Extension of DMRG to 3D classical lattice models

(phase diagram of the 3D ANNNI model)

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http://aulimo.phys.sci.kobe-u.ac.jp/Leiden/seminar.pdf

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1. Tensor Product Variational Approach (TVPA)

For simplicity, let us consider the 3D Ising model.

Our aim is to compute

$$T|\Psi\rangle = \lambda_{\max}|\Psi\rangle$$
$$\langle\Psi|T|\Psi\rangle = \lambda_{\max}\langle\Psi|\Psi\rangle$$

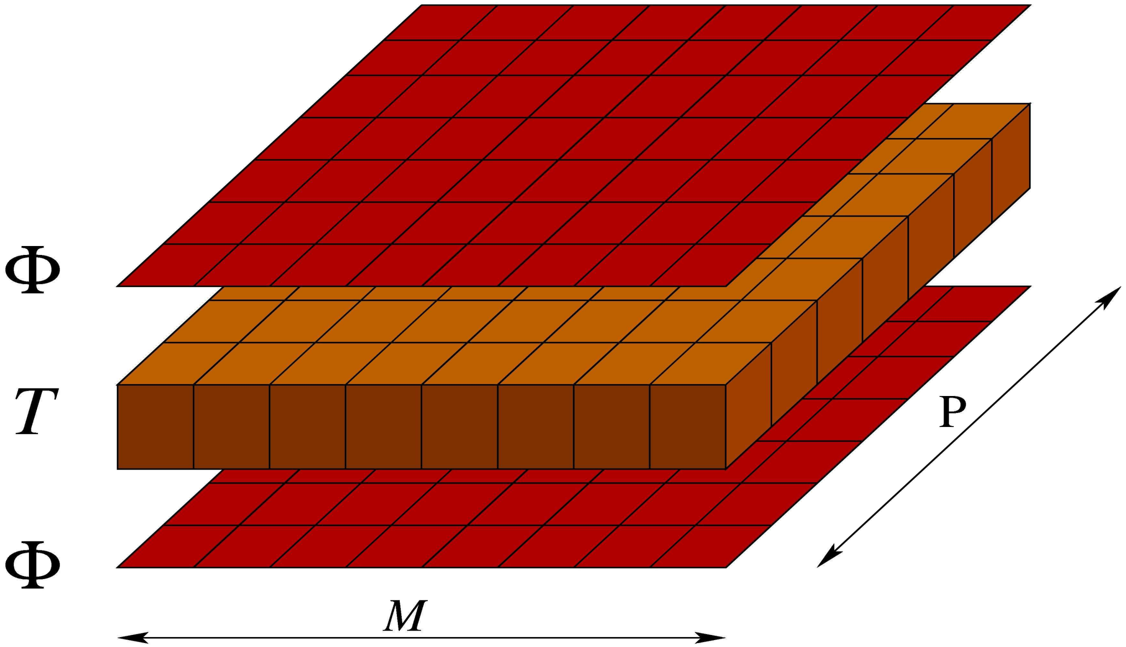
with the transfer matrix dimension: 2^{MP}**.**

Assuming an arbitrary trial function $|\Phi\rangle$ ***, we can write the relation***

$$\lambda_{\max} \geq \lambda_{\mathrm{var}} = \frac{\langle\Phi|T|\Phi\rangle}{\langle\Phi|\Phi\rangle}$$

A way to solve this non-trivial task is to study it from the variational point of view.

However, this is a hopelessly difficult task since the trial function contains 2^{MP} ***parameters.***



We introduce an approximation in order to decrease the number of parameters in the trial function $|\Phi\rangle$

$$|\Psi\rangle \approx |\Phi\rangle = \prod_{i=1}^{M}\prod_{j=1}^{P} V\left(\sigma_{i,j}\sigma_{i+1,j}\sigma_{i,j+1}\sigma_{i+1,j+1}\right) \equiv \prod_{i=1}^{M}\prod_{j=1}^{P} V_{i,j}$$

The number of parameters is decreased from 2^{MP} *down to* $2^4=16$.

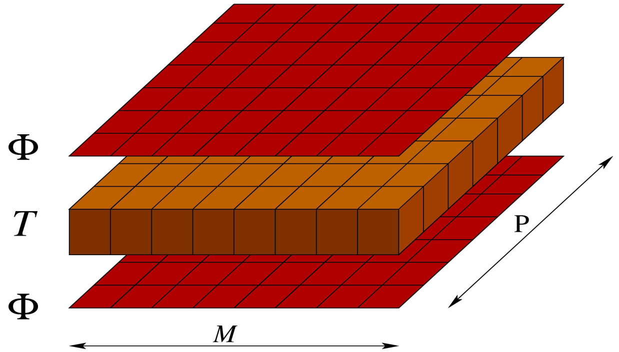
Here we assume the product of the equivalent *local variational weights* $V_{i,j}$ *(because of the translational invariance of the Ising model).*

The variational partition function (the so-called Raileigh ratio) can then be consequently simplified into the form:

$$\lambda_{\mathrm{var}} = \frac{\langle\Phi|T|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \frac{\sum_{\{\sigma\},\{\overline{\sigma}\}}\prod_{i=1}^{M}\prod_{j=1}^{P} V_{i,j} W_B^{i,j} \overline{V}_{i,j}}{\sum_{\{\sigma\},\{\overline{\sigma}\}}\prod_{i=1}^{M}\prod_{j=1}^{P} V_{i,j} \overline{V}_{i,j}}$$

2-layer system (2D)

1-layer system (2D)



Both expressions can be accurately calculated by means of DMRG (or CTMRG) as they represent two-dimensional classical lattice systems.

Simple algorithm: maximize λ_{var} *for given parameters in* $V_{i,j}$.

How to derive an algorithm which computes $V_{i,j}$ automatically?

In order to maximize λ_{var} , let us first consider its variation

$$\delta\,\lambda_{\text{var}} \equiv \sum_{i,j} \frac{\partial \lambda_{\text{var}}}{\partial V_{i,j}} \delta\, V_{i,j} + \sum_{i,j} \frac{\partial \lambda_{\text{var}}}{\partial \overline{V}_{i,j}} \delta\, \overline{V}_{i,j}$$

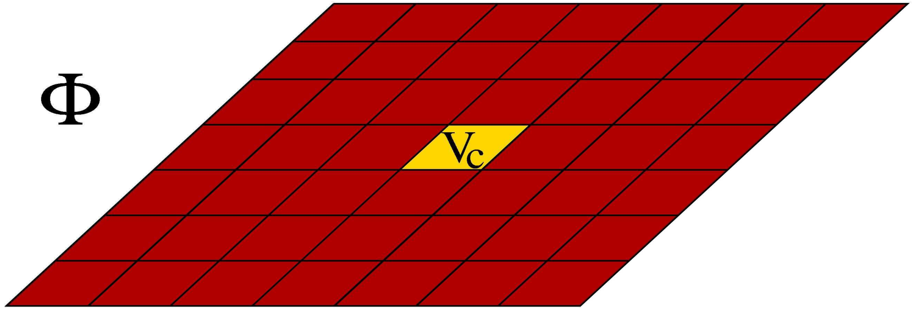
with respect to infinitesimal changes of $V_{i,j}$, i.e.,

$$V_{i,j} \rightarrow V_{i,j} + \delta\, V_{i,j} \quad \text{and} \quad \overline{V}_{i,j} \rightarrow \overline{V}_{i,j} + \delta\, \overline{V}_{i,j}$$

Suppose the lattice size is large enough. Most of the terms $\frac{\partial \lambda_{\text{var}}}{\partial V_{i,j}} \delta\, V_{i,j}$ are then identical because the boundary effects become negligible. For this reason, we can treat the variation of λ_{var} in the central part of the system.

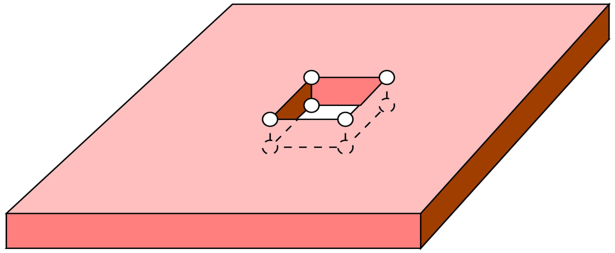
$$\delta_c\,\lambda_{\text{var}} \equiv \frac{\partial \lambda_{\text{var}}}{\partial V_c} \delta\, V_c + \frac{\partial \lambda_{\text{var}}}{\partial \overline{V}_c} \delta\, \overline{V}_c ,$$

where $V_c \equiv V_{M/2,P/2}$.



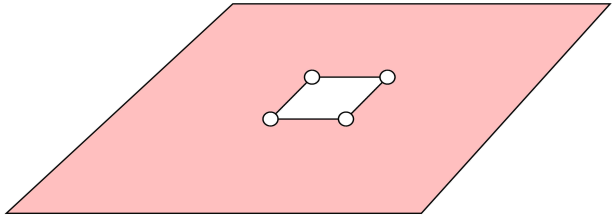
Let us write λ_{var} in terms of V_c and define the two new matrix functionals

$$B_c = W_B^c \sum_{\{\sigma\}'} \sum_{\{\overline{\sigma}\}'} \prod_{i\neq M/2} \prod_{j\neq P/2} V_{i,j} W_B^{i,j} \overline{V}_{i,j}$$



and

$$A_c = \sum_{\{\sigma\}'} \sum_{\{\overline{\sigma}\}'} \prod_{i\neq M/2} \prod_{j\neq P/2} V_{i,j} \overline{V}_{i,j}$$



With these matrix functionals, we can simplify the notation for the variational partition function λ_{var}.

Then, the numerator is $$\left\langle \Phi \middle| T \middle| \Phi \right\rangle = \sum_{\{\sigma_c\}} \sum_{\{\overline{\sigma}_c\}} V_c B_c \overline{V}_c \equiv \left(V_c \middle| B_c \middle| V_c \right)$$

and the denominator is $$\left\langle \Phi \middle| \Phi \right\rangle = \sum_{\{\sigma_c\}} \sum_{\{\overline{\sigma}_c\}} V_c A_c \overline{V}_c \equiv \left(V_c \middle| A_c \middle| V_c \right)$$

Inserting $\lambda_{\text{var}} = \dfrac{\left(V_c \middle| B_c \middle| V_c\right)}{\left(V_c \middle| A_c \middle| V_c\right)}$

into the expression $\delta_c\, \lambda_{\text{var}} \equiv \dfrac{\partial \lambda_{\text{var}}}{\partial V_c} \delta V_c + \dfrac{\partial \lambda_{\text{var}}}{\partial \overline{V}_c} \delta \overline{V}_c \overset{!}{=} 0$, ***we obtain***

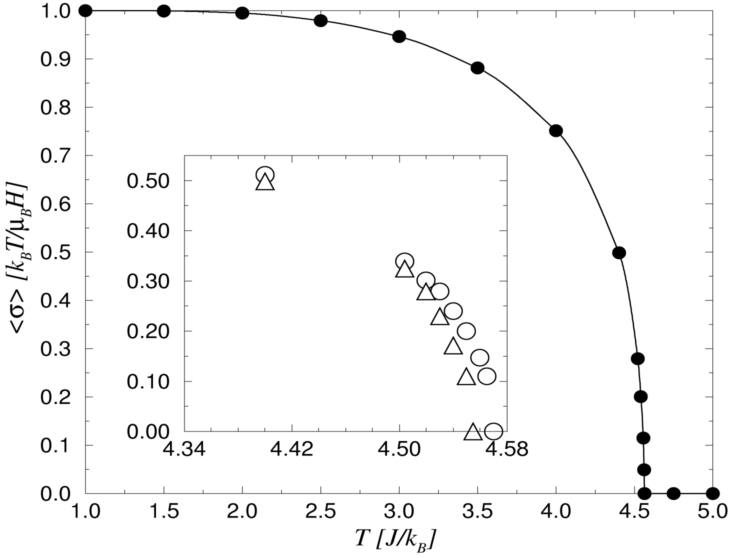
$\sum_{\{\sigma_c\}} B_c V_c = \lambda_{\text{var}} \sum_{\{\sigma_c\}} A_c V_c$ ***or in a simplified form as*** $\boxed{\dfrac{B_c}{A_c} \left| V_c \right) = \lambda_{\text{var}} \left| V_c \right)}$

It is a non-linear equation in terms of V because the matrix functionals themselves depend on V. It is a self-consistent equation and should be solved by means of consequent iterations.

We call this algorithm Tensor Product Variational Approach (TPVA).

