Propagator for the wetting transition in 1+1 dimensions

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The partition function or propagator $Z(y_2,y_1;x_2-x_1)$ of a solid-on-solid interface with fixed endpoints $(y_1,x_1),(y_2,x_2)$, fluctuating in the half-plane $y>0$ with an attractive contact force at $y=0$, is evaluated in terms of elementary functions. Finite-size-scaling properties are discussed. Expressed in terms of rescaled position variables $\xi_\perp^{-1}y,\xi_\parallel^{-1}x$, the propagator appears to be a universal quantity. The scaling function for energy-energy correlations obtained by Ko and Abraham for the wetting transition in the two-dimensional Ising model is derived from the propagator. An analogous scaling function for spin-spin correlations is given. The shape of a droplet adjacent to the wall is studied as the temperature is lowered through the wetting temperature.

I. INTRODUCTION

The wetting transition in the two-dimensional Ising model with a short-range interface-pinning force at the boundary was first studied in detail by Abraham.[1] He and many other authors[2–9] have pointed out that solid-on-solid (SOS) models exhibit depinning transitions with the same general characteristics as the wetting transition in the Ising model. The characteristic lengths $\xi_\perp,\xi_\parallel$ of interface fluctuations diverge as $(T_W-T)^{-1}$, $(T_W-T)^{-2}$, respectively, as the wetting temperature T_W is approached from below, and the second temperature derivative of the interface free energy is discontinuous at T_W. Vallade and Lajzerowicz[7] and Abraham and Huse[10] have found that exact results for the magnetization of the semi-infinite Ising model with various boundary conditions are also reproduced by SOS interface or droplet models.

In Sec. II of this paper a closed expression is given for the partition function or propagator $Z(y_2,y_1;x_2-x_1)$ of a continuum SOS interface with fixed end points (y_1,x_1), (y_2,x_2), fluctuating in the half-plane $y>0$ and subject to a contact pinning force at $y=0$. Recently Privman and Švrakić[11] discussed the finite-size scaling properties of a lattice SOS model of wetting with displacement variables restricted to integer values $y_i=1,2,\ldots,N$ in the limit of a large transverse dimension N. Information on finite-size behavior in the complementary limit of a large longitudinal distance x_2-x_1 follows from the explicit expression for the propagator given below.

Expressed in terms of scaled position variables $y/\xi_\perp,x/\xi_\parallel$, the propagator no longer depends explicitly on microscopic quantities and is presumably universal. It is shown in Sec. III that the SOS propagator implies the same scaling function for energy-energy correlations as obtained by Ko and Abraham[12] for the two-dimensional Ising model of wetting. An analogous scaling function for spin-spin correlations is derived. Finally in Sec. IV the shape of a droplet adjacent to the wall is determined as a function of temperature from the SOS propagator.

II. THE SOS PROPAGATOR

Following Vallade and Lajzerowicz,[7] we define the partition function or propagator of an SOS interface with fixed endpoints (y_1,x_1), (y_2,x_2) by the path integral

$$Z(y_2,y_1;x_2-x_1)=\int Dy\,\exp\left\{-\int_{x_1}^{x_2}dx\left[\tfrac{1}{2}K\left[\frac{dy}{dx}\right]^2+V(y)\right]\right\}. \tag{1}$$

Here K is a stiffness parameter, and $V(y)$ is the potential energy associated with the pinning potential and the hard wall.

As in the path-integral formulation of quantum mechanics,[13] Eq. (1) implies the Schrödinger equation

$$\left[\frac{\partial}{\partial x}+V(y_2)-\frac{1}{2K}\frac{\partial^2}{\partial y_2^2}\right]Z(y_2,y_1;x)=0\,. \tag{2}$$

The solution to Eq. (2) can be expressed as

$$Z(y_2,y_1;x)=\sum_\alpha \psi_\alpha(y_2)\psi_\alpha^*(y_1)e^{-E_\alpha x} \tag{3}$$

in terms of a complete orthonormal set of solutions $\psi_\alpha(y)$ to the time-independent Schrödinger equation

$$\left[-E_\alpha+V(y)-\frac{1}{2K}\frac{\partial^2}{\partial y^2}\right]\psi_\alpha(y)=0\,. \tag{4}$$

Here the initial condition

$$Z(y_2,y_1;0)=\delta(y_2-y_1) \tag{5}$$

has been imposed. Equation (3) implies the useful relation

$$Z(y_2,y_0;x_2-x_0)=\int_{-\infty}^{\infty}dy_1\,Z(y_2,y_1;x_2-x_1)\times Z(y_1,y_0;x_1-x_0)\,. \tag{6}$$

