty$

  (Brandt & Mielsch '89)

MAIN DIFFICULTY :

SOLVE THE 1-SITE PB. FOR AN ARBITRARY $G_0(\tau)$. ?

"CAVITY - METHOD" DERIVATION



Bethe lattice coordination z

$t_{ij} = \frac{1}{\sqrt{z}}$ n.n

$z \to \infty$

$$Z = \int \prod_i Dc_i Dc_i^+ e^{-S} \qquad S = S_0 + S' + S_{0-n}$$

$$\begin{cases} S_0 = \int_0^\beta d\tau \left[\sum_\sigma c_{0\sigma}^+ (\partial_\tau + \mu) c_{0\sigma} - U n_{0\uparrow} n_{0\downarrow} \right] \\ S' = \int_0^\beta d\tau \sum_{i,j \neq 0} c_{i\sigma}^+ \left[(\partial_\tau + \mu)\delta_{ij} - t_{ij} \right] c_{j\sigma} - U \sum_{i \neq 0} n_{i\uparrow} n_{i\downarrow} \\ S_{0-n} = - \int_0^\beta d\tau \sum_{i,\sigma} t_{i0} (c_{i\sigma}^+ c_{0\sigma} + h.c) \end{cases}$$

Integrate over $\{c_{i\sigma}, c_{i\sigma}^+\}$ for $i \neq 0$: S_{0-n} is a source t°

$$S_{eff} = S_0 - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{i,j,\sigma} t_{i0} t_{j0} c_{i\sigma}^+(\tau) G'_{ij}(\tau - \tau') c_{j\sigma}(\tau')$$
$$- \int d\tau_1 .. d\tau_4 \sum_{ijkl} t_{i0} t_{j0} t_{k0} t_{l0} c^+ c^+ G'(1,2,3,4) c c$$
$$+ \cdots$$

But : $\sum_i t_{i0}^2 = z \cdot \frac{1}{z} = 1$, $\sum_i t_{i0}^4 = \frac{1}{z}$ etc ...

Thus :

$$S_{eff} = \int_0^\beta d\tau \left[\sum_\sigma c_{0\sigma}^+ (\partial_\tau + \mu) c_{0\sigma} - U n_{0\uparrow} n_{0\downarrow} \right] - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_{0\sigma}^+(\tau) G'_{ii}(\tau - \tau') c_{0\sigma}(\tau')$$

Thus :

$$\underline{i\omega_n + \mu - \mathcal{G}_0^{-1} = G'_{ii} = G_{ii}} \qquad (\infty \text{ lattice})$$

boils down to $G = \int \frac{d\varepsilon D(\varepsilon)}{\cdots}$ for semi-circular $D(\varepsilon)$)

MAIN TASK:

SOLVE FOR A COUPLED (G_0, G)-
Iterative procedure:

$$\begin{tikzcd} G_0 \arrow[rr, bend left, "\text{solution of impurity pb.}\ (S)"] & & G \arrow[ll, bend left, "\text{self-consistency eq.}"] \end{tikzcd}$$

$\longrightarrow$ is the hard part (non-linear, non local)

Methods:

① GUESSING... (w/ G.K)

② "ITERATED PERTURBATION THEORY" in U

(w/ G.K, then X.Y Zhang et al

③ FULL NUMERICAL SOLUTION

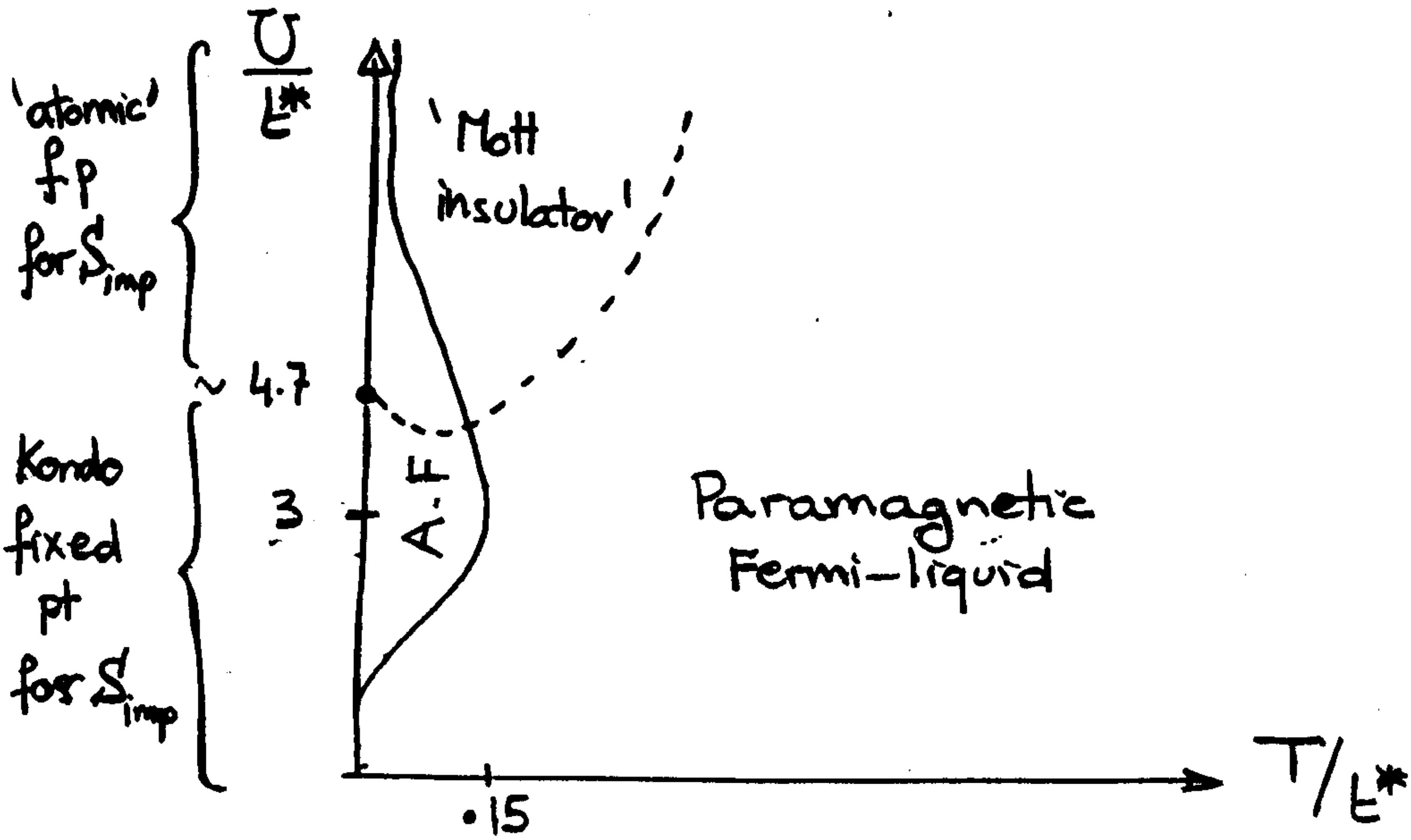
$\Longleftrightarrow$ 1d Ising problem w/ LR. int

$$e^{-\Delta\tau U n_\uparrow n_\downarrow} = \frac{1}{2}\mathop{Tr}_{\sigma}\, e^{\lambda\sigma(\tau)[n_\uparrow - n_\downarrow]} + -$$

A.G + W. KRAUTH exact enumeration

$\left.\begin{array}{l}\text{Zhang, Rozenberg, Kotliar} \\ \text{M Jarrell}\end{array}\right\}$ M. Carlo

PHASE-DIAGRAM AT HALF-FILLING.



N.B: The paramagnetic Mott insulator can be stabilised as the ground-state of an alternative model (w/disorder).

(A.G w/ S. Sachdev, D.S Fisher)

cf 3D T_N vs. U

CONNECTION w/ 1-impurity ANDERSON MODEL

Write a spectral representation for G_0^{-1}:

$$i\omega_n + \mu - G_0^{-1}(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega\, \Delta(\omega)}{i\omega_n - \omega}$$

Then S_{imp} describes the dynamics of a d-orbital hybridized w/ a conduction band of d.o.s $\Delta(\omega)$:

$$H_{AM} = \sum_{k\sigma} \omega_k a^+_{k\sigma} a_{k\sigma} - \mu \sum_{\sigma} d^+_\sigma d_\sigma + U n_{d\uparrow} n_{d\downarrow}$$
$$+ \sum_{k\sigma} V_k a^+_{k\sigma} d_\sigma + h.c$$

with $\Delta(\omega)_{A.M} = \sum_k |V_k|^2 \delta(\omega - \omega_k)$

But here $\Delta(\omega)$ is not known a-priori: it is self-consistently related to the <u>solution</u> of S_{imp}!

(Bethe lattice: $\Delta(\omega) = \rho(\omega)$)

POSSIBLE FIXED POINTS FOR THE PARAMAGNETIC SOLUTION AT HALF-FILLING

$\left(\epsilon_d = -\mu = -\frac{U}{2} \right)$

* FERMI-LIQUID FIXED POINT

(as long as $\Delta(0) \neq 0$ and $W_0 \neq 0$)

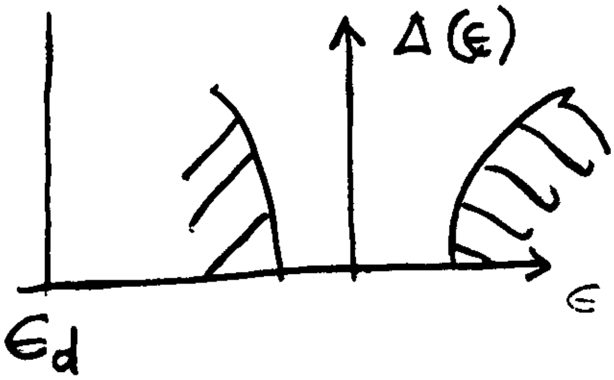
Local moment quenched by Kondo effect

virtual hybridization $\rightarrow J_K \sim \frac{V^2}{|\epsilon_d|}$ (Schrieffer-Wolff)

R.G flow to STRONG KONDO COUPLING

* INSULATING FIXED POINT

($\Delta(\epsilon)$ has zero weight around $\varepsilon = 0$)



NO Kondo effect $\rightarrow$ local moment

R.G flow to WEAK KONDO COUPLING –

THE F.L REGIME **MUST** BE UNSTABLE FOR LARGE ENOUGH U $\rightarrow$ Mott insulator

(Recall : within the paramagnetic solution)

A.G+W. Krauth ; Rozenberg, Zhang, Kotliar

- When U increases, one has to solve a Kondo problem in which the width of $\Delta(\epsilon)$, W_0, is the smallest scale.

