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Interface models and the bulk phase transition of Ising systems

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The validity of calculating the interface free energy of Ising systems near the bulk phase transition directly in terms of a Hamiltonian dependent only on interface coordinates is considered. It is shown that interface models which exclude the effects of bubbles and overhangs lack the appropriate rotational invariance for the Ising model. A generalized self-avoiding-walk model is introduced, in which overhangs are permitted and rotational invariance restored. However, the critical exponents found do not belong to the Ising universality class. We conclude that bubble excitations in the bulk phases are crucial for a correct calculation of the interface free energy.

Models for calculating the interface free energy between two phases coexisting with one another in thermal equilibrium have been extensively studied in recent years.[1-7] The interface free energy (or surface tension) σ is expected to be positive below the transition temperature T_c of the bulk system. If this transition is continuous, one expects the interface free energy to vanish at T_c. Scaling arguments[8] indicate that for $T \lesssim T_c$, σ should behave like $\sigma \sim \xi^{-(d-1)} \sim t^{\nu(d-1)}$, where ξ is the correlation length, $t=(T_c-T)/T_c$, and d is the dimensionality of the (bulk) system. In fact, this relation between σ and ξ provides one of the motivations for studying the interface free energy. It enables one to calculate the properties (e.g., the critical exponent ν) of the *bulk* phase transition. However, calculating the interface free energy is, in principle, not simpler than calculating that of the bulk. For an Ising system with N^d spins, σ is defined by $\sigma=\lim_{N\to\infty} N^{-(d-1)}\ln(Z_{+-}/Z_{++})$, where Z_{+-} and Z_{++} are the partition functions of the system calculated with antiperiodic and periodic boundary conditions, respectively. One therefore has to calculate both (bulk) partition functions in order to evaluate σ. In order to bypass this rather complicated bulk problem, models for calculating the interface free energy directly have been introduced. In such models one considers an interface variable $f(\mathbf{x})$, which gives the height of the interface at $\mathbf{x}$, where $\mathbf{x}$ is a point in $(d-1)$-dimensional space. In order to evaluate the interface free energy one introduces a Hamiltonian $\mathscr{H}[f(\mathbf{x})]$ associated with the interface configuration $f(\mathbf{x})$. The surface tension σ is then given by $\sigma=-N^{-(d-1)}k_B T\ln Z$, where

$$Z=\int D[f(\mathbf{x})]e^{-\beta H[f(\mathbf{x})]} \quad . \tag{1}$$

Usually the integral in (1) is taken over all possible single-valued functions $f(\mathbf{x})$. In such models one therefore does not consider interface configurations with bubbles or overhangs. Although this approach incorporates some uncontrolled approximations it leads to some remarkable results for two-dimensional (2D) Ising models. It has been noted[1] that by taking $\mathscr{H}[f(\mathbf{x})]$ to be a solid-on-solid (SOS) model one can reproduce the exact interface free energy of the 2D Ising model on a square lattice, when the interface lies along the principal axis of the lattice. However, when the interface is tilted with respect to the lattice one does not obtain the exact free energy in this way.[6,9] This approach also yields the exact transition temperature of the 2D Ising model on a triangular lattice with nearest-neighbor interactions.[3] By applying the same method to the square-lattice Ising antiferromagnet in a magnetic field,[2] the critical field $H_c(T)$ has been calculated. However, it turned out that the expression for $H_c(T)$, while a good approximation, is not exact.[10] More recently, Wallace and Zia, in a very interesting work,[4] introduced a continuum version of the SOS model. They considered a rotationally invariant Hamiltonian

$$\mathscr{H}[f(\mathbf{x})]=\int d^{d-1}x(1+(\nabla f)^2)^{1/2} \quad , \tag{2}$$

and studied it using renormalization-group techniques in $d=1+\epsilon$ dimensions, where $\epsilon>0$. An ϵ expansion for the critical exponent ν was obtained in this way.

In the present paper we examine some of the difficulties in defining an interface model for the interface free energy of Ising systems. One of the requirements for such a model is that it should yield a free energy which at $T=T_c$ becomes rotationally invariant. Such invariance must result in the divergence of the susceptibility with respect to a slope-inducing field. As was noted, the standard SOS models, for which the interaction between nearest-neighbor columns is of the form $|\Delta f|^p$, $p>0$, where $\Delta f=f(\mathbf{x}_i)-f(\mathbf{x}_j)$, do not satisfy this requirement. We find, in fact, that the SOS models are not singular at any T unless one takes an interaction which for large Δf behaves as $\ln|\Delta f|$. It is not clear, however, how such an interaction can arise in an Ising model. In order to overcome this problem, we introduce a rotationally invariant model which allows for interface configurations with overhangs. We show that for 2D systems (namely, a 1D interface), this model yields a critical exponent $\nu=\frac{3}{4}$, which is not the expected one for the 2D Ising model. We also consider the continuum interface model (2) and demonstrate explicitly that at lowest order in T it does not yield a rotationally invariant free energy for any finite ϵ.

