Phase transitions of Blume-Emery-Griffiths Model on a Cellular Automata

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Outline

- Blume-Emery-Griffiths (BEG) Model
- Model on Cellular Automata and algorithm
- Simulations and results

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BLUME-EMERY-GRIFFITHS(BEG) MODEL

BEG model(1971): He^3-He^4 mixtures and other physical systems

Hamiltonian of the model

$$H_I = J\sum_{<ij>} S_i S_j + K\sum_{<ij>} S_i^2 S_j^2 + D\sum_i S_i^2$$

Si= -1, 0, 1

J bilinear and K biquadratic interaction constants
D single-ion anisotropy constant

The model has been studied by different techniques. Most of these analysis predict that, the model on three dimension shows a variety of interesting features:

- single and double re-entrancy region
- ferrimagnetic phases
- including a tricitical point, critical end point or bicritical end point for certain model parameters

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- The model is simulated on a cellular automata by using improved algorithm(it is improved from Creutz algorithm)
- The calculations are done on a simple cubic lattice of the linear dimensions L=12,16,18 and 24 with periodic boundary conditions.

Blume-Emery-Griffiths Model on a cellular automata

Each site of the lattice has three variables:

All variables are an integer

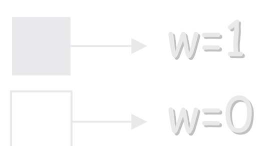
The first one is Ising spin Bi,

Bi = Si + 1, Si= -1, 0 and 1 Bi= 0, 1 and 2

The second one is H_k (kinetic energy associated with the demon) It is equal to the changing in the Ising energy for any spin flip. It takes integer values in the interval (0,m)

The third variable, w, is parity its value may be 0 or 1.

it provides a checkboard style updating



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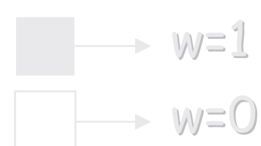

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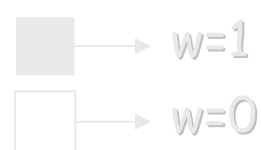

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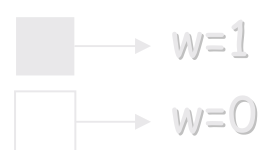

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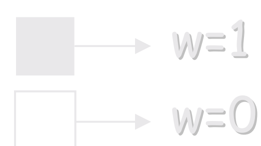

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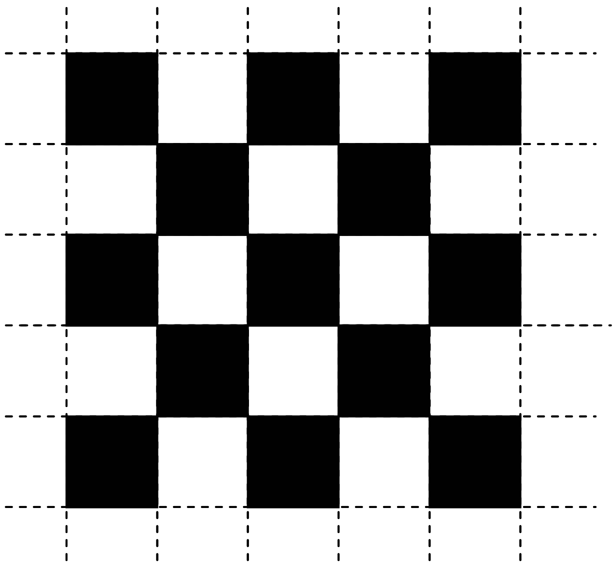

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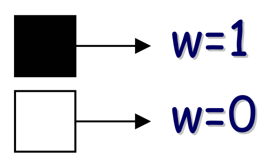

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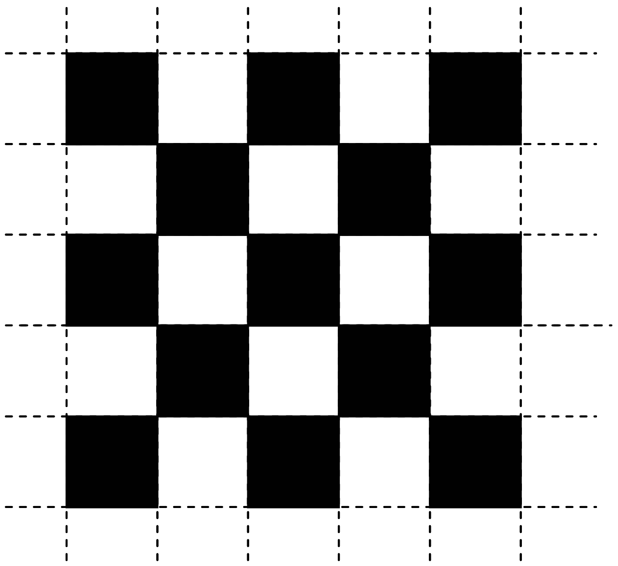

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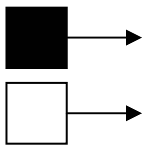

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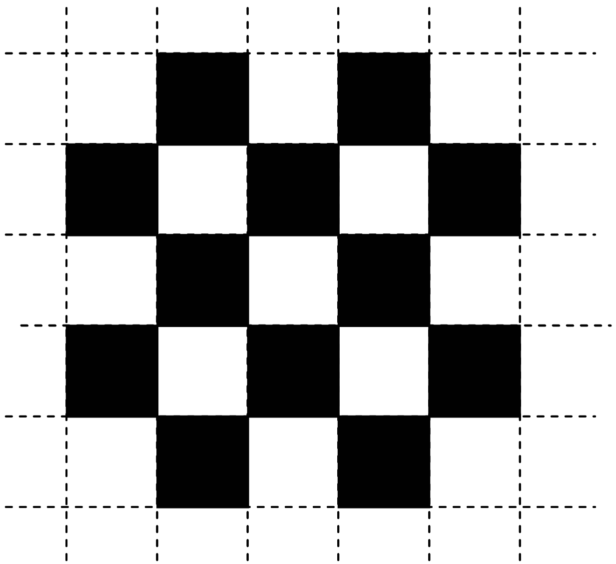

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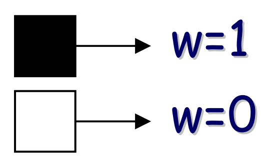

updating rule:

- For a site to be updated, its spin is changed to one of the other two states with ½ probability.
- The change in the Ising energy, dH_I is calculated.
- If this energy is transferable to or from the momentum variable(H_k) associated with this site, this change is done and the momentum is appropriately changed. Otherwise, the spin and momentum are not changed.
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updating rule:

- For a site to be updated, its spin is changed to one of the other two states with $\frac{1}{2}$ probability.
- The change in the Ising energy, dH_I is calculated.
- If this energy is transferable to or from the momentum variable(H_k) associated with this site, this change is done and the momentum is appropriately changed. Otherwise, the spin and momentum are not changed.
- During the updating process, total energy of the system $H=H_I+H_k$ is conserved.

Heating algorithm

- All spins take the F/SQ ordered structure according to the selected (J,K,D) parameter set.
- Kinetic energy per site is given to the certain percent of the lattice via second variable.
- This configuration is run during 10000 *CA* time steps.
- At the end of this step, the configuration at low temperature is obtained.
- This configuration has been chosen as a starting configuration for the heating run.
- During the heating cycle, energy is added to the system through the second variable of each site(Hk) after "t" cellular automaton steps. This process is realized by increasing of certain values in the kinetic energy of each site.

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Detail of simulations

For estimating the kind of PTs, the temperature variations of the some quantites are calculated:

- **order parameters,**

$$m = \frac{1}{N}\sum_{i=1}^{N} S_i \qquad q = \frac{1}{N}\sum_{i=1}^{N} S_i^2$$

- **susceptibility,**

$$\chi = \frac{\partial m}{\partial h} = N(< m^2 > - < m >^2)/kT$$

Detail of simulations

- **internal energy,**

$$U = H_I / H_0 \qquad H_I = J\sum_{<ij>} S_i S_j + K\sum_{<ij>} S_i^{\,2} S_j^{\,2} + D\sum_i S_i^2$$

