Reply to "Comments on Abraham's intrinsic interface structure"

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The definition of intrinsic structure commented on by Huse is extended. This removes Huse's objection and agrees better with Widom's original phenomenological ideas on interfacial structure.

Huse¹ is certainly correct in his observation that the intrinsic interface profile calculated in Ref. 2 is not monotonic. [In what follows, we shall denote by Eq. (I.m) and Eq. (II.m) the corresponding Eq. (m) in Refs. 1 and 2, respectively.] Equation (II.14) is correct; the O(1/y) term is proportional to -1/y. The idea that any intrinsic structure function must be monotonic is by no means universally accepted. The theory of Stillinger, for instance, also gives an oscillatory profile.³

In the authors opinion, the failure to recapture the anomalous inverse correlation length for the pair-correlation function of $4(K - K^*) = 2 \ln B$ (Ref. 4) (rather than simply $\ln B$) [see (I.4) *et seq.*] is far more serious.

Huse also discusses (II.4) in his (I.2). Equation (I.3) cannot be solved in a nontrivial way with an expansion of (I.2) valid for $y \ll N$ truncated at the quadratic (the capillary wave approximation). This is because large fluctuations must be taken into account. Even then, it is not clear that the convolution procedure introduced could ever work. From a physical point of view, domain wall configurations with macroscopically distinct multiple intersections with the line $x = x_0$ might be significant. Mathematically, it is quite trivial to construct counterexamples which have, e.g., $\hat{m}_{int}(\infty, \omega) = 0$. As pointed out in Ref. 2, the ansatz

$$\hat{P}_{cap}(n,\omega) = \exp\{-n\left[\gamma(\omega) - \gamma(0)\right]\}$$
(1)

works mathematically, and it agrees to quadratic approximation with (I.2) and (II.4). If we recall the definition of angle-dependent surface tension,⁵ then it is natural to set

$$P_{\rm cap}(n,y) = Z^{+-}(n,y) / \sum_{y=-\infty}^{\infty} Z^{+-}(n,y) \quad , \tag{2}$$

where Z(n,y) is the partition function for an infinite length

⁵D. B. Abraham and P. Reed, J. Phys. A 10, L212 (1977); D. S.

strip of width *n* crossed by a domain wall going from (0,0) to (n,y) (suitably normalized to remove the bulk free energy term which cancels out). The restricted ensemble implied by (2) was used in a rigorous version⁶ of the Weeks columnar model.⁷ The exponent in the large *n* development of (2) is the same as in (I.2) and (II.4). But this does not suffice to give the anticipated length scale of $(2 \ln B)^{-1}$ or monotonicity.

It is not clear to the authors precisely what Huse means by edge effects; presumably (2) takes them into account and yet it is still unsatisfactory.

A satisfactory resolution of the problem can be given as follows: Consider an interface running from (-N, 0) to (N, 0) and set

$$m(x,y|N) = \sum_{y'} m_{\text{int}}(x,y-y'|N)P(x,y'|N) , \qquad (3)$$

with P(x,y|N) the obvious two-sided generalization of (2). Then look at $N \to \infty$ with fixed x, in other words, stay near the center of the strip, unlike in Ref. 2. This problem is much harder, but we have solved it for $m_{int}(x,y|\infty)$, which is independent of x, as it should be; further, it is monotonic in y and has the Wu length scale of $(2\ln B)^{-1}$ (Ref. 4). If we put x = N, $-1 < \beta < 1$ then we encounter a variable length scale which recaptures the one of Ref. 2 if $\beta \to \pm 1$. The details of this work will be published elsewhere.

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⁶D. B. Abraham, Phys. Rev. Lett. 47, 585 (1981).

⁷J. D. Weeks, J. Chem. Phys. 67, 3106 (1977).