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Microscopic approach to critical phenomena at interfaces: An application to complete wetting in the Ising model

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We study how the formalism of the hierarchical reference theory (HRT) can be extended to inhomogeneous systems. HRT is a liquid-state theory which implements the basic ideas of the Wilson momentum-shell renormalization group (RG) to microscopic Hamiltonians. In the case of homogeneous systems, HRT provides accurate results even in the critical region, where it reproduces scaling and nonclassical critical exponents. We applied the HRT to study wetting critical phenomena in a planar geometry. Our formalism avoids the explicit definition of effective surface Hamiltonians but leads, close to the wetting transition, to the same renormalization group equation already studied by RG techiques. However, HRT also provides information on the nonuniversal quantities because it does not require any preliminary coarse graining procedure. A simple approximation to the infinite HRT set of equations is discussed. The HRT evolution equation for the surface free energy is numerically integrated in a semi-infinite three-dimensional Ising model and the complete wetting phase transition is analyzed. A renormalization of the adsorption critical amplitude and of the wetting parameter is observed. Our results are compared to available Monte Carlo simulations.

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I. INTRODUCTION

Effective interfacial Hamiltonians are widely used to describe the large-scale fluctuations that occur near surface critical phenomena such as wetting [1]. Of course these models are not truly microscopic but are usually considered valid for length scales larger than some appropriate cutoff. The prevailing belief is that interfacial models may be derived from more microscopic approaches if the bulk degrees of freedom are integrated out. Needless to say, this is an extremely difficult task and interfacial models still retain a partly phenomenological status. Therefore it is interesting to develop a genuine microscopic approach to study interfacial behaviors. Effective Hamiltonians are used to describe the critical behavior also in homogeneous systems because they allow a direct implementation of renormalization group (RG) ideas. For such bulk systems, the hierarchical reference theory (HRT) [2,3] provides a systematic way to derive an effective Hamiltonian from a given microscopic model [4]. This theory, which implements the basic ideas of the Wilson momentum-space renormalization group for microscopic Hamiltonians, allows us to derive an exact hierarchy of differential equations describing the evolution of the free energy and of the n-point correlation functions of the system when fluctuations on larger and larger length scales are included. This hierarchy of differential equations can be closed, for example, by imposing an approximation for the pair correlation function, usually of Ornstein-Zernike (OZ) form. Already at this level of approximation, the HRT shows genuine nonclassical critical behavior.

The extension of the HRT formalism to inhomogeneous systems would enable us to study the interfacial phase transition starting from the microscopic model, without the explicit introduction of effective interfacial Hamiltonians. Given two homogeneous phases α and β, in contact with a third passive phase (a wall), we study the particular case of complete wetting in planar geometry [1]—i.e., the phase transition which corresponds to the growth of an infinitely thick liquid layer close to the wall when bulk phase coexistence is approached at fixed temperature. The standard fluctuation theory of the wetting transition, beyond the mean-field approximation, is described by using the capillary-wave (CW) effective Hamiltonian in d dimensions [5,6]:

$$H_{CW} = \int d^{d-1}\mathbf{x}\left[\frac{\Sigma}{2}[\nabla l(\mathbf{x})]^2 + W(l(\mathbf{x}))\right], \tag{1}$$

where $l(\mathbf{x})$ is a collective coordinate which represents the distance of the α-β interface from the wall, $W(l)$ is the effective interface potential which describes the effective interaction between the wall and the α-β interface, and Σ is the stiffness coefficient of the interface. For isotropic models Σ can be identified with the surface tension, but it may also depend on the curvature of the interface. The form of effective interfacial potential $W(l)$ depends on the range of the microscopic interaction. In the case of short-range potentials, for large l it is parametrized as [5,6,8–11]

$$W(l) \simeq -A\exp(-ml/\xi) + B\exp(-nl/\xi), \tag{2}$$

where m, n are two dimensionless constants with $n > m$. The parameter ξ can be identified with the bulk correlation length. It is important to note that the use of such an effective surface Hamiltonian can be justified only when bulk fluctua-

