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MINIWORKSHOP ON STRONG ELECTRON CORRELATIONS
"Disorder and Interaction in Quantum Systems and Their Classical Analogs"

(1 - 19 July 1996)

"Plaguette Resonating-Valence-Bond Ground State of CaV_4O_9"

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

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Plaquette Resonating-Valence-Bond Ground State of CaV_4O_9

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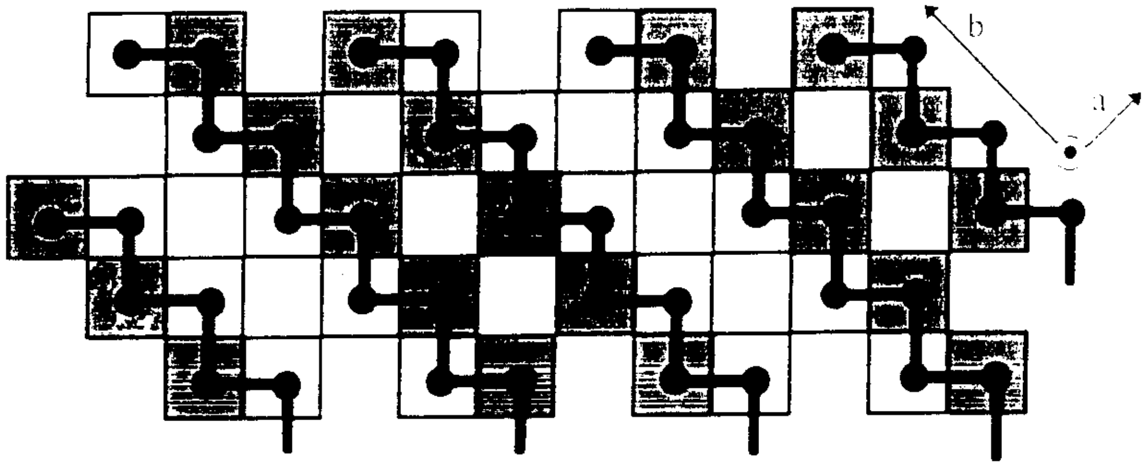
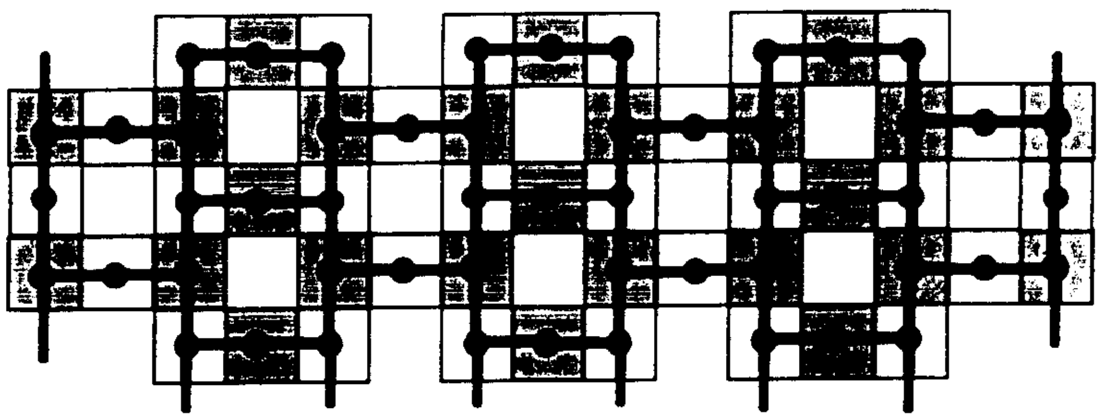
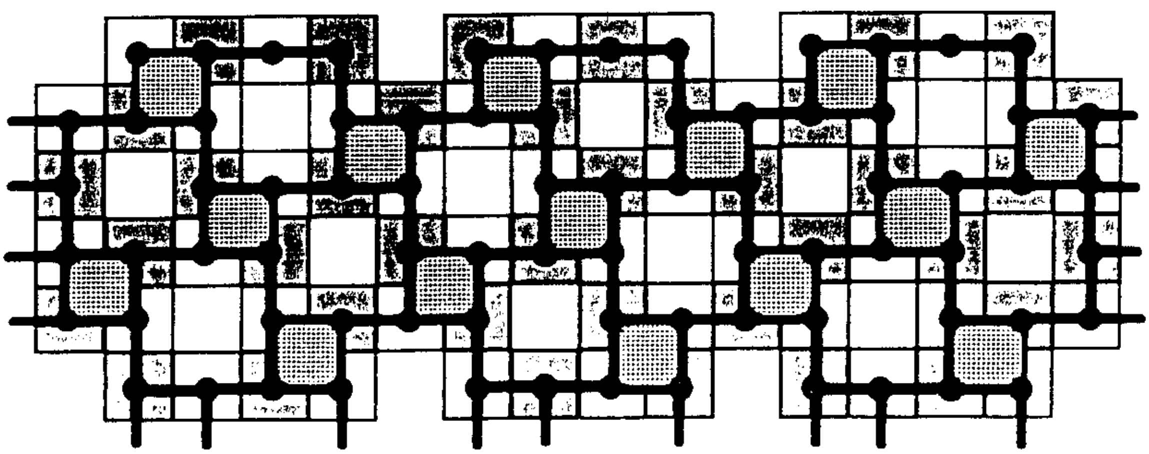
CaV_2O_5