- **specific heat**

$$C = \partial H_I / \partial T = N(< U^2 > - < U >^2)/(kT)^2$$

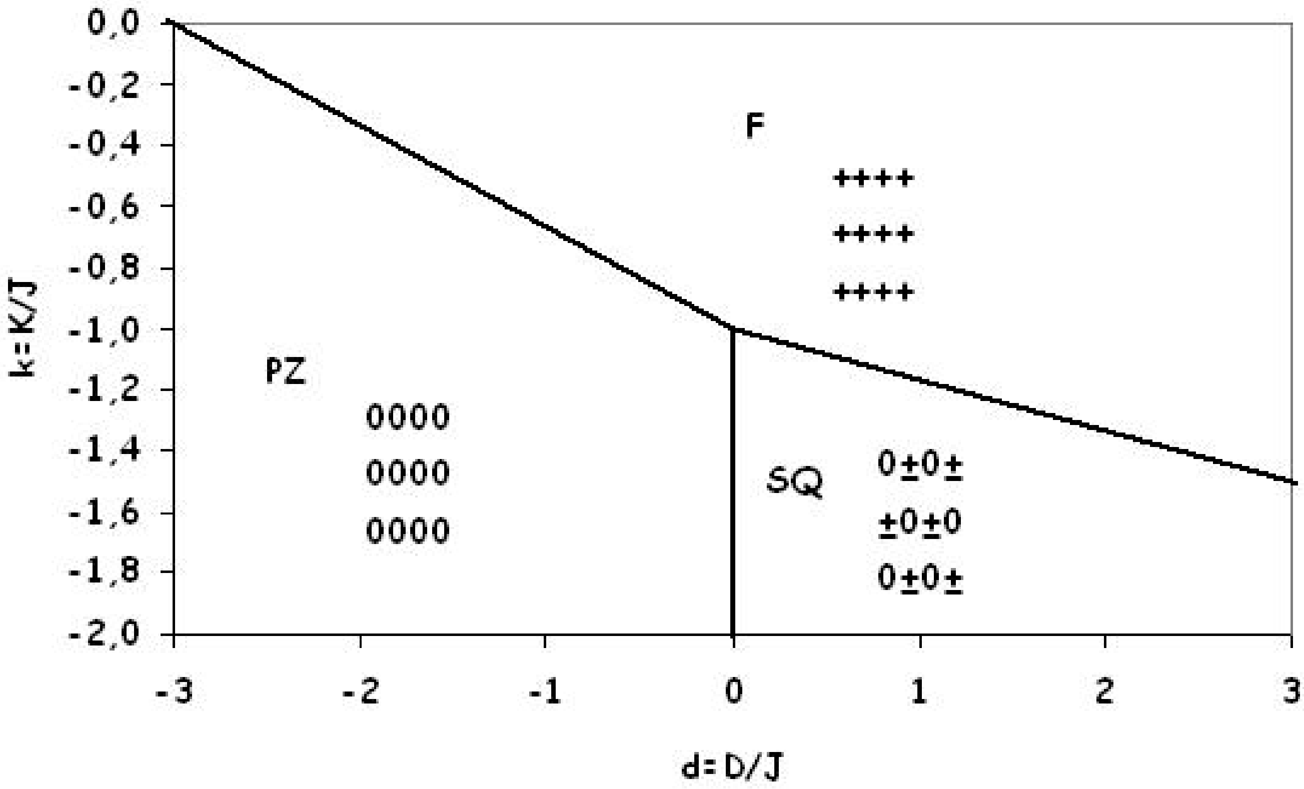
- **Binder cumulant**

$$g_L = 1 - \frac{< M^4 >}{< M^2 >^2}$$

- **In addition, finite-size scaling theory is used for estimating the static critical exponents.**

The results of simulations

The phase diagram in the ground state of model on a simple cubic lattice



Ferromagnetic order(F), all spins are "+1" or "-1"

Perfect zero order(S), "0"

Stagger quadrupolar (SQ), two sublattice(A and B), randomly, in A Si=±1 and in B Si=0

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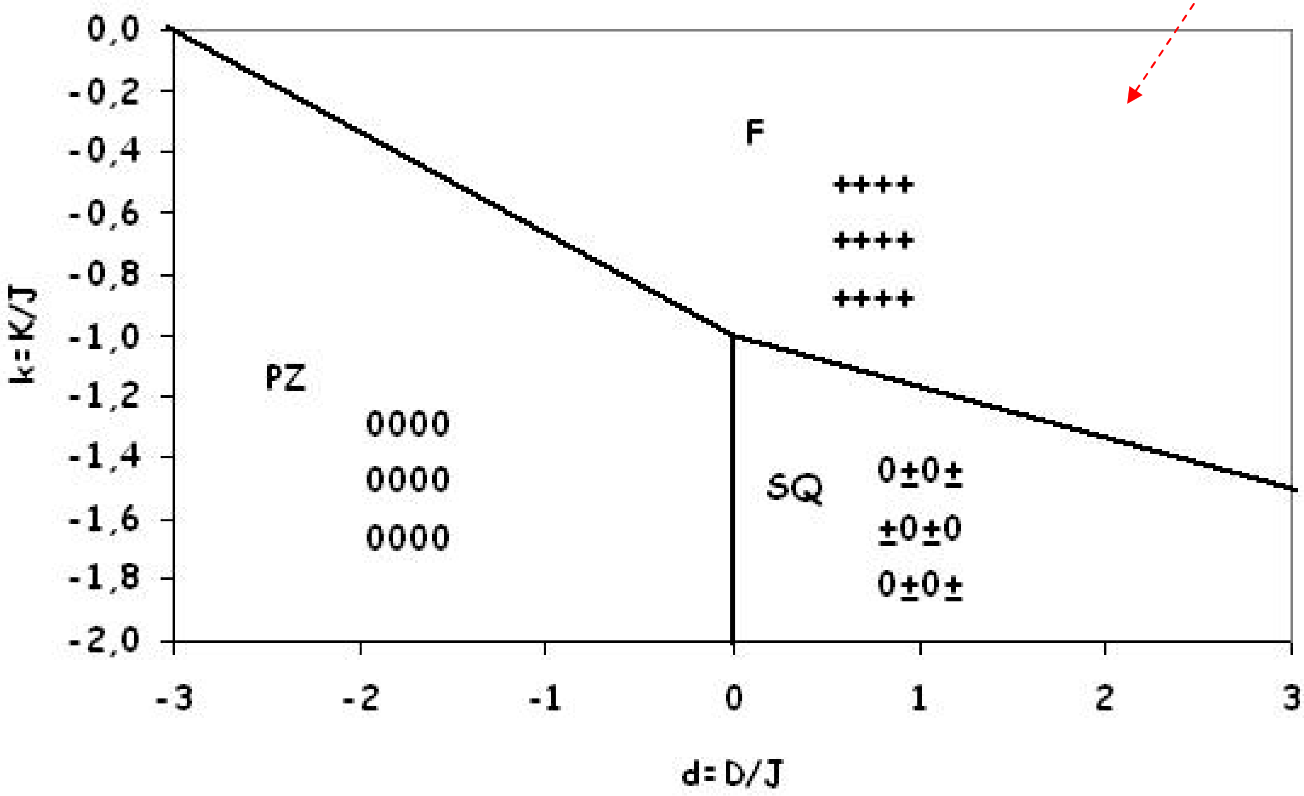

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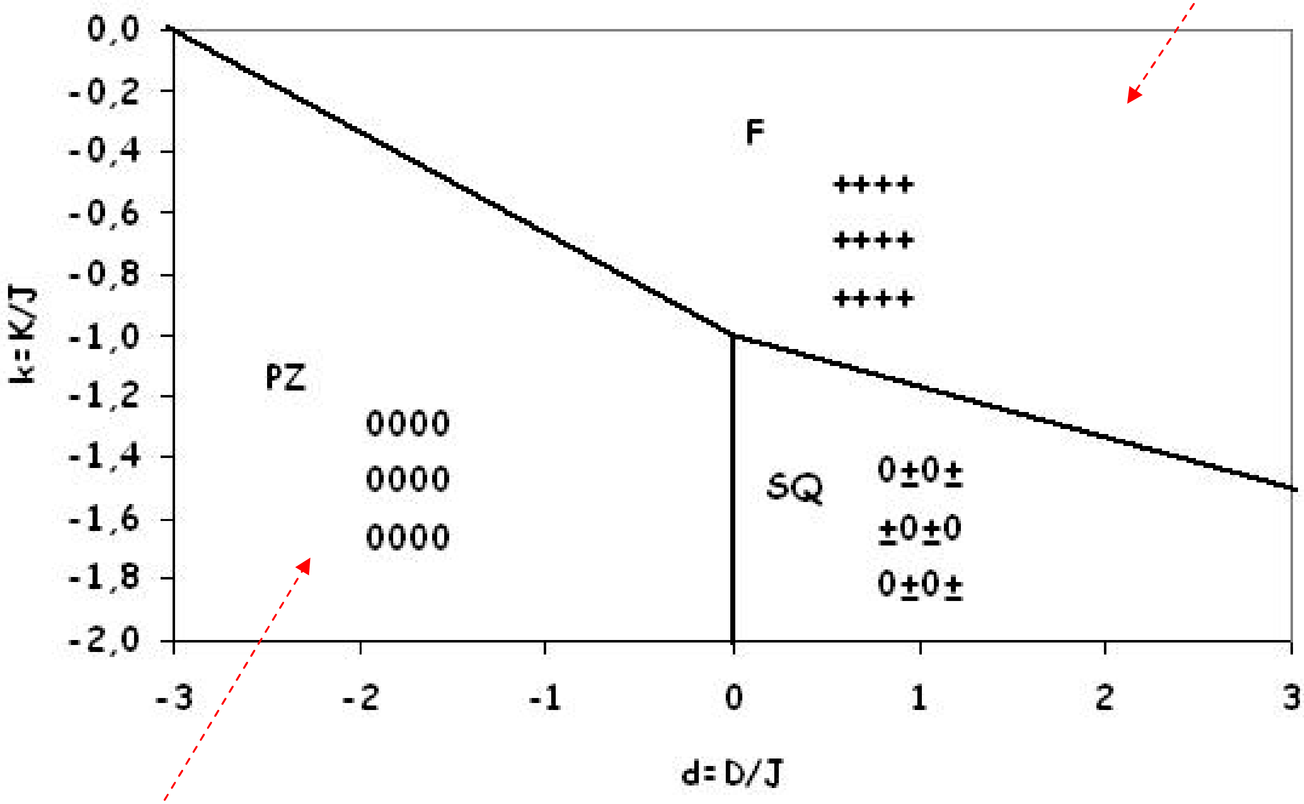