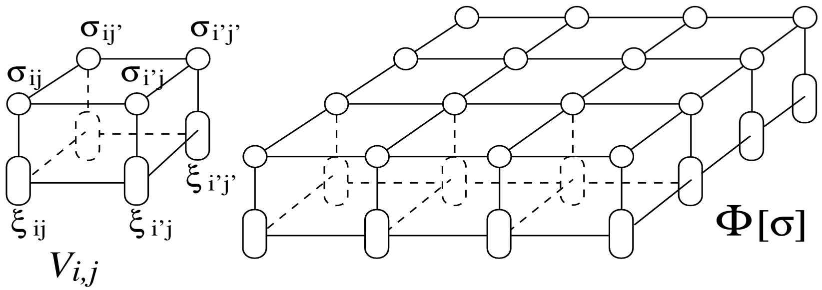
Example: 3D Ising and Potts models on the simple cubic lattice.

method	**type**	**T_c**	**rel. error**
TPVA	*Ising IRF*	***4.570***	***1.28%***
TPVA	*Ising vertex*	***4.533***	***0.47%***
TPVA	*3-state Potts*	***1.819***	***0.18%***
MC simul.	*IRF*	***4.512***	***---***



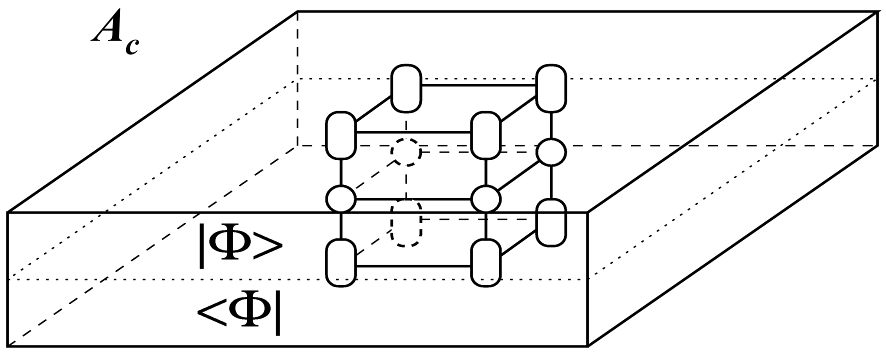
Auxiliary variables implemented in the local variational weight $V_{i,j}$

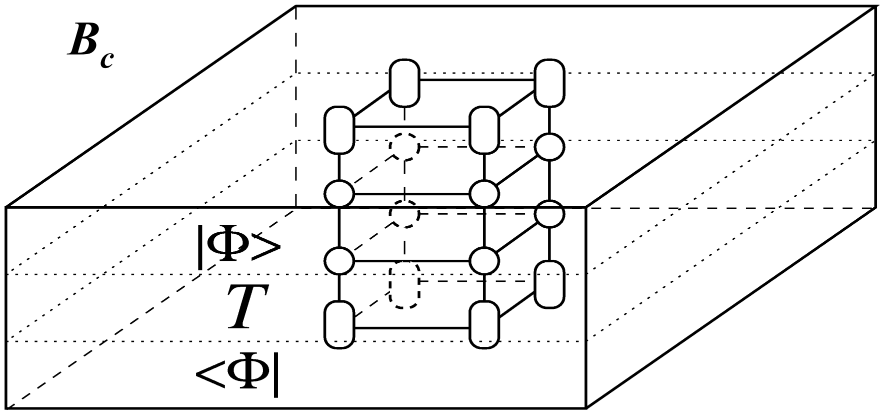
3D Ising model on a simple cubic lattice.



method	type	T_c	rel. error
TPVA	*IRF*	***4.570***	***1.28%***
TPVA aux.	*IRF*	***4.550***	***0.84%***
TPVA	*Vertex*	***4.533***	***0.47%***
TPVA aux.	*Vertex*	***4.525***	***0.29%***
MC simul.	*IRF*	***4.512***	***---***

Number of variational parameters: $(2n)^4$.





A. Gendiar, N. Maeshima, and T. Nishino, *Prog. Theor. Phys.* **110** (2003), 691

2. The ANNNI model

- *Axial Next-Nearest-Neighbor Ising (ANNNI) model with Hamiltonian*

$$H = -J_1 \sum_{\{i,j,k\}} (\sigma_{i,j,k}\sigma_{i+1,j,k} + \sigma_{i,j,k}\sigma_{i,j+1,k} + \sigma_{i,j,k}\sigma_{i,j,k+1}) + J_2 \sum_{\{i,j,k\}} \sigma_{i,j,k}\sigma_{i+2,j,k}$$

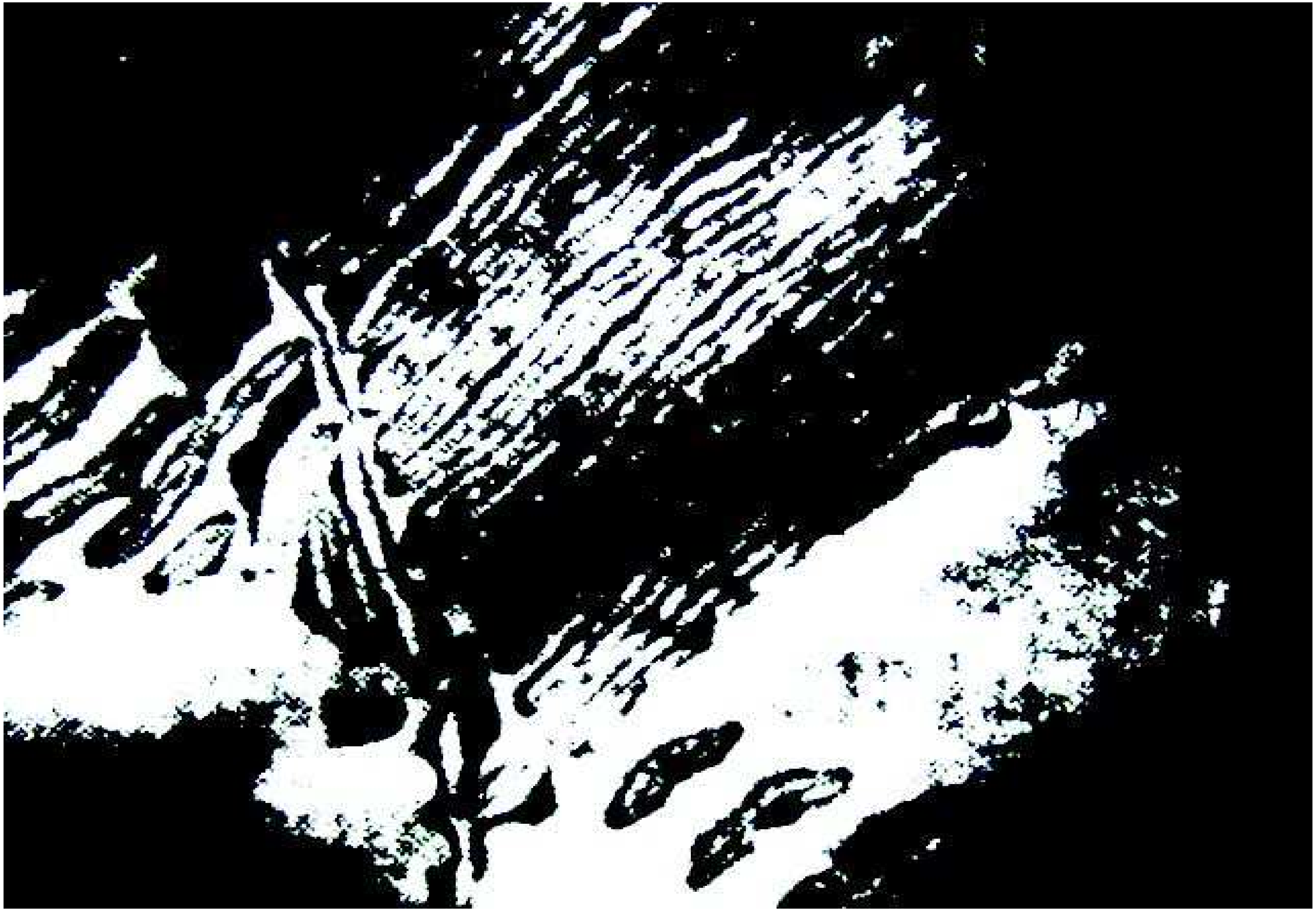
- *Invented by Elliott (1961) in order to describe the modulated magnetic structures of erbium.*

- *There are no "exact" theories of the global phase diagram neither in 2D nor in 3D.*

- *Although the model is too simple to mimic real systems, it does reproduce most of the features encountered in experiment.*

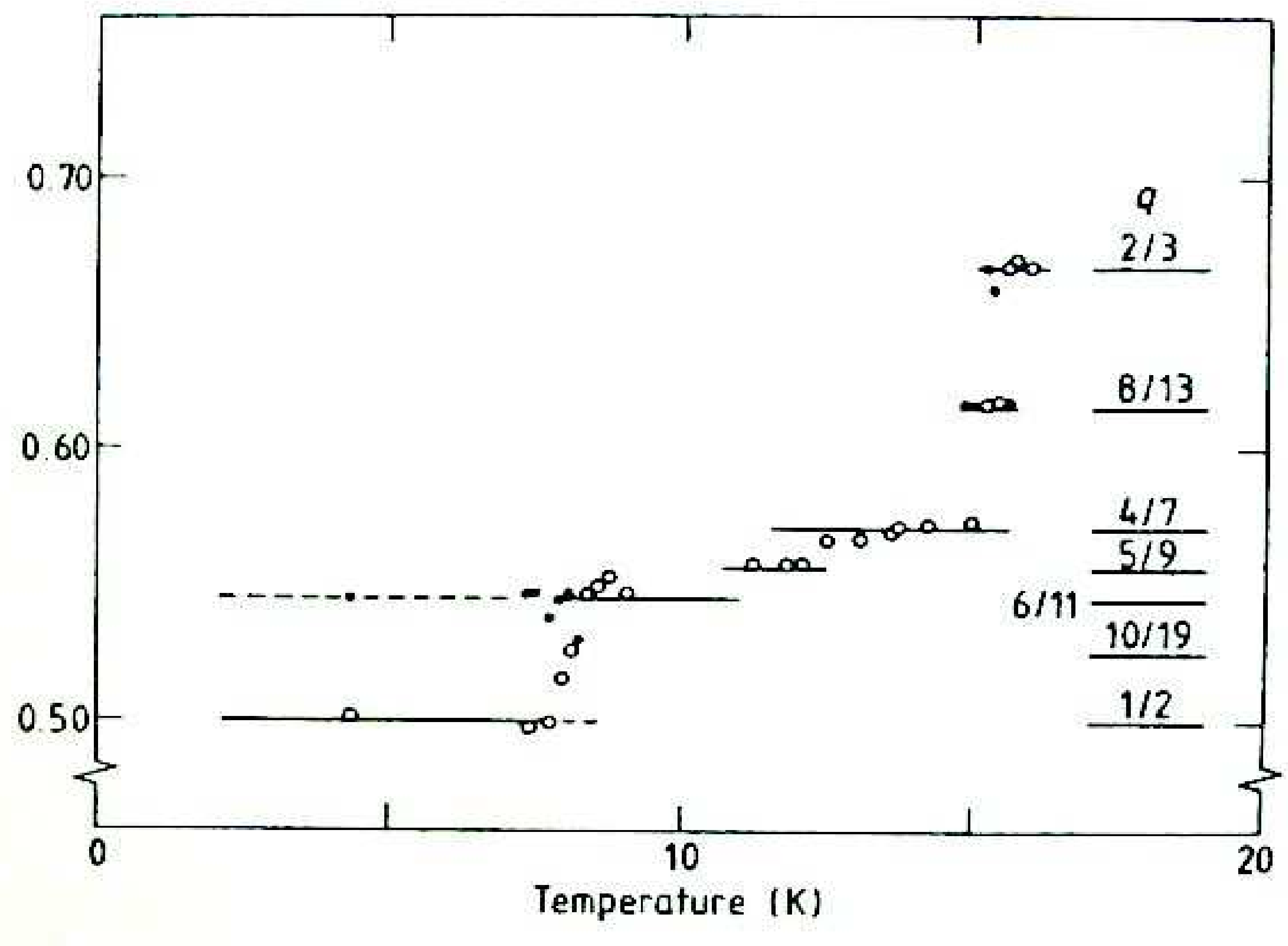
- *The 3D ANNNI model exhibits*
  - * *ferromagnetic (ordered) phase*
  - * *paramagnetic (disordered) phase*
  - * *low-order commensurate (periodic) phases*
  - * *high-order commensurate phases*
  - * *truly incommensurate phase*

Incommensurate system



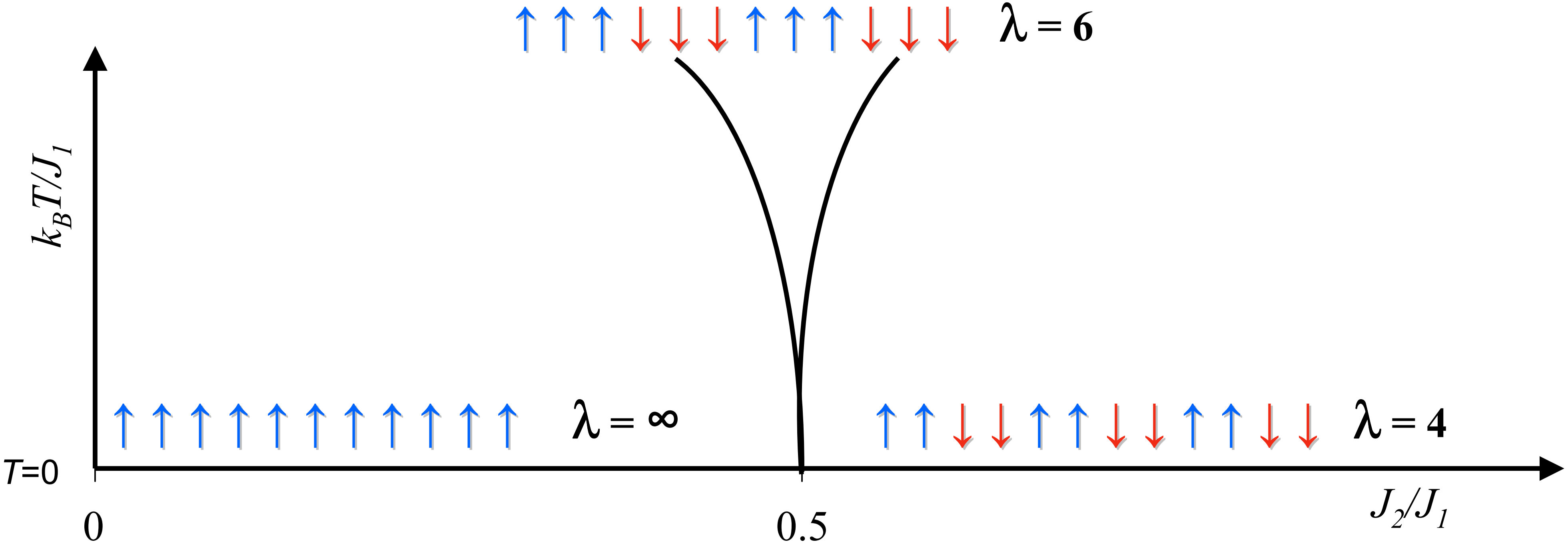
Electron microscope picture of domain wall structure in 2H-TaSe$_2$

- *Fisher et al. (1978) found the temperature dependence of the wave vector for CeSb, where the wave vector jumps between multitude of commensurate values*



