

Research Article

Bicritical Central Point of $J_{\text{FN}} - J_{\text{SN}}$ Ising Model Phase Diagram

**Yahia Boughaleb,^{1,2} Mohammed Nouredine,¹ Mohamed Snina,¹ Rachid Nassif,^{1,2}
and Mohamed Bennai¹**

¹Laboratoire de Physique de la Matière Condensée, Faculté des Sciences Ben M'sik, Université Hassan II, Casablanca, Morocco

²Laboratoire de Physique de la Matière Condensée, Faculté des Sciences El Jadida, Université Chouaib Doukkali, Casablanca, Morocco

Correspondence should be addressed to Rachid Nassif, nassif_rachid@yahoo.fr

Received 16 September 2010; Accepted 6 November 2010

Academic Editor: Harold Zandvliet

Copyright © 2010 Yahia Boughaleb et al. This is an open access article distributed under the Creative Commons Attribution License, which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited.

We deal with a 2D half occupied square lattice with repulsive interactions between first and second neighboring particles. Despite the intensive studies of the present model the central point of the phase diagram for which the ratio of the two interaction strengths $R = J_{\text{SN}}/J_{\text{FN}} = 0.5$ is still open. In the present paper we show, using standard Monte Carlo calculations, that the situation corresponds to a phase of mixed ordered structures quantified by an “algebraic” order parameter defined as the sum of densities of the existing ordered clusters. The introduced grandeur also characterizes the transitions towards the known pure ordered phases for the other values of R as mentioned by the agreement of our results with those of the literature. The computation of the Cowley short range order parameter against R suggests that the central point is bicritical and is a state to cross when passing between the two pure phases.

1. Introduction

The study of frustrated magnetic systems always arouses the interest [1–7]. It is known that the nature of the ordering at low temperatures regime of these materials depends on the concentration of the magnetic species and on the relative magnitude of competing energy scales [8, 9]. The $J_{\text{FN}} - J_{\text{SN}}$ Ising model offers a valuable framework for dealing with the phenomena involved as has been confirmed by recent discovery of high- T_c superconductivity in pnictides [10, 11] (the model helps in dealing with the magnetism of the square Fe sublattice). However, when the interactions between first and second neighboring particles are repulsive in a square lattice the approximations adopted to solve the Ising model give rise to a controversial phase diagram [12–18]. In fact nowadays everyone agrees that the transition line from the disordered to the ordered $p(2 \times 2)$ phase is continuous when the ratio between the second “ J_{SN} ” and the first “ J_{FN} ” neighboring interactions $R = J_{\text{SN}}/J_{\text{FN}} < 0.5$. The situation $R > 0.5$ where the degenerate $p(2 \times 1)/p(1 \times 2)$ ordered phase holds is still under debate, particularly the extent of interaction rate for which the transition is first order

[1, 2, 14–17, 19]. In both cases, the characterization of phase transition is done by means of order parameters that quantify the breakdown of lattice occupation symmetry. This cannot be applied to the system with $R = 0.5$ as to this interaction strength corresponds three ground states: the two ordered phases ($p(2 \times 2)$ and $p(2 \times 1)$) and a third “2d-honeycomb $p(4 \times 2)/p(2 \times 4)$ ” structure joining a central particle to one first and to two second neighboring particles.

Numerical calculations using relaxation processes based on the jump of unique particles are far from being sufficient to alter the stability of clusters formed. To overcome the status quo and reach a stable low temperature pure phase, it was suggested to improve the jump algorithm by considering parallel tempering method [20]. Here the finite size scaling analysis on the obtained effective critical temperatures concludes an absence of phase transition in the thermodynamic limit [14, 15]. In the present, we argue that no pure phase holds rather there are clusters with different ordered structures and sizes that interpenetrate each other well. In other words, the low temperature phase lets appear a kind of long range order with mixed structures. By expecting the local environment of a given site, one easily recognizes