CaV_3O_7

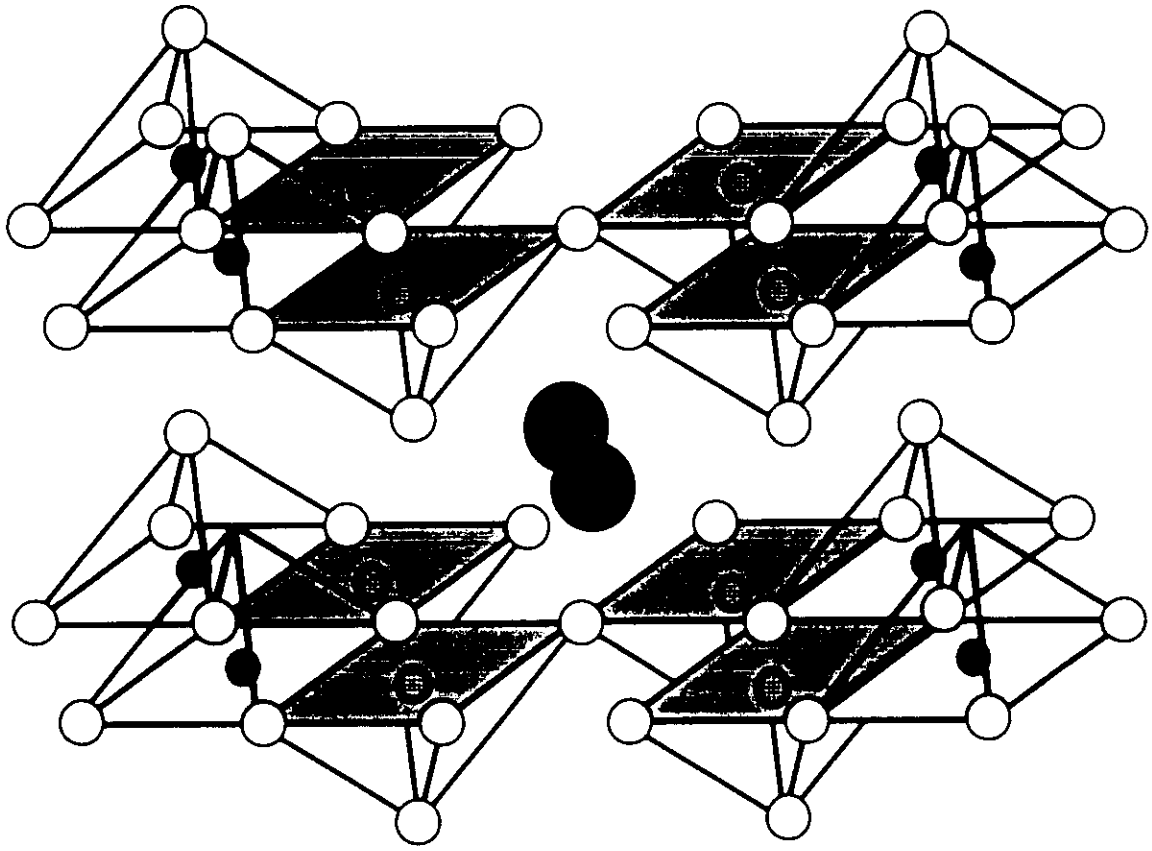


CaV_4O_9

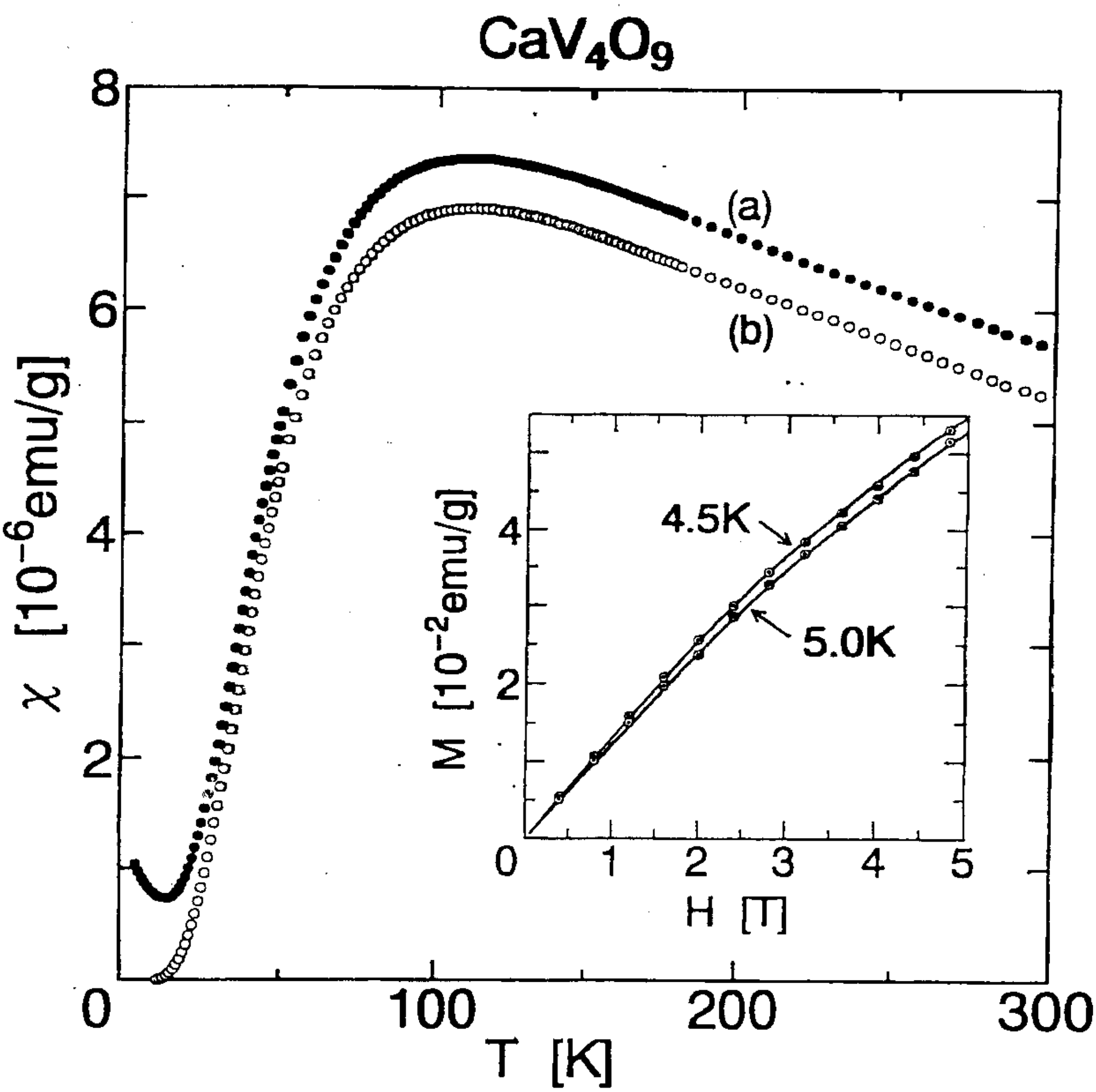


made by Yasuoka 2.