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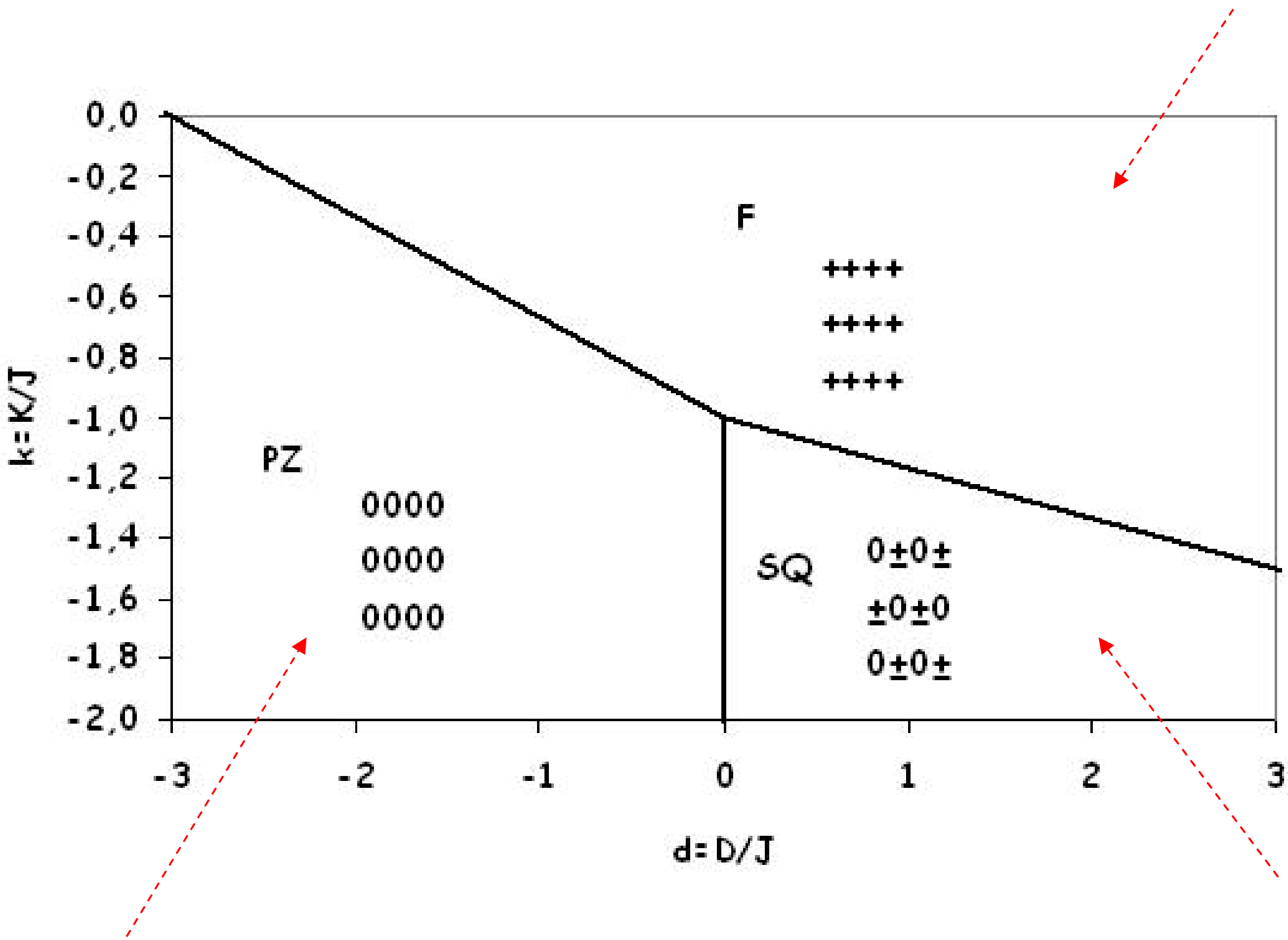

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At $T \neq 0$, the variaous phases of the model are defined according to the order parameters at a selected model parameter set:

For F region,

Ferromagnetic phase (F)
$m \neq 0, q \neq 2/3$

Quadrupolar phase (Q)
$m = 0, q \neq 2/3;$

For SQ region,

Ferromagnetic phase (F)
$mA = mB \neq 0$ and $qA = qB$

Quadrupolar phase (Q)
$mA = mB = 0$ and $qA = qB$

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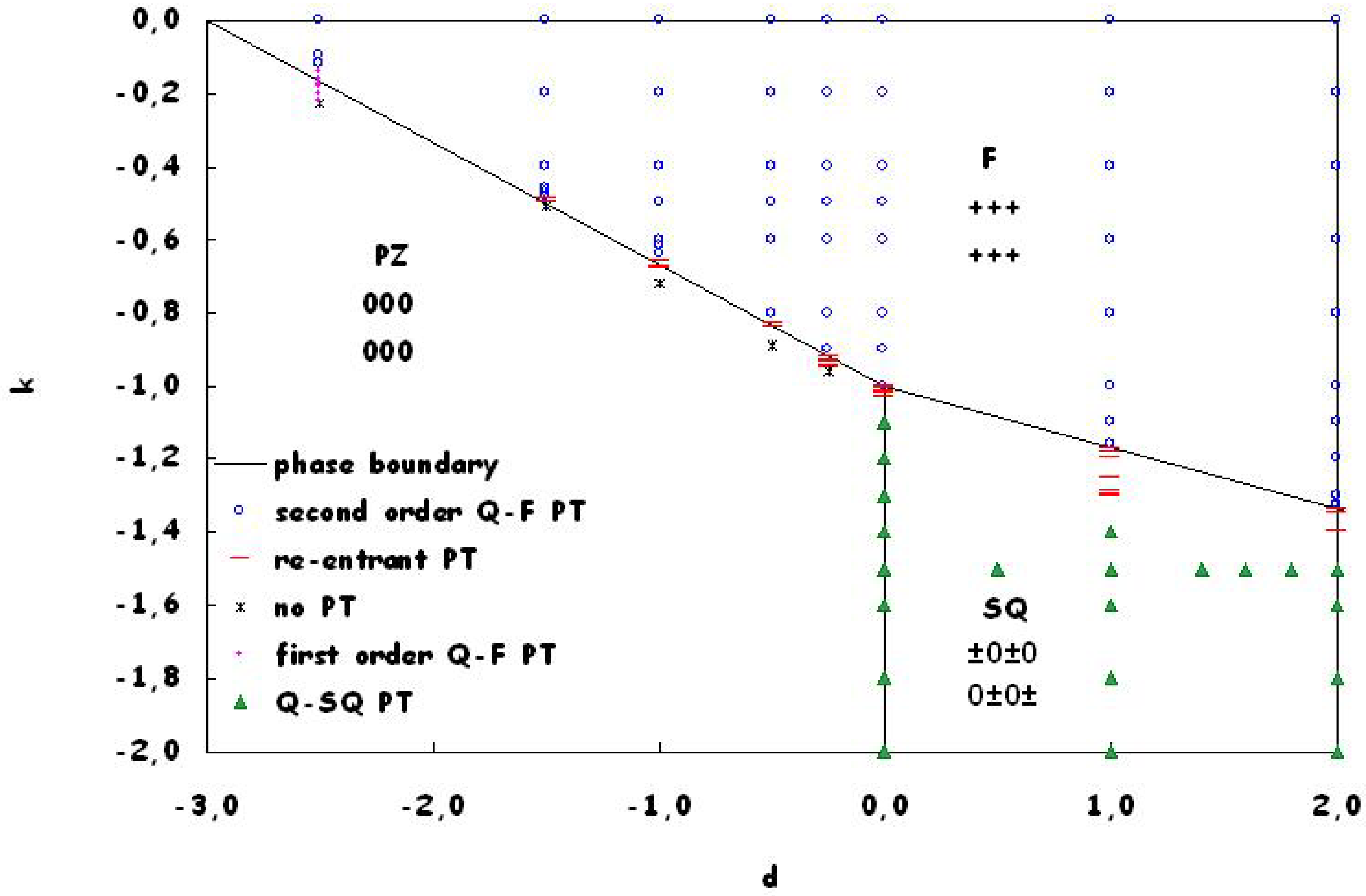
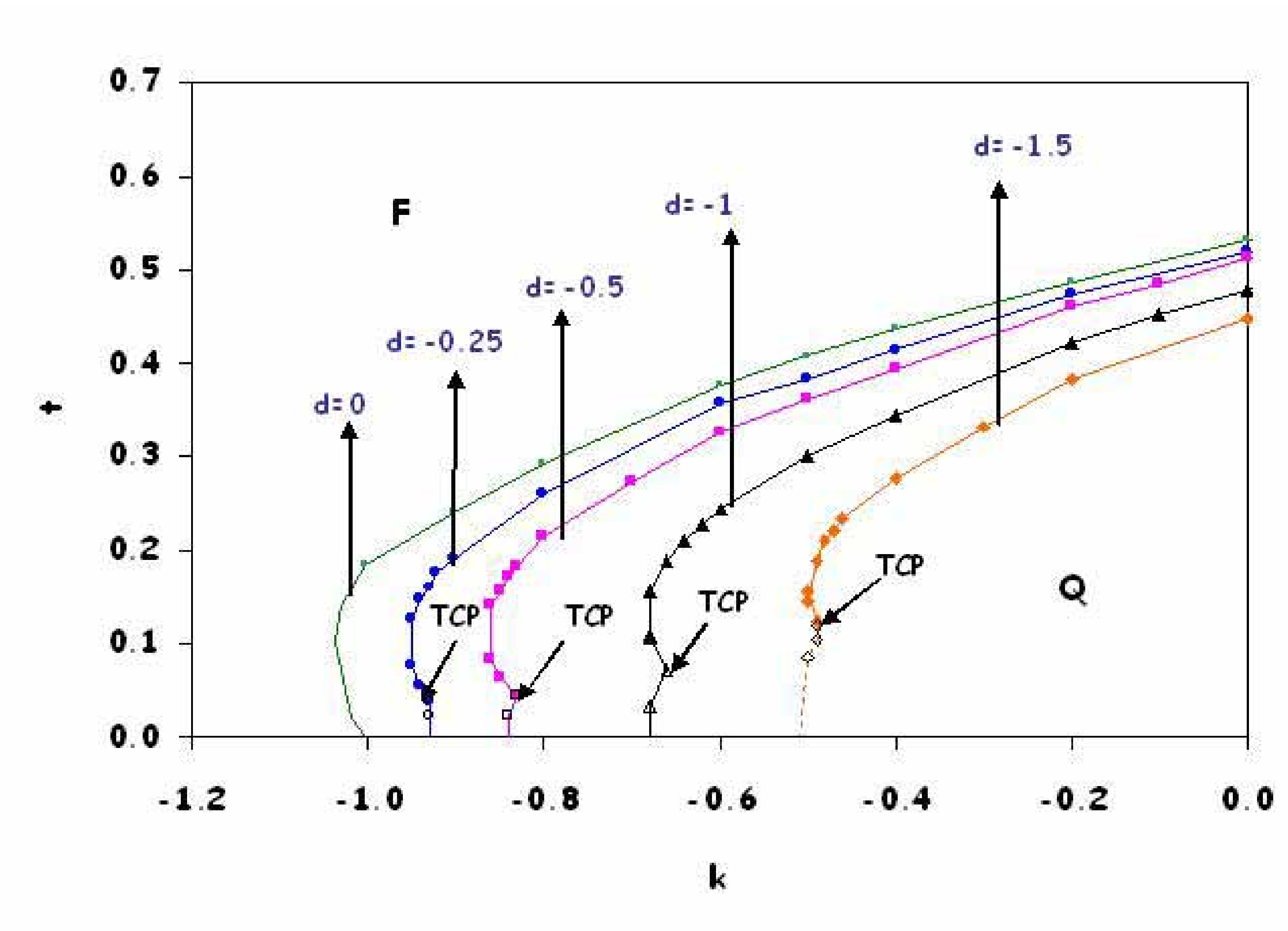
Phase transition in BEG model



