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LETTER TO THE EDITOR

Honeycomb Ising antiferromagnet in a magnetic field: interface tension and critical temperature

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Abstract. By extending the method due to Müller-Hartmann and Zittartz, we calculate the interface tension for the nearest-neighbour antiferromagnetic ising model on the honeycomb lattice at finite magnetic fields. The calculation reproduces exact interface tension at zero field. From the zero point of the interface tension we derive a compact analytic form of the 'critical frontier' in the (H, T) plane (H: magnetic field, T: temperature), which agrees excellently with the recent 'quasi-analytical' result presented by Wu, Wu and Blöte.

The phase diagram of the two-dimensionl (2D) antiferromagnetic (AF) nearest-neighbour (NN) Ising model on square lattice was investigated by Müller-Hartmann and Zittartz (MZ) (1977). They presented an analytic form for the 'critical frontier' separating regimes of ordered and disordered phases in the (H, T) plane where H is external field and T is temperature. The analytic form derived by MZ reproduces the exact results at zero field (Onsager 1944) and the exact critical field at zero temperature. Even at non-zero magnetic field, the form is in close agreement with results obtained by other methods (Rapaport and Domb 1971, Rapaport 1978, Sneddon 1979). Thus, the analytic form is conjectured to be exact, and the MZ method is believed to produce reliable results for other models (Lin and Wu 1979). For other 2D lattices with non-trivial unit cell structure, the naive application (Slotte and Hemmer 1985) of the MZ method have not succeeded in giving a satisfactory result for the critical frontier. In this letter, for the NN honeycomb AF Ising model, we calculate the interface tension and derive a closed form of the critical frontier in the (H, T) plane. The present method is the same as that of MZ in spirit, but is extended so as to handle the unit cell structure of the honeycomb lattice properly. We shall show that our result reproduces the exact interface tension and critical temperature at zero field (Wannier 1945, Fisher and Ferdinand 1967, Zia 1986). We shall also show that, for general (H, T), the present result is in excellent agreement with the recent 'quasi-analytical' result of Wu, Wu and Blöte (WWB) (1989) where numerical calculation is combined with mapping of the model into the honeycomb eight-vertex model.

Consider an Ising antiferromagnet on a honeycomb lattice. Expecting Néel-state spin configuration at low temperatures, we decompose the honeycomb lattice into two triangular sublattices A and B. The Hamiltonian $\mathcal{H}$ of the system with the NN coupling constant J and the external field H is

$$\mathcal{H} = \sum_{i=1}^{N/2} \sum_{j} \left[J\sigma_{A_i}\sigma_{B_j} - (\sigma_{A_i} + \sigma_{B_j})\frac{H}{z} \right] \qquad (\sigma_A, \sigma_B = \pm 1) \tag{1}$$

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where N is total number of lattice sites, σ_{A_i} (respectively σ_{B_i}) is the Ising spin variable at the A (respectively B) sublattice site i, and $z=3$ is the NN coordination number of the honeycomb lattice. In the above, i runs over all A sublattice sites whereas j runs over B sublattice sites adjacent to the A sublattice site i. Note that the terms in a square bracket gives an energy per bond. For NN spin combinations $(\sigma_{A_i}, \sigma_{B_j}) = (\pm 1, \mp 1)$, the energy per bond is $E_b = -J$, and for combinations $(\pm 1, \pm 1)$, $E_b = J \mp (2/z)H$. The ground state combination $(\sigma_{A_i}, \sigma_{B_j})$ depends on H. When $|H|$ is less than the critical value $H_c(T=0) = zJ$, combinations $(\pm 1, \mp 1)$ are selected for the ground state and $(\pm 1, \pm 1)$ are considered as excited states. We introduce 'excited bond strengths' w_+ and w_- as

$$w_- = \frac{1}{k_B T}\left(2J - \frac{2}{z}H\right) \qquad w_+ = \frac{1}{k_B T}\left(2J + \frac{2}{z}H\right) \tag{2}$$

where k_B is the Boltzmann constant.