Skeleton of CaV_2O_5

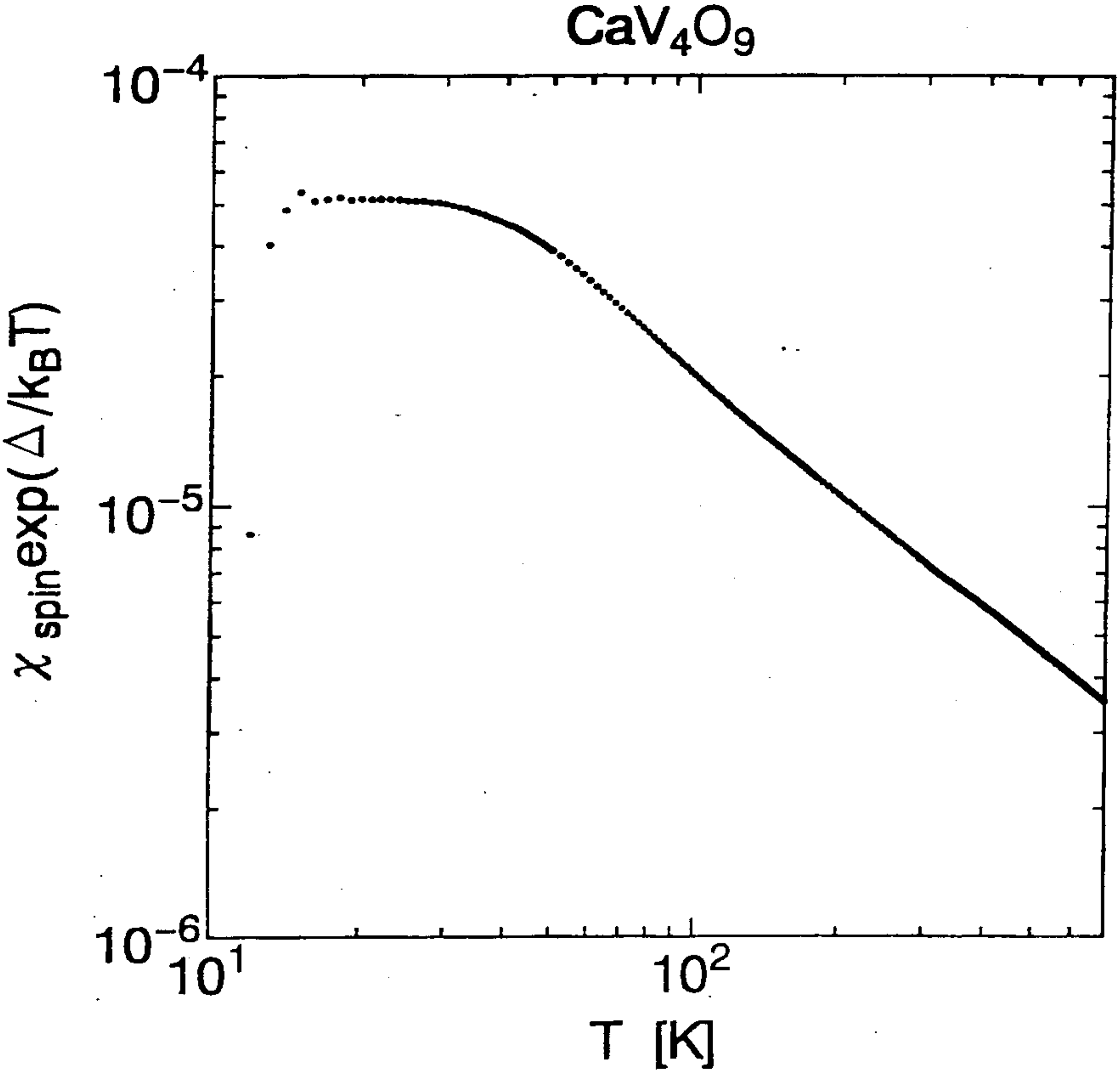


- Oxygen
- Vanadium in up Pyramid
- Vanadium in dowm Pyramid
- Calcium

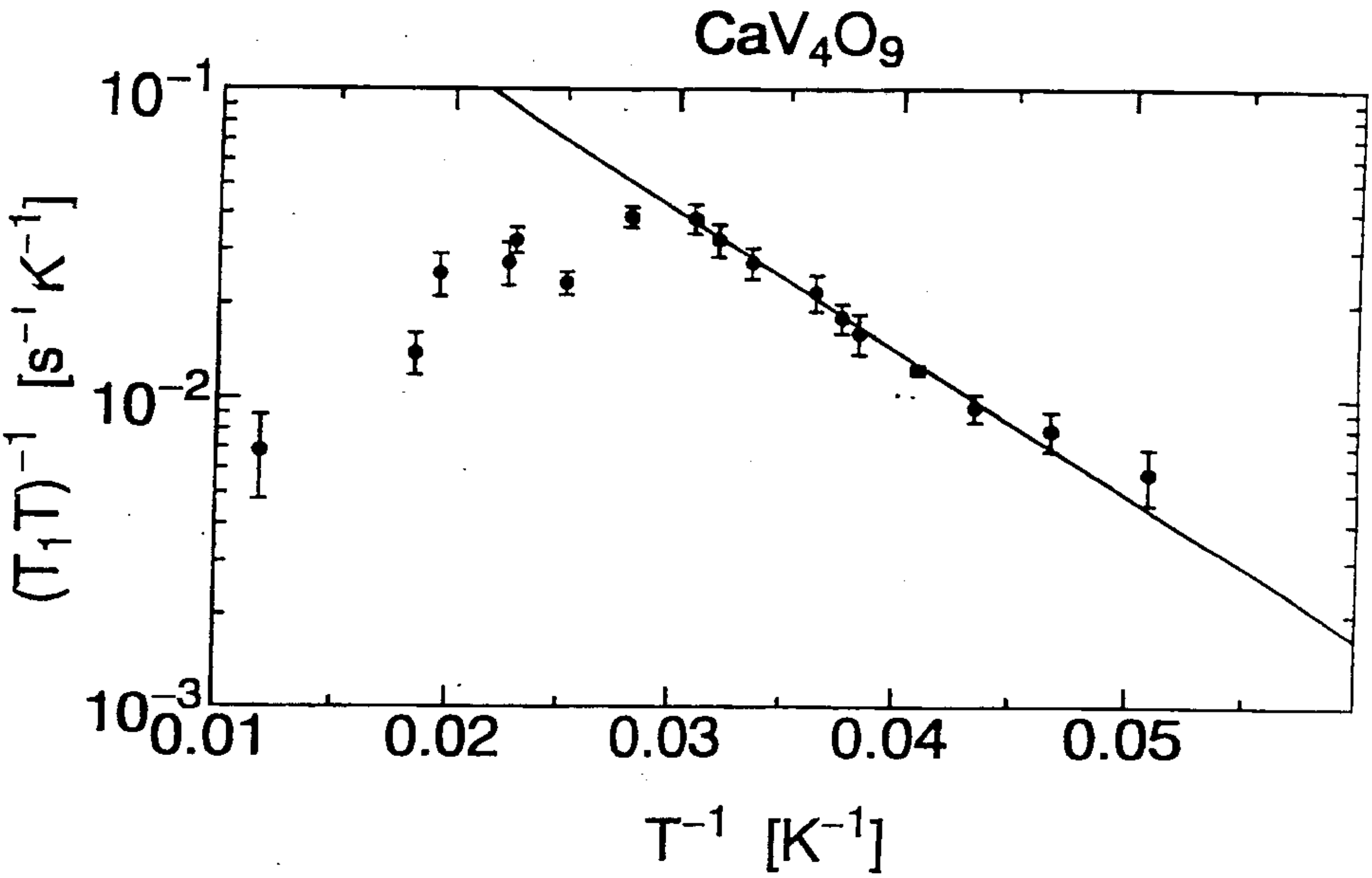


S. Taniguchi et al

J. Phys. Soc. Jpn 64, 2758 (1995)

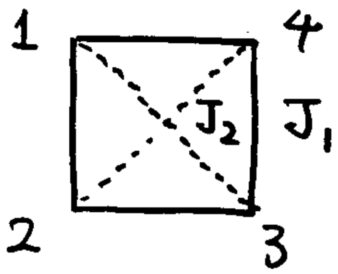


$\Delta/k_B \sim 107$ K



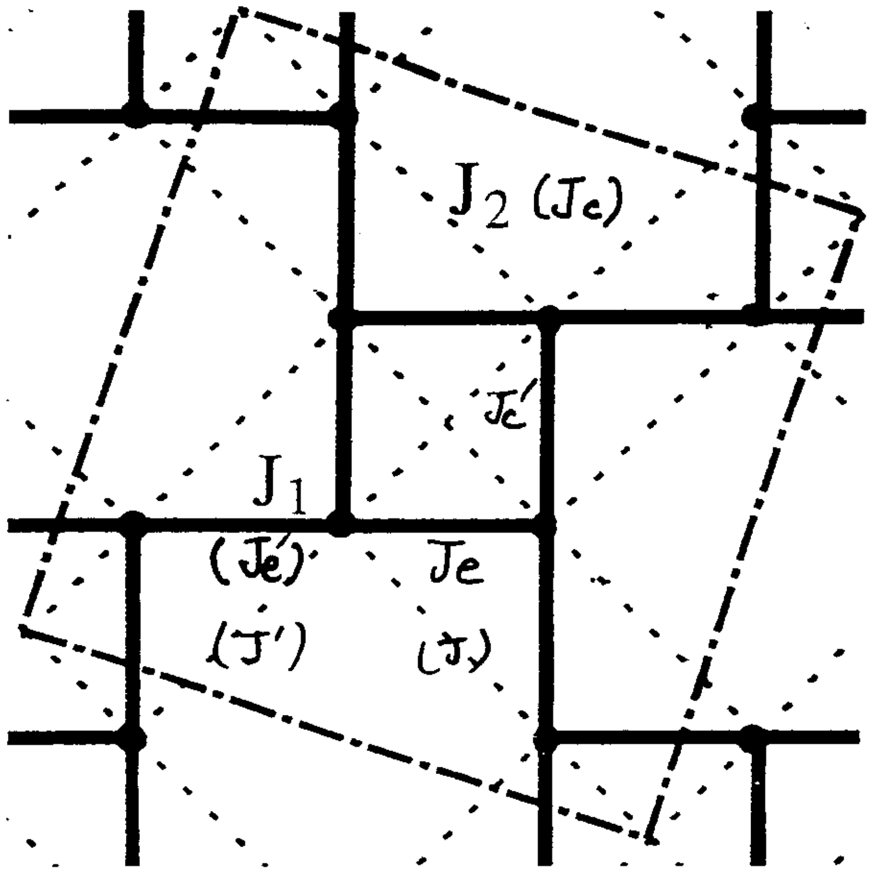
CaV_4O_9
$(T_1T)^{-1}$ $[s^{-1}K^{-1}]$
10^{-1}
10^{-2}
10^{-3}
0.01
0.02
0.03
0.04
0.05
T^{-1} $[K^{-1}]$

Eigenstates of a plaquette



$$\mathcal{H}_{\text{plaquette}} = J_1 (\vec{S}_1 + \vec{S}_3)\cdot(\vec{S}_2 + \vec{S}_4) + J_2 (\vec{S}_1\cdot\vec{S}_3 + \vec{S}_2\cdot\vec{S}_4)$$

S_{13}	S_{24}	S	
0	0	0	$-\frac{3}{2}J_2$
1	0	1	$-\frac{1}{2}J_2$
0	1	1	$-\frac{1}{2}J_2$
1	1	0	$-2J_1 + \frac{1}{2}J_2$
		1	$-J_1 + \frac{1}{2}J_2$
		2	$J_1 + \frac{1}{2}J_2$



model for CaV_4O_9

$$\mathcal{H} = J_1 \sum_{n.n.} \vec{S}_i \vec{S}_j + J_2 \sum_{n.n.n.} \vec{S}_i \cdot \vec{S}_j$$

estimation of parameters

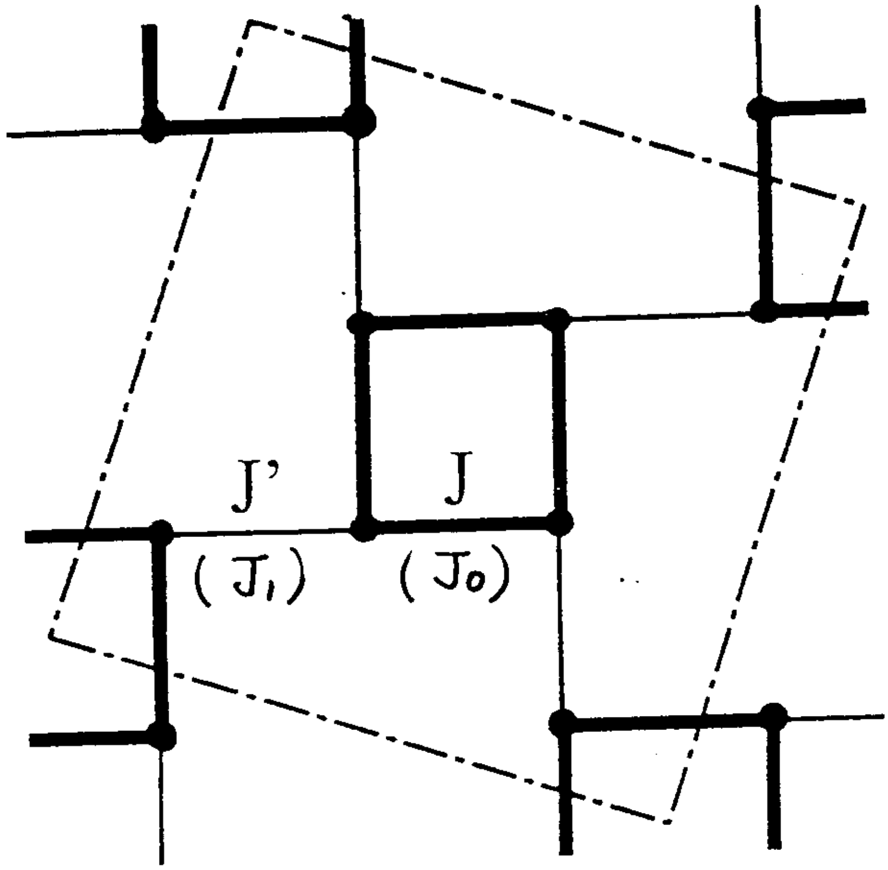
$$J_2 \sim \frac{1}{2} J_1$$

Weiss constant

$$k_B \theta = \frac{1}{3} S(S+1)(z_1 J_1 + z_2 J_2)$$

$$\theta = 220\,K \Rightarrow J_1 \sim 200\,K$$

} consistent with high temperature expansion (Gelfand et al).



