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The Uniaxial Brickwork Model, Exact Results, and CVM Approximation

Alphonse Finel[1,2] and D. de Fontaine[1]

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A complete phase diagram of the uniaxial brickwork lattice is determined first by using exact results, and then by using the cluster variation method. Both results are in very good agreement, which demonstrates the reliability of the CVM for two-dimensional systems. A well-defined maximum in the exact specific heat and a divergence of the CVM susceptibility provide strong indication for the occurrence of a floating phase.

KEY WORDS: Hexagonal network model; floating phase.

The anisotropic next-nearest-neighbor Ising (ANNNI) model has been the object of many studies, since it is one of the simplest models for exhibiting commensurate or incommensurate modulated phases; for a recent review see Refs. 1, 2. In particular, much attention has been paid to the two-dimensional version of the model since there is some evidence for an incommensurate floating phase possessing no long-range order and characterized by algebraically decaying correlation functions.

The transition between the incommensurate phase and the disordered one is believed to be similar to that of the X–Y model. Dislocation-like spin configurations[(3,4)] (in the 2-d ANNNI model) play the role of the vortices of the Kosterlitz–Thouless theory.[(5,6)] As in the X–Y model, no exact results are presently available for the ordinary 2-d ANNNI model. This has led some authors[(7,8,9)] to the study of a new model, the uniaxial brickwork lattice (UBL) which is exactly soluble. The purpose of this Communication is twofold: to present evidence for the existence of a floating phase in the

[1] University of California, Department of Materials Science and Mineral Engineering, Berkeley, California 94720.
[2] Permanent Address: ONERA, BP72, 92322 Chatillon, Cedex, France.

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UBL, although it has been argued previously[8] that no such phase should exist in this case, and to compare the exact phase diagram to the one determined by the CVM. We shall determine the temperatures T_m where the transition between the floating and disordered phases occurs and the temperature T_2 where the susceptibility diverges. But first, the locus of second-order transitions T_c between disordered and ordered phases will be determined. Temperatures T_c and T_m, as functions of interaction parameter ratios, are determined exactly, T_2 in an approximate manner. There will result a complete phase diagram.

The UBL is represented in Fig. 1. Along the vertical direction, connected nearest-neighbors interact with ferromagnetic ($J_0 < 0$) coupling while, along the horizontal direction, ferromagnetic interactions between nearest neighbors (alternatively J_1 and J_3) compete with antiferromagnetic interactions ($J_2 > 0$) between next-nearest neighbors. If $|J_3| \leqslant |J_1|$, the ground state is ferromagnetic for $K = J_2/|J_3| < \frac{1}{2}$ and goes over, for $K > \frac{1}{2}$, to a $\langle 2 \rangle$ antiphase state (see Fig. 1). The point $K = \frac{1}{2}$ is infinitely degenerate. Unlike the second ANNNI model, there is no crossing between interactions J_0 and J_2; the UBL is then a planar Ising model which is exactly soluble. The partition function can be evaluated by a generalization of the Kac and Ward method,[10] equivalent to the Pfaffian method used in Refs. 7 and 8. For the singular part of the free energy, we obtain

$$F_{\text{sing}} = -\frac{k_B T}{4} \int_0^1 \int_0^1 \ln \det M(p, q, J_i, t)\, dp\, dq \tag{1}$$

where J_i represents the set (J_0, J_1, J_2, J_3) and $M(p, q, J_i, T)$ is a 10×10 matrix (this matrix is smaller than the one used in the Pfaffian method).

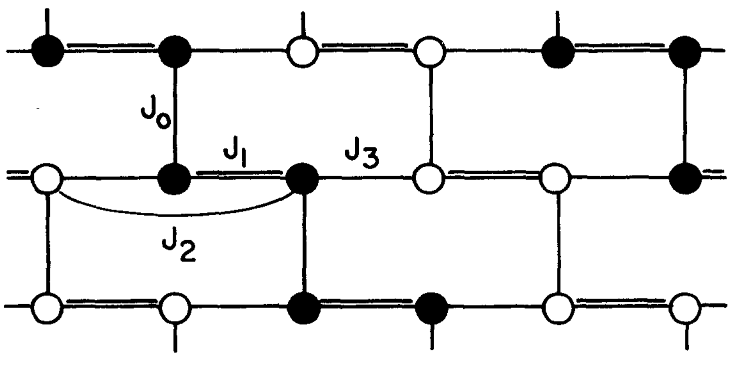

Fig. 1. The uniaxial brickwork lattice. Full circles (open) represent "up" ("down") spins in the $\langle 2 \rangle$ phase.

