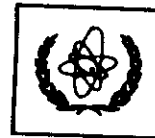




UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL ATOMIC ENERGY AGENCY
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
I.C.T.P., P.O. BOX 586, 34100 TRIESTE, ITALY, CABLE: CENTRATOM TRIESTE



SMR.998a - 4

Research Workshop on Condensed Matter Physics
30 June - 22 August 1997
MINIWORKSHOP ON
QUANTUM MONTE CARLO SIMULATIONS OF LIQUIDS AND SOLIDS
30 JUNE - 11 JULY 1997
and
CONFERENCE ON
QUANTUM SOLIDS AND POLARIZED SYSTEMS
3 - 5 JULY 1997

**"Magnetism of ^3He on graphite:
From ferromagnetism to spin liquid"**

G. MISGUICH
Laboratoire de Physique Theorique des Liquides
Universite Pierre et Marie Curie
Case 121, 4 Place Jussieu
75252 Paris Cedex
URA 765 of CNRS
France

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

MAIN BUILDING STRADA COSTIERA, 11 TEL. 2240111 TELEFAX 224163 TELEX 460392 ADRIATICO GUEST HOUSE VIA GRIGNANO, 9 TEL. 224241 TELEFAX 224531 TELEX 460449
MICROPROCESSOR LAB. VIA BEIRUT, 31 TEL. 2249911 TELEFAX 224600 TELEX 460392 GALILEO GUEST HOUSE VIA BEIRUT, 7 TEL. 2240311 TELEFAX 2240310 TELEX 460392

Magnetism of ^3He on graphite: From ferromagnetism to spin liquid

G. Misguich *, B. Bernu *, C. Lhuillier * and
D.Ceperley †

June 27, 1997

* Laboratoire de Physique Théorique des Liquides, Université P.
et M. Curie, case 121, 4 Place Jussieu, 75252 Paris Cedex.
URA 765 of CNRS

† National Center for Supercomputer Applications, Dept. of
Physics, University of Illinois, Champaign, IL 61820 USA

Objective: understanding the competing effects of many-body exchange processes in the 2D solid ^3He .

- Multi spin exchange theory
- Classical phase diagram,
PIMC & experiments
- Exact diagonalizations: **A spin liquid phase**

Multi spin exchange

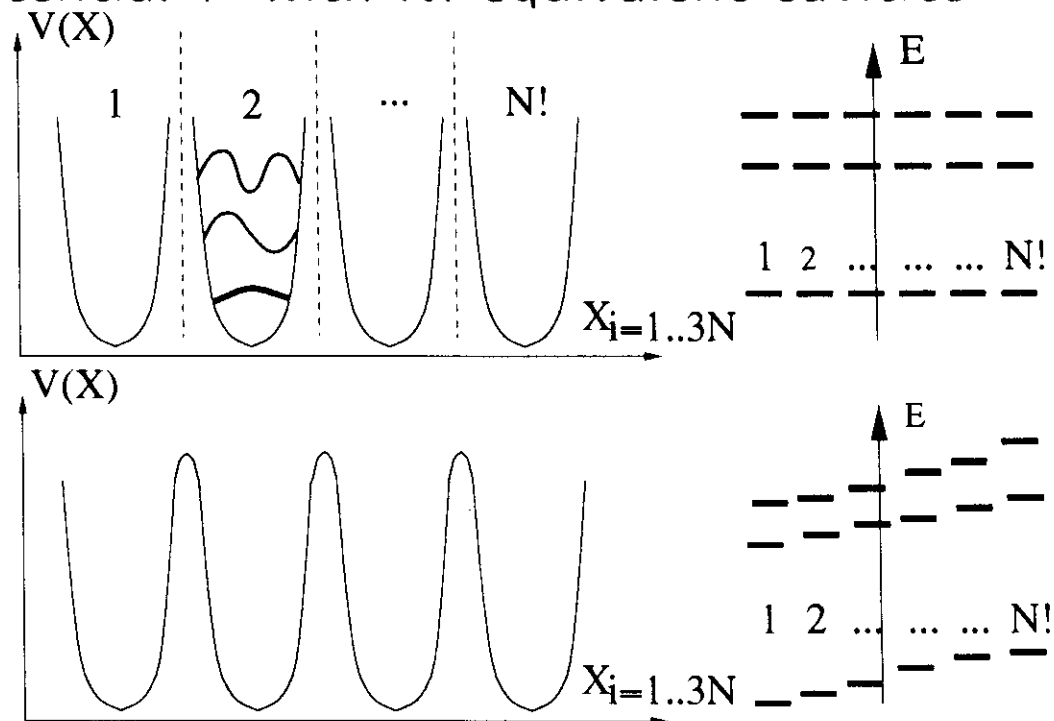
Dirac and Heisenberg (1926), Thouless (1965)

= Effective description of interactions + Pauli principle for quasi localized fermions.

N distinguishable interacting particles:

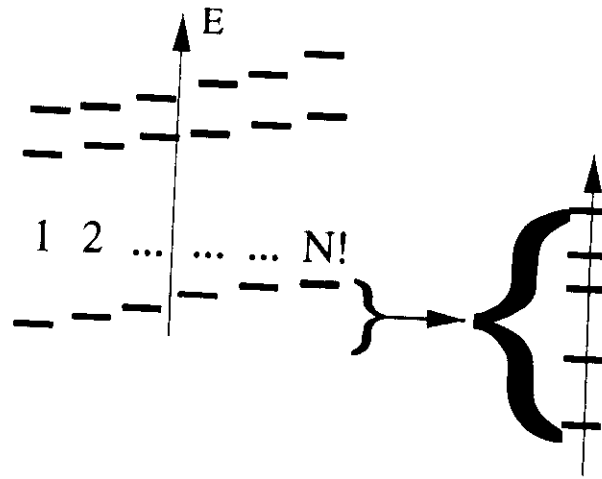
$$H = \sum_{i=1}^N \frac{\mathbf{p}_i^2}{2m} + E_1(\mathbf{x}_i) + \sum_{i<j} E_2(\mathbf{x}_i, \mathbf{x}_j)$$