Then $T_K[W_0] \propto \underline{\underline{W_0}}\, f(U)$ (eg poor man's scaling)

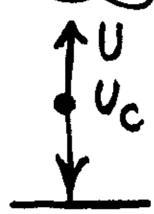
- But self-consistency eq. implies $W_0^{n+1} \sim T_K^{(n)}$

Therefore $W_0^{(n+1)} \propto W_0^{(n)} f(U)$ and $W_0^{(n)} \xrightarrow[n\to\infty]{} 0$ if $f(U) < 1$ (which holds for large U).

$\Delta(\epsilon)$ acquires a gap $U > U_c$:

NO Kondo effect (magnetic imp in an insulator) $\rightarrow$ local moment

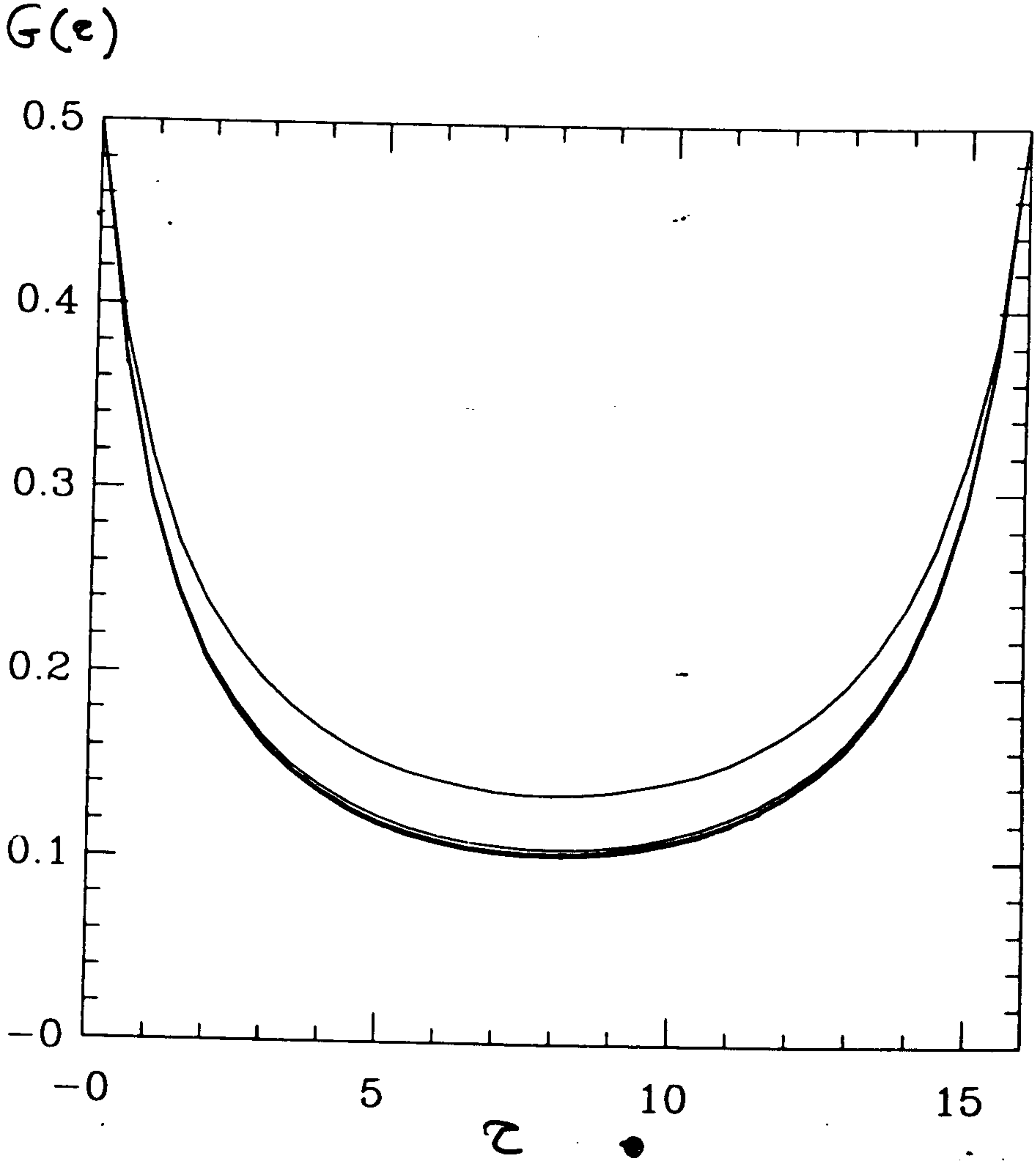
Physics is controlled by WEAK KONDO coupling fixed point (i.e ATOMIC limit)



U = 1 β = 16 Δτ = .5

20.000 M.C sweeps.

w/ W. KRAUTH
dec '91



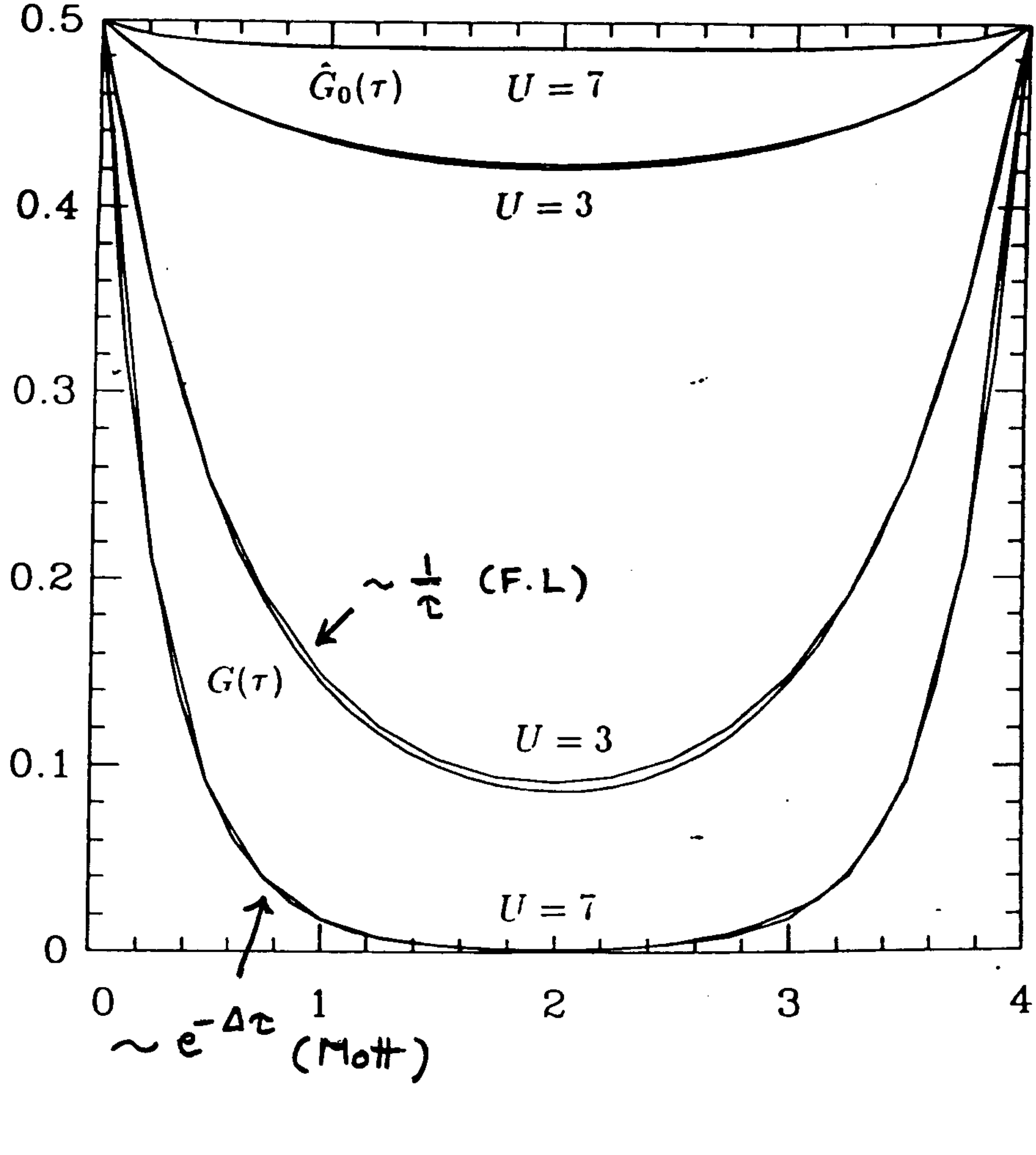

0.5
0.4
0.3
0.2
0.1
0
0
1
2
3
4
$\hat{G}_0(\tau)$
$U = 7$
$U = 3$
$\sim \frac{1}{\tau}$ (F.L)
$G(\tau)$
$U = 3$
$U = 7$
$\sim e^{-\Delta\tau}$ (Mott)

fig. 1

FL behaviour of the paramagnetic solution for moderate U ($\frac{1}{2}$ filled-case).