The obtained results in the F region and near the F and PZ phase boundary

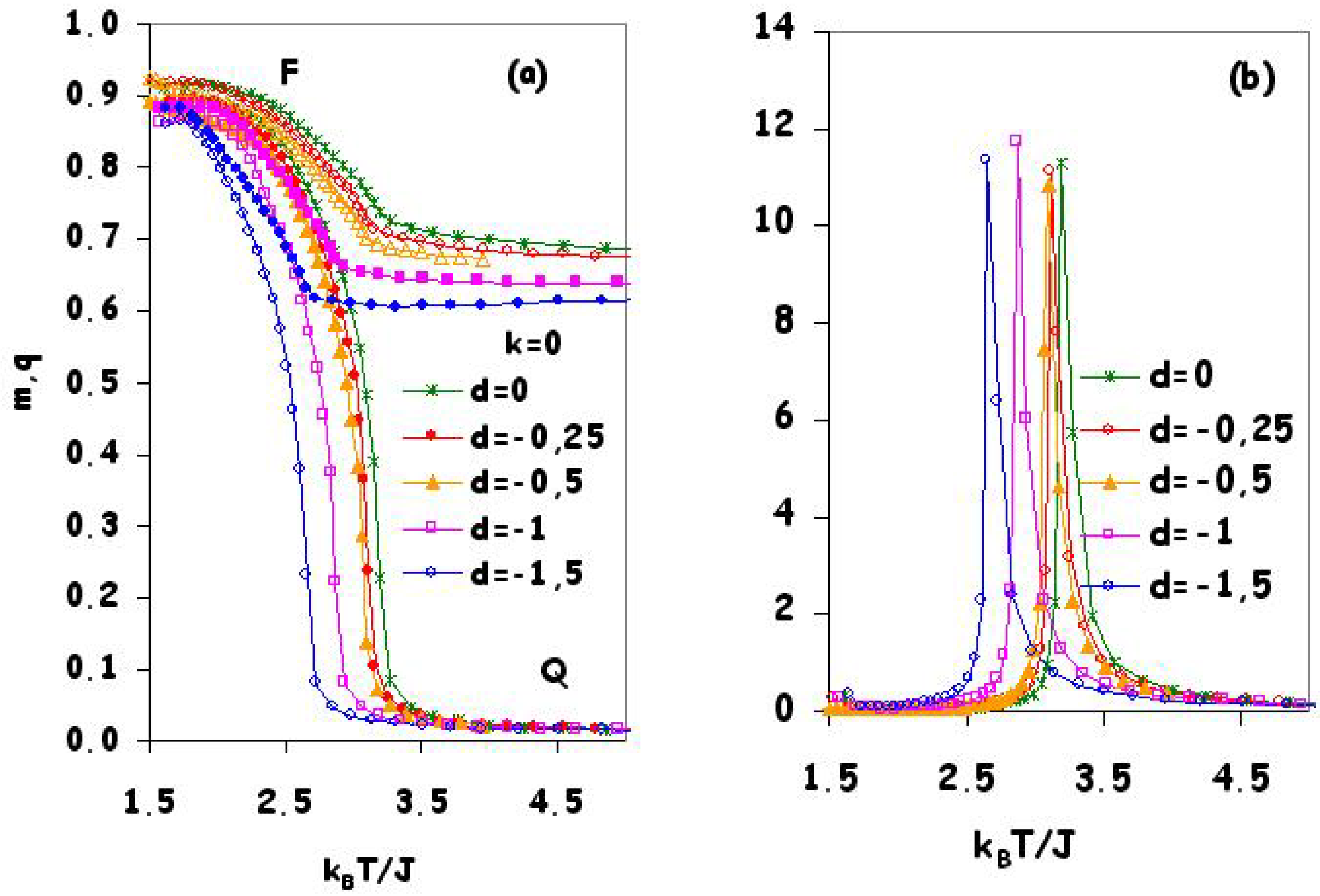
• Phase diagrams are obtained for certain model parameters



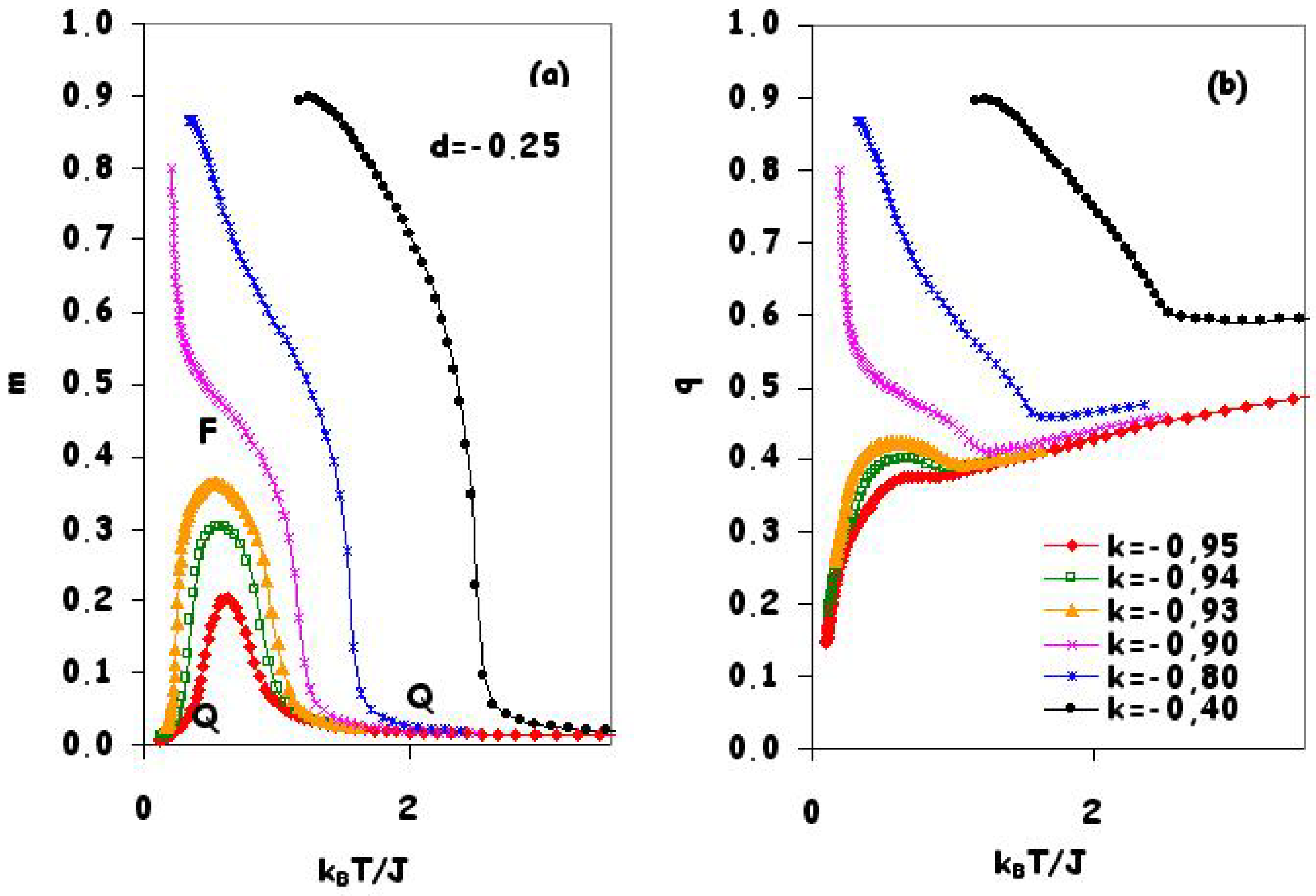
TCP: at which the PT changes from second order to first order

second-order Q→F (at certain parameters)

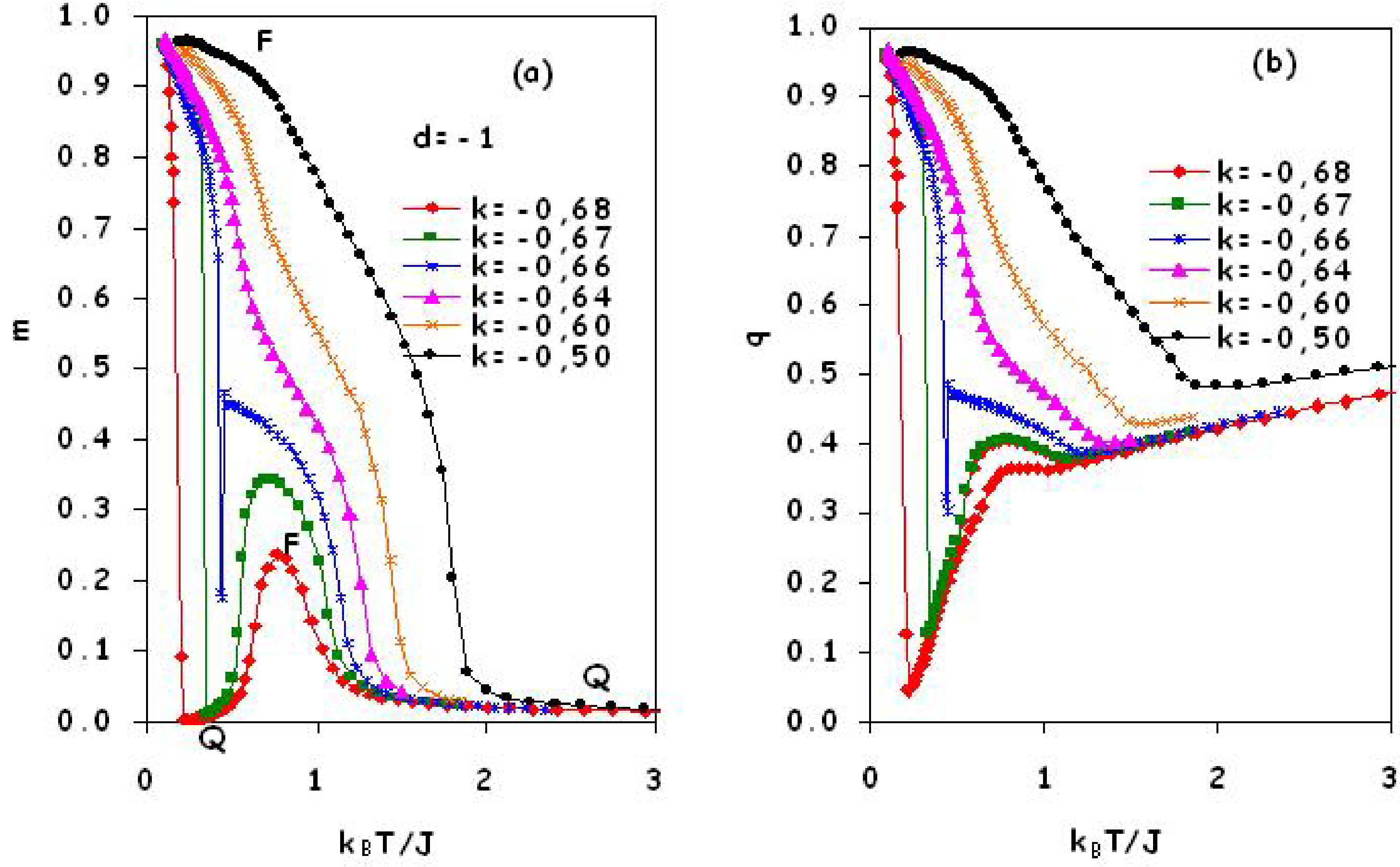
Q: $m=0$, $q \neq 2/3$;
F: $m \neq 0$, $q \neq 2/3$



