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Interface Structures and Hamiltonians: Exact Results[1]

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There have been many recent applications of interface models and Hamiltonians to problems in the theory of wetting. These models help to understand more abstract calculations on the type of problem which can be treated on the one hand, and on the other, to extend the type of problem which can be treated. A very recent example of this is corner wetting, also known as filling. This contribution discusses the validity of such concepts from first principles using exactly calculated interface structures and phase diagrams. The planar Ising model, with boundary conditions and surface fields imposed to bring in wetting, is used. The well-known Jordan–Wigner transformation to lattice fermions is composed of a product of spin reversals to one side (on a strip) of the point at which the lattice Fermi operator acts. Such spin reversals introduce a domain wall in a natural way which can be exploited to bring in interface Hamiltonians in a natural and precise way. The perennial problem of intrinsic structure is discussed. The findings do not support the notion of such a structure attached to capillary waves by convolution. In a sense to be made precise, kinks have to be taken into account.

KEY WORDS: exact solvable models; Ising model; interfaces; wetting.

1. INTRODUCTION

Some time ago, one might have been excused for thinking that there was nothing more to the scientific study of interfaces than determining incremental free energies such as surface tension. Following Onsager's advice that "preoccupation with partition functions maketh a dull man," the study of correlation functions in interfaces between coexisting phases in uniaxial ferromagnets has produced a number of surprises. These have been exposed by calculations on the planar Ising model.

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This article is organized as follows: first, some exact results about interfacial structure and wetting will be presented. After this, a coarse-grained representation of interfaces will be introduced; this brings in interface Hamiltonians.

2. INTERFACIAL STRUCTURE

Consider a planar Ising model with spins $\sigma(\mathbf{i}) = \pm 1$ at the vertices $\mathbf{i}$ of a quadratic lattice with unit side, coupled by a Hamiltonian

$$\mathscr{H}_\Lambda = -J \sum_{|\mathbf{i}-\mathbf{j}|} \sigma(\mathbf{i})\,\sigma(\mathbf{j}) - H \sum_{\mathbf{i}} \sigma(\mathbf{i}) \tag{1}$$

In Eq. (1), Λ specifies a finite subset of the quadratic lattice that is rectangular and has no holes in it.

Let the Ising model be equilibrated with a heat bath at a temperature T. Then it is well known that the probability of any configuration of spins denoted by $\{\sigma\}$ is given by

$$p(\{\sigma\}) = \frac{1}{\mathscr{Z}_\Lambda} \exp(-\beta \mathscr{H}_\Lambda(\{\sigma\})) \tag{2}$$

where $\beta = 1/(kT)$. Here, the notation $\beta J = K$ and $\beta H = h$ will be used. $\mathscr{Z}_\Lambda$ is the canonical partition function which normalizes $p(\{\sigma\})$ in Eq. (2). The basic theory of this model shows that only for $h = 0$ and $\sinh 2K > 1$ is there an ordered phase [1–4], which is characterized by two coexisting phases [3, 4] of equal and opposite magnetization $\pm m^*$, with

$$m^* = \left(1 - \frac{1}{\sinh^4 2K}\right)^{1/8} \tag{3}$$

A crucial fact is that phase transitions only occur in the thermodynamic limit as $\Lambda \to \infty$ (in a manner to be specified). Clearly, there is a problem about the meaning of Eq. (2) in such a limit, but this can be circumvented by considering expectation values for finite Λ, followed by a limit. A more subtle problem is how the coexistence of oppositely magnetized phases comes about. The resolution of this was first given by Peierls [5]; the mathematics was improved later [6, 7]. The correct procedure is to fix the boundary spins on Λ to be $\sigma(\mathbf{i}) = +1$ on $\delta\Lambda$; this prescribes the $+$-magnetized state as $\Lambda \to \infty$. Equally well, the opposite one is prescribed by $\sigma(\mathbf{i}) = -1$ on $\delta\Lambda$. To produce an interface, a reasonable candidate is to fix $\sigma(\mathbf{i})$ on the boundary $\delta\Lambda$ as follows: $\sigma(\mathbf{i}) = +1$ for $\mathbf{i} = (i_1, i_2) \in \delta\Lambda$ and $i_2 \geqslant 0$, but $\sigma(\mathbf{i}) = -1$ for $\mathbf{i} \in \delta\Lambda$, $i_2 < 0$. Let the partition function in this case be denoted by $\mathscr{Z}_{\Lambda}^{+-}$, and, for the case, $\sigma(\mathbf{i}) = +1$, $\mathbf{i} \in \delta\Lambda$, $\mathscr{Z}_{\Lambda}^{+}$. Then, the surface tension is defined by

$$\tau = \lim_{M \to \infty} \frac{1}{2M+1} \lim_{N \to \infty} \log\left(\frac{\mathscr{Z}_{\Lambda}^{+}}{\mathscr{Z}_{\Lambda}^{+-}}\right) \tag{4}$$