Impurity model:

Local moment quenched by Kondo effect $T \lesssim T_K$

$\Sigma(\omega) \sim \Sigma(0) + \left(1 - \frac{1}{z}\right)\omega + i\gamma\omega^2 + \cdots$ $\omega \to 0$ $T \to 0$: FL

$z \sim T_K$ low energy scale for spin fluctuations

Lattice model: 3 temperature regimes

$T \lesssim T_K$ FL description applies

$$\frac{m^*}{m} = z^{-1} \sim T_K^{-1} \qquad C_v \propto \frac{T}{T_K} \qquad S \to \sim N \ln 2 \text{ at } T \sim T_K$$

$$\sum_{\vec{q}} \chi(\vec{q}) \simeq \chi_{imp} \propto \frac{1}{T_K}$$

? $\chi(\vec{q} = \vec{0})$ involves another energy scale ?

$T_K < T \lesssim U$ INCOHERENT SPIN-FLUCTUATION REGIME

charge frozen; $|\uparrow\rangle \rightleftarrows |\downarrow\rangle$ dominate the physics

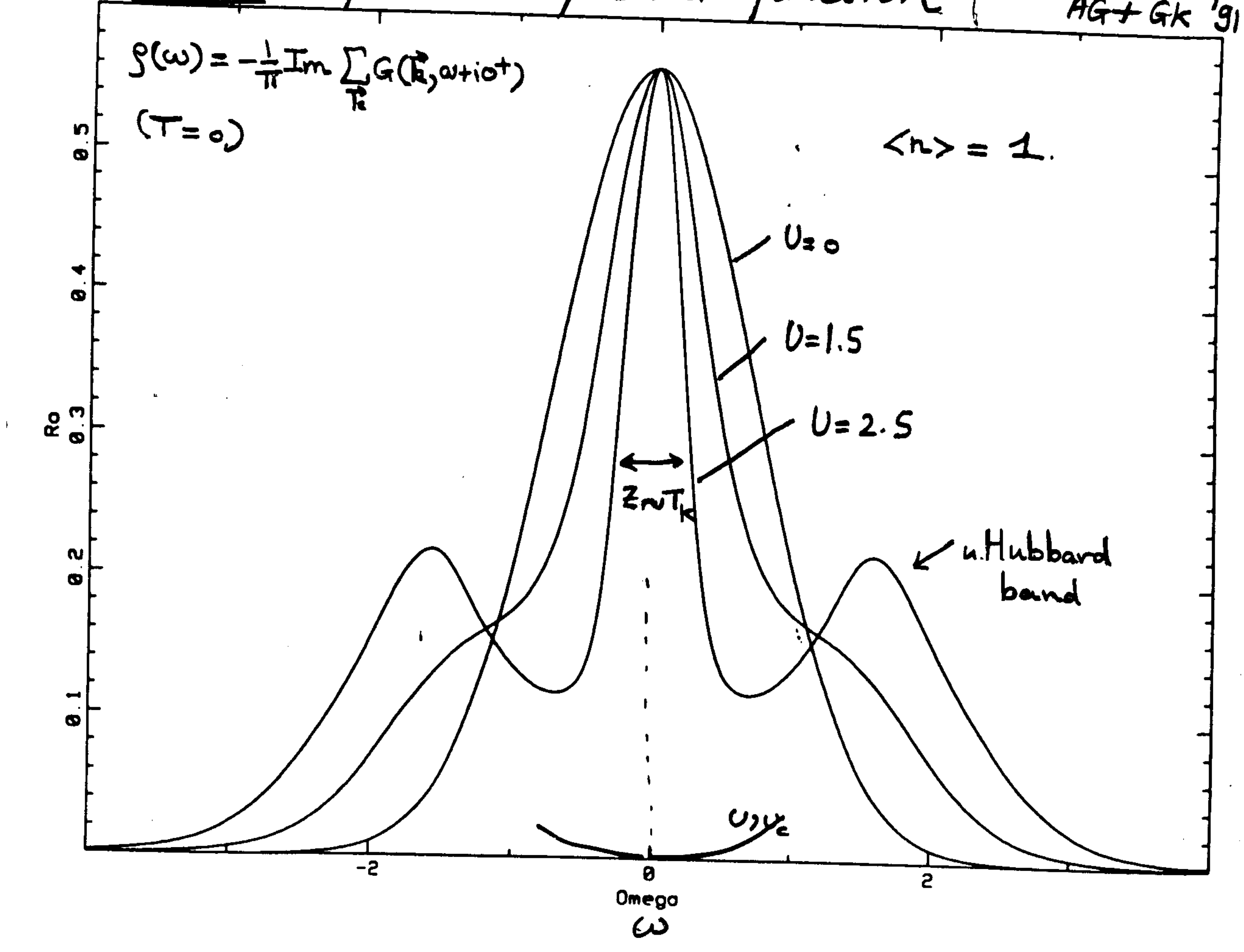
depleted C_v ? $\chi \propto 1/T$?

