Comments

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Comments on Abraham's intrinsic interface structure

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Abraham has proposed a definition for and calculated exactly an *intrinsic interface structure* for phase separation in the planar Ising model. Here I wish to argue that the definition actually is rather arbitrary and that the exact result is not a plausible realization of the intrinsic interface structure hypothesized by Widom's scaling theory.

Abraham[1] considers a strip of width N of a square-lattice Ising model with nearest-neighbor couplings only. The spins, $s(x,y)=\pm 1$, are situated at sites specified by the integers $0 \leq x \leq N$ and $-\infty < y < \infty$. Fixed-spin boundary conditions,

$$\begin{aligned} s(0,y) &= s(N,y) = 1, \quad y \geq 0 \\ &= s(N,y) = -1, \quad y < 0 \ , \end{aligned} \tag{1}$$

are imposed and result in an interface running horizontally across the system from the point (0,0) to $(N,0)$ (see Fig. 1 of Ref. 1). A naive estimate at the probability of the interface crossing the column $x=n$ at height y is

$$P(n,y|N) = Z^{-1} \exp\left\{ -\left[(n^2+y^2)^{1/2} \sigma\left(\frac{y}{n}\right) + [(N-n)^2+y^2]^{1/2} \sigma\left(\frac{y}{N-n}\right) \right] \right\} , \tag{2}$$

where $\sigma(w)$ is the reduced surface tension of an interface running at angle $\theta = \tan^{-1}(w)$ to the x axis, and Z is chosen so $\sum_y P(n,y|N)=1$. The exponent in (2) is simply the thermodynamic free energy of an interface running from (0,0) to (n,y) and then to $(N,0)$. Note that (2) neglects the free energies of the bend in the interface at (n,y) and of its ends at (0,0) and $(N,0)$.

Abraham[1] calculates exactly the local magnetization $m(n,y) \equiv \langle s(n,y) \rangle$ in the limit $N \to \infty$. This local magnetization is then equated to a convolution of the interface fluctuations specified by (2) and an *intrinsic* interface structure M_{int} via[1]

$$m(n,y) = \sum_{y'} P(n,y') m_{\text{int}}(n,y-y') \ , \tag{3}$$

where $P(n,y) = P(n,y|\infty)$. In the limit $n \to \infty$ this definition yields a unique interface structure

$$m_{\text{int}}(y) = \lim_{n \to \infty} m_{\text{int}}(n,y) \ . \tag{4}$$

For convenience, let us consider the discrete derivative of $m_{\text{int}}(y)$, namely,

$$m'_{\text{int}}(y) = m_{\text{int}}(y) - m_{\text{int}}(y-1) \ , \tag{5}$$

and its Fourier series, $\hat{m}'_{\text{int}}(\omega)$. If $m_{\text{int}}(y)$ is the type of intrinsic interface structure discussed by Widom,[2] then we expect it to be a monotonic function, which smoothly connects positive and negative magnetizations over a length scale of order ξ, the bulk correlation length. If $m_{\text{int}}(y)$ is indeed monotonic, then $m'_{\text{int}}(y)$ is non-negative definite and its Fourier series $\hat{m}'_{\text{int}}(\omega)$ has its maximum at $\omega=0$. However, an examination of the results [Eqs. (10) and (11) of Ref. 1] reveals that $\hat{m}'_{\text{int}}(\omega)$, which is proportional to Abraham's $g(\omega)$, actually has a minimum at $\omega=0$ and a larger value at $\omega=\pi$ than $\omega=0$. Thus the proposed $m_{\text{int}}(y)$ is a non-monotonic or oscillatory function, which is certainly not what we expect of the intrinsic interface structure, particularly near the critical point.[2]

What is the source of this strange result? Examination of the exact magnetization profile $m(n,y)$ reveals that it is actually *narrower* than the profile we would obtain from (3) with a perfectly sharp interface structure (a step function) replacing m_{int}. This is because the function $P(n,y)$ ignores the energies associated with the bends and ends of the interface. The fixed-spin boundary conditions at $x=0$ certainly inhibit the interfacial fluctuations out to distances of order ξ from the boundary. Thus one can quite reasonably argue that the interface is effectively starting not at the point (0,0) but at $(c\xi,0)$, where c is a number of order unity specifying how the boundaries inhibit the interfacial fluctuations. This would suggest that we might replace (3) with

$$m(n,y) = \sum_{y'} P(n-c\xi,y') m_{\text{int}}(n,y-y') \ . \tag{6}$$

This new definition of m_{int} will give a different result in the limit $n \to \infty$ for each value of c. If c is taken to be large enough, then the resulting $m_{\text{int}}(y)$ can be made monotonic. However, simply replacing n with $(n-c\xi)$ cannot be an ex-

act description of the effects due to boundary conditions, so the definition (6) must still be considered to be arbitrary.

In conclusion, a proper deconvolution of an intrinsic interface structure from $m(n,y)$, if possible, must certainly take into account the interaction between the interface and the boundaries of the system. In principle, this edge effect can be calculated; however, one might also need to take account of the free energy of the bend in the interface at the column $x = n$, a quantity whose precise definition is not obvious.

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[1]D. B. Abraham, Phys. Rev. B **29**, 525 (1984).
[2]B. Widom, J. Chem. Phys. **43**, 3892 (1965); in *Phase Transitions and Critical Phenomena,* edited by C. Domb and M. S. Green (Academic, London, 1972), Vol. 2.