With the square-well hard-wall potential

$$V(y)=\begin{cases}\infty, & y<0\\ -U_0/kT, & 0<y<a\\ 0, & y>a\,,\end{cases} \tag{7}$$

Eq. (4) has both bound and scattering solutions[2–9] at sufficiently low temperatures. On increasing T the last bound state vanishes into the continuum at the wetting temperature T_W. As noted by de Gennes[14] in the context of polymer adsorption, an important quantity for T near T_W is the logarithmic derivative of the ground-state wave function

$$\frac{\partial \ln\psi_0(a)}{\partial y} \equiv -\tau = -c(T_W - T) , \tag{8}$$

which changes sign at T_W. Near the wetting transition the ground-state wave function extends much further from the wall than the distance a. Since we are interested in large-distance behavior, we take the limit $a \to 0$ corresponding to a contact potential and replace Eqs. (2) and (4) by

$$\left[\frac{\partial}{\partial x} - \frac{1}{2K}\frac{\partial^2}{\partial y_2^2}\right] Z(y_2,y_1;x) = 0 , \qquad \frac{\partial}{\partial y_2}\ln Z(0,y_1;x) = -\tau , \tag{9}$$

$$\left[-E_\alpha - \frac{1}{2K}\frac{\partial^2}{\partial y^2}\right]\psi_\alpha(y) = 0 , \qquad \frac{\partial}{\partial y}\ln\psi_\alpha(0) = -\tau . \tag{10}$$

The set of equations (9) is well known in surface magnetism[15,16] and in polymer adsorption.[14,17] The solution to Eqs. (5) and (9) has the expansion

$$Z(y_2,y_1;x) = 2\Theta(\tau)\tau e^{-\tau(y_2+y_1)+\tau^2 x/2K} + \int_{-\infty}^{\infty}\frac{dp}{2\pi} e^{-p^2 x/2K}\left[e^{ip(y_2-y_1)} + \frac{ip+\tau}{ip-\tau} e^{-ip(y_2+y_1)}\right] \tag{11}$$

in terms of bound and scattering solutions to Eq. (10). Performing the p integration[18] gives

$$Z(y_2,y_1;x) = \left[\frac{K}{2\pi x}\right]^{1/2}\left(e^{-K(y_2-y_1)^2/2x} + e^{-K(y_2+y_1)^2/2x}\right) + \tau e^{\tau^2 x/2K - \tau(y_2+y_1)}\,\mathrm{erfc}\left[\left[\frac{K}{2x}\right]^{1/2}(y_2+y_1) - \left[\frac{x}{2K}\right]^{1/2}\tau\right] . \tag{12}$$

Here

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}}\int_z^{\infty} e^{-t^2}dt \tag{13}$$

is the complementary error function.[19]

Two special cases are of interest. In the limits $\tau \to -\infty$ and $\tau \to 0$, corresponding to $T \gg T_W$ (pure hard-wall potential) and $T = T_W$, respectively, Eq. (12) becomes

$$Z(y_2,y_1;x) = \left[\frac{K}{2\pi x}\right]^{1/2}\left(e^{-K(y_2-y_1)^2/2x} \mp e^{-K(y_2+y_1)^2/2x}\right) , \tag{14}$$

respectively. These superpositions of object and image solutions to the diffusion equation satisfy Dirichlet and Neumann boundary conditions at $y_2 = 0$, respectively. The two expressions (14) were obtained as fixed points of an exact renormalization group by Huse.[20]

$$\xi_\parallel = 2K\tau^{-2}, \quad \xi_\perp = |\tau|^{-1} \tag{15}$$

appear. From the initial condition (5) it follows that $Z(y_2,y_1;x)$ has the dimensions of an inverse length. The dimensionless quantity $\xi_\perp Z(y_2,y_1;x)$ only depends on the scaling variables

$$Y = (y_2-y_1)/\xi_\perp, \quad \bar{Y} = (y_2+y_1)/\xi_\perp, \quad X = x/\xi_\parallel \tag{16}$$

and is given by

$$\xi_\perp Z(y_2,y_1;x) = \frac{1}{2\sqrt{\pi X}}\left(e^{-Y^2/4X} + e^{-\bar{Y}^2/4X}\right) \pm e^{X \mp \bar{Y}}\,\mathrm{erfc}\left[\frac{\bar{Y}}{2\sqrt{X}} \mp \sqrt{X}\right] \tag{17}$$

for $\tau > 0$ and $\tau < 0$, respectively. By taking the limit $a \to 0$ of a contact potential, we have eliminated a microscopic length and obtained exact scaling for all τ, x, y_1, y_2. For pinning potentials with a nonzero range a, Eq. (17) is also expected to hold in the scaling limit $T \to T_W$ and $y, x \to \infty$ with $y/\xi_\perp$, $x/\xi_\parallel$ fixed. Expressed in terms of the rescaled position variables, the propagator of Eq. (17) appears to be a universal quantity. Some indirect evidence for the universality is given in Secs. III and IV, where exact results for the Ising model of wetting are derived from the SOS propagator.

