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Universality in two-point functions at wetting: Exact scaling function for energy-density correlations

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The scaling function at the wetting transition for the two-point energy-density correlation function is computed exactly for two-dimensional Ising models with interfaces in the [10] and [11] directions. The two-point separations perpendicular and parallel to the wall are scaled by $\xi_{\perp} \sim (T_w - T)^{-1}$ and $\xi_{\parallel} \sim (T_w - T)^{-2}$, respectively; and the energy-density operator scales as $T_w - T$. The resulting scaling function is independent of the microscopic couplings, boundary interactions, wall orientation, and specifics of the operator. Furthermore, the result is simple and consists of Gaussians and error functions, suggestive of random walk.

The wetting transition, or the unbinding of interfaces, is a subject of much recent interest. (See reviews in Refs. 1-5). Despite the tremendous understanding that has been achieved through these works, no exact result from microscopic models on correlation functions for wetting⁶ has been computed. Effort in this direction has been inhibited by the expectation that the results may be complicated, hence unilluminating. However, we will present below an exact result which is simple and may be reproduced by other approaches, such as the random-walk method.

The last few years have seen an important development⁷ in the applications of conformal algebra to twodimensional systems. The method has been successfully used to derive correlation functions at the critical temperature T_c , and there has been much interest in extending the method to⁸ $T \neq T_c$ and to defect systems.⁹ Twodimensional wetting naturally falls in the regime of concern, for wetting generally occurs at $T_w < T_c$ and the defect representing wall interactions is the mechanism of interface pinning. If it is possible to extend conformal algebra to treat wetting, one would expect the results to possess some universal character. However, it is well known¹⁰ that noncritical correlations in general depend very explicitly on the detailed couplings. Furthermore, two-point scaling functions for $T \rightarrow T_c$ for the Ising model with linear defects has been computed in Ref. 11 for energy densities, and in Ref. 12 for spins; it was shown that the universal scaling forms are destroyed by the defect. The energy-density correlation is a simple expression in terms of Bessel functions for the homogeneous system,¹³

but that for the defect system is rather complicated, with the explicit dependence on the defect persisting to the at- T_c limit, even though the critical exponent α remains universal.¹⁴ In view of these known results, it is not *a* priori clear how universality can arise for wetting in the Ising model, even though it is expected from generally accepted principles. Our result shows that the answer lies in the following two points: First, how to isolate the interfacial contribution to the correlations in a microscopic model and second, how to scale the distances as well as the operators as $T \rightarrow T_w$.

The answer to part of the second point has been suggested in fluctuation theory¹⁵ and solid-on-solid walks,¹⁶ where it has been proposed that the scaling behaviors of correlation lengths perpendicular and parallel to the wall are $\xi_{\perp} \sim (T_w - T)^{-1}$ and $\xi_{\parallel} \sim (T_w - T)^{-2}$. And indeed these are consistent with the exact result to be shown. On the other hand, the answer to the first point comes out of our exact calculation. It is found that the proper "net energy-density correlation" for wetting is

$$\langle \varepsilon_{1}\varepsilon_{2}\rangle_{c} = \langle \varepsilon_{1}\varepsilon_{2}\rangle_{+-} - \langle \varepsilon_{1}\varepsilon_{2}\rangle_{++} - \langle \varepsilon_{1}\rangle_{c}\langle \varepsilon_{2}\rangle_{++} - \langle \varepsilon_{1}\rangle_{++}\langle \varepsilon_{2}\rangle_{c},$$
(1)

where ++ denotes the boundary condition for pure phase. The net one-point function $^{16} \langle \varepsilon \rangle_c = \langle \varepsilon \rangle_{+-} - \langle \varepsilon \rangle_{++}$ decreases exponentially from the wall to the bulk in the partially wet phase, and changes to a power-law decay at the transition. Note that this subtraction removes the disconnected part as well as the pure phase contributions.

Consider two infinite cylindrical Ising lattices, one

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oriented in the [10] direction, and the other in the [11] direction. The reduced interactions between nearestneighbor spins are K_1 and K_2 , except they are modified to \tilde{K}_1 and \tilde{K}_2 in the bottom row, as shown in Fig. 1. The boundary condition at the top and bottom of the cylinder is that all spins are +1 in the top row and -1 in the bottom row. An interface is imposed by this boundary condition. The thermodynamics of the [11] interface has recently been calculated;¹⁶ a large entropic freedom is associated with this geometry and it results in lower T_w compared with that of the well-known [10] case, calculated in Ref. 17. The incremental free energy τ for the two lattices has the form

$$\cosh \tau = \cosh \tau_0 - \frac{1}{2} F(T) , \qquad (2)$$

with τ_0 the bulk incremental free energy,

$$\tau_0^{[10]} = 2K_1 + \ln \tanh K_2,$$
(3)

