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## The commensurate–disordered phase transition in the 2D classical ATNNI model studied by DMRG

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**Abstract.** The classical two-dimensional anisotropic triangular nearest-neighbour Ising (ATNNI) model is studied by the density matrix renormalization group (DMRG) technique when periodic boundary conditions are imposed. Applying the finite-size scaling to the DMRG results, a commensurate–disordered (CD) phase transition line as well as temperature and magnetic critical exponents are calculated. We conclude that the CD phase transition in the ATNNI model belongs to the same universality class as the ordered–disordered phase transition of the Ising model.

Analysis of semi-finite systems of small size in one or more directions has been used as a powerful tool in extracting critical properties of 2D classical models and corresponding 1D quantum models. Although finite or 1D systems themselves do not display any critical behaviour, it is, however, possible to extract critical parameter values as well as critical exponents. Temperature, ordering magnetic field and finite-size deviations from criticality are all described by the same set of the critical exponents [1]. This paper is focused on infinite strips of finite width where the relevant numerical data are obtained from the transfer matrix methods, in particular, the density matrix renormalization group (DMRG) method.

In 1992 the DMRG technique was invented by White [2] in real space for 1D quantum spin Hamiltonians. Three years later Nishino [3] applied this numerical technique to classical spin 2D models based on the renormalization group transformation for the transfer matrix for the open boundary conditions. DMRG treatment of 2D classical systems exceeds the classical Monte Carlo approach in accuracy, speed and size of the systems [4].

Recently, we have modified the DMRG method for the 2D classical models, imposing periodic boundary conditions (PBCs) on strip boundaries, and found a relation that helped to determine an optimal strip width  $L^{\text{opt}}$  in order to obtain correct values of critical temperature and exponents [5] using finite-size scaling (FSS). We have obtained results of very high accuracy exceeding the DMRG method with standard open boundary conditions. Our method does not require any extrapolation analysis of the data.

The use of DMRG for 2D classical models may follow one of two different approaches: (i) the DMRG method is applied to strips of finite width and, from two largest transfer-matrix eigenvalues or the free energy estimated with high precision, the critical properties of the system are calculated by the FSS analysis (here, we use this approach).

(ii) The strip width is enlarged until a steady state is reached (in the thermodynamic limit) when the output from the DMRG does not depend on the lattice size. Then, the DMRG yields properties of the 2D infinite system with spontaneously broken symmetry and mean-field-like

behaviour close to the criticality. This approach was used recently to study the high-field part of the anisotropic triangular nearest-neighbour Ising (ATNNI) model phase diagram [6], where approach (i) ran into convergence problems. We were able to show that the phase transition between the commensurate phase and the disordered phase proceeds via a narrow strip of an incommensurate phase. This approach also gives accurately the low-field part of the phase diagram, but it is not convenient for determination of the critical properties of the system by FSS. In distinction to the finite-width approach (i), it explicitly undergoes the phase transition, but its critical behaviour is mean-field-like and the speed of calculation suffers from critical slowing-down at the phase transition line. Therefore, we use here approach (i) to find the low-field critical behaviour of the ATNNI model.

The FSS approach should give the correct critical properties of the system in the limit of infinite strip width. Nevertheless, it was shown in [5] that in the approximate DMRG treatment for given size of the transfer matrix (limited by computer capacity), it is not useful to enlarge the strip width to too large values, because here the the DMRG results do not satisfy the scaling laws assumed by the FSS. Thus, an optimal width, up to which the results systematically improve, must exist. It was also shown that the estimation of critical properties of the Ising and Potts models by DMRG with the periodic boundary conditions are much better than those with the open ones, although the latter yields better results for the finite-width strips [5].

Below the optimal strip width  $L^{\text{opt}}$  the ratio

$$R \equiv \frac{\frac{\partial}{\partial L} T_C^*(L)}{\frac{\partial^2}{\partial L^2} T_C^*(L)} \quad (1)$$

is an almost linear function of  $L$  while, above it, it is not. ( $L$  in (1) is the width of the strip and  $T_C^*(L)$  is the critical temperature for given  $L$ .)