re-entrant Q→F→Q (at certain parameters)



double re-entrant Q→F→Q→F (at certain parameters)



double re-entrant
Q→F→Q→F
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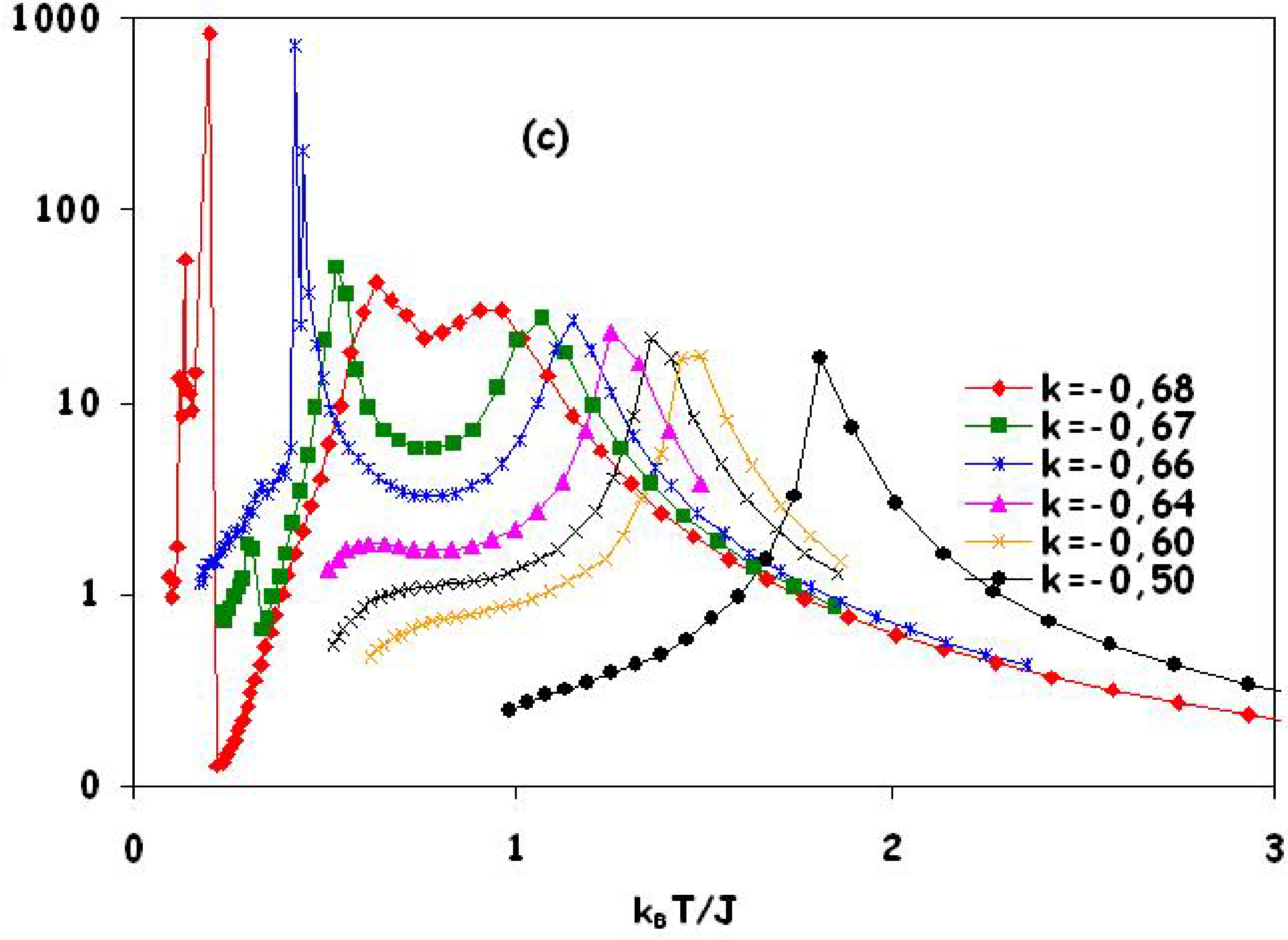

The obtained results in the SQ region and near the F and SQ phase boundary

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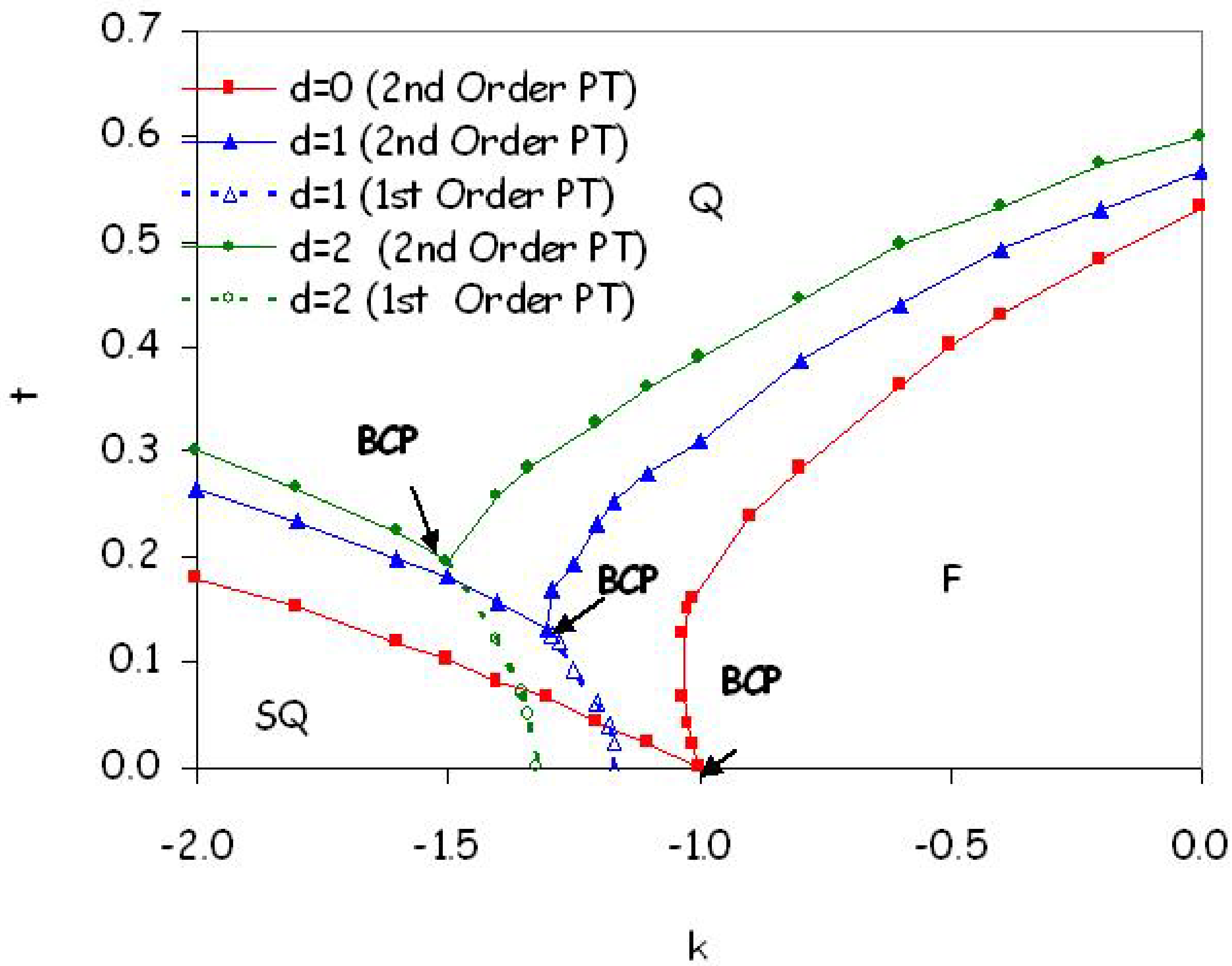
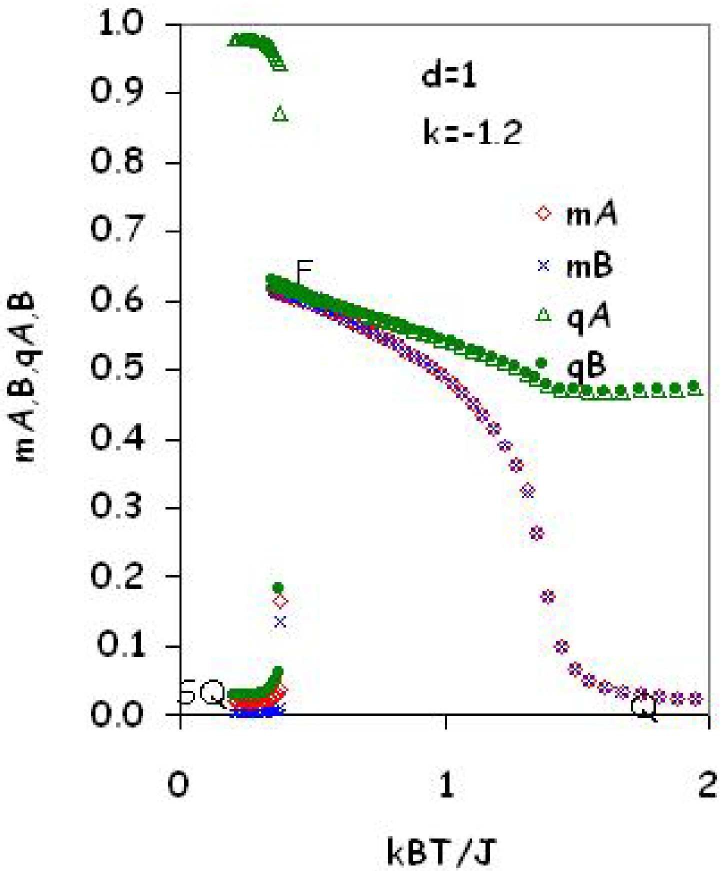
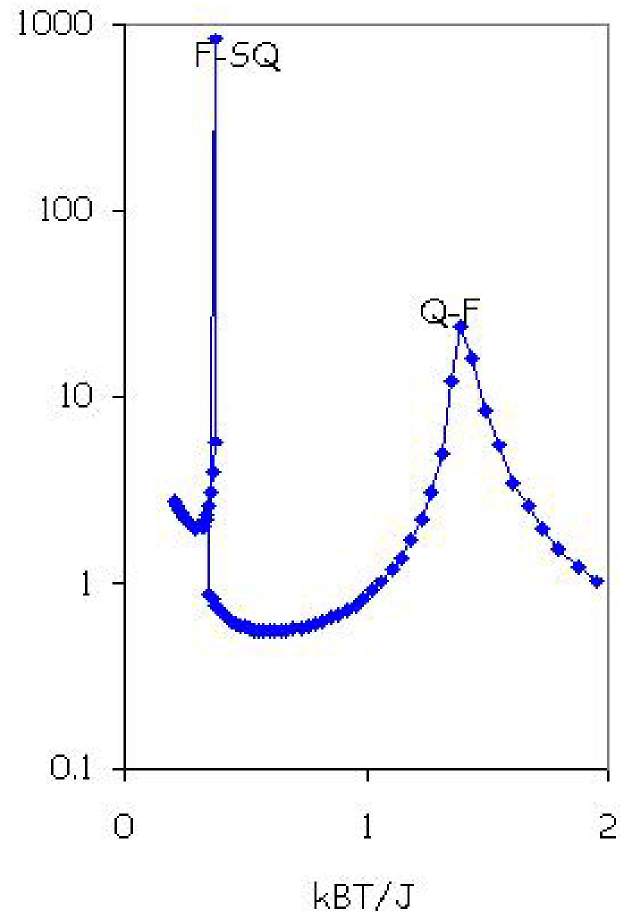