spin ½ Heisenberg model on
the ⅕-depleted square lattice

J : plaquette covering

J' : dimer covering

simplest approximations

parametrization

$$\begin{cases} J = \tilde{x} \\ J' = 1 - \tilde{x} \end{cases}$$

$$E_{PRVB} = -\frac{1}{2} J = -\frac{1}{2}\tilde{x}$$

$$E_{dimer} = -\frac{3}{8} J' = -\frac{3}{8}(1-\tilde{x})$$

$$E_{Néel} = -\frac{1}{4} J - \frac{1}{8} J' = -\frac{1}{8}(1+\tilde{x})$$

perturbation calculations

$$E_{PRVB} = -\frac{1}{2} J \left[1 + \frac{43}{576} \left(\frac{J'}{J}\right)^2 \right]$$

$$E_{dimer} = -\frac{3}{8} J' \left[1 + \frac{1}{4} \left(\frac{J}{J'}\right)^2 \right]$$

spin wave approximation $(J = J')$

$$E_{Néel} = -J \left[\frac{3}{2} S^2 + 0.325\, S \right]$$

$$\delta S = 0.288$$

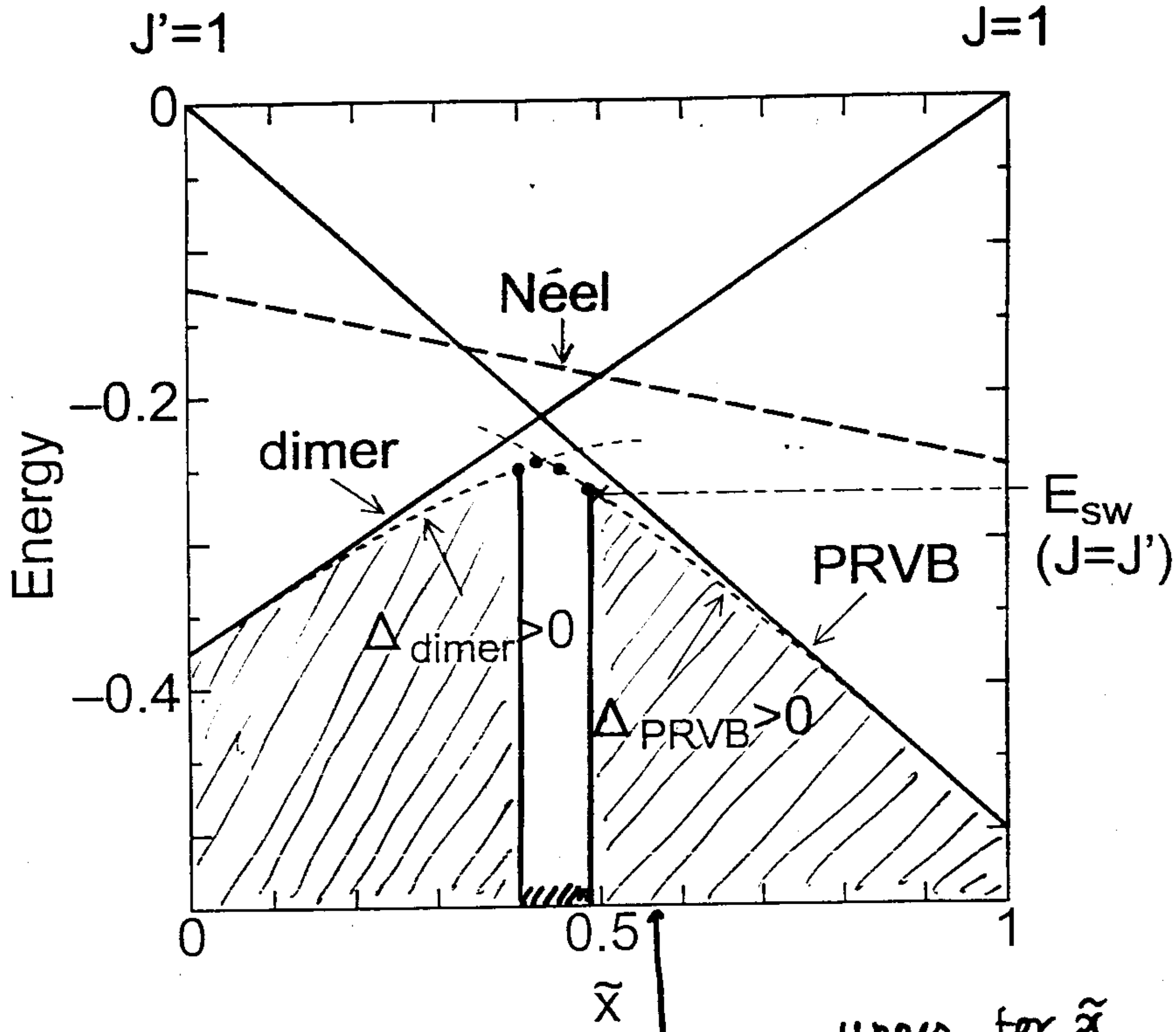
spin gap

$$\Delta_{PRVB} = J \left[1 - \frac{2}{3}\left(\frac{J'}{J}\right) - \frac{31}{96}\left(\frac{J'}{J}\right)^2 \right]$$

$$\Delta_{dimer} = J' \left[1 - \frac{J}{J'} - \frac{3}{4}\left(\frac{J}{J'}\right)^2 \right]$$

$$\Delta_{PRVB} = 0 \Rightarrow \left(\frac{J'}{J}\right)_c = 0.992$$

$$\Delta_{dimer} = 0 \Rightarrow \left(\frac{J}{J'}\right)_c = 0.667$$



upper for $\tilde{x}$

$\tilde{x} = \frac{4}{7}$ a (lower) bound for the critical point $\left(\frac{J'}{J}\right)_c$ by the cluster mean field theory

What is the ground state at the symmetric point ?

(1) perturbation theory

(M.P. Gelfand et al, K.U. et al)

gap $\Delta = 0.01$ J

(2) spin wave theory (K.U. et al)

Long Range Order

(3) Quantum Monte Carlo Simulations

(Katoh and Imada)

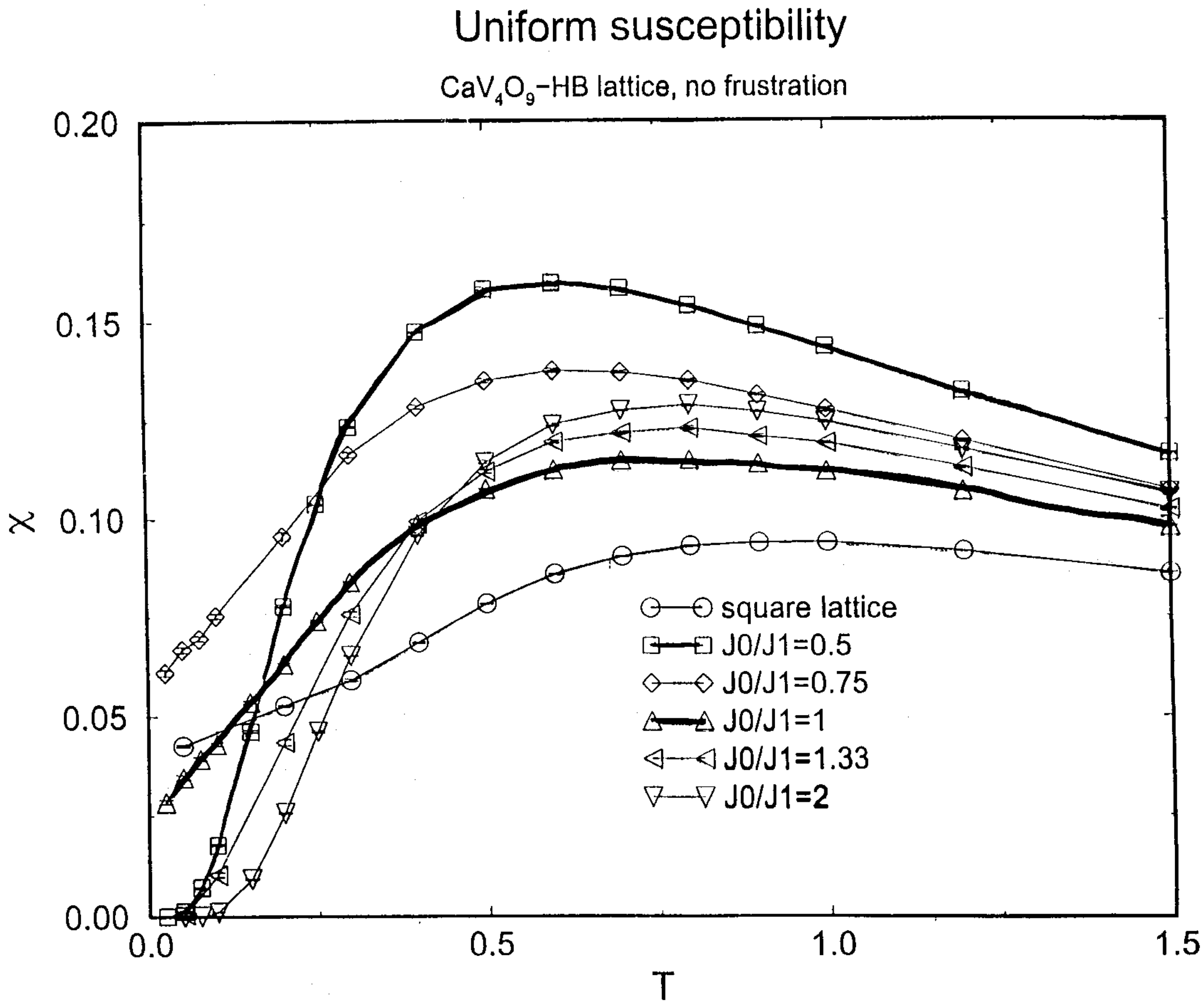
gap $\Delta \cong 0.11$ J

(4) exact diagonalization

Yes and No "Difficulty in extrapolation"