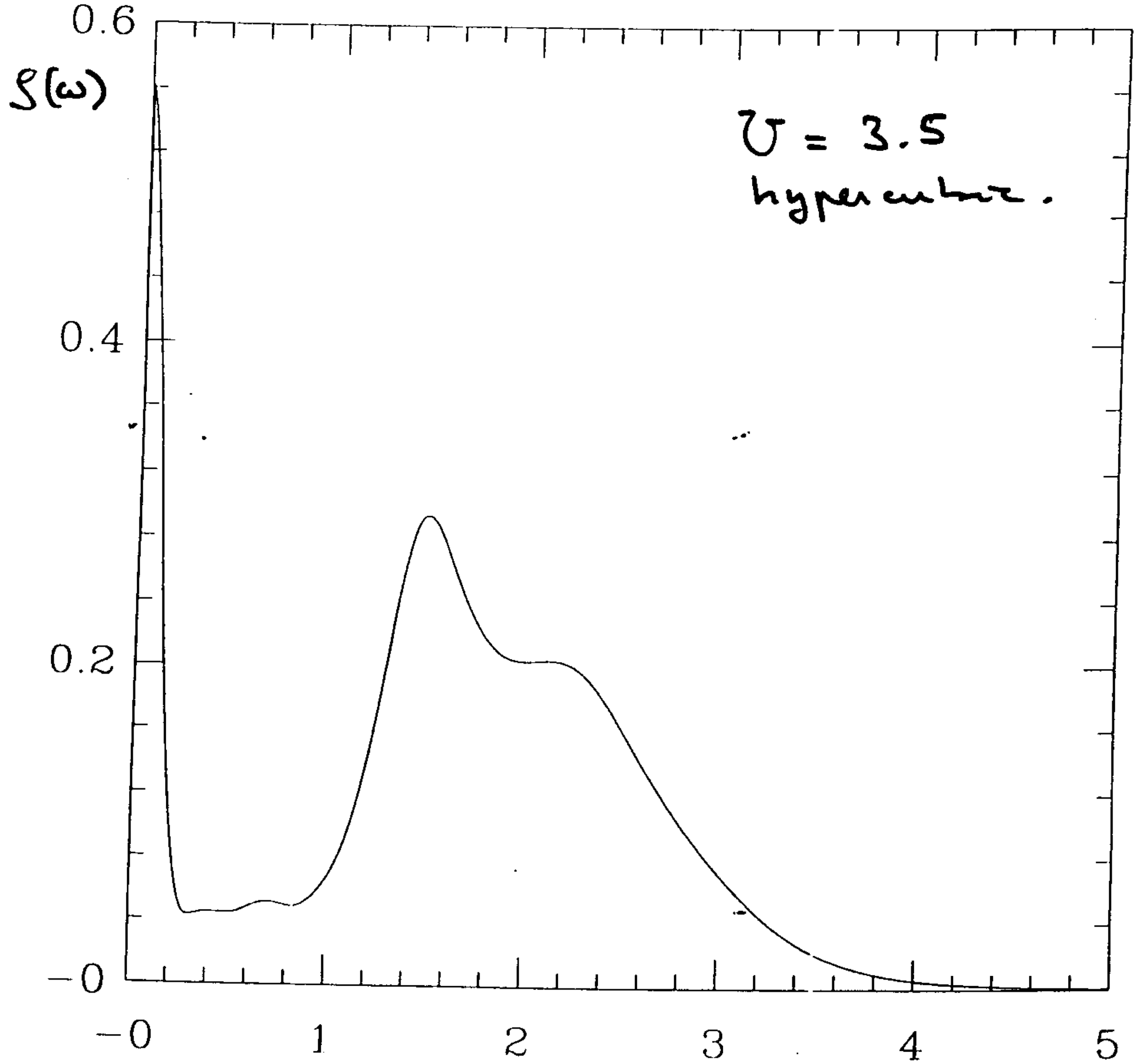
$T \gtrsim U$ Almost atomic regime

$S \to N \ln 4$: charge no longer frozen

N.B: Gutzwiller Appx misses the high-energy scale

<u>LOCAL</u> 1-particle spectral function (AG + GK '91



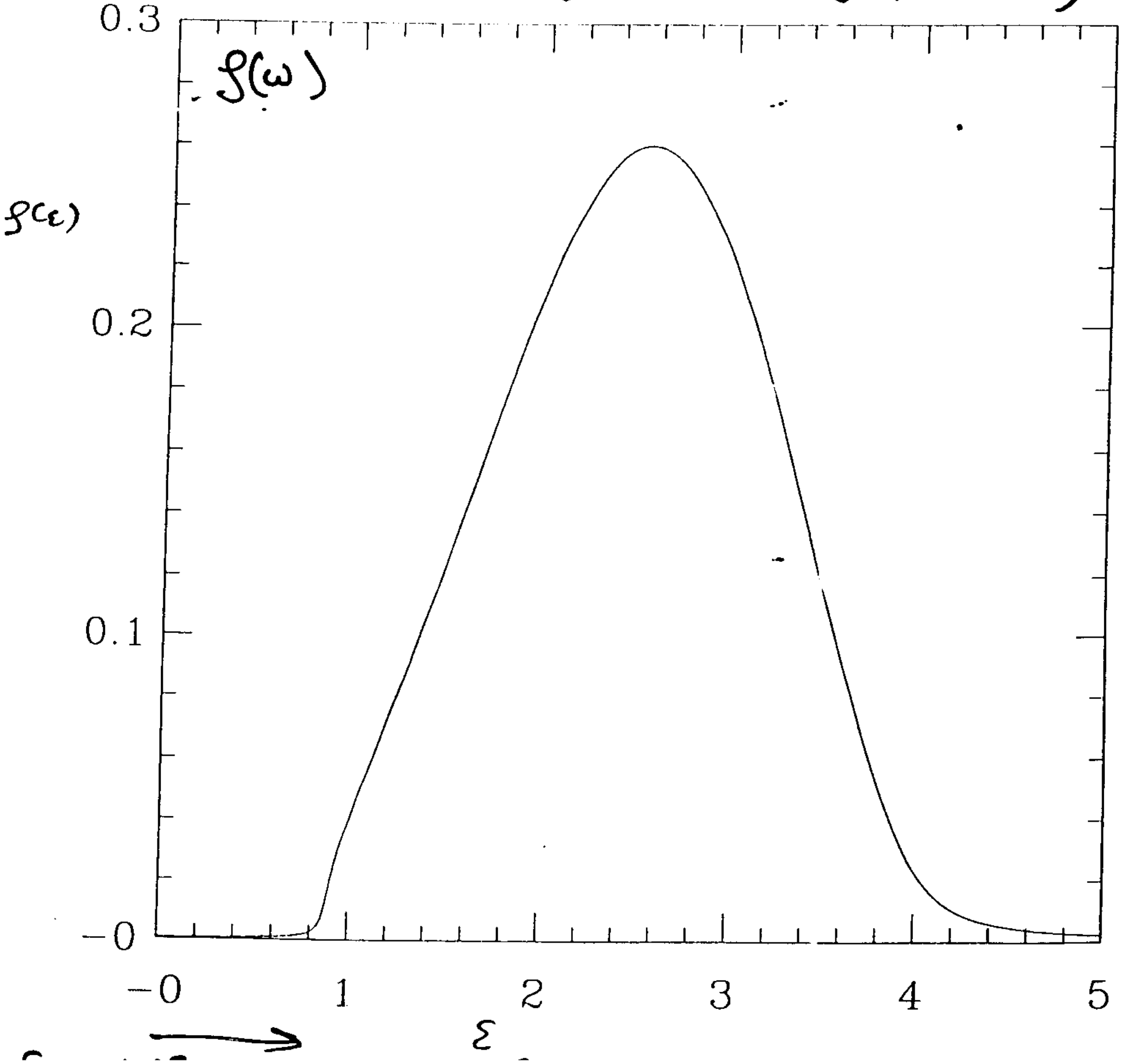


0.6
$\rho(\omega)$
$U = 3.5$
hypercubic.
0.4
0.2
−0
−0
1
2
3
4
5

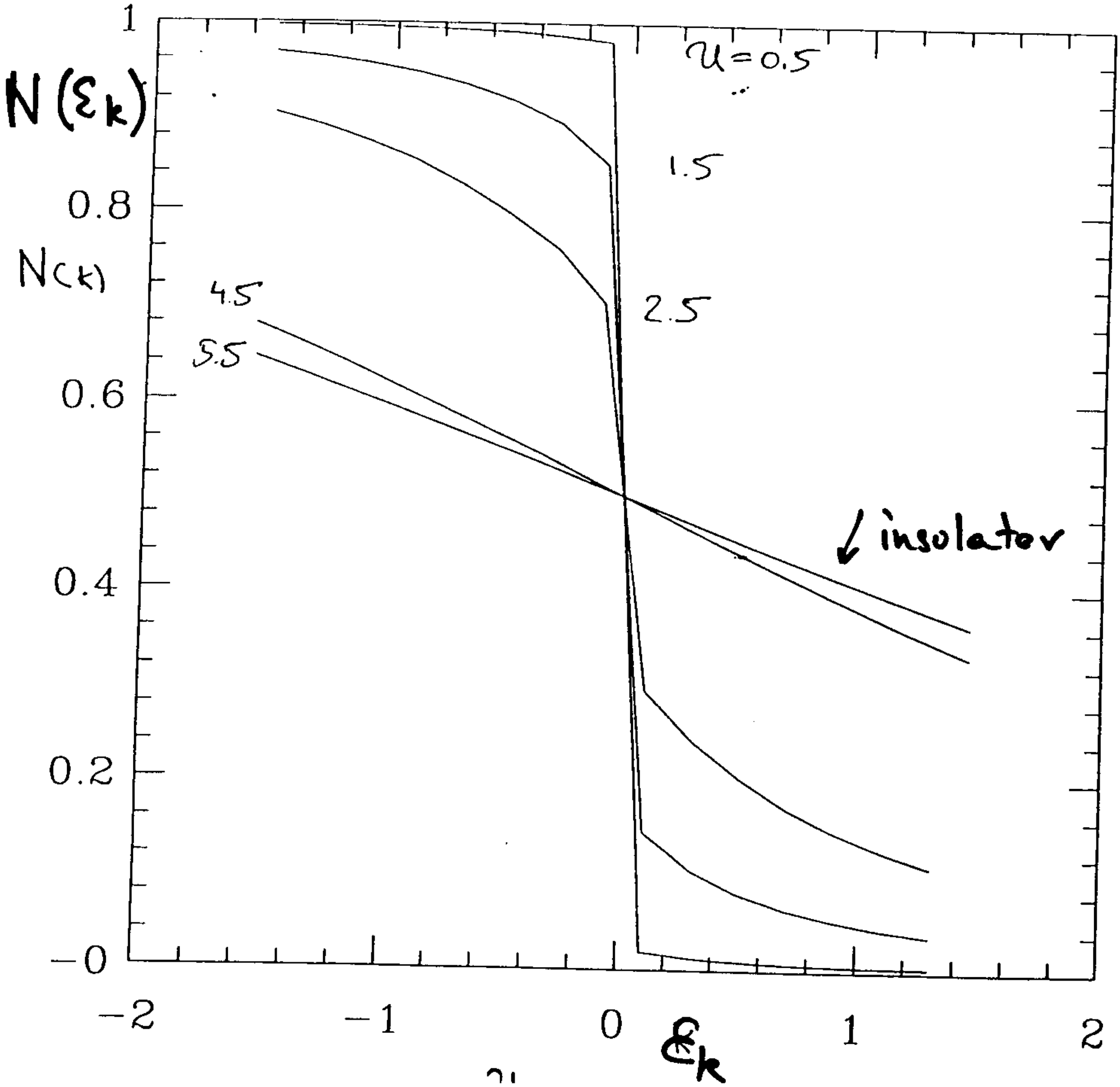
Densité d'états

U = 5 gauss

U = 5 (Insulating phase)