This can be calculated, giving [9, 10]

$$\tau = 2(K - K^*) \tag{5}$$

where the involution K^* of K is defined by

$$e^{-2K^*} = \tanh K \tag{6}$$

This satisfies Widom scaling [8], and one might be forgiven for thinking Onsager's dictum to be inappropriate, but for the following result: calculate the magnetization $\lim\langle\sigma(x, y)\rangle_{\Lambda}^{+-}$ [10]. The results are

$$\lim_{M \to \infty} \lim_{N \to \infty} \langle\sigma(x, y)\rangle^{+-} = 0 \tag{7}$$

for all (x, y), and $\sinh 2K > 1$. This invites the following question: Where is the interface? It is recaptured by scaling x and y with M, the width of the strip, giving

$$\lim_{M \to \infty} \lim_{N \to \infty} \langle\sigma(\beta M, \alpha M^{\delta})\rangle = m^* \operatorname{sgn} \alpha \begin{cases} 1 & \delta > 1/2 \\ 0 & \delta < 1/2 \\ \Phi(b\,|\alpha|/\sqrt{1-\beta^2}) & \end{cases} \tag{8}$$

where

$$\Phi(u) = \frac{2}{\sqrt{\pi}} \int_0^u e^{-t^2}\, dt \tag{9}$$

and

$$b = \sqrt{\sinh 2(K - K^*)} \tag{10}$$

So the loci of constant modulus of magnetization are elliptical, with a semi-major axis βM $(-1 < \beta < 1)$ and a semi-minor axis $C\alpha M^{1/2} b^{-1}$, where c is determined by the value of the magnetization. To understand Eq. (10), a further argument is needed: suppose that the point at which the spin reverses on the right-hand side of the lattice is moved upwards. This allows investigation of an angle-dependent surface tension denoted by $\tau(\theta)$ [11]. A tedious calculation shows that

$$b^2 = \tau(0) + \tau^{(2)}(0) \tag{11}$$

The generalization of Eqs. (8)–(10) to the interface at angle θ is obtained with rotated axes, one lying along the lines connecting the points of spin reversal, the other along a perpendicular to that line, with the intersection point defining an appropriate value of b. Equation (8) is recaptured with but one change—b is replaced by $b(\theta)$. Provided the angle dependence of $\tau(\theta)$ is taken into account, a fluctuation theory also gives Eqs. (8)–(10) [12]. This theory assumes that there is a sharp line separating regions of opposite magnetization $\pm m^*$; this line has no overhangs and is controlled by a fluctuation theory of the Helmholtz type. That such a simple model "works" is very reassuring, but one should not be deluded into concluding that the physics is the same. Before going on to examine this point critically, it should be noted that this phenomenology appears to work whenever $\tau(\theta) > 0$. Trying to understand Eqs. (8)–(10) from the point of view of low-temperature series is unduly restrictive and has the disadvantage that the factor $b(\theta)$ in Eqs. (8) and (10) cannot be identified with $\tau(\theta)$ and $\tau^{(2)}(\theta)$ since they are approximated by polynomials in e^{-2K}.

The objective is to develop an analogue of Peierls contours expressed in a language appropriate for the exact solution of the planar Ising model by "transfer matrix" and "fermionic" methods. The description given here will be qualitative; the reader who wants mathematical precision is referred to the references [13].

Since the interactions in Eq. (1) are nearest-neighbor, expectations with respect to the canonical probability in Eq. (2) can be expressed in terms of a Markov chain between states of vertical columns of spins. The transition matrix (un-normalized!) is taken as a representation in a prescribed basis of an operator on the finite-dimensional Hilbert space $\mathscr{H}_M$ of spin-$\frac{1}{2}$ states:

$$\mathscr{H}_M = \mathbb{C} \times \cdots \times \mathbb{C} \tag{12}$$

where each $\mathbb{C}$ is a two-dimensional spin space. The object is to "diagonalize" symmetrised versions of the transfer operator. This has been done in the "classical" period [14]. The maximum eigenvalue gives the free energy in the thermodynamic limit; the submaximal ones (excited states) together with matrix elements of local observables [15] such as spin $\sigma(x, y)$ at position y in column x, with some method of implementing the boundary conditions [16], give correlation functions such as Eqs. (7) and (8).