Our first purpose is to determine the lines of second-order phase transitions, T_c. The only possibility for F to be singular for any values of the interactions J_i and T is given by setting det $M(p, q, J_i, T) = 0$. If $J_1 = J_3$, we find only one critical temperature for $K < \frac{1}{2}$ and no transition for $K > \frac{1}{2}$ due to infinite degeneracy at $T = 0$. If $J_1 \neq J_3$, this degeneracy is removed and there is one and only one critical temperature for all K (with $T_c = 0$ for $K = \frac{1}{2}$). These results agree with those of Refs. 7–9. In order to handle the entire range of frustration effects ($K = 0$ to ∞) we introduce a different parameter α to determine the competing effect along the anisotropic direction

$$J_2/J_0 = -\alpha, \qquad J_3/J_0 = 1 - \alpha, \qquad J_1/J_0 = 1$$

Thus, as α varies from 0 to 1, our model changes continuously from a honeycomb lattice at $\alpha = 0$ to a square lattice at $\alpha = 1$ with isotropic nearest-neighbor interactions. The results are summarized in the phase diagram presented in Fig. 2, where we note that the transition lines $T_c(\alpha)$ go down to the multiphase point $\alpha = \frac{1}{3}$, $T = 0$.[3]

[3] T_c is given by $p = q = 0$ for $\alpha < \frac{1}{3}$, $p = q = \frac{1}{4}$ for $\alpha > \frac{1}{3}$; this is related to the ground states: ferromagnetic phase for $\alpha < \frac{1}{3}$ and $\langle 2 \rangle$ phase for $\alpha > \frac{1}{3}$.

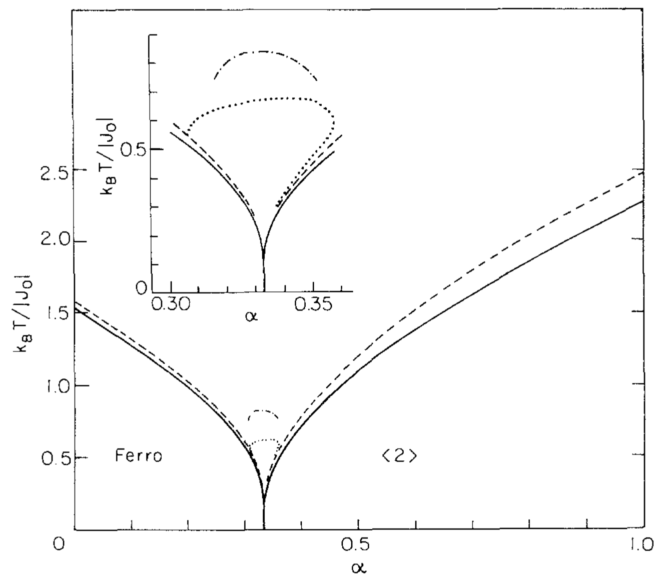

Fig. 2. Phase diagram of the uniaxial brickwork model. Full lines represent the exact critical temperatures T_c, dashed lines the CVM results. The exact locations $T_m(\alpha)$ of maxima of the specific heat are shown by the dot-dashed line, and $T_2(\alpha)$ by the dotted line. The insert shows the region of the multiphase point $\alpha = \frac{1}{3}$ on an expanded scale.

