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SMR. 758 - 15

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

QUANTUM ANTIFERROMAGNETS: FIELD-THEORY METHODS

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QUANTUM ANTIFERROMAGNETS

FIELD THEORY METHODS

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I) SOME SIMPLE QUANTUM SPIN SYSTEMS
SPIN-WAVE THEORY : GOLDSTONE MODES

II) THE QUANTUM NONLINEAR SIGMA MODEL
ITS R-G FLOW.

III) MORE SIGMA MODELS. BETA FUNCTION
FOR AN ARBITRARY MANIFOLD
SOME PERTURBATIVE PROPERTIES.

IV) SPIN CHAINS : HALDANE'S CONJECTURE
UNBROKEN SYMMETRY V.S. ALMOST L.R.O.

V) EXPERIMENTS ON REAL SPIN-1
CHAINS : CONFRONTING THEORY AND EXP.

SOME SIMPLE QUANTUM SPIN SYSTEMS

• IONS WITH LOCALIZED MOMENTS $\vec{S}_n$
INTERACTING THROUGH THE EXCHANGE
INTERACTION :

$$\hat{H} = \sum_{ij} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

• [illegible] D = 1 CHAINS
• D = 2 POPULAR (CuO_2)
D = 3

• [illegible] MAY BE FRUSTRATING !!

2D LATTICES : SQUARE
_TRIANGULAR
_KAGOME

TRY FIRST "SPIN-WAVE THEORY"
START FROM CLASSICAL GROUND STATE

Table 1. One-dimensional magnets with characteristic properties (note that, in section 4, we use $H = -J\sum S\cdot S$ while, in section 5, $H = -\frac{1}{2}J\sum \sigma\sigma = -2J\sum S\cdot S$ is used).

Substance	S	J/k (K)	T_c, T_N (K)	T_c/Θ_p	Model
$CuSO_4.5H_2O$	$\frac{1}{2}$	−2·9	0·03	0·02	Heisenberg
$CuSeO_4.5H_2O$	$\frac{1}{2}$	−1·6	0·045	0·056	Heisenberg
$Cu(NH_3)_4SO_4.H_2O$	$\frac{1}{2}$	−6·3	0·37	0·12	Heisenberg
$Cu(NH_3)_4SeO_4.H_2O$	$\frac{1}{2}$	−4·72	1·2	?	Heisenberg
$Cu(NH_3)_4(NO_3)_2$	$\frac{1}{2}$	−7·4	1·4	?	Heisenberg
$CuCl_2.2NC_5H_5$	$\frac{1}{2}$	−26	1·7	0·13	Heisenberg
CHAB	$\frac{1}{2}$	131·6	1·5		Heisenberg (weak x–y)
$KCuF_3$	$\frac{1}{2}$	−380	38	0·2	Heisenberg
$CsNiCl_3$	1	−16·6	4·65	0·13	Heisenberg
$RbNiCl_3$	1	−34	11·0	0·24	Heisenberg
$CsMnCl_32H_2O$	$\frac{5}{2}$	−7·2	4·89	0·12	Heisenberg
TMMC	$\frac{5}{2}$	−13	0·84	0·011	Heisenberg
$CsCuCl_3$	$\frac{1}{2}$	+?	10·4	?	Heisenberg
$(CH_3)_4NCuCl_3$	$\frac{1}{2}$	60	< 2	?	Heisenberg
$((CH_3)_3NH)Cu_2Cl_7$	$\frac{1}{2}$	100	< 2	?	Heisenberg
$(CH_3)_4NNiCl_3$	1	+4	1·2?	0·5?	Heisenberg
$K_3Fe(CN_6)$	$\frac{1}{2}$	−0·23	0·129	0·56	Ising
$CsCoCl_3$	$\frac{1}{2}$	−75	21·5	0·08	Ising
$(NH_4)_2MnF_5$	$\frac{1}{2}$	−12	7·5	0·08	Ising
$CsCoCl_3.2H_2O$	$\frac{1}{2}$		3·8	?	Ising
$CoCl_2.2NC_5H_5$	$\frac{1}{2}$	+11·5	3·2	0·37	Ising
$CsCoBr_3$	$\frac{1}{2}$	−78	28·3		Ising
$RbCoBr_3$	$\frac{1}{2}$		36	?	Ising
$Fe(N_2H_5)_2(SO_4)_2$	2	−2·0	6·0		Ising
$FeC_2O_4.2H_2O$	$\frac{1}{2}$	−82·6	11·7		Ising
$Fe(biPy)Cl_3$	$\frac{5}{2}$	−3·0	?		Ising
$RbFeCl_3.H_2O$	$\frac{1}{2}$	39	12·0		Ising
$FeCl_2Py_2$	$\frac{1}{2}$	+25	6·6		Ising
$NiCl_2Py_2$	$\frac{1}{2}$	+21·4	6·8		Ising
$RbFeCl_3$	2		2·55	?	Planar Heisenberg
$CsNiF_3$	1	23·6	2·65	0·08	Planar Heisenberg

4.1. *Spin Hamiltonians and magnetic chain model substances*

4.1.1. *The ferromagnetic Heisenberg chain with easy-plane anisotropy*

The Hamiltonian of this system is given by

$$H = -J\sum_n S_n\cdot S_{n+1} + D\sum_n (S_n^z)^2 - \mu B\sum_n S_n^x, \tag{4.1}$$

with nearest-neighbour exchange interaction $J>0$ and single-ion anisotropy $D>0$. The single-ion anisotropy provides the easy-plane character of the system at sufficiently low temperatures, whereas at higher temperatures the system becomes more and more equivalent to the isotropic Heisenberg chain. For vanishing external magnetic field

S2

...remote from each other, well isolated by the per... ...anions. The nickel (II)-ions are covalently linked ...nitrite groups bonded on one side by the nitro... atom and on the other side by one of the oxygen atoms.

S3

5

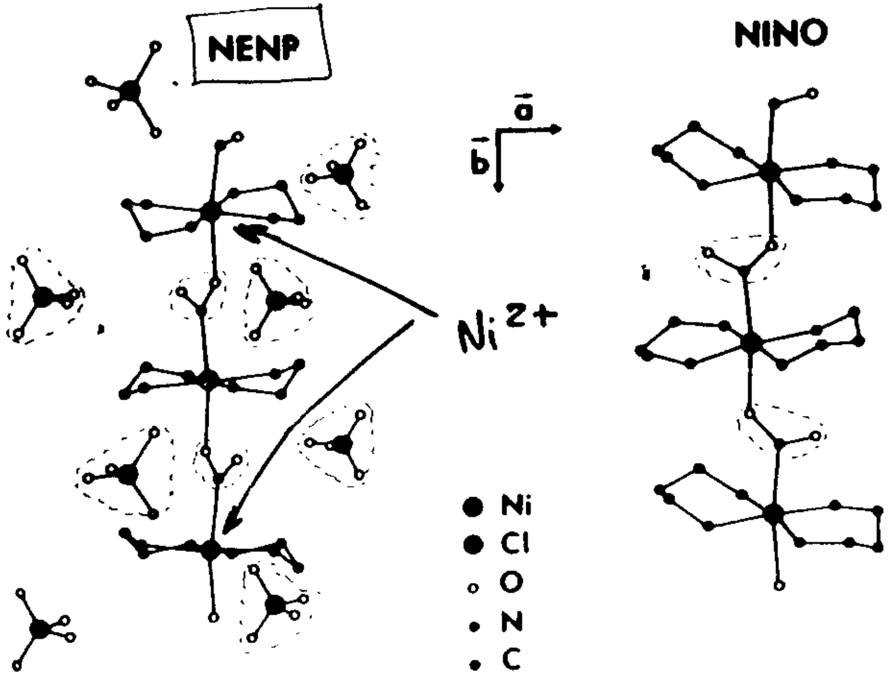


FIG. 1. Schematic view of the chain structure of $Ni(C_2H_8N_2)_2NO_2(ClO_4)$ (NENP) and $Ni(C_3H_{10}N_2)_2NO_2(ClO_4)$ (NINO).

4

✡ SEARCH FOR CLASSICAL GROUND STATE:

- FOURIER TRANSFORM

$$\sum_{i-j} J_{ij}\, e^{i\vec{K}\cdot(\vec{R}_i-\vec{R}_j)}$$

D-dimensional Lattice nearest-neighbor

$$J(K) = \frac{1}{D}\left(\cos k_1 + \dots + \cos k_D\right)$$

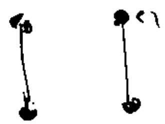
MINIMUM ENERGY REACHED BY A SPIRAL (HELICAL) ARRANGEMENT

$$\vec{S}_n = \quad \cos(\vec{Q}\cdot\vec{R}_n) + \quad \sin(\vec{Q}\cdot\vec{R}_n)$$

where $\vec{Q}$ minimizes $J(K)$ [HEISENBERG CASE]

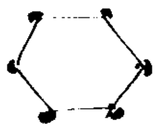
EXAMPLES

nearest neighbor J_{ij} → SQUARE

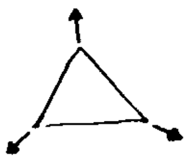


$\vec{Q} = (\pi,\pi)$ NEEL ORDER

→ TRIANGULAR



← $\vec{Q}$



120° NEEL ORDER

SEMICLASSICAL EXPANSION:

MAP SPINS ONTO BOSONS:

HOLSTEIN PRIMAKOV

$$\begin{cases} S_n^z = S - a_n^\dagger a_n \\ S_n^+ = \sqrt{2S - a_n^\dagger a_n}\; a_n \\ S_n^- = a_n^\dagger \sqrt{2S - a_n^\dagger a_n} \end{cases}$$

- BEST WITH AXIS OF QUANTIZATION ALONG CLASSICAL SPIN DIRECTION

→ EXPANSION IN POWERS OF $1/S$ ...

THE HAMILTONIAN BECOMES:

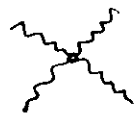
$$\hat{H}_{HEIS.} = S^2(\dots) + JS\left[\sum_k B_k a_k^\dagger a_k + A_k\left(a_k a_k + h.c.\right)\right]$$

+ interactions between Bosons

- FROSTRATED NONCOLINEAR

$1/\sqrt{S}$

- SQUARE LATTICE



$1/S$

USE BOGOLYUBOV ROTATION TO DIAGONALIZE FREE PART :

$$H_{Free} = JS \sum_k \omega_k \left[\underbrace{\alpha_k^\dagger \alpha_k}_{\text{normal modes}} + \frac{1}{2} \right]$$

normal modes
SPIN WAVES .

D-dimensional cubic lattice

$$\omega_k = \sqrt{1-\gamma_k^2} \quad , \quad \gamma_k = \frac{1}{z} \sum_{\vec{\delta}} e^{i \vec{k} \cdot \vec{\delta}}$$

Note that $k \to 0$ $\quad \omega_k \sim c\,|\vec{k}|$

[Ferro has $\omega_k \sim \vec{k}^2$] $\qquad$ c spin-wave velocity

ZERO MODES ARE GOLDSTONE MODES

SURVIVE TO ALL ORDERS IN PERT. THEORY.

CONSEQUENCE OF LONG-RANGE ORDER

$$\langle S_n^z \rangle = S - \langle a_n^\dagger a_n \rangle \doteq S - \int \frac{d^D k}{\omega_k}$$

FINITE IN D = 2 AF CASE $\Rightarrow$ ORDER ?

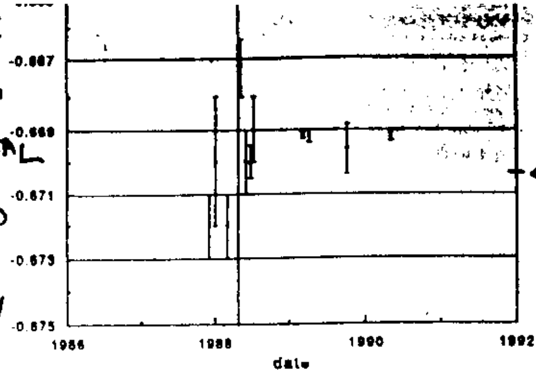
DIVERGES IN D = 1 AF !

AT THE I.R END OF $\int$

BIS

ENERGIE DU FONDAMENTAL

GROUND STATE ENERGY



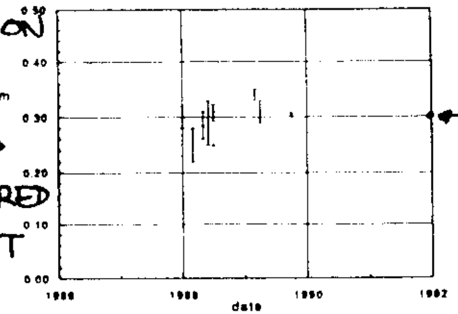
← SW

Fig. 3. 2D Heisenberg antiferromagnet ground state energy per spin.

