PHYSICAL REVIEW B VOLUME 37, NUMBER 7 1 MARCH 1988

Interface at general orientation in a two-dimensional Ising model

D. B. Abraham
Department of Theoretical Chemistry, 1 South Parks Road, Oxford, OX1 3TG, England

P. J. Upton
Department of Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, England
(Received 12 November 1987)

The magnetization profile of a two-dimensional Ising model, containing an interface with general orientation, is obtained exactly in the thermodynamic limit for all subcritical temperatures. At zero temperature the interface is found to be *rough* if it is not oriented in one of the lattice directions. The results are compared with those of a construction of the Wulff type.

Recently there has been much interest in the statistical mechanics of two-dimensional interface models. In particular, it has been proposed[1,2] that the rms displacement $w(\theta)$ of an interface, whose mean position is at an angle of θ from one of the axial lattice directions is given by

$$w^2(\theta)=L[\tau(\theta)+\tau''(\theta)]^{-1}\;, \tag{1}$$

where L is its mean length and $\tau(\theta)$ is its angle-dependent surface tension. This is a generalization of an earlier observation by Fisher *et al.*[3] for $\theta=0$ which was obtained from fluctuation theory and an exact result.[4,5] Akutsu and Akutsu[1] showed that (1) it is true for the solid-on-solid model and assumed its validity for the Ising model. De Coninck and Ruiz considerated generalizations of the solid-on-solid model.[2]

In this Rapid Communication we demonstrate that (1) is indeed correct for the two-dimensional Ising model using exact methods. We provide only a brief account of the calculation here, leaving details to a further publication.[6] We start by defining the model.

Spin-$\frac{1}{2}$ Ising spins occupy sites (n,m) of a $2N\times M$ square lattice Λ and interact through the following Hamiltonian

$$\mathcal{H}_\Lambda\{\sigma\}=-J\sum_{n,m}\sigma_{n,m}(\sigma_{n+1,m}+\sigma_{n,m+1})\;,$$
$$\sigma_{n,m}=\pm 1,\; J>0\;. \tag{2}$$

An interface is introduced into the system by imposing boundary conditions along all four edges of Λ as shown in Fig. 1. Let Z_Λ^{+-} be the canonical partition function for the system with the interfacial boundary conditions and Z_Λ^{+} be that for the same lattice with all boundary spins set at $\sigma_{n,m}=+1$. Then the surface tension is defined by

$$\tau(\theta)=-\lim_{N\to\infty}(2N\sec\theta)^{-1}\lim_{M\to\infty}\ln(Z_\Lambda^{+-}/Z_\Lambda^{+}) \tag{3}$$

and the magnetization at position $(n=\beta N,\; m=p)$ is defined as

$$m(\beta N,p)=\lim_{M\to\infty}\langle\sigma_{\beta N,p}\rangle,\quad -1<\beta<1\;, \tag{4}$$

where $\langle\cdots\rangle$ denotes the ensemble average with respect to (2). $\tau(\theta)$ has already been evaluated by Abraham and Reed[7] and a partial result along the lines of (4) was stated there. In order to evaluate (4) we use a transfer matrix method.[5,8] Cyclic boundary conditions are set up by introducing a second interface into the system passing through boundary spins at $(n,m)=(-N,s)$ and $(n,m)=(N,t+s-1)$ and then joining the two horizontal edges together to produce a cylinder of circumference M. The single-interface properties are then recovered by taking $s\to\infty$. A transfer matrix V operates in the direction parallel to the symmetry axis of the cylinder from which we can write

$$m(\beta N,p)=\lim_{s\to\infty}\lim_{M\to\infty}\Sigma_M(s\,|\,\beta N,p)/Z_M^{+-}(s)\;, \tag{5a}$$

$$\Sigma_M(s\,|\,\beta N,p)=\langle -\,|\,R_1(s)V^{(1+\beta)N}\sigma_p^xV^{(1-\beta)N}R_t(s)\,|\,-\rangle\;, \tag{5b}$$

$$Z_M^{+-}(s)=\langle -\,|\,R_1(s)V^{2N}R_t(s)\,|\,-\rangle\;, \tag{5c}$$

$$V=V_2^{1/2}V_1V_2^{1/2},\quad V_1=\exp\left(-K^*\sum_1^M\sigma_j^z\right)\;,$$
$$V_2=\exp\left(K\sum_1^M\sigma_j^x\sigma_{j+1}^x\right)\;, \tag{5d}$$