$$\tau_0^{[11]} = \ln(\sinh 2K_1 \sinh 2K_2);$$

and F(T), the vanishing of which determines T_w and, hence, the phase diagram, is given by 16,17

$$F(T)^{[10]} = \frac{\left[e^{K_2}(\cosh 2K_1 - \cosh 2\tilde{K}_1) - \sinh 2K_1 e^{-K_2}\right]^2}{(\cosh 2K_1 - \cosh 2\tilde{K}_1)\sinh 2K_1},$$

$$F(T)^{[11]} = \frac{(\sinh 2K_1 \sinh 2K_2 - 1 - 2\sinh 2\tilde{K}_1 \sinh 2\tilde{K}_2)^2}{\sinh 2K_1 \sinh 2K_2}.$$
(4)

We calculate the correlation function between two energy densities $\varepsilon_1 = \varepsilon_{n_1,m_1}$ and $\varepsilon_2 = \varepsilon_{n_2,m_2}$ with $\varepsilon_{i,j} = \sigma_{i,j}\sigma_{i,j+1}$. The precise coordinates in each lattice are



FIG. 1. The two-dimensional Ising lattices with boundary oriented in the [10] and [11] directions. The boundary conditions are periodic on the side and all spins are -1 (+1) at the bottom (top). The reduced couplings are K_1 and K_2 except near the wall at the bottom where they are \tilde{K}_1, \tilde{K}_2 . The coordinations of the energy-density operator $\varepsilon_{n,m}$ are indicated.

shown in Fig. 1. Note that the term "energy density" is used in a loose sense in the [11] lattice, for it is really the next-nearest-neighbor spin pair. Clearly the presence of the wall destroys some symmetries enjoyed by correlations in the bulk. The translational invariance in the horizontal direction remains valid, and only $m=m_2-m_1>0$ is relevant; but both n_1 and n_2 will appear in the correlation, and the natural vertical separations are $n=n_2-n_1>0$ and $\bar{n}=n_2+n_1$. We use the method of transfer matrix to compute this two-point function in both lattices. In the following we show the net two-point functions for the two Ising lattices in a notation which brings out the similarity of the results in the two lattices for arbitrary temperature below transition. Then we proceed to show how to obtain the scaling function.

The exact result for the net energy-density correlations is

$$\langle \varepsilon_1 \varepsilon_2 \rangle_c = L(\omega_p) \frac{1}{2\pi} \int_{-\pi}^{\pi} d\omega (i \sin[\delta^*(\omega) - \delta^*(\omega_p)] L_{-}(\omega) - \{1 - \cos[\delta^*(\omega) - \delta^*(\omega_p)]\} L_{+}(\omega)) [1 + O(e^{2im\omega_p})], \quad (5)$$

with $\omega_p = i\tau$, the incremental free energy, and

$$L(\omega) = \frac{2e^{-\bar{n}\gamma(\omega) - im\omega}}{C(\omega)A'(-\omega)}, \quad L_{-}(\omega) = e^{-n\gamma(\omega) - im\omega}, \quad L_{+}(\omega) = \frac{iB(\omega)}{A(\omega)}e^{-\bar{n}\gamma(\omega) - im\omega}.$$
(6)

A term of $O(e^{2im\omega_p})$ in (5) has been ignored because we shall concentrate on the limit $m, n \to \infty$. An anisotropy factor which differs from unity only for one lattice has also been suppressed, being irrelevant in the scaling limit. The m, n dependence in (5) has a simple form which only appears in $L(\omega)$, $L_{-}(\omega)$, and $L_{+}(\omega)$. The combination $\exp[-n\gamma(\omega) - im\omega]$ is a familiar one^{10,18} in the infinite homogeneous Ising model. The functions $\gamma(\omega)$ and $\delta^{*}(\omega)$ for the [10] lattice are the elements of Onsager's hyperbolic triangle,¹⁸

$$\sinh \gamma(\omega) = \frac{\sinh 2K_2}{2\sinh 2K_1} [(\alpha_1^{-1} - e^{i\omega})(1 - \alpha_1 e^{-i\omega})(\alpha_2^{-1} - e^{i\omega})(1 - \alpha_2 e^{-i\omega})]^{1/2},$$

$$e^{i\delta^*(\omega)} = \left(\frac{(1 - \alpha_1 e^{i\omega})(1 - \alpha_2 e^{-i\omega})}{(1 - \alpha_2 e^{i\omega})(1 - \alpha_1 e^{-i\omega})}\right)^{1/2},$$
(7)

where $\alpha_1^{-1} = \exp(K_1 + K_2^*)$, $\alpha_2^{-1} = \exp(K_1 - K_2^*)$. These are presented in their factored form so that the analytic structures are easily discerned. Similarly, for the [11] lattice,¹⁹