AIMANTATION

$\langle S^z \rangle$

STAGGERED MOMENT



← VALEUR SW
SEMI CLASSICAL VALUE
$\langle S^z \rangle = 0.303$

Fig. 6. Ground state staggered magnetisation of the 2D Heisenberg antiferromagnet.

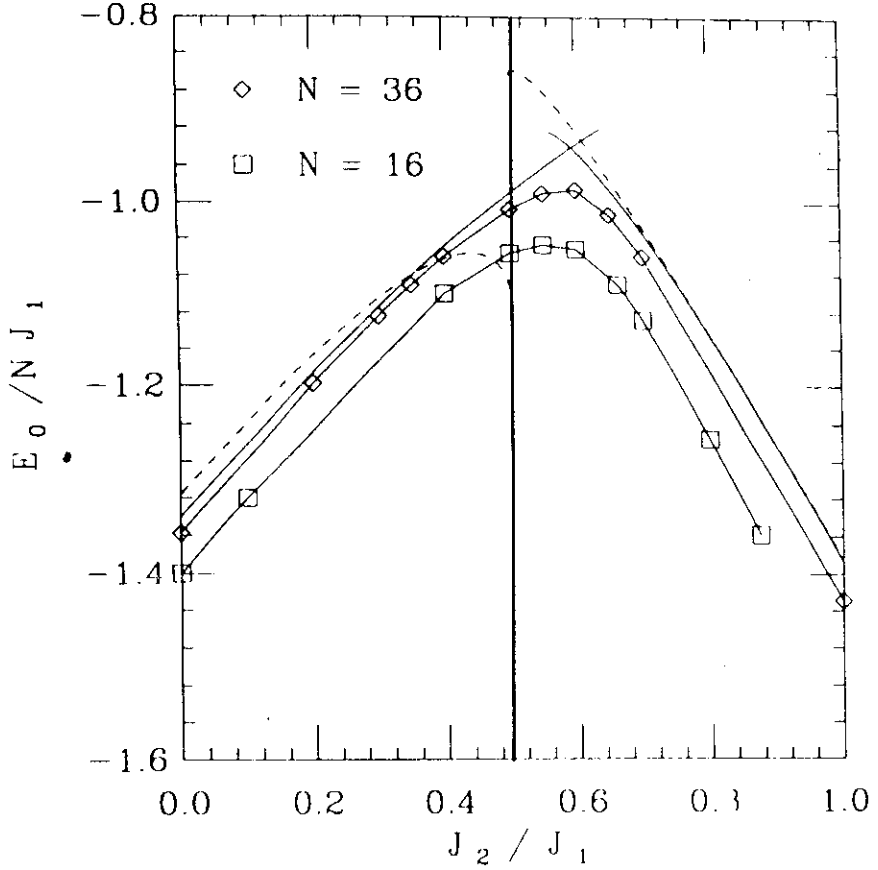
Table 2 Numerical results for the RMS ground state staggered magnetisation.

$m^{rms}(L \to \infty)$	Date	Method	Reference
0.43 ± 0.01	11/77	Lanczos	[Oit78] Oitmaa and Betts
0.30 ± 0.02	1/88	MC(Suzuki-Trotter)	[Reg88] Reger and Young
0.29 ± 0.03	3/88	Lanczos	[Tan88a] Tang and Hirsch
0.305 ± 0.025	5/88	MC(Suzuki-Trotter)	[Gro88a] Gross, Sánchez-Velasco and Siggia
0.29 ± 0.04	6/88	MC(Suzuki-Trotter)	[Oka88a,b] Okabe and Kikuchi
0.308 ± 0.014	7/88	MC(Suzuki-Trotter)	[Reg89] Reger, Riera and Young
$m^{rms} \approx 0.28$	7/88	MC(DGRW)	[Bar89a] Barnes, Kotchan and Swanson
0.34 ± 0.01 ± sys	3/89	MC(GFMC)	[Car89] Carlson
0.31 ± 0.02 ± sys	4/89	MC(GFMC)	[TC89] Trivedi and Ceperley
0.304 ± 0.004	10/89	MC(RVB-PMC)	[Lia90b] Liang

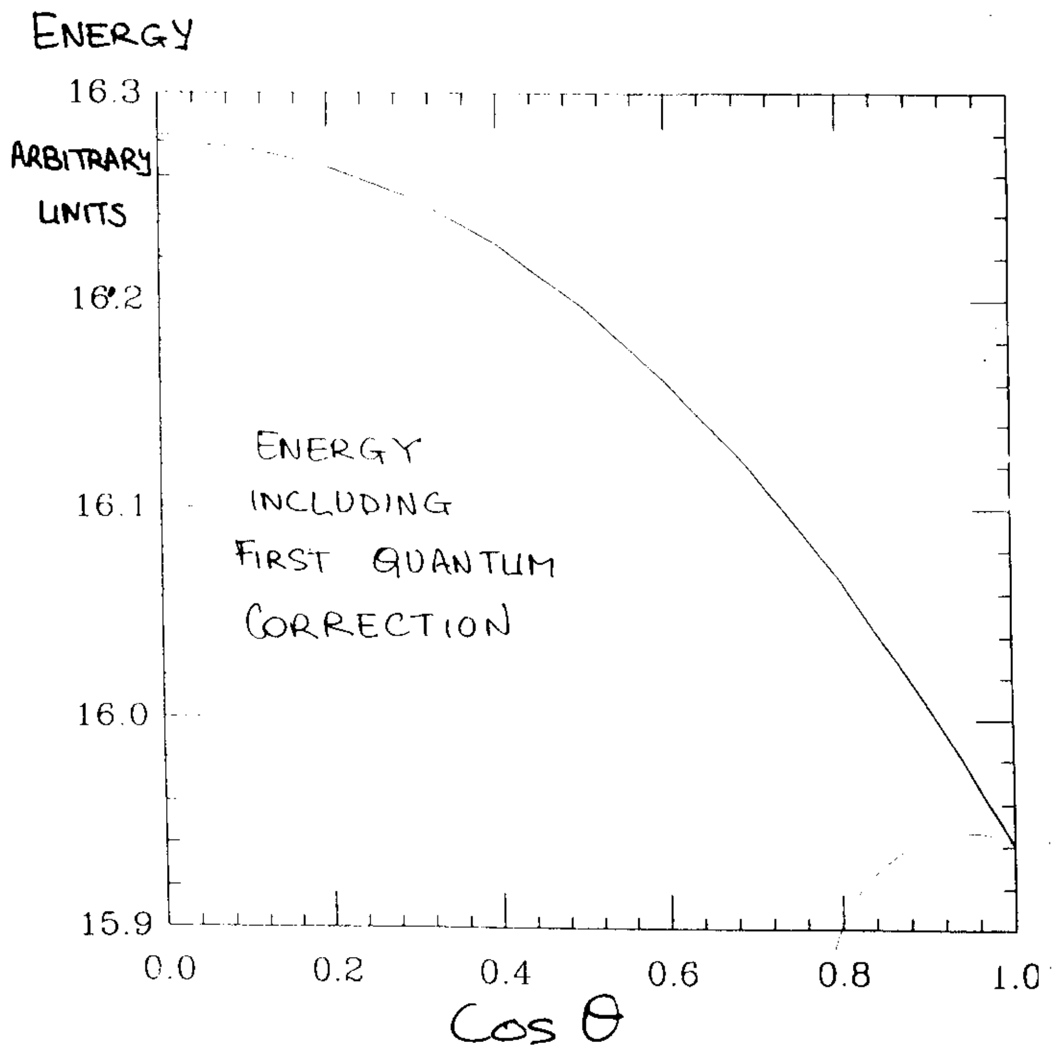
SPIN LATTICE DATA

T. BARNES Int J Mod Phys C 2 (91) 659

GROUND STATE ENERGY



SÉLECTION DES ÉTATS COLLINÉAIRES SUR LE RÉSEAU CARRÉ : $\frac{J_2}{J_1} > \frac{1}{2}$.



SQUARE LATTICE AF SPIN-$1/2$ $\boxed{\text{nearest neighbor}}$
ORDER IS LIKELY

$S \geq 1$ ORDER IS PROVEN RIGOROUSLY

BUT

NEEL ORDER
\+ QUANTUM FLUCTUATIONS $\Rightarrow$ LIQUID ?

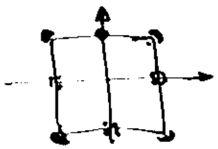
FRUSTRATED SYSTEMS ?

SIMPLE "$J_1 - J_2$" MODEL

$$H = J_1 \sum_{\text{nearest neighb.}}' \vec{S}_i \cdot \vec{S}_j + J_2 \sum_{\text{next to nearest}}' \vec{S}_i \cdot \vec{S}_k$$

ONLY ONE PARAMETER J_2/J_1

CLASSICAL GROUND STATES



$J_2/J_1 < \frac{1}{2}$: NEEL STATE

$J_2/J_1 > \frac{1}{2}$: TWO NEEL SUBLATTICES

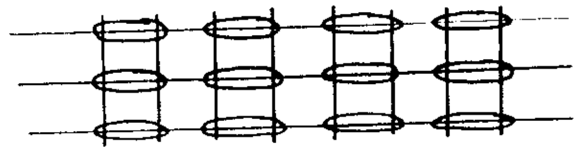
QUANTUM SELECTION OCCURS

↑ ↑ ↑ ↑ ↑   ↑ ↓ ↑ ↓ ↑ ↓
↓ ↓ ↓ ↓ ↓   ↑ ↓ ↑ ↓ ↑ ↓
↑ ↑ ↑ ↑ ↑   ↑ ↓ ↑ ↓ ↑ ↓

- THERE IS A WINDOW WITHOUT ANY OBVIOUS MAGNETIC LRO

$\Rightarrow$ DIMERIZATION IS LIKELY
CRYSTAL OF SPIN SINGLETS:

COLUMNAR DIMER STATE

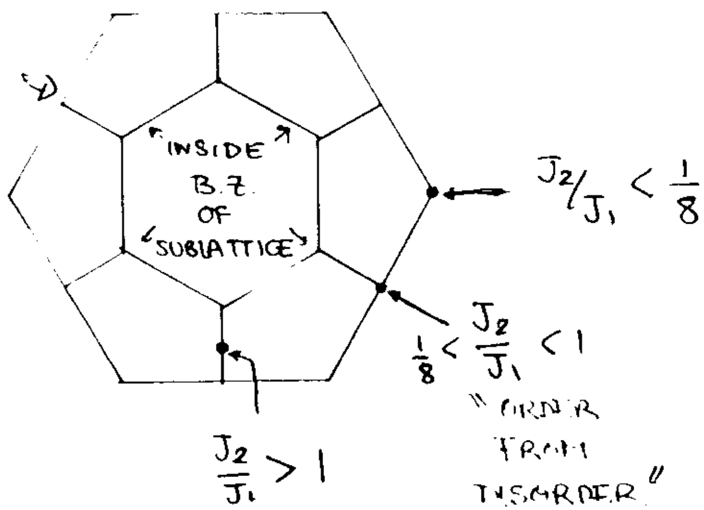


★ THE TRIANGULAR CASE:
HISTORICAL CANDIDATE FOR SPIN LIQUID

$J_1 - J_2$ TRIANGULAR HEISENBERG

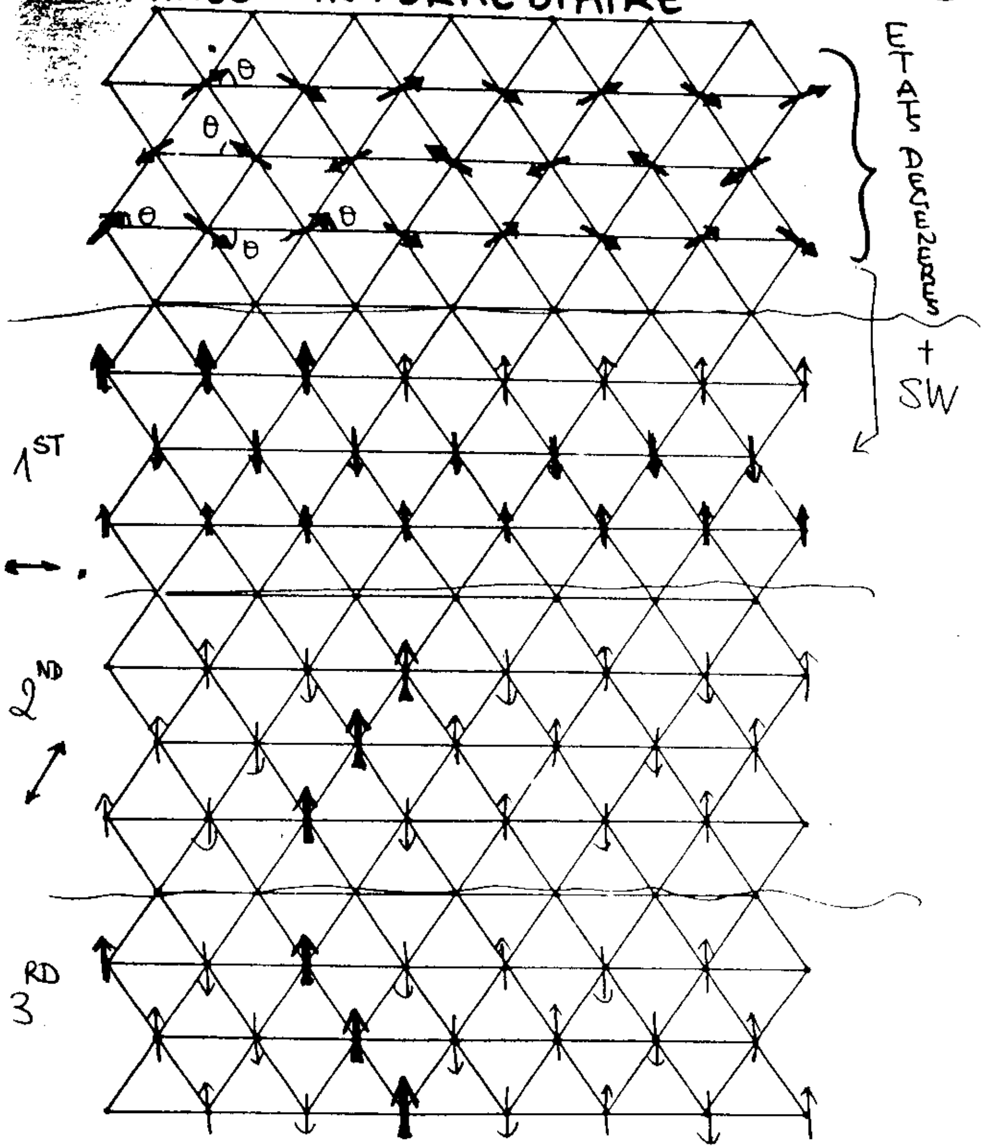
MINIMIZE $J(K)$

1ST BRILLOUIN ZONE OF TRIANGULAR LATTICE



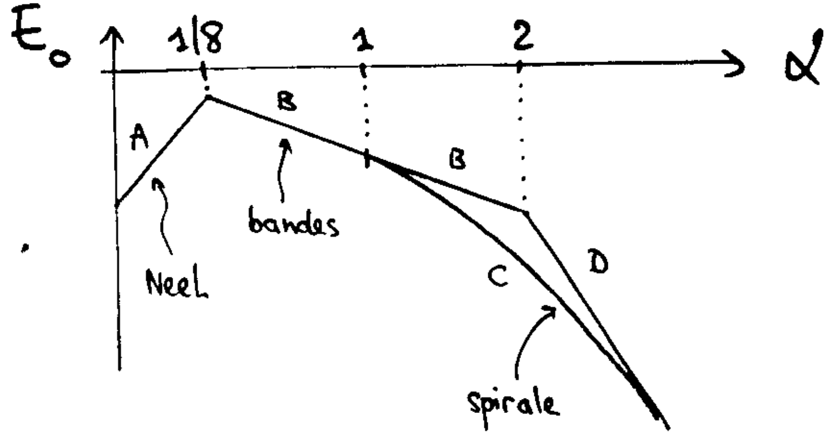
$\frac{1}{8} < \frac{J_2}{J_1} < 1$ (5) 8

PHASE INTERMEDIAIRE



Energies classiques :

$$\left.\begin{aligned} A &: \ \alpha - 1/2 \\ B &: \ -\frac{1}{3} - \frac{1}{3}\alpha \\ C &: \ -\frac{\alpha}{2} - \frac{1}{6\alpha} \end{aligned}\right\} \text{ en unités } NS^2$$



D : sous-réseaux à 120°, énergie $-\frac{\alpha}{2}$

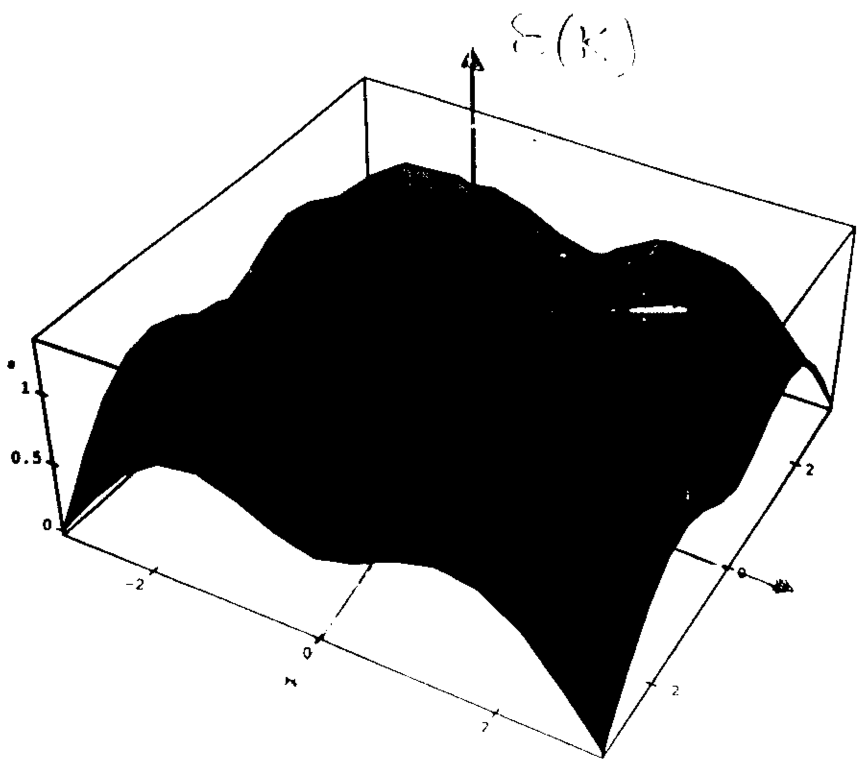
A → B : 1^{er} ordre

B → C : 2^{nd} ordre

SW :

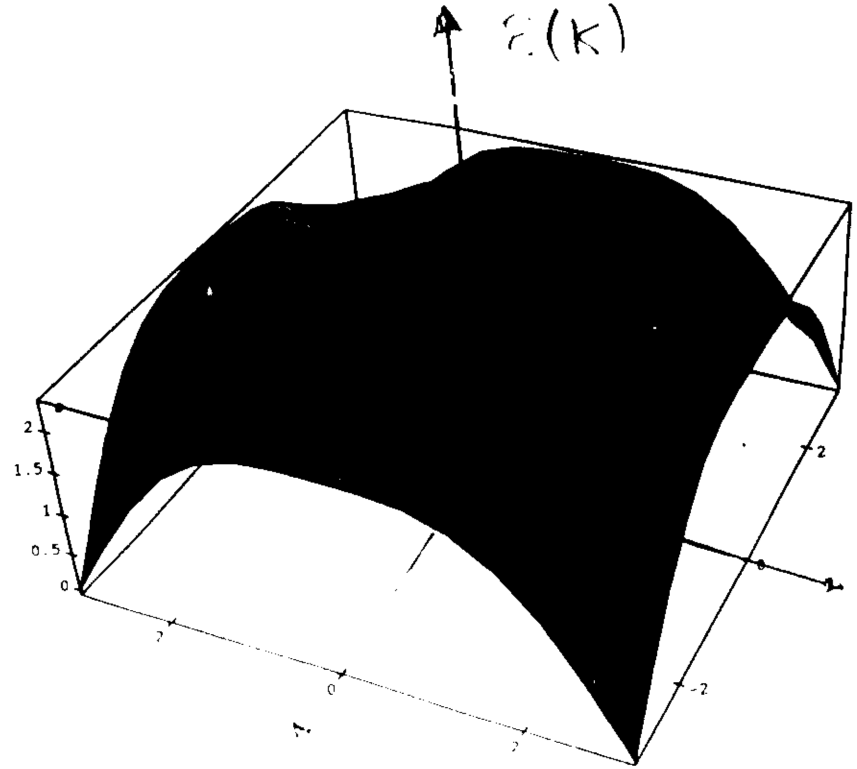
$$\omega_k \approx \sqrt{(J(k) - J(Q_0))\left(\frac{J(k+Q_0) + J(Q_0-k)}{2} - J(Q_0)\right)}$$