BCP: at which two second order lines meet on the first order line

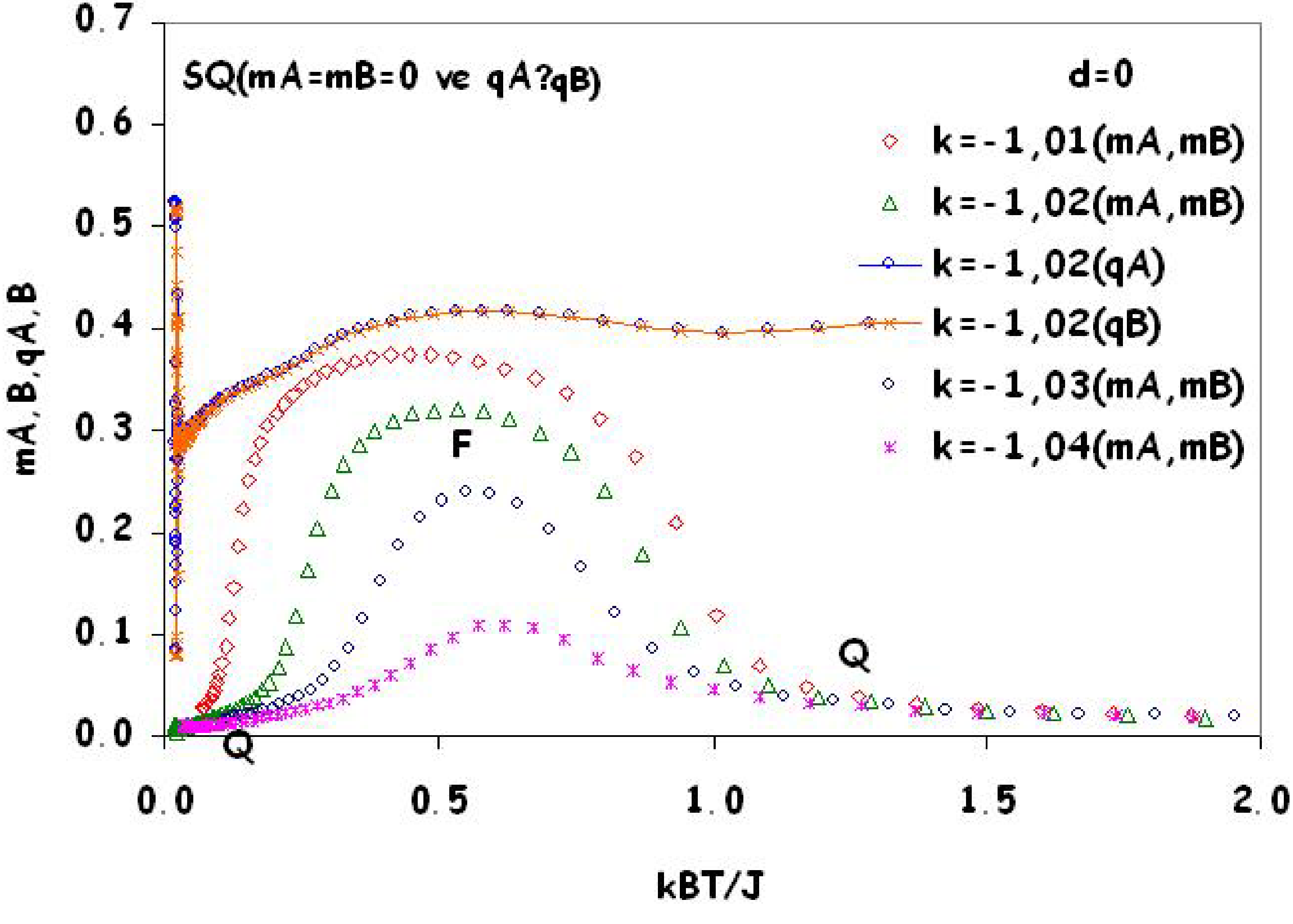
successive Q → F → SQ PT



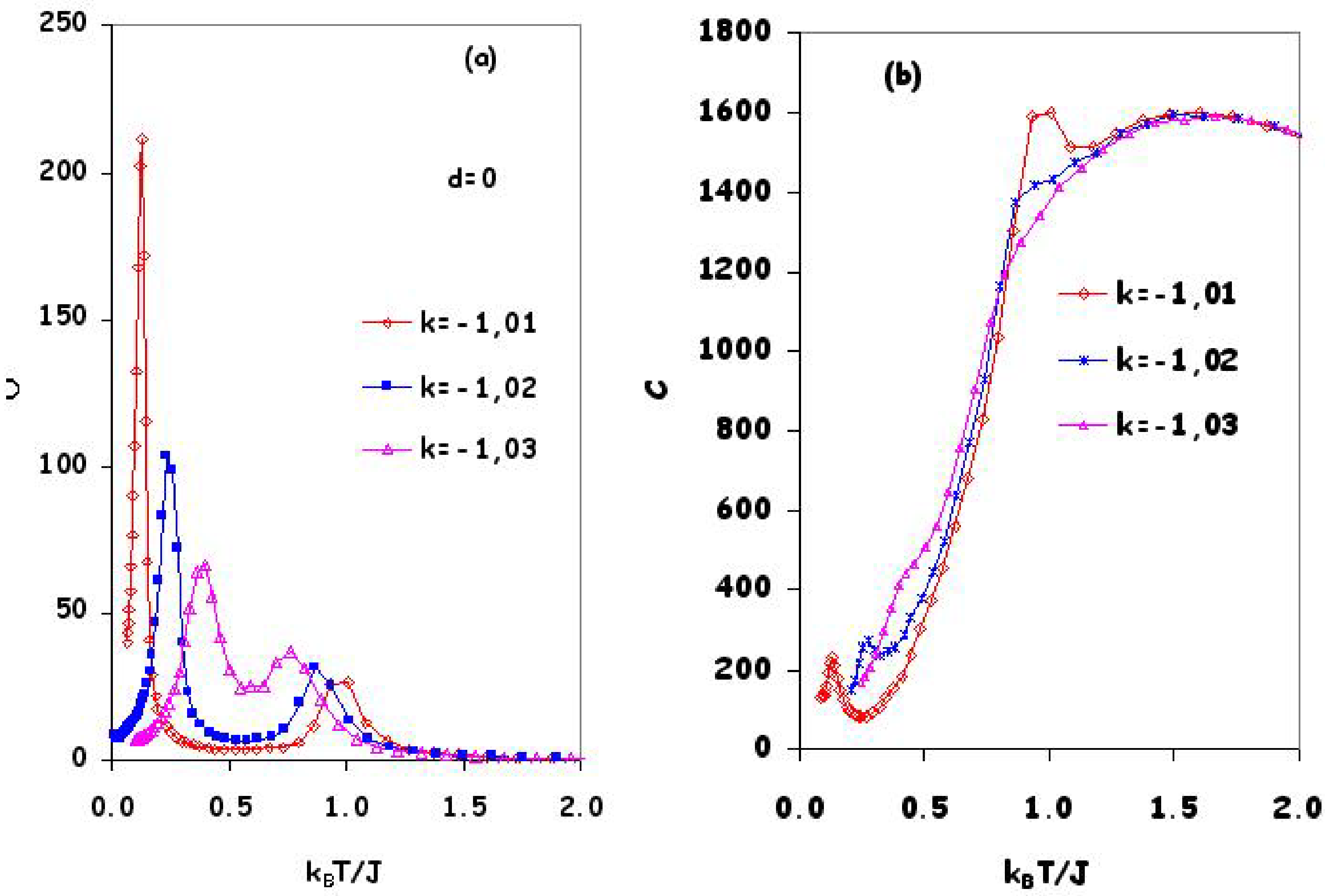


Q→F second order
F→SQ first order

re-entrant Q → F → Q → SQ PT

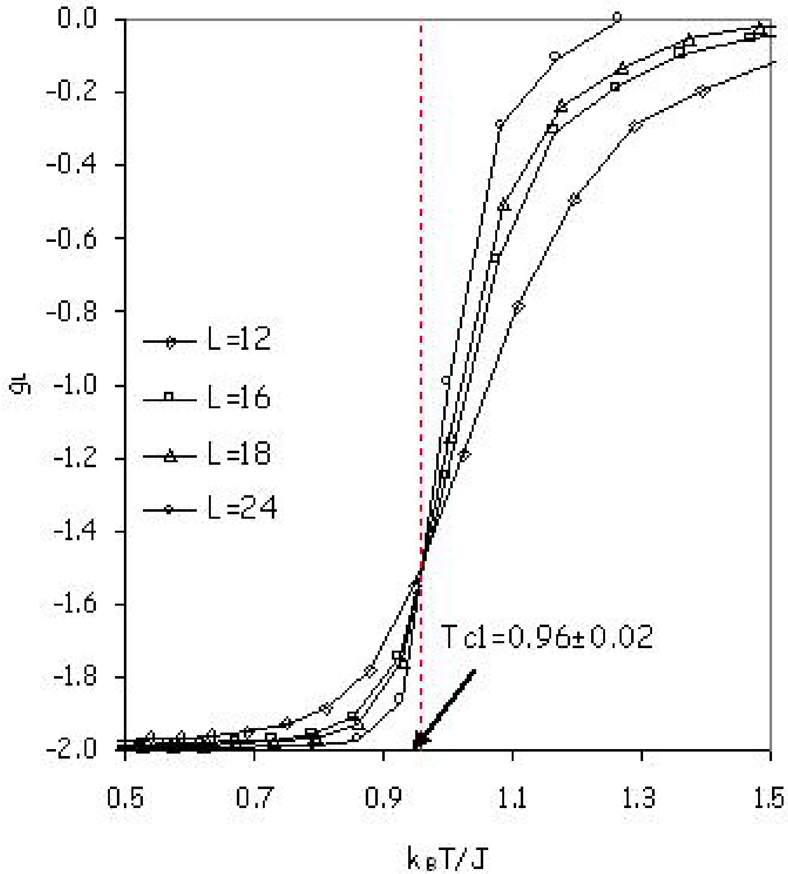


re-entrant Q → F → Q → SQ PT

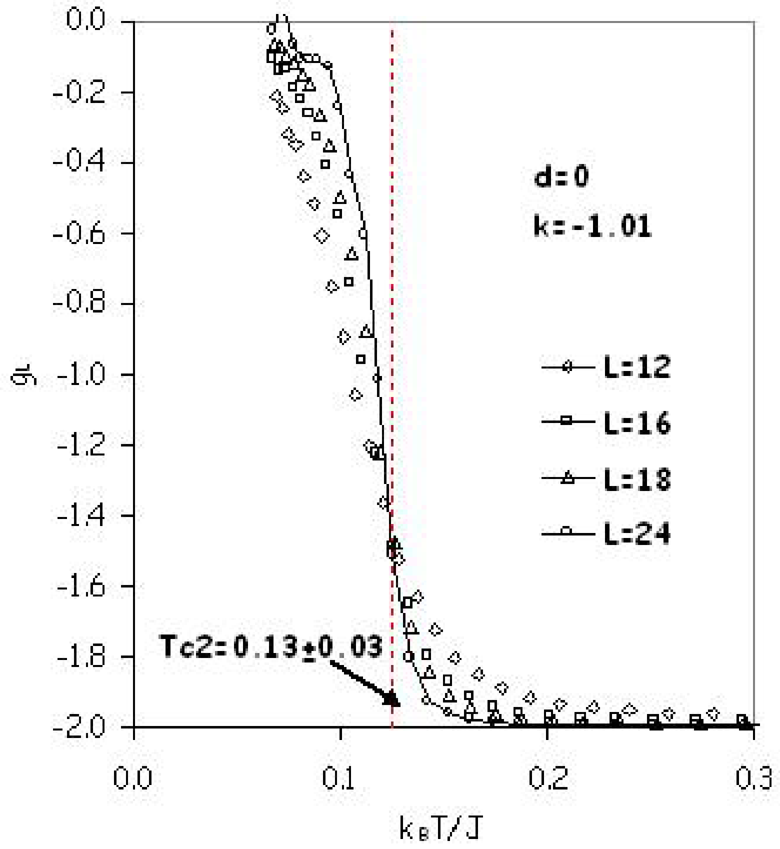


Static critical exponents

