# Intrinsic structure and long-ranged correlations in interfaces

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An intrinsic interface structure for phase separation in the planar Ising model is defined and calculated exactly. This structure is scaled by the bulk correlation length in accordance with Widom scaling theory. The pair correlation function with one of the points conditioned to lie in the interface decays as the inverse square root of the separation when this is parallel to the flat interface direction. This is an exactly solved example of the Wertheim phenomenon.

The structure of the interface between phases in a statistical-mechanical treatment at a molecular level has been the subject of much controversy in recent years. On the one hand, the theory of van der Waals[1] as developed by Cahn and Hilliard[2] and by Fisk and Widom[3] predicts an interface between phases which varies on the scale of the bulk correlation length, as Widom scaling[4] hypothesizes. On the other hand, such exact solutions and rigorous results as there are for systems in two or more dimensions indicate, depending on the parameters, large fluctuations of the position of the interface; these fluctuations diverge with increasing system size.[5–7] For instance, referring to Fig. 1 for notation, let the magnetization at the point $(x,y)$ in the strip of width $N$ be $m(x,y|N)$. Then the limiting result

$$\lim_{N\to\infty} m((1+\beta)N/2,\alpha N^{\delta}|N)=\begin{cases} m^{*}\,\mathrm{sgn}\alpha, & \delta>\frac{1}{2}\\ 0, & \delta<\frac{1}{2}\\ m^{*}\,\mathrm{sgn}\alpha\,\phi(|\alpha|b/(1-\beta^2)^{1/2}), & \delta=\frac{1}{2}\end{cases} \tag{1}$$

has been obtained[5] for $\beta\epsilon(-1,1)$ with

$$\phi(x)=\frac{1}{\sqrt{\pi}}\int_0^x e^{-u^2}du \ , \tag{2}$$

$m^*$ the usual spontaneous magnetization,[8] and

$$b^2=\sinh 2(K_1^*-K_2) \ , \tag{3}$$

where $\exp 2x^*=\coth x$ defines the usual dual variable. Equation (1) shows that $\sqrt{N}$ is a natural length scale in the problem; the result for $\delta=\frac{1}{2}$, however, cannot be derived from simple capillary wave theory,[9] but can be recaptured as shown by Fisher, Fisher, and Weeks[10] using the angle-dependent surface tension of the planar Ising model.[11] The idea is that the magnetization jumps abruptly between its extremal values $\pm m^*$ on crossing the interface along any vertical line (see Fig. 1). The probability of finding the interface at $(n,y)$ is given by simple fluctuation theory as

$$P_{\mathrm{cap}}(n,y|N)=Z^{-1}\exp-[\tau(\theta_1)L_1+\tau(\theta_2)L_2] \ , \tag{4}$$

where $\tau(\theta)$ is the surface tension for an interface at an angle $\theta$ to the $x$ axis. The magnetization in this model is then

$$\tilde{m}(n,y|N)=m^*\sum_{y'}P_{\mathrm{cap}}(n,y'|N)\,\mathrm{sgn}(y-y') \ . \tag{5}$$

Taking the leading term in the expansion in (4) of the exponent in powers of $y^2$ for $y^2<<N$ gives exactly the limiting result of (1). It is vital to notice that any reasonable function increasing from $-1$ to $+1$ could replace sgn in (5), and still yield (1).

By extending Ref. 5, the magnetization $m(n,y)=m(n,y|\infty)$ has been obtained *exactly* in the present work. An intrinsic structure $m_{\mathrm{int}}$ is *defined* by

$$m(n,y)=\sum_{y'}P_{\mathrm{cap}}(n,y|\infty)m_{\mathrm{int}}(n,y-y') \tag{6}$$

and

$$m_{\mathrm{int}}(y)=\lim_{n\to\infty}m_{\mathrm{int}}(n,y) \ . \tag{7}$$

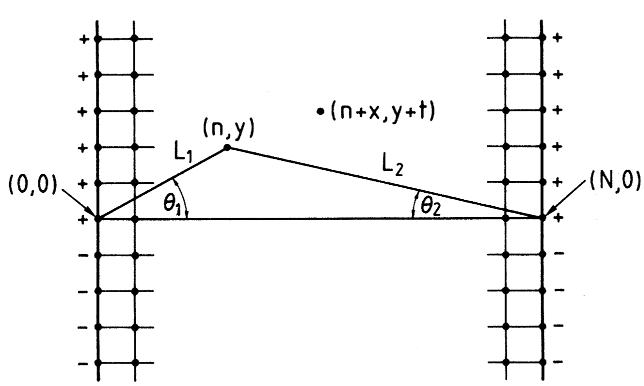


FIG. 1. Ising strip lattice with boundary conditions to achieve phase separation perpendicular to $y=-\frac{1}{2}$. The fluctuation probability is computed by considering the lengths $L_1$ and $L_2$ of the straight lines from $(n,y)$ to $(0,0)$ and to $(N,0)$ and by using an angle-dependent surface tension $\tau(\theta)$, as given in (4). The horizontal and vertical nearest-neighbor ferromagnetic couplings are $K_1$ and $K_2$ in units of $kT$.