The key features of the diagonalization process is the appearance of fermion operators f_j and $f_j^\dagger$ through the Jordan–Wigner transformation,

$$f_j = \prod_{k=1}^{j-1} (-\sigma_k^z)\, \sigma_j^- \tag{13}$$

These operators display Fermi anticommutation relations, and a unitary transformation diagonalizes the transfer matrices, which are in the representation with σ_j^x diagonal. Thus Eq. (13) has a "tail" which reverses all x-quantized spins between $j-1$ and reference point at $k=1$. A pair of operators $f_j f_l$ reverses spins between j and l; this is a collective effect and is not surprisingly important in investigating submaximal eigenvectors of the transfer matrix. These remarks are merely a tour d'horizon, and the reader who wants to go further should consult the references. The key feature needed is that for $\sinh 2K > 1$ and cylindrical boundary conditions there are two-particle states generated by the "diagonal" Fermi operators. In order to be able to wrap the setup onto a cylinder, we need two interfaces which become infinitely separated, and thus independent, in the infinite volume limit. Each interface is generated by a single fermion (multi-fermion states are suppressed in the $M \to \infty$ limit). What is desired now is a real-space version of such an argument, in which we can track the location of the interface as it crosses the lattice. It is not obvious that this can be accomplished without including overhangs; this turns out to be possible.

Suppose such a domain-wall state $|j\rangle$ exists, and that such states span the 1-particle subspace. Then the following properties are generated

$$\langle j \mid k \rangle = \delta_{jk} \tag{14}$$

$$T\,|j\rangle = |j-1\rangle \tag{15}$$

where T is the unit translation in the column, and

$$\mathbb{M}\,|j\rangle = -(2j-1)\, m^*\, |j\rangle \tag{16}$$

where $\mathbb{M}$ is the total magnetization between points $\pm p$ in a column (with $p \to \infty$). Clearly, the fluctuations in the local magnetization should be localized. Thus,

$$\langle j_1 |\, \sigma^x(j)\, | j_2 \rangle \tag{17}$$

should have the value $m^* \operatorname{sgn}(j-\frac{1}{2})\, \delta_{j_1, j_2}$ as $j \to \pm\infty$ for any finite j. A detailed analysis of this matrix element shows that it is nonconstant whenever the j's are closer together than about a correlation length.

The magnetization profile is given in terms of the domain wall states (the result is restricted to the 1-particle spectrum, which suffices for the limit) by

$$\langle \sigma(x, j) \rangle = \frac{\sum_{j_1, j_2} \langle b | V^{N+x} | j_1 \rangle \langle j_1 | \sigma^x(j) | j_2 \rangle \langle j_2 | V^{N-x} | b \rangle}{\langle b | V^{2N} | b \rangle} \tag{18}$$

Were the SOS approximation correct, the central matrix element would be given by

$$\langle j_1 | \sigma^x(j) | j_2 \rangle = m^* \delta_{j_1, j_2} \operatorname{sgn}(j - j_1 - \tfrac{1}{2}) \tag{19}$$

This would give the results of Eqs. (8)–(10) but does not agree with the exact calculation. Similarly, the notion that

$$\langle j_1 | \sigma^x(j) | j_2 \rangle = m^* \delta_{j_1, j_2} g(j - j_1 - \tfrac{1}{2}) \tag{20}$$

for some possibly monotonic function $g(x)$ (with $\lim_{x \to \infty} g(\pm x) = \pm 1$) is not correct either. This is the vehicle for the usual ideas of *intrinsic structure* and *unfreezing of capillary waves*, represented by the two other matrix elements with the boundary states. The matrix element $\langle j_1 | \sigma^x(j) | j_2 \rangle$ has off-diagonal elements; this renders the usual formulation of intrinsic structure invalid, and with it, the idea of unfreezing capillary waves appears to be misleading.