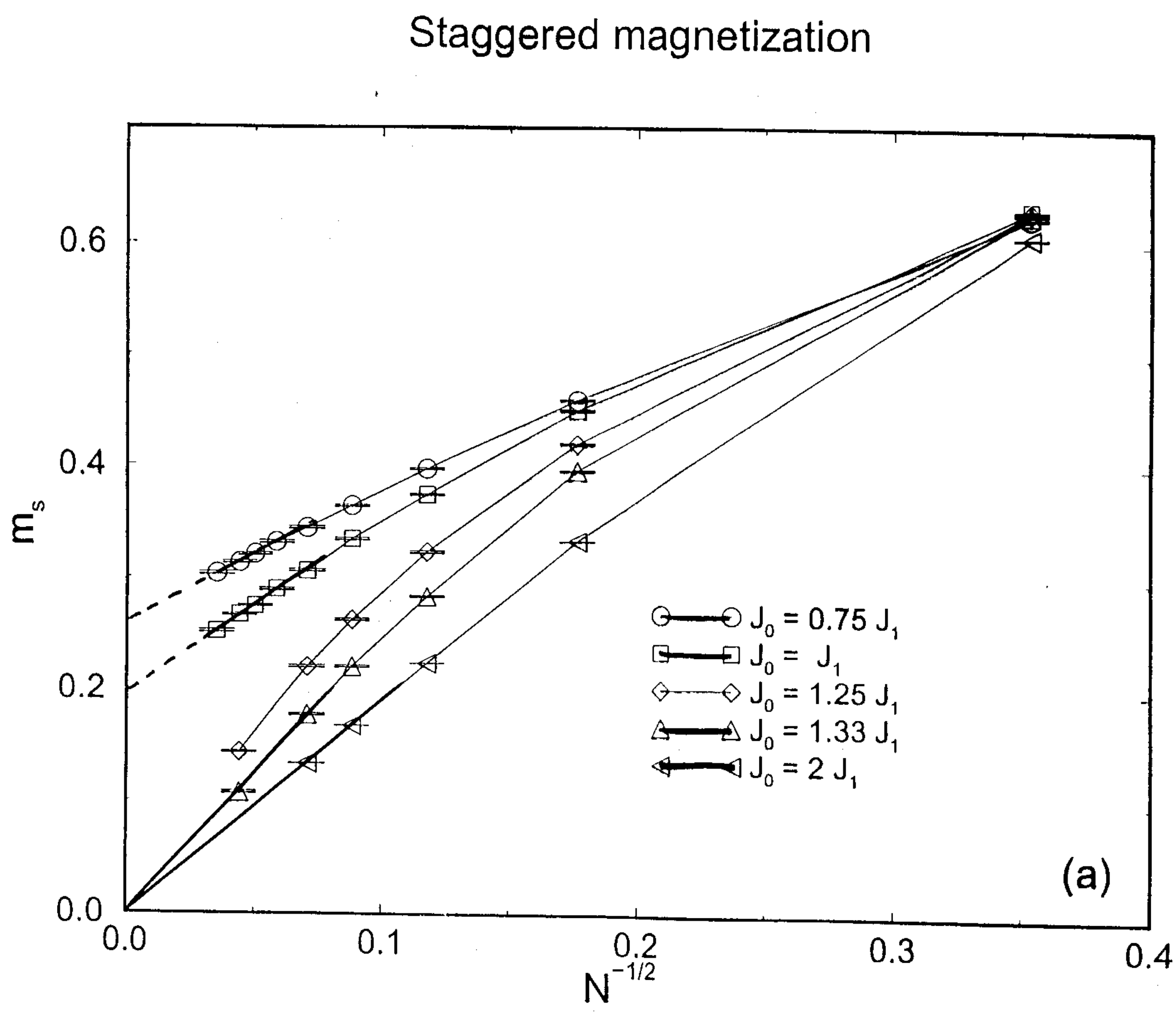
Extensive QMC by using the loop algorithm

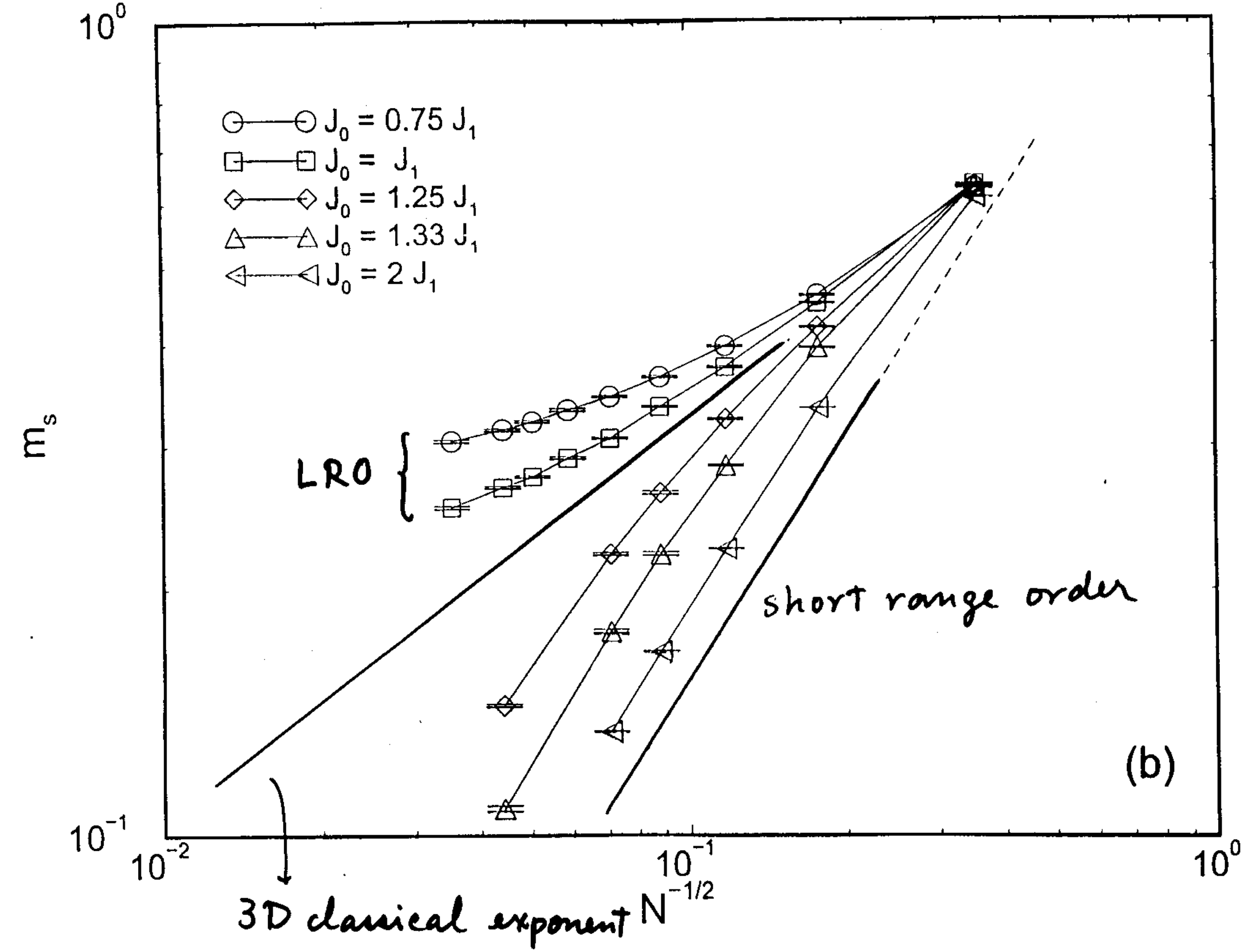
up to 800 spins (Troyer and K.U)


Uniform susceptibility
CaV_4O_9–HB lattice, no frustration
χ
T
0.20
0.15
0.10
0.05
0.00
0.0
0.5
1.0
1.5
square lattice
J0/J1=0.5
J0/J1=0.75
J0/J1=1
J0/J1=1.33
J0/J1=2