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tions are small—i.e., far from the bulk critical point [7]. In three dimensions, renormalization group studies of the Hamiltonian (1) [8,10] predict that the wetting critical behavior is nonuniversal depending on the value of the wetting parameter:

$$\omega = \frac{k_B T}{4\pi\Sigma\xi_b^2}, \tag{3}$$

where ξ_b is the *true* bulk correlation length which governs the exponential decay of correlations in real space [12,13]. At the critical wetting transition (i.e., wetting at coexistence) the critical exponents depend on this parameter [8] while at complete wetting (i.e., wetting approaching coexistence) the critical exponents are predicted to remain mean-field-like but critical amplitudes are ω dependent. For example, the interface height l grows as

$$\frac{l}{\xi_b} \sim \left(1 + \frac{\omega}{2}\right)\ln(\Delta\mu), \tag{4}$$

where $\Delta\mu = \mu - \mu_0$ is the deviation of the chemical potential from the value at coexistence. The mean-field approximation to an effective ϕ^4 Hamiltonian provides a value $\omega_{mf} = 0$ via Eq. (4).

The three-dimensional semi-infinite Ising model is one of the simplest microscopic models which may be simulated to test the RG predictions. The value of the wetting parameter ω is a function of the temperature and has been theoretically estimated [12,14]: $\omega \sim 0.8$ for $T_c > T \geqslant 0.6T_c$. Extensive Monte Carlo [15] simulation studies appear to be consistent with $\omega \sim 0.3$ at $T_{sim} \simeq 0.663T_c$ [16], a much smaller value than the predicted one. One possible solution of this discrepancy between the simulations and RG results is the inadequacy of the CW Hamiltonian and the introduction of more general effective interfacial Hamiltonians [17–20].

The HRT, suitably generalized to deal with inhomogeneous systems, can be used to study the effects of thermal fluctuations beyond the mean-field behavior without reference to the CW approach and so without introducing ω as an external parameter. We first obtain the HRT surface evolution equation for the Ising model which is then numerically solved in the case of complete wetting in three dimensions. The divergence of the adsorption Γ is studied when coexistence is approached and the critical amplitude is evaluated and compared to simulations. This work is organized as follows: in Sec. II we extend the HRT approach to the case of inhomogeneous systems with planar geometry. We derive the evolution equation for the bulk and surface free energy. We also show that in the asymptotic region the HRT equations reduce to the known RG approach. In Sec. III we study complete wetting for a lattice gas model with nearest-neighbor interactions (which is equivalent to the Ising model). We investigate how fluctuations modify the mean-field picture by integrating the HRT surface equation. In Sec. IV we briefly summarize the most relevant results and compare them to the avaliable simulation data.

II. HRT FOR INHOMOGENEOUS SYSTEMS

A. Evolution equations

The starting point in the derivation of HRT equations is the separation of the interatomic potential $v(r)$ into two parts:

$$v(\mathbf{r}) = v_R(\mathbf{r}) + w(\mathbf{r}), \tag{5}$$

where $v_R(\mathbf{r})$ is the short-range repulsive part of $v(\mathbf{r})$. The thermodynamic and structural properties of the system with interaction $v_R(\mathbf{r})$, the "reference system," are considered known, at least numerically. It is also assumed that there is no phase transition in the reference system. Instead $w(\mathbf{r})$ is a (mostly) attractive term, which triggers the liquid-vapor phase transition. Using this separation and performing a Legendre transformation on the grand partition function, a formal diagrammatic expansion for the Helmholtz free energy can be written to all orders in perturbation theory [3]. We implement the basic ideas of Wilson's RG approach [21] within such a formal perturbative expansion to study how the bulk and surface thermodynamic quantities evolve due to the inclusion of fluctuations. This can be done by introducing a sequence of intermediate potentials characterized by an infrared cutoff in Fourier space, depending on a parameter Q. In the HRT for (off-lattice) bulk systems this cutoff is spherical in Fourier space, thereby respecting the isotropy of the interaction. Here we want to consider the case of inhomogeneous systems in the presence of a planar wall, where only cylindrical symmetry survives in wave vector space. Moreover, in wetting phenomena the correlation length parallel to the surface, $\xi_\parallel$, and the correlation length perpendicular to the surface, $\xi_\perp$, are related by [1,10]

$$\xi_\perp \sim \begin{cases} [\ln(\xi_\parallel)]^{1/2}, & d = 3, \\ \xi_\parallel^{(3-d)/2}, & d < 3. \end{cases} \tag{6}$$