$\Leftrightarrow$ 1 particle in a $3N$ -dimensional space + potential V with $N!$ equivalent cavities

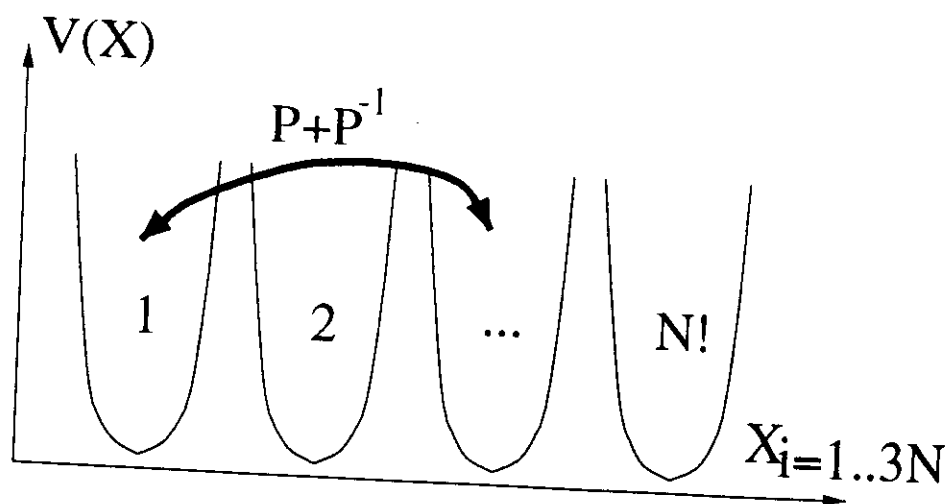


$N!$ -fold degeneracy lifted by tunneling processes

Permutation = Hopping in phase space



$$H \longrightarrow H_{eff} = - \sum_{P \in \sigma_N} J_P (P + P^{-1})$$



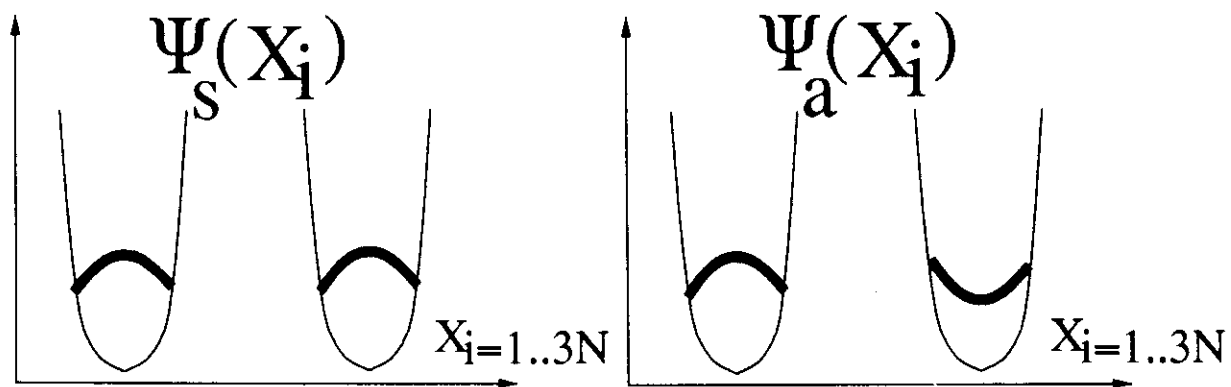
$$J_P > 0$$

Since tunneling events $\sim$ rare+independent
 $\Rightarrow$ We focus on one **single** event.

- Consider a single term $-J_P (P + P^{-1})$ when the system starts from the 1st cavity.

$$\{|1\rangle, P|1\rangle\}$$

- 2 eigenstates in the restricted Hilbert space:



$$|\Psi_s\rangle = |1\rangle + P|1\rangle \quad E_s = -J_P$$

$$|\Psi_a\rangle = |1\rangle - P|1\rangle \quad E_a = J_P$$

- $|\Psi_s\rangle$ (nodeless) has the lowest energy

$$\Rightarrow J_P > 0$$

Pauli principle

$|\Psi\rangle$ is a fermion wave function $\Leftrightarrow$

$$\forall P \quad P_{spin} P_{space} |\Psi\rangle = (-1)^P |\Psi\rangle$$

$$\begin{aligned} H_{eff} |\Psi\rangle &= - \sum_{P \in \sigma_N} J_P (P_{space} + P_{space}^{-1}) |\Psi\rangle \\ &= - \sum_{P \in \sigma_N} (-1)^P J_P (P_{spin}^{-1} + P_{spin}) |\Psi\rangle \end{aligned}$$

$$\Rightarrow H_{eff}^{spin} = - \sum_{P \in \sigma_N} (-1)^P J_P (P_{spin}^{-1} + P_{spin})$$

From now, $P_{spin} \longrightarrow P$

$$\begin{aligned} H_{eff}^{spin} &= J_2 \sum_{\text{---}} P_{1,2} - J_3 \sum_{\text{---}} (P_{1...3} + P^{-1}) \\ &\quad + J_4 \sum_{\text{---}} (P_{1...4} + P^{-1}) - J_5 \sum_{\text{---}} (P_{1...5} + P^{-1}) \\ &\quad + \dots \end{aligned}$$

^3He on graphite: 2^{nd} layer

= spins $1/2$ on a triangular lattice.

Heisenberg hamiltonian = 2-spins exchange:

$$\mathbf{S}_i \mathbf{S}_j = \frac{1}{2} \left(P_{i,j} - \frac{1}{2} \right)$$

But experimental $C_V(T)$ and $\chi(T)$ data are incompatible with a pure Heisenberg hamiltonian.