Known features of the ANNNI model at T=0

- *Ferromagnetic structure* ↑↑↑↑ *for* $J_2 / J_1 < 0.5$
- *Anti-phase structure* ↑↑↓↓ *for* $J_2 / J_1 > 0.5$
- *A highly degenerated spin structure for* $J_2 / J_1 = 0.5$ *consists of successive* ↑ *and* ↓ *domains separated by walls perpendicular to the direction of competing interactions (an infinity of commensurate phases is possible)*



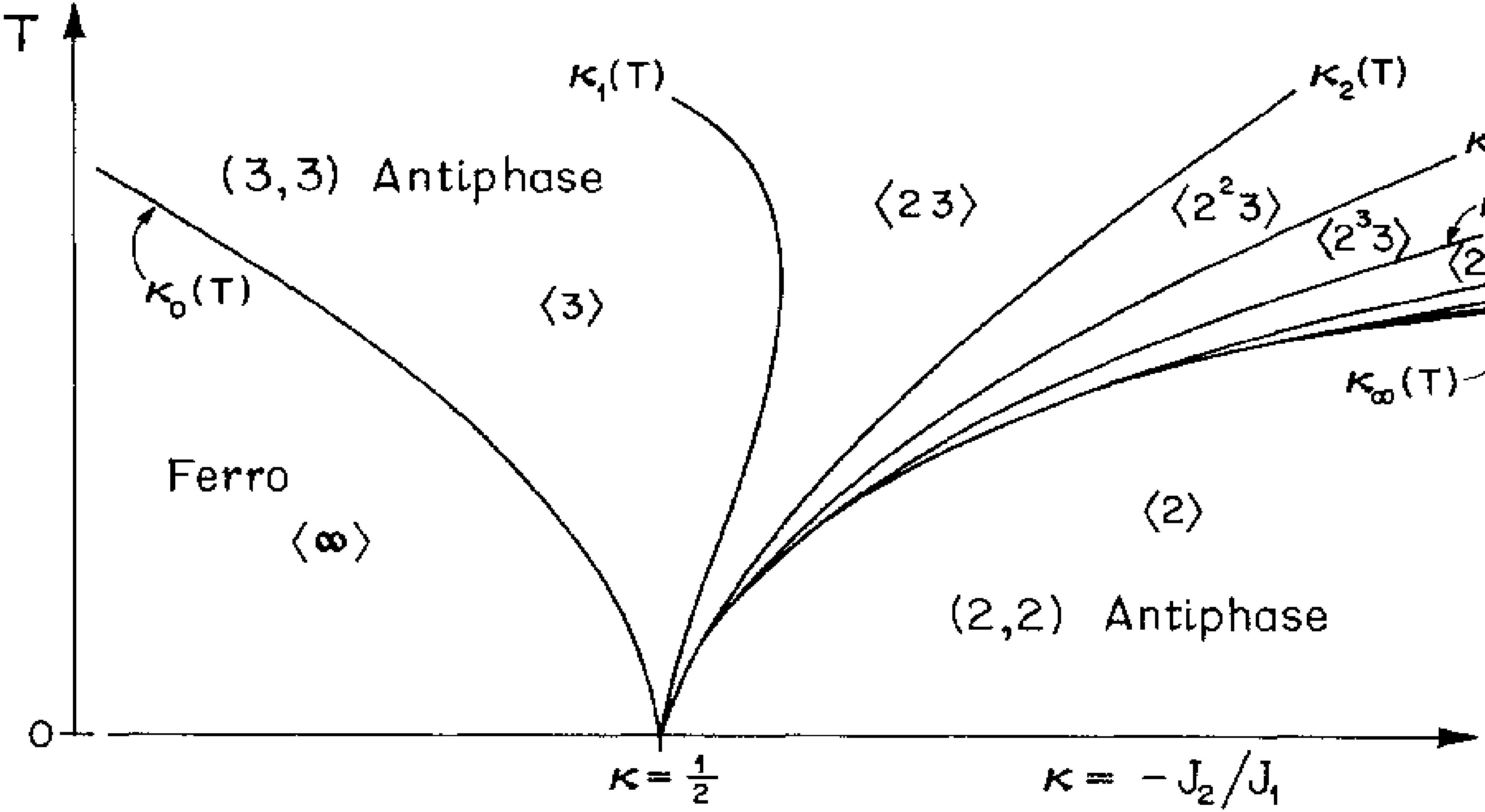
Notations: wavelength λ *with corresponding wave vector* $q = \dfrac{2\pi}{\lambda}$

- *Ferromagnetic phase* ↑↑↑↑↑↑↑↑↑↑↑↑ $\lambda=\infty$
- *Anti-phase structure* ↑↑↓↓↑↑↓↓↑↑↓↓ $\lambda=4$ or **<2>**
- *Commensurate phase* ↑↑↑↓↓↓↑↑↑↓↓↓ $\lambda=6$ or **<3>**
- *Commensurate phase* ↑↑↓↓↑↑↓↓↑↑↑ $\lambda=22/5$ or **<2^4,3>**
- *Commensurate phase* ↑↑↓↓↑↑↓↓↓↑↑↓↓↑↑↑ $\lambda=32/7$ or **<2^3,3,2^2,3>**

M. Fisher and W. Selke, *Phys. Rev. Lett.* **44**, 1502 (1980)

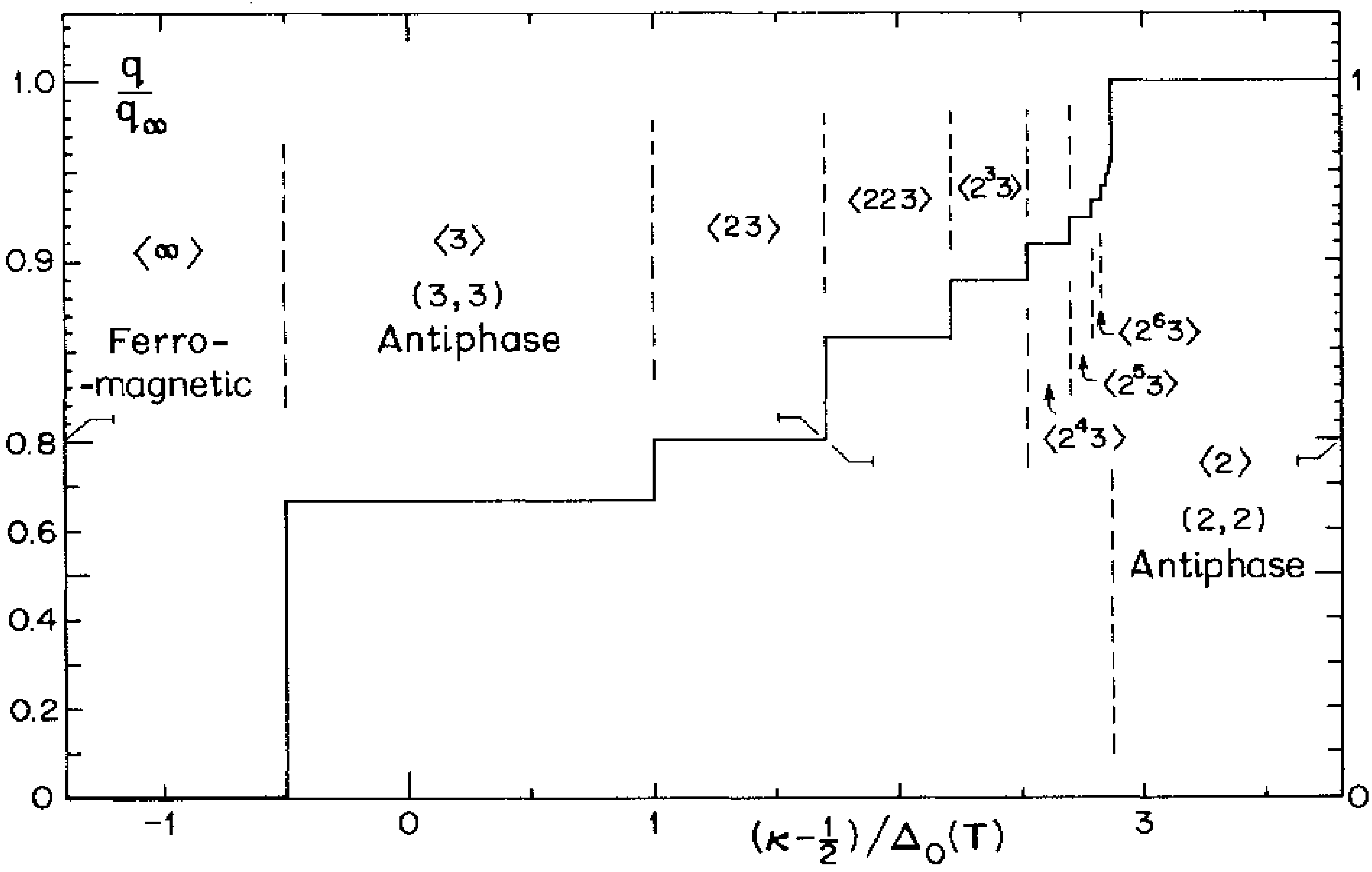
- low-temperature series expansions

$\langle 2^2 3 \rangle \equiv (2,2,3) \Rightarrow \cdots \uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\downarrow\cdots$



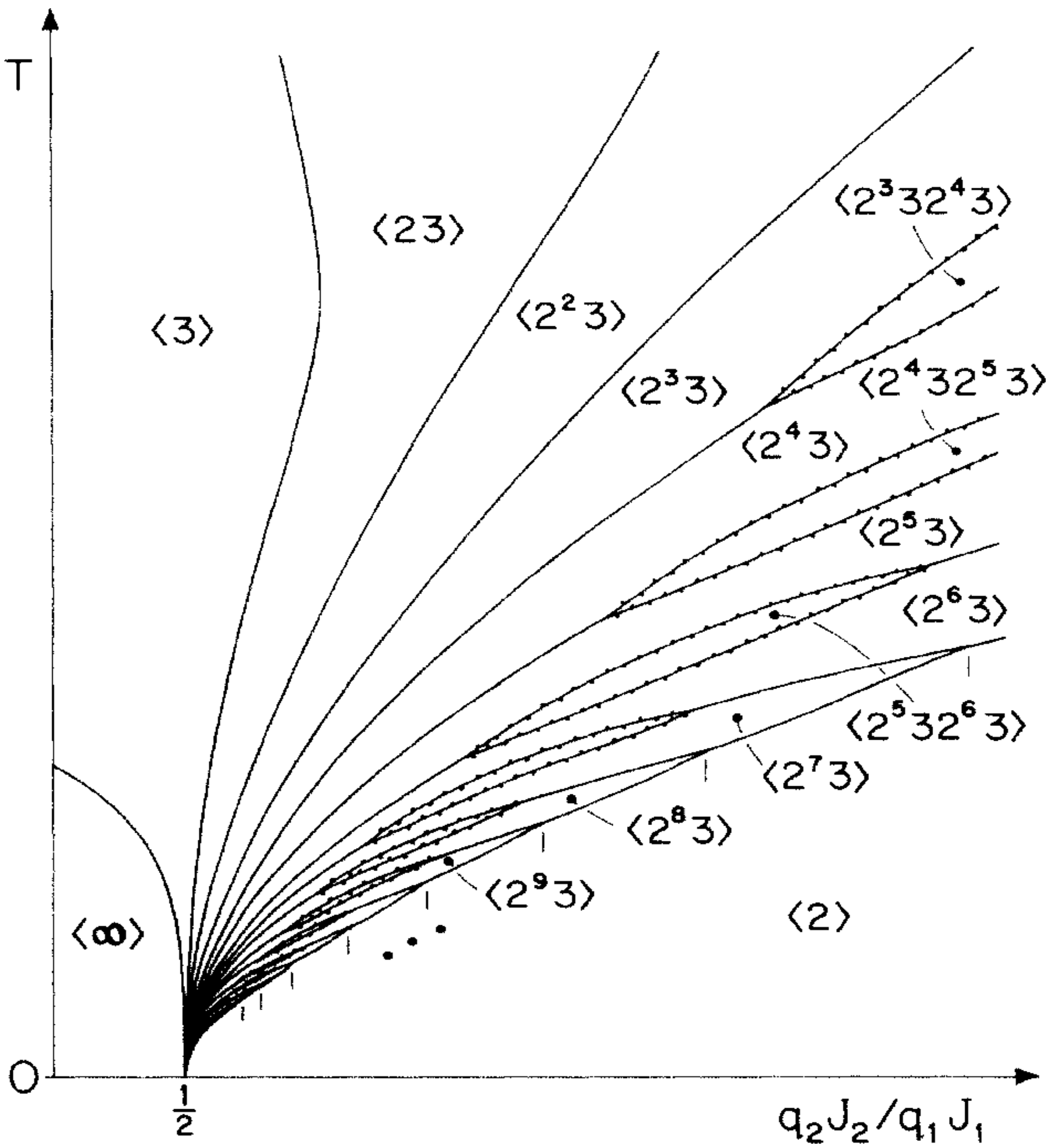
M. Fisher and W. Selke, *Phys. Rev. Lett.* **44**, 1502 (1980)

