Path-Summation Representations in Planar Uniaxial Ferromagnets

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(Received 25 March 1996)

We construct path-summation representations for the planar Ising ferromagnet at subcritical temperatures. The paths are Gibbs dividing surfaces on the scale of the bulk correlation length, and are controlled by coarse-grained quantities such as the surface tension and the surface stiffness. We recapture the phenomenological bubble model of correlation functions in a controlled way, and we are able to consider the scaling limit and the influence of a bulk field. [S0031-9007(96)00531-5]

PACS numbers: 75.40.–s, 05.50.+q, 64.60.Fr

Applications of the solid-on-solid (SOS) model to the statistical mechanical treatment of fluctuations in interfaces are widespread [1,2] and important in the theory of surface phase transitions [3–5]. The restrictions inherent in this model are easily appreciated by considering an interface in two dimensions, which separates two coexisting uniaxially ordered thermodynamic phases, and which is pinned at $(-N, \frac{1}{2})$ and $(N, \frac{1}{2})$, but otherwise free to fluctuate under the control of surface tension. The minimum energy state is a straight line connecting $(-N, \frac{1}{2})$ to $(N, \frac{1}{2})$. The shape of the fluctuating interface is restricted so that it intercepts any line $x = i$ with $-N \le i \le N$ precisely once. Such an apparently gross but computationally convenient approximation could only possibly be valid in a coarse-grained sense, in which fluctuations up to the typical spatial extent found in a pure phase are summed out. Under these circumstances, the putative interface Γ divides the space sharply into pure-phase regions. The shape of the interface is followed by giving its intercept y_i with each line $x = i$ for $-N \le i \le N$. The statistical weight of any configuration $\Gamma = \{y_{-N}, y_{-N+1}, \dots, y_N\}$ is then given by

$$W(\Gamma) = Z^{-1} \exp\left[-\beta\left(E_{-N}(y_{-N}) + E_N(y_N) + \sum_{i=-N}^{N-1} E(y_{i+1} - y_i)\right)\right], \qquad (1)$$

where β is the inverse temperature, $E(y) = \tau\sqrt{1 + y^2}$ where τ is the surface tension, and the functions $E_{\pm N}$ correspond to the boundary conditions at $x = \pm N$. This may be generalized for small y to include an angle-dependent surface tension $\tau(\theta)$ [6,7]: In a quadratic approximation, $E(y) = \tau(0) + \Sigma y^2/2$ where $\Sigma = \tau(0) + \tau''(0)$ is the surface stiffness [8]. Notice that only neighboring y variables are coupled. In order to evaluate the partition function Z, or expectation values with the probability distribution (1), sums over configurations must be performed. To do this the *a priori* weight of the y variables must be known.

The wide applicability of SOS interface models to fluids (the columnar model of Weeks [9]), solid surfaces (TLK [10] and multiziggurat models [11]), and bubble models of correlation functions [12–16] motivates investigating whether it is anything more that a lucky approximation of unspecified accuracy, derived by a rather shaky gedanken renormalization. By considering the interface between coexisting thermodynamic phases in the planar Ising model, we shall show first how a path representation comes about exactly, and then explicitly how it is approximated to get the Fisher-Fisher-Weeks discrete Gaussian form [8]. The correct *a priori* weighting in the sums over the y_i is stipulated. Further, the precise interpretation of the y_i variables is given, allowing inclusion of an external magnetic field in the discussion. Finally, we describe the pair correlation function below the critical temperature in terms of droplets, again in a controlled way.

First, consider a subcritical planar Ising model strip with edges $x = \pm N$ parallel to the y axis, and with spins fixed at $+1$ for $x = \pm N$ and $y \ge 1$, but fixed at -1 for $x = \pm N$ and $y \le 0$. This induces an interface, or long Peierls contour on the dual lattice running from $(-N, \frac{1}{2})$ to $(N, \frac{1}{2})$. The magnetization in such a system is known to display extensive spatial fluctuations: For $-1 < \beta < 1$ we have [17,18]

$$\lim_{N\to\infty} \langle \sigma(\beta N, \alpha N^\delta)\rangle = m^*(\mathrm{sgn}\alpha) \begin{cases} 0 & \text{for } \delta < 1/2 \\ \Phi\left(|\alpha|\sqrt{\frac{\Sigma}{1-\beta^2}}\right) & \text{for } \delta = 1/2 \\ 1 & \text{for } \delta > 1/2 \end{cases} \qquad (2)$$

0031-9007/96/77(1)/171(4)$10.00

where m^* is the spontaneous magnetization, and Φ is a Gaussian error function:

$$\Phi(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2}\, du\,. \tag{3}$$

The earliest phenomenological evidence for large fluctuations of the interface comes from applying equipartition to the Fourier modes of a fluid interface [19].