SPIN WAVE DISPERSION NEEL BOUNDARY



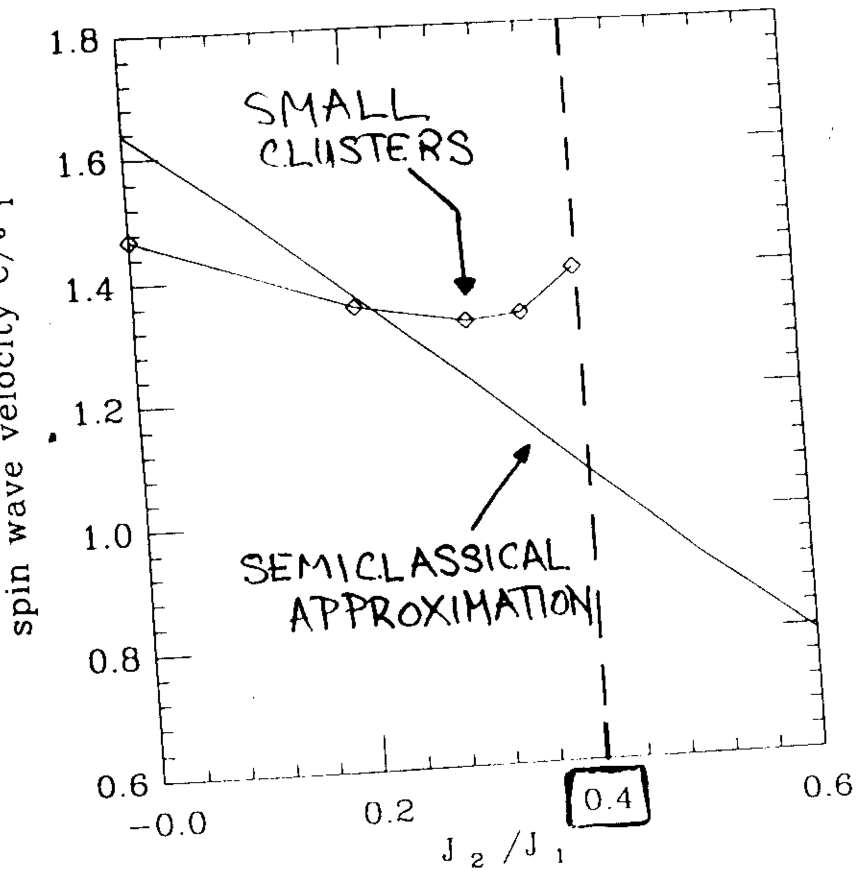
$\frac{J_2}{J_1} = 0.6$

SPIN WAVE DISPERSION



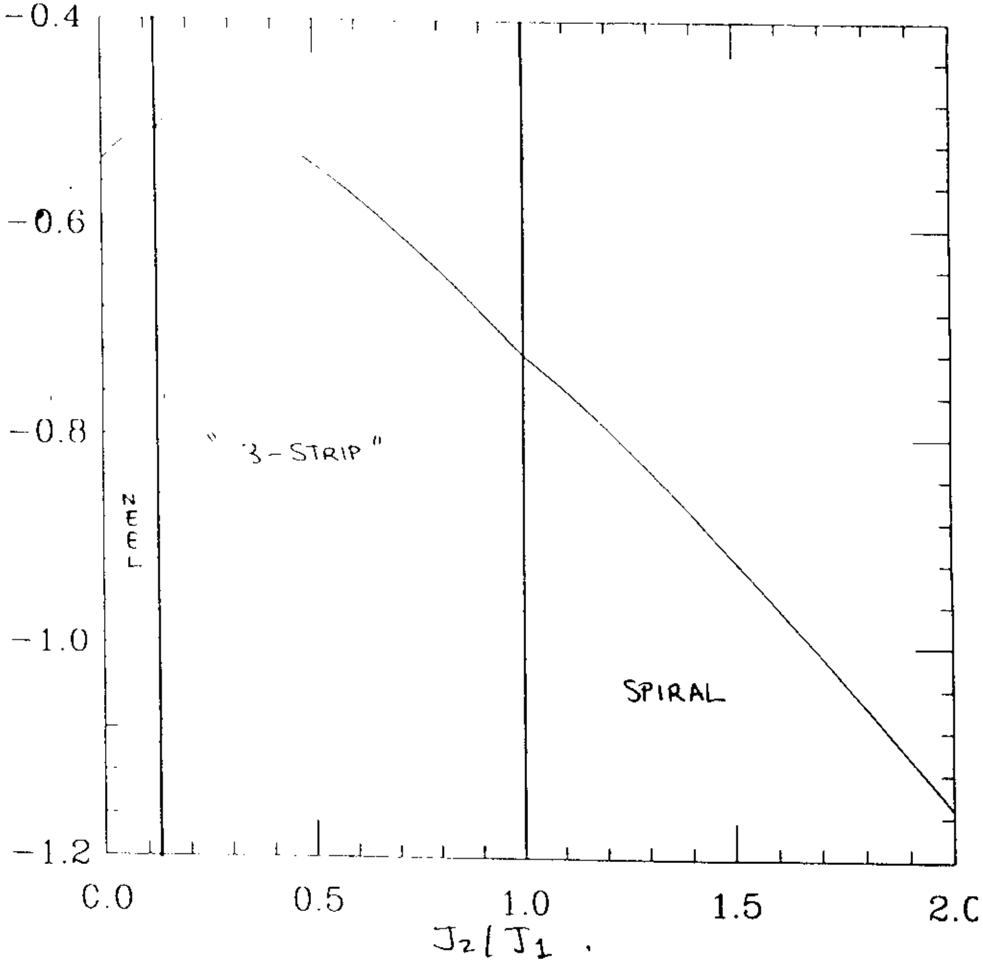
$J_2 = 0$

SPIN WAVE VELOCITY



TRIANGULAR LATTICE

GROUND-STATE ENERGY PER SITE IN UNITS OF J_1.



USING THE NON-LINEAR SIGMA MODEL

[STAGGERED] ORDER PARAMETER $\vec{\Omega}$

A UNIT VECTOR — N-Compont

LANDAU FREE ENERGY IS THEN

$$F = \frac{1}{2g} \int d^D x \, (\nabla_\alpha \vec{\Omega})^2 + \text{higher gradients}$$

ALL INVARIANT IN POTENTIAL ENERGY ARE FORBIDDEN ($\vec{\Omega}^2 = 1$)

PERTURBATIVE CONTENT OF NLσM ?

SOLVE THE CONSTRAINT

where has N-1 components

$$F = \frac{1}{2g} \int d^D x \left[(\nabla_\alpha \vec{\pi})^2 + \frac{(\vec{\pi} \cdot \nabla_\alpha \vec{\pi})^2}{1 - \vec{\pi}^2} \right]$$

THE π'S ARE UNCONSTRAINED ...

EXPANSION AROUND $\vec{\Omega}_0 = [1, 0, \dots, 0]$

⇒ THE π'S ARE THE N-1 GOLDSTONE BOSONS

WITH $1/p^2$ PROPAGATOR

AND INTERACTIONS

, etc...

SYMMETRY OF F is O(N)

AND $\vec{\Omega}_0$ IS INVARIANT UNDER

$$\begin{array}{ccccc} & O(N) & & O(N-1) & \\ \# \text{ générators} & \frac{1}{2} N(N-1) & \ominus & \frac{1}{2}(N-1)(N-2) & = N-1 \end{array}$$

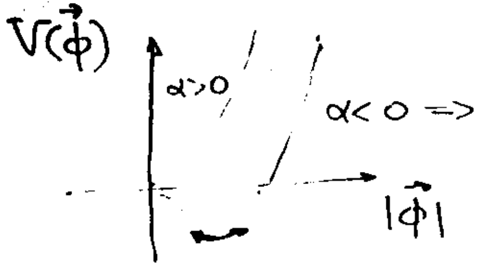
SIMPLEST EFFECTIVE THEORY OF THE SYMMETRY BREAKDOWN

$$O(N) \to O(N-1)$$

If Ordinary Landau Theory

$$F = \frac{1}{2g} (\nabla \vec{\phi})^2 + \alpha \vec{\phi}^2 + \beta (\vec{\phi}^2)^2$$

PHASE TRANSITION VARYING α



$\alpha < 0 \Rightarrow$ BROKEN SYMMETRY

$O(N) \to O(N-1)$

THERE IS AN ADDITIONAL RADIAL MODE CALLED σ WHICH IS MASSIVE

PROPAGATOR. $1/(p^2+M^2)$

FORGET IT IN THE I.R $\Rightarrow$ NON-LINEAR SIGMA MOD.

CRITICAL PHYSICS CAN BE REACHED BY BOTH MODELS

- LINEAR THEORY $(\vec{\phi}^2)^2$ RENORMALIZABLE $D=4$
- NON-LINEAR THEORY RENORMALIZABLE $D=$ [illegible]

BOTH CAN BE STUDIED FOR LARGE N AT [illegible]

- THE CASE $N=3$, $D=3$ IS DIFFICULT TO STUDY [$4-\epsilon$ RG studies, high-T series, numerics, fixed-D RG]

CLASSICAL FERRO CASE

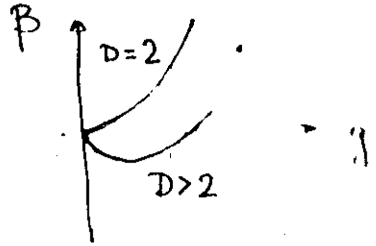
$$\beta H = -\frac{1}{T}\sum \vec{S}_i \cdot \vec{S}_j \Rightarrow \frac{1}{2T}\int d^D x \, (\nabla_\alpha \vec{S})^2$$

DO PERTURBATIVE RG

WILSON'S WAY $\Lambda \to \Lambda e^{-\ell}$

THEN $g(\ell)$ GIVEN BY:

$$\underbrace{\frac{dg(\ell)}{d\ell} = -(D-2)g + \frac{N-2}{2\pi}g^2 + O(g^3)}_{\text{THE } \beta \text{ FUNCTION}}$$



$D>2$: THERE IS A ZERO g^* AT WHICH THE THEORY IS SCALE INVARIANT

$\xi = \infty$ 2^{ND} ORDER AT T_c

$D=2$. $g^* = 0$

FLOW TO STRONG COUPLING

ALWAYS DISORDERED

OK WITH MERMIN-WAGNER

UNBROKEN SYMMETRY

$\boxed{\text{NOTE THE } N=2 \text{ CASE IS SPECIAL!}}$

BEHAVIOUR OF THE CORRELATION LENGTH :

$$\xi \equiv \xi(g(\ell))$$

UNDER RESCALING

$$\Lambda \to \Lambda/b$$

$$\xi \to \xi/b = \xi\, e^{-\ell}$$

THUS SIMPLE SCALING

$$\frac{d\xi}{d\ell} = -\xi = \frac{d\xi(g)}{dg} \cdot \underbrace{\frac{dg(\ell)}{d\ell}}_{\beta(g)}$$

$$\rightarrow \frac{d}{dg} \ln \xi(g) = \frac{-1}{\beta(g)}$$

IN $D = 2$ $\quad \beta(g) = \frac{N-2}{2\pi} g^2 + O(g^3)$

LEADING TERM : $\frac{d}{dg} \ln \xi(g) = -\frac{2\pi}{N-2} \frac{1}{g^2}$

$$\Rightarrow \quad \xi(g) = C^{ST} \cdot e^{\frac{2\pi}{N-2} \cdot \frac{1}{g}}$$

ESSENTIAL SINGULARITY AT $g = 0$ $[T = 0]$

HIGHER ORDER CALCULATION :

$$\Rightarrow \quad \xi(g) = C^{ST} \cdot g^{\frac{1}{N-2}} \cdot e^{\frac{2\pi}{N-2} \cdot \frac{1}{g}} \left[1 + O(g)\right]$$

THE C^{ST} IS <u>NOT</u> FIXED BY PERT. THEORY

IN $D > 2$ ONE HAS NEAR g^*

$$\frac{d}{d(g-g^*)} \ln \xi \simeq -\frac{1}{\beta'(g^*)} \frac{1}{(g-g^*)}$$

AND THUS $\xi \sim |g - g^*|^{-1/\beta'(g^*)}$

$$\boxed{\nu = \frac{1}{\beta'(g^*)}}$$

(ν begins by $\nu = \frac{1}{D-2}$)

IN $D = 2$ $\quad T \to 0$ TRANSITION.

<u>MORE TECHNICAL</u> : THE SO-CALLED SCHEME DEPENDENCE OF THE C^{ST} IN $\xi(g)$

SEVERAL WAYS TO IMPOSE A CUT-OFF NECESSARY SINCE PERT. THEORY IS DIVERGENT

EXAMPLES : LATTICE $\quad \Lambda = \frac{\pi}{a}$ $\quad a$: spacing

PAULI-VILLARS $\quad \frac{1}{p^2 + M} \to \frac{1}{p^2 + M} - \frac{1}{p^2 + M^2}$

COUPLING CONSTANT RENORMALIZATION

$$g_R = Z_{PV}^{-1}\, g \quad , \quad g_R = Z_{LAT}^{-1}\, g$$

where

$$\begin{cases} Z_{PV} = 1 + B(M)\,g^2 + O(g^4) \\ Z_{LAT} = 1 + B_L(a)\,g_L^2 + \cdots \end{cases}$$

There are logarithmic divergences in B's

$$\begin{cases} B(M) = -\beta_0 \ln M + C_{PV} \\ B_L(a) = -\beta_0 \ln\left(\frac{1}{a}\right) + C_{LAT} \end{cases}$$

We hold g_R fixed :

$$M \frac{\partial}{\partial M}\left(\frac{1}{g_R}\right) = 0 = M \frac{\partial}{\partial M}\left(\frac{1}{g} + B(M)\right)$$

leads to $M \frac{\partial g}{\partial M} = -\beta_0 g^2$

$$\begin{cases} g = \dfrac{1}{\beta_0 \ln \frac{M}{\Lambda_{PV}}} \\ g_L = \dfrac{1}{\beta_0 \ln \frac{1}{a\Lambda_L}} \end{cases}$$

Integration constant in Λ_{PV}, Λ_L for each scheme.

They are related since

$$\frac{1}{g_R} = \frac{Z_{PV}}{g} = \frac{Z_{LAT}}{g_L}$$

$$\frac{1}{g} + B(M) = \frac{1}{g_L} + B_L(a)$$

$$\beta_0 \ln \frac{M}{\Lambda_{PV}} + B(M) = \beta_0 \ln \frac{1}{a\Lambda_L} + B_L(a)$$

$$\boxed{\frac{\Lambda_{PV}}{\Lambda_{LAT}} = \exp\left[\frac{1}{\beta_0}\left(C_{PV} - C_{LAT}\right)\right]}$$

needs only finite parts in B's functions

Now $\xi = c^{st}.\, a .\, e^{+\frac{1}{\beta_0 g_L}}$

becomes $\xi = c^{ST}.\ \Lambda_{LAT}^{-1}$

If c^{ST} KNOWN IN ONE SCHEME THEN APPLY FORMULA IN $\boxed{}$ TO GET IT ELSEWHERE

THE $O(N)$ - NLσM model $\quad \sigma 9$

IS KNOWN FROM BETHE-ANSATZ

ξ^{-1} is THE MASS GAP m

$$m = \left(\frac{8}{e}\right)^{\frac{1}{N-2}} \frac{\Lambda_{\overline{MS}}}{\Gamma\left(1+\frac{1}{N-2}\right)}$$

for $O(3)$ case $\boxed{m = \frac{8}{e} \cdot \Lambda_{\overline{MS}}}$

ON A LATTICE $\boxed{m = 80.0864.. \Lambda_{LAT}}$

$\xi(T)$ IS KNOWN INCLUDING PREFACTOR.