Path Integral Monte Carlo calculations of J_n :

$3N$ 	$J_2 P_{1,2}$	$J_2 = 10.9 \pm 0.6 mK$
$2N$ 	$J_3 (P_{1...3} + P_{3...1})$	$J_3 = 8.3 \pm 0.5 mK$
$3N$ 	$J_4 (P_{1...4} + P_{4...1})$	$J_4 = 5.8 \pm 0.4 mK$
$6N$ 	$J_5 (P_{1...5} + P_{5...1})$	$J_5 = 2.4 \pm 0.3 mK$
N 	$J_6 (P_{1...6} + P_{6...1})$	$J_6 = 2.6 \pm 0.5 mK$

($\rho = 0.179 \text{ atom}/\text{\AA}^{-2}$, Bernu and Ceperley)

From permutations to classical spins

$$2 \text{ (triangle)} = \text{ (V-shape)} + \text{ (inverted V-shape)} + \text{ (horizontal line)} - 1 \Rightarrow J_2^{eff} = J_2 - 2J_3$$

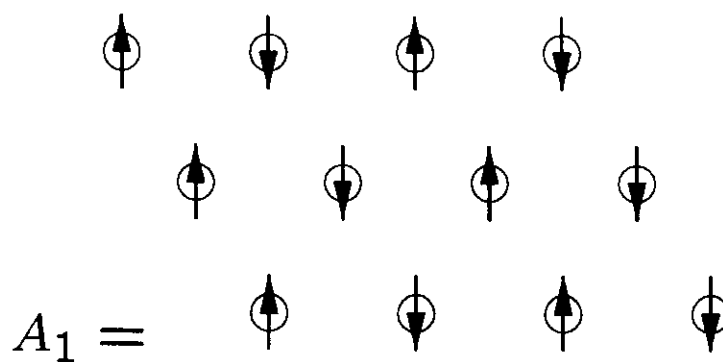
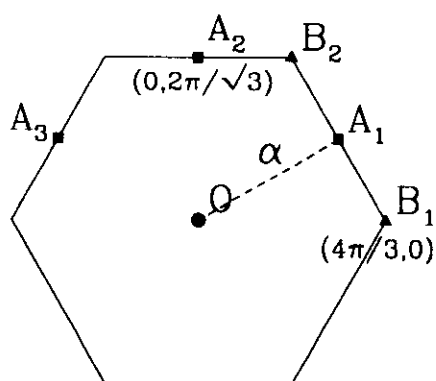
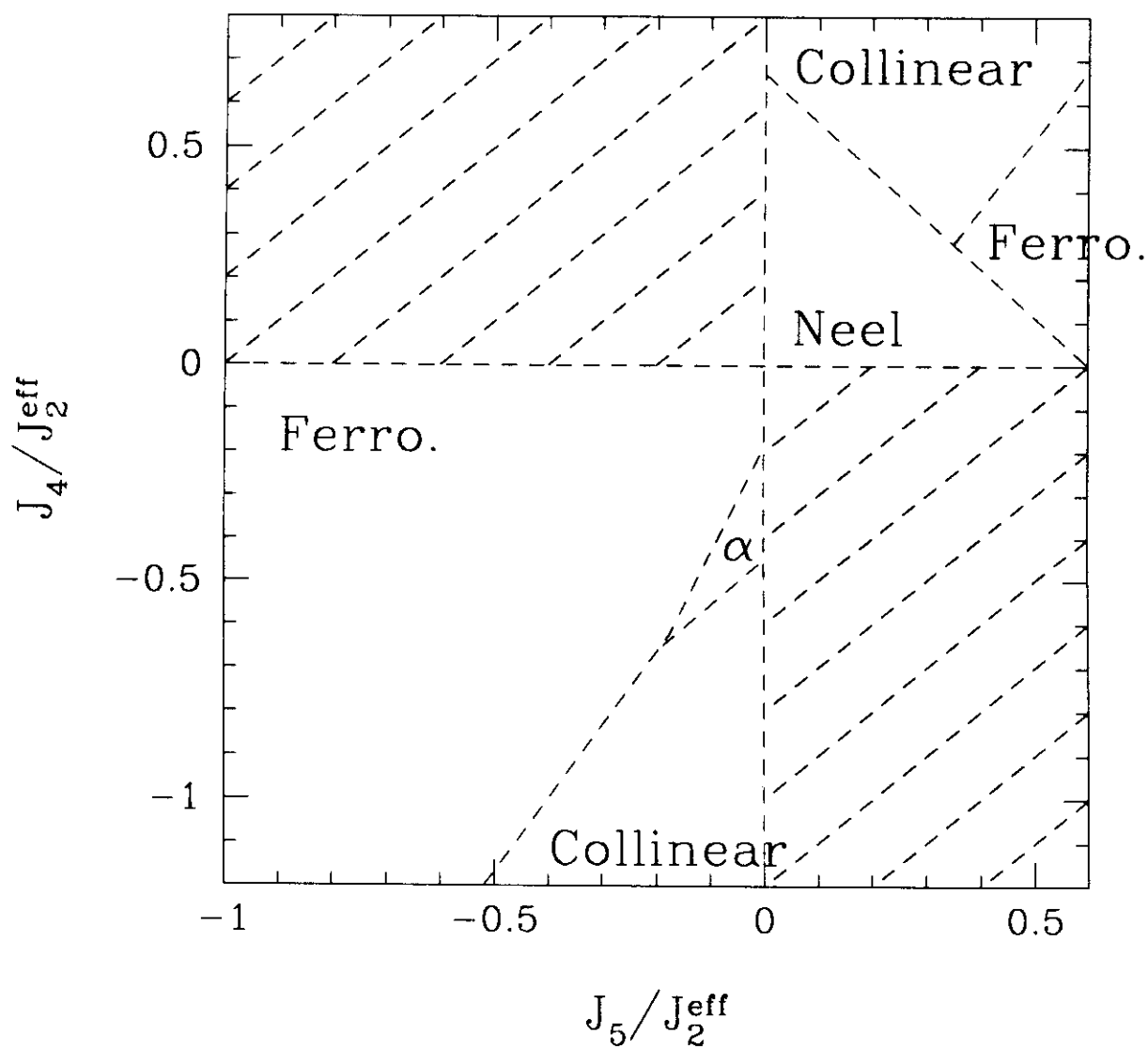
$$2 \text{ (parallelogram)} = \text{ (horizontal line)} + \text{ (two V-shapes)} - \text{ (crossed lines)} + \text{ (two diagonal lines)} + \text{ (two separate dots)} - 1$$

$$2 \text{ (pentagon)} = -\frac{1}{2} \left(\text{ (V-shape)} + \dots \right) + \frac{1}{2} \left(\text{ (diagonal line)} + \dots \right) + \frac{1}{2} \left(\text{ (two V-shapes)} + \dots \right) + \frac{1}{2} \left(\text{ (crossed lines)} + \dots \right)$$

