The Ising bilayer honeycomb lattice: a cluster mean-field study

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1) Abstract

We study the Ising model on a bilayer honeycomb lattice with frustrated antiferromagnetic interactions using the cluster mean-field method. We investigate the role of exchange couplings and thermal fluctuations, providing a picture for the global phase diagram of the model and its thermodynamics. Our findings indicate that the model hosts a highly frustrated regime, in which no long-range order takes place and a finite entropy is found at absolute zero. Near the highly frustrated regime, signatures of frustration can be spotted in the specific heat above the ordering temperature. In addition, our results support that the model exhibits order-by-disorder state selection and tricriticality for a wide range of parameters. A comparison of the cluster mean-field outcomes with literature data is given.

2) Model and Method

We consider the Ising model on a honeycomb lattice bilayer described by the Hamiltonian

$$H = J_1 \sum_{\langle i,j\rangle} \sigma_i\sigma_j + J_p \sum_{(i,j)} \sigma_i\sigma_j + J_x \sum_{((i,j))} \sigma_i\sigma_j,$$

where $\sigma_i = \pm 1$ is the Ising variable of site i. The first sum runs over intralayer first-neighbours while the second and third sums run over interlayer first- and second-neighbours, respectively. In the present work, we consider only antiferromagnetic interactions (i.e., J1 , Jp and Jx are positive), which allows us to compare our findings with those of Ref. [1].

We employ a variational cluster mean-field theory [2] that allows us to describe the thermodynamics as well as the role of thermal fluctuations on the phase transitions of the present model. In this approach, we employ the Bogoliubov inequality for the system free energy

$$F \leq F_{ub} = F_r + \langle H - H_r \rangle_r,$$

This variational approach allows us to write the cluster mean-field Hamiltonian:

$$H_{\mathrm{CMF}} = H_{intra} + H_{inter}$$

where H intra incorporates the intracluster interactions of a given cluster and

$$H_{inter} = J_1 \sum_{\langle i,j\rangle_{dc}} (\sigma_i m_j - m_i m_j/2) + J_x \sum_{((i,j))_{dc}} (\sigma_i m_j - m_i m_j/2)$$

incorporates the mean-field contribution from the neighbour clusters. Here,

$$m_i = (\mathrm{Tr}\, \sigma_i\, e^{-\beta H_{\mathrm{CMF}}})/(\mathrm{Tr}\, e^{-\beta H_{\mathrm{CMF}}})$$

is the local magnetization of site i. It is also worth to note that for the three types of long-range order found in this model, the clusters considered exhibit an identical pattern of local magnetizations throughout the entire system. It means one can obtain the local magnetizations of a given cluster from any other cluster. Therefore, the many-body problem is reduced to a self-consistent single-cluster problem.