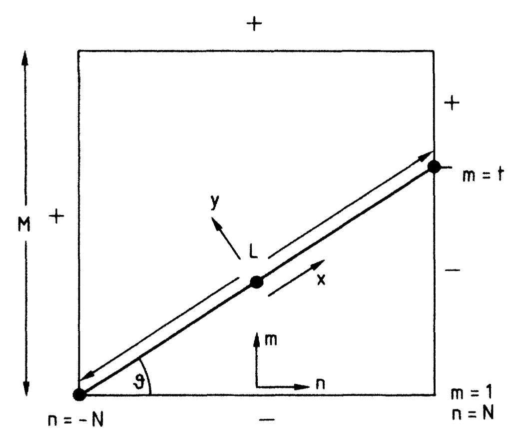

FIG. 1. The boundary conditions of the lattice under consideration. Spins along edges labeled + (−) are kept in the up (down) state. Here and throughout this Rapid Communication $t=2N\tan\theta$.

where $K=J/k_BT$ and $\exp(-2K^*)=\tanh K$. σ_j^a are the usual Pauli matrices operating on the direct product of M two-dimensional Hilbert spaces. $|-\rangle$ is defined as the state where $\sigma_j^x|-\rangle=-|-\rangle$ for $1\le j\le M$. $R_i(s)$ is the block rotation operator which, when applied to $|-\rangle$, reverses all spins from i to $i+s$ inclusive. $\Sigma_M(s\,|\,\beta N,p)$ and $Z_M^{+-}(s)$ are evaluated using Ref. 8 and the standard fermion methods of Schultz *et al.*[9]

A Jordan-Wigner transformation is used to convert the system into one involving fermions. As usual, one has to separate V into V_+ and V_- which operate on states containing only even and odd numbers of fermions, respectively. Equation (5b) then becomes

$$\Sigma_M(s\,|\,\beta N,p)=\tfrac{1}{2}\sum_{\epsilon=-,+}\langle\Phi_\epsilon^0|\,R_1(s)V_\epsilon^{(1+\beta)N}\sigma_p^x V_{-\epsilon}^{(1-\beta)N}R_t(s)\,|\Phi_{-\epsilon}^0\rangle \tag{6}$$

and similarly for $Z_M^{+-}(s)$. $|\Phi_\epsilon^0\rangle$ is the state associated with the largest eigenvalue of V_ϵ. The translational symmetry of the system is exploited by Fourier transforming the fermion operators and writing $\sigma_p^x=T^{-p}\sigma_1^xT^p$, $R_t(s)=T^{-t}R_1(s)T^t$ where T is the linear translation operator. $V_\pm$ is diagonalized by using the Bogoliubov-Valatin transformation which produces new fermion operators $G^\dagger(\alpha_i)$, $G^\dagger(-\beta_i)$ $(i=1,2)$ where $\alpha_i(\beta_i)$ is the wave number belonging to a state containing odd (even) number of fermions in the site representation. It now follows that the $\epsilon=-$ term in (6) (and similarly for $\epsilon=+$) becomes

$$\begin{aligned}\tfrac{1}{4}\sum_{\alpha_1\alpha_2\beta_1\beta_2}&\exp\{-N(1+\beta)[\gamma(\alpha_1)+\gamma(\alpha_2)]-N(1-\beta)[\gamma(-\beta_1)+\gamma(-\beta_2)]\}\exp[i(\beta_1+\beta_2)t-i(\alpha_1+\alpha_2)p-i(\beta_1+\beta_2)p]\\&\times\langle\Phi_-^0|\,R_1(s)G^\dagger(\alpha_1)G^\dagger(\alpha_2)\,|\Phi_-\rangle\langle\Phi_-|\,G(\alpha_2)G(\alpha_1)\sigma_1^xG^\dagger(-\beta_1)G^\dagger(-\beta_2)\,|\Phi_+\rangle\\&\times\langle\Phi_+|\,G(-\beta_2)G(-\beta_1)R_1(s)\,|\Phi_+^0\rangle\ ,\end{aligned}\tag{7}$$

where $|\Phi_\pm\rangle$ are the G-particle vacuum states and we have used the fact that only states containing exactly two particles contribute. $\gamma(\omega)$ is the usual Onsager function.[10] The factors containing t and p arise from the translations. As $M\to\infty$ the sum becomes an integral. The matrix element containing four G operators has been evaluated using a generalized Wick theorem.[8] The remaining matrix elements, which were evaluated by Abraham and Reed,[5] give a factor of $\exp[is(\alpha_1+\beta_1)]$ which forces $\Sigma_M(s\,|\,\beta N,p)\to 0$ as $s\to\infty$ unless there is a pole at $\alpha_1=-\beta_1$. Thus, the only nonvanishing term in (7) in this limit is that coming from the pair contractions represented by the diagram in Fig. 2. The diagram can be thought of as representing two "dressed" domain walls.