Let us set a grid upon the honeycomb lattice as shown in figure 1. Impose a proper boundary condition so that a phase separation line, an interface between the two co-existing phases, runs across the lattice. We calculate the interface tension under the solid-on-solid (SOS) approximation (Temkin 1966) where the 'overhang' interface configurations are discarded. It should be remarked that the SOS approximation often reproduces exact 1D interface tensions if the orientation of the interface is appropriately chosen (Müller-Hartmann and Zittartz 1977, Chalheiros *et al* 1987). We describe the SOS interface configuration by a set of variables $\{h_x, h'_x, \alpha_x, \alpha'_x\}$, where h_x (respectively h'_x) is the unit-cell height at the horizontal site x (respectively x'), and α_x (respectively α'_x) $= A$ or B denotes the position in the unit cell. The interface Hamiltonian $\mathcal{H}_I$ is then expressed as

$$\frac{1}{k_B T}\mathcal{H}_I = \sum_{x=0}^{n} [V_{\alpha_x,\alpha'_x}(h_x - h'_x) + V'_{\alpha'_x,\alpha_{x+1}}(h'_x - h_{x+1})] \tag{3}$$

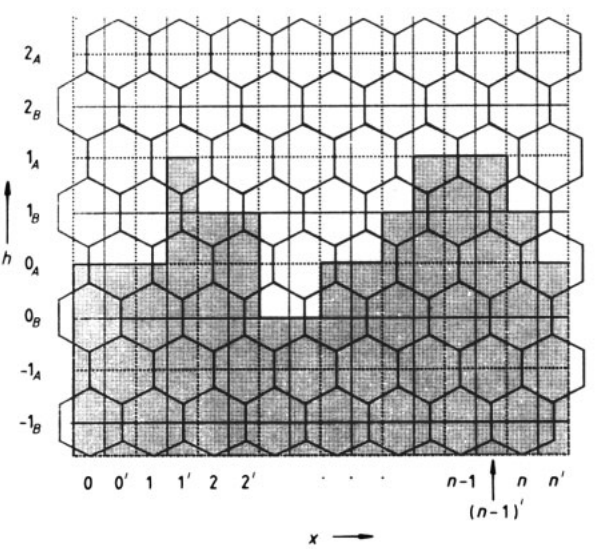

Figure 1. Example of interface configuration. We set a rectangular grid over the honeycomb lattice to indicate column site (horizontal direction) and interface height (vertical direction). The non-trivial unit cell structure of the honeycomb lattice is considered by 'inner degree of freedom' (A or B) for heights and by primes for column site positions.

where n is a half of the total number of columns, $\{V_{\alpha,\beta}(h)\}$ and $\{V'_{\alpha,\beta}(h)\}$ are:

$$V_{A,A}(h) = \frac{w_+}{2} + |h|(w_+ + w_-)$$

$$= V_{B,B}(h) = V'_{A,A}(h) = V'_{B,B}(h) \tag{4a}$$

$$V_{A,B}(h) = \begin{cases} 2w_+ + (h-1)(w_+ + w_-) & (h > 0) \\ 2w_+ + |h|(w_+ + w_-) & (h \leq 0) \end{cases} \tag{4b}$$

$$V_{B,A}(h) = \begin{cases} w_- + h(w_+ + w_-) & (h \geq 0) \\ w_- + |h+1|(w_+ + w_-) & (h < 0) \end{cases} \tag{4c}$$

$$V'_{A,B}(h) = \begin{cases} w_- + (h-1)(w_+ + w_-) & (h > 0) \\ w_- + |h|(w_+ + w_-) & (h \leq 0) \end{cases} \tag{4d}$$

$$V'_{B,A}(h) = \begin{cases} 2w_+ + h(w_+ + w_-) & (h \geq 0) \\ 2w_+ + |h+1|(w_+ + w_-) & (h < 0). \end{cases} \tag{4e}$$