This relationship suggests that the fluctuations perpendicular to the wall diverge much more slowly than the fluctuations parallel to the wall. Therefore it is natural to define a sharp *cylindrical* cutoff [22] which prevents long-wavelength CW critical fluctuations. Within the HRT approach, this is implemented by defining the sequence of intermediate potentials:

$$w^Q(\kappa, q) = \begin{cases} w(\kappa, q), & \kappa \geqslant Q, \\ 0, & \kappa < Q, \end{cases} \tag{7}$$

where κ is the component of the wave vector parallel to the surface and q is the component normal to the wall. The system characterized by the potential $v^Q(\mathbf{r}) = v_R(\mathbf{r}) + w^Q(\mathbf{r})$ will be named the Q system. For $Q \to \infty$, v^Q reduces to v_R while for $Q \to 0$ the full interaction is recovered. Therefore it is natural to look for evolution equations governing the change in the physical properties of the Q system as the cutoff is varied. In order to derive such evolution equations, we consider the structure of the perturbative series which defines the free energy of the model. In the perturbative diagrammatic expansion of the free energy of the Q system A^Q, every loop contains one or more $\phi = -\beta w^Q$ bonds [2]. Therefore, due to the vanishing of $w^Q(\kappa, q)$ for $\kappa < Q$, A^Q is defined by the same perturbative expansion as the full free energy of the model, A, where each (longitudinal) momentum integration is limited by an inferred cutoff Q. The correspondence between a cutoff in the potential and a cutoff in fluctuations (i.e., in the momentum integrations) is valid with the single exception of the first, mean-field, diagram of the perturbation series which does not contain any loop. This contribution is in fact discontinuous in Q because it contains just the $\kappa=0$ Fourier component of the attractive potential (7) which is zero for every $Q\neq 0$ and finite for $Q=0$. However, we can introduce a modified free energy $\mathcal{A}^Q$ which is continuous in Q and is simply related to A^Q:

$$-\beta\mathcal{A}^Q = -\beta A^Q - \frac{1}{2}[\phi(\mathbf{r}=0) - \phi^Q(\mathbf{r}=0)]\int d^d\mathbf{r}\,\rho(\mathbf{r}) + \frac{1}{2}\int d^d\mathbf{r}_1 d^d\mathbf{r}_2[\phi(\mathbf{r}_1,\mathbf{r}_2) - \phi^Q(\mathbf{r}_1,\mathbf{r}_2)]\rho(\mathbf{r}_1)\rho(\mathbf{r}_2). \tag{8}$$

Analogously, we can introduce the direct correlation functions C_n^Q for each Q system by functional derivation of the free energy A^Q with respect to the local density $\rho(\mathbf{r})$. These correlation functions are continuous in Q for $n\geqslant 3$ because there are no zero-loop contributions in the corresponding perturbative expansion, but the two-point direct correlation function is discontinuous at $\kappa=Q$. So we introduce a modified function which is continuous, being the second functional derivative of $\mathcal{A}^Q$ with respect to the density:

$$\mathcal{C}_2^Q(q,\kappa) = C_2^Q(q,\kappa) + [\phi(q,\kappa) - \phi^Q(q,\kappa)]. \tag{9}$$

It is apparent from the definitions (8) and (9) that $\mathcal{A}^Q$ and $\mathcal{C}_2^Q$ coincide with the free energy and direct correlation function of the fully interacting system, respectively, when $Q\to 0$. On the other hand, in the limit $Q\to\infty$ these modified quantities reproduce the mean-field approximation for the free energy and the direct correlation function, contrary to A^Q and C_2^Q, which reduce to the reference system quantities. This suggests that the HRT procedure does indeed describe the growth of fluctuations on top of the mean-field approximation, as in the RG approach.