- * low-temperature series expansions



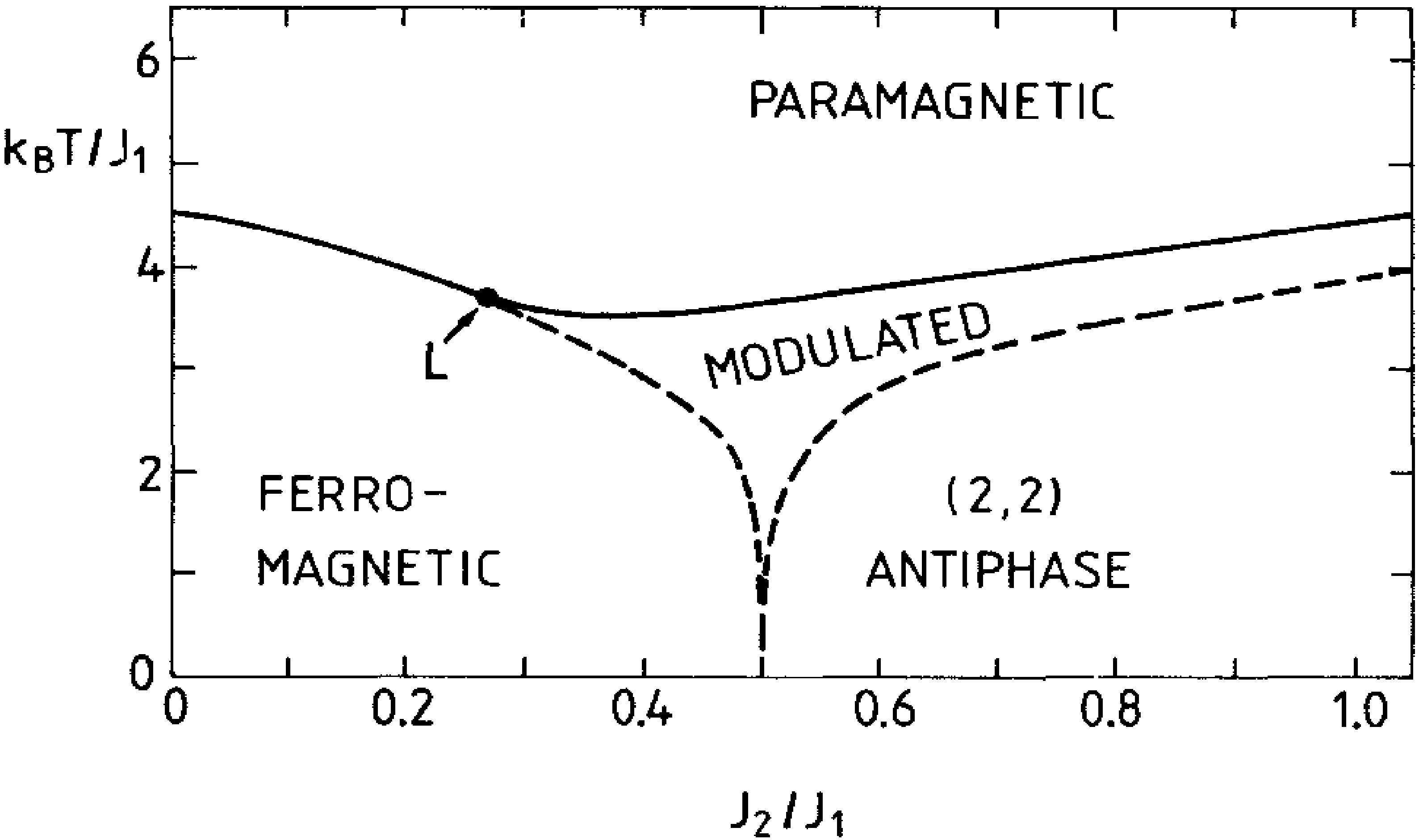
A. Szpilka and M. Fisher, *Phys. Rev. Lett.* **57**, 1044 (1986)

low-temperature series expansions



W. Selke and M. Fisher, *Phys. Rev. B* **20**, 257 (1979)
K. Kaski and W. Selke, *Phys. Rev. B* **31**, 3128 (1985)

Monte Carlo studies of C-I transition in 3D ANNNI model
* wave vector jumps (many computational difficulties)



High-temperature series expansions – *Lifshitz point*

S. Redner and H.E. Stanley, *J. Phys. C: Solid State Phys.* **10** (1977) 4756

S. Redner and H.E. Stanley, *Phys. Rev. B* **16** (1977) 4901

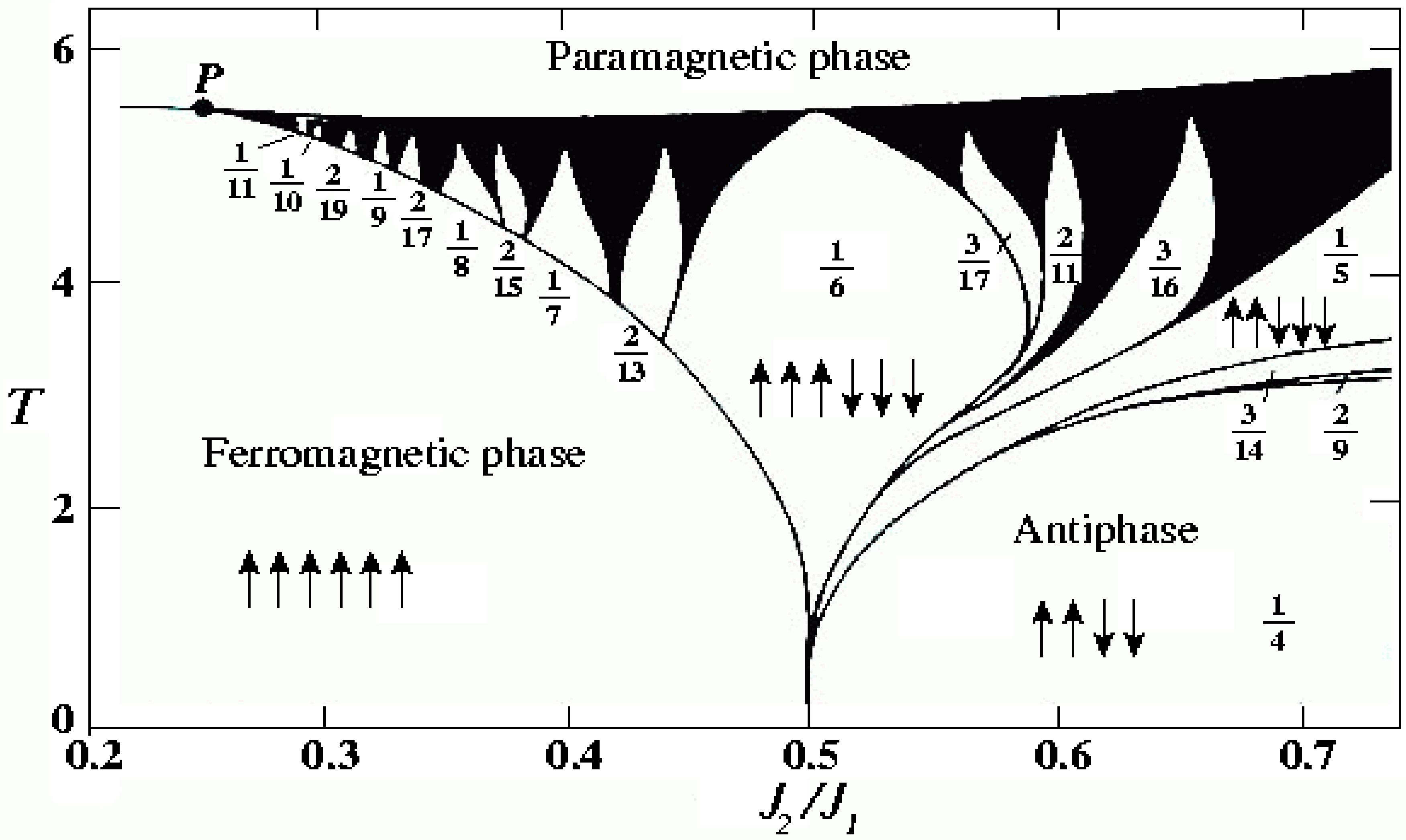
Monte Carlo simulations

(critical exponent calculations at the Lifshitz point)

M. Pleimling and M. Henkel, *Phys. Rev. Lett.* **87** (2001) 125702
W. Selke, M. Pleimling and D. Cartain, *Eur. Phys. J. B* **27** (2002) 321

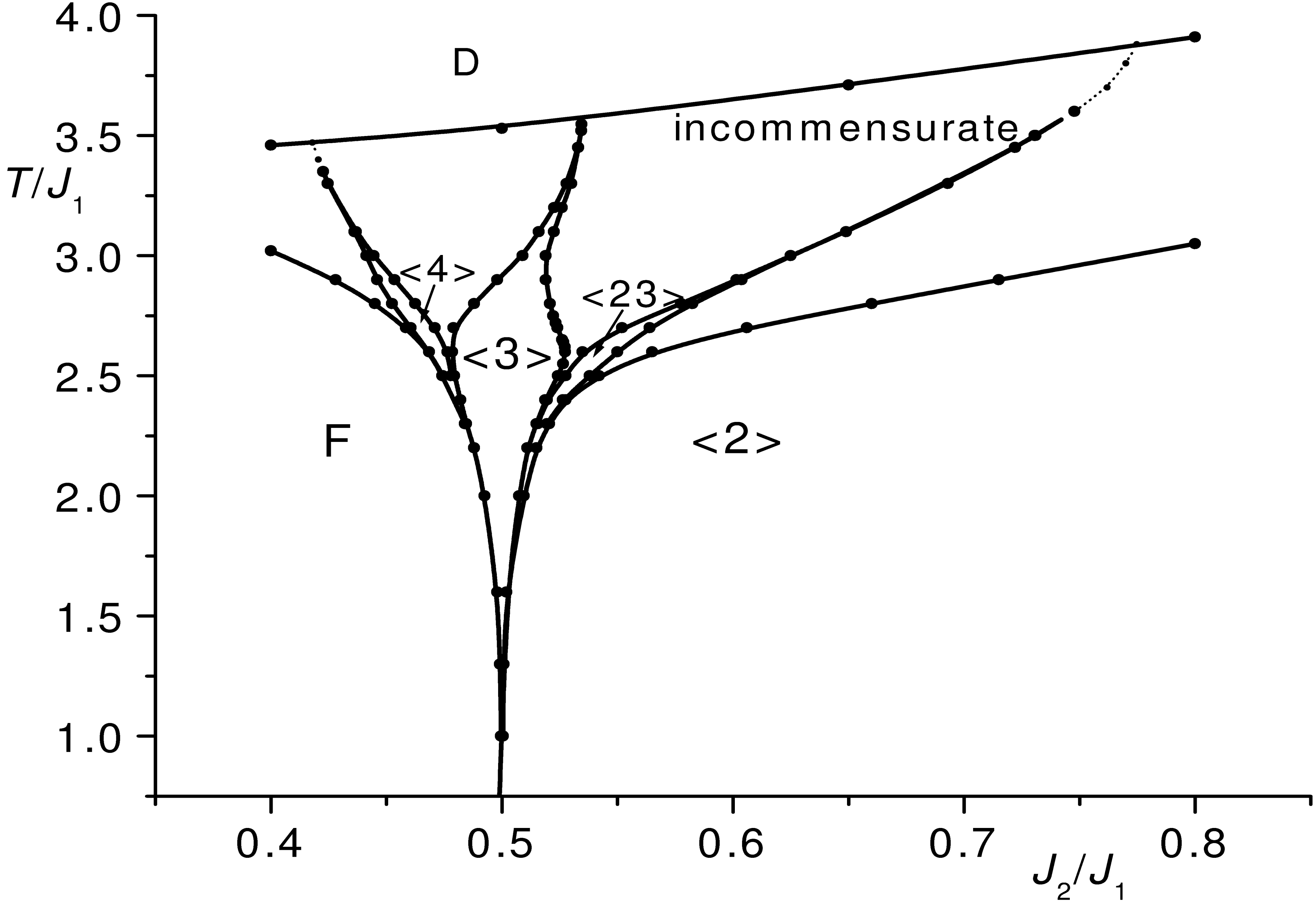
P. Bak and J. von Boehm, *Phys. Rev. B* **21** (1980) 5297

* Mean-field calculations



A. Šurda, *Phys. Rev. B* **69** (2004) 134116

Effective field approximation (the cluster transfer matrix method)



3. Application of TPVA to the ANNNI model

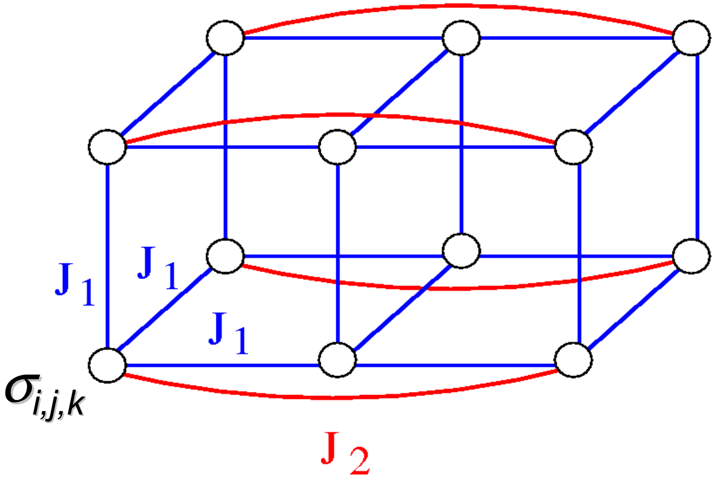
3D ANNNI model on a simple cubic lattice with size $N \times \infty \times \infty$

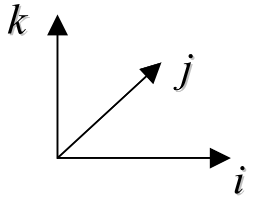
$$H = -J_1 \sum_{\{i,j,k\}} (\sigma_{i,j,k}\sigma_{i+1,j,k} + \sigma_{i,j,k}\sigma_{i,j+1,k} + \sigma_{i,j,k}\sigma_{i,j,k+1}) + J_2 \sum_{\{i,j,k\}} \sigma_{i,j,k}\sigma_{i+2,j,k}$$