$$\sinh\gamma(\omega) = |\sinh 2K_1 + \sinh 2K_2 e^{i\omega}|^{-1} [(\alpha_0^{-1} - e^{i\omega})(\alpha_0^{-1} - e^{-i\omega})]^{1/2}, \quad e^{i\delta^*(\omega)} = \left(\frac{1 - \alpha_0 e^{-i\omega}}{1 - \alpha_0 e^{i\omega}}\right)^{1/2}, \quad (8)$$

where $\alpha_0^{-1} = \sinh 2K_1 \sinh 2K_2$. The branch selected for each square root in (7) and (8) takes a positive value at $\omega = 0$. Comparison between (7) and (8) shows that they both have the structure of a branch cut inside and outside the unit circle in the complex $e^{i\omega}$ plane, and the branch points α_1 , α_2 , α_2^{-1} , and α_1^{-1} in the [10] lattice are replaced by 0, α_0 , α_0^{-1} , and ∞ in the [11] lattice. Below the bulk critical temperature, α_0 , $\alpha_2 < 1$ and they are related to the bulk incremental free energy by $\omega_0 = i\tau_0$, where $\exp i\omega_0 = \alpha_2$, α_0 for the [10], [11] lattice, respectively. To complete the definition of Eq. (5), we have

$$A(\omega) = Z_{+}(\omega)[-f_{+}(\omega) + \tan\theta(\omega)],$$

$$B(\omega) = Z_{+}(\omega)[f_{+}(\omega)\tan\theta(\omega) + 1],$$
 (9)

$$C(\omega) = Z_{-}(\omega)[f_{-}(\omega)\tan\theta(\omega) + 1],$$

where $\theta(\omega) = \delta^*(\omega)/2$, $\delta^*(\omega)/2 + \omega/2$ for the [10], [11] lattice, respectively; and

$$f_{\pm}^{[10]}(\omega) = \mp (\operatorname{coth} 2\tilde{K}_1 \mp \cos\omega) \operatorname{csc} \omega e^{\pm 2K_2},$$

$$f_{\pm}^{[11]}(\omega) = \tanh^{\pm 2} (\tilde{K}_1 \pm \tilde{K}_2) \tan \frac{\omega}{2}, \qquad (10)$$

$$Z_{\pm}^{[10]}(\omega) = \pm \sinh 2\tilde{K}_{1} \sin \omega e^{\mp K_{2}} \cos \frac{\delta^{*}(\omega)}{2} ,$$

$$Z_{\pm}^{[11]}(\omega) = \frac{\cosh 2(\tilde{K}_{1} \pm \tilde{K}_{2}) \mp 1}{\sinh K_{1} + \sinh K_{2} e^{-i\omega}} \cos \frac{\omega}{2} \cos \theta(\omega) . \quad (11)$$

Note that $A(\pm \omega_p) = 0$; this adds two poles to the branch points in the singularities of the integrand of (5).

As $T \to T_w^-$, the incremental free energy approaches the bulk value, $\tau \to \tau_0$, thus $\gamma(\omega_p) \to \gamma(\omega_0) = 0$. In the limit $n, m \to \infty$ and $T \to T_w^-$, we obtain the scaling function for (5) by defining the scaled distances $x = m(\tau_0 - \tau)$, $y = n\gamma(\omega_p)$ and $\bar{y} = \bar{n}\gamma(\omega_p)$. Thus, the vertical¹⁷ and horizontal correlation lengths are given by

$$\xi_{\perp}^{-1} = \gamma(\omega_p) \sim T_w - T, \quad \xi_{\parallel}^{-1} = \tau_0 - \tau \sim (T_w - T)^2.$$
(12)

The above scaling is implemented in the two-point function in (5) in the following steps. The contour of integration in ω from $-\pi$ to π is deformed down to the lower complex ω plane; there is a contribution from the pole at $\omega = -\omega_p = -i\tau$, and a contribution from the contour along the branch cut from $\omega = -\omega_0 = -i\tau_0$ to $\omega \rightarrow -i\infty$. Since the latter is dominated by $\omega \sim \omega_0$ due to the factor $\exp -im\omega$, we expand ω around $-\omega_0$ and scale it by $z^2 = (\omega + \omega_0)/(\omega_p - \omega_0)$. This reduces (5) to the following scaling form.

$$\langle \varepsilon_{1}\varepsilon_{2} \rangle_{c} = We^{-\bar{y}} \left[2e^{-\bar{y}} + \frac{e^{-x}}{\pi} \int_{0}^{\infty} dz e^{-xz^{2}} \left[\cos yz - \frac{(1-z^{2})\cos \bar{y}z + 2z\sin \bar{y}z}{1+z^{2}} \right] \right],$$
(13)

where

$$W = \lim_{\omega_p \to \omega_0} 2e^{-2i\delta^*(\omega_p)} / \xi_{\parallel} C(\omega_p) A'(-\omega_p) \sim (T_w - T)^2$$