Consider first the SOS model in $d=2$ dimensions. Let f_i be the integer height of the interface at site i. The fact that the heights f_i are taken to be integers is not crucial for the following considerations. The Hamiltonian is given by

$$\mathscr{H}=\sum_{i=1}^{N} V(f_{i+1}-f_i)-\eta\sum_{i=1}^{N}(f_{i+1}-f_i) \quad , \tag{3}$$

where for the standard model the interaction may be taken as $V(z)=2J_2+2J_1|z|$ and where we have introduced a field η conjugate to the difference $(f_N-f_1)\equiv Nh$. h measures the tilt of the interface. With free boundary conditions the free energy density $\tilde{F}(\eta)$ is easily calculated. One finds

$$\tilde{F}(\eta)=F(0)-\tfrac{1}{2}\chi\eta^2+O(\eta^4)\ , \tag{4}$$

where

$$\chi=\beta\sum_{z=-\infty}^{\infty}e^{-\beta V(z)}z^2\Big/\sum_{z=-\infty}^{\infty}e^{-\beta V(z)} \tag{5}$$

is the susceptibility with respect to η. The corresponding Legendre-transformed free energy is then given by

$$F(h)=F(0)+\tfrac{1}{2}\chi^{-1}h^2+O(h^4)\ . \tag{6}$$

For the surface free energy to vanish for interfaces of any slope h at the same temperature T_c, one must have $\chi^{-1}(T_c)=0$. This divergence of χ at T_c is just the reflection of the singular behavior of the bulk system at T_c. However, it is easy to see from (5) that for the general SOS model χ does not diverge at finite T unless $V(z)\sim\ln|z|$ for large z. This is clearly not the case for the standard potential $V(z)\sim|z|^p$, $p>0$. These models do not exhibit any singular behavior at all. In particular, the model of Wallace and Zia (2), when discretized and studied in $d=2$, does not yield any phase transition.

The lack of self-consistency in the SOS models, in their failure to yield a rotationally invariant (i.e., h-independent) free energy density at $T=T_c$, may be traced to the restriction of averaging only over those interfaces without bubbles and overhangs, namely, only those expressible as single-valued functions in the coordinate frame of the lattice axes. Such a set of interfaces lacks the rotational symmetry of the underlying lattice. To correct this defect we now consider a generalized interface model, where we average over a set of interfaces preserving the symmetry of the lattice. For the isotropic case ($J_1=J_2\equiv J$), we take the energy of an interface, as in (2), proportional to its length. We consider first the set of all interfaces on the square lattice, which do not intersect themselves, i.e., may have overhangs but no bubbles. The partition function of this model for a lattice of length L is thus

$$Z_L=\sum_N C(N)e^{-\beta JN}\ , \tag{7}$$

where $C(N)$ is the number of ways to connect the ends of the lattice with a "string" N-bonds long. This problem is just that of the self-avoiding random walk which has been solved in the context of the polymer problem.[11] The partition function (7) as $L\to\infty$ can be expressed in terms of the correlation function of an n-component spin model in the limit $n\to 0$. $Z_L=c^{-\beta LF}=\langle\mathbf{S}(L)\cdot\mathbf{S}(0)\rangle=e^{-L/\xi}$, where F is the free energy density. The coupling constant $\bar{\beta}\bar{J}$ of the spin model is related to βJ by $e^{-\beta J}=\bar{\beta}\bar{J}$. The rotational invariance of the correlation functions as $T\to T_c$ guarantees the rotational invariance of the surface free energy and hence the self-consistency of our interface model. We thus have $\beta F=\xi^{-1}$ and the divergence of the spin-correlation length ξ at T_c gives $F\sim t^\nu$. Unfortunately, the exponent ν for the $\eta\to 0$ spin model is $\frac{3}{4}$, as opposed to $\nu=1$ for the 2D Ising model.[12]

One can now generalize the set of interfaces to include those which intersect themselves, i.e., include connected bubbles. However, a recent paper by Shapir and Oono[13] shows the exponent ν to remain $\frac{3}{4}$. (Note that for walks on a honeycomb lattice, which would describe interfaces of a triangular Ising model, there are no connected bubbles. Thus, that their inclusion in the square lattice produces no change is reassuring). Our interface model thus clearly is not a description of the 2D Ising model. Moreover, we know of no bulk model for which it might be the appropriate description.