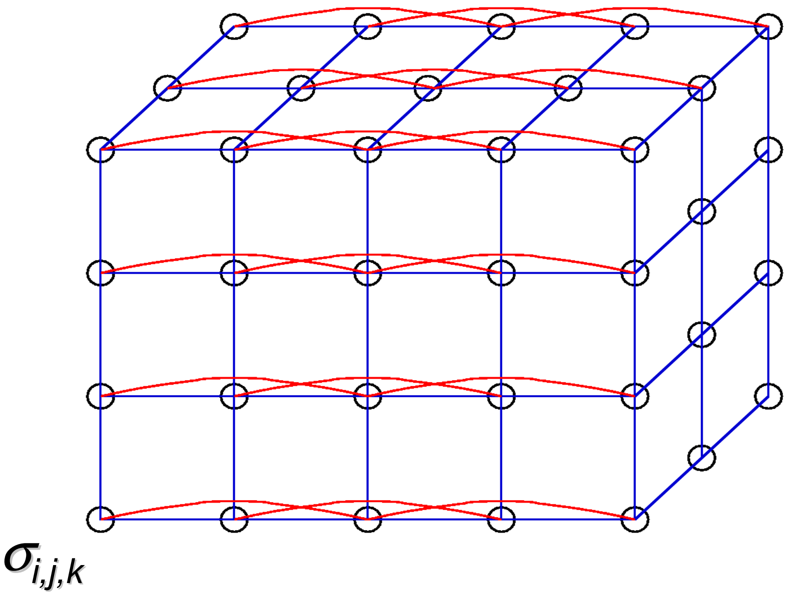
$\sigma_{i,j,k} = \pm 1$ (↑↓)

J_1 – ferromagnetic interaction

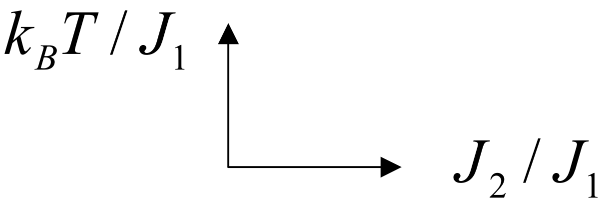
J_2 – antiferromagnetic interaction







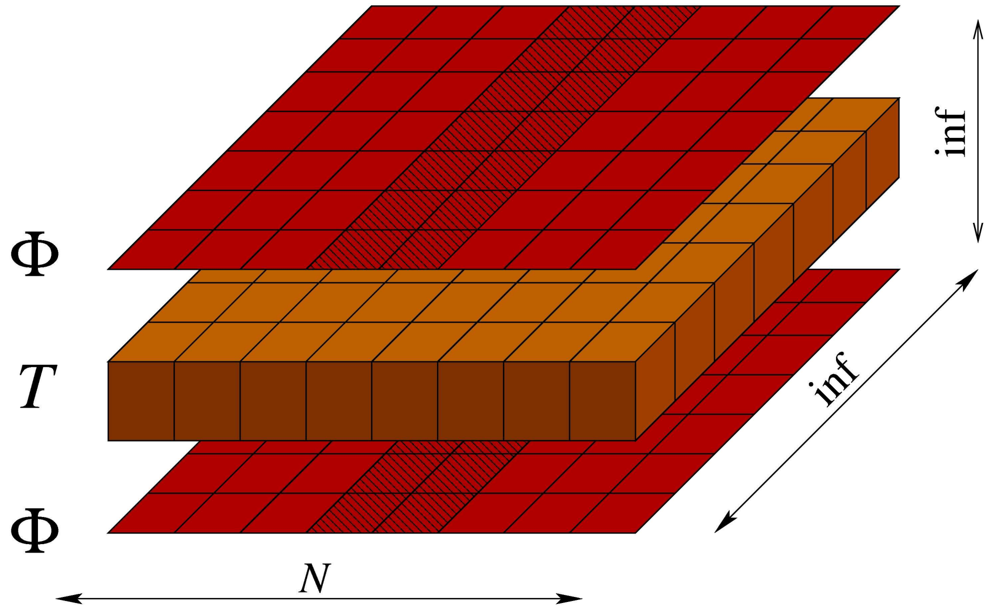
Boltzmann weight $W = \exp\left[-\frac{H(J_1, J_2)}{k_B T} \right]$

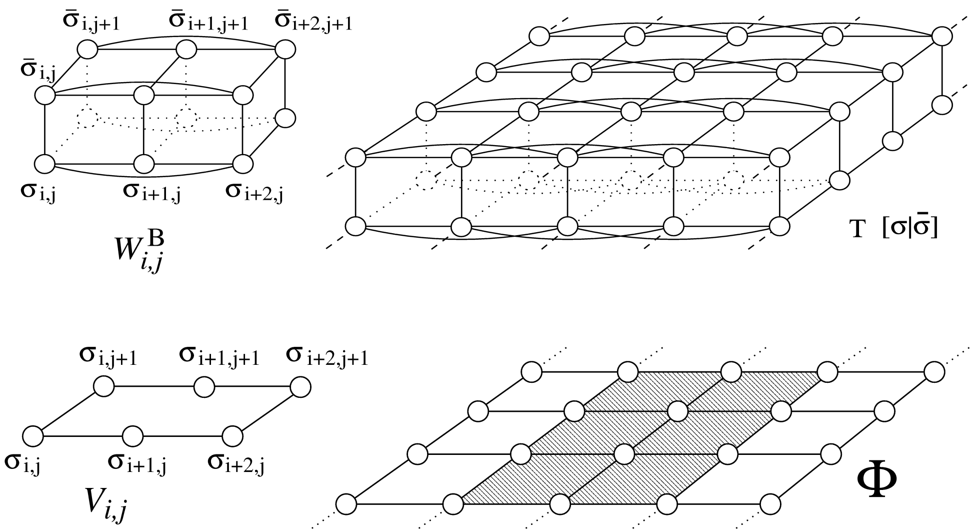


The aim is to maximize the variational partition function $\lambda_{\max}$

$$\lambda_{\max} = \frac{\langle \Phi \,|\, T \,|\, \Phi \rangle}{\langle \Phi \,|\, \Phi \rangle} = \frac{\sum\limits_{[\sigma],[\sigma']} \prod\limits_{i=1}^{N} \prod\limits_{j=-\infty}^{+\infty} V_{i,j}\{\sigma\} W^{B}_{i,j}\{\sigma|\sigma'\} V_{i,j}\{\sigma'\}}{\sum\limits_{[\sigma]} \prod\limits_{i=1}^{N} \prod\limits_{j=-\infty}^{+\infty} V_{i,j}\{\sigma\} V_{i,j}\{\sigma\}}$$

and calculate the free energy $f = -\frac{1}{N} k_B T \ln \lambda_{\max}$ ***and magnetization*** $\langle \sigma_i \rangle = \langle \Phi | \sigma_i | \Phi \rangle$

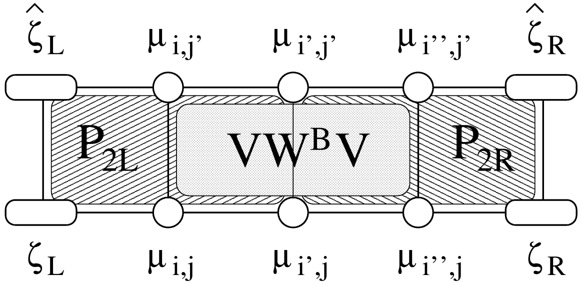


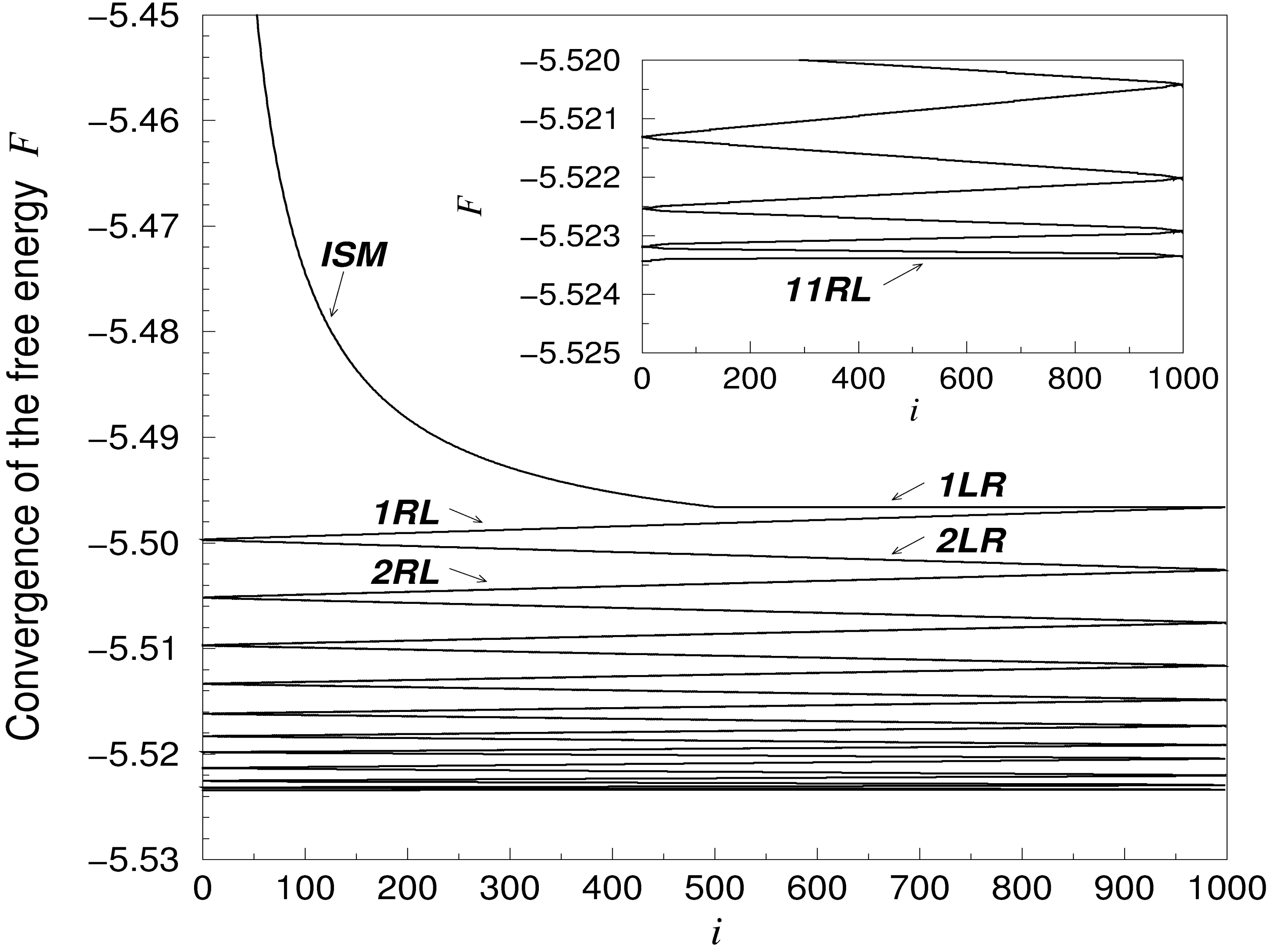


Convergence process of the TPVA

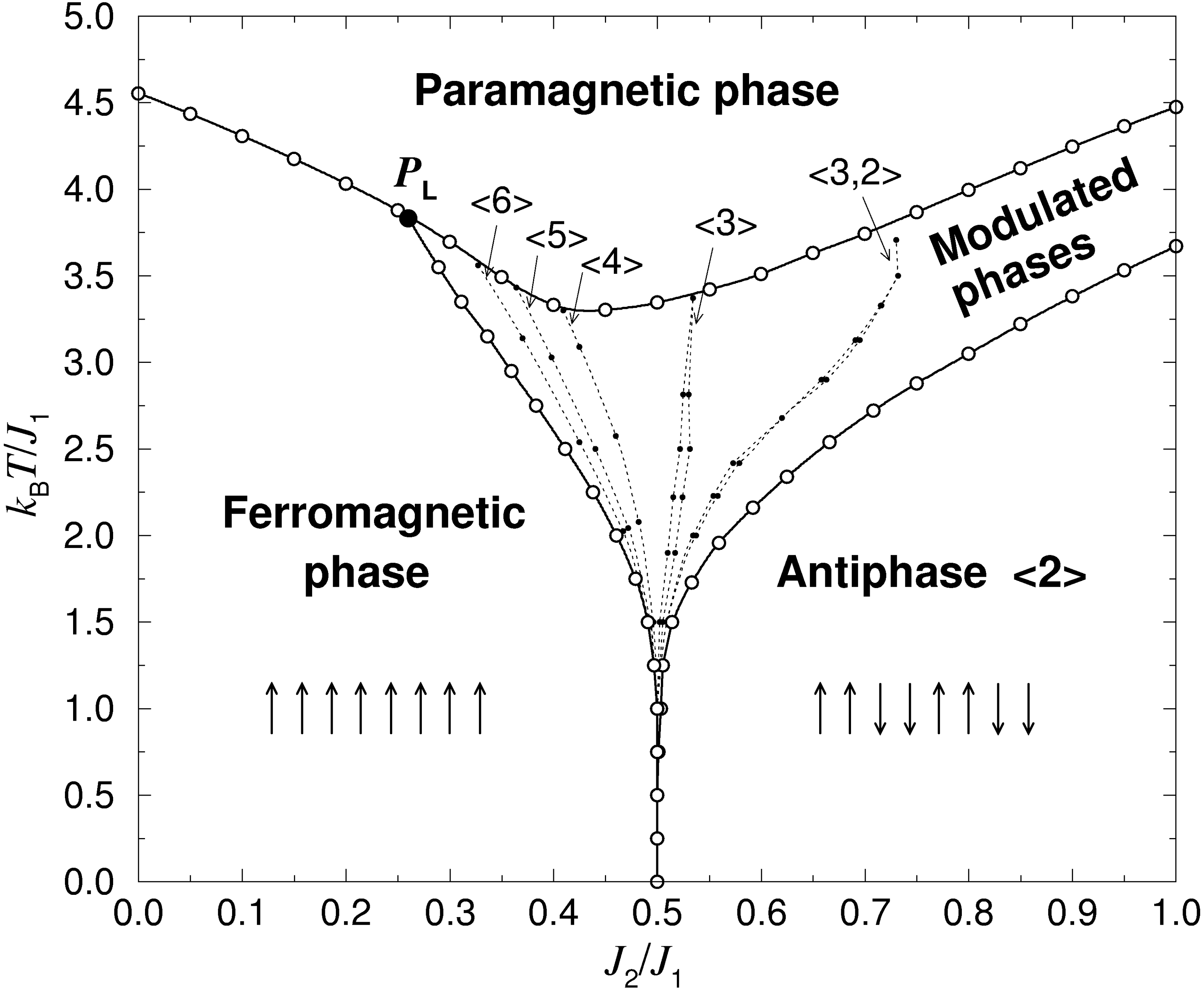
Infinite System Method (ISM)