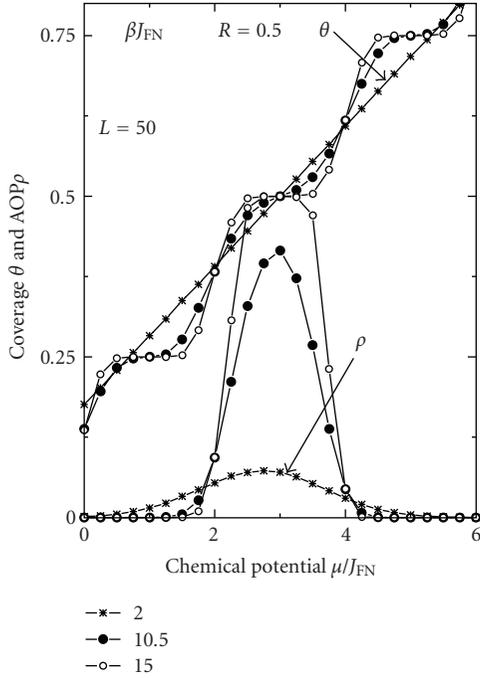


FIGURE 1: Variation of adsorption isotherms and density of ordered structures versus chemical potential for different interaction regimes at $R = 0.5$. Size of the lattice is fixed to $L = 50$.

the ordered structure's the site belongs to and calculates the density of each ordered structure. The sum of densities of the existing structures is a nonconservative stochastic variable we introduce to play the role of an order parameter. Standard Monte Carlo calculations using the Metropolis algorithm are performed and conclude the existence of a nonvanishing critical temperature when freezing the initial disordered lattice. We then generalize the application of the present grandeur to all values of R ratio and discuss the agreement with results of the literature. Next we consider the Cowley Short Range Order Parameter "SROP" that we compute versus the strength of the competing interaction energies at fixed temperatures. The calculations lead to the same results except for the central point where the discontinuity in the behavior of SROP reflects that the phase transition is first order. We notice here that the bicriticality does not originate from mixture of different particles as in references [21, 22].

2. Model and Method

The study is performed in the framework of lattice gas model. We consider a bidimensional square lattice with lateral size L for which interaction energy is insured by the following Hamiltonian of static interactions:

$$H = -\frac{1}{2}J_{FN} \sum_{\langle i,j \rangle} n_i n_j - \frac{1}{2}J_{SN} \sum_{\langle\langle i,k \rangle\rangle} n_i n_k - \mu \sum_i n_i. \quad (1)$$

" n_i " is a Boolean occupation number, R denotes the ratio between interaction energies of second " J_{SN} " and first " J_{FN} "

neighboring particles, and μ is the chemical potential and number of angle brackets indicates number of the neighbors.

Adsorption/desorption processes on periodically bounded lattices are insured meaning standard Metropolis transition rate applied to the state of single site of the lattice

$$W = \min(1, e^{-\beta\Delta H}). \quad (2)$$

β denotes the inverse reduced temperature and ΔH corresponds to the energy difference between the final and the initial configurations. We recall that in the Metropolis algorithm a site is allowed to change its state if the global energy of the system is reduced or as a response to a local deformation of the lattice represented by the comparison of the adsorption/desorption length to a number chosen at random. For each given size of the lattice ($L = 40, 60, 80$) the relaxation is controlled by computing at fixed temperature the energy, the average concentration, and the introduced algebraic order parameter "AOP". The later grandeur characterizes the sum of densities of the ordered clusters on the lattice $\rho = \sum_i \rho_i$, where " i " designates the structure and $\rho_i = \sum n_r^i / L^2$. Here the summation is performed once constraints relative to establishment of a type of order are fulfilled (e.g., a site belongs to the $p(2 \times 2)$ ordered structure whenever its first neighboring sites are all empty)

$$i \equiv 2 \times 2 = \left\{ n_r^p = 1; \sum_{\langle r \rangle} n_r^p = 0, \sum_{\langle\langle r \rangle\rangle} n_r^p = 4 \right\},$$

$$i \equiv 2 \times 1 = \left\{ n_r^p = 1; \sum_{\langle r \rangle \perp} n_r^p = 2; \sum_{\langle r \rangle \parallel} n_r^p = 2, \sum_{\langle\langle r \rangle\rangle} n_r^p = 0 \right\},$$

$$i \equiv 4 \times 2 = \left\{ n_r^p = 1; \sum_{\langle r \rangle} n_r^p = 1; \sum_{\langle\langle r \rangle\rangle \parallel} n_r^p = 2, \sum_{\langle\langle r \rangle\rangle} n_r^p = 2 \right\}. \quad (3)$$

Brackets designate the neighbours and the number of the brackets the number of the neighbours and the symbols \perp and \parallel denote perpendicular and parallel direction of the given site.

3. Results and Discussions

Figure 1 reports adsorption isotherm as well as the behavior of AOP for different temperature regimes. For high temperatures adsorption isotherm presents the known Langmuir gas behavior. Absence of ordering is characterized by weak values of AOP. This can be understood by existence of ordered clusters of limited sizes as a consequence of the equal probability of occupying lattice sites.