The first new result is that

$$m(n,y)=\frac{m^*}{2\pi}\mathscr{P}\int_{\pi}^{\pi}d\omega\, e^{-n[\gamma(\omega)-\gamma(0)]}e^{i\omega y}g(\omega)/(e^{i\omega}-1)+O(e^{-2n\gamma(0)}) \ , \tag{8}$$

where $\mathscr{P}$ is the Cauchy principal part,

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

$[\gamma(\omega)\geq 0$ for real $\omega]$ and

$$g(\omega)=\frac{1}{e^{i\delta^*(\omega)}+1}\left(\frac{B}{A}\right)^{1/2}\left[\left(\frac{e^{i\omega}-A}{e^{i\omega}-B}\right)^{1/2}\left(\frac{1-B^{-1}}{1-A^{-1}}\right)^{1/2}+\left(\frac{e^{i\omega}-B^{-1}}{e^{i\omega}-A^{-1}}\right)^{1/2}\left(\frac{1-A}{1-b}\right)^{1/2}\right] \tag{10}$$

with

$$e^{i\delta^*(\omega)}=\left(\frac{(e^{i\omega}-A)(e^{i\omega}-B^{-1})}{(e^{i\omega}-A^{-1})(e^{i\omega}-B)}\right)^{1/2}\left(\frac{B}{A}\right)^{1/2} ,$$

where

$$A=\coth K_1^*\coth K_2,\quad B=\coth K_1^*\tanh K_2 \ . \tag{11}$$

To obtain decay as $y\to\pm\infty$, the partial difference $\partial_y$ is applied to (6). This removes the singularity at $\omega=0$ in (8). Since (6) is a convolution, it can be solved by standard Fourier series methods. The fluctuation theory gives

$$\hat{P}_{\rm cap}(n,\omega\,|\,\infty)=\exp-n[\gamma(\omega)-\gamma(0)] \ , \tag{12}$$

where $\hat{f}(\omega)$ is the function having $f(y)$ as its Fourier series coefficients (in $e^{iy\omega}$). The limiting solution as $n\to\infty$ is

$$\partial_y\hat{m}_{\rm int}(\omega)=g(\omega) \tag{13}$$

from which $(y\geq 0)$

$$m^*-m_{\rm int}(y)\sim e^{-\kappa y}y^{-3/2}[1+O(1/y)] \ , \tag{14}$$

where $\kappa=\ln B$ is the bulk inverse correlation length. This is in accord with Widom scaling theory,[4,12] although (14) is not a solution of Fisk-Widom theory[3,12] which would have a pure exponential decay as $y\to\pm\infty$.

We now make a number of remarks about the solution.

(i) Equation (6) is a tautology until $P_{\rm cap}$ is defined. The Fisher-Fisher-Weeks fluctuation theory gives a physically natural choice which turns out to be mathematically sufficient to get a nontrivial limit $m_{\rm int}(y)$ to exist.

(ii) Unlike the conclusions reached earlier,[13] (12) implies no restriction of ensemble on the line $x=n$ in Fig. 1. It is of interest, nevertheless, that the results are qualitatively similar.

(iii) A convolution structure such as (6) has also been suggested by Jasnow and Rudnick,[14] but with a pure Gaussian for $P_{\rm cap}$. This will not do to solve (6) in an interesting way; (4) in fact contains a more careful estimate of large fluctuations. What appears here as a mathematical necessity may well prove useful in analyzing light scattering data from interfaces.

(iv) As stated above, (14) is not in accord with Fisk-Widom theory.[3] This could well be connected with the anomalous decay of the truncated pair function

$$u_2(r)\sim(m^*)^2e^{-2\kappa r}/r^2$$

obtained by Wu[15] in place of the usual Ornstein-Zernike result.

(v) Other definitions of intrinsic structure are available[14,16,17] which are not based on the convolution idea, but they do not appear to be amenable to exact analysis at all temperatures below the critical value.

We now return to another aspect of the problem, the existence of long-ranged correlations within the interface originally proposed by Wertheim[18] and found within the columnar model.[19,20] An intrinsic pair function $C(x,y)$ is defined by the solution of

$$\lim_{N\to\infty}\langle\sigma(n,y)\sigma(n+x,y)\rangle=\sum_{y'}C(x,y'|n)P_{\rm cap}(n,y-y'|\infty)$$

with $C(x,y)=C(x,y|\infty)$. The reasoning is the same as before and the solution is

$$C(x,y)\sim m^*m_{\rm int}(y)\frac{1}{2\pi}\int_{\pi}^{\pi}d\omega\exp-x[\gamma(\omega)-\gamma(0)]+O(e^{-2x\gamma(0)}) \ ,$$

which has a $1/\sqrt{x}$ behavior as $x\to\infty$, as was obtained using the restricted ensemble.[13]

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