Finite System Method (FSM)

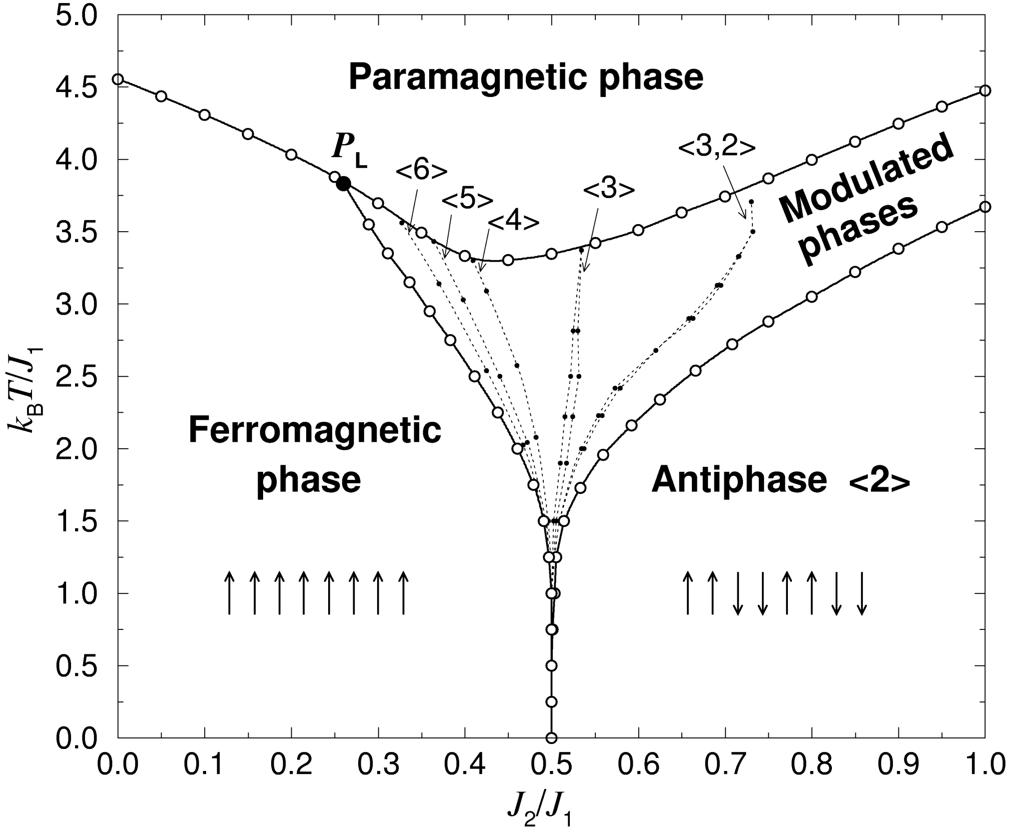




4. *Phase diagram of the 3D ANNNI model*



TPVA



Critical point (Ising):

$T_c\ (J_2/J_1) = 4.554 \quad (\varepsilon = 0.9\%)$

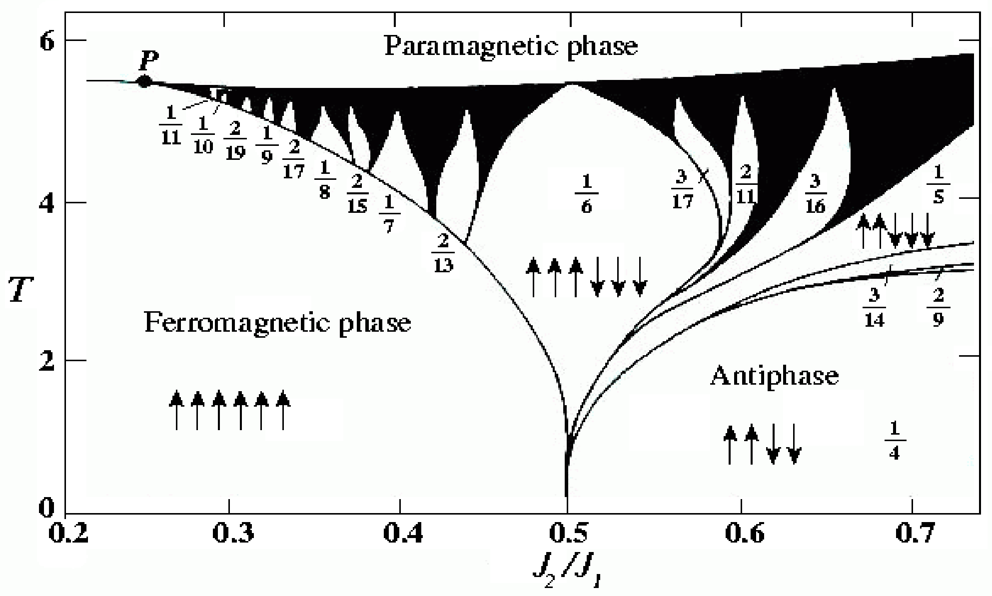
Lifshitz point (by TPVA):

$P_L = (J_2/J_1 = 0.26\ ;\ k_BT/J_1 = 3.83)$

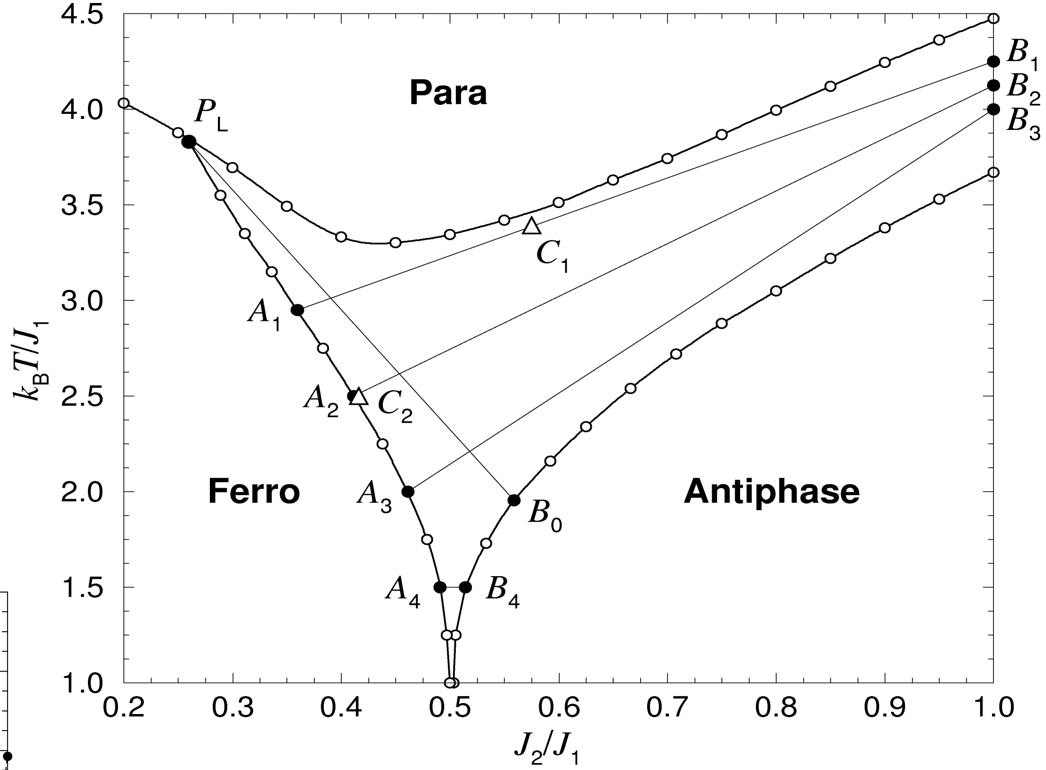
Lifshitz point (by MC, Henkel 2002):

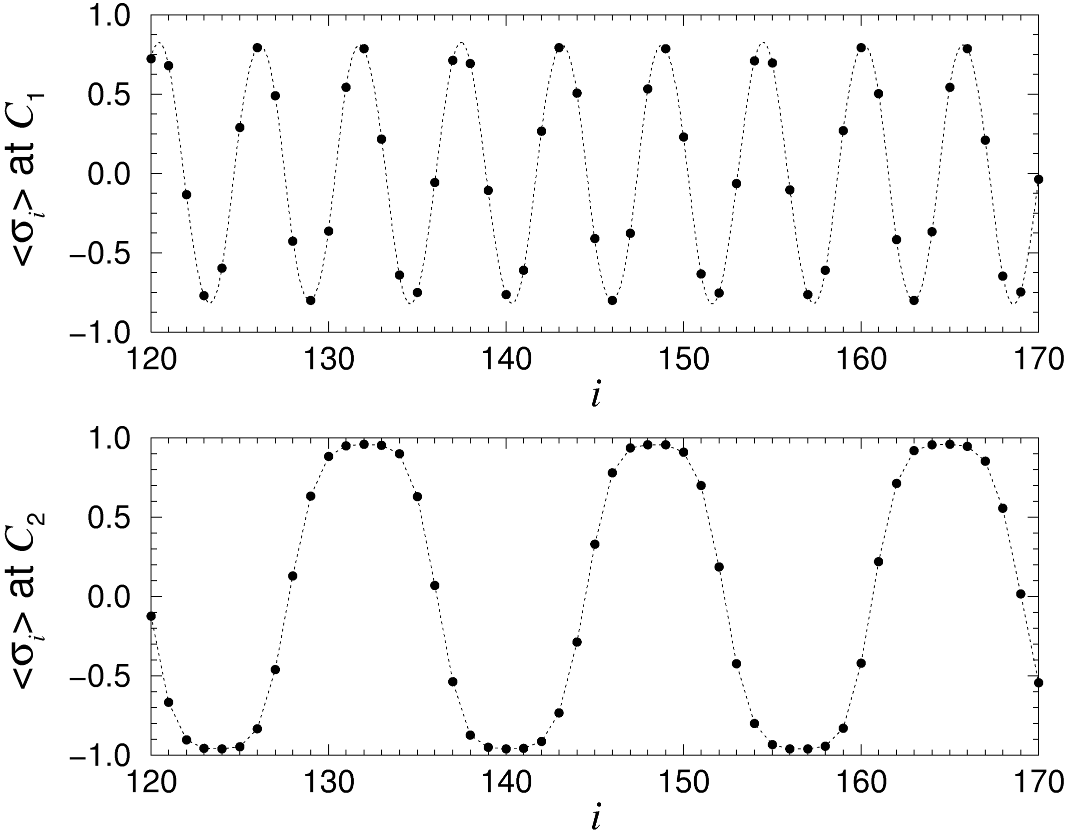
$P_L = (J_2/J_1 = 0.27\ ;\ k_BT/J_1 = 3.75)$

The mean-field approximation



Applying Fourier transform to the spontaneous magnetization, we obtain the wavelength λ.