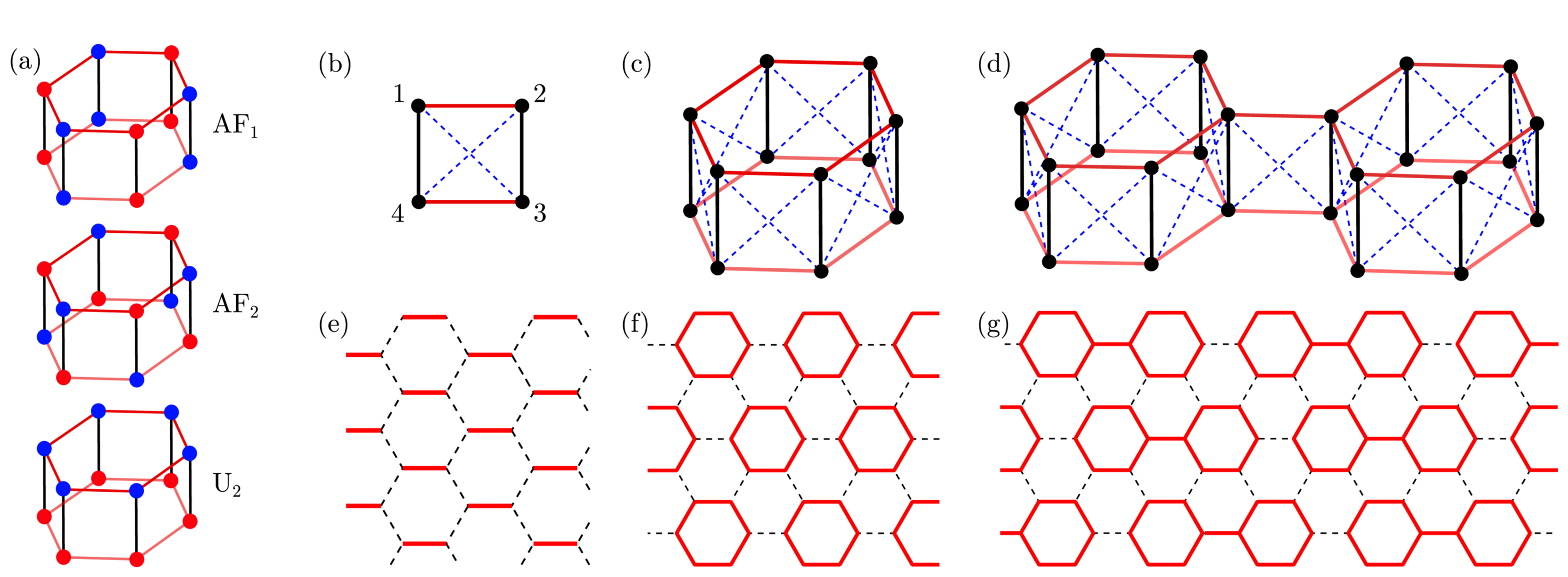

FIGURE 1: Panel (a) shows the ordered ground-states of the frustrated honeycomb Ising model. The cluster structures used in the CMF theory are shown in panels (b), (c) and (d), in which the exchange couplings adopted in the model are also shown. Red solid lines indicate J1 couplings, blue dashed lines denote Jx interactions and black lines represent Jp interactions. Panels (e), (f) and (g) exhibit a single layer divided into the clusters adopted within the approximation for ns spins per cluster, with ns = 4, 12 and 24, respectively. The clusters are delimited by solid red lines and dashed black lines representing intercluster interactions.

4) Conclusions

- Frustration brings the ordering temperature to zero when J1 = Jx < Jp/3, which is a consequence of the macroscopic degeneracy of the model.
- Round maximum in the specific heat and residual entropy can be found in this highly frustrated scenario.
- Our findings are in very good agreement with the results from Bethe lattice calculations and Monte Carlo simulations [1].
- Findings **indicate** the **existence** of a **tricritical point** in the phase boundary between AF1 and PM phases, that takes place when J1/Jp > 1/3 and Jx/Jp > 1/3. More importantly, our results support that the tricritical point can be found for a wide range of J1/Jp.