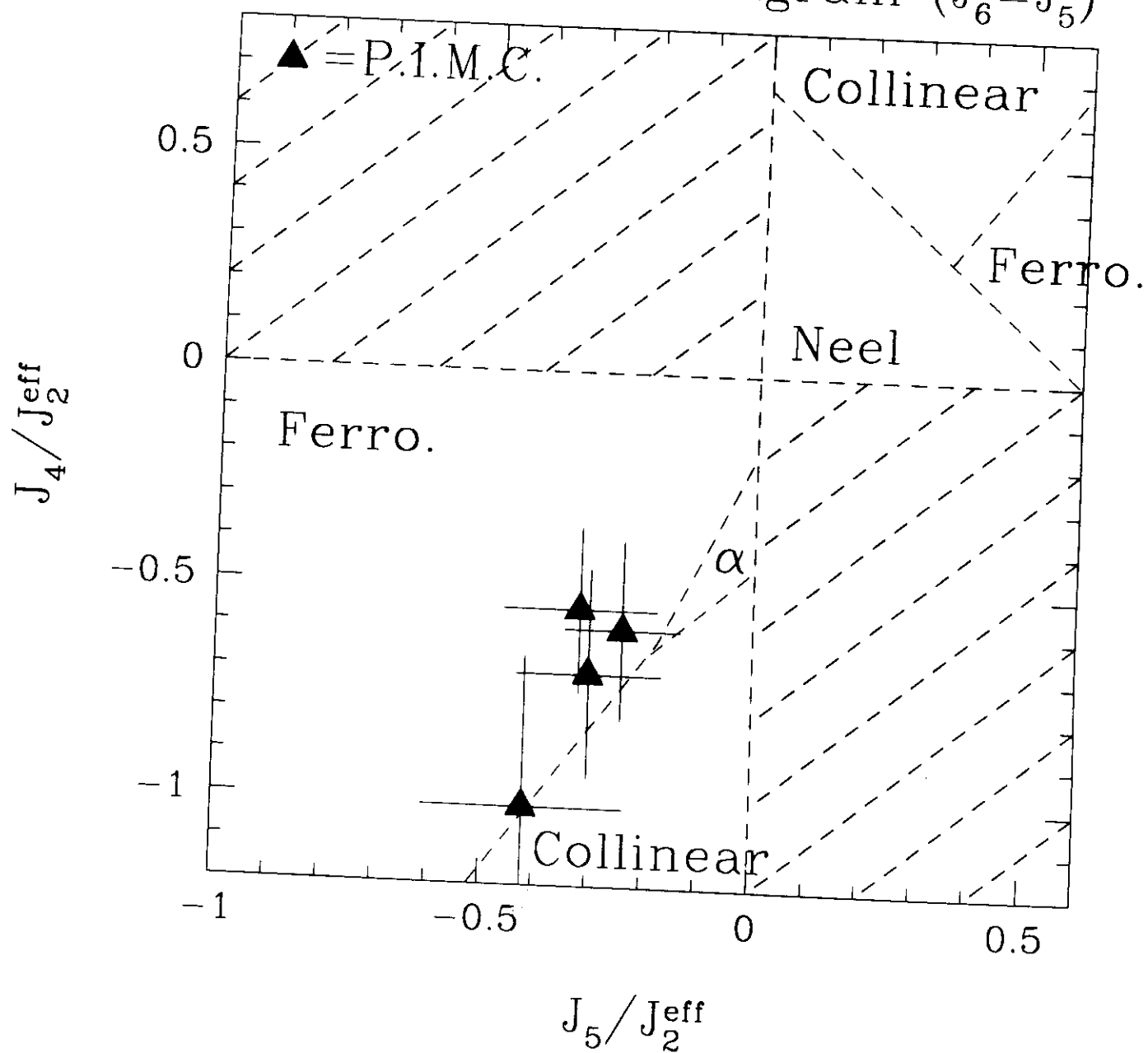
$$2 \text{ (hexagon)} = \text{ (horizontal line)} + \text{ (two V-shapes)} + 41 \text{ terms}$$