The simple relationship between the cutoff-dependent modified quantities ($\mathcal{A}^Q$ and $\mathcal{C}_2^Q$) and the Q-system properties (A^Q and C_2^Q) allows us to derive the evolution equations describing how $\mathcal{A}^Q$ and C_n^Q change when Q is decreased from infinity to zero—i.e., when fluctuations on larger and larger length scales are included. The perturbative expansion of the free energy can be specialized to the case where the reference system is the Q system and the perturbation potential is

$$\delta v^Q(q,\kappa) = v^{Q-\delta Q}(q,\kappa) - v^Q(q,\kappa) = \begin{cases} v(q,\kappa), & Q-\delta Q < \kappa < Q, \\ 0, & \text{elsewhere}, \end{cases} \tag{10}$$

where $\delta Q > 0$ is an infinitesimal shift in the cutoff. By summing all terms linear in δQ in the diagrammatic expansion of the free energy and taking the limit $\delta Q\to 0$ one obtains the evolution equation for the free energy. Until now we have formally considered the total free energy, but for an inhomogeneous system it is useful to separate the bulk quantities, which refer to the homogeneous system without an external potential, from the surface terms due to the presence of the wall:

$$\mathcal{A}^Q = \mathcal{A}_b^Q + \Delta\mathcal{A}^Q,$$

$$\rho(\mathbf{r}) = \rho_b + \Delta\rho(\mathbf{r}),$$

$$F_2^Q(\mathbf{r}_1,\mathbf{r}_2) = F_{2b}^Q(z_1 - z_2, |\mathbf{s}_1 - \mathbf{s}_2|) + \Delta F_2^Q(\mathbf{r}_1,\mathbf{r}_2),$$

where the two-point correlation function $F_2^Q(\mathbf{r}_1,\mathbf{r}_2)$ is the functional inverse of $-C_2^Q(\mathbf{r}_1,\mathbf{r}_2)$—i.e.,

$$\int d\mathbf{r}^d F_2^Q(\mathbf{r}_2,\mathbf{r}_3) C_2^Q(\mathbf{r}_3,\mathbf{r}_2) = -\delta(\mathbf{r}_1 - \mathbf{r}_2). \tag{11}$$

This differs from the known Ornstein-Zernike equation for inhomogeneous fluids because of the inclusion of the ideal gas terms. Note that, due to the cylindrical cutoff, F_{2b}^Q has lost the full rotational symmetry of the physical system for every $Q\in(0,\infty)$. The separation in bulk and surface terms may be inserted in the diagrammatic expansion of the total Helmholtz free energy. We begin with the derivation of the evolution equation for the bulk contribution to the free energy. Only the one-loop diagrams containing "bulk" F_{2b}^Q bonds alone in the diagrammatic expansion contribute to the leading order in δQ. The sum of these term can be carried out in closed form [2] and reproduces the known random phase formal expression

$$\beta\boldsymbol{\mathcal{A}}_b^Q - \beta\boldsymbol{\mathcal{A}}_b^{Q-\delta Q} = -\frac{V}{2}\int\frac{dq}{2\pi}\int_{(Q,Q-\delta Q)}\frac{d^{d-1}\kappa}{(2\pi)^{d-1}} \times \ln[1 - \phi(q,\kappa)F_{2b}^Q(q,\kappa)]. \tag{12}$$

This equation is not yet suitable for taking the $\delta Q\to 0$ limit because it contains the discontinuous function $F_{2b}^Q(q,\kappa) = -1/C_{2b}^Q(q,\kappa)$. Expressing F_{2b}^Q in terms of the continuous function $\mathcal{F}_{2b}^Q(q,\kappa) = -1/\mathcal{C}_{2b}^Q(q,\kappa)$ via Eqs. (9) and (11) we obtain

$$\frac{\partial}{\partial Q}\left(\frac{\beta\mathcal{A}_b^Q}{V}\right) = \frac{1}{2}K_{d-1}Q^{d-2}\int\frac{dq}{2\pi}\ln[1 + \mathcal{F}_{2b}^Q(q,Q)\phi(q,Q)], \tag{13}$$

where K_{d-1} is a geometric factor defined by

$$\int\frac{d^{d-1}\kappa}{(2\pi)^{d-1}}\delta^{d-1}(\kappa - Q) = K_{d-1}Q^{d-2}.$$