Consider next the interface model (2) studied by Wallace and Zia. In this model the Hamiltonian is proportional to the area of the interface, and therefore it is rotationally invariant. It has been argued that since the Hamiltonian is rotationally invariant, the resulting total free energy will be isotropic. If true, this would ensure the divergence of the susceptibility at the same temperature at which the interface free energy vanishes. However, we point out that although the Hamiltonian (2) is rotationally invariant the resulting free energy is *not* isotropic. This is due to the fact that the set of interface functions $f(\mathbf{x})$ integrated over in (1) is *not* rotationally invariant. This set includes all functions $f(\mathbf{z})$ which are single valued in a given reference frame, and is clearly not invariant under rotations. By performing momentum-shell renormalization-group iterations in $d=1+\epsilon$, one generates terms which break the symmetry, and the square-root form need not be preserved. In order to demonstrate this point, we explicitly evaluate the total free energy as a function of the average slope h to lowest order T, but for arbitrary finite ϵ. Let $f(\mathbf{x})=\mathbf{h}\cdot\mathbf{x}+\Delta f(\mathbf{x})$ when $\Delta f(\mathbf{x})$ are functions which vanish at the boundaries. Expanding (2) in Δf, keeping terms to $O((\Delta f)^2)$, and evaluating the resulting Gaussian integrals in the partition function, we find that the free energy to $O(T)$ is given by

$$F=\sqrt{1+h^2}-\frac{k_BT}{\epsilon}\left[1+\sum_{n=1}^{\infty}\frac{(-1)^n}{2n}h^{2n}\frac{K_{\epsilon-1}}{2\pi}B\left(n-\frac{1}{2}+\frac{\epsilon}{2},\frac{1}{2}\right)\right]+\frac{3}{4}k_BT\ln(1+h^2)+C\ , \tag{8}$$

where $(2\pi)^\alpha K_\alpha$ is the area of a sphere in α-dimensional space, B is the beta function, and C is a constant independent of h. This procedure is equivalent to summing all one-loop diagrams.[14] For an isotropic surface tension, the last two h-dependent terms of the free energy (8) must sum up to be proportional to $\sqrt{1+h^2}$. One can verify, however, that this is only true in the limit $\epsilon\to 0$. Thus to lowest order in ϵ, F is rotationally invariant and χ diverges at $k_BT_c=\epsilon$. However, at any finite ϵ, to $O(T)$, F is no longer rotationally invariant.

In $d=2$ dimensions, continuum SOS-like interface models can be dealt with by an explicit real-space renormalization group. We consider the generalized SOS model (3) with arbitrary potential V, taking the heights f_i to be continuous variables and letting the lattice constant go to zero. By performing a decimation a renormalization equation is obtained for the potential V. The variable $h=f_{i+1}-f_i$ rescales as a length as in the work of Wallace and Zia. The renormalization equation can easily be solved by Fourier transforms, and we find for the fixed-point potential

$$-\beta_c V^*(h) = \ln\left(\frac{2\alpha/\pi}{\alpha^2+h^2}\right) , \qquad (9)$$

for arbitrary α. This fixed point is clearly not rotationally invariant, and has the required logarithmic behavior at large h as noted previously.

To conclude, we have considered several interface models. In two dimensions we demonstrated the failure of the class of generalized SOS models in providing a consistent description of the bulk Ising transition. We have considered the continuum model of Wallace and Zia and find that it is not isotropic at low T for finite ϵ. This raises questions as to whether or not it is, in fact, an appropriate model for an Ising system. These failures were traced to the lack of proper rotational invariance of the interfaces averaged over. We have introduced a new model in $d=2$ which properly takes into account all possible interface configurations. Although self-consistent (i.e., rotationally invariant), this model fails to give the known critical exponent of the Ising model. This failure thus illustrates the crucial importance of bulk bubbles in computing the interfacial free energy. The entropy of these bubbles with respect to the interface produces a nontrivial contribution which cannot be accounted for by any model which is dependent on interface variables alone.

Note added in proof. Results similar to those of this paper were recently obtained by D. A. Huse, W. V. Saarloos, and J. D. Weeks [Phys. Rev. B **32**, 233 (1985)]. In a recent work, R. K. P. Zia (unpublished) has shown that within the context of the $1+\epsilon$ expansion, the isotropic fixed point is stable to a wide class of anisotropic perturbations.

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