To the transition to ordering marked by plateau in adsorption isotherm corresponds a clear increase of AOP values. All sites of the lattice contribute to the appearance of the order as can be seen by the collapse of both adsorption isotherm and AOP curves in the interval corresponding to the coverage fixed at $\theta = 0.5$. Signature of this kind of long range order constituted by mixture of different types

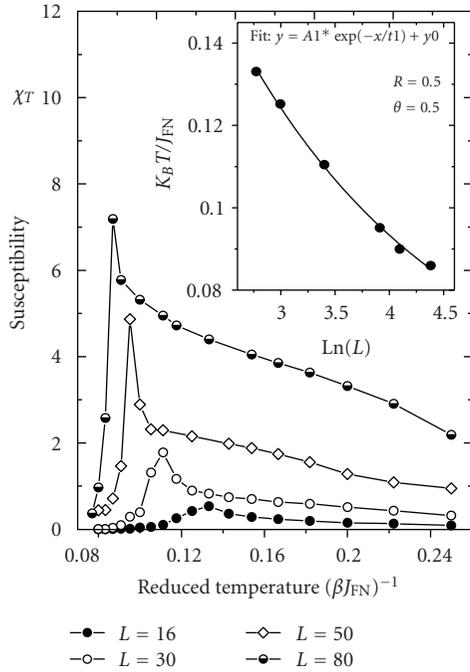


FIGURE 2: Validity of algebraic order parameter ρ hypothesis: behavior of the susceptibility defined as fluctuations of ordered structures density versus reduced temperature for different sizes of the lattice and finite size scaling analysis (the inset: we notice that the error bars have the same size of the symbols used in the graph).

of ordered clusters is also revealed by the behavior of the susceptibility of the system. The later is defined as a measure of the autocorrelation function of the AOP:

$$\chi_T \equiv \frac{1}{K_B T} \langle \rho^2 \rangle - \langle \rho \rangle^2. \quad (4)$$

In Figure 2 we report the susceptibility for different sizes of the lattice as well as the finite size scaling analysis joining the effective critical temperatures (the inset). Maxima of the curve are related according to the formula

$$T_L = T_C + A \cdot L^{-1/\nu}. \quad (5)$$

This leads to a nonvanishing critical temperature at the thermodynamic limit ($T_C = 0.039$). The obtained critical exponents suggest that the phase transition is nonuniversal ($\nu = 0.94$ and $\gamma = 1.56 \pm 0.13$).

Another proof of the validity of our hypothesis lies in characterizing the phase transition to all R values. The phase diagram of Figure 3 shows that obtained critical temperatures agree with the results of studies within Monte Carlo technique [12–15, 23]. Once again finite size scaling analysis confirms an Ising-like behavior with universal critical exponents of the system with $R < 0.5$ and that order/disorder phase transition for $R > 0.5$ is nonuniversal ($\nu = 0.70$ and $\gamma = 1.726 \pm 0.08$ for $R = 0.75$ for example, the value has to be compared with the one in [12, 13]).

Now that transition to ordered phase at $R = 0.5$ has nonnull temperature in the thermodynamic limit, it would

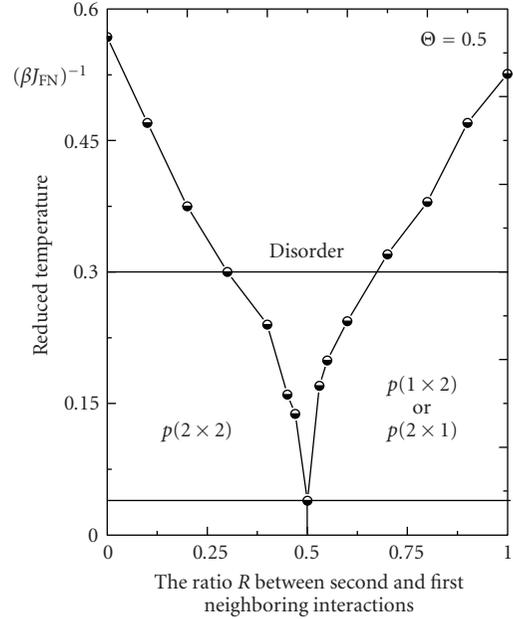


FIGURE 3: Phase Diagram of the half full lattice obtained by means of the algebraic order parameter fluctuations.

be interesting to characterize transition from $p(2 \times 2)$ ordered phase to $p(2 \times 1)/p(1 \times 2)$ one as a response of varying the relative magnitude of competing interaction energies. For this reason we compute the Cowley [24] short range order parameter $\alpha = (\langle n_i n_j \rangle - \theta^2) / \theta(1 - \theta)$ versus intensity of R ratio for different temperatures of the system. The situation corresponds to crossing over the phase diagram. One distinguishes plateaus in the low temperature regime (Figure 4) that quantify the appearance of ordered structures in the lattice with a $p(2 \times 2)$ structure when $R < 0.5$ and a $p(2 \times 1)/p(1 \times 2)$ phase for $R > 0.5$.