The initial condition must be imposed at $Q=\infty$ and coincides with the mean-field approximation for the Helmholtz free energy of the fully interacting system. Unfortunately, Eq. (13) is not written in closed form because the evolution of the free energy depends on knowledge of the two-particle correlation function $\mathcal{F}_{2b}^Q(q,Q)$ at a generic value of the cutoff Q. However, we can study how the two-particle function $\mathcal{F}_{2b}^Q$ itself (or equivalently $\mathcal{C}_{2b}^Q$) is modified owing to the inclusion of fluctuations by performing the same analysis leading to Eq. (13). In this way we obtain an evolution equation for the pair correlation function, but this equation contains the three-particle and four-particle correlation functions. The procedure may be iterated to higher orders, thereby obtaining an infinite hierarchy of coupled differential equations. This hierarchy may be truncated at the level of the first equation by introducing a suitable ansatz for the two-particle correlation function and using the compressibility sum rule [23] which relates the second density derivative of the free energy to the zero-wave-vector limit of the pair correlation function

$$\mathcal{C}_{2b}^{Q}(\mathbf{k}=0)=\frac{\partial^2(-\beta\mathcal{A}_b^Q/V)}{\partial\rho_b^2}. \qquad (14)$$

Note that this equation is exact for each Q; system, it provides an extremely useful link between thermodynamics and the long-wavelength limit of correlation functions but it is not sufficient to close the hierarchy because it does not give information about the momentum dependence of $\mathcal{F}_{2b}^Q(q,\kappa)$.

In the derivation of the bulk evolution equation, translational invariance allowed us to perform an analytical resummation of the one-loop diagrams leading to Eq. (13) without specifying the form of $\mathcal{F}_{2b}^Q$. Instead, in order to express in closed form the sum of the required diagrams in the expansion of the surface free energies, we need to specialize to a particular form of the inhomogeneous two-point correlation function $\Delta F_2^Q(\mathbf{r}_1,\mathbf{r}_2)$. Therefore, it is important to understand what type of fluctuations are described by $\Delta F_2^Q(\mathbf{r}_1,\mathbf{r}_2)$. Let us consider the case of a wetting transition between two bulk phases β and α in contact with a wall. At a temperature larger than the wetting temperature and slightly off coexistence, the system will consist of a slab of the wetting phase, with density ρ_β, an interfacial region, and the bulk ρ_α phase. If F_{2b}^α, which is the bulk correlation function of the α phase, is not equal to F_{2b}^β, then $\Delta F_2^Q(\mathbf{r}_1,\mathbf{r}_2)$, which is defined as $F_2(\mathbf{r}_1,\mathbf{r}_2)-F_{2b}(\mathbf{r}_1-\mathbf{r}_2)$, describes not only the correlations in the interfacial region, but also in the slab. In this case it is difficult to find a suitable ansatz for the form of ΔF_2^Q. However, in systems where the bulk correlation functions are the same for the two phases the problem simplifies and ΔF_2^Q just describes the interfacial region. This is precisely the case of the lattice gas model with nearest-neighbor interaction (i.e., of the Ising model) due to the symmetry $\rho_\beta=1-\rho_\alpha$. If the inhomogeneous part of the two-point correlation function describes only the interfacial region, we can parametrize $\Delta\mathcal{F}_2^Q$ according to the standard factorized form [24]

$$\Delta\mathcal{F}_2^Q(q_1,q_2,\kappa)=g^Q(q_1)g^Q(q_2)F_s^Q(\kappa), \qquad (15)$$

where $g^Q(z)$, the Fourier transform of $g^Q(q)$, is usually identified as the first spatial derivative of the density profile and we have taken the wall perpendicular to the z axis. Using this parametrization it is possible to perform the summation of the one-loop diagrams which allows us to obtain the evolution equation for the surface free energy:

$$\frac{\partial}{\partial Q}\left(\frac{\beta\Delta\mathcal{A}^Q}{S}\right)=\frac{K_{d-1}}{2}Q^{d-2}\ln[1+F_s^Q(Q)\alpha^Q(Q)], \qquad (16)$$

where α^Q is

$$\alpha^Q(\kappa)=\int\frac{dq}{2\pi}g^Q(q)\frac{\phi(\kappa,q)}{1+\phi(\kappa,q)\mathcal{F}_{2b}^Q(\kappa,q)}g^Q(-q). \qquad (17)$$

Note that the evolution of the surface free energy is coupled to the bulk evolution through the α^Q coefficient.