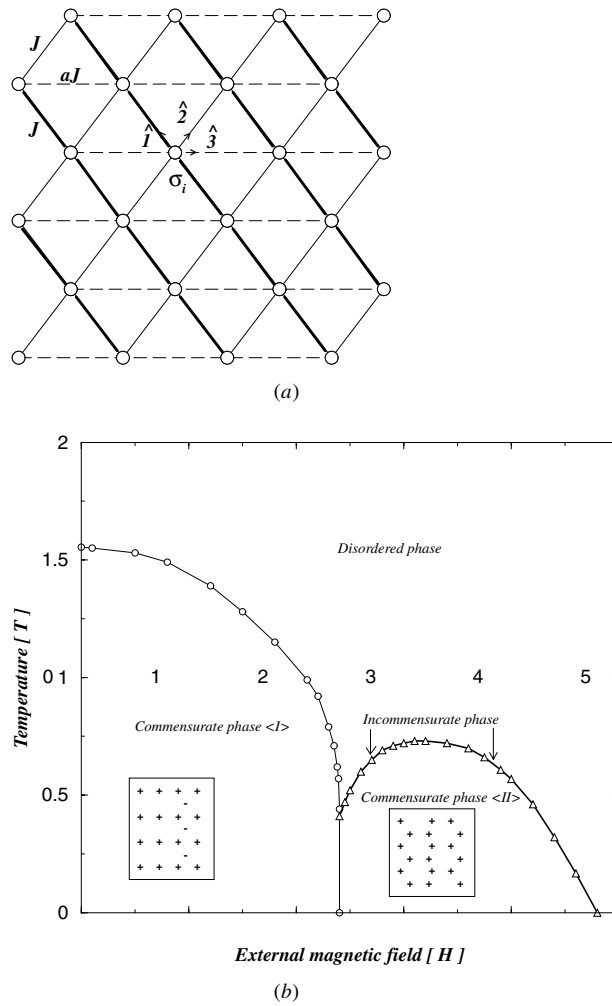
The deviation of  $R$  from linearity above the optimal strip width is very fast and the ratio  $R$  becomes zero or infinity within enlargement of the strip by one lattice constant. Thus, if  $R = 0$  or  $R \rightarrow \infty$  (i.e. if the numerator or the denominator tends to zero or changes its sign), we accept  $L$  as the strip width for further calculations and call it the optimal width  $L^{\text{opt}}$  of the strip. The critical temperature for the optimal width  $T_C^*(L^{\text{opt}})$  is taken as the best approximation of the critical temperature of the 2D system studied, and at this temperature the critical exponents of the system are calculated. The values of the critical exponents are sensitive to  $T_C^*$  and must be determined with due care.

In the FSS approach, the critical exponents are derived from the scaling behaviour of the correlation length and free energy at the critical point, where they depend on strip width  $L$  in the following way [1]:

$$K_L^h \sim L^{2y_h^{(\beta)}} \quad K_L^T \sim L^{y_T^{(\alpha)}} \quad c_L \sim L^{2y_T^{(\alpha)} - d} \quad (2)$$

where  $K_L^T$  and  $K_L^h$  are the derivatives of inverse correlation length  $K$  with respect to temperature  $T$  and the second derivative with respect to ordering (magnetic) field  $h$ , respectively, and  $c_L$  is the specific heat, i.e. the second derivative of the free energy with respect to temperature. The two temperature exponents  $y_T^{(\alpha)}$  and  $y_T^{(\nu)}$  should be equal to each other. The exponents  $y_T$  and  $y_h$  determine the critical behaviour of all statistical quantities characterizing the system. The critical exponents of specific heat, magnetization and correlation length can be calculated from  $y_T$  and  $y_h$  as follows:  $\alpha = 2 - \frac{2}{y_T}$ ,  $\beta = \frac{2 - y_h}{y_T}$  and  $\nu = y_T^{-1}$ . Other critical exponents can be obtained from the scaling equations  $y_h = \beta + \gamma$ ,  $\gamma = \beta(\delta - 1)$  and  $\eta = 2 - \gamma y_T$  [7].