Up to this point, and according to the previous analysis in terms of nonanalycity of the free energy, the phase diagram of the UBL seems not to display a floating phase. However, the transition between a floating phase and the disordered one could be of an unusual type. Inside a floating phase, by definition, the pair correlation function $\xi(\mathbf{R})$ follows an algebraic decay law[11]

$$\xi(\mathbf{R}) \simeq |\mathbf{R}|^{-\eta} \cos k_0 \cdot \mathbf{R} \tag{2}$$

where $\mathbf{R}$ is a lattice vector and k_0 a wave vector which defines the modulation in the floating phase. In all generality, the singular exponent η and k_0 are functions of T and the parameter α. If the analogy with the X–Y model is relevant, there is in fact no reason a priori for the transition between the floating and the disordered phases to give rise to a singularity in the free energy as a function of T. A rigorous analysis of the X–Y model by Zittartz[12] has shown that the singular exponent $\eta(T)$ which governs the algebraic decay of the correlation functions is a smooth monotonic function of T which increases from 0 at $T=0$ and diverges for some T_m, the transition temperature between the floating phase and the disordered one. This indicates presumably a rather smooth change to exponential decay above T_m, leading Zittartz to conclude that the free energy is analytic in T except possibly weakly singular at T_m, where $F(T)$ is, however, infinitely differentiable. The specific heat is then a smooth (possibly analytic) function in agreement with the results of a Monte Carlo study of the X–Y model.[14] An exact treatment[13] of an approximate analogy of the X–Y model with a two-dimensional plasma[5,13] confirms this general picture. In previous studies of the two-dimensional ANNNI model[3] and the asymmetric three-state clock model[15] using Monte-Carlo simulations, it was shown that a transition between a floating phase and the disordered one was related to a broad maximum in the specific heat curve. We suggest that this maximum is related to the smooth change of law for the pair correlation function.

Our purpose is then to determine the exact specific heat and to determine whether there exists, besides the singularity at T_c and for some values of α, a maximum which, according to the analysis presented above, could well correspond to a change in decay law, and hence would mark the transition to the floating phase. We shall denote by $T_m(\alpha)$ the temperatures at which such a maximum occurs. If a maximum does exist and corresponds to a transition between a floating phase and the disordered one, the susceptibility $\chi(k)$ in k space should diverge for $\eta(\alpha, T) \leqslant 2$ and $k = k_0$, according to (2). Therefore, as the temperature is lowered, the susceptibility should first become infinite for some temperature, say T_2, smaller than T_m. For

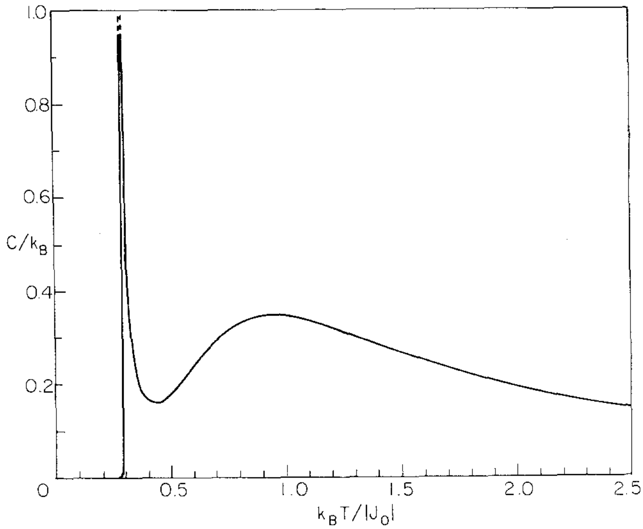

Fig. 3. Exact specific heat curve for $J_1/|J_0| = -1.1$, $J_2/|J_0| = 0.55$, $J_3/|J_0| = -1$ $(J_0 < 0)$. The exact critical temperature is $k_B T/|J_0| = 0.2880$.

fixed α, we denote by $T_2(\alpha)$ and $k_2(\alpha)$ the temperature and k vector at which this divergence takes place.