ALL THIS IS FOR $D=2$ CLASSICAL NLσM

THEORY IS N degenerate massive particles with non trivial scattering

THE QUANTUM NONLINEAR SIGMA MODEL

$$S = \frac{1}{2}\rho \int_0^\beta d\tau \int d^D x \left[(\nabla \vec{\Omega})^2 + \frac{1}{c^2}(\partial_\tau \vec{\Omega})^2 \right]$$

$$+ \quad \vec{\Omega}^2 = 1$$

$\omega \sim k$: a relativistic theory appropriate to $O(N) \Rightarrow O(N-1)$ breakdown.

MATSUBARA TIME $\beta = 1/T$ IS A FINITE-SIZE EFFECT ONTO A $D+1$ "ORDINARY" NLσM.

$\Rightarrow$ INTERPLAY BETWEEN $\boxed{\xi \text{ AND } \beta}$

PERTURBATIVE CONTENT IS THE SAME GOLDSTONE $(N-1)$ WITH $\omega_k = ck$

$\Rightarrow$ LOOK AT R.G BEHAVIOUR OF THE COUPLINGS

$$g = \frac{c}{\rho}\Lambda^{D-1} \quad \text{and} \quad t = \frac{T}{\rho}\Lambda^{D-2}$$

$$\hookrightarrow g(\ell) \qquad\qquad \hookrightarrow t(\ell)$$

where $\vec{\Omega} = \left[\sqrt{1-\vec{\pi}^2},\ \vec{\pi}\right]$ as before

$$\vec{\pi}(x_0, x) = \sum_{n=-\infty}^{+\infty} \int \frac{d^D k}{(2\pi)^D}\, \vec{\pi}(\omega_n, \vec{k})\, e^{i\omega_n x_0 + i\vec{k}\cdot\vec{x}}$$

$$\vec{\pi}(\omega_n, \vec{q}) = \begin{cases} \vec{\pi}_<(\omega_n, q) & 0 < |\vec{q}| < \Lambda e^{-l} \\ \vec{\pi}_>(\omega_n, q) & \Lambda e^{-l} < |\vec{q}| < \Lambda \end{cases}$$

INTEGRATE OUT $\vec{\pi}_>$: $\int \mathcal{D}\vec{\pi}_>$

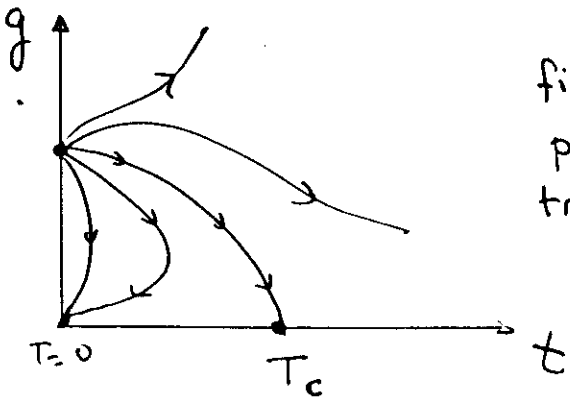
- EFFECTIVE ACTION FOR $\vec{\pi}_<$
- RESCALE q's BACK TO Λ

$$\begin{cases} \dfrac{dg(l)}{dl} = (1-D)g + \dfrac{1}{2} g^2 \coth\left(\dfrac{g}{2t}\right) \\[2ex] \dfrac{dt(l)}{dl} = (2-D)t + \dfrac{1}{2} g t \coth\left(\dfrac{g}{2t}\right) \end{cases}$$

$1 < D \leq 2$ ONE ZERO-TEMPERATURE FIXED POINT $g^* \neq 0$

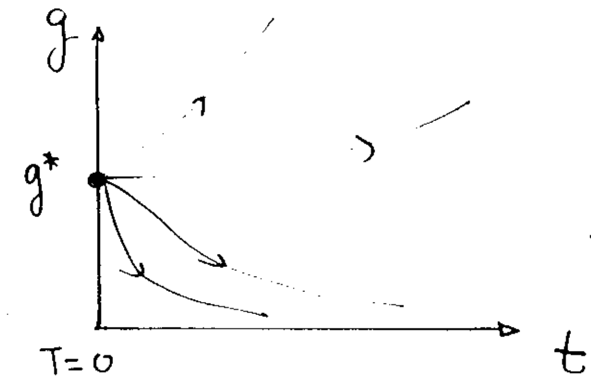
$D > 2$ TWO FP's

D = 3



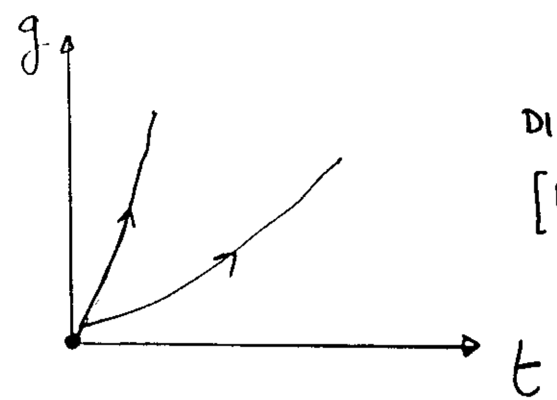
finite-T phase transition

D = 2



NO finite-T phase transition

D = 1



ALWAYS DISORDERED

[INTEGER SPINS ONLY]

ξ D=2 QUANTUM CASE

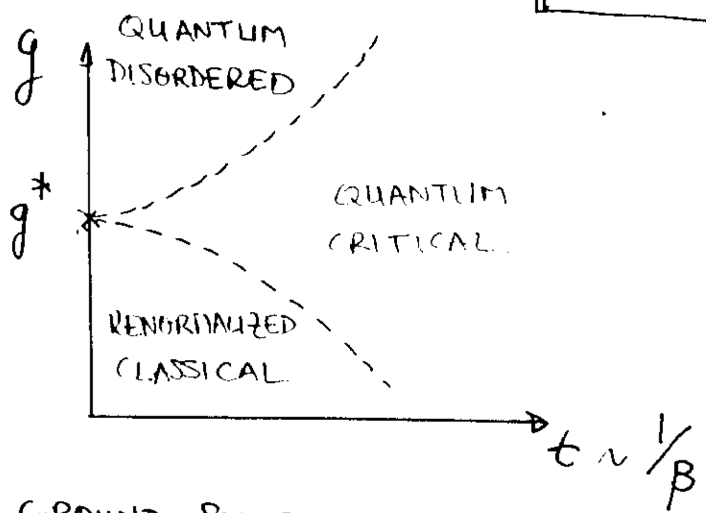
A QUANTUM (T=0) PHASE TRANSITION

ORDERED / NONORDERED

WHICH IS $\begin{cases}\text{HEISENBERG} & D=3\\ \text{CLASSICAL}\end{cases}$

AT $\boxed{T=0} \Rightarrow \xi \sim |g-g|^{-\nu_3}$

THERE ARE CROSSOVER LINES $\boxed{\xi \sim \beta}$



$g<g^*$ GROUND STATE IS ORDERED

SPIN-$\frac{1}{2}$ SQUARE LATTICE $\Rightarrow g<g^*$

CORRELATION LENGTH ξ(T)

AT $g=g^*$ β FIXES THE SCALE

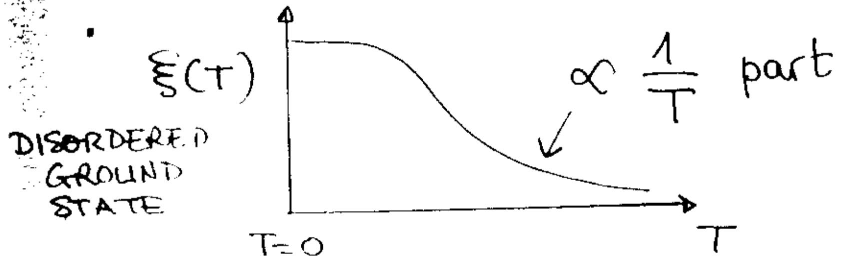
$$\xi(T) \sim \beta \sim \frac{1}{T}$$

TRUE AS LONG AS $\beta \gtrless \xi_\infty(T=0)$

DEFINES THE "QUANTUM CRITICAL REGIME"

– IF $g>g^*$ THERE IS A LIMITING VALUE

$\xi(T=0)$ ξ SATURATES AS $T \to 0$



IN QNLσM finite $\xi \Rightarrow$ $\boxed{\text{finite} \neq 0 \text{ GAP AT } T=0}$

NOTE: IN THE ORDERED PHASE

ξ DEFINED A LA JOSEPHSON

MASSLESS MAGNONS / CRITICAL FLUCTUATIONS

THE RENORMALIZED CLASSICAL REGIME

INTEGRATE OUT QUANTUM FLUCTUATIONS

IN THIS REGIME : SMALL EFFECT !!!

$$\vec{\pi}(\omega_n, q) = \begin{cases} \vec{\pi}_<(q) & \omega_n = 0 \\ \vec{\pi}_>(\omega_n, q) & \omega_n \neq 0 \end{cases}$$

$\int \mathcal{D}\vec{\pi}_>(\omega_n, q)$ gives

$$S_{RC} = \frac{1}{2t_{RC}} \int d^2x \, (\nabla \vec{\Omega})^2$$

where :

$$\frac{1}{t_{RC}} = \frac{1}{T}\left[\underbrace{\rho - \frac{(N-2)}{4\pi} c\Lambda}_{\tilde{\rho}} + T \, \frac{N-2}{4\pi} \ln\left(\frac{\Lambda c}{T}\right) + \ldots \right]$$

$\Rightarrow$ BACK TO A D-dimensional CLASSICAL NLσM WITH t_{RC} coupling

USE FORMULA FOR ξ WITH t_{RC} COUPLING AND RELATE SCHEME THROUGH 1-LOOP FINITE-PARTS

$$\hookrightarrow \boxed{\xi(T) = 0.35 \times \frac{c}{2\pi\tilde{\rho}} \times \exp\left[\frac{2\pi\tilde{\rho}}{T}\right]}$$

EXPONENTIAL DIVERGENCE AS $T \to 0$ (GS ORDERED)

- SEEN IN La_2CuO_4 ABOVE T_{NEEL} !
- THE PARAMETERS c AND $\tilde{\rho}$ FROM SPIN-WAVE THEORY OR SERIES OR QMC | LANCZOS
- SQUARE LATTICE SPIN-$1/2$ $\begin{cases} \tilde{\rho} \simeq 0.15 \, J \\ c \simeq 0.64 \, J \end{cases}$
- ABSOLUTE PREDICTION.
- UNDOPED CuO_2 PLANES HAVE AT $T=0$ NEEL ORDER.
- NUMERICAL ESTIMATES OF $\xi(T)$ FOR SPIN-$\frac{1}{2}$ SQ. LAT ARE IN AGREEMENT WITH R.G PREDICTIONS.
- TRIANGULAR LATTICE $\Rightarrow$ ANOTHER SIGMA MODEL LEADS ALSO TO $\xi(T) \sim e^{A/T}$ (ABSOLUTE PREFACTOR NOT KNOWN) BUT A-AMPLITUDE FROM SWT NOT OK WITH SERIES.

MORE SIGMA MODELS

THE COOKBOOK WAY

FRUSTRATED SYSTEMS (NON COLLINEAR)
LOCALIZATION

MANIFOLD WITH A METRIC

ϕ^i SOME COORDINATES ON THE MANIFOLD

METRIC IS GIVEN BY

$$ds^2 = g_{\mu\nu}(\phi)\, d\phi^\mu d\phi^\nu$$

[ex $ds^2 = c^2 dt^2 - d\vec{x}^2$ IN MINKOVSKI SPACE]

THERE ARE GOOD OBJECTS

$\phi \rightsquigarrow \phi'$ $\quad \phi^i = \phi^i(\phi')$

$$V^i(\phi) = \frac{\partial \phi^i}{\partial \phi'^j} V^j(\phi')$$

V IS A CONTRAVARIANT VECTOR

WITH $\frac{\partial \phi'}{\partial \phi} \to$ COVARIANT $V_i \leftarrow$ LOWER INDEX

($d\phi^i$ is vector, NOT ϕ^i !!!)