The result (2) was obtained using the transfer matrix along the x axis: This matrix has free-fermionic eigenstates [20], and (2) comes entirely from the one-particle sector of the spectrum, which contains the eigenvectors $G_k^\dagger|\Phi_\pm\rangle$, where the $|\Phi_\pm\rangle$ describe the bulk spontaneously magnetized phases and

$$G_k^\dagger = M^{-1/2} \sum_{j=1}^{M} e^{ijk}[\cos\theta(k)\sigma_j^+ - i\sin\theta(k)\sigma_j^-] \prod_{l=1}^{j-1}(-\sigma_l^z)\,, \tag{4}$$

where $2\sigma_j^\pm = \sigma_j^x \pm i\sigma_j^y$ and the spins are chosen x quantized, giving the following interpretations for the Pauli matrices: σ_j^x measures the jth spin in the column and $-\sigma_j^z$ is the spin-flip operator. Thus $G_k^\dagger$ is a weighted sum over lattice positions j of operators which reverse x-quantized spins between positions 1 and $j \leq M$. The particular choice of weight is stipulated by the diagonalization of V, which specifies $\theta(k)$. This procedure regrettably does not allow a useful formulation in terms of Peierls contours.

The factor e^{ijk} in (4) and Fourier-transform ideas suggest the following change of basis:

$$|j\rangle = M^{-1/2} \sum_k e^{-ijk} e^{i\varphi(k)} G_k^\dagger |\Phi_\pm\rangle\,, \tag{5}$$

where $\varphi(k)$ is an as yet unspecified phase. We require invariance under reversal of the horizontal direction, giving $e^{i\varphi(-k)} = e^{-i\varphi(k)}$. Note that $\langle j_1|j_2\rangle = \delta_{j_1,j_2}$, and that inserting (4) in (5) relates $|j\rangle$ directly to combinations of block-rotated states: If $e^{i\varphi(k)+i\theta(k)}$ is analytic in a strip containing the real axis, as will turn out to be the case below, then $|j\rangle$ is a linear combination of states that have reversed spins from 1 to l, with coefficients that decay exponentially in $|l - j|$.

Consider now the partition function

$$Z_N = \langle b|V_{(1)}^{2N}|b\rangle\,, \tag{6}$$

where $|b\rangle$ describes the Dobrushin boundary conditions alluded to above, and $V_{(1)}$ is the transfer matrix restricted to the one-particle subspace. Using the $|j\rangle$ basis, (6) becomes

$$Z_N = \sum_{\{j_{-N},\ldots,j_N\}} \langle b|j_{-N}\rangle \left(\prod_{i=-N}^{N-1} \langle j_i|V_{(1)}|j_{i+1}\rangle\right) \langle j_N|b\rangle\,. \tag{7}$$

This change of basis achieves a path representation with no overhangs, just as the SOS ideas require. To put this further to the test, consider the matrix elements in the product: Using (5) and the diagonal form of $V_{(1)}$ gives

$$t_1^n(j_1, j_2) = \langle j_1|V_{(1)}^n|j_2\rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-n\gamma(k)} e^{i(j_2-j_1)k}\, dk\,, \tag{8}$$

where we have allowed matrix elements to be taken for every run of n factors $V_{(1)}$ in (6) (assume N is a multiple of n), and $\gamma(k)$ is Onsager's function [21] given by

$$\cosh\gamma(k) = \cosh 2K_1^* \cosh 2K_2 - \sinh 2K_1^* \sinh 2K_2 \cos k\,, \tag{9}$$

where $\tanh K_1^* = e^{-2K_1}$, and K_1 and K_2 are the Ising model's coupling constants: $K_1^* < K_2$ for subcritical temperatures $T < T_c$.