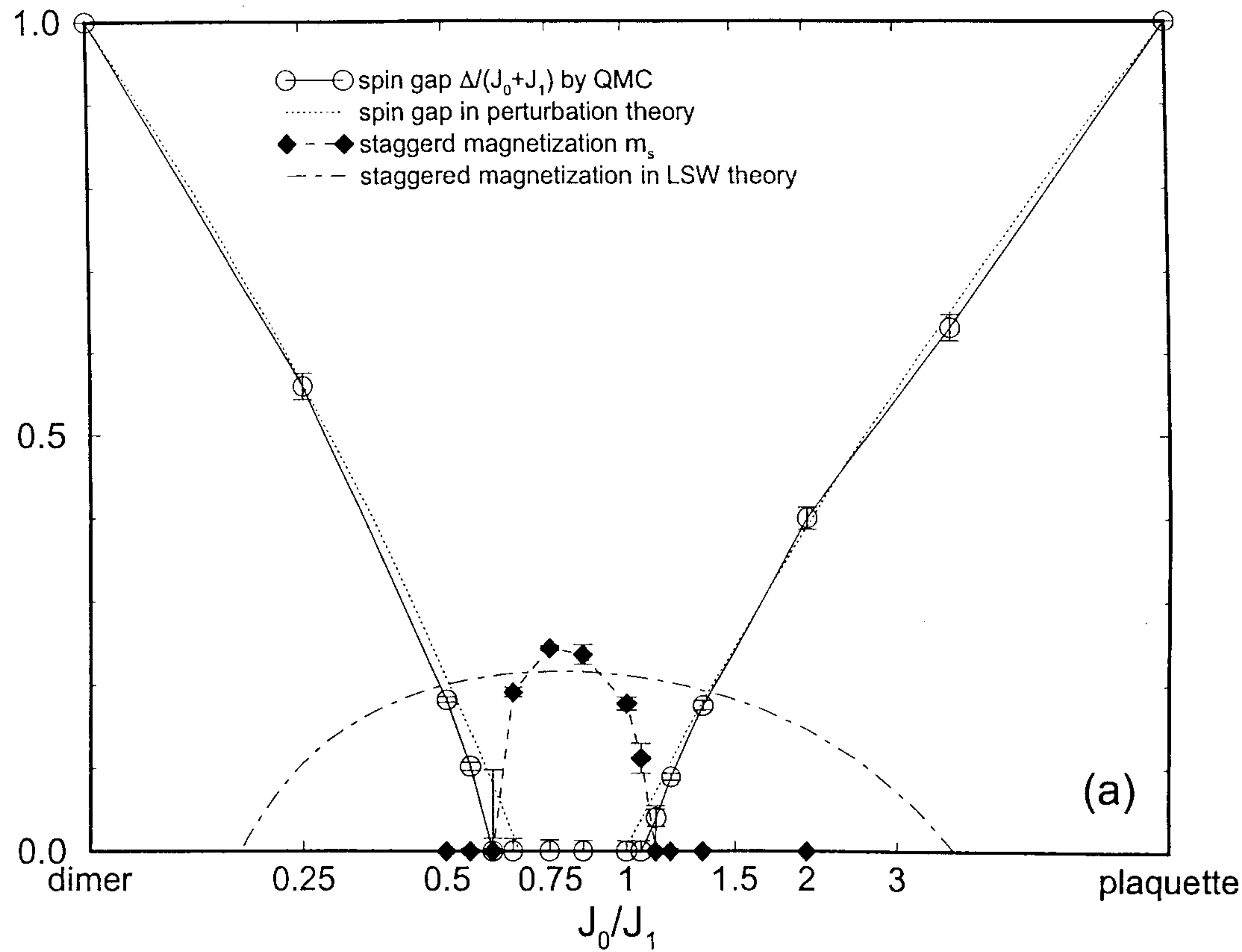
$J_0 = J$

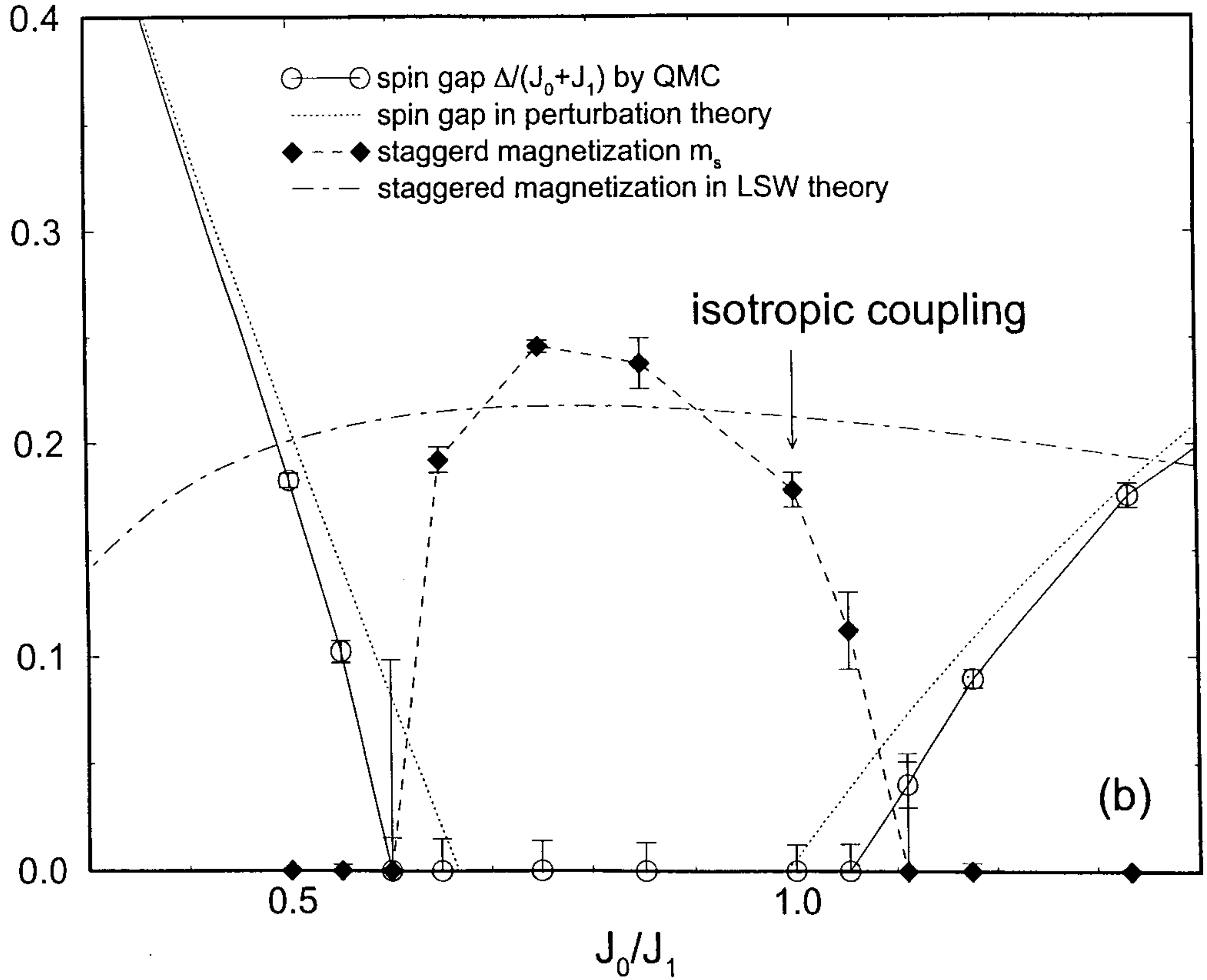
$J_1 = J'$


Staggered magnetization
m_s
0.0
0.2
0.4
0.6
0.0
0.1
0.2
0.3
0.4
$N^{-1/2}$
J_0 = 0.75 J_1
J_0 = J_1
J_0 = 1.25 J_1
J_0 = 1.33 J_1
J_0 = 2 J_1
(a)



(b)
$J_0 = 0.75\ J_1$
$J_0 = J_1$
$J_0 = 1.25\ J_1$
$J_0 = 1.33\ J_1$
$J_0 = 2\ J_1$
LRO
short range order
3D classical exponent
m_s
$N^{-1/2}$
10^0
10^{-1}
10^{-2}
10^{-1}
10^0


spin gap Δ/(J0+J1) by QMC
spin gap in perturbation theory
staggerd magnetization ms
staggered magnetization in LSW theory
(a)
1.0
0.5
0.0
dimer
0.25
0.5
0.75
1
1.5
2
3
plaquette
J0/J1



spin gap Δ/(J0+J1) by QMC
spin gap in perturbation theory
staggerd magnetization ms
staggered magnetization in LSW theory
isotropic coupling
(b)
0.0
0.1
0.2
0.3
0.4
0.5
1.0
J0/J1

effect of frustration

$J''(J_2)$: next neighbor exchange

$$\Delta_{PRVB} = J\left\{1 - \frac{2}{3}(x-2y) - \frac{1}{108}(23x^2 - 20xy + 20y^2)\right.$$

$$- \frac{1}{12}\frac{4x^2-3xy}{2-y} + \frac{7}{18}\frac{(x-y)^2+y^2}{3-y} - \frac{1}{6}\frac{x^2}{3-2y}$$

$$\left. - \frac{5}{72}\frac{(x-y)^2+y^2}{4-y}\right\}$$

$$x = \frac{J'}{J}, \quad y = \frac{J''}{J}$$

$$\Delta_{dimer} = J'\left\{1 - \frac{1}{x}\left(1 - \frac{3}{2}y\right) - \frac{1}{8}\frac{1}{x^2}(4 - 4y + 9y^2)\right.$$