$\partial_i V^j$ IS NOT A GOOD OBJECT

THE RIGHT ONE IS

$$D_i V^j = \partial_i V^j + \Gamma^j_{ik} V^k$$

where the Christoffel symbol Γ means

$$\Gamma^i_{jk} = \frac{1}{2} g^{il}\left[\partial_j g_{lk} + \partial_k g_{lj} - \partial_l g_{jk}\right]$$

CURVATURE IS ENCODED IN $\mathbb{R}$ TENSOR

$$[D_i, D_j] V^k = \mathbb{R}^k_{lij} V^l$$

$$\mathbb{R}^k_{lij} = \partial_i \Gamma^k_{jl} - \partial_j \Gamma^k_{il} + \Gamma^k_{im}\Gamma^m_{jl} - \Gamma^k_{jm}\Gamma^m_{il}$$

A SIMPLER OBJECT IS THE RICCI TENSOR

$$\mathbb{R}_{ij} = \mathbb{R}^k_{ijk}$$

and the scalar curvature

$$R = R^i_i = R^{kl}_{kl}$$

an arbitrary SIGMA MODEL

$$x\text{- space} \xrightarrow{\phi^i(x)}$$

TARGET SPACE OF ϕ

$$S = \int d^D x \; g_{\mu\nu}(\phi(x))\, \partial_\alpha \phi^\mu(x)\, \partial_\alpha \phi^\nu(x)$$

BEWARE OF INDEX GAMES in x-space.

THEN β-function is known

$$\beta(g) = (D-2)\, g^{\mu\nu} - \frac{1}{2\pi} R^{\mu\nu} - \frac{1}{8\pi^2} R^{\mu\rho\sigma\tau} R^{\nu}{}_{\rho\sigma\tau} + O(g^4)$$

USE MATH PACKAGE ...

REMEMBER $O(N)$ NLσM

$$S = \int d^D x \left[(\nabla_\alpha \vec{\pi})^2 + \frac{(\vec{\pi}\nabla_\alpha \vec{\pi})^2}{1-\vec{\pi}^2} \right]$$

THIS CASE

TREAT π AS N-1 COORDINATES

AND

$$g^0_{\mu\nu} = \delta_{\mu\nu} + \frac{\pi_\mu \pi_\nu}{1-\vec{\pi}^2}$$

IS A NONTRIVIAL METRIC ON π-SPACE

IF LUCKY $\beta(g) \propto g^0$

$\to$ RENORMALIZABLE THEORY

ONLY CHANGE OF COUPLING CONSTANT...

HEISENBERG SPIN CHAINS AND THE HALDANE CONJECTURE

RIVING THE NLσM FOR A SPIN CHAIN

$$= \frac{1}{2g}\int dt\,dx\,(\nabla\vec{\Omega})^2 + (\theta\text{-term})$$

$$g = \frac{2}{S} \quad \text{and}$$

$$\text{term} = 2\pi S \times \underbrace{\frac{1}{8\pi}\int dt\,dx\,\epsilon_{\mu\nu}\,(\vec{\Omega}\,|\,\partial_\mu\vec{\Omega}\,|\,\partial_\nu\vec{\Omega})}_{\text{INTEGER}}$$

COUNTING $\pi_2(S^2)$

TH BC's $\vec{\Omega}$ maps S^2 ONTO S^2

EYNMANN'S AMPLITUDE

$$\sum_{\vec{N}} \int \mathcal{D}\vec{\Omega}\,\delta(\vec{\Omega}^2-1)\, e^{i\cdot 2\pi S\cdot N}\, e^{i\frac{1}{2g}\int dt\,dx\,(\nabla\vec{\Omega})^2}$$

S INTEGER $\Rightarrow$ NLσM O(3) "STANDARD" ONE

DPOLOGICAL TERM REMAINS MYSTERIOUS ...

INTEGER $\to$ GAP PHASE "HALDANE" GAP.

S $\frac{1}{2}$-INTEGER ? LOOK AT SPIN-$\frac{1}{2}$

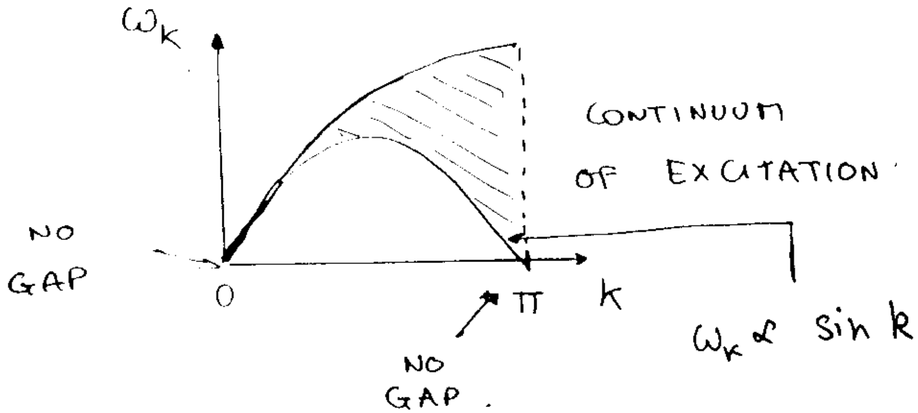
MUCH IS KNOWN FROM BETHE-ANSATZ + BOSONIZATION

THERE IS ALMOST LONG-RANGE ORDER

$$\langle \vec{S}_0 \cdot \vec{S}_x \rangle \sim \frac{(-)^x}{|x|}$$

ALGEBRAIC DECAY (NOT $e^{-x/\xi}$!!!)

THERE IS NO GAP : ALMOST-GOLDSTONE MODES !!!



EASY FROM A FERMION PICTURE OF XY SPIN-$\frac{1}{2}$: $\sum_i S_i^x S_{i+1}^x + S_i^y S_{i+1}^y$

FROM NLσM + θ-term

EXPECT. SUCH PICTURE FOR ALL

$\frac{1}{2}$-INTEGER SPIN CHAINS.

• FOR SPIN-1 CHAIN:

HALDANE GAP SEEN IN NUMERICS

AND $Ni(C_2H_8N_2)_2NO_2ClO_4$ [NENP]

OTHER CANDIDATES SUCH AS

$Ni(C_3H_{10}N_2)_2NO_2ClO_4$ [NINO]

• QUANTUM-MECHANICAL STUDY FOR

SPIN-$\frac{1}{2}$ XY:

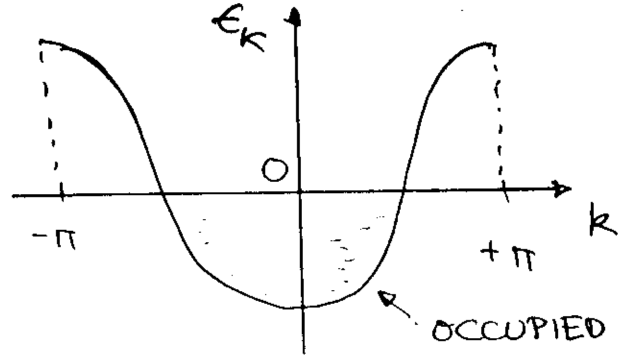
USE JORDAN-WIGNER SPINS ⇒ FERMIONS

$$\begin{cases} S^z = c_n^+ c_n - \frac{1}{2} \\ S_n^+ = e^{i\pi \sum_{m<n} c_m^+ c_m} c_n \\ S_n^- = (S_n^+)^n \end{cases}$$

$$\text{XY-CHAINS} \Rightarrow H = -\sum_n c_n^+ c_{n+1} + c_{n+1}^+ c_n$$

SPINLESS FREE

FERMIONS.



HALF-FILLED: $\langle S^z \rangle = 0$

PARTICLE-HOLE GAPLESS EXCITATIONS

AT $K=0$ AND $K=\pi$

FOR XXZ SPIN CHAIN ⇒ INTERACTING FERMIONS

$\Delta S_n^z S_{n+1}^z \Rightarrow$ 4-fermi term.

PICTURE STILL TRUE FOR NOT TOO

STRONG ANISOTROPY $\Delta \leq 1$

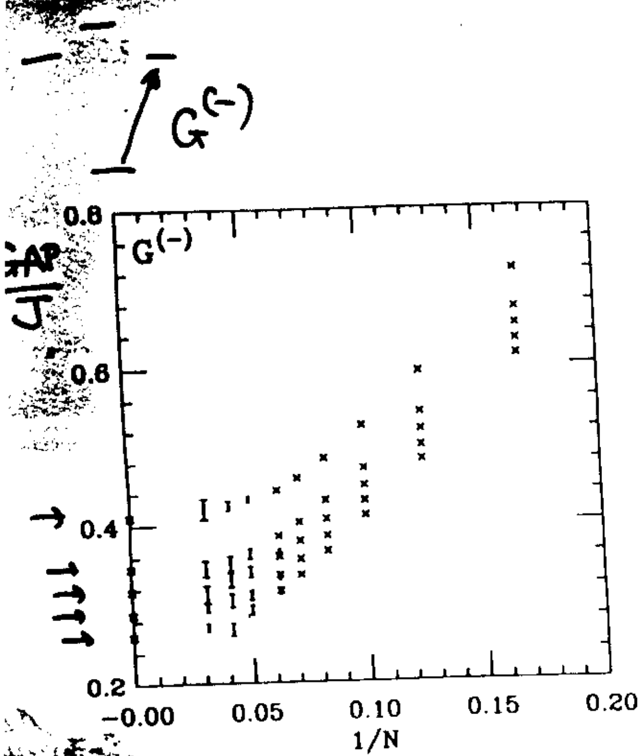
THE SPIN-1 CHAIN AND VBS STATES

SPIN-1 = TWO SYMMETRIZED SPIN-$\frac{1}{2}$

SPIN-1   2 SPIN-$\frac{1}{2}$

sc4 9

A NUMERICAL CALCULATION



N = # SPINS

Fig. 3

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sc5

CONSTRUCT A WAVEFUNCTION

$$|VBS\rangle = \cdots$$

means

$$\psi_{VBS} = \cdots \underbrace{\psi_{\alpha\beta}}_{\text{symmetrized two spin-}\frac{1}{2}} \epsilon^{\beta\gamma} \psi_{\gamma\delta} \epsilon^{\delta\rho} \psi_{\rho\mu} \epsilon^{\mu\nu} \psi_{\nu\sigma} \cdots$$

ALL BONDS ARE SINGLET STATES

NOTE THAT $\hat{\mathbb{P}}_{S=2}\left[\;\underset{i}{\odot}\;\;\underset{i+1}{\odot}\;\right] = 0$

THUS

$$\left\{ \sum_i \hat{\mathbb{P}}^{S=2}_{i,i+1} \right\} |VBS\rangle = 0$$

IN TERMS OF SPINS

$$\hat{H}_{VBS} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2$$

HAS EXACT GROUND STATE $|VBS\rangle$!!!

[AKLT CONSTRUCTION]

CORRELATION LENGTH IS SHORT:

$$\langle VBS | \vec{S}_0 \cdot \vec{S}_n | VBS \rangle = (-3)^{-n} \quad \text{(exact)}$$

THERE IS A GAP $\approx 0.38 \times J$ (VBS)

IN THE FAMILY

$$\hat{H}_\theta = \cos\theta \sum_n \vec{S}_n \cdot \vec{S}_{n+1} + \sin\theta \sum_n (\vec{S}_n \cdot \vec{S}_{n+1})^2$$

VBS Hamiltonian and nearest-neighbor are close ($\frac{1}{3}$ is small)

- $$\hat{H} = J \sum_n \vec{S}_n \cdot \vec{S}_{n+1}$$

has $\underbrace{\text{gap}}_{\downarrow} = \boxed{0.41 \times J}$ and $\boxed{\xi \cong 6.2\, a}$

- EXACT DIAGONALIZATION UP TO 22 SITES
- QUANTUM MONTE-CARLO IN A GOOD BASIS [LIEB-MATTIS]

GROUND STATE WAVEFUNCTION HAS ALL WEIGHTS POSITIVE : Can be interpreted as transition probability

AIN LENGTH IS NO PROBLEM BUT STATISTICAL FLUCTUATIONS AND INTRINSIC BIAS

- REAL-SPACE R.G IS ALSO VERY EFFICIENT
- The THERMODYNAMIC LIMIT IS APPROACHED EXPONENTIALLY ON A CLOSED SPIN CHAIN Very favorable!
- Use Accelerated Convergence Tricks

$$G_N^{(K+1)} = \frac{G_{N+1}^{(K)} G_{N-1}^{(K)} - G_N^{(K)2}}{G_{N+1}^{(K)} + G_{N-1}^{(K)} - 2\, G_N^{(K)}}$$

[Shanks (remember π), Aitken's Δ_2, ϵ-algorithm of Wynn ..]

Very usefull to know ...