Further, we demonstrate the capabilities of our approach to find the critical properties of the 2D spin lattice model on the Ising model with different symmetries of the lattice, where critical temperatures and critical indices are known from exact solutions, and the ATNNI



**Figure 1.** (a) The triangular lattice of the ATNNI model. (b) The phase diagram of the ATNNI model for  $a = 0.4$  obtained by the DMRG method [6].

model where the phase diagram is generally unknown and the critical indices are predicted from symmetry considerations.

The 2D classical ATNNI model is given by the Hamiltonian

$$\mathcal{H} = \sum_i -J \left( \sum_{\hat{\delta}=\hat{1},\hat{2}} \sigma_i \sigma_{i+\hat{\delta}} + a \sigma_i \sigma_{i+\hat{3}} \right) - H \sum_i \sigma_i \quad (3)$$

with the antiferromagnetic coupling  $J < 0$  and spins  $\sigma_i = \pm 1$ . The numbers  $\hat{1}$ ,  $\hat{2}$  and  $\hat{3}$  are lattice directions in the ATNNI model. The coupling  $J$  is multiplied by the parameter  $a$  ( $0 < a < 1$ ) along the direction  $\hat{3}$  as depicted in figure 1(a).

This model was studied by Domany and Schaub [8] and in [6], and it was shown that its phase diagram, as a plot of temperature  $T$  and external magnetic field  $H$  (for  $a = 0.4$ ), exhibits four different phases: two commensurate phases  $\langle I \rangle$  and  $\langle II \rangle$ , a disordered phase and an incommensurate phase (see figure 1(b)). Commensurate phase  $\langle I \rangle$  occurs at magnetic

**Table 1.** Critical temperatures  $T_C^*$  obtained from (1) with DMRG compared with the exact ones  $T_C^{(\text{exact})}$ . The symbols  $\square$  and  $\triangle$  describe square and triangular lattices, respectively.

Model	$H$	$T_C^*$	$T_C^{(\text{exact})}$
$\square$ Ising	0.0	2.269 1851	2.269 1853
$\square$ AF Ising	0.0	2.269 1848	2.269 1853
$\triangle$ Ising	0.0	3.640 955	3.640 957
$\triangle$ ATNNI	0.0	1.553 52	1.553 62
$\triangle$ ATNNI	0.5	1.528 67	unknown
$\triangle$ ATNNI	1.0	1.451 35	unknown
$\triangle$ ATNNI	1.5	1.311 05	unknown
$\triangle$ ATNNI	2.0	1.070 09	unknown

field  $H < 2.4$ . This structure satisfies the Lifshitz condition, and it is characterized by a 1D representation of the lattice symmetry group, i.e. its phase transition is predicted to belong to the Ising universality class [9]. Domany and Schaub tried to confirm this prediction by numerical calculation of the exponent  $y_T$ , but due to the low-order approximation it differed from the expected value by more than 10% and the magnetic exponent was not calculated at all.

We have calculated critical properties of the ATNNI model at the phase transition line between the commensurate  $\langle I \rangle$  and the disordered phase. To illustrate the accuracy of the method, we have calculated critical properties of the exactly solvable models: ferromagnetic and antiferromagnetic Ising models on square and triangular lattices at zero magnetic field as well as the zero-magnetic-field ATNNI model, for which the critical temperature is given by the equation [10]