$$H[\dots P_n \dots] \longrightarrow H[\dots (S_i \cdot S_{j \neq i}) \dots]$$

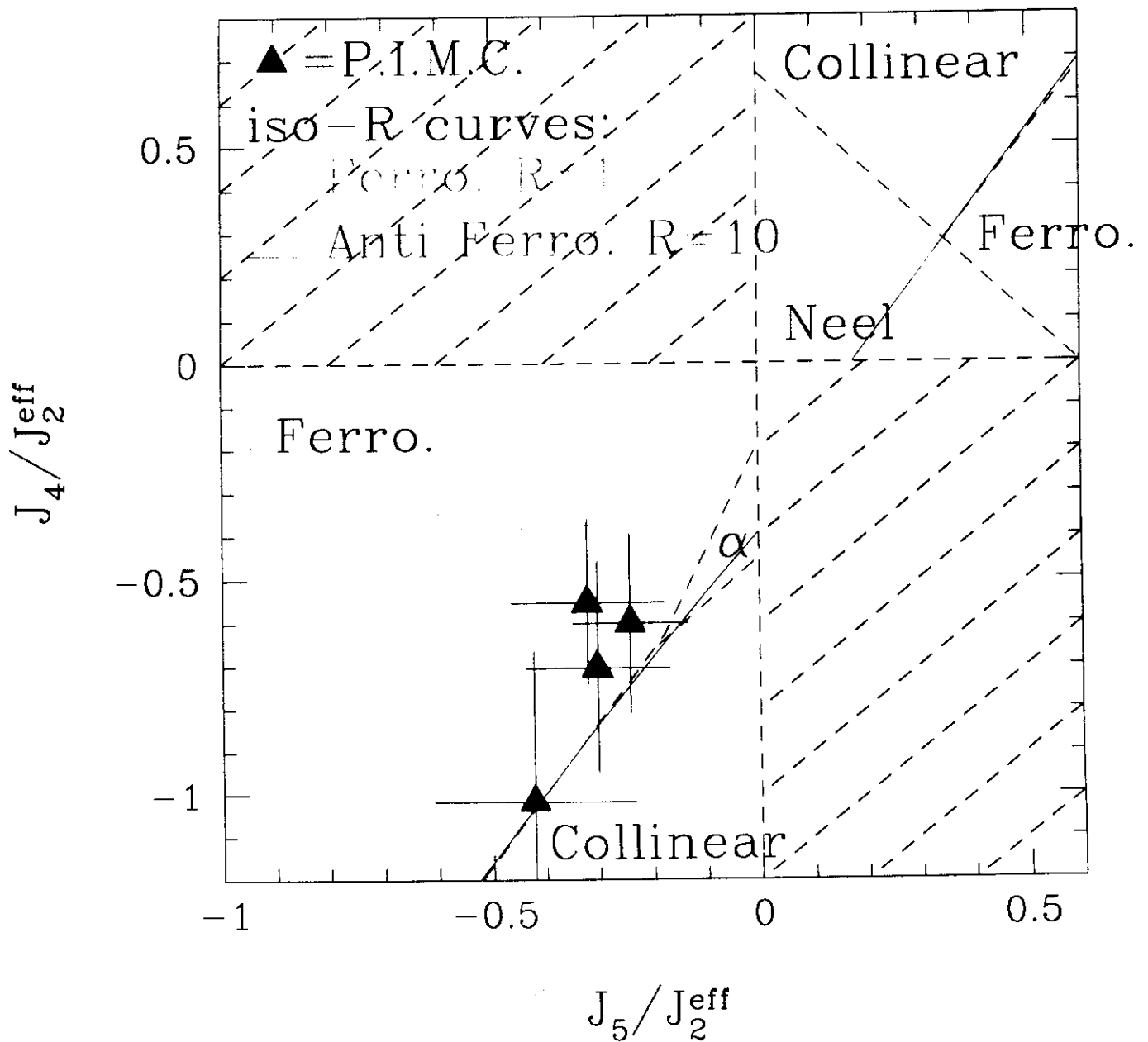
Classical Phase Diagram ($J_6=J_5$)



Classical Phase Diagram ($J_6=J_5$)



Classical Phase Diagram ($J_6=J_5$)



$$C_V = \frac{9N}{4} \left(\frac{J_{CV}}{T} \right)^2 + O(1/T^3)$$

$$\frac{4\chi}{N} = \frac{1}{T} + \frac{3J_\chi}{T^2} + O(1/T^3) \quad R := \left(\frac{J_{CV}}{J_\chi} \right)^2$$

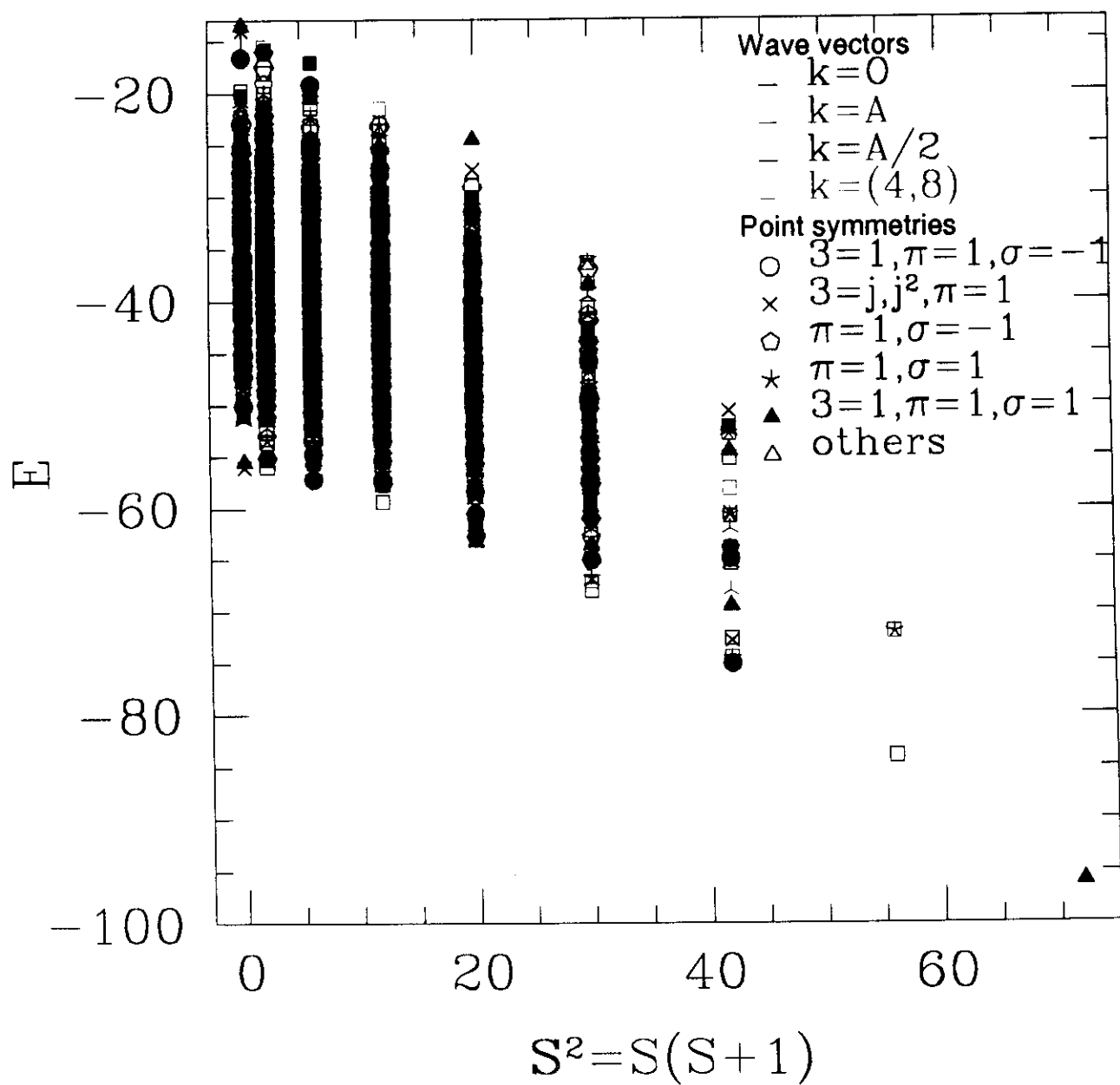
Exact diagonalizations: spin liquid phase