TABLES

D	N	$G^{(0)}$	$G^{(1)}$	$G^{(2)}$	$G^{(3)}$
0.00	4	1.0000000			
	6	0.7200374	0.4076324		
	8	0.5935553	0.4437764	0.4126206	
	10	0.5240000	0.4253773	0.4152913	0.4107742
	12	0.4841965	0.4176742	0.4109213	
	14	0.4600053	0.4130413		
	16	0.4437000			
0.10	4	0.9561081			
	6	0.6716110	0.4327300		
	8	0.5410006	0.3863721	0.3500700	
	10	0.4700600	0.3683023	0.3464963	0.3407451
	12	0.4286764	0.3500570	0.3474703	
	14	0.4021143	0.3622272		
	16	0.3847610			
0.15	4	0.9363447			
	6	0.6501495	0.4097091		
	8	0.5103640	0.3622356	0.3232136	
	10	0.4479770	0.3400061	0.3183048	0.3174152
	12	0.4051510	0.3301904	0.3180702	
	14	0.3770060	0.3243021		
	16	0.3500610			
0.20	4	0.9170223			
	6	0.6300006	0.3409209		
	8	0.4993425	0.3406023	0.2967202	
	10	0.4374912	0.3170041	0.2916224	0.2864543
	12	0.3940400	0.3053027	0.2905016	
	14	0.3560694	0.2984033		
	16	0.3372277			
0.25	4	0.9000057			
	6	0.6120073	0.3700198		
	8	0.4814006	0.3210606	0.2718349	
	10	0.4091656	0.2902431	0.2645361	0.2611069
	12	0.3661006	0.2823130	0.2622753	
	14	0.3363528	0.2740957		
	16	0.3106475			

Table I

ORDER PARAMETERS & ANISOTROPIES

$$\hat{H} = J\sum_n S_n^x S_{n+1}^x + S_n^y S_{n+1}^y + \underbrace{\Delta S_n^z S_{n+1}^z}_{\text{EXCHANGE}} + \underbrace{D\sum_n (S_n^z)^2}_{\text{SINGLE ION}}$$

HALDANE PHASE FINALLY SHOULD DISAPPEAR !! for LARGE Δ or D.

THE "SURFACE" LANGUAGE :
TRANSLATE $|VBS\rangle$ IN $\{S_i^z\}$-EIGENSTATES

$$|VBS\rangle = \sum_{\text{states}} |\cdot\cdot 0 \uparrow\downarrow 0 \cdot\cdot 0 \uparrow 0 \cdot\cdot 0 \downarrow\uparrow 0 \cdot\cdot 0 \downarrow 0 \cdots\rangle$$

$\exists$ Strict AF order diluted by <u>zeros</u>

A "DISORDERED FLAT" SURFACE

ISING LIMIT $\Delta \to +\infty$

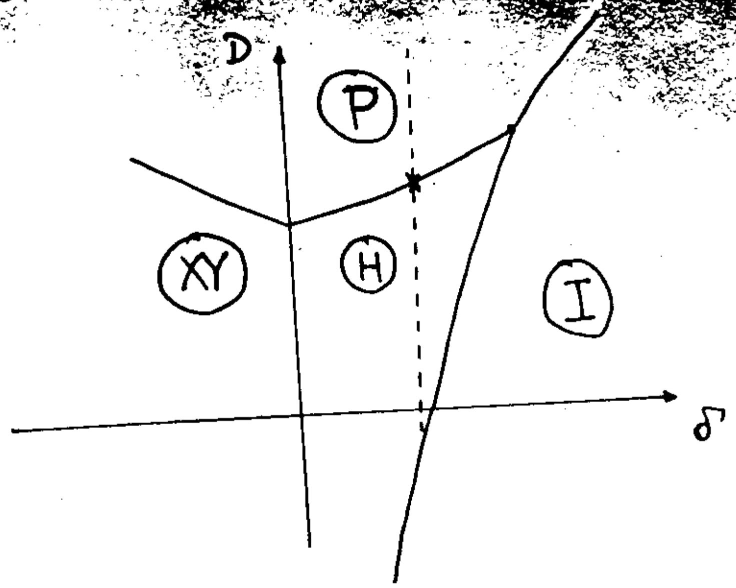
$|0\rangle = |\uparrow\downarrow\uparrow \cdots\rangle$

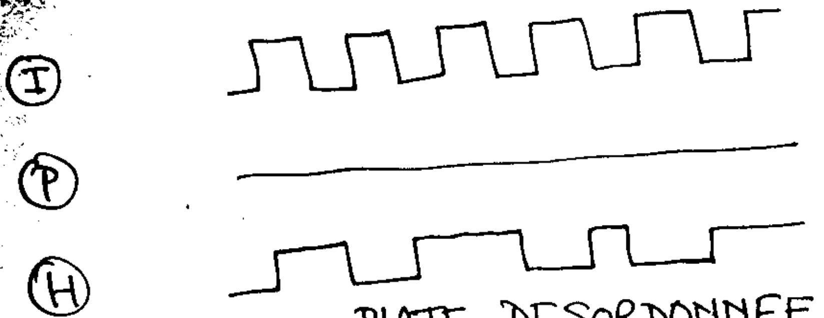
LARGE-D PHASE $D \to +\infty$

$|GS\rangle = |00\ldots0\cdots\rangle$

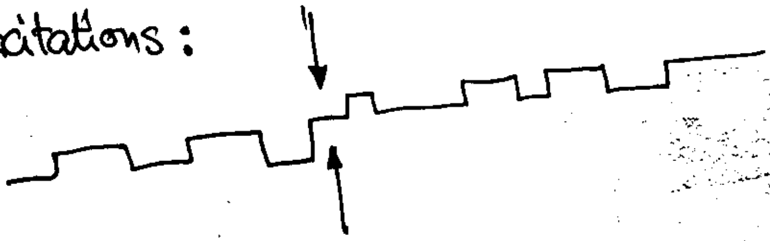
…ME DE PHASE DANS LES ANISOTROPES

Rommelse Den Nijs 89





excitations :



REAL HALDANE GAP MATERIAL

SHOULD HAVE Δ AND D SMALL ENOUGH

IN THE THERMODYNAMIC LIMIT:

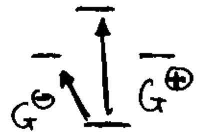
$S=1$ — — — $K=\pi$ FINITE CHAIN GAP

$S=0$ — $K=0$ GROUND STATE

If Anisotropy ⇒ SPLITTING OF THE TRIPLET

$\underbrace{- - -}_{S=1} \xrightarrow{D\neq 0}$ — $S^z=0$, — — $S^z=\pm 1$

THERE ARE <u>TWO GAPS</u>



TILL $D/J = 0.4$ ALMOST LINEAR SPLIT

$$\begin{cases} G^{(+)}(D) = 0.41 + 1.41\,D \\ G^{(-)}(D) = 0.41 - 0.57\,D \end{cases}$$

PHASE TRANSITION TO LARGE-D PHASE

AT $\left(\frac{D}{J}\right)_{crit} = 1.00(1)$

...NENF GAP IS SEEN IN
...HERMODYNAMICS $C_V(T)$, $\chi(T)$
...AND NEUTRON SCATTERING

GAPS AT $K=\pi$ $\quad G^{(+)} = 2.5$ meV
$\quad G^{(-)} = 1.25$ meV

...EADS TO $\boxed{J = 44\,K}$ $\boxed{D/J = 0.18}$

...SHOULD PREDICT ALL MAGNETIC PROPERTIES

...NEUTRON SCATTERERS MEASURE
DYNAMICAL STRUCTURE FACTOR

$$S^{\alpha\alpha}(Q,\omega) = \sum_n \underbrace{|\langle n|\, S^\alpha_Q \,|0\rangle|^2}_{\text{matrix element non-trivial}} \delta(\omega - \epsilon_n)$$

ϵ_n: excited state energy

...N GENERAL

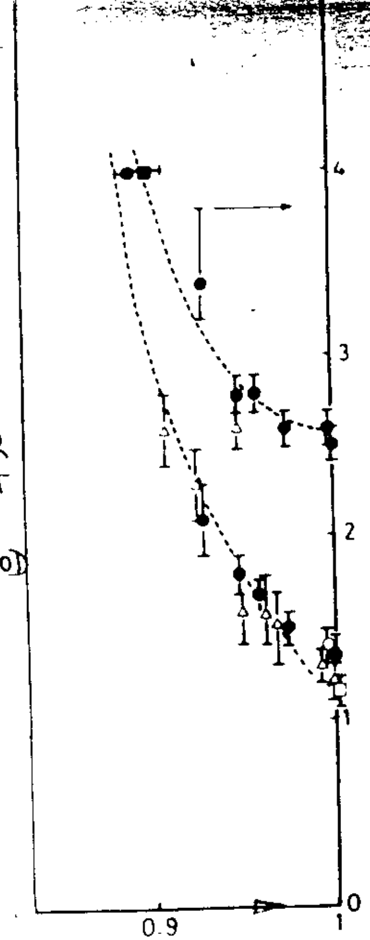
$$I(Q\,\omega) = C^{st} \sum_{\alpha,\beta}{}' \left(\delta_{\alpha\beta} - \frac{Q^\alpha Q^\beta}{\vec{Q}^2}\right) S^{\alpha\beta}(Q,\omega)$$

...INCE $|0\rangle$ SINGLET (UNBROKEN SYMMETRY)

$S^\alpha_{Q=0}\,|0\rangle = 0$ $\quad Q \Rightarrow 0$ $\quad S^{\alpha\alpha}$ should vanish

ENERGIE

meV



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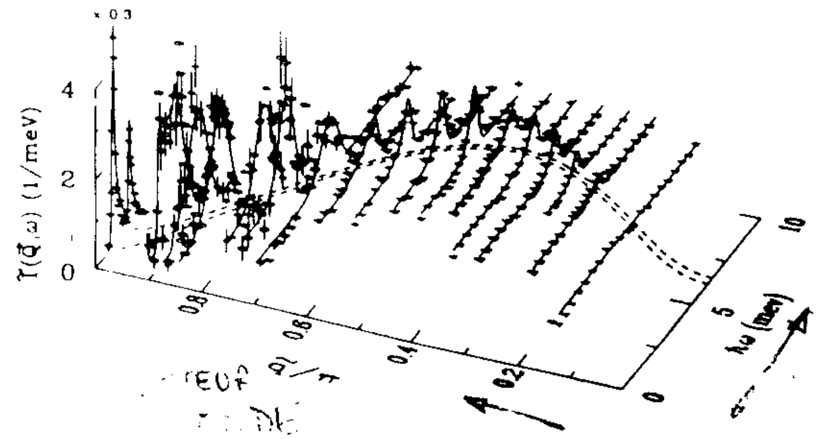
DISPERSION DES EXCITATIONS MAGNETIQUES

[GRAND] VECTEUR D'ONDE $\frac{q}{\pi}$

STRUCTURE FACTOR



MA
BROHOLM
REICH
STERNLIEB
ERWIN 1992

THE WOULD-BE SPIN-WAVE

IS $\begin{cases} \text{TRIPLET } S=1 \text{ - UNBROKEN SYMMETRY} \\ \text{GAPPED (NL}\sigma\text{M) } \Delta_H \end{cases}$

→ SOME MODE $\omega_H(k)$ $\begin{cases} \text{"MASSIVE"} \\ \text{MAGNON} \end{cases}$

TWO-MAGNON

CONTINUUM START AT $2\Delta_H$ FOR $K=0$

$\left((K=\pi) + (K=\pi) \text{ have mass } 2\Delta_H \right)$

WITH ANISOTROPY TWO GAPPED MODES

$\begin{cases} \text{IN } S^z=0 \text{ SECTOR} \\ \text{IN } S^z=\pm1 \text{ SECTOR} \end{cases}$

CONTINUUM IN $S^z=0$ $\begin{cases} (S^z=0)+(S^z=0) \\ (S^z=+1)+(S^z=-1) \end{cases}$

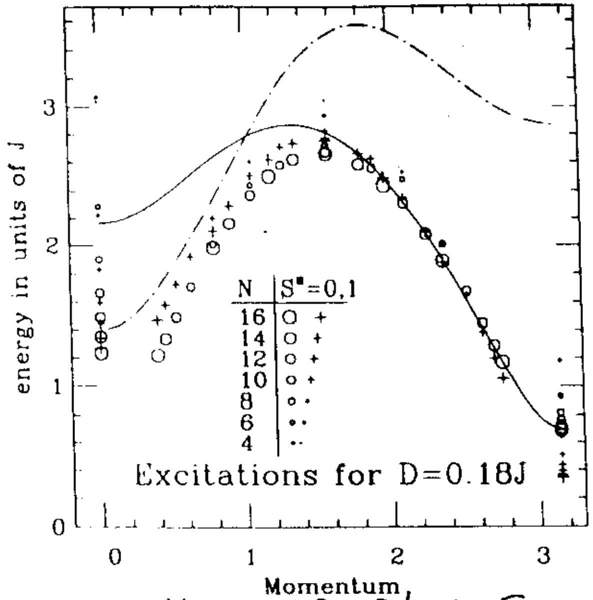
CONTINUUM IN $S^z=\pm1$ $\left\{ (S^z=0) + (S^z=\pm1) \right.$