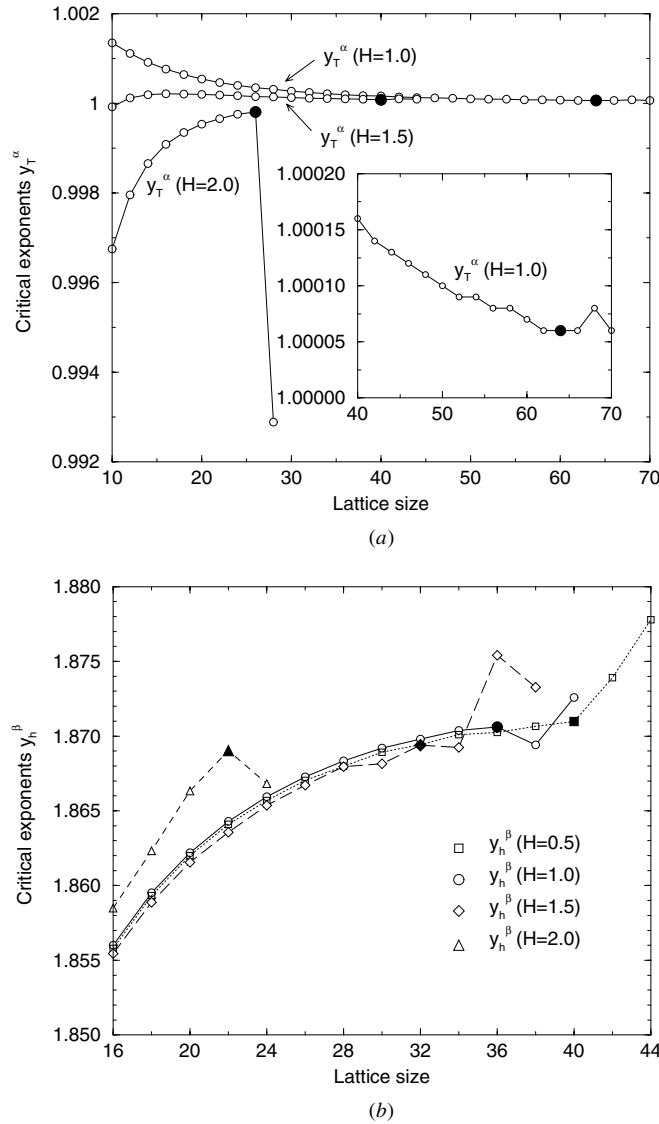
$$\sinh^2 \left( \frac{2J}{T_C} \right) = \exp \left( -\frac{4aJ}{T_C} \right). \quad (4)$$

We have used the FSS analysis of DMRG results with a superblock consisting of eight Ising spins and four multi-spin variables, each acquiring 85 values ( $m = 85$ ). The computational effort at this approximation is less than for the classical transfer matrix method of strip width equal to 17 lattice constants. However, the DMRG enables us to treat a wider strip (of tens of lattice constants) up to the optimal width, further improving the values of the critical parameters.

The first, important step of the calculations is determination of the critical temperature  $T_C^*$  (see table 1), of which the best estimation for given  $m$  is  $T_C^*(L^{\text{opt}})$  calculated from the FSS approach [5]. At this temperature the values of the critical exponents are derived from the scaling laws (2).

As the quantities appearing in (2) are first and second derivatives of the free energy and correlation length, the effect of approximation starts to be manifest at a strip width lower than  $L^{\text{opt}}$ . The criterion determining the strip width at which the value of the critical exponent may be still acceptable was taken as completely analogous to that for critical temperature, equation (1). The accepted values of the critical exponents are denoted by filled symbols in figures 2(a) and (b).

The critical exponent  $y_T$  is determined more precisely from the free energy  $y_T^{(\omega)}$  than from the correlation length  $y_T^{(v)}$ , as for the evaluation of the former only the largest eigenvalue of the superblock matrix is needed in distinction to the correlation length, calculation of which the ratio of the largest and the second largest eigenvalue is necessary. This point is irrelevant for the models with a symmetric transfer matrix (Ising models in table 1), but significant for the ATNNI model with a non-symmetric transfer matrix [11]. The plot of thermal critical exponent



**Figure 2.** (a) The plot of thermal critical exponents  $y_T^{(\alpha)}$  for different fields in the ATNNI model. (b) The plot of magnetic critical exponents  $y_h^{(\beta)}$ . The filled symbols denote the accepted critical exponents satisfying equation (1).