The domain wall states allow a rigorous formulation of the domain wall problem as a sum over paths without overhangs with a transition amplitude between nth neighbor columns of

$$T^n(j_1, j_2) = \frac{1}{2\pi} \int_0^{2\pi} d\omega \, e^{-n\gamma(\omega)} e^{i(j_1 - j_2)\omega} \tag{21}$$

This allows an exact formulation of the Weeks columnar model [16] in this case. Note that it is not required to bring in the scaling limit, and that the usual Gaussian type of approximation to Eq. (21) arises naturally and in a controlled way.

3. WETTING PHENOMENA

The next topic which will be investigated is particularly appropriate, namely, exact solutions for wetting and the relevance of domain walls states for setting up interface Hamiltonians. First, the exact solution for pinning-depinning will be overviewed. If there is a domain wall, or long contour in the Peierls sense, to be precise, should the bonds normal to the edge be weakened from the bulk value, then the interface will be stabilized by lying at the boundary, but will lose entropy as a result. This is the classical transition scenario. There is indeed a phase transition at a temperature intermediate between zero and the two-dimensional bulk value given by $\sinh 2K_c = 1$ depending on the degree of bond weakening. Let the surface bonds have value aK, $0 < a < 1$. Then the transition occurs when (see Figs. 2 and 3)

$$e^{2K}(\cosh 2K - \cosh 2aK) = \sinh 2K \tag{22}$$

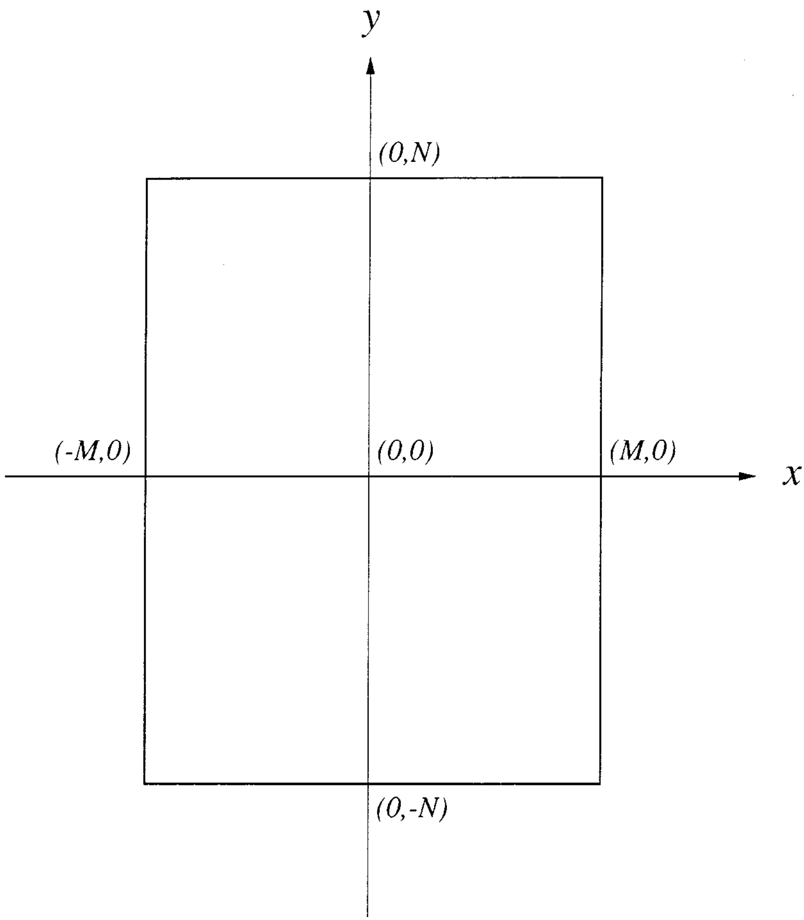

Fig. 1. Geometry of the lattice.