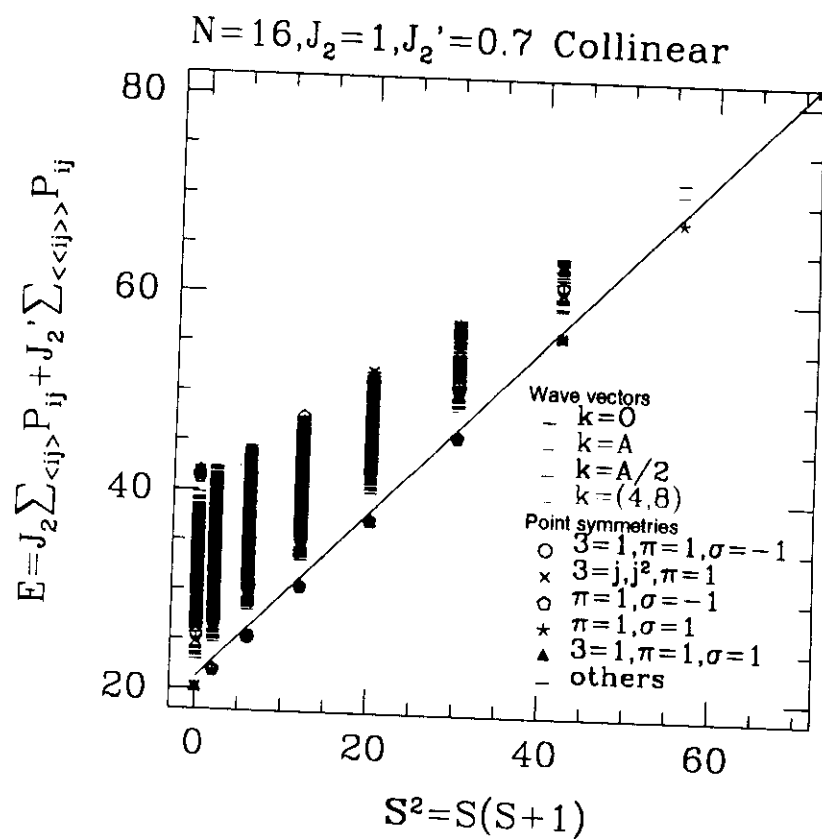
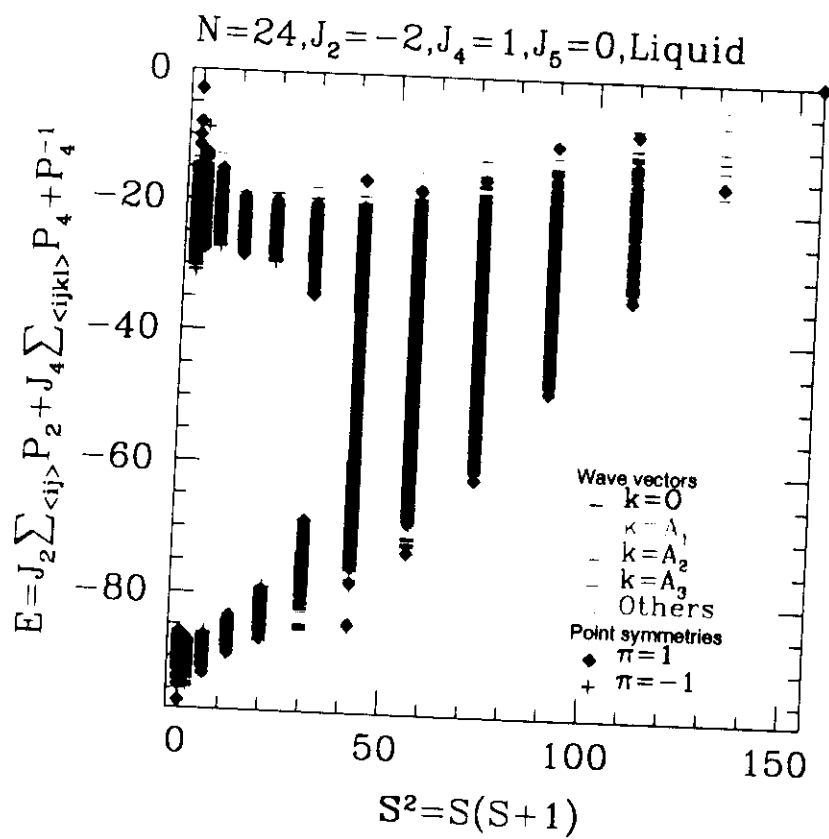
Performed for $N=12, 16, 18, 20, 24$ and 28

- Ferromagnetic region $\rightarrow$ OK
- Collinear region $\rightarrow$ Classical long range order destroyed by quantum fluctuations
 $\Rightarrow$ spin liquid phase