In order to determine the specific heat $C = -T(\partial^2 F/\partial T^2)$, we have to evaluate numerically the integral in (1) and to differentiate twice with respect to T.[4] We present a typical result of the specific heat in Fig. 3. Besides the singularity at T_c, a well-defined maximum exists at T_m. In Fig. 2, we report the temperatures where these maxima occur as a function of α. For $\alpha < 0.316$ and $\alpha > 0.352$ the specific heat curve no longer shows this well-defined maximum, but there still exists a broad shoulder on the specific heat curve, indicating that the maximum of the specific heat could be hidden by the singularity at T_c. The determination of the specific heat maximum T_m does not unambiguously prove the existence of the floating phase, however. To accomplish that, it would be necessary to establish that correlations decay according to the algebraic law (2), which cannot be done readily within the present framework. Instead, we shall determine $T_2(\alpha)$, the temperature at which the susceptibility $\chi(k)$ diverges, according

[4] As F is evaluated numerically, we have to use a discrete method to determine the specific heat $C = -T(\Delta^2 F/\Delta T^2)$. The error is expected to be small except near the critical temperature. This is verified as follows: We determine C first with $\Delta T = 10^{-1}$ and $\delta F = 10^{-4}$ (precision on the numerical value of F) and then with $\Delta T = 10^{-2}$ and $\delta F = 10^{-6}$. The difference between the results is always smaller than 10^{-2} for $|T - T_c| > 5 \times 10^{-2}$. We used Gauss integration to evaluate F.

to an approximate method, the cluster variation method (CVM). The technique used for calculating the susceptibility is described briefly in a companion paper.[16]

The approximate CVM entropy was determined by using two clusters: centered lozenge and rectangle.[5] First, the accuracy of the CVM must be established. For that purpose, a critical test is provided by how well the critical lines of second-order transitions for the ferromagnetic and $\langle 2 \rangle$ phases are reproduced. A second-order transition between the disordered phase and an ordered one is characterized by the divergence of the susceptibility $\chi(k)$ for the k vector which determines the periodicity of the ordered phase. Hence, if k^x and k^y are the components of the k vector (in units of $2\pi/a$), the critical lines T_c are located at temperatures where $\chi(k)$ becomes infinite at $k^x = k^y = 0$ for the ferromagnetic phase and at $k^x = k^y = \frac{1}{4}$ for the $\langle 2 \rangle$ phase. The results are presented in Fig. 2. The agreement with the exact results is very good, especially near $\alpha = \frac{1}{3}$.

The interesting question now is to find out whether the susceptibility diverges for some k vector in the region of the phase diagram between the ferromagnetic and the $\langle 2 \rangle$ phases, where maxima of the specific heat were located. As explained above, this divergence should take place at T_2 smaller than T_m. Moreover, we expect the k value for which $\chi(k)$ is (first) infinite when T is lowered to be a continuous function of α. For fixed α, we find that the k vector where the susceptibility reaches its maximum varies continuously with T. The maximum increases as T decreases and eventually becomes infinite. We report in Fig. 2 the temperatures $T_2(\alpha)$ and in Fig. 4 the k vectors $k_2(\alpha)$ where this divergence occurs. On the ferromagnetic side, the $T_2(\alpha)$ curve meets the CVM critical line for $\alpha = 0.306$, which indicates a direct transition between the ferromagnetic and floating phases for α between 0.306 and $\frac{1}{3}$. Therefore, we expect the existence of a Lifshitz point, namely a point where the floating, disordered, and ferromagnetic phases meet. As the transition between the floating and disordered phases is indicated by the maximum of the specific heat, the Lifshitz point should be located where $T_m(\alpha)$ intersects the line separating the ferromagnetic and floating phases. By extrapolating the exact curve $T_m(\alpha)$, we surmise that the Lifshitz point should be close to $\alpha = 0.306$. On the $\langle 2 \rangle$ side, $T_2(\alpha)$ seems to drop down to $\alpha = \frac{1}{3}$ where it meets the CVM transition line for the $\langle 2 \rangle$ phase. Therefore, it is possible for the exact $T_m(\alpha)$ curve to drop down to the multiphase point $\alpha = \frac{1}{3}$, through the small gap between $T_2(\alpha)$ and the $\langle 2 \rangle$ phase boundary. Hence, we can draw no conclusion concerning the existence of a Lifshitz point on the $\langle 2 \rangle$ side of the phase diagram. Due to the particular topology of the UBL, a modulation along the anisotropy

[5] The choice of these clusters was proposed to us by R. Kikuchi and J. Kulik.