The interface partition function is

$$Z_n = \sum_{\{h_\chi, h'_\chi\} = -\infty}^{\infty} \sum_{\{\alpha_\chi, \alpha'_\chi\} = A,B} \exp[-\mathcal{H}_1 / k_B T] \qquad (h_0 = 0) \tag{5}$$

from which the interface tension $\gamma(H, T)$ is calculated as

$$\gamma(H, T) = -k_B T \lim_{n \to \infty} \frac{1}{n} \ln Z_n. \tag{6}$$

The partition function Z_n is re-expressed in terms of transfer matrices $\mathscr{Z}$ and $\mathscr{Z}'$ after taking a partial sum with respect to $\{h_x\}$ and $\{h'_x\}$:

$$Z_n = \sum_{\alpha_n} \langle \alpha_0 | (\mathscr{Z} \cdot \mathscr{Z}')^n | \alpha_n \rangle \tag{7}$$

where

$$\mathscr{Z}_{\alpha,\beta} = \sum_h \exp[-V_{\alpha,\beta}(h)] \qquad \mathscr{Z}'_{\alpha,\beta} = \sum_{h'} \exp[-V'_{\alpha,\beta}(h')]. \tag{8}$$

More explicitly,

$$\mathscr{Z} = \begin{pmatrix} \mathscr{Z}_1 & \mathscr{Z}_3 \\ \mathscr{Z}_4 & \mathscr{Z}_1 \end{pmatrix} \qquad \mathscr{Z}' = \begin{pmatrix} \mathscr{Z}_1 & \mathscr{Z}_4 \\ \mathscr{Z}_3 & \mathscr{Z}_1 \end{pmatrix} \tag{9}$$

$$\mathscr{Z}_1 = \exp\left(-\frac{w_+}{2}\right)\left(\frac{1 + \exp(-w_+ - w_-)}{1 - \exp(-w_+ - w_-)}\right) \tag{10a}$$

$$\mathscr{Z}_3 = \frac{2\exp(-2w_+)}{1 - \exp(-w_+ - w_-)} \tag{10b}$$

$$\mathscr{Z}_4 = \frac{2\exp(-w_-)}{1 - \exp(-w_+ - w_-)}. \tag{10c}$$

It is interesting to note that the system described by the combined transfer matrix $\mathscr{Z} \cdot \mathscr{Z}'$ is equivalent to a one-dimensional Ising model in a staggered field with the Hamiltonian:

$$\mathscr{H}^{(1D)} = -J^{(1D)} \sum_i \sigma_i \sigma_{i+1} - H^{(1D)} \sum_{i:\text{even}} \sigma_i + H^{(1D)} \sum_{i:\text{odd}} \sigma_i \tag{11}$$

where

$$J^{(1D)} = k_B T \tfrac{1}{4} \log \frac{\mathscr{Z}_1^2}{\mathscr{Z}_3 \mathscr{Z}_4} \ (>0) \qquad H^{(1D)} = k_B T \tfrac{1}{2} \log \frac{\mathscr{Z}_3}{\mathscr{Z}_4}. \tag{12}$$

The maximum eigenvalue λ of the transfer matrix $\mathscr{Z} \cdot \mathscr{Z}'$ is

$$\lambda = \left[\sqrt{\mathscr{Z}_1^2 + \left(\frac{\mathscr{Z}_3 - \mathscr{Z}_4}{2} \right)^2} + \frac{\mathscr{Z}_3 + \mathscr{Z}_4}{2} \right]^2. \tag{13}$$

From equation (6), we obtain $\gamma(H, T)$ as

$$\gamma(H, T) = -k_B T \ln \lambda. \tag{14}$$

In particular at $H = 0$, we have

$$\gamma(0, T) = 2J - 2k_B T \ln \left[\frac{1}{2 \sinh K} \left(\sqrt{4 \sinh^2 K + 1} + 1 \right) \right] \tag{15}$$

which reproduces the exact expression (Zia 1986).