Transition to the disordered phase is signalled by the intersection between the critical curve and the line of constant temperature. Extent of the plateaus increases by cooling while phase with mixed structures constitutes remarkable point. Jump in short range order parameter reflects the transition is first order. Then the central point presents bicritical behaviour and constitutes the only one way between the two ordered pure phases.

4. Conclusion

We can conclude from the results obtained that within the definition of the AOP it is possible to envisage—for the frustrated square lattice with repulsive interactions—a transition to an ordered phase with a mixture of structures constituted by ground state configurations of a same energy. This phase transition presents a bicritical behavior depending on whether the establishment phase is carried out by cooling at $R = 0.5$ or by varying the ratio of exchange constants at fixed temperature. AOP grandeur can also be applied to characterize ordinary ordered/disordered phase transition. The critical universal behavior for $R < 0.5$ is

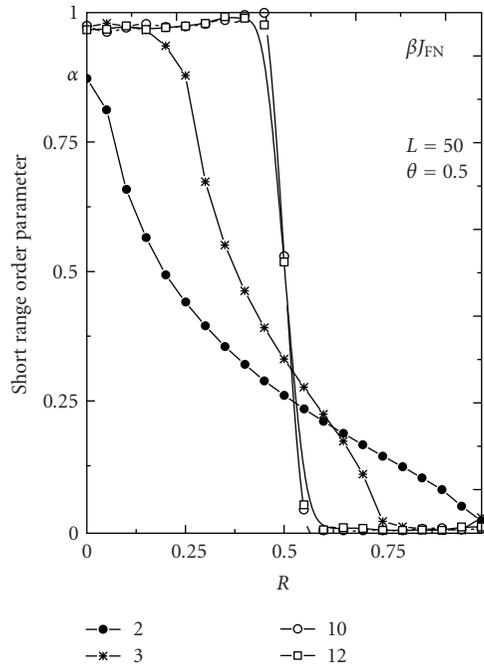


FIGURE 4: Behavior of short range order parameter while crossing the phase diagram. The curve shows bicritical character of the remarkable phase diagram central point.

found. For $R > 0.5$ the calculations lead to nonuniversal critical behavior and support then the absence of any first-order phase transition.

Acknowledgment

The authors are grateful to Pr. J. Prost for fruitful discussions and suggestions.

