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Ising-Model Surface Tension Using Real-Space Renormalization-Group Methods

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Approximate real-space (cell-type) renormalization-group methods are used to calculate the surface tension between coexisting phases in two- and three-dimensional Ising models. The results are physically reasonable and show the expected scaling properties near a critical point. However, there are some problems in reconciling the three-dimensional results with the existence of a roughening transition.

An important problem in studying phase equilibria is to understand the structure of the interface separating two phases. It is very difficult to calculate the density distribution at an interface and the interfacial free energy, or surface tension, from the first principles of statistical mechanics. We present here an approximate calculation of the surface tension γ^{σ} of an Ising ferromagnet, or lattice gas, based on a real-space (cell-type) renormalization-group (RG) transformation.[1,2]

The results are encouraging in that very simple approximations yield results in fair agreement with the exact answers already available for the Ising model on a square lattice.[3,4] The same approximations yield sensible results for three-dimensional Ising models, for which exact answers are not known, and even reliable approximations based on exact series expansions do not seem to be available. The dependence of γ^{σ} on the temperature T near the critical temperature T_c is consistent with the predictions of scaling arguments.[5]

Our calculations for the simple cubic (sc) lattice show no evidence for an anomaly in γ^{σ} at a roughening transition[6] temperature T_R below T_c. While it is easy to suggest some reasons for this, there are some troublesome questions of principle involved. These are discussed further at the end of the paper.

Two RG calculations of the interfacial profile and tension for the Landau-Ginzburg-Wilson model using the $\epsilon = 4 - d$ expansion, with d the dimensionality, have recently appeared.[7] While it seems unlikely that such a model shows a roughening transition, the presumed divergence[8] of the interface thickness raises certain other questions of principle about the applicability of such calculations to $d = 3$.

The surface tension of an Ising ferromagnet on a square lattice with nearest-neighbor interactions can be computed as follows. Consider a square piece of the lattice containing L^2 spins, with periodic boundary conditions. Assume that all the vertical nearest-neighbor interactions in a particular row (hereafter called the "seam") have their signs reversed, as indicated in Fig. 1, so that they represent antiferromagnetic rather than ferromagnetic coupling.[4] The dimensionless free energy F, equal to the logarithm of the partition function, can be written as

$$F = L^2 f + L f^{\sigma}, \tag{1}$$

where f and f^{σ} are normalized bulk and interfacial contributions to F, and terms diverging less rapidly than L as L tends to infinity have been omitted from (1). The surface tension is given

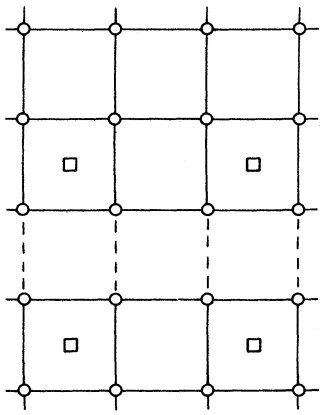

FIG. 1. The solid lines indicate ferromagnetic, the dashed lines antiferromagnetic bonds on a square lattice, while the small squares are cell spins.

by

$$\gamma^{\sigma} = -kTf^{\sigma} \tag{2}$$

if the lattice constant is unity.

In the RG procedure[2] a new set of $L^2/4$ cell spins, indicated by small squares in Fig. 1, are introduced, each of which may be thought of as coupled, by suitable weight factors, to the four spins (small circles) closest to it on the original lattice. The RG transformation replaces the original interactions with a new set of interactions among the cell spins which preserves their correlation functions and leaves the value of the partition function unchanged. If the new values of the various free energies, referring now to the cell spins, are indicated with primes, we have

$$F = F' = (L/2)^2 f' + (L/2) f^{\sigma\prime}. \tag{3}$$

Hence, by comparison with (2), f' is $4f$ and

$$f^{\sigma\prime} = 2f^{\sigma}. \tag{4}$$

Note that since the (bulk) correlation length ξ is reduced by a factor of 2 in the RG transformations, (4) and its generalization to d dimensions may be written in the form

$$\xi^{d-1} f^{\sigma} = \text{const} \tag{5}$$

along a RG trajectory.[9]

In order to calculate f^{σ} explicitly we have used the first-order cumulant approximation[2,10] to the RG transformation in which the dimensionless nearest-neighbor coupling K (the exchange energy J divided by kT) is mapped onto itself by the equation

$$K' = 2K\left(\frac{e^{4K}+2}{e^{4K}+6+e^{-4K}}\right)^2. \tag{6}$$

In this approximation the interaction between nearest-neighbor cell spins is $+K'$ if they are on the same and $-K'$ if they are on opposite sides of the seam, preserving the same structure of interactions as on the original lattice, Fig. 1.