Momentum distribution



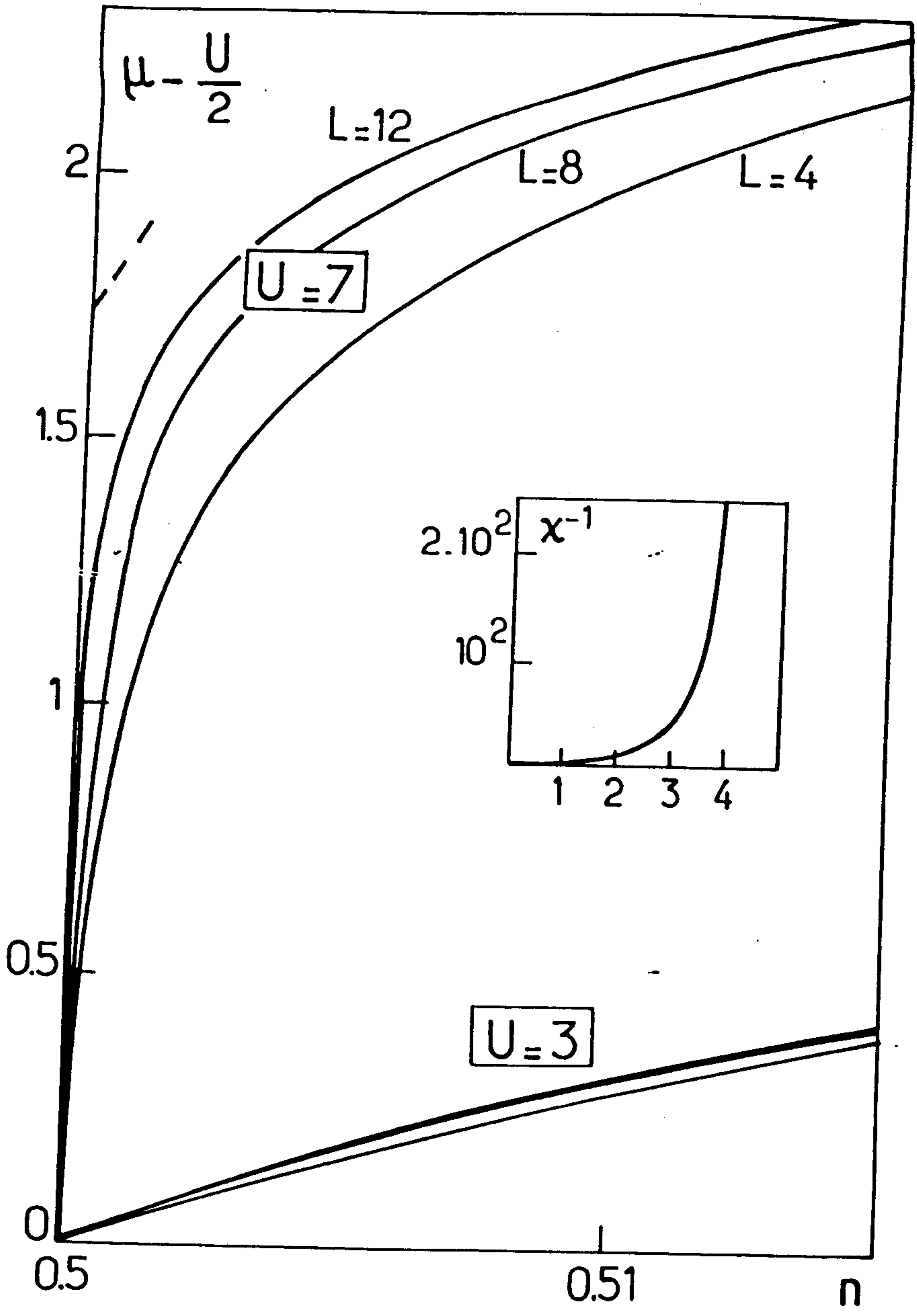
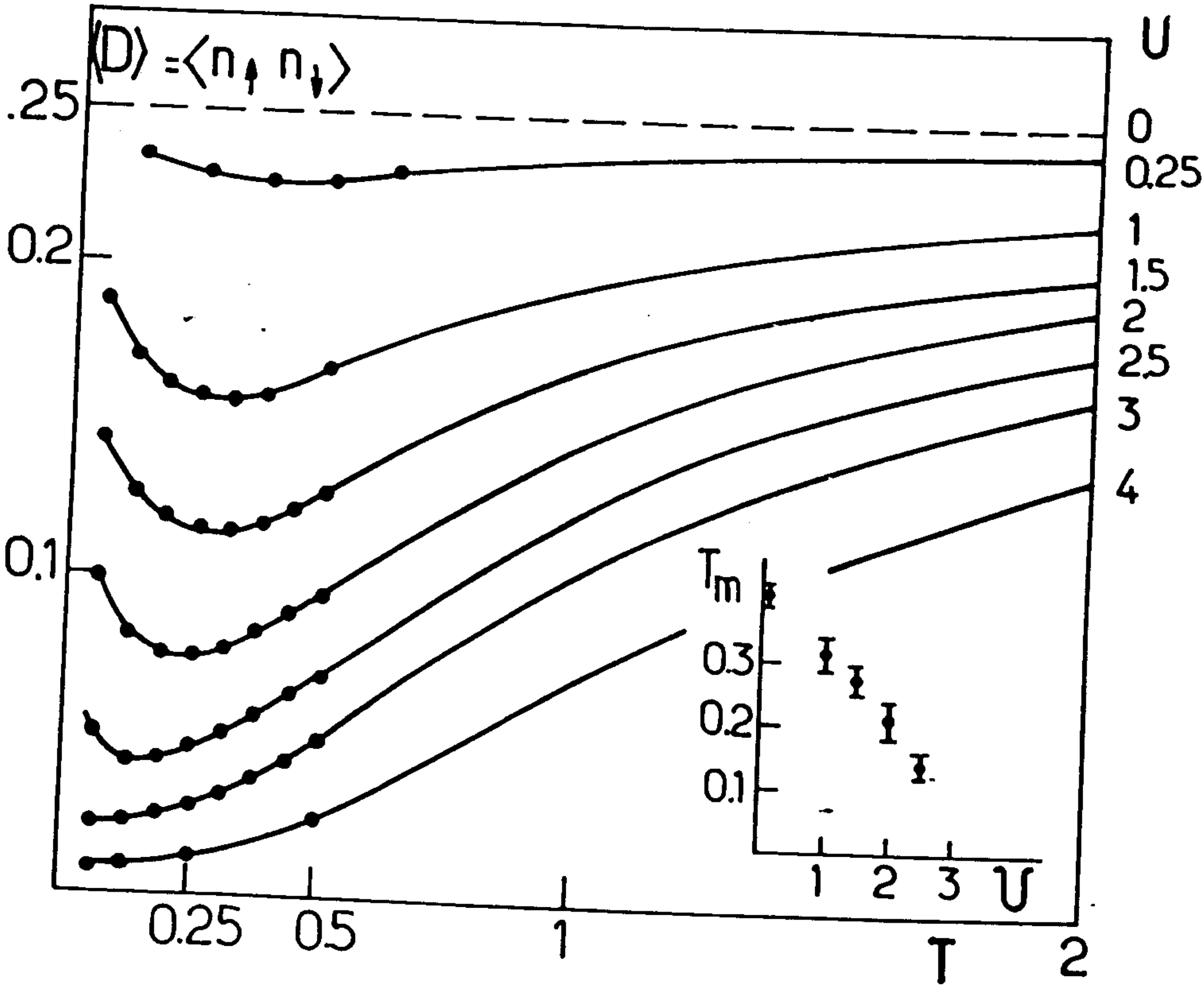


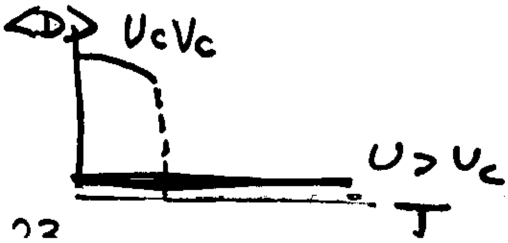
fig. 3

Fraction de sites doublement occupés :

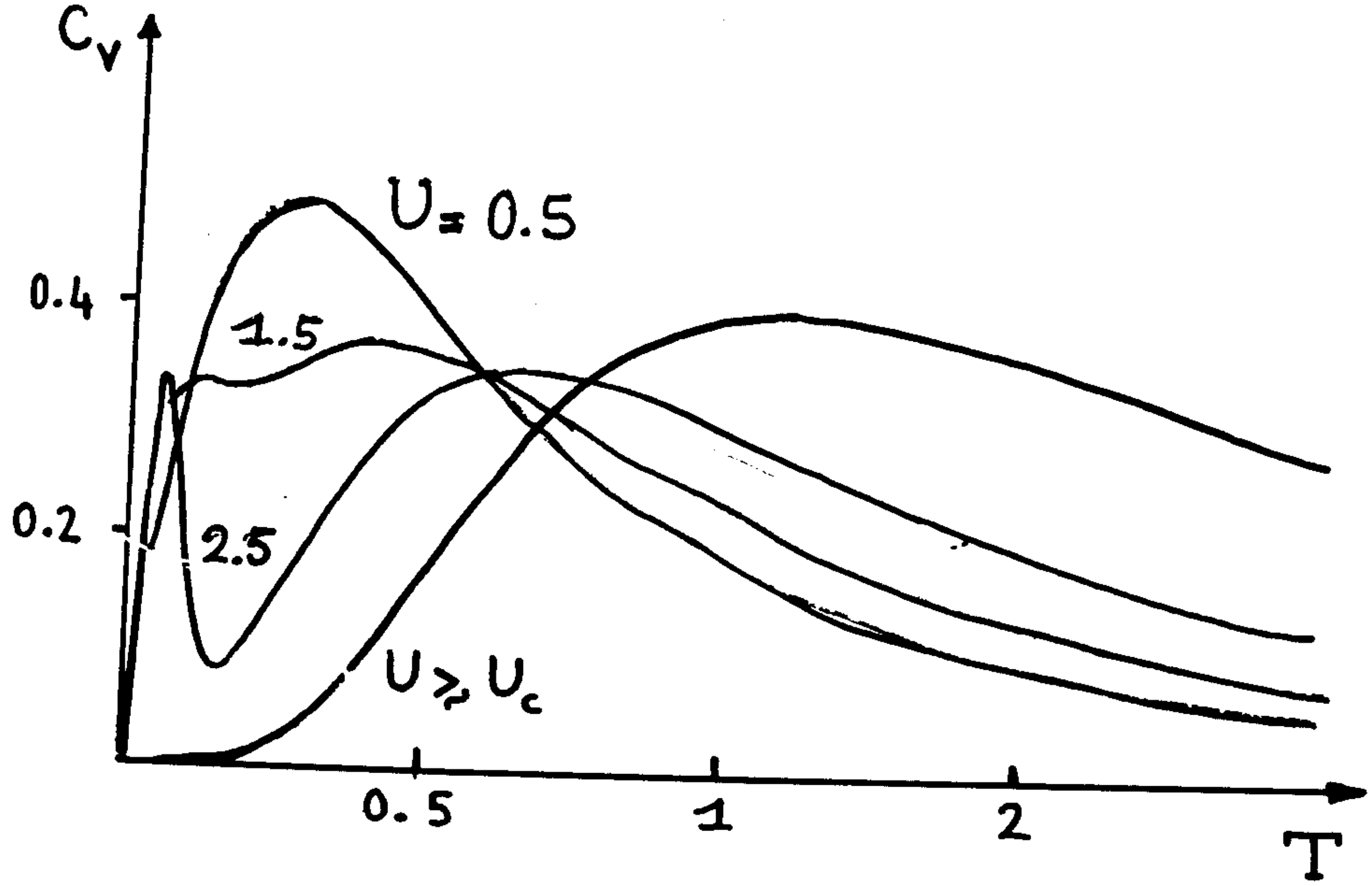
~ mesure du 'degré de localisation'.