3) Results

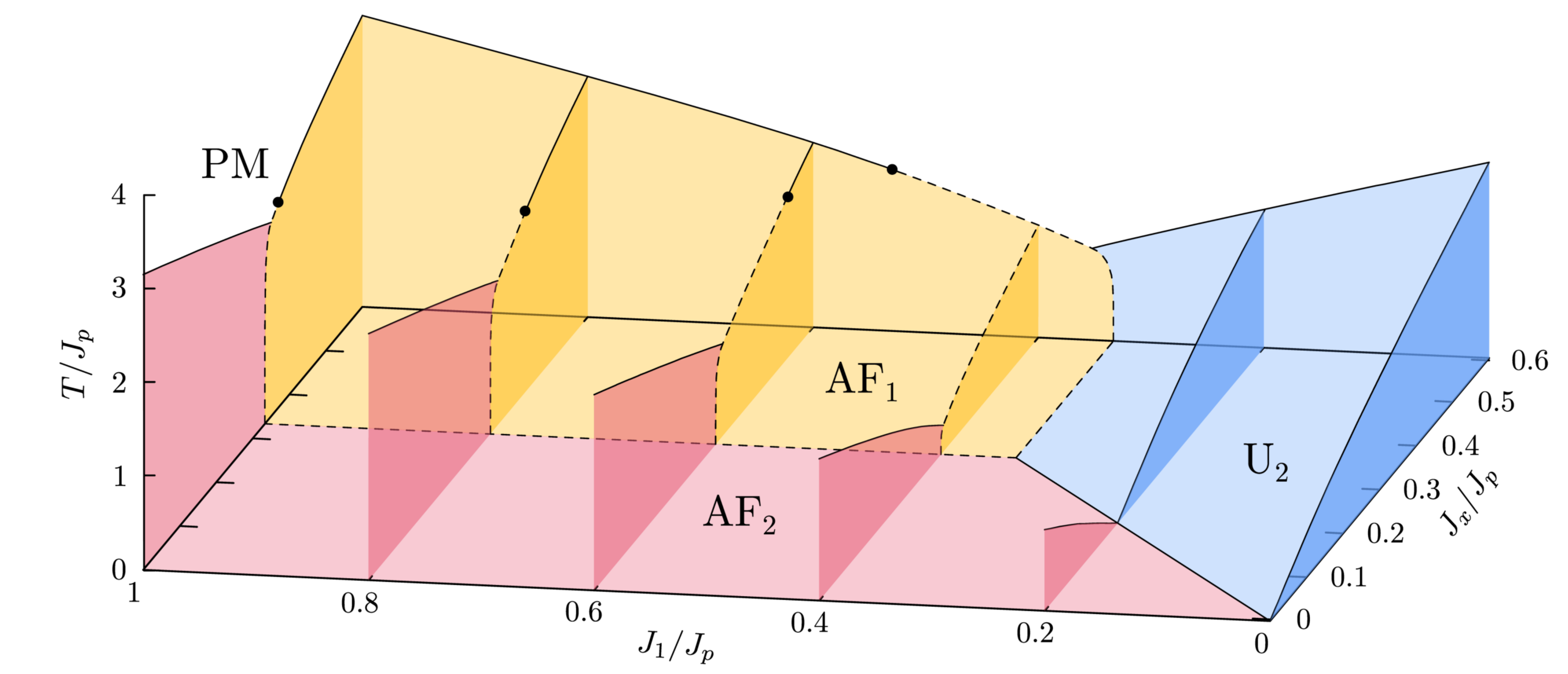

FIGURE 2: Global phase diagram evaluated within the 12-site CMF theory with first- and second-order phase transitions indicated by dashed and solid lines, respectively. The filled circles indicate the location of the tricritical points. In the ground-state, the boundary between phases U2 and AF2 takes place at Jx = J1 for Jx/Jp < 1/3. For Jx/Jp > 1/3, phases U2 and AF1 ground-state boundary occurs at J1/Jp = 1/3. The boundary between phases AF1 and AF2 is located at Jx/Jp = 1/3 when J1/Jp > 1/3.