References

- [1] A. Malakis, S. S. Martinos, I. A. Hadjiagapiou, N. G. Fytas, and P. Kalozoumis, "Entropic sampling via Wang-Landau random walks in dominant energy subspaces," *Physical Review E*, vol. 72, no. 6, Article ID 066120, 2005.
- [2] A. Malakis, A. N. Berker, I. A. Hadjiagapiou, and N. G. Fytas, "Strong violation of critical phenomena universality: Wang-Landau study of the two-dimensional Blume-Capel model under bond randomness," *Physical Review E*, vol. 79, no. 1, Article ID 011125, 2009.
- [3] P. Carretta, M. Filibian, R. Nath, C. Geibel, and P. J. C. King, "Fluctuations and correlations in a frustrated $S = 1/2$ square lattice with competing ferromagnetic and antiferromagnetic interactions studied by muon-spin relaxation," *Physical Review B*, vol. 79, no. 22, Article ID 224432, 2009.
- [4] N. G. Fytas, A. Malakis, and I. Georgiou, "Wang-Landau study of the random bond square Ising model with nearest- and next-nearest-neighbor interactions," *Journal of Statistical Mechanics: Theory and Experiment*, vol. 2008, no. 7, Article ID L07001, 2008.
- [5] O. R. Salmon, J. R. de Sousa, and F. D. Nobre, "Phase diagram of the two-dimensional Ising model with random competing interactions," *Physics Letters A*, vol. 373, no. 30, pp. 2525–2528, 2009.
- [6] L. M. Volkova and S. A. Polyshchuk, "The study of nearest- and next-nearest-neighbour magnetic interactions in seven tetragonal compounds of V(IV) containing linear chains and square lattices," *Journal of Physics Condensed Matter*, vol. 18, no. 49, pp. 11177–11193, 2006.
- [7] A. A. Tsirlin and H. Rosner, "Extension of the spin-1/2 frustrated square lattice model: the case of layered vanadium phosphates," *Physical Review B*, vol. 79, no. 21, Article ID 214417, 2009.
- [8] H. V. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, "Fermi-liquid instabilities at magnetic quantum phase transitions," *Reviews of Modern Physics*, vol. 79, no. 3, pp. 1015–1075, 2007.
- [9] S. T. Bramwell, M. J. P. Gingras, and P. C. W. Holdsmorth, "Spin Ice," in *Frustrated Spin Systems*, H. T. Diep, Ed., p. 367, World Scientific, Singapore, 2005.
- [10] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, "Iron-based layered superconductor $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ ($x = 0.05 - 0.12$) with $T_c = 26$ K," *Journal of the American Chemical Society*, vol. 130, no. 11, pp. 3296–3297, 2008.
- [11] X. H. Chen, T. Wu, G. Wu, R. H. Liu, H. Chen, and D. F. Fang, "Superconductivity at 43 K in $\text{SmFeAsO}_{1-x}\text{F}_x$," *Nature*, vol. 453, no. 7196, pp. 761–762, 2008.
- [12] D. P. Landau, "Phase transitions in the Ising square lattice with next-nearest-neighbor interactions," *Physical Review B*, vol. 21, no. 3, pp. 1285–1297, 1980.
- [13] K. Binder and D. P. Landau, "Phase diagrams and critical behavior in Ising square lattices with nearest- and next-nearest-neighbor interactions," *Physical Review B*, vol. 21, no. 5, pp. 1941–1962, 1980.
- [14] A. Kalz, A. Honecker, S. Fuchs, and T. Pruschke, "Phase diagram of the Ising square lattice with competing interactions," *European Physical Journal B*, vol. 65, no. 4, pp. 533–537, 2008.
- [15] A. Kalz, A. Honecker, S. Fuchs, and T. Pruschke, "Monte Carlo studies of the Ising square lattice with competing interactions," in *Proceedings of the Conference on Highly Frustrated Magnetism*, Journal of Physics: Conference Series 145, (2009)012051, September 2008.
- [16] A. Malakis, P. Kalozoumis, and N. Tyraskis, "Monte Carlo studies of the square Ising model with next-nearest-neighbor interactions," *European Physical Journal B*, vol. 50, no. 1-2, pp. 63–67, 2006.
- [17] J. L. Monroe and S.-Y. Kim, "Phase diagram and critical exponent ν for the nearest-neighbor and next-nearest-neighbor interaction Ising model," *Physical Review E*, vol. 76, no. 2, Article ID 021123, 2007.
- [18] R. A. dos Anjos, J. Roberto Viana, and J. Ricardo de Sousa, "Phase diagram of the Ising antiferromagnet with nearest-neighbor and next-nearest-neighbor interactions on a square lattice," *Physics Letters A*, vol. 372, no. 8, pp. 1180–1184, 2008.
- [19] J. L. Moran-Lopez, F. Aguilera-Granja, and J. M. Sanchez, "Phase transitions in Ising square antiferromagnets with first- and second-neighbour interactions," *Journal of Physics: Condensed Matter*, vol. 6, no. 45, pp. 9759–9772, 1994.
- [20] D. J. Earl and M. W. Deem, "Parallel tempering: theory, applications, and new perspectives," *Physical Chemistry Chemical Physics*, vol. 7, no. 23, pp. 3910–3916, 2005.
- [21] J. Strečka, "Weak universality, bicritical points and reentrant transitions in the critical behaviour of a mixed spin-1/2 and spin-3/2 Ising model on the Union Jack (centered square) lattice," *Physica Status Solidi (B)*, vol. 243, no. 3, pp. 708–715, 2006.

- [22] J. Strečka, L. Čanová, and J. Dely, “Weak universal critical behaviour of the mixed spin-(1/2, S) Ising model on the Union Jack (centered square) lattice: integer versus half-odd-integer spin-S case,” *Physica Status Solidi (B)*, vol. 243, no. 8, pp. 1946–1955, 2006.
- [23] M. Noureddine, R. Nassif, K. Saadouni, and Y. Boughaleb, *International journal of Modern Physics B*, vol. 24, no. 23, Article ID 05530, 2010.
- [24] J. M. Cowley, “An approximate theory of order in alloys,” *Physical Review*, vol. 77, no. 5, pp. 669–675, 1950.



Hindawi

Submit your manuscripts at
<http://www.hindawi.com>