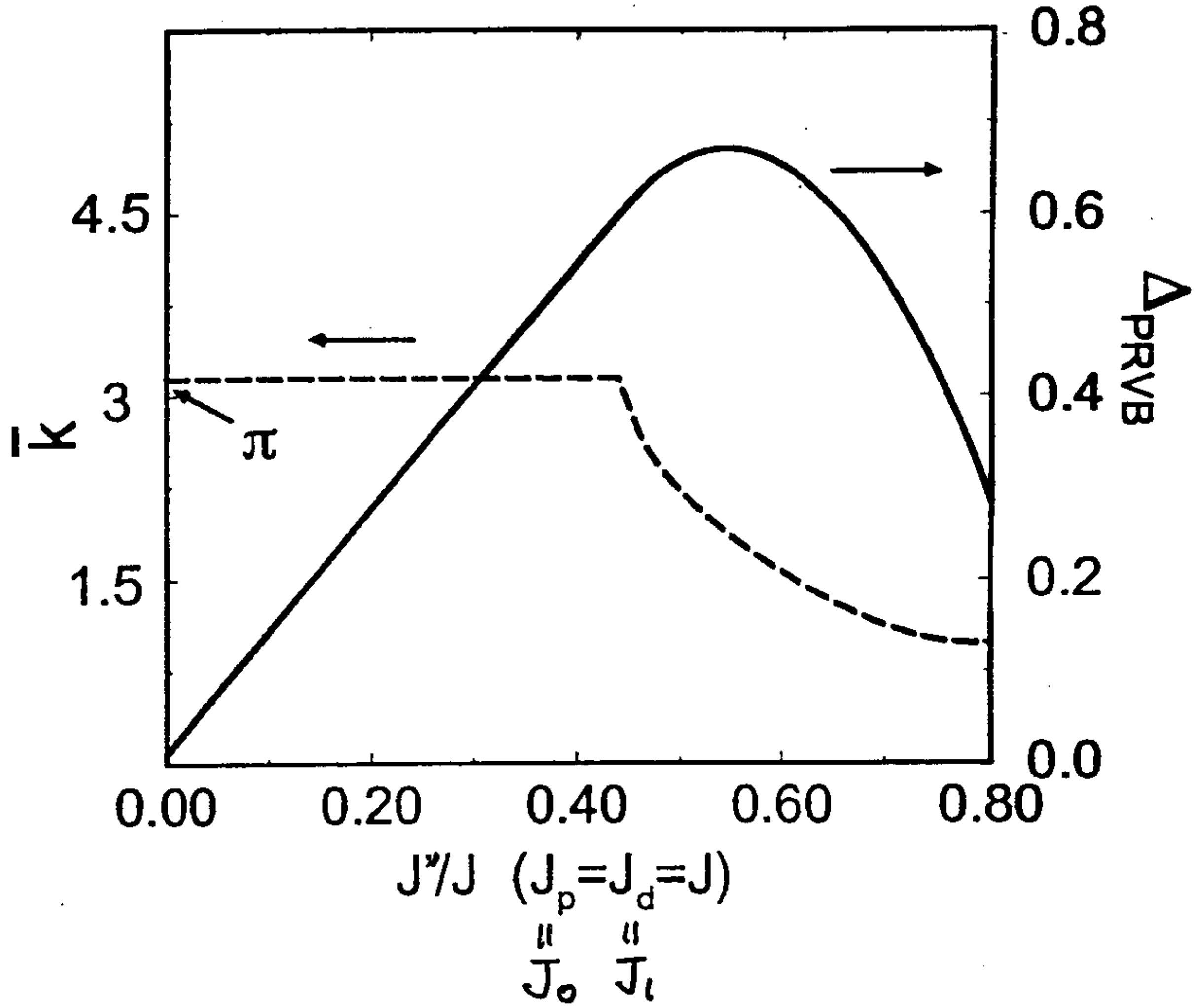
the gap increases for both PRVB and dimer singlet states

another method — cluster mean field theory

lower bound for the critical point from PRVB

$$\left(\frac{J' - 2J''}{J}\right)_c = \frac{3}{4}$$

this condition is easily fulfilled



minimum of the dispersion $(\bar{k}, \bar{k})$

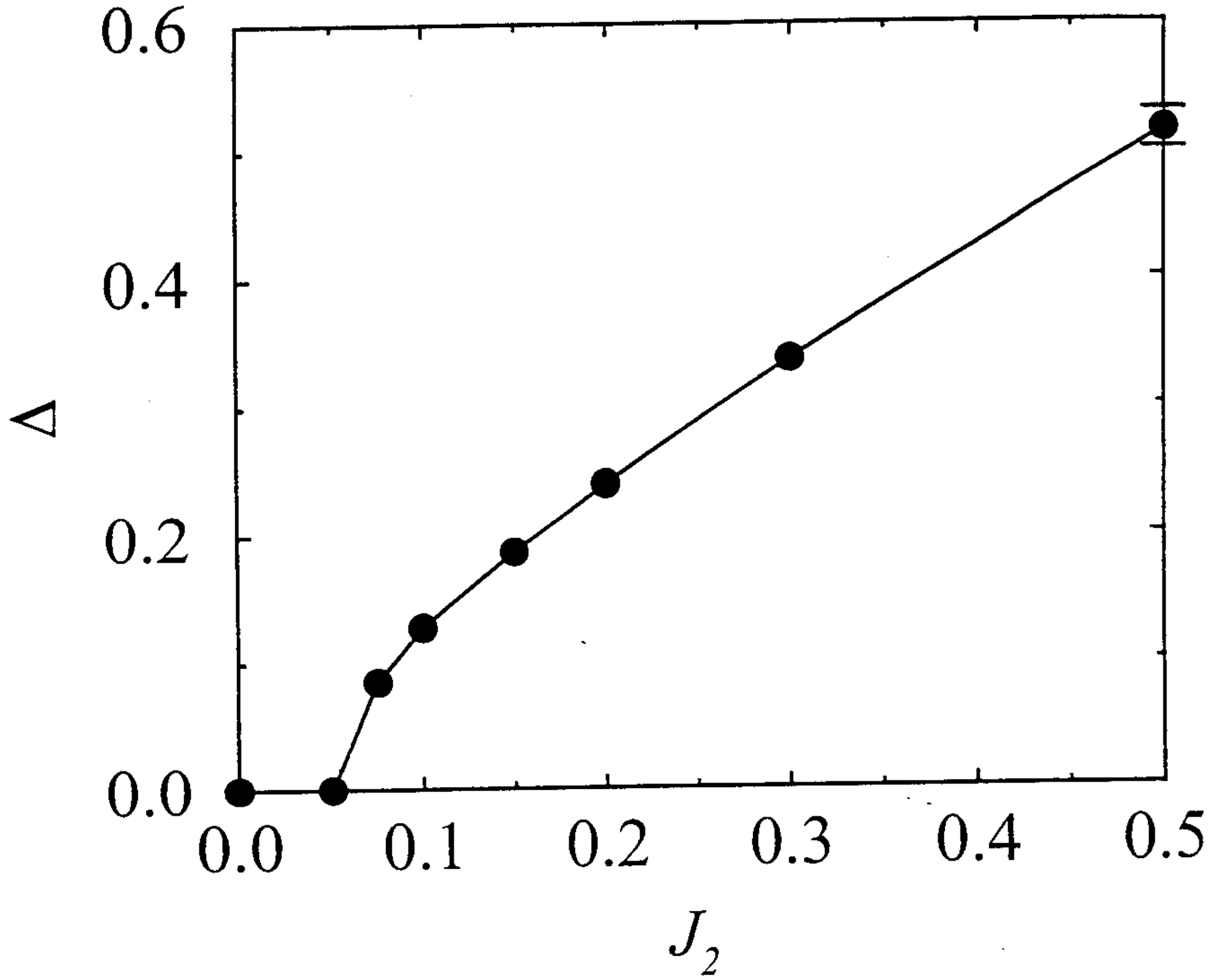


Fig. 4

White

Conclusions

(1) The spin-$\frac{1}{2}$ Heisenberg model on the $\frac{1}{5}$-depleted square lattice is presented as a theoretical model for the spin gap of CaV_4O_9.

(2) The $\frac{1}{5}$-depleted square lattice is favorable for the quantum disordered phase which may be characterized as the PRVB singlet. However at the symmetric point ($J = J'$) the ground state has AF LRO when only the nearest neighbor coupling is considered.

(3) It is possible to explain the large spin gap observed experimentally by including the frustrating exchange for the corner sharing bonds.

Effect of Quantum Fluctuations on Magnetic Ordering in CaV_3O_7

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in collaboration with

Hiroshi KONTANI

M. E. ZHITOMIRSKY

neutron scattering experiments

H. Harashina, K. Kodama, S. Shamoto,

S. Taniguchi, T. Nishikawa, M. Sato

K. Kakurai, M. Nishi

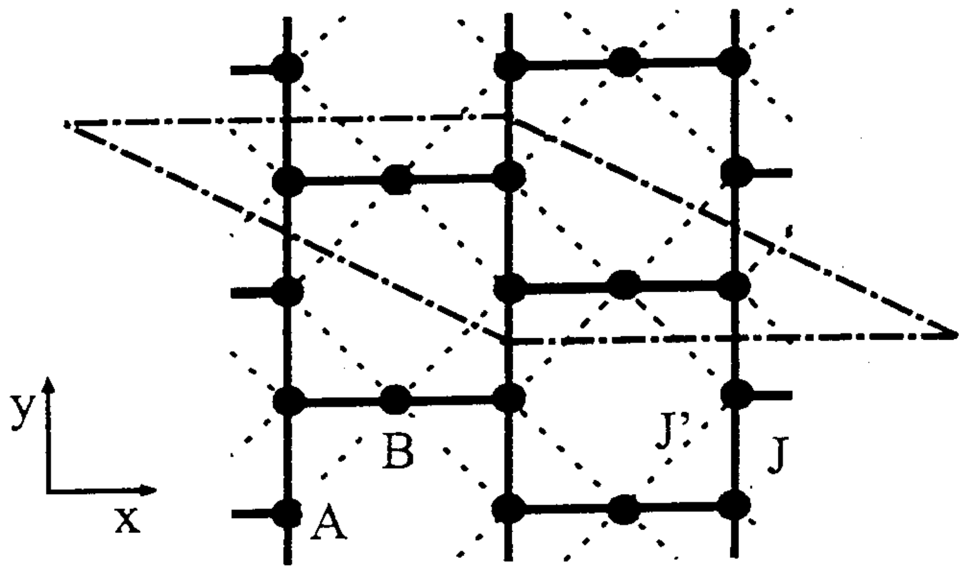


FIG. 1. A model for CaV_3O_7 of the spin-1/2 Heisenberg model with the nearest neighbor (solid lines) and the next nearest neighbor (broken lines) exchange interactions. The dot dashed lines show the six-spin unit cell of the 1/4 depleted square lattice.