The infinite lattice critical point(Tc) are obtained from the intersection of the Binder cumulant curves for different lattice sizes.



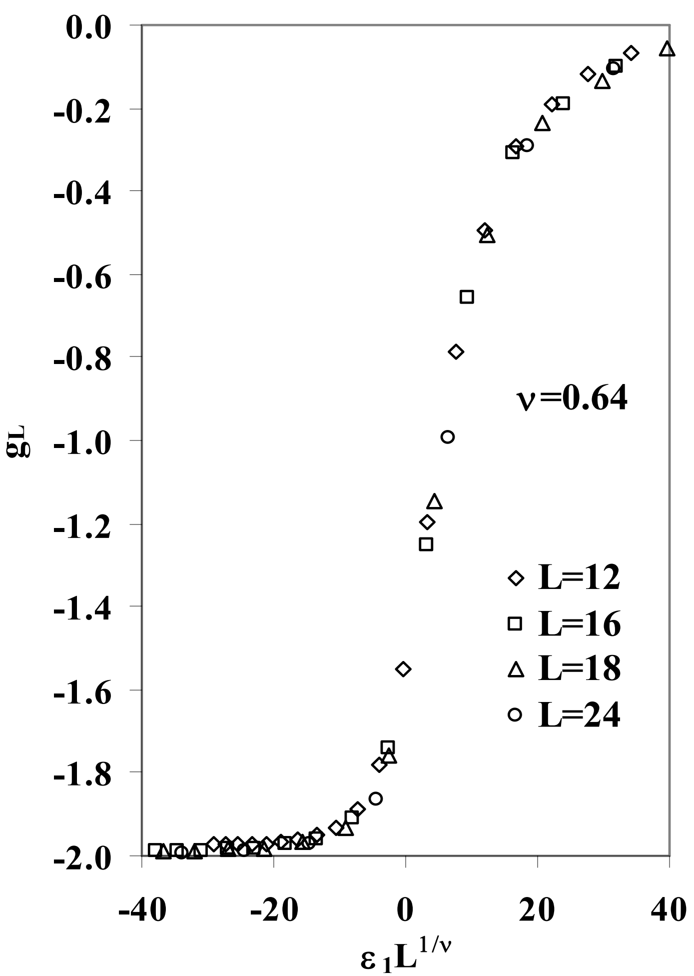
for the Q→F PT



for the F→Q PT

Exponent ν:

ν can be obtained using the finite size scaling relation for Binder cumulant, which is defined by $g_L = g(\varepsilon L^{1/\nu})$ $\varepsilon=(T-T_c)/T_c$