* Gutzwiller : fig. 2

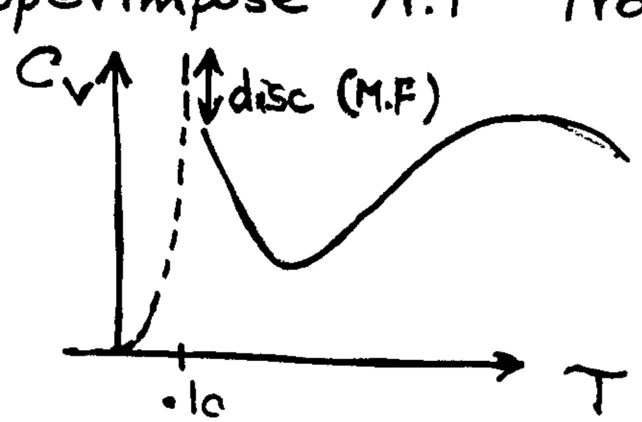


Specific Heat vs. T



métal $(m^*/m \sim 1)$
métal très corrélé $(m^*/m \gg 1)$
(isolant (gap)

+ superimpose A.F transition discontinuity:



gauss

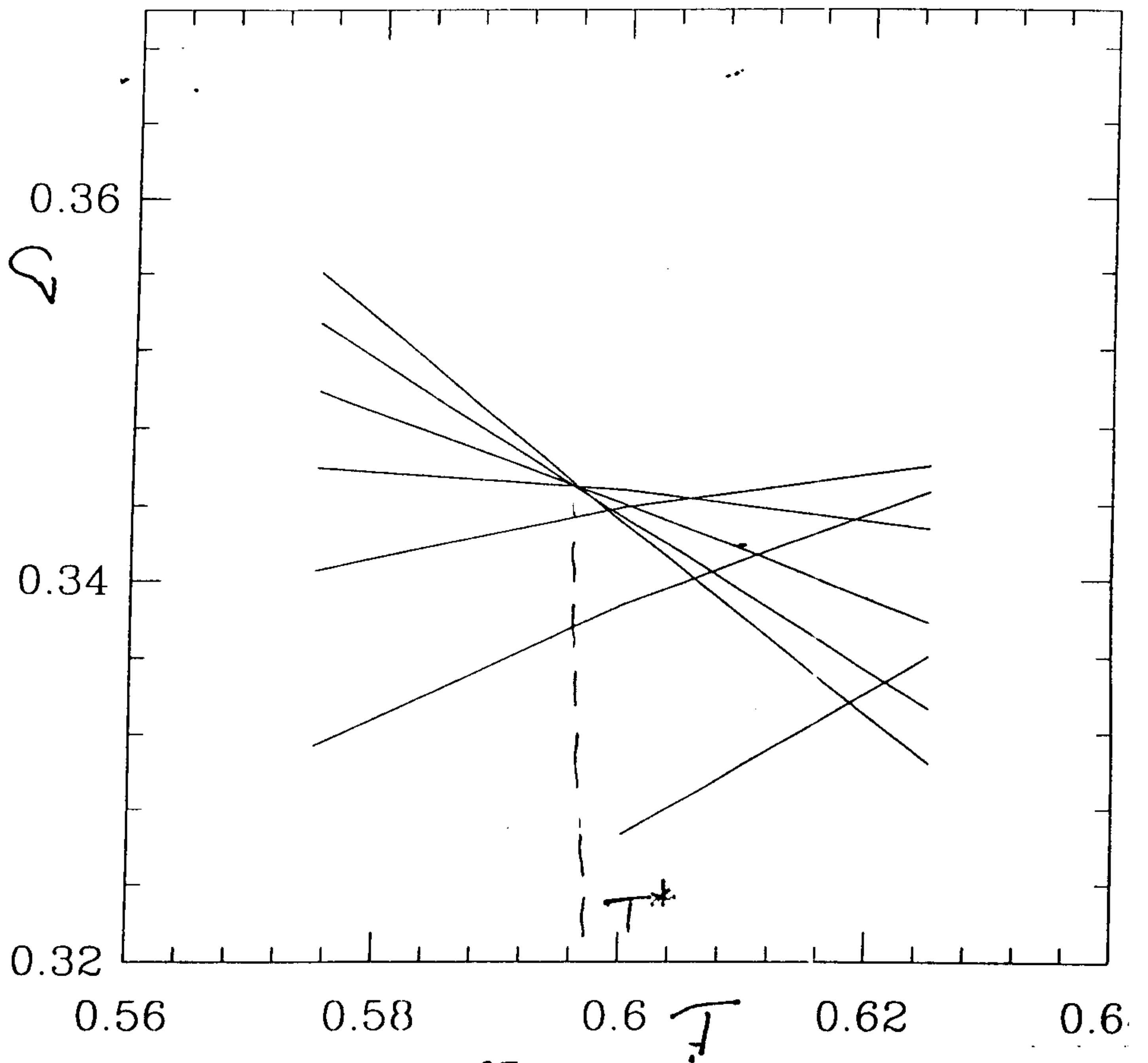
$C_v(T)$

pour $U = 0.5, 1, 1.5 \ldots$

coleétoil !

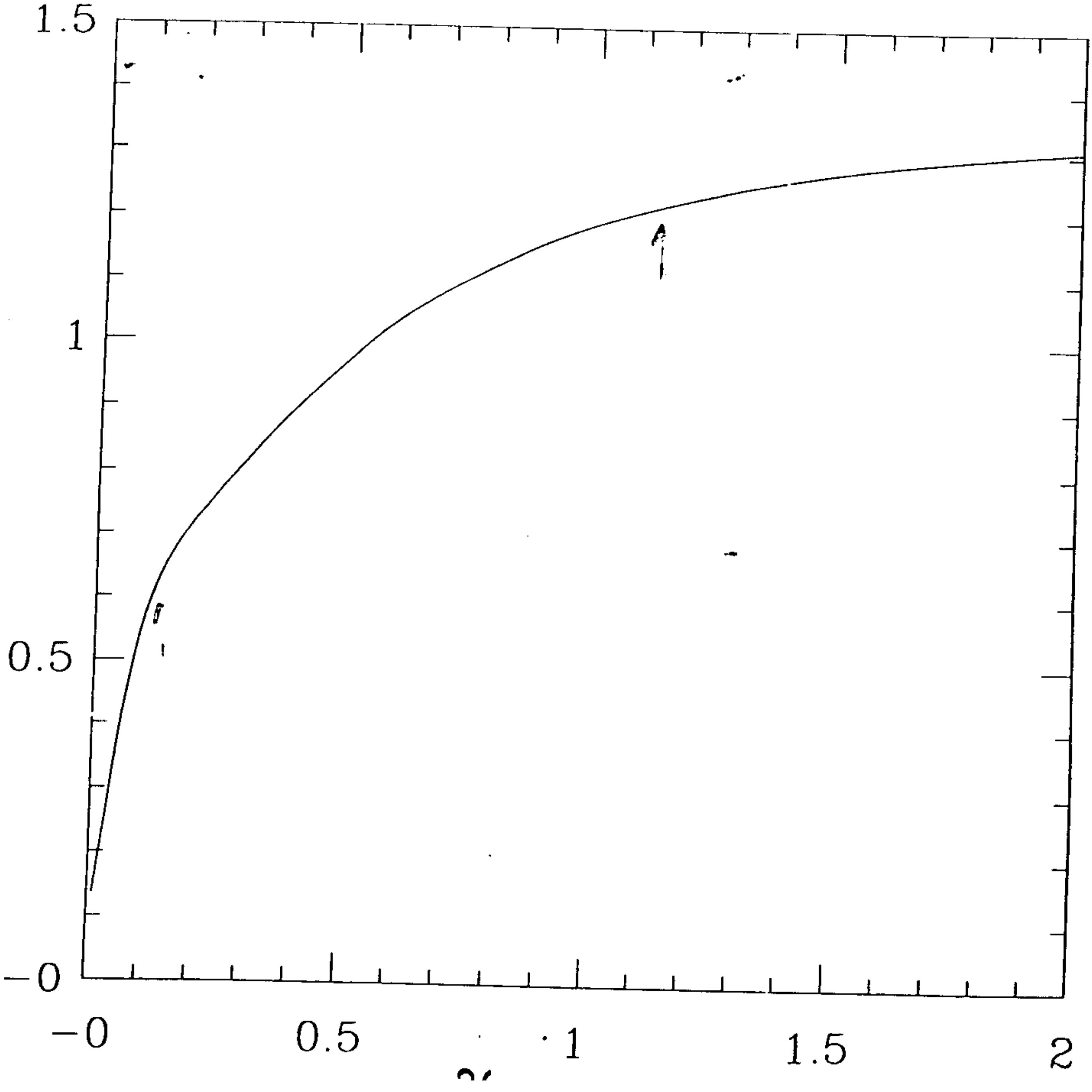
$C_v(T^*) \sim$ independent of U as long as $U<T$

(also seen in liquid ^3He ! ($p \sim U$))



Entropie à $\mathcal{U}=2$
(détail)