DETAILED INS EXPERIMENTS IN AGREEMENT

CONTINUUM NOT YET SEEN

ENERGY

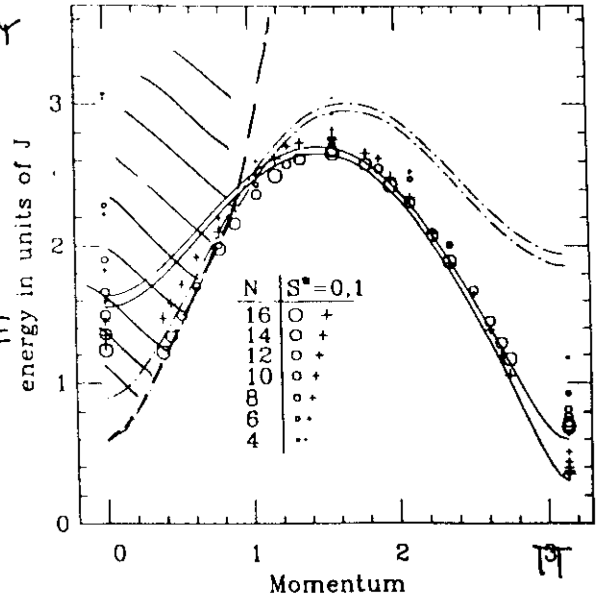
THEORIE + THEORIE



VECTEUR D'ONDE ⟹

ENERGY

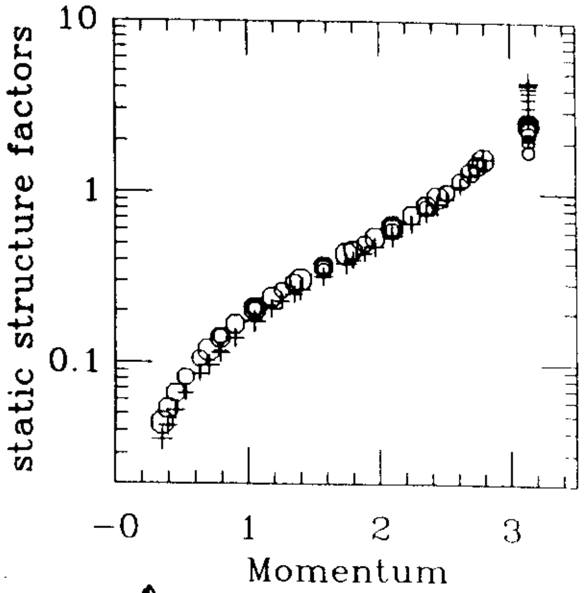
THEORIE + EXPERIENCE



WAVEVECTOR

$S(q) = \int d\omega \, S(q, \omega)$

INTEGRATED INTENSITY



THE $\frac{D}{J} = 0.18$ CASE

(AS NENP)

VERY SMALL FOR $K \to 0$

A SIMPLE FERMIONIC APPROXIMATION

IN $|VBS\rangle$ KEEP ONLY THE ZEROS

$\to$ FERMIONS $\boxed{S^z = 0 \text{ Sector}}$

$\uparrow\downarrow \longrightarrow 0\,0 \quad : \quad c_i^+ c_{i+1}^+$

$0\,0 \longrightarrow \uparrow\downarrow \quad : \quad c_i c_{i+1}$

$$\hat{H}_f = \sum c_n^+ c_{n+1} + c_{n+1}^+ c_n + c_n^+ c_{n+1}^+ + c_n c_{n+1} + \dots$$

USE a BCS-approximation

$$|\psi_0\rangle = \prod_k \left(u_k + v_k c_k^+ c_{-k}^+\right) |0\rangle$$

EXCITED STATES ($S^z = 0$ ONLY)

$$\gamma_q^+ |\psi_0\rangle = c_q^+ \prod_{k \neq q} \left(u_k + v_k c_k^+ c_{-k}^+\right) |0\rangle$$

HAVE GAPPED DISPERSION LAW $E(K)$ (SEE FIG.) $\Rightarrow$ GOOD APPROXIMATION !!!

TAILED HIGH-RES NEUTRON

THREE GAPS $\begin{cases} 1.05 \\ 1.25 \quad \text{meV} \\ 2.5 \end{cases}$

"PARASITIC" SPLITTING BETWEEN $S^z = +1$ & -1

$$D(S^z_n)^2 + E\left[(S^x_n)^2 - (S^y_n)^2\right]$$

In fact $\frac{E}{J} \simeq 0.012$ $(E << D)$

PERTURBATION THEORY ON THE HALDANE TRIPLET STATE

$\vec{H}$ ALONG γ-direction

then Δ_γ unchanged

$$\Delta_\pm = \frac{1}{2}\left[\Delta_\alpha + \Delta_\beta \pm \left[(\Delta_\alpha - \Delta_\beta)^2 + 4H_\gamma^2\right]^{1/2}\right]$$

Hyperbolic splitting

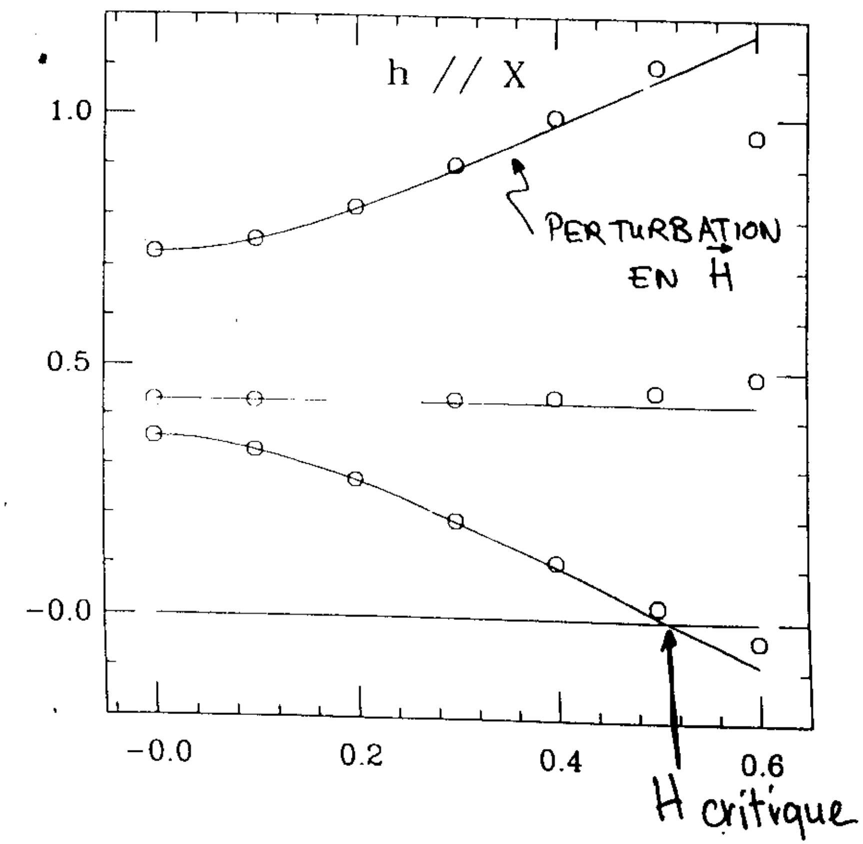
in agreement with Lanczos Studies

INFLUENCE D'UN CHAMP MAGNETIQUE

$$D[S^z_i]^2 + E\left[(S^x_i)^2 - (S^y_i)^2\right] - \vec{H}\cdot\vec{S}_i$$

triplet de Haldane $\begin{cases} \text{— } 2.5 \text{ meV} \\ \\ \text{= } 1.25 \text{ meV} \\ \text{= } 1.05 \text{ meV} \end{cases}$ E D

$\overline{S=0}$



GAP DE HALDANE

SOUS CHAMP MAGNETIQUE

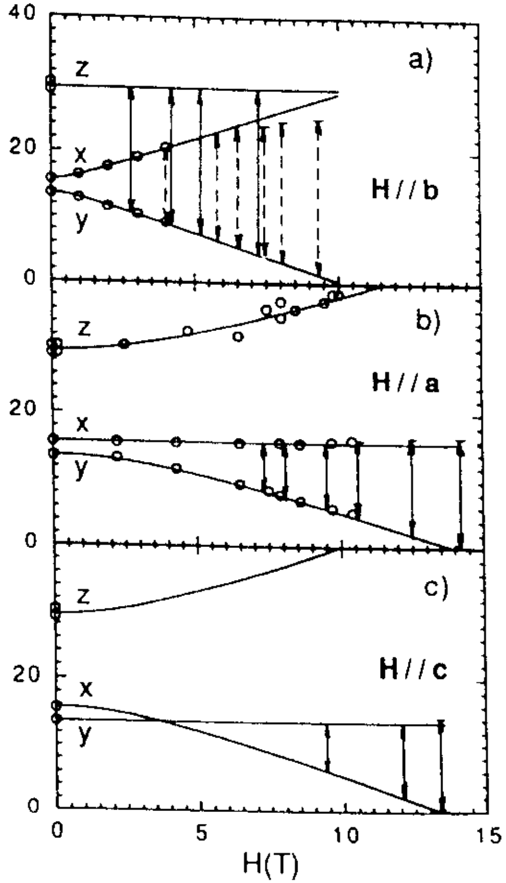
[SUITE]

TRANSITIONS
ESR

TRAITS VERTICAUX

• NEUTRONS
○

LIGNES:
perturbation
en $\vec{H}$
= Diagonalization
exacte



USE OF QNLσM [ALL INTEGER SPINS]

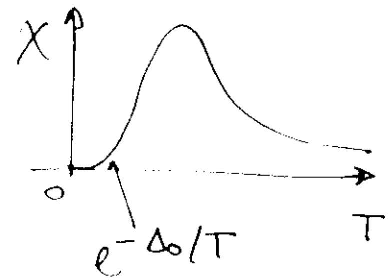
FP AT THE ORIGIN

TREAT BY LARGE-N LIMIT

- $\Delta(T) = \Delta_0 + \sqrt{2\pi\Delta_0 T}\, e^{-\Delta_0/T}$
- χ AND C ACTIVATED BEHAVIOUR
- IN NMR $T_1^{-1} \propto e^{-\Delta_0/T}$
- QUASIPARTICLE LINEWIDTH
- $\Gamma(T) \sim e^{-\Delta_0/T}$

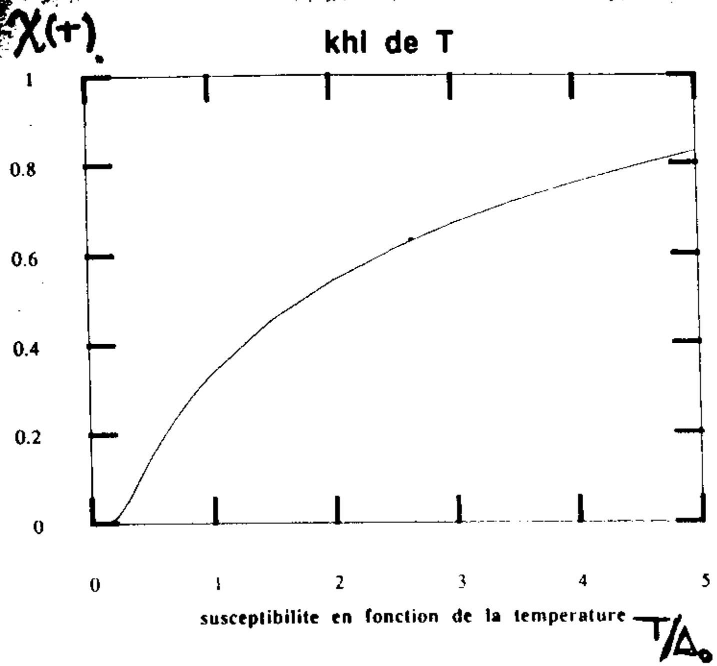
BUT BREAKS DOWN EARLY !!!
WHEN T ↗

REAL $\chi(T)$
FOR SPIN-1



NO QUANTUM CRITICAL WINDOW
FOR S=1 SPIN CHAIN.

DICTIONS DU MODELE σ NON-LINEAIRE



susceptibilite en fonction de la temperature