The finite-size-scaling properties[11,21] of an interface with length x follow directly from Eq. (12). For finite x the partition function is an analytic function of the temperature τ, i.e., an interface of finite length does not have a sharp wetting transition. The nonanalyticity at $\tau = 0$ arises in the limit $x \to \infty$ since the argument of the error function in Eq. (12) tends to $+\infty$ for $\tau < 0$ and $-\infty$ for $\tau > 0$. Utilizing asymptotic properties of the error function, one obtains

$$f(\tau) = \lim_{x\to\infty} x^{-1}\ln Z(y_2,y_1;x) = \begin{cases} 0, & \tau < 0 \\ \dfrac{\tau^2}{2K} = \xi_\parallel^{-1}, & \tau > 0 \end{cases} \tag{18}$$

for the interface free energy. Equation (18) implies the well-known discontinuity of $\partial^2 f/\partial T^2$ at the wetting transition.[1-9]

The probability $P(y)dy$ that an infinitely long SOS interface crosses the line $x = \text{const}$ with y coordinate between y and $y+dy$ is determined by

$$P(y)=\lim_{\substack{x_0\to-\infty\\ x_1\to\infty}}\frac{Z(y_1,y;x_1-x)Z(y,y_0;x-x_0)}{Z(y_1,y_0;x_1-x_0)} . \tag{19}$$

The normalization $\int_0^\infty P(y)dy=1$ is implied by Eq. (6). Substituting from Eq. (12), one finds that $P(y)=2\tau e^{-2\tau y}$ for $\tau>0$ or $T<T_W$. Thus, as pointed out in Refs. 1–9, the average y coordinate of the interface $\langle y\rangle=\frac{1}{2}\xi_\perp=(2\tau)^{-1}$ diverges as $(T_W-T)^{-1}$ as the wetting temperature is approached from below.

III. CORRELATION FUNCTIONS

One may compute correlation functions for the Ising model in the SOS approximation by assigning values $\pm m^*$ to spins located above and below the SOS interface, respectively. The product of a pair of neighboring spins has the constant value m^{*2} unless the SOS interface passes between the two spins. The interfacial contribution $\langle\epsilon(y_2,x_2)\epsilon(y_1,x_1)\rangle_c$ to the energy-energy correlation function of the Ising model of wetting, considered by Ko and Abraham,[12] corresponds, apart from a proportionality constant, to the probability

$$P(y_2,y_1;x_2-x_1)=\lim_{\substack{x_0\to-\infty\\ x_3\to\infty}}\frac{Z(y_3,y_2;x_3-x_2)Z(y_2,y_1;x_2-x_1)Z(y_1,y_0;x_1-x_0)}{Z(y_3,y_0;x_3-x_0)} \tag{20}$$

that an infinitely long SOS interface passes through the points (y_1,x_1) and (y_2,x_2). From Eq. (6) one sees that

$$\int_0^\infty dy_2\int_0^\infty dy_1 P(y_2,y_1;x_2-x_1)=1 .$$

Substituting Eq. (17) into Eq. (20) yields

$$\xi_\perp^2 P(y_2,y_1;x_2-x_1)=(\pi X)^{-1/2}\times e^{-X-\bar{Y}}(e^{-Y^2/4X}+e^{-\bar{Y}^2/4X})+2e^{-2\bar{Y}}\operatorname{erfc}\left[\frac{\bar{Y}}{2\sqrt{X}}-\sqrt{X}\right] \tag{21}$$

for $\tau>0$. This is the same as the result of Ko and Abraham[12] for the Ising model of wetting in the scaling regime below the wetting temperature. The quantity $P(y_2,y_1;x_2-x_1)$ vanishes for $\tau<0$, as expected for an unbound interface.

That the SOS scaling function in Eq. (21) coincides with the exact Ising result is consistent with the conjectured universality of the SOS propagator (17). Analogous scaling functions that correspond to the spin-spin correlation function and magnetization profile of the Ising model of wetting will now be derived.