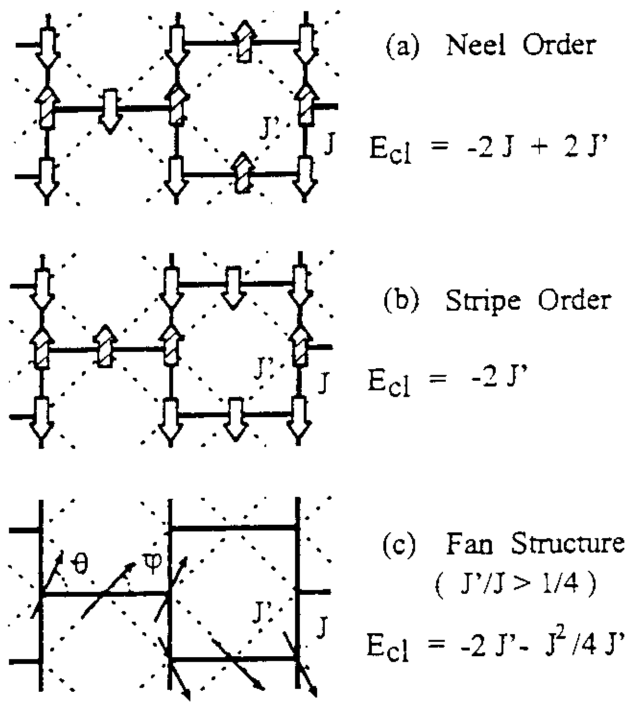


FIG. 2. Typical classical magnetic structures. The fan phase is the ground state for $J'/J > 1/4$ and the Néel phase is the ground state for smaller frustrations. In the classical treatment, the stripe phase is a saddle point and thus always unstable.

Modified Spin Wave Theory

(M. Takahashi, 1989)

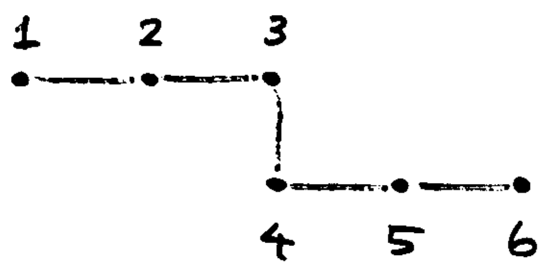
Dyson - Maleev transformation

$$S_i^z = \frac{1}{2} - a_i^+ a_i$$

$$S_i^+ = (1 - a_i^+ a_i)\, a_i$$

$$S_i^- = a_i^+$$

mean field treatment for the interaction term



$$\langle a_1^+ a_2^+ \rangle$$

$$\langle a_2^+ a_4 \rangle$$

$$\langle a_3^+ a_4^+ \rangle$$

$$\frac{1}{2} = \langle a_i^+ a_i \rangle_{QF} + \langle a_i^+ a_i \rangle_{BC}$$

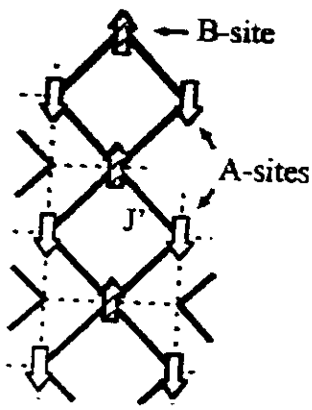


FIG. 3. The chain Heisenberg model constructed only by the next-nearest-neighbor coupling J'.

Table I The ground state properties for $J' = 1$, $J = 0$. E_g is the ground state energy per six spins.

	LSW	MSW	ED
M_A	0.3476	0.3955	0.3961
M_B	0.1951	0.2910	0.2922
E_g	-2.873	-2.910	-2.908

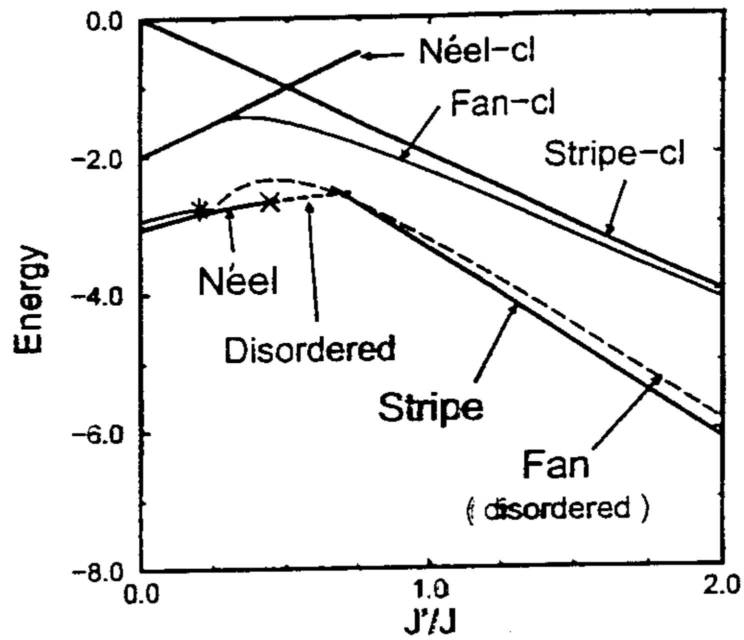


FIG. 4. Comparison between energies of different states. In this figure, 'Stripe-cl', 'Néel-cl' and 'Fan-cl' represent the classical energies of the corresponding magnetic orderings. 'Stripe' and 'Néel' represent the energy calculated by the MSW theory, respectively. 'Fan' represents the energy calculated by the LSW theory, whose spin reduction however is always divergent. Energy of the disordered state is shown by the thick dashed line.

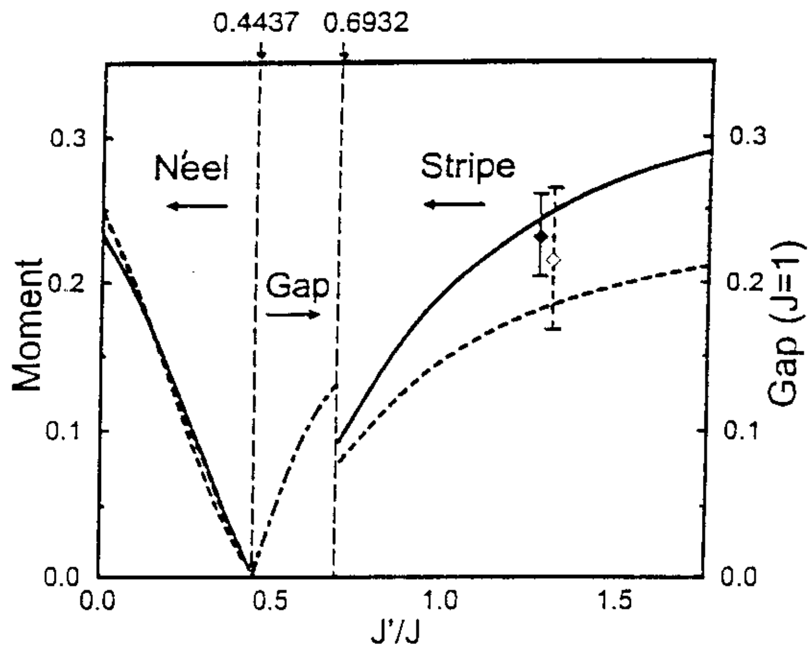


FIG. 5. Phase diagram obtained by the MSW theory, considering the Néel, stripe and the disordered phases. Solid (broken) lines represent the sublattice magnetization for A(B)-sites, respectively. For the disordered phase the magnitude of the spin gap is shown by the dot-dashed line. The experimental data by the neutron diffraction[2] are also shown, where the form factor of d_{xz} (or d_{yz}) is assumed.

Conclusions

(1) The collinear stripe phase experimentally observed in CaV_3O_7 is not stable in the classical theory.

(2) The stripe phase is stabilized by quantum fluctuations.
The modified spin wave theory predicts that this state is stable for $J'/J > 0.69$

(3) The ordered moment is reduced significantly by quantum fluctuations.
In CaV_3O_7, J and J' are estimated to be nearly equal.