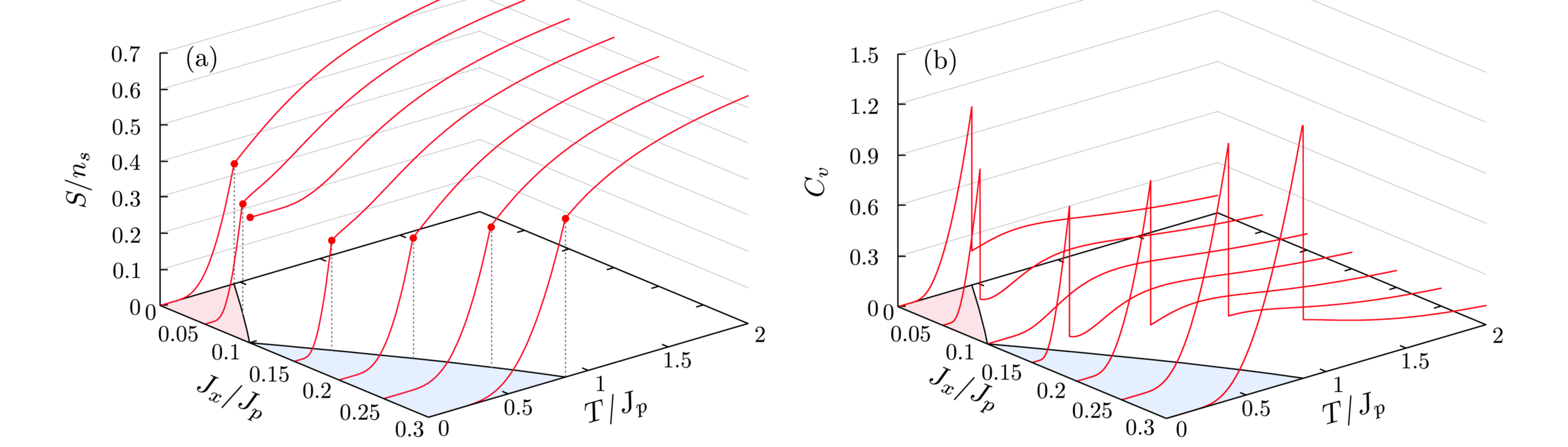

FIGURE 3: Thermal dependence of (a) entropy per spin and (b) specific heat (in units of kB) for J1/Jp = 0.1 and several strengths of the crossing interaction Jx/Jp for ns = 12. Filled circles indicate the entropy at the critical temperature, where the dotted lines are guides for the eyes to the critical points in the Jx/Jp × T/Jp plane. In the Jx/Jp-T/Jp plane, the phase diagram is shown using the color scheme of Fig. 2.

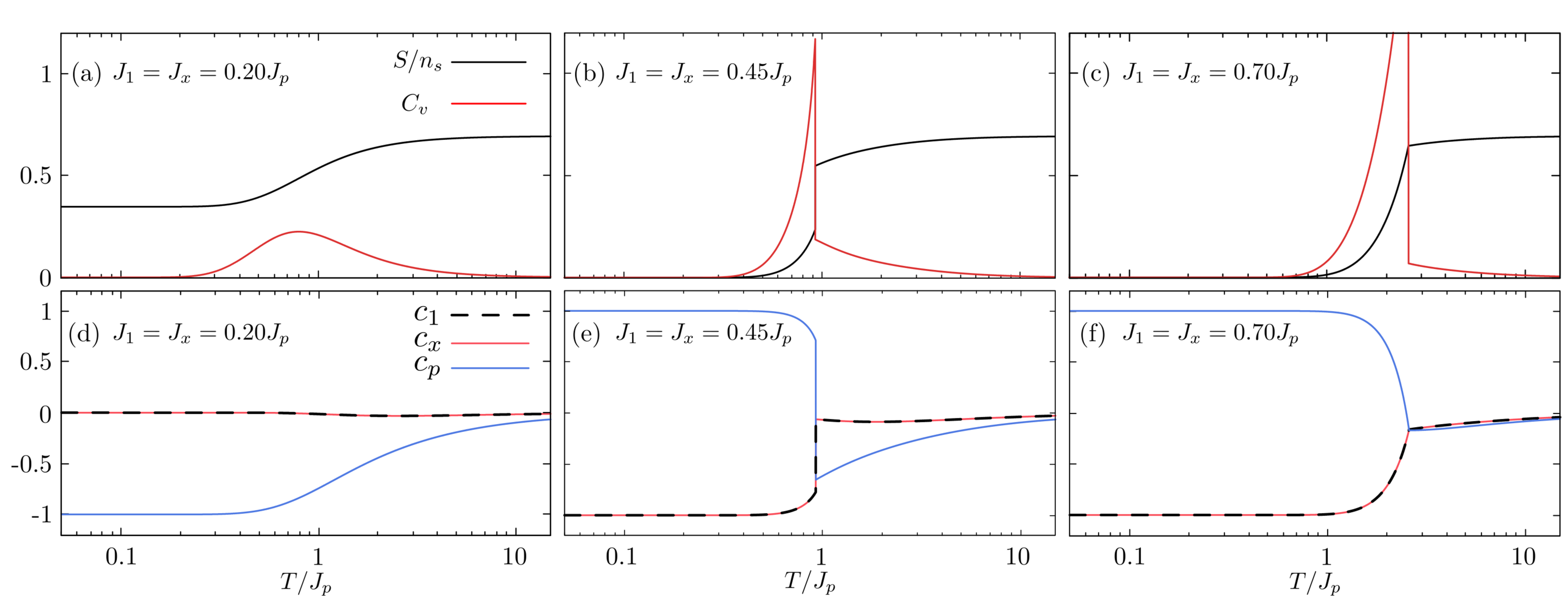

FIGURE 4: Thermodynamic quantities for several strengths of J1 = Jx within the CMF for a cluster of size ns = 12. The upper panels show the thermal dependence of entropy per spin and specific heat (in units of kB) and lower panels show the thermal dependence of correlations.