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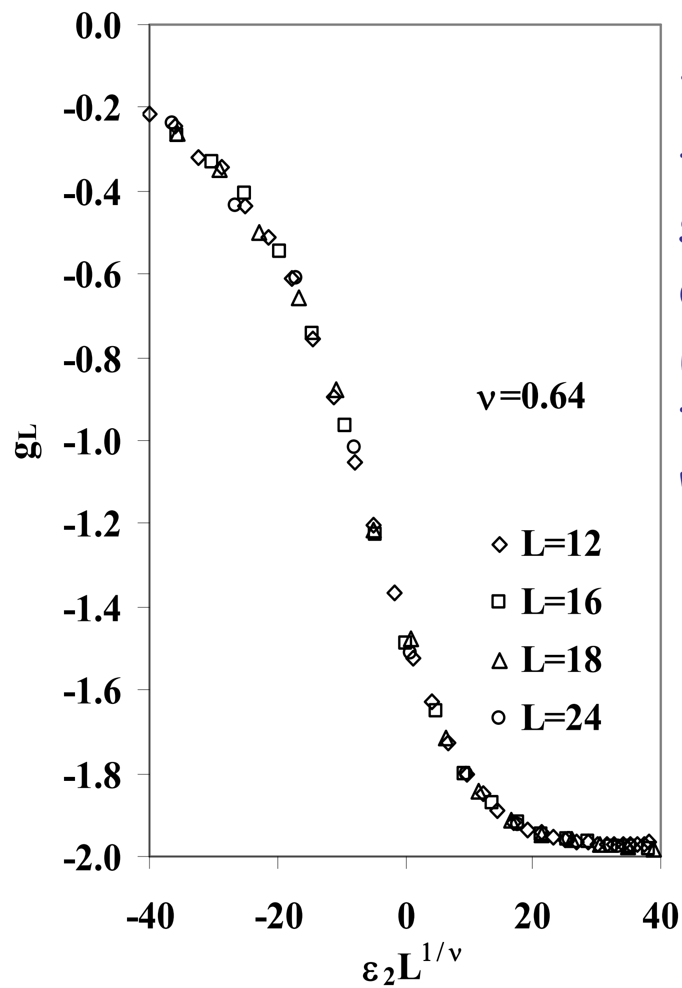
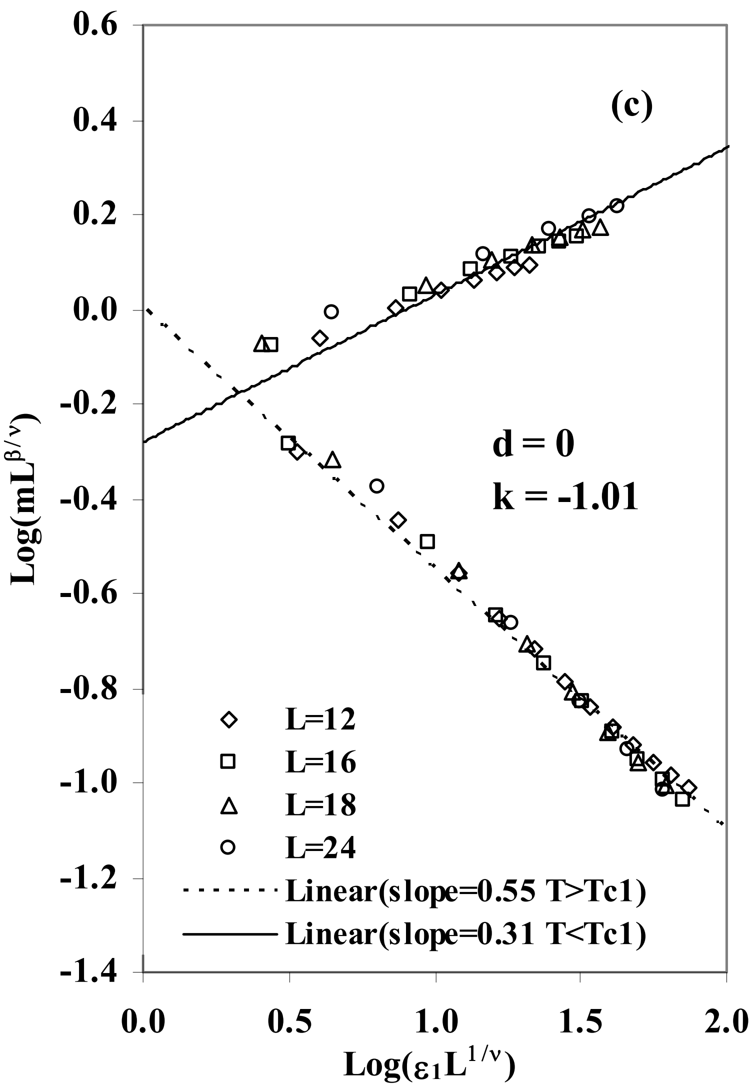


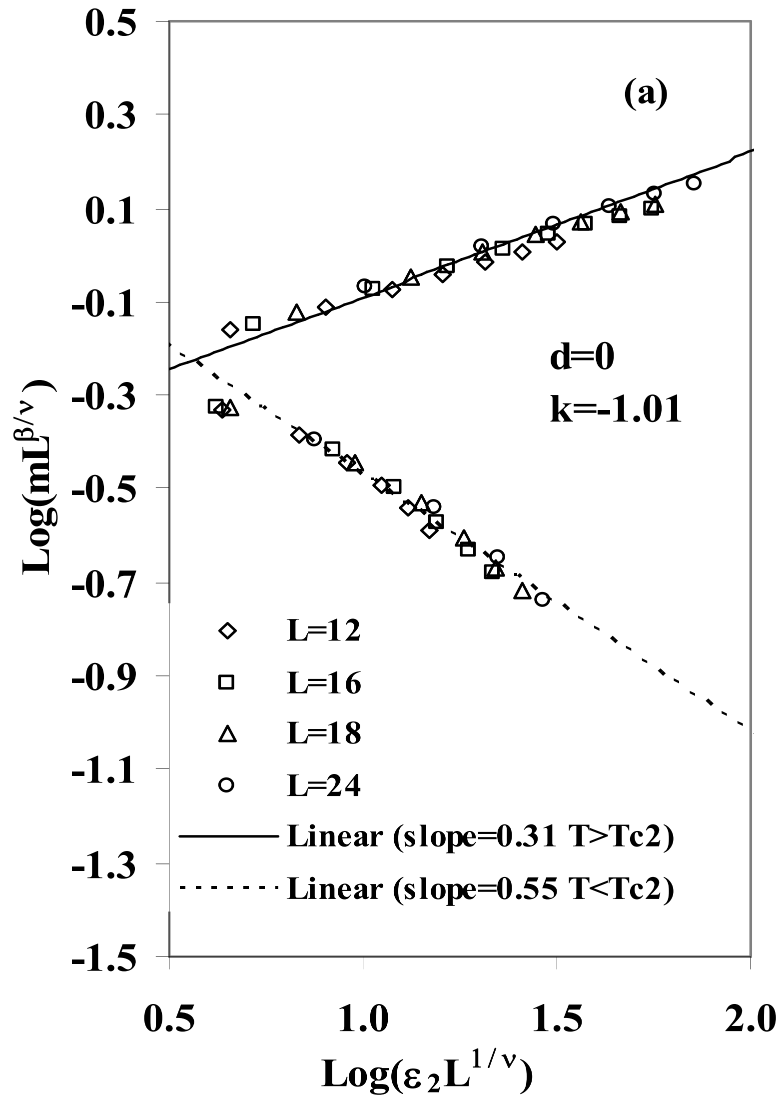
for the F→Q PT

The scaling data for the finite-size lattices lies on a single curve near the critical temperatures when ν=0.64

exponent β: $m = L^{-\beta/\nu} X(\varepsilon L^{1/\nu})$

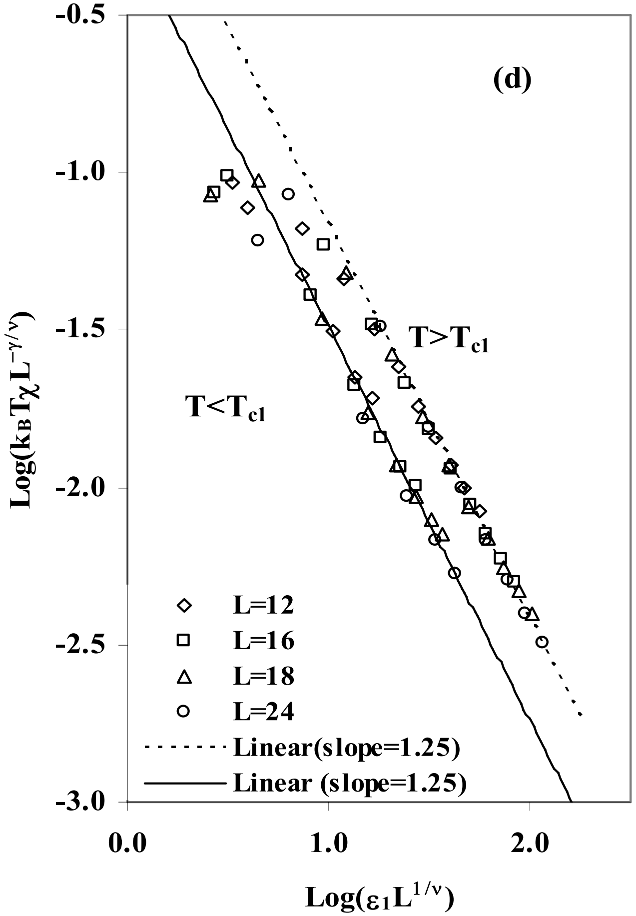


for the Q→F PT

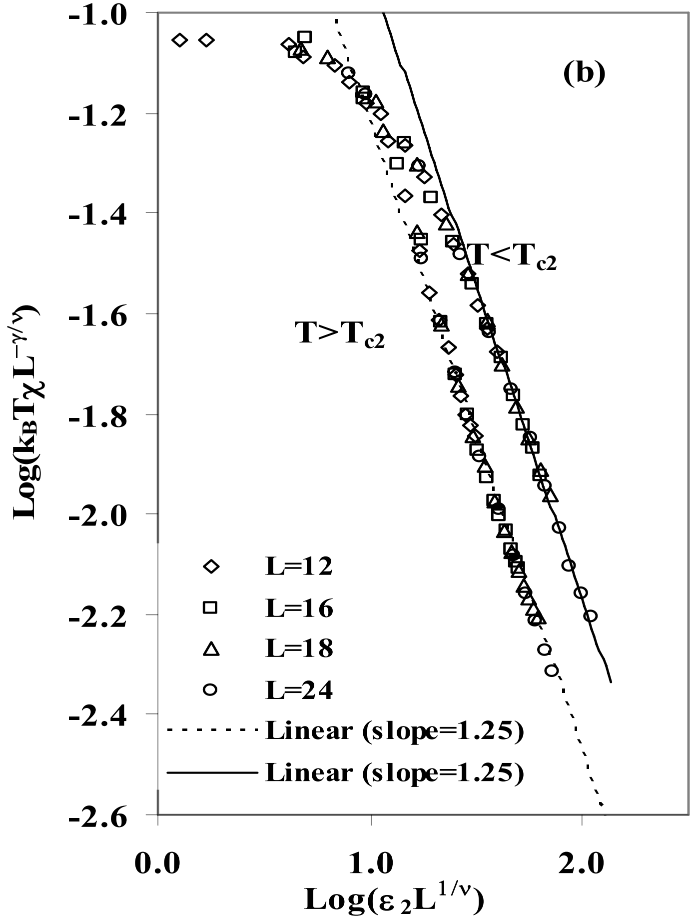


for the F→Q PT

exponent γ : $kT\chi = L^{\gamma/\nu} Y(\varepsilon L^{1/\nu})$



for the Q→F PT



for the F→Q PT

For the all continous Q $\rightarrow$F PT, the estimated values of critical exponents are equal to universal values (β=0.31, γ=1.25, α=0.12, ν = 0.64)

Thank you for your attention!