Since spins above and below the SOS contour are assigned the values $\pm m^*$, the interfacial contribution to the spin-spin correlation function of the Ising model corresponds, apart from a proportionality constant, to the quantity

$$Q(y_2,y_1;x_2-x_1)=\int_0^\infty dy_2'\int_0^\infty dy_1'\operatorname{sgn}(y_2-y_2')\times\operatorname{sgn}(y_1-y_1')P(y_2',y_1';x_2-x_1) \tag{22}$$

in the SOS model. An explicit expression for $Q(y_2,y_1;x_2-x_1)$ in the scaling regime may be obtained by substitution of Eq. (21) into Eq. (22).

IV. DROPLET SHAPES

We now consider the local magnetization of the two-dimensional Ising model of wetting defined on the half-space $y>0$ with fixed boundary spins on the line $y=0$ directed down in the interval $|x|<L/2$ and directed up for $|x|>L/2$. These boundary conditions produce a droplet of negative spins adjacent to the wall with a fixed base length L.

In the SOS approximation the probability $P_L(y,x)dy$ that the edge of the droplet passes between the points (y,x) and $(y+dy,x)$ is determined by the quantity

$$P_L(y,x)=\frac{Z(0,y;L/2-x)Z(y,0;L/2+x)}{Z(0,0;L)} . \tag{23}$$

The magnetization at point (y,x) is proportional to the quantity

$$M_L(y,x)=\int_0^\infty dy'\operatorname{sgn}(y-y')P_L(y,x) . \tag{24}$$

From Eq. (6) one sees that $\int_0^\infty dy\, P_L(y,x)=1$ and that $M_L(y,x)\to\pm1$ in the limits $y\to\infty$ and $y\to0$. In the limiting cases $\tau\to-\infty,0,+\infty$, which we now consider, the droplet shape can be derived analytically.

The predictions of the SOS model in the limit $\tau\to-\infty$ $(T\gg T_W)$, corresponding to a pure hard-wall potential, have been discussed by Vallade and Lajzerowicz[7] and by Fisher.[8] In this limit Eqs. (12) or (14), (23), and (24) reduce to

$$P_L(y,x)=\frac{4}{\sqrt{\pi}}\lambda^{3/2}y^2e^{-\lambda y^2} , \tag{25}$$

$$M_L(y,x)=1-\frac{4}{\sqrt{\pi}}\lambda^{1/2}ye^{-\lambda y^2}-2\operatorname{erfc}(\lambda^{1/2}y) , \tag{26}$$

$$\lambda=\frac{KL}{2(L^2/4-x^2)} . \tag{27}$$

Abraham[1] has calculated $M_L(y,0)$ for the Ising model in the absence of a pinning potential and with y large in comparison with the lattice constant. Equation (26) reproduces his exact result when the stiffness parameter K is chosen[22] according to

$$Ka=\cosh 2K_2-\cosh 2K_1^* ,\quad \exp(2K_1^*)=\coth K_1 . \tag{28}$$

Here K_1 and K_2 denote Ising coupling constants perpendicular and parallel to the x axis, and a is the lattice constant.

In the special case $\tau=0$ or $T=T_W$, Eqs. (12) or (14), (23), and (24) yield

$$P_L(y,x)=\frac{2}{\sqrt{\pi}}\lambda^{1/2}e^{-\lambda y^2} , \tag{29}$$

$$M_L(y,x)=1-2\,\mathrm{erfc}(\lambda^{1/2}y) , \tag{30}$$

where λ is again given by Eq. (27). In the limit $\tau\to\infty$ or $T\ll T_W$, corresponding to a contact potential with infinite strength, $P_L(y,x)$ is infinite at $y=0$ and vanishes for $y>0$.

One may characterize the typical droplet shape in several ways. The most-probable shape $y_{\mathrm{mp}}(x)$ follows from the relation $\partial P_L(y_{\mathrm{mp}},x)/\partial y=0$, and the average shape $y_{\mathrm{av}}(x)$ from the definition $y_{\mathrm{av}}=\int_0^\infty dy\, yP_L(y,x)$. The half-value shape $y_{1/2}(x)$ is defined by

$$M_L(y_{1/2},x)=0 \text{ or } \tfrac{1}{2}=\int_0^{y_{1/2}} dy\, P_L(y,x) .$$

In the special cases $\tau\to-\infty$ and $\tau=0$ considered in Eqs. (25)–(30), these three definitions of the typical shape yield ellipses of the form $\lambda^{1/2}y=c$ or

$$x^2+\frac{KL}{2c^2}y^2=\frac{L^2}{4} . \tag{31}$$

For $\tau=-\infty$

$$c=\begin{cases}1, & \text{most-probable}\\ \dfrac{2}{\sqrt{\pi}}=1.128, & \text{average}\\ 1.088, & \text{half-value}\end{cases} \tag{32}$$

and for $\tau=0$

$$c=\begin{cases}0, & \text{most-probable}\\ \dfrac{1}{\sqrt{\pi}}=0.5642, & \text{average}\\ 0.4769, & \text{half-value .}\end{cases} \tag{33}$$

The value $c=0$ corresponds to $y_{\mathrm{mp}}=0$.