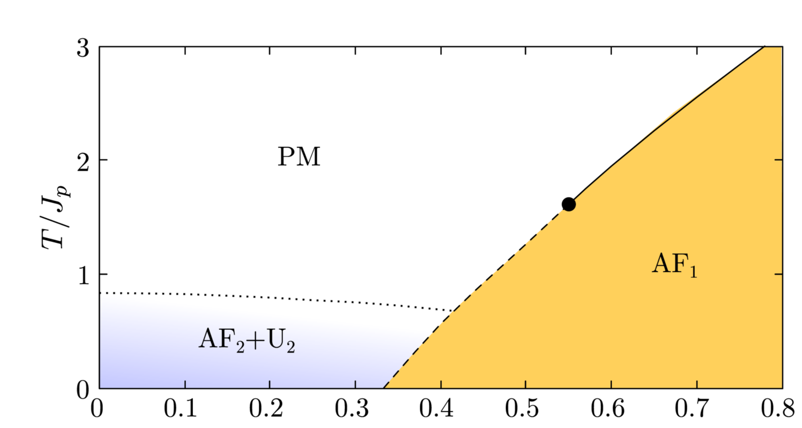

FIGURE 5: Phase diagram for J1 = Jx within the CMF for a cluster of size ns = 24. The dashed and solid lines indicate first- and second-order phase transitions, respectively. The filled circle indicates the tricritical point and the dotted line indicates a crossover between the high-temperature paramagnet and the correlated paramagnet at lower temperatures in which short-range correlations are consistent with both AF2 and U2 phases.

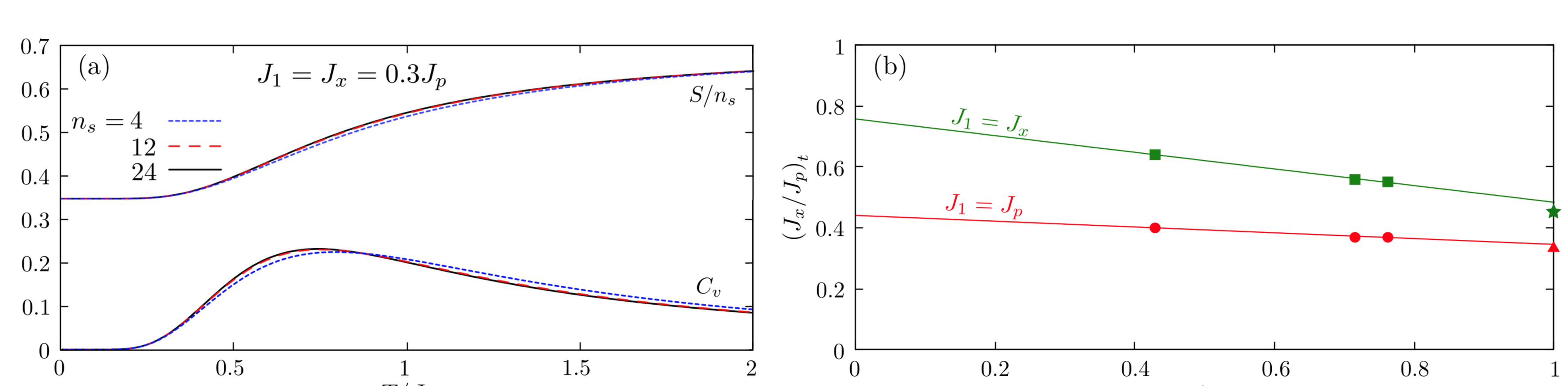

FIGURE 6: Comparison of CMF outcomes for different cluster sizes. Panel (a) shows the specific heat and entropy per spin (in units of kB) for ns = 4, 12 and 24 when J1 = Jx = 0.3Jp. Panel (b) shows a scaling for the coupling coordinate of the tricritical point (details are provided in the text). Squares are CMF estimates of (Jx/Jp)t for the highly frustrated scenario J1 = Jx. The Monte Carlo result for this scenario is indicated by a star. Circles are estimates of the tricritical point for J1/Jp = 1. The triangle indicates the limit case Jx/Jp = 1/3. Lines are the linear fits of the CMF data.

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