The function $t_1^n(j_1, j_2)$ is positive and depends only on the difference $j_2 - j_1$. Its asymptotics are revealing: For $|j_2 - j_1| \ll \sqrt{n\gamma''(0)}$,

$$t_1^n(j_1, j_2) \approx e^{-n\gamma(0)}[2\pi n\gamma''(0)]^{-1/2} \exp\left(-\frac{(j_2 - j_1)^2}{2n\gamma''(0)}\right). \tag{10}$$

Examination of (9) and the exact result for the angle-dependent surface tension [6,7] give $\tau(0) = \gamma(0)$ and $\Sigma = \gamma''(0)^{-1}$; therefore (10) is indeed a discrete Gaussian with the fluctuations controlled by the surface stiffness as Fisher, Fisher, and Weeks suggested in [8]. Moreover, the *a priori* weights in the sums over the j_i are specified by the prefactors.

It is also of interest to get the scaling limit, at least formally. Take $T \to T_c$ in (8), holding $l = n\gamma(0)$ and $L = N\gamma(0)$ fixed. We define $B = \coth K_1^* \tanh K_2$ (note that $B = e^{\gamma(0)}$ in the case $K_1 = K_2$). Both $\gamma(0)$ and $\ln B$ vanish as $(T_c - T)/T_c$. We use $u = k/\ln B$ as a momentum variable and set $y_i = j_i \ln B$, which becomes a continuous variable. This gives

$$t_1^n(j_1, j_2) \approx \frac{\ln B}{2\pi} \int_{-\infty}^{\infty} e^{-l\sqrt{1+u^2}} e^{i(y_2-y_1)u}\, du \tag{11}$$

asymptotically as $T \to T_c$, reducing the path sum to a path integral [22] for a relativistic free particle.

We now develop the path summation approach to include an external magnetic field. Consider the total magnetization of the portion of a column comprised between q and $p - 1$, denoted by

$$M^{pq} = \sum_{j=q}^{p-1} \sigma_j^x\,. \tag{12}$$

There is a unique choice of the phase factor $e^{i\varphi(k)} = e^{-ik/2}$ in (5) for which the matrix elements of M^{pq} for the $|j\rangle$ basis have the simple asymptotic expression

$$\langle j_1|M^{pq}|j_2\rangle = m^*\delta_{j_1,j_2}(p + q - 2j_1 - 2) + O(B^{-p} + B^{-|q|}). \qquad (13)$$

Here we have set the system up so that the bulk magnetization far above the interface is $+m^*$ by careful handling of $|\Phi_+\rangle$ and $|\Phi_-\rangle$ in a rather technical way which is explained in Ref. [18]. This choice of phase factor is also the only one for which the $|j\rangle$ basis is covariant under a reflection transformation. If we take $p + q = 0$, followed by the limit $p \to \infty$, then we have

$$\langle j_1|M^{\infty}|j_2\rangle = -2m^*\delta_{j_1,j_2}(j_1 + 1). \qquad (14)$$

This is what we would get if the magnetization jumped abruptly from $-m^*$ to m^* when crossing the point $j_1 + \frac{1}{2}$: This is reminiscent of a Gibbs dividing surface.

It is also interesting to look at the matrix elements $\langle j_1|\sigma_j^x|j_2\rangle$, since the local magnetization with the Dobrushin boundary conditions is given by

$$\langle\sigma(n,j)\rangle = \frac{\sum_{j_1,j_2}\langle b|V^{N+n}|j_1\rangle\langle j_1|\sigma_j^x|j_2\rangle\langle j_2|V^{N-n}|b\rangle}{\langle b|V^{2N}|b\rangle}. \qquad (15)$$

In the usual SOS approximation it is assumed that

$$\langle j_1|\sigma_j^x|j_2\rangle = m^*\delta_{j_1,j_2}\,\mathrm{sgn}(j - j_1 - \tfrac{1}{2}). \qquad (16)$$