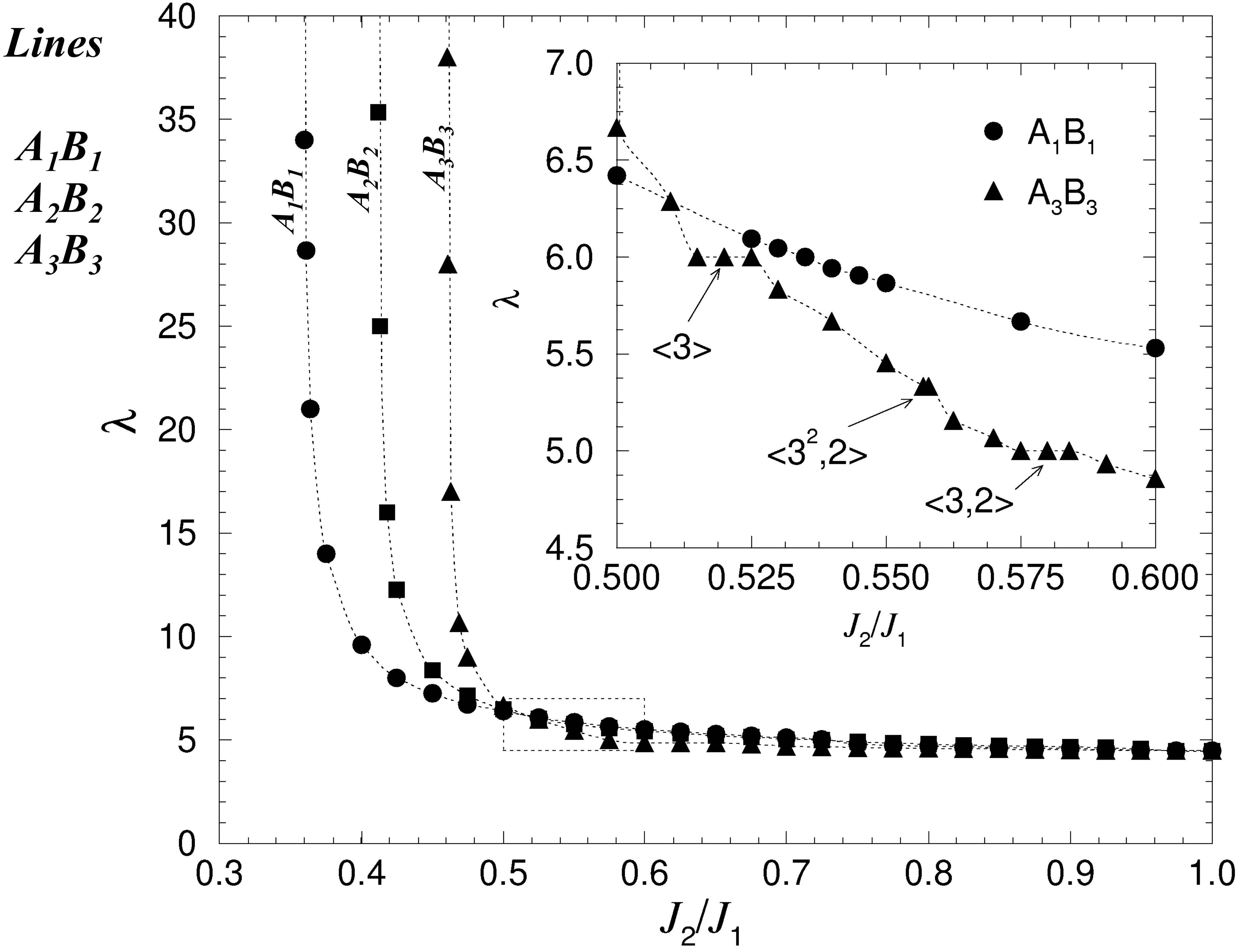


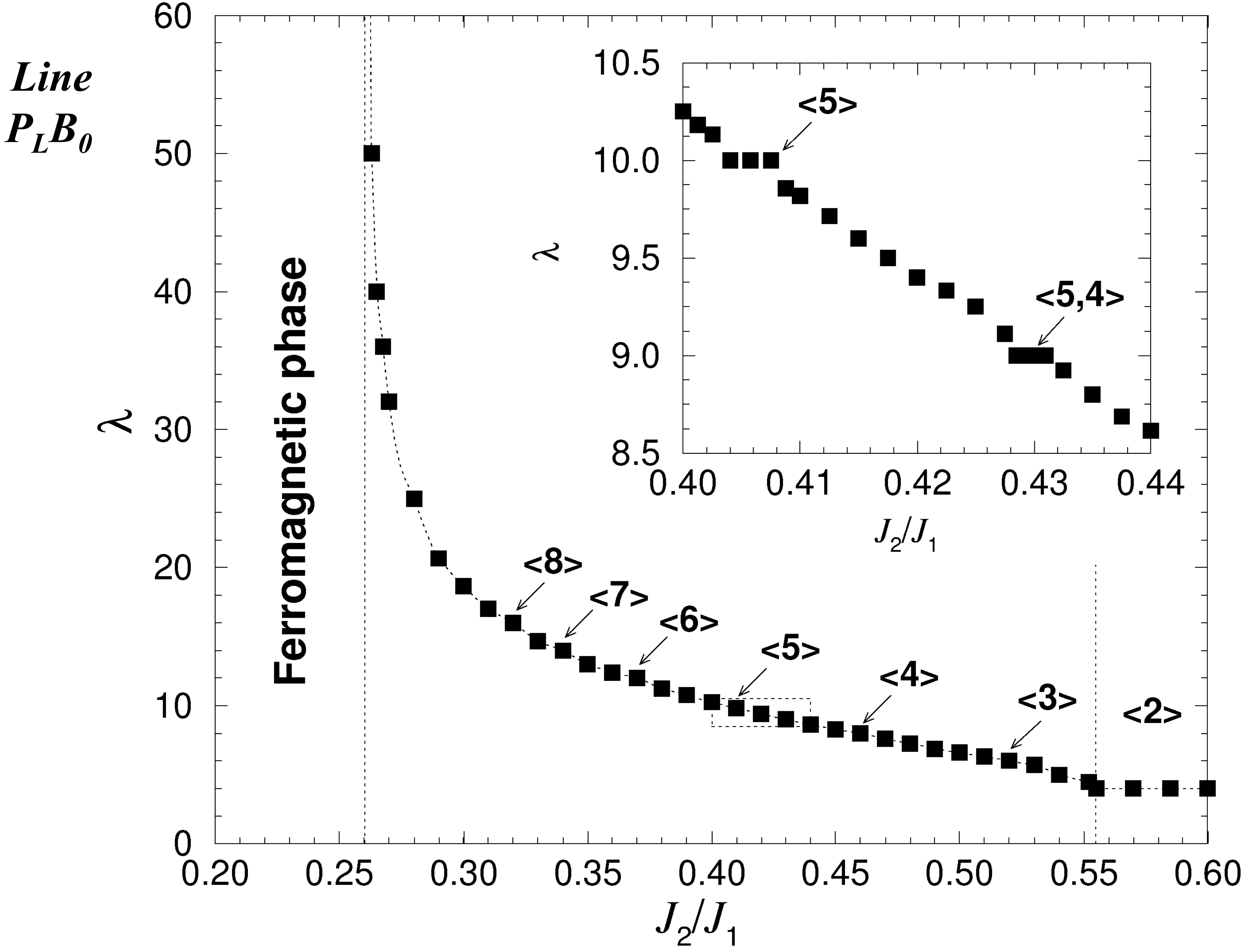


Lattice size: $401\times\infty\times\infty$

$\lambda\,(C_1) = 17/3 \quad < 2, 3^5 >$

$\lambda\,(C_2) = 16.7$


Lines
A1B1
A2B2
A3B3
λ
J2/J1
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0
5
10
15
20
25
30
35
40
A1B1
A2B2
A3B3
λ
J2/J1
0.500
0.525
0.550
0.575
0.600
4.5
5.0
5.5
6.0
6.5
7.0
A1B1
A3B3
<3>
<3^2,2>
<3,2>


Line
$P_L B_0$
Ferromagnetic phase
λ
60
50
40
30
20
10
0
0.20
0.25
0.30
0.35
0.40
0.45
0.50
0.55
0.60
J_2/J_1
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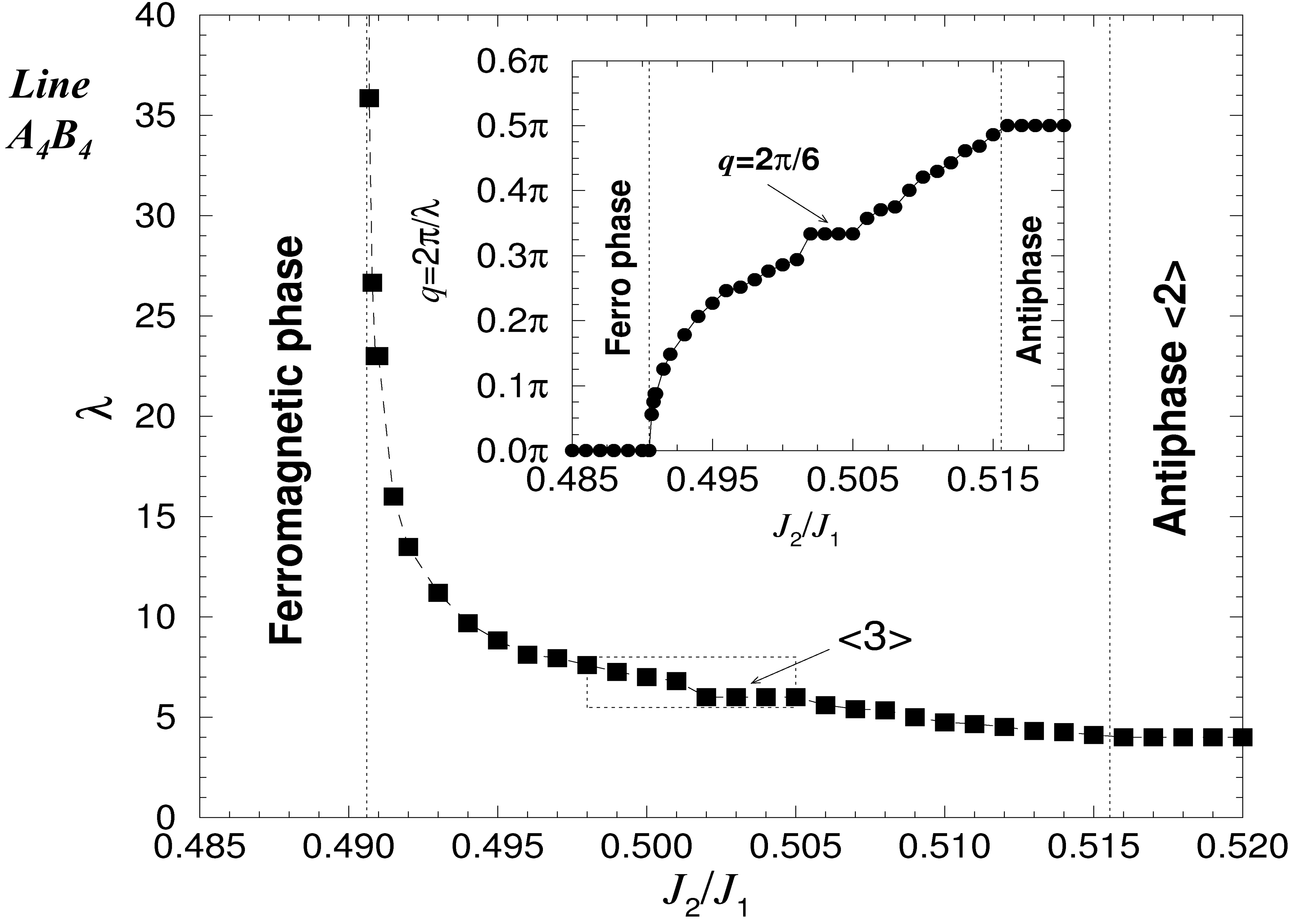
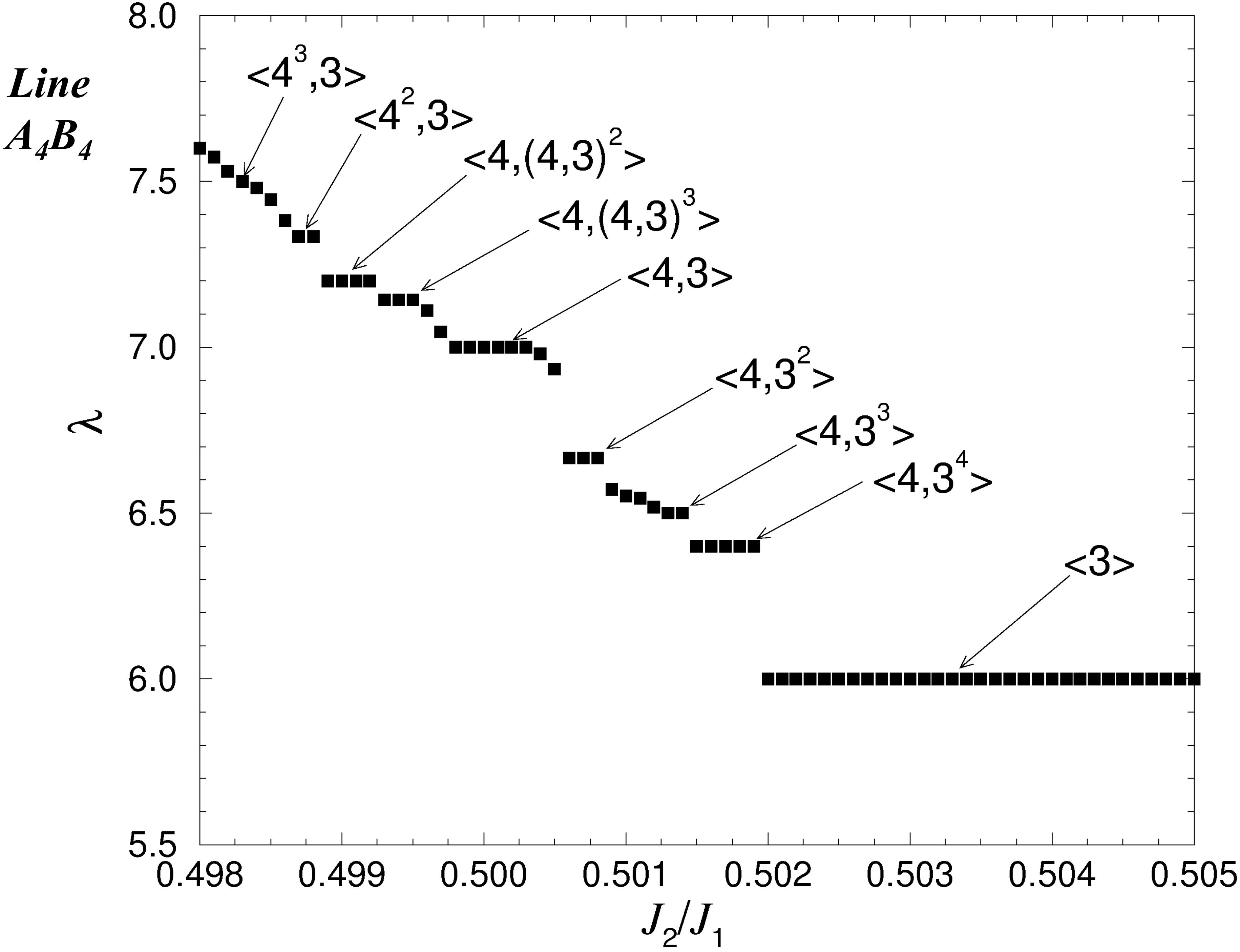
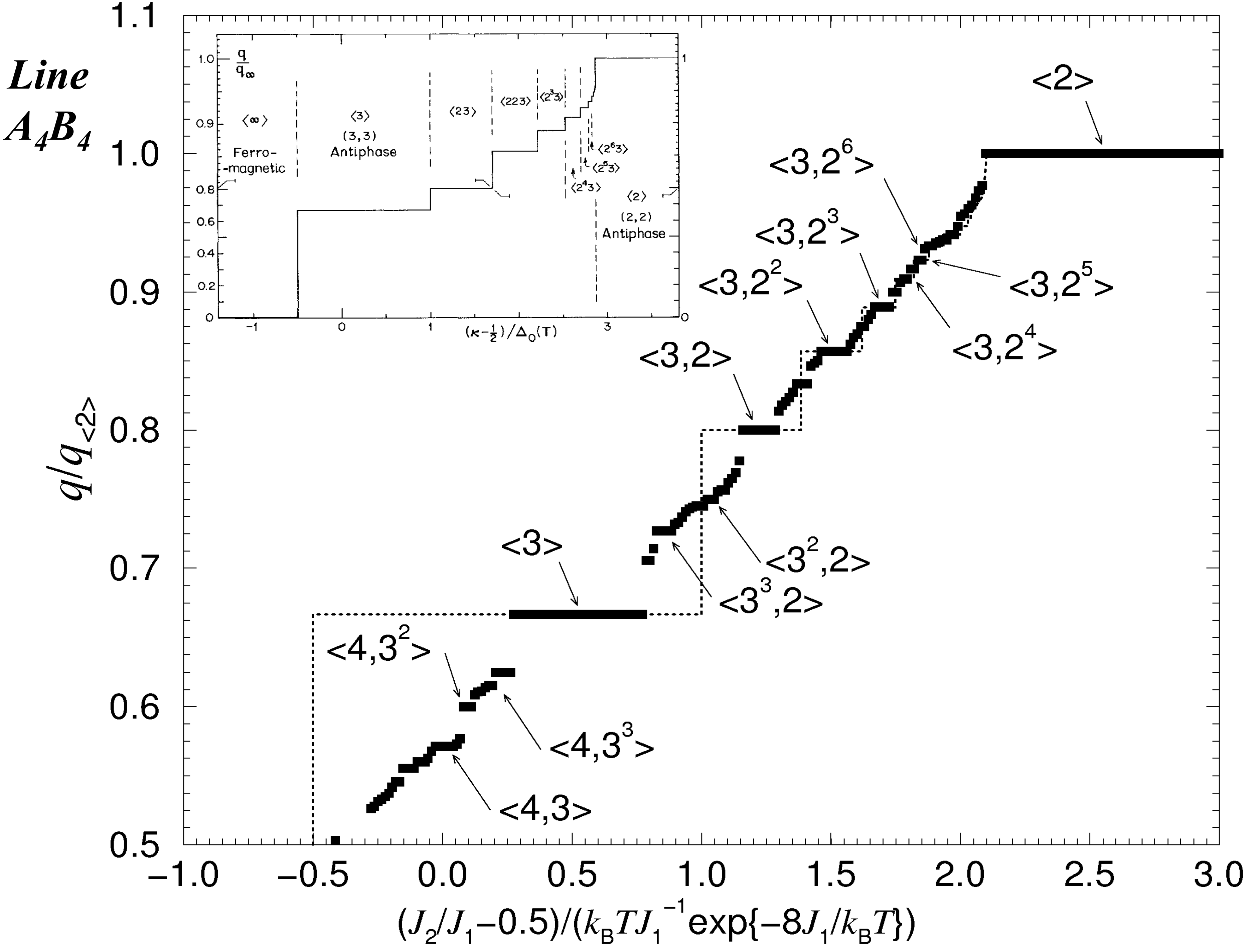
<7>
<6>
<5>
<4>
<3>
<2>
10.5
10.0
9.5
9.0
8.5
0.40
0.41
0.42
0.43
0.44
<5>
<5,4>