Entropy vs. T in the strongly correlated metal



Entropie à $U=5$

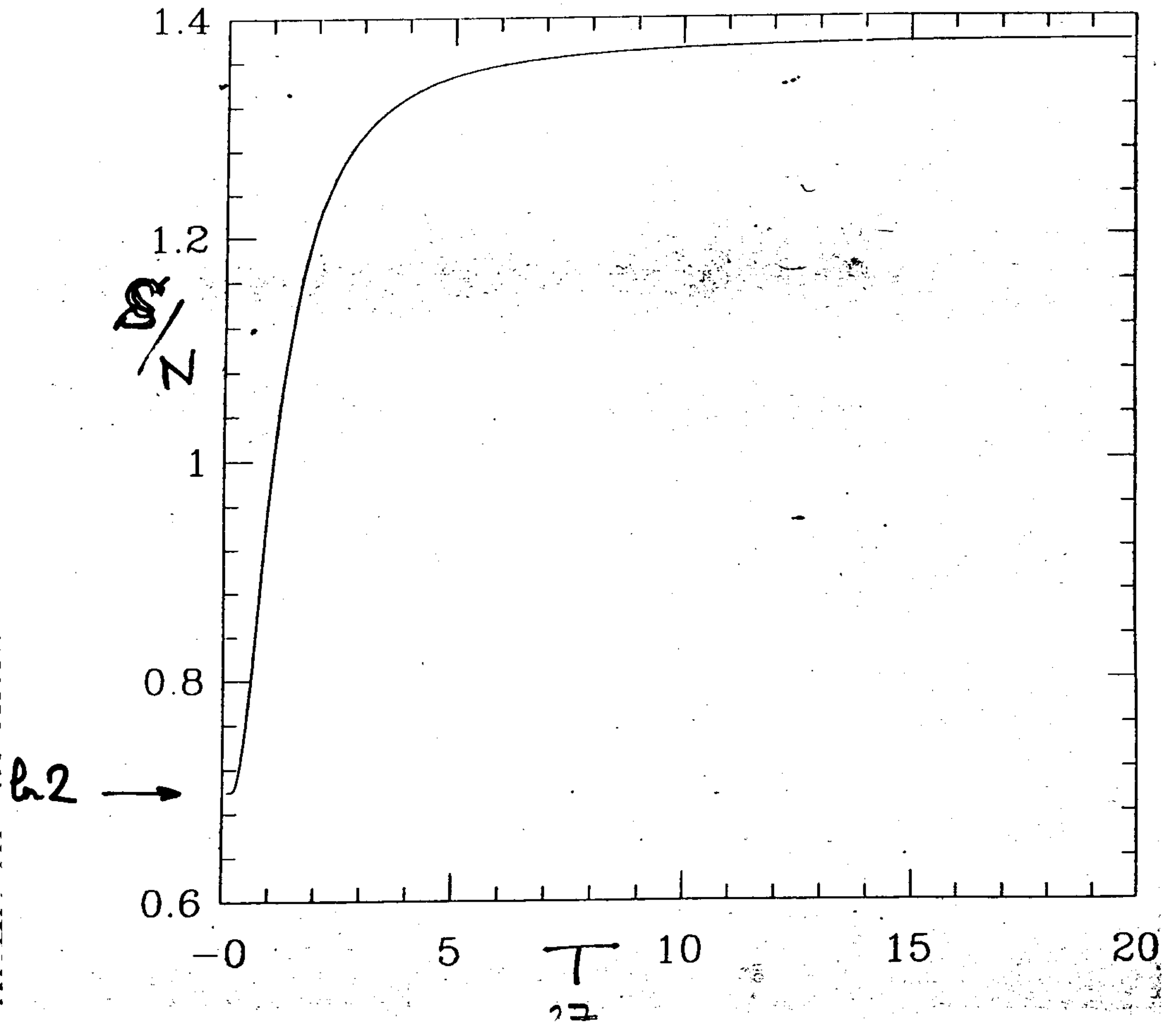
$\int_0^{20} dt \frac{c_V}{T} = 0.678$ $\qquad$ $\ell(2) = 0.693$

T Pert

$2^{13}/2^{9}$

+ corrections

Entropy vs. T in the insulator $U > U_c$.



V_2O_3

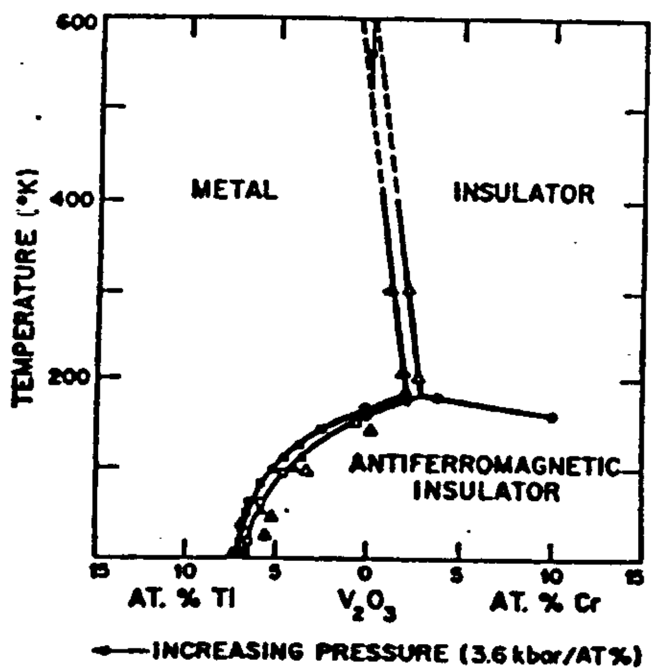


Figure 6: Phase diagram of V_2O_3 and various alloys. The effects of alloying is similar to the application of external pressure. After [18]

The finite-T crossover is made first-order (by coupling to lattice ?)

Mc Whan et al.

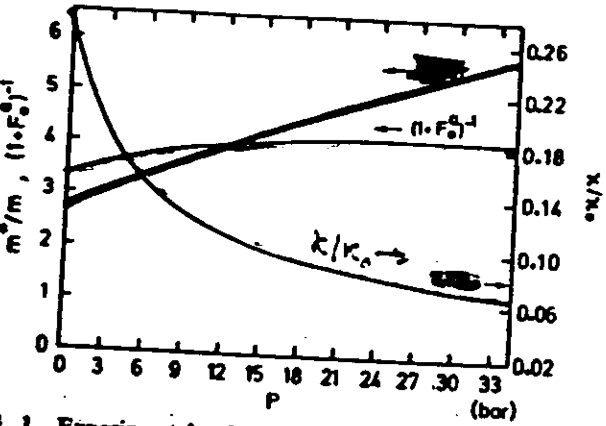


FIG. 1. Experimental values (Greywall, 1983) of the normalized effective mass m^*/m, the ratio between spin susceptibility and effective mass, $(1+F_0^a)^{-1}$, and the normalized compressibility κ/κ_0.

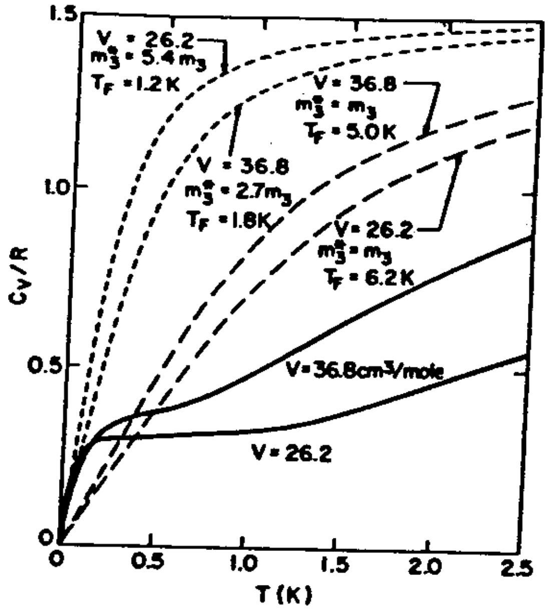


FIG. 6. Smoothed results for the ³He specific heat (in units of the gas constant R) measured at molar volumes corresponding to nominal sample pressures of 0 and 29 bar. For comparison, long-dashed curves show the ideal-Fermi-gas specific heat at the same two densities. Short-dashed curves were also computed using the ideal-gas relations but with the particle mass adjusted to give the correct limiting slopes at $T=0$.

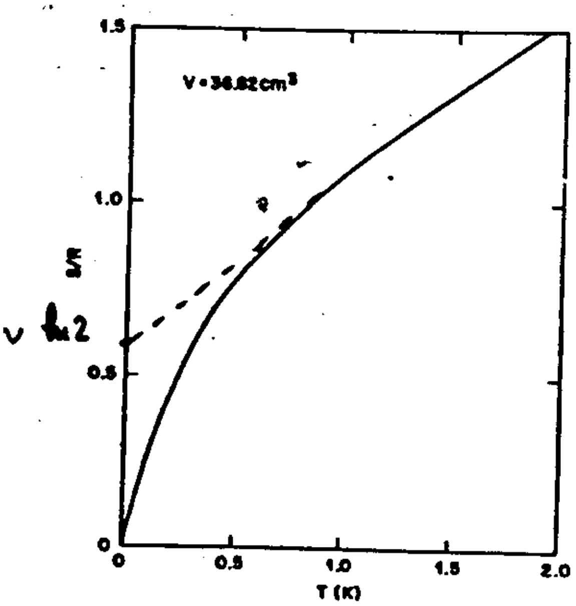


FIG. 10. ³He entropy at a molar volume of 36.82 cm³.

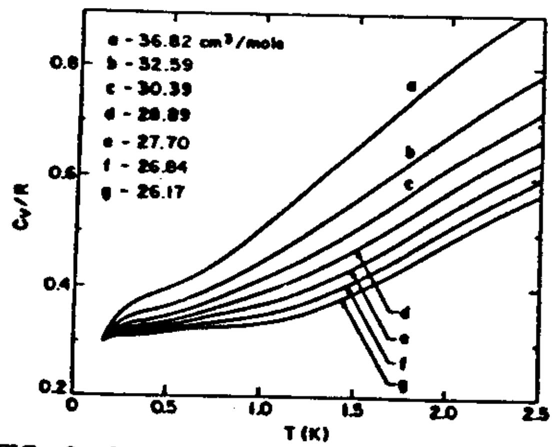
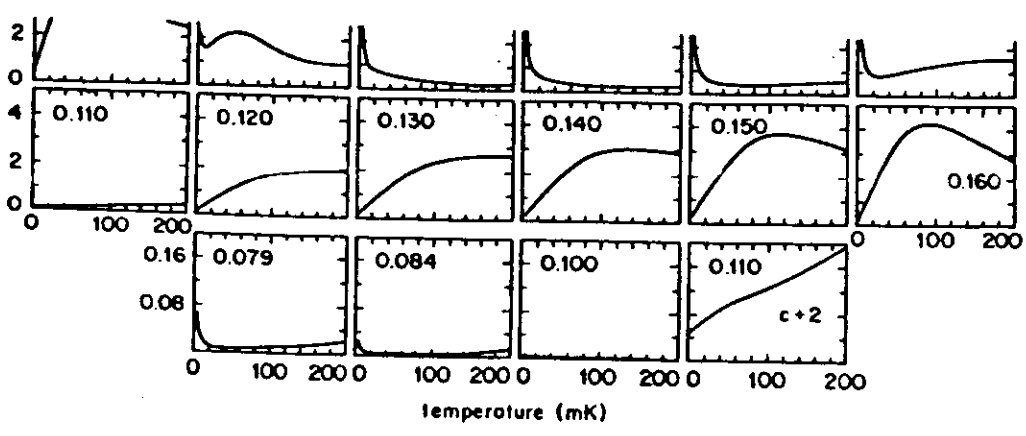