Ferromagnetism: ground state $S = \frac{N}{2}$

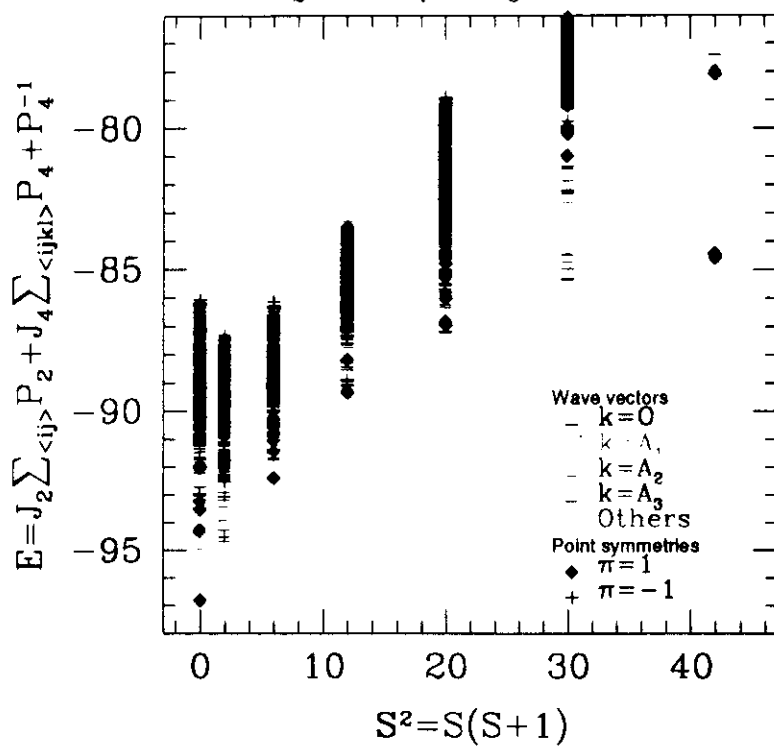
$N=16, J_2=-2, J_4=1, J_5=-0.5, \text{Ferro.}$



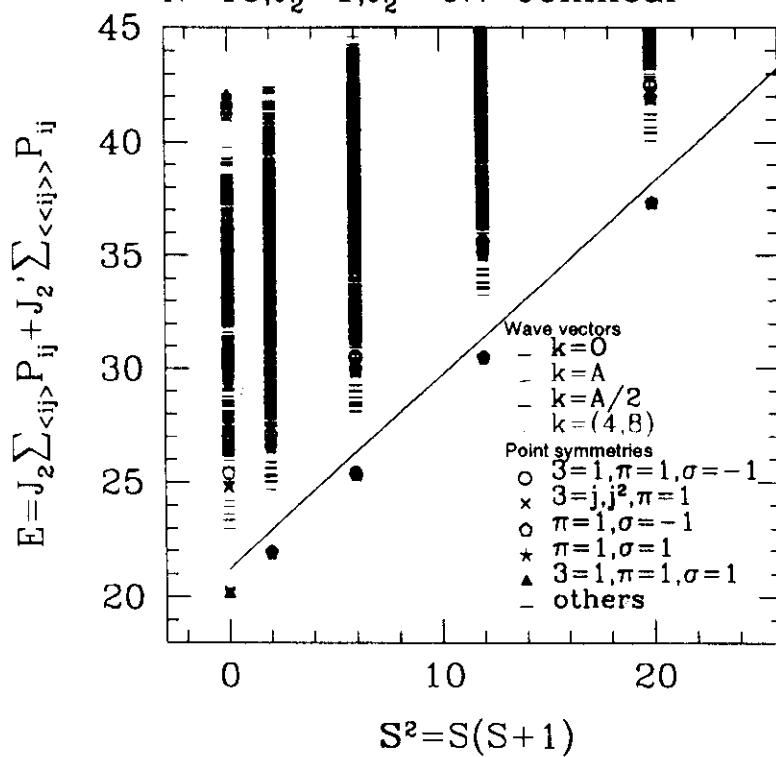


No tower of states:

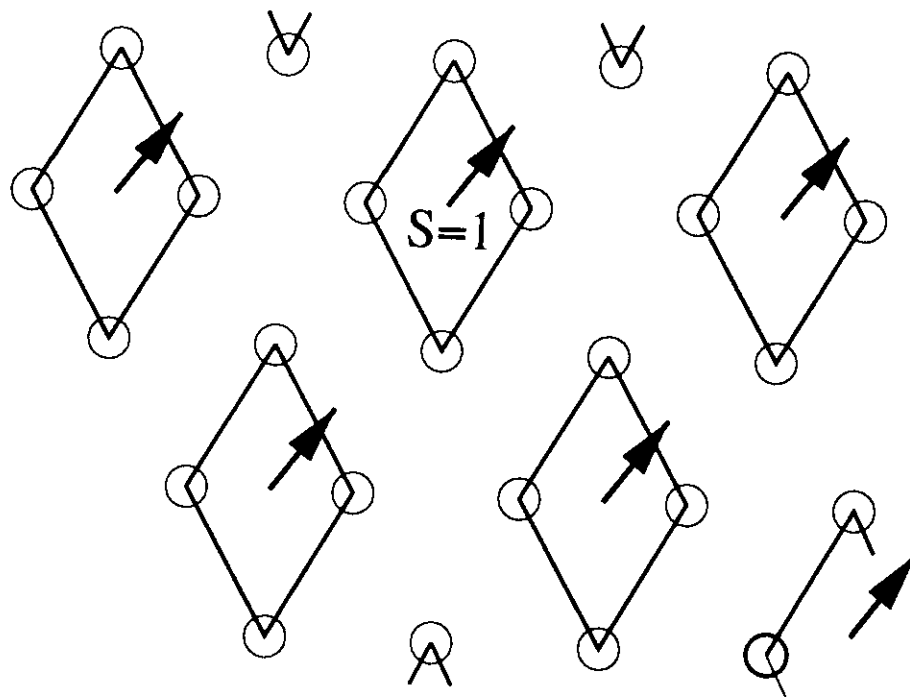
$N=24, J_2=-2, J_4=1, J_5=0, \text{Liquid}$