When K exceeds the fixed-point value K^*, successive iterations of (6) carry K towards infinity, or T towards zero. If K is large enough, f^{σ} is $-2K$ to a good approximation, and thus f^{σ} for any $K > K^*$ can be computed by successive iterations using (4) and (6). The results are shown in Fig. 2 together with the exact answer.[3,4]

If near the critical point

$$\gamma^{\sigma} \sim (T_c - T)^{\mu}, \quad \xi \sim (T_c - T)^{-\nu}, \tag{7}$$

then (5) leads to the result

$$\mu = (d-1)\nu \tag{8}$$

predicted by scaling arguments.[5] In the first-order cumulant approximation on a square lattice, $\mu = \nu = 0.994$, which should be compared with the exact values of $\mu = \nu = 1$. For the sc lattice the same approximation yields $\nu = 0.803$ in place of the generally accepted value of 0.63. However, the calculated γ^{σ}, Fig. 3, has a temperature dependence which is at least qualitatively reasonable.

Other RG approximations may be employed in conjunction with (5) to calculate γ^{σ}. For example, Fig. 4 shows the results obtained for a (100) surface in a body-centered cubic Ising model with nearest-neighbor interactions using the Kadanoff lower-bound approximation.[11] However, it was necessary, in order to obtain sensible results, to make a choice of the Kadanoff p parameter which minimizes f^{σ} rather than f. And even so, the value of $-d\gamma^{\sigma}/dT$ (surface entropy) at $T = 0$ is not correct.[12] [Note that an RG approximation which yields an upper or lower bound for f will not, at least in general, yield a corresponding bound for f^{σ}, as the latter must be obtained by subtraction, Eq. (1).] It has been our experience that f^{σ} is rather more sensitive than the bulk f to details of the approximation scheme at low temperatures, and a method which gives good results for one surface orientation may yield poor results for another.

Whereas the difficulties just mentioned can easily be ascribed to the relatively crude approximations necessary to construct an explicit RG

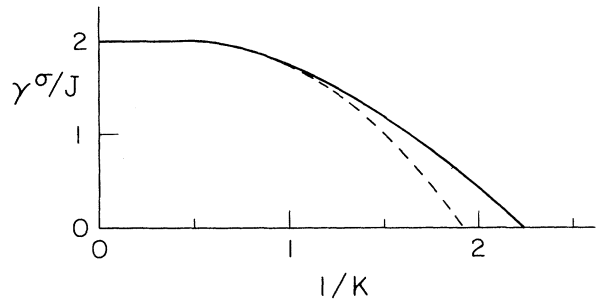

FIG. 2. Exact result (solid) and first-order cumulant approximation (dashed) for γ^σ for the (10) interface on a square lattice.

transformation, the absence of any indication of a roughening transition in an sc lattice at a temperature $T_R < T_c$ cannot be dismissed so easily. The reason is that the derivation of (5) makes no (obvious) use of these approximations. If (5) is valid for an *exact* RG transformation, it seems somewhat surprising, though of course not impossible, that f^σ should exhibit some nonanalytic behavior at a temperature where ξ, the bulk correlation length, is generally assumed to be analytic function of temperature. Of course, it has not been rigorously established that a roughening transition actually occurs, and it is conceivable that, even if it does, there is still no anomaly in f^σ at T_R.[13] Nor should one ignore the possibility that (5) breaks down for an exact RG, though this in turn raises some intriguing questions, such as whether long-range interactions play an important role.

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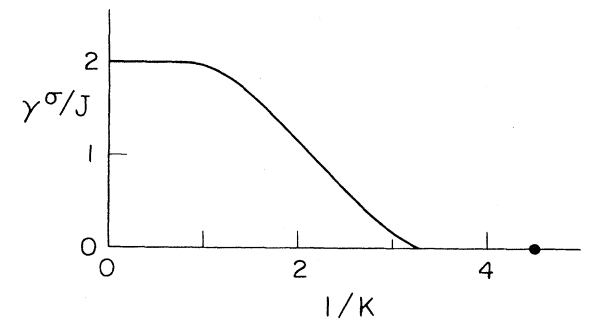

FIG. 3. First-order cumulant approximation for γ^σ for the (100) interface in a simple cubic lattice. The series-expansion T_c is indicated by a dot.