This misses significant local structure: The exact result which replaces the difference form

$$\langle j_1|\sigma_{j+1}^x - \sigma_j^x|j_2\rangle = 2m^*\delta_{j_1,j_2}\delta_{j,j_1} \qquad (17)$$

equivalent to (16) is

$$\langle j_1|\sigma_{j+1}^x - \sigma_j^x|j_2\rangle = m^*[a_-(j_1 - j)a_+(j_2 - j) + a_+(j_1 - j)a_-(j_2 - j)], \qquad (18)$$

where

$$a_\pm(j) = \frac{1}{2\pi}\int_{-\pi}^{\pi}[\tanh(\gamma/2)]^{\pm 1/2}e^{ijk}\,dk. \qquad (19)$$

However, the recapture of (2) does not differentiate between the two because the limit $N \to \infty$ is taken, and (14) shows that the local structure (18) disappears when considering the total magnetization of a column. Since $\gamma(k)$ is analytic in the strip $|\mathrm{Im}k| < \ln B$ containing the real axis, the functions $a_\pm(j)$ decay exponentially on the scale of the correlation length in the vertical direction $\xi = (\ln B)^{-1}$: The only information lost by the SOS approximation is on that scale. Nevertheless, (18) and (19) strongly support the view that there is an inhomogeneity of size about the correlation length associated with the interface, and, with that, the validity of Widom scaling [23].

Another important application of this path representation is the droplet model of subcritical spin correlation functions [12]. For large enough separations x (with respect to the correlation length), the decay of the truncated pair function is dominated by the two-particle sector since the sum of the remaining terms is bounded above by $e^{-4x\gamma(0)}$. We can change the basis to the two-domain-wall states $|\mathbf{j}\rangle$ defined by analogy with (5) by

$$|\mathbf{j}\rangle = \frac{M^{-1}}{\sqrt{2}}\sum_{k^<,k^>} e^{-j^<k^< - ij^>k^>}e^{i\varphi(k^<)+i\varphi(k^>)}G_{k^<}^\dagger G_{k^>}^\dagger|\Phi\rangle, \qquad (20)$$

where $\mathbf{j}$ is any pair $\mathbf{j} = \{j^<, j^>\}$ ordered by $j^< < j^>$. Then we have

$$\langle\sigma(1,1)\sigma(1 + x, 1 + y)\rangle - (m^*)^2 = \sum_{\{\mathbf{j}_1,\ldots,\mathbf{j}_{1+x}\}}\langle\Phi_+|\sigma_1^x|\mathbf{j}_1\rangle\left(\prod_{i=1}^{x}\langle\mathbf{j}_i|V_{(2)}|\mathbf{j}_{i+1}\rangle\right)\langle\mathbf{j}_{1+x}|\sigma_{1+y}^x|\Phi_+\rangle. \qquad (21)$$

The constraint $j_i^< < j_i^>$ is characteristic of nontouching paths. The matrix elements $\langle\mathbf{j}_1|V_{(2)}^n|\mathbf{j}_2\rangle$ are given by

$$\langle\mathbf{j}_1|V_{(2)}^n|\mathbf{j}_2\rangle = t_1^n(j_1^<, j_2^<)t_1^n(j_1^>, j_2^>) - t_1^n(j_1^<, j_2^>)t_1^n(j_1^>, j_2^<) \qquad (22)$$

in terms of the one-particle case (8), and the obvious generalization of (21) to the slab case $n \geq 2$ enables us to recover the Gaussian approximation to each path separately using (10), or the scaling limit as in (11). The new feature is the second term on the right of (21) which implies a repulsive interaction between the paths—normally neglected—supplementary to the nontouching restriction $j_i^< < j_i^>$. Further, the matrix elements $\langle j^<, j^>|\sigma_j^x|\Phi_+\rangle$, which appear as terminating factors in (21), have a local structure similar to (18):

$$\langle j^<, j^>|\sigma_j^x - \sigma_{j+1}^x|\Phi_+\rangle = m^*[a_-(j^< - j)a_+(j^> - j) - a_+(j^< - j)a_-(j^> - j)]. \qquad (23)$$

This implies that $\langle j^<, j^>|\sigma_j^x|\Phi_+\rangle$ is insignificant whenever either $|j^< - j|$ or $|j^> - j|$ is large compared to the correlation length ξ, justifying the SOS approximation of holding the ends of the bubble fixed at 1 and at $1 + y$, respectively.