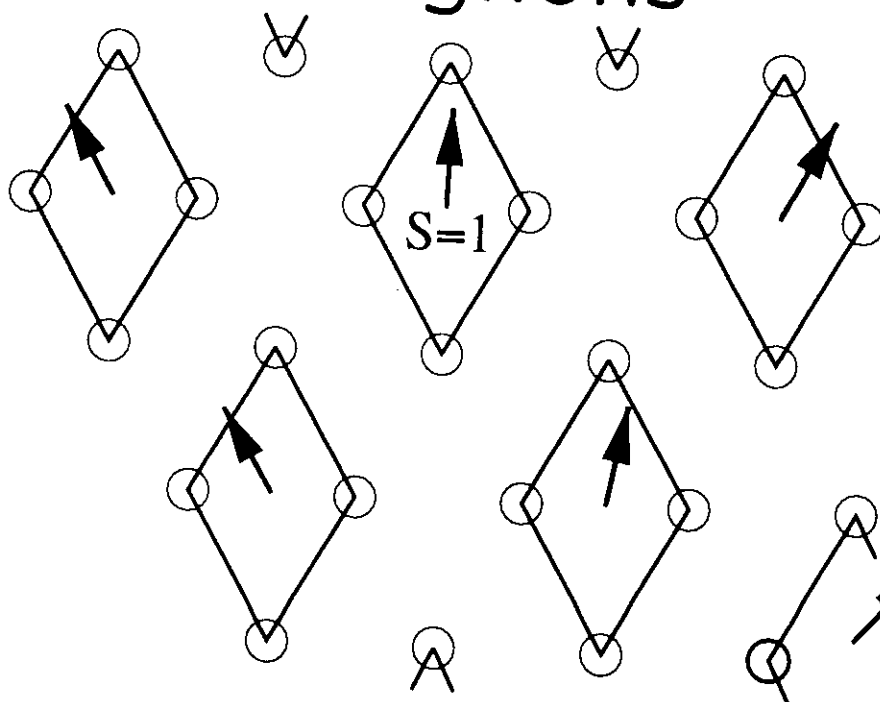
$N=16, J_2=1, J_2'=0.7 \text{ Collinear}$



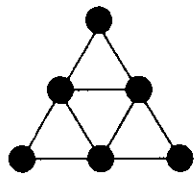
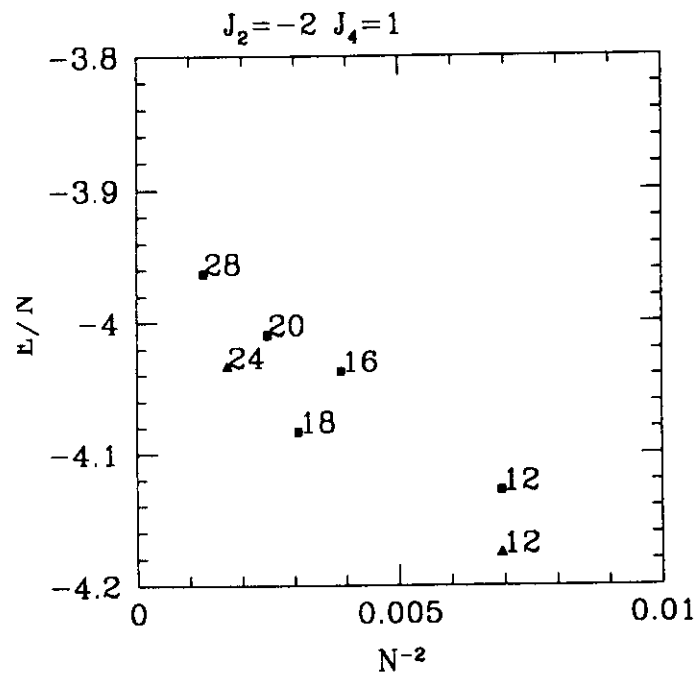
4-spins plaquettes



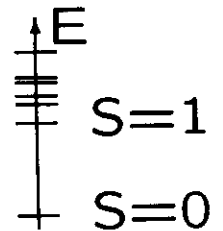
Magnons



Ground state: 6-spins arrangements ?



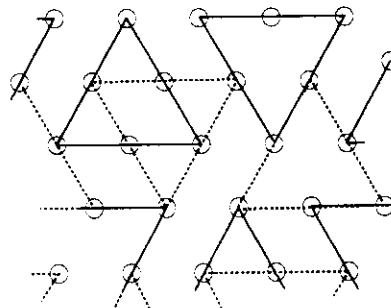
= The only $N \leq 8$ pattern with:



$\Rightarrow$ Toy-model with a tight-binding calculation

Result: First $S = 1$ excitation is found with a gap $= .4J_4$ (for $J_2^{eff} = -2J_4$)

Mean-field failure $\Rightarrow \exists$ large resonances:



Results: A RVB-like spin liquid

- No long range order: none of the spectra (In the classical collinear region) display any 'tower of states'.
- $S=0$ ground state and gap
- Stabilized states in the $S = N/4$ and $S = N/4 - 1$ subspaces:
4-spins plaquettes.

Conclusions:

We determined the physical range of parameters relevant for the description of the 2nd layer magnetism of ^3He and pointed out the possibility of a **gaped spin liquid phase**.

We recognized the presence of low energy **plaquettes degrees of freedom**. These states might be observed experimentally. NMR ?

A few references

D.J. Thouless, *Proc. Phys. Soc.* **86**, 893-904 (1965)

M. Roger, J.H. Hetherington and J.M Delrieu, *Rev. of Modern Phys.* **55**, 1-63 (1983)

C. Bauerle, Ph.D. thesis, Grenoble France (1996)

H. Godfrin and H.-J Lauter, *Pogress in Low Temp. Phys.* **XIV**, 213-320 (1995) and references therein.

M. Siqueira, J. Nyeki, B. Cowan and J. Saunders, *Phys. Rev. Lett.* **78**, 2600-2603 (1997) and references therein.

P. Lecheminant, B. Bernu, C. Lhuillier and L. Pierre *Phys. Rev. B* **52**, 6647-6652 (1995)