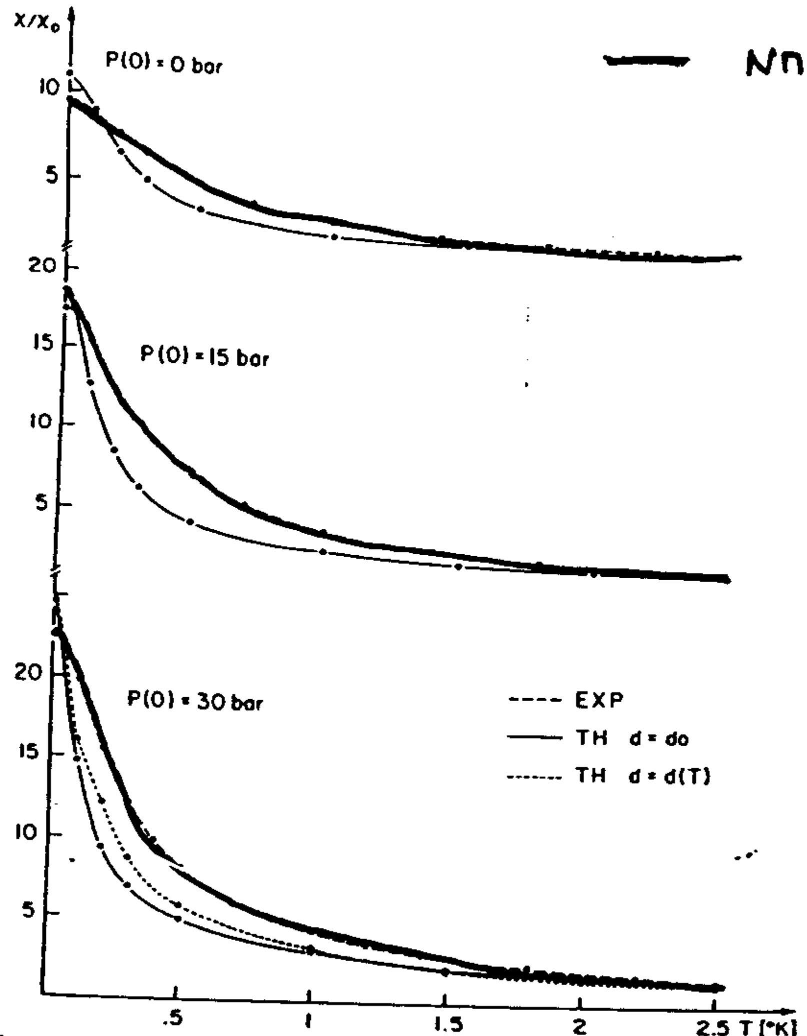
FIG. 9. High-temperature specific-heat results at several molar volumes.



← 2D data

ALL DATA FROM GREYWALL.

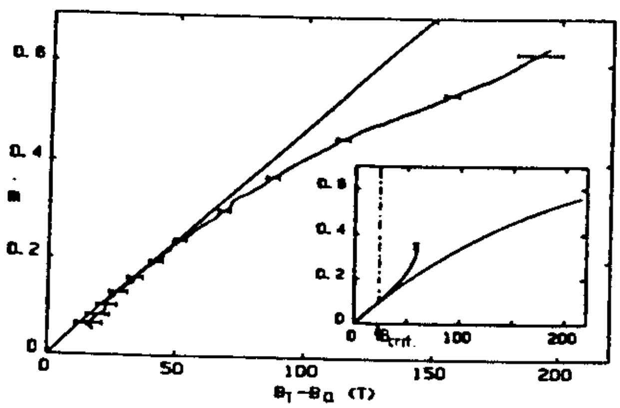
χ/χ_0 — NMR expts. Ramm et al.



T

Fig. 7. Temperature dependence of the spin susceptibility of normal ^{3}He below 2.5 K. (--) Experiment (Ramm *et al.*[21]); (—) theory (d = const); (···) theory [$d = d(T)$].

m



B (T)

FIG. 3. $m(t)-m(\infty)$ vs $(B_T-B_a)(t)$ for the melting experiment of Fig. 2(a), curve 1. The error bars are displayed each 15 s. The straight line is the expected behavior at low m. Inset: m vs B_m as predicted by the RPA (lower trace) and for the Gützwiller ansatz (Ref. 1) (upper trace), for a twentyfold-enhanced initial susceptibility (corresponding to 25 bars). Also shown is the spinode (×) and the field B_{crit} at which the transition occurs in the latter model.

Wiegers, Wolf and Puech '92.

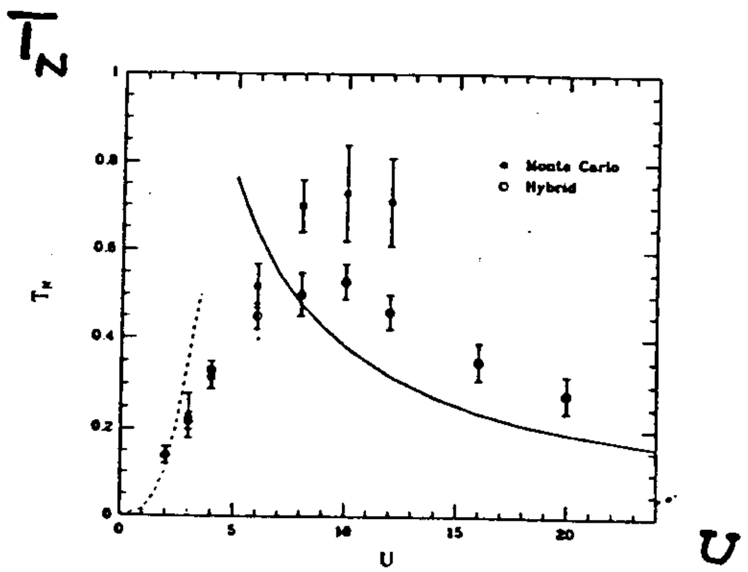


FIG. 6. The Néel temperature T_N vs U. The dashed curve is the weak-coupling RPA obtained from Eq. (4) and the solid line is the strong coupling expression, Eq. (5). The open circles represent data from the hybrid molecular dynamic algorithm, and the filled squares are values obtained in Ref. 3 using exact updating algorithms on a 4^3 lattice with self-consistent mean-field boundary conditions.

Néel temperature for the 3D Hubbard model ~ QMC.

Scalettar et al.

Remarks on $U \lesssim U_c$ and / ^3He.

- $T_F^* = Z T_F$ ($\sim T_K$) spin fluctuation scale

  $S/N \sim \ln 2$ at $T \sim T_F^*$

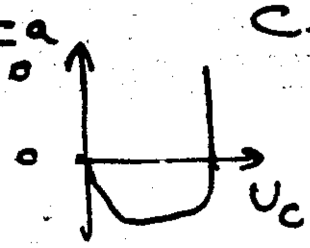
  C_v has a plateau

  ($\sim$ "Kondo peak" in 2D ^3He)

- In contrast to Gutzwiller appx and Brinkman - Rice picture:

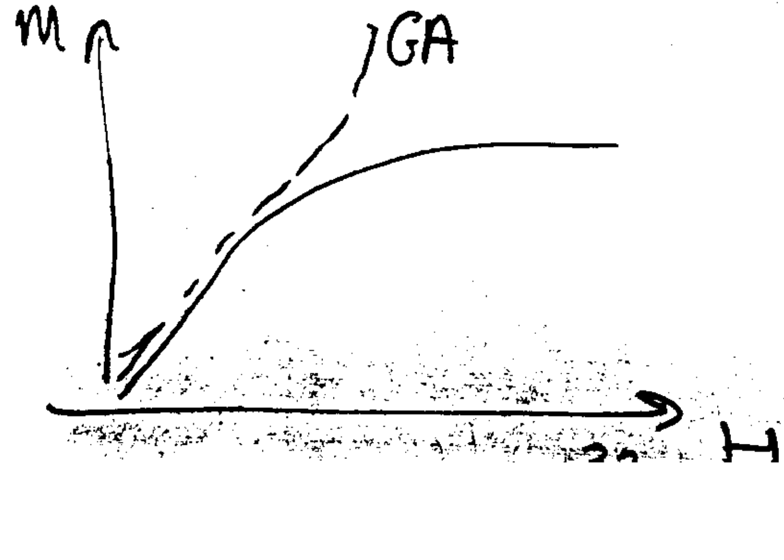
* $\frac{m^*}{m} \to \infty$ at U_c but $\chi < \infty$ (note: $\sum_{\vec q} \chi(\vec q) \sim$

Hence Wilson Ratio $\frac{\chi T}{C_v} = \frac{1}{1+F_0^a}$ is not constant.



?

* NO metamagnetism close to U_c:



CONCLUSION AND PROSPECTS_

$d = \infty$ provides a highly non-trivial "mean-field theory" of strongly correlated systems which describes accurately <u>on-site temporal fluctuations</u>

A number of problems may benefit from this approach:

- X-ray edge w/ finite mass
- Kondo lattice
- Many-band models w/ excitonic effects

etc...

A fundamental goal would be to reintroduce <u>long-wavelength spatial fluctuations</u> (spin-wave, etc...) into the picture.

$\rightsquigarrow$ "Loop expansion" ?