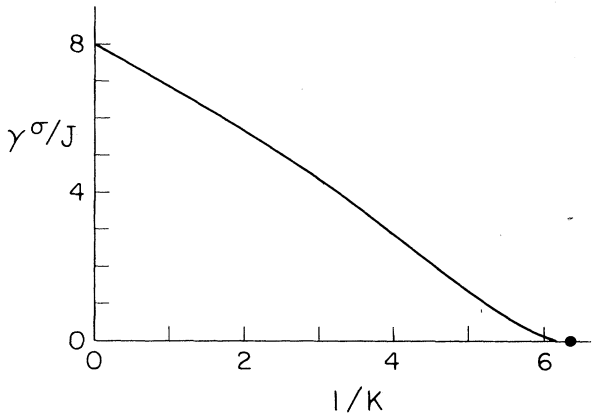

FIG. 4. Kadanoff lower-bound approximation (see text) for γ^σ for a (100) interface in a body-centered cubic lattice, with cube edge of length 1. The series-expansion T_c is indicated by a dot.

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Spontaneous Symmetry Breaking and Blocking of Metastable States

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A mechanism for spontaneous symmetry breaking and related phenomena and the corresponding blocking of metastable states is discussed. It is based on the interaction of an object with a background of "probes" like photons or particles, etc., in its natural surrounding. Applications include quasilocalization of macroscopic bodies, spontaneous parity nonconservation of sugar crystals, localization of atoms in molecules (Born-Oppenheimer approximation), stability of metastable compounds, and perhaps also intrinsic symmetries of elementary particles.

The object of this Letter is to discuss a quantum mechanical mechanism of spontaneous symmetry breaking and related phenomena and the corresponding blocking of states which are not eigenstates of the Hamiltonian of the object in question. This mechanism differs from, and is much more powerful than, the one usually discussed in the current literature based on nonsymmetric solutions to symmetric equations.

Consider an object O and a probe P described in Hilbert spaces H^O and H^P, respectively. For simplicity H^O is assumed to be two dimensional; generalizations will be mentioned at the end. Consider further two orthogonal states $\varphi_1{}^O$ and $\varphi_2{}^O$ of the object and an interaction between object and probe leading to the following transitions of the combined system:

$$\varphi_i{}^O\otimes\varphi_0{}^P\rightarrow\varphi_i{}^O\otimes\varphi_i{}^P,\quad i=1,\ 2, \tag{1}$$

where $\varphi_0{}^P$ is the assumed initial state of the probe. By linearity this gives the transition for arbitrary initial state $a\varphi_1{}^O+b\varphi_2{}^O$. If no further observation is performed on the probe, and the object alone is considered after separation of the two, the object has to be described by a density matrix ρ^O on H^O and the trace has to be taken over H^P.

Taking $\varphi_1{}^O,\varphi_2{}^O$ as basis in H^O and assuming $(\varphi_1{}^P,\varphi_2{}^P)=0$, the transition (1) for an initial superposition $a\varphi_1{}^O+b\varphi_2{}^O$ with $|a|^2+|b|^2=1$ leads then for the density matrix ρ^O of the object to

$$\begin{pmatrix}|a|^2 & ab^*\\ a^*b & |b|^2\end{pmatrix}\rightarrow\begin{pmatrix}|a|^2 & ab^*(\varphi_2{}^P,\varphi_1{}^P)\\ a^*b(\varphi_1{}^P\varphi_2{}^P) & |b|^2\end{pmatrix}$$
$$=\begin{pmatrix}|a|^2 & 0\\ 0 & |b|^2\end{pmatrix}. \tag{2}$$

This constitutes a "reduction of the state vector" of a pure initial to a mixed final state of the object.

There are two important aspects in this connection. One is the compatibility of this reduction with the linearity of the law of motion. This is the case by construction. The second is the assessment of the relevance and frequency of occurrence of this phenomenon. This may be judged from its connection to the process of measurement. Indeed Eq. (1) is a (simplified) model of a measurement, in which information is transferred from the object to the probe in such a way that subsequent observation of the probe alone *could* discriminate exactly between the two cases where the object is initially in the state $\varphi_1{}^O$ or $\varphi_2{}^O$. The *possibility* of this discrimination requires $\varphi_1{}^P$ and $\varphi_2{}^P$ in Eq. (1) to be orthogonal and thus leads to the exact depletion of the off-diagonal elements of ρ^O in Eq. (2) if the object alone is considered, i.e., even, and in particular, *in*