A similar analysis follows for $Z_M^{+-}(s)$ so that we are eventually left with

$$m(\beta N,p)=m^*I_N^{-1}(2\pi)^{-2}\int\int_0^{2\pi}d(\omega)_2\frac{\exp\{-N[(1+\beta)\gamma(\omega_1)+(1-\beta)\gamma(\omega_2)]+i[\omega_1t-p(\omega_1+\omega_2)]\}f_+(e^{i\omega_1},e^{i\omega_2})}{\cos[\tfrac{1}{2}\delta^*(\omega_1)]\cos[\tfrac{1}{2}\delta^*(\omega_2)]}, \tag{8a}$$

$$I_N=\pi^{-1}\int_0^{2\pi}d\omega\frac{\exp(i\omega t)\exp[-2N\gamma(\omega)]}{1+\cos\delta^*(\omega)}, \tag{8b}$$

where $\delta^*(\omega)$ and $f_+(z_1,z_2)$ are defined in Abraham and Reed[5] and m^* is the usual spontaneous magnetization for the system with homogeneous boundary conditions.

As $N\to\infty$ [(8a) and (8b)] can be evaluated using the saddle-point method. We present the result below in terms of the coordinate system (x,y) defined *along* and *normal* to the mean position of the interface (see Fig. 1)

$$\lim_{L\to\infty}m(x=\tfrac{1}{2}\beta L,y=aL^\delta)=\begin{cases}0,\ \ 0\le\delta<\tfrac{1}{2},\\ m^*\,\mathrm{sgn}(a),\ \ \delta>\tfrac{1}{2},\\ m^*\,\mathrm{sgn}(a)\Phi(|a|\{2[\tau(\theta)+\tau''(\theta)]/(1-\beta^2)\}^{1/2}),\ \ \delta=\tfrac{1}{2}\ ,\end{cases} \tag{9}$$

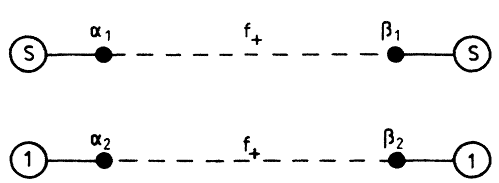

FIG. 2. The only Feynman diagram contributing to $\Sigma_M(s\,|\,\beta N,p)$ as $s\to\infty$.

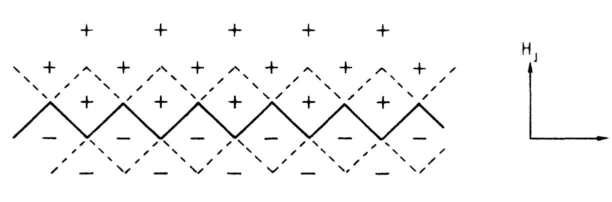

FIG. 3. A possible ground-state configuration for the case when $\theta=\pi/4$. The broken lines denote the positions each V segment in the solid line can jump to without changing the energy.

where Φ is the standard error function and we have used the known result for $\tau(\theta)$.[7] L is the mean length of the interface as shown in Fig. 1. By taking the second moment of (9) we obtain (1) thus proving the conjecture made by Akutsu and Akutu[1] for the Ising model.

The zero-temperature properties of this model can be alternatively derived from random-walk arguments. To see this, consider the case when $\theta=\frac{1}{4}\pi$. A possible ground state is illustrated in Fig. 3. Spins adjacent to the interface are fully frustrated (i.e., they can flip without changing the energy). Therefore each section of the interface is free to flip to one of the positions denoted by the broken line. So, if we define h_j as being the height of the jth section above its mean position (the solid line in Fig. 3), then the set $\{h_j\}$ can be treated as a Markov chain.[11] We define the following generating function (now for general θ):

$$\langle\exp(ih_j\phi)\rangle=\frac{\sum\limits_{h_0}\cdots\sum\limits_{h_{2N}}\delta(h_0,0)\delta(h_{2N},t')\exp(ih_j\phi)W(h_1-h_0)\cdots W(h_{2N}-h_{2N-1})}{\sum\limits_{h_0}\cdots\sum\limits_{h_{2N}}\delta(h_0,0)\delta(h_{2N},t')W(h_1-h_0)\cdots W(h_{2N}-h_{2N-1})}\ , \tag{10}$$