Finally, we come to the role of the magnetic field in the droplet model which we have constructed. By analogy with (13), consider the matrix element $\langle\mathbf{j}_1|\tilde{M}^{pq}|\mathbf{j}_2\rangle$ where $\tilde{M}^{pq}$ is defined by $\tilde{M}^{pq} = M^{pq} - m^*(p - q)$ and (12).

This comes out in the limit $p \to \infty$ and $q \to -\infty$ as

$$\langle \mathbf{j}_1|\tilde{M}|\mathbf{j}_2\rangle = -2m^*\delta_{\mathbf{j}_1,\mathbf{j}_2}(j_1^> - j_1^<) + O(e^{-\gamma(0)(j_1^> - j_1^<)}). \quad (24)$$

This vindicates the phenomenological contention that the expected magnetization of the correlation droplet is proportional to its area, and entirely so when its opposite sides are sufficiently separated for the error term in (24) to be negligible.

In the case of a nonzero bulk field h, the expression replacing (21) for the two-point function will contain iterates of $Ve^{h\tilde{M}}$. It is important to note that $\tilde{M}$ scatters significantly into the many-particle sectors. The problem which this implies for treating nonzero fields can be obviated by going to the scaling limit. We choose $K_1 = K_2$ and denote $t = \gamma(0) = \ln B$. The function t_1^1 coming into expressions such as (22) for matrix elements of V is then given by (11). The magnetization term also has scaling with the scaled field variable $\overline{h} = \lim_{t\to 0} t^{-2}hm^*$ [24]. Thus the two-point function becomes

$$\lim_{t\to 0} \frac{\langle \sigma(1,1)\sigma(1 + t^{-1}\overline{x}, 1 + t^{-1}\overline{y})\rangle}{(m^*)^2} = \langle \Phi|\sigma e^{-\overline{x}H}e^{i\overline{y}P}\sigma|\Phi\rangle, \quad (25)$$

where P is the momentum operator, $|\Phi\rangle$ is the ground state eigenvector of H, and σ is the scaled local magnetization at the origin. The two-particle sector of the Hamiltonian, which dominates the low-energy behavior, is given in terms of position and momentum operators by

$$H_{(2)} = \sqrt{1 + p_<^2} + \sqrt{1 + p_>^2} + 2\overline{h}(y^> - y^<). \quad (26)$$

The nonrelativistic limit of (26) permits separation of the problem into center of mass and relative motion; it leads us back to the important work of McCoy and Wu on the "breakup of the cut" in the Fourier transform of the truncated two-point spin correlation [25]. This breakup replaces the Kadanoff-Wu anomalous decay [26,27] in scaled separation $\overline{r}$, with a prefactor $\overline{r}^{-2}$, by a sum of Ornstein-Zernike forms

$$h\overline{r}^{-1/2}\sum_{j=1}^{\infty}\exp[-(2 + h^{2/3}\gamma_j)\overline{r}], \quad (27)$$

where the γ_j are related to the zeros of the Airy function Ai [12,25,28].

We now summarize our results. We have shown that path representations without overhangs are achieved exactly without, we emphasize, any local mutilations of the lattice. The fluctuations of these paths are controlled by coarse-grained quantities such as the surface stiffness, and the paths are Gibbs dividing surfaces provided that they do not come too close together on the scale of the bulk correlation length. Thus we recapture the phenomenological bubble model of correlation functions in a controlled way.

The authors thank Professor T. Spencer and the Institute for Advanced Study very much for hospitality and excellent facilities. They also thank Professor J. L. Lebowitz, Professor E. Speer, Professor M. E. Fisher, and Dr. P. J. Upton for many informative discussions on these and related topics. D. B. A. acknowledges financial support from the EPSRC and the EU under Grants GR/J78044, GR/L15357, and ERBHBICT941666. He also thanks Professor É. Brézin and the Laboratoire de Physique Théorique of the École Normale Supérieure for hospitality and support. F. T. L. is very grateful to Merton College, Oxford, for the award of a Senior Scholarship. He also thanks the EPSRC for the award of a Research Studentship, and acknowledges a travel grant from Merton College and the Committee for Graduate Studies, Oxford University.

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