Let us proceed to derive the analytic form of the critical frontier from condition $\gamma(H, T) = 0$, i.e. $\lambda = 1$. From equation (13), we have

$$\mathscr{Z}_1^2 = (1 - \mathscr{Z}_3)(1 - \mathscr{Z}_4). \tag{16}$$

Substituting (10) into (16), we have

$$\cosh\left(\frac{w_+ + w_-}{2} \right) - 2 \cosh\left(\frac{w_+ - w_-}{2} \right) = 0. \tag{17}$$

Note that the equation (17) explicitly shows that the critical frontier is symmetric in w_+ and w_-. Inserting (2) into (17), we obtain an equation to determine the critical frontier

$$2 \cosh(\tfrac{2}{3} L) = \cosh 2K \tag{18}$$

or, equivalently,

$$L = \tfrac{3}{2} \ln[\tfrac{1}{2} \cosh 2K \pm \sqrt{\tfrac{1}{4} \cosh^2 2K - 1}]. \tag{18'}$$

where $L = H/k_B T$ and $K = J/k_B T$. We show the curve (18) in figure 2.

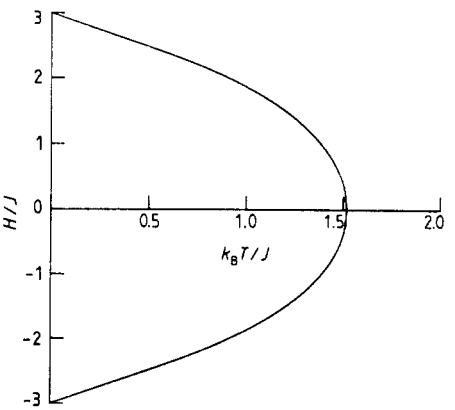

Figure 2. Critical frontier in the (H, T) plane obtained from equation (18). There is no perceptible difference between this curve and that of Wu *et al* (1989).

Table 1. Critical values of $L = H/k_B T$. The present results are shown in the second column. For comparison, values of Wu *et al* (1989) are listed in the third column.

	L	
K	Equation (18)	Wu *et al* 1989
0.7	0.579 082 014	0.582 429 186
0.8	1.114 082 143	1.119 888 647
0.9	1.513 520 819	1.520 610 887
1.0	1.868 121 505	1.875 996 047
1.2	2.521 452 338	2.530 156 031
1.5	3.448 969 759	3.458 127 977

In the $L \to 0$ limit, the exact critical temperature (Wannier 1945) $k_B T_c/J = 2/\ln(2+\sqrt{3})$ is obtained from (18). In the $T \to 0$ limit, the exact critical field $H_c = \pm 3J$ is also reproduced. In the second column of table 1, we show the values of critical fields calculated from (18) for several temperatures. In the third column, the results of WWB (1989) are shown. Our results are in good agreement with those of WWB within 1%. The slope of the critical frontier near $T = 0$ is $\pm(3/2)\ln 2 = \pm 1.0397$, which is also consistent with the value $\pm 1.030\,3701$ obtained by WWB.

We have seen that our approximate treatment gives a fairly simple but accurate formula (18) for the critical frontier. We must say, however, that (18) may not be exact for $H \neq 0$; the discrepancy ($\sim 1\%$) far exceeds the numerical error ($\sim 10^{-8}$) of WWB. Morevoer, (18) does not satisfy the $n = 4$ critical condition $f_{4+}(a, b, c, d) = 0$ in WWB (see equations (10) and (14) of Wu *et al* (1989)).

The present honeycomb AF Ising model can be mapped to a two-component lattice gas model on the {111} surface of GaAs. The field H then relates to the partial vapour pressure. Since a step of unit height on the surface can be regarded as a 1D interface, the interface tension obtained in this letter gives the step tension for various partial vapour pressure. The critical frontier gives an estimate of roughening temperature T_R (Jayaprakash *et al* 1983, Akutsu and Akutsu 1987) of the {111} surface as a function of the partial vapour pressure. The partial-vapour-pressure dependence of T_R, which has been actually observed in Ag_2S (Ohachi and Taniguchi 1983, 1988), is a common feature of two- (or more-) component systems. With suitable extension of the present treatment introducing extra 'inner degrees of freedom' (like $\{\alpha_x\}$), we can calculate the interface tension for various realistic systems with complicated unit cell structure.

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