For general τ the quantities $y_{\mathrm{mp}}(x)$, $y_{\mathrm{av}}(x)$, and $y_{1/2}(x)$ can be calculated numerically from Eqs. (12), (23), and (24). Typical results are shown in Fig. 1. As the temperature is lowered, i.e., as τ increases, the droplets flatten against the boundary. For $\tau\geq 0$, $y_{\mathrm{mp}}(x)=0$. The quantities $y_{\mathrm{av}}(x)$ and $y_{1/2}(x)$ vanish in the limit $\tau\to\infty$. Only in the special cases $\tau=-\infty$ and $\tau=0$ are the curves ellipses.

Monte Carlo results of Selke[23] for droplet shapes in the two-dimensional Ising model in the absence of a pinning potential are in good agreement with the SOS results (28), (31), and (32) for $\tau\to-\infty$, which, as noted above, reproduce Abraham's exact result for $M_L(y,0)$. It would be nice to have Monte Carlo results for the Ising model of wetting for comparison with the droplet shapes derived from the SOS propagator for general τ.

V. DISCUSSION OF THE RESULTS

The SOS propagator and each of the quantities we have calculated from it can be expressed in a form that looks universal by expressing the microscopic parameters K and τ in terms of the correlation lengths $\xi_\parallel$ and $\xi_\perp$ of Eq. (15), as in Eq. (17). The agreement of the quantities $P(y_2,y_1;x_2-x_1)$ and $M_L(y,0)$ given in Eqs. (21) and (26) with exact results for the Ising model of wetting is consistent with universality. As a further check it would be useful to have exact results in the scaling regime for the spin-spin correlation function and droplet shapes in the Ising model of wetting for comparison with Eqs. (22) and (24). The logarithm of the propagator (17) is the free energy or tension of the SOS interface. It would also be instructive to compare this quantity with the interface free energy of the Ising model of wetting defined on the half-strip $y>0$, $x_1<x<x_2$ with boundary conditions that fix the endpoints of the interface at (y_1,x_1) and (y_2,x_2).

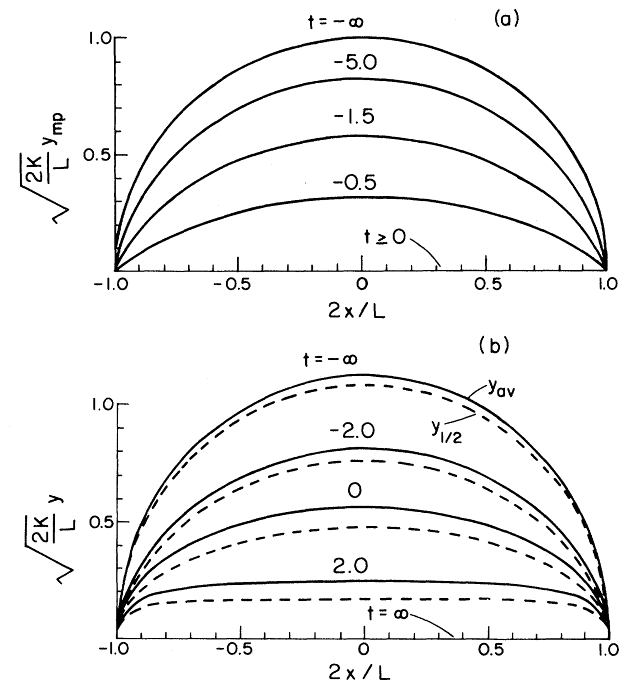

FIG. 1. Droplet shapes for representative values of $t=\tau\sqrt{L/2K}\propto T_W-T$. The most probable shape y_{mp} is shown (a). The solid and dashed lines (b) indicate the average and half-value shapes, y_{av} and $y_{1/2}$, respectively.

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$$\int_{-\infty}^{\infty} \frac{dp}{2\pi}(ip-\tau)^{-1}\exp[-p^2x/2K-ip(y_2+y_1)]$$

may be evaluated by elementary contour integration after the substitution

$$\exp(-p^2x/2K)=\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} du\, \exp(-u^2-i\sqrt{2x/K}pu)\ .$$

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