$y_T^{(\alpha)}$  versus strip width is shown in figure 2(a). For increasing lattice size they both tend to the Ising value 1. The convergence also depends on the magnetic field. It worsens for magnetic field close to the multi-critical point  $H = 2.4$ . Here the reliability of the DMRG breaks down at rather small strip width, as well. The accepted values depicted by black symbols are listed in table 2.

The critical exponent  $y_h^{(\beta)}$  describes the decay of the order parameter at the phase transition line from the commensurate phase  $\langle I \rangle$  to the disordered phase. The structure  $\langle I \rangle$  consists of two ferromagnetically ordered sublattices each with different magnetization. As the external

**Table 2.** Critical exponents of various 2D spin models calculated by the DMRG method with PBC and FSS analysis. The exact critical exponents of the Ising models are as follows:  $y_T = 1$  and  $y_h = 1.875$ .

Model	$H$	$y_T^{(\alpha)}$	$y_T^{(\nu)}$	$y_h^{(\beta)}$	$\alpha$	$\beta$	$\nu$
□ Ising	0.0	1.000 0009	0.999 999 94	1.875 002	0.000 0017	$\frac{1}{8.00012}$	1.000 000 06
□ AF Ising	0.0	1.000 0009	0.999 999 94	1.875 126	0.000 0017	$\frac{1}{8.00804}$	1.000 000 06
△ Ising	0.0	1.000 0014	0.999 999 43	1.875 030	0.000 0027	$\frac{1}{8.00192}$	1.000 000 57
△ ATNNI	0.0	1.000 0022	0.994 7	1.870 05	0.000 004	$\frac{1}{7.70}$	1.005 27
△ ATNNI	0.5	1.000 0280	0.990 2	1.870 98	0.000 056	$\frac{1}{7.75}$	1.009 93
△ ATNNI	1.0	1.000 0580	0.990 2	1.870 62	0.000 116	$\frac{1}{7.73}$	1.009 93
△ ATNNI	1.5	1.000 0767	0.991 1	1.869 39	0.000 153	$\frac{1}{7.66}$	1.008 93
△ ATNNI	2.0	0.999 8366	1.012 2	1.869 02	0.000 327	$\frac{1}{7.63}$	0.987 95

magnetic field  $H$  is generally non-zero in the ATNNI model, the total magnetization (sum of both sublattice magnetizations) is non-zero, as well. The difference between the two magnetizations is taken as the order parameter in this case. The small ordering field  $h$  used for calculation of the derivative  $K_L^h$  acquires the opposite sign at each of the two sublattices. The accuracy of the calculations of the magnetic exponent is smaller than that of the thermal exponent in the case of the exactly solvable models listed in table 2. Thus, we can expect a lower accuracy also for the ATNNI model. All the exponents depicted in figure 2(b) are below 1.871. Extrapolations to  $L \rightarrow \infty$  for  $H = 0.5$ – $1.5$  give values of  $y_h^{(\beta)}$  of about 1.872, i.e.  $\beta = \frac{1}{7.81}$ , which still differs from the Ising value  $y_h^{(\beta)} = 1.875$  and corresponding  $\beta = \frac{1}{8}$ . Note that the value of  $y_h^{(\beta)}$  is extremely sensitive to the correct determination of the critical temperature. A very small decrease of its value would shift  $y_h^{(\beta)}$  to the expected Ising value. At modest magnetic field, where our calculations are assumed to be more accurate, the plots of  $y_h^{(\beta)}$  for different magnetic field lie on the same curve, which suggests that not only is  $y_h^{(\beta)}$  a universal quantity independent of  $H$ , but the corrections to it for finite  $L$  are universal, as well.

In conclusion, it can be stated that the DMRG method with periodic boundary conditions reproduces with a high accuracy the critical properties of exactly solvable models and confirms the prediction that the CD phase transition for magnetic fields  $H = 0$ – $2.4$  belongs to the universality class of the Ising model.

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