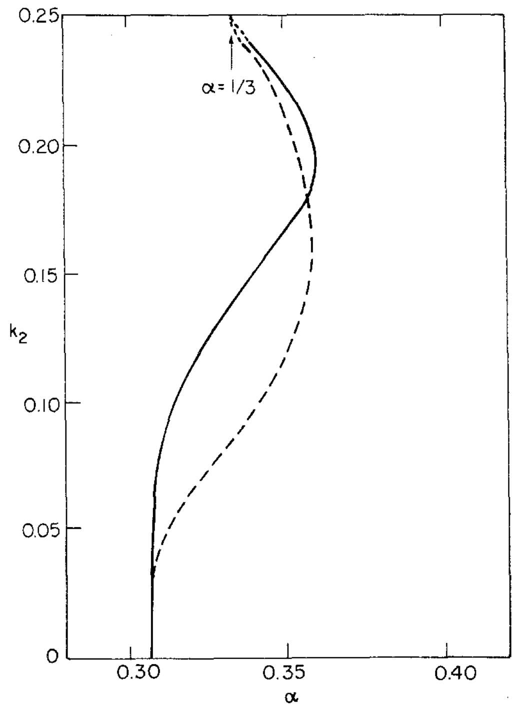

Fig. 4. Variation of the components of $k_2(\alpha)$ (in units of $2\pi/a$) along the line $T_2(\alpha)$. The full line represents k_2^x, the dashed one k_2^y.

direction creates another modulation along the perpendicular axis if $J_1 \neq J_3$. Thus, two components of $k_2(\alpha)$ are reported in Fig. 4. The two curves are continuous functions, which indicates that k_2^x and k_2^y are incommensurate almost everywhere. The lines come together for $\alpha = 0.306$, with $k_2^x = k_2^y = 0$ as $T_2(\alpha)$ meets the transition line of the ferromagnetic phase. At the other end, they also seem to meet for $\alpha = \frac{1}{3}$ with $k_2^x = k_2^y = \frac{1}{4}$.

In conclusion, we have shown the existence of a well-defined maximum in the specific heat of the UBL for suitable values of the interaction parameters. By using the CVM, we have related this maximum to the divergence of the susceptibility at lower temperatures, supporting the idea that a floating phase is present in this model. The comparison between the exact and the CVM results for the critical lines proves that the CVM is an effective and accurate method, even in two-dimensional space. Two-dimensional ANNNI model results are reported in a companion paper in this volume.

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REFERENCES

1. W. Selke, in *Nato Advanced Study Institute on Modulated Structure Materials*, T. Tsakalakos, ed. (Maleme-Chania, Crete, 1983).
2. D. de Fontaine and J. Kulik, *Acta Metall.* **33**:145 (1985).
3. W. Selke and M. E. Fisher, *Z. Physik* **B40**:71 (1980); W. Selke, *Z. Physik* **B43**:335 (1981).
4. J. Villain and P. Bak, *J. Physique* **42**:657 (1981).
5. J. M. Kosterlitz and D. J. Thouless, *J. Phys.* **C6**:1181 (1973).
6. J. M. Kosterlitz, *J. Phys.* **C7**:1046 (1974).
7. R. Bidaux and L. de Seze, *J. Phys.* **42**:371 (1981).
8. I. Morgenstern, *Phys. Rev.* **B26**:5296 (1982); I. Morgenstern, *Phys. Rev.* **B29**:1458 (1984).
9. W. F. Wolff and J. Zittartz, *Z. Physik* **B49**:139 (1982).
10. M. Kac and J. C. Ward, *Phys. Rev.* **88**:1332 (1952).
11. D. R. Nelson and B. I. Halperin, *Phys. Rev.* **B19**:2457 (1979).
12. J. Zittartz, *Z. Physik* **B23**:55 (1976).
13. J. Zittartz, *Z. Physik* **B23**:63 (1976).
14. J. Tobochnik and G. V. Chester, *Phys. Rev.* **B20**:3761 (1979).
15. W. Selke and J. M. Yeomans, *Z. Physik* **B46**:311 (1982).
16. A. Finel and D. de Fontaine, *J. Stat. Phys.* **43**:645 (1986).