Line
A_4B_4
λ
40
35
30
25
20
15
10
5
0
0.485
0.490
0.495
0.500
0.505
0.510
0.515
0.520
J_2/J_1
Ferromagnetic phase
Antiphase <2>
<3>
$q=2\pi/\lambda$
0.6π
0.5π
0.4π
0.3π
0.2π
0.1π
0.0π
0.485
0.495
0.505
0.515
J_2/J_1
Ferro phase
Antiphase
$q=2\pi/6$

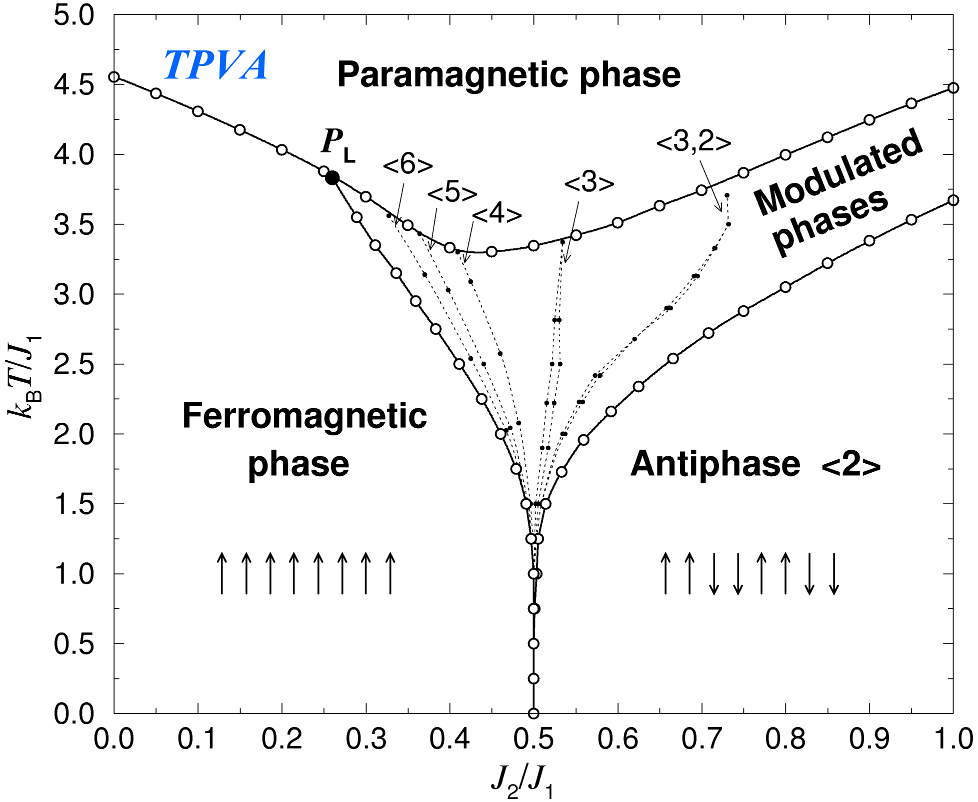


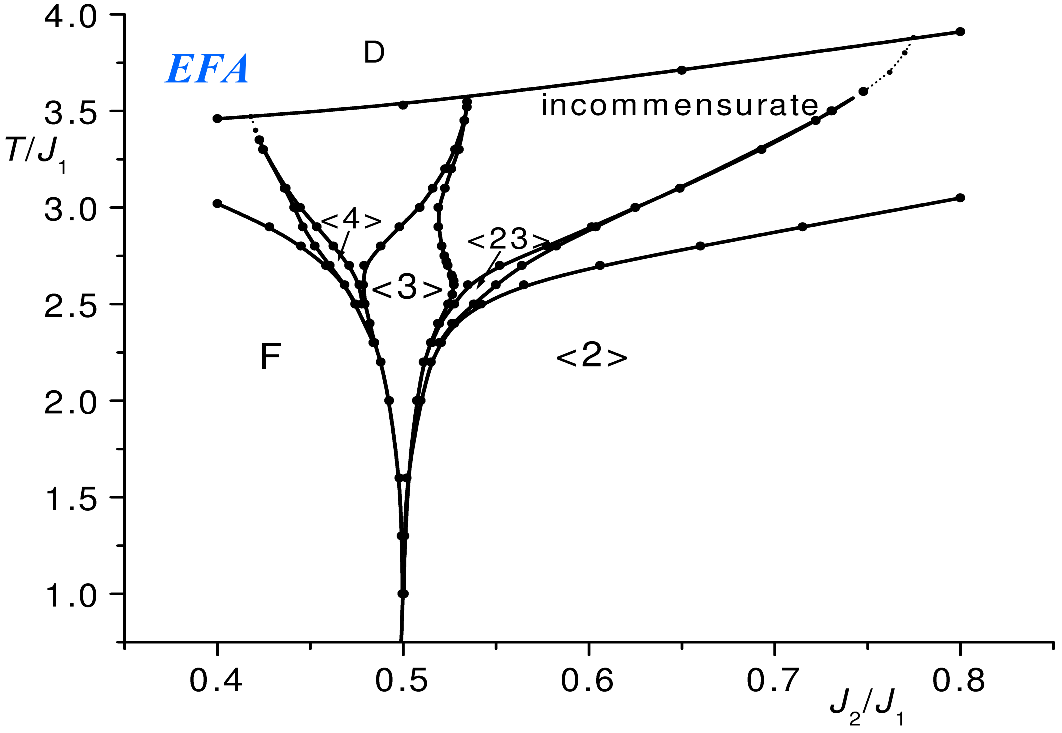
Line
A_4B_4
$<4^3,3>$
$<4^2,3>$
$<4,(4,3)^2>$
$<4,(4,3)^3>$
$<4,3>$
$<4,3^2>$
$<4,3^3>$
$<4,3^4>$
$<3>$
λ
8.0
7.5
7.0
6.5
6.0
5.5
0.498
0.499
0.500
0.501
0.502
0.503
0.504
0.505
J_2/J_1

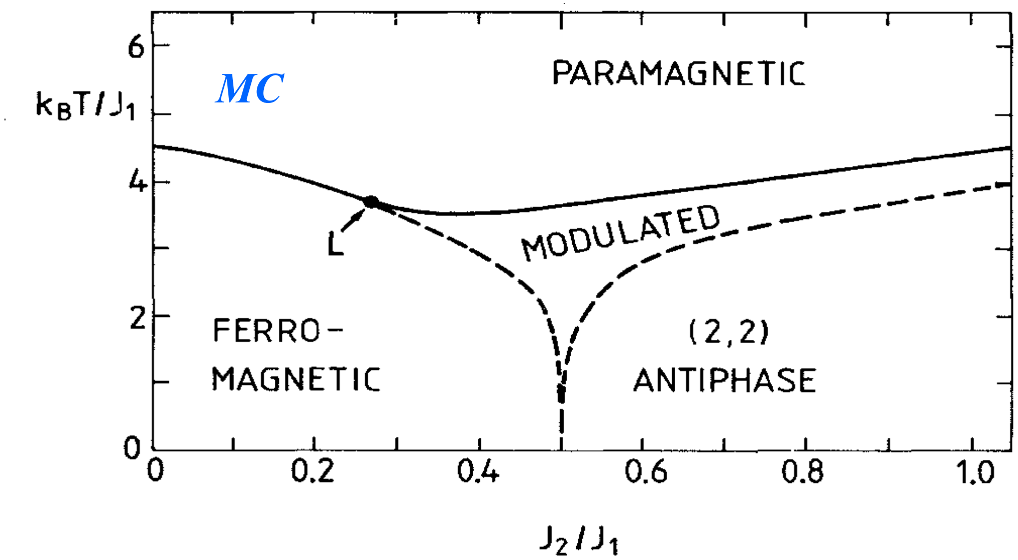

Line A_4B_4
$q/q_{<2>}$
1.1
1.0
0.9
0.8
0.7
0.6
0.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
$(J_2/J_1-0.5)/(k_BTJ_1^{-1}\exp\{-8J_1/k_BT\})$
<2>
<3,2^6>
<3,2^3>
<3,2^5>
<3,2^2>
<3,2^4>
<3,2>
<3^2,2>
<3>
<3^3,2>
<4,3^2>
<4,3^3>
<4,3>
$\frac{q}{q_\infty}$
1.0
0.9
0.8
0.6
0.4
0.2
0
1
0
−1
0
1
3
$(\kappa-\frac{1}{2})/\Delta_0(T)$
⟨∞⟩
Ferro-
-magnetic
⟨3⟩
(3,3)
Antiphase
⟨23⟩
⟨223⟩
⟨2^3 3⟩
⟨2^6 3⟩
⟨2^5 3⟩
⟨2^4 3⟩
⟨2⟩
(2,2)
Antiphase

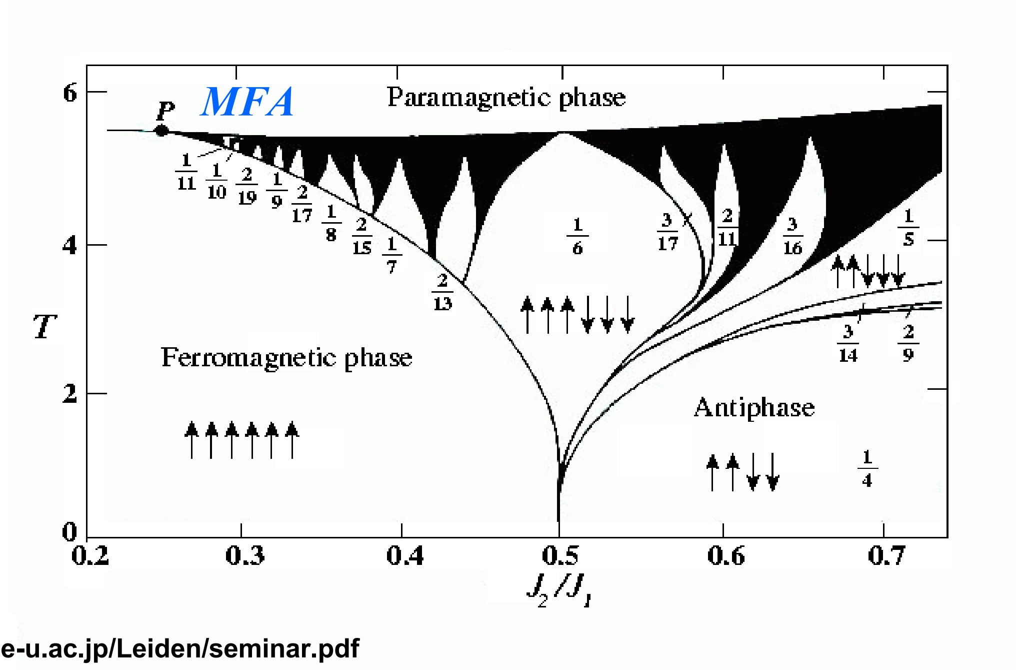
5. Concluding remarks

- *The 3-dimensional ANNNI model reveals an infinity of commensurate structures in the modulated phase. The devil's stairs behavior is observed.*
- *The wavelength λ diverges near the boundary with the ferromagnetic phase.*
- *The stable commensurate structures with $\lambda > 6$ are found at low temperatures.*
- *The position of the Lifshitz point $P_L=(0.26\ ;\ 3.83)$ is in qualitative agreement with $P_L^{MC}=(0.27\ ;\ 3.75)$.*
- *Additional interesting problems in 3D:*
  - *external magnetic field applied to $S=1/2$ ANNNI*
  - *frustrated $S=5/2$ (ANNNI) model,*
  - *frustrated q-state Potts model,*
  - *competing interactions imposed along more than one coordination axis*









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