The consequence of this factor is that the scaling dimension of the energy density is one. This is the same scaling dimension for energy density at T_c ; whether or not it is only a coincidence remains open. We scale the operator by $\hat{\varepsilon}_j = \varepsilon_j / \sqrt{W}$, and carry out the integral²⁰ in (13) to obtain the final result

$$\langle \hat{\varepsilon}_{1} \hat{\varepsilon}_{2} \rangle_{c} = \frac{1}{2} (x\pi)^{-1/2} e^{-x - \bar{y}} (e^{-y^{2}/4x} + e^{-\bar{y}^{2}/4x}) + e^{-2\bar{y}} \left[1 + \Phi \left[\sqrt{x} - \frac{\bar{y}}{2\sqrt{x}} \right] \right], \qquad (14)$$

where $\Phi(x)$ is the error function, and x and $y(\bar{y})$ are the scaled horizontal and vertical (image) separation between the two scaled energy densities $\hat{\epsilon}_1$ and $\hat{\epsilon}_2$, respectively.

Clearly the above result is universal: any dependence on the microscopic couplings K_1, K_2 , the wall interactions \tilde{K}_1, \tilde{K}_2 , as well as any reference to the orientation of the boundary or the difference between nearest- and nextnearest neighbor pair operators has been scaled away, and is implicit through $\xi_{\perp}, \xi_{\parallel}$, and W only. Furthermore, the appearance of Gaussians and error functions is very suggestive of random walk and may be reproduced by methods such as those reviewed in Ref. 5. The randomwalk feature is expected to be general and valid for more complicated correlations even if spins are involved. While the spin- and energy-density correlations are profoundly different at T_c , we expect them to be quite similar at T_w , provided proper subtraction and scaling are taken.

Note added in proof. Professor T. W. Burkhardt kindly informed us that he has recently produced our results with a solid-on-solid model.

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- ¹M. E. Fisher, J. Chem. Soc. Faraday Trans. 2 82, 1569 (1986).
- ²D. B. Abraham, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1986), Vol. 10, p. 1.
- ³S. Dietrich, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1988), Vol. 12.
- ⁴R. Lipowsky (unpublished).

- ⁵M. E. Fisher, J. Stat. Phys. **34**, 667 (1984); V. Privman and N. M. Švrakić, *ibid.* **51**, 1111 (1988).
- ⁶M. S. Wertheim, J. Chem. Phys 65, 2377 (1976); P. Tarasona and R. Evans, Mol. Phys. 47, 1033 (1982); S. M. Foiles and N. W. Ashcroft, Phys. Rev. B 25, 1366 (1982); P. Tarazona, R. Evans, and U. Marini Bettolo Marconi, Mol. Phys. 54, 1357 (1985).
- ⁷A. A. Belavin, A. M. Polyakov, and A. B. Zamolodchikov, J.

Stat. Phys. 34, 763 (1984); J. L. Cardy, in *Phase Transitions* and *Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1987), Vol. 11, p. 55.

- ⁸H. Itoyama and H. B. Thacker, Phys. Rev. Lett. **58**, 1395 (1987); J. Cardy, *ibid.* **60**, 2709 (1988).
- ⁹L. Turban, J. Phys. A **18**, L325 (1985); T. W. Burkhardt and I. Guim, Phys. Rev. B **36**, 2080 (1987); M. Henkel and A. Patkos, J. Phys. A **20**, 2199 (1987).
- ¹⁰See B. M. McCoy and T. T. Wu, *The Two-Dimensional Ising Model* (Harvard, Cambridge, MA, 1973).
- ¹¹L. F. Ko, Au-Yang, and J. H. H. Perk, Phys. Rev. Lett. 54, 1091 (1985).
- ¹²L. F. Ko, J. Stat. Phys. 52, 795 (1988); 52, 815 (1988).

- ¹³J. Stephenson, J. Math. Phys. 7, 1123 (1966); R. Hecht, Phys. Rev. 158, 557 (1967).
- ¹⁴M. E. Fisher and A. E. Ferdinand, Phys. Rev. Lett. **19**, 169 (1967).
- ¹⁵D. S. Fisher, M. P. A. Fisher, and J. D. Weeks, Phys. Rev. Lett. 48, 369 (1982).
- ¹⁶D. B. Abraham, L. F. Ko, and N. M. Švrakić, Phys. Rev. B 38, 12011 (1988).
- ¹⁷D. B. Abraham, Phys. Rev. Lett. 14, 1165 (1980).
- ¹⁸L. Onsager, Phys. Rev. 65, 117 (1944).
- ¹⁹D. B. Abraham and B. Davis (unpublished).
- ²⁰I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products, Fourth edition* (Academic, New York, 1980).