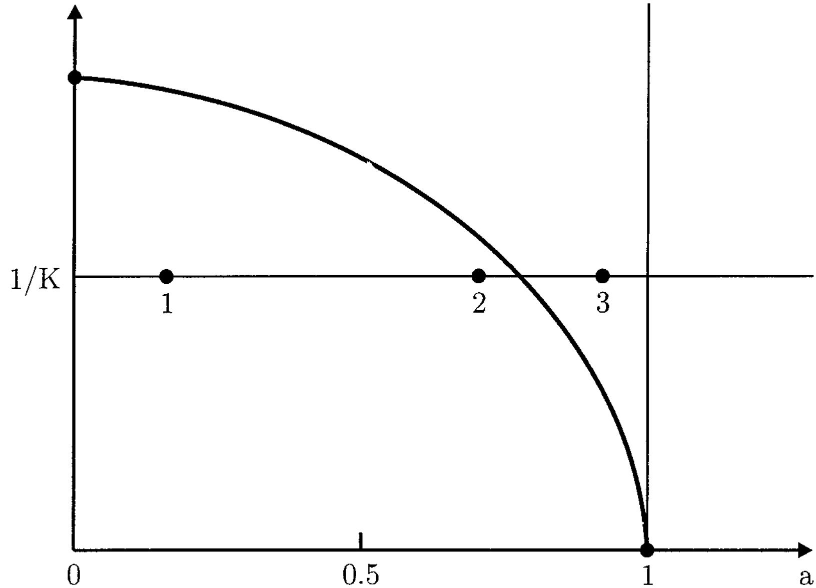

Fig. 2. Phase diagram for wetting. Between the axes and the curve there is partial wetting, represented by points 1 and 2 on the line of constant *K*. Point 3 is characteristic of the completely wet substrate.

At a thermodynamic level, there is a singularity of the incremental free energy. This transition is associated with a new length scale $\xi^x(a, K)$ which diverges on approaching the transition line from one side. On the other side, the interface is detached from the wall. Some care is needed in setting up this transition: boundary conditions must be chosen so that the bulk state is fully magnetized, with a value $+m^*$. It turns out that domain wall states can be defined in this case as well, but now in terms of eigenstates of a transfer matrix working parallel to the edge of the system. Let the state $|j\rangle$ now describe a domain wall at a distance j from the edge of the lattice. The transfer matrix elements are

$$\langle j_1 | \, V^n \, | j_2 \rangle = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-n\gamma(\omega)} \{ e^{i\omega(j_1 - j_2)} - e^{i\omega(j_1 + j_2)} e^{i\phi(\omega)} \} \tag{23}$$

Some remarks are in order. Firstly, only a single interface appears. This is at variance with the ideas of Parry and coworkers [18]. The interfacial stiffness once again acts to flatten the interface in the Gaussian approximation.

The interface stiffness does not have a correction depending on $(j_1 + j_2)/2$, as the work *in three dimensions* of Fisher and Jin [19] suggests:

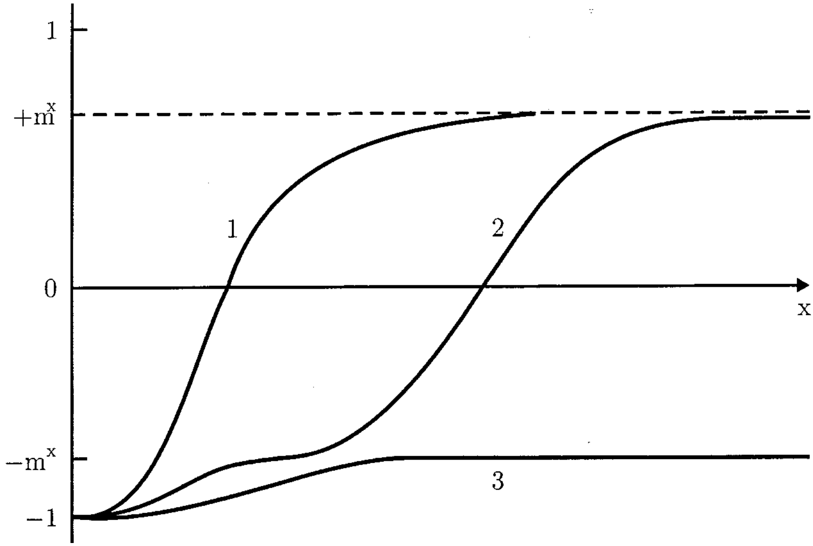

Fig. 3. Curves of magnetization as a function of distance from the substrate, for constant K but with variable pinning factor a. For the point 2 (see Fig. 2), $m(x)$ first approaches $-m^*$ on the scale of the bulk correlation length. On a new larger length scale, $m(x)$ goes through zero and attains m^*.

this absence may well be a special feature of the planar Ising model. The question of the matrix elements $\langle j_1 | \sigma^x(j) | j_2 \rangle$ in the wetting case is under active consideration; the problem is much more difficult than the free interface one, but will hopefully prove tractable.

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