where $W(h)=\frac{1}{2}[\delta(h,-1)+\delta(h,1)]$, $t'=2N\tan\theta'$, and $\theta'=\frac{1}{4}\pi-\theta$. Also $0\leq j\leq 2N$ and the N used here is different from that of the previous calculation. The magnetization at lattice position (j,H_j) (see Fig. 3) is obtained from

$$m(j,H_j)=2\int_0^{H_j}p(h_j)dh_j,\ \ p(h_j)=\frac{1}{2\pi}\int_0^{2\pi}d\phi\exp(-ih_j\phi)\langle\exp(ih_j\phi)\rangle\ , \tag{11}$$

where $p(h_j)$ is the probability that the interface will pass through (j,h_j).

The generating function was evaluated using Fourier transforms and the remaining integrals were evaluated for $N\to\infty$ using the saddle-point method. After transforming the coordinates onto the (x,y) system of Fig. 1 we obtain the following expression for the zero-temperature magnetization:

$$\lim_{L\to\infty}m(\tfrac{1}{2}\beta L,aL^{\delta})=\begin{cases}0, & 0\leq\delta<\frac{1}{2},\\ \operatorname{sgn}(a), & \delta>\frac{1}{2},\\ \operatorname{sgn}(a)\Phi(|a|[\frac{1}{2}(1-\beta^2)\sin\theta\cos^2\theta(1+\tan\theta)^{-1/2}, & \delta=\frac{1}{2}\ .\end{cases} \tag{12}$$

This is, of course, the zero-temperature limit of (9). Note that at $T=0$, $w(\theta)=0$ for $\theta=0,\frac{1}{2}\pi$ only. The zero-temperature roughening for all other values of θ is due to the presence of fully frustrated spins at the interface. The pair-spin correlation function has also been evaluated at $T=0$ via $\langle\exp(h_j\phi_1+h_{j+r}\phi_2)\rangle$ (Ref. 6).

Finally, we discuss the relevance of our results to the Wulff construction[12] for equilibrium crystal shapes. If we assume that the equilibrium crystal shape is differentiable with fixed ends at (0,0) and $(L,L\tan\theta)$ then a simple variational calculation for the surface free energy functional, along Wulff lines, gives a straight line shape, *exactly* as given by the mean direction from (9) and (12). The form of the fluctuations *proves* faceting at $T=0$ for $\theta=0,\pm\frac{1}{2}\pi$, exactly as the Wulff phenomenology requires. There is, however, one snag at $T=0$. If we allow discontinuous solutions, then at $T=0$ any nondecreasing function $f:\mathbb{Z}\cap[-N,N]\to\mathbb{Z}$ with $f(0)=0$ and $f(L)=L\tan\theta$ will minimize the energy; it is therefore a Wulff solution in a general sense; (12) shows which of these solutions are significant.

The authors thank Professor R. J. Ball very much for a helpful discussion on the Wulff construction at $T=0$ and one of us (P.J.U.) acknowledges support from the Science and Engineering Research Council, United Kingdom.

[1]Y. Akutsu and N. Akutsu, J. Phys. A **19**, 2813 (1986).
[2]J. De Coninck and J. Ruiz (unpublished).
[3]M. P. A. Fisher, D. S. Fisher, and J. D. Weeks, Phys. Rev. Lett. **48**, 368 (1982).
[4]D. B. Abraham and P. Reed, Phys. Rev. Lett. **33**, 377 (1974).
[5]D. B. Abraham and P. Reed, Commun. Math. Phys. **49**, 35 (1976).
[6]D. B. Abraham and P. J. Upton (unpublished).
[7]D. B.Abraham and P. Reed, J. Phys. A **10**, L121 (1977).
[8]D. B. Abraham, Commun. Math. Phys. **59**, 17 (1978).
[9]T. D. Shultz, D. C. Mattis, and E. H. Lieb, Rev. Mod. Phys. **36**, 856 (1964).
[10]L. Onsager, Phys. Rev. **65**, 117 (1944).
[11]W. Feller, *An Introduction to Probability Theory and its Applications,* Vol. 1 (Wiley, New York, 1950).
[12]G. Wulff, Z. Kristallogr. **34**, 449 (1901); recent results are discussed by C. Rottmann and M. Wortis, Phys. Rep. **103**, 59 (1984); R. K. P. Zia, in *Statistical Physics and Particle Physics, Common Problems and Techniques,* edited by K. C. Bowler and A. J. M. McKane, Proceedings of 26th Scottish Universities Summer School in Physics, NATO ASI (SUSSP Publications, Edinburgh, 1984).