In the general case of $F_{2b}^\alpha\neq F_{2b}^\beta$ the derivation of the evolution equation is more involved: By introducing further simplifying assumptions in the spirit of the local density approximation, it is still possible to obtain a decoupled evolution equation identical to Eq. (16) with a slightly different coefficient α^Q [25]

$$\alpha_{LDA}^Q(\kappa)=\int\frac{dq}{2\pi}g^Q(q)\phi(\kappa,q)g^Q(-q). \qquad (18)$$

Equation (16) has been obtained by starting from an expansion of the free energy at constant density profile: every Q system has the same $\rho(\mathbf{r})$. It means that the external potential which stabilizes the density profile changes with Q. In the case of wetting or drying this procedure is clearly artificial: we would rather want to study how the density profile is modified by the inclusion of fluctuations at *fixed* external potential. In order to allow the change in $\rho(\mathbf{r})$ when fluctuations are included, it is convenient to perform a Legendre transform of the total free energy $\mathcal{A}^Q$. In this way, it is possible to obtain the evolution equations at fixed fugacity—i.e., by keeping fixed the quantity

$$\gamma(z)=\beta[\mu-U(z)],$$

where $U(z)$ is the microscopic interaction between the wall and molecules of the fluid. We first define the (modified) grand free energy by

$$-\beta\omega^Q=-\beta\mathcal{A}^Q+\int d^3\mathbf{r}\rho^Q(z)\gamma(z). \qquad (19)$$

Here $\gamma(z)$ is fixed to the physical value, while the density profile changes with the cut off wave vector Q. The Q-dependent density profile is related to ω^Q by

$$\rho^Q(z)=-\frac{\delta\beta\omega^Q}{\delta\gamma(z)}. \qquad (20)$$

As usual, for $Q\to\infty$ ω^Q reduces to the mean-field grand free energy and $\rho^Q(z)$ approaches the density profile in the mean-field approximation. From the properties of the Legendre transform we obtain

$$\left(\frac{\partial\beta\omega^Q}{\partial Q}\right)_\gamma=\left(\frac{\partial\beta\mathcal{A}^Q}{\partial Q}\right)_\rho. \qquad (21)$$

As a consequence, the evolution equation for the grand free energy formally coincides with that of the Helmholtz free energy and the surface tension $\sigma^Q=\Delta\omega^Q/S$ obeys the evolution equation

$$\frac{\partial(\beta\sigma^Q)}{\partial Q}=\frac{1}{2}K_{d-1}Q^{d-2}\ln[1+F_s^Q(Q)\alpha^Q(Q)]. \qquad (22)$$

Note that now α^Q is given again by Eq. (17) in terms of $g^Q(q)$ and $F_s^Q(\kappa)$. Analogously to the bulk case, also surface quantities obey a hierarchy of coupled differential equations which can be closed at the free energy level (22) by a suitable ansatz for $F_s^Q(\kappa)$ and $g^Q(z)$. Two surface sum rules will provide the link between the free energy and the correlation functions [1]:

$$-\frac{\partial\sigma^Q}{\partial\mu} = \Gamma^Q = \int dz[\rho^Q(z) - \rho_b^Q] = \int dz\Delta\rho^Q(z), \qquad (23)$$

$$-\frac{\partial^2\sigma^Q}{\partial\mu^2} = \int dz_1 dz_2 \Delta\mathcal{F}_2^Q(z_1,z_2,\kappa=0) = \beta F_s^Q(0)\left|\int dz g^Q(z)\right|^2. \qquad (24)$$

Equation (24) can be identified as a "surface compressibility" sum rule while Eq. (23) constrains the form of the density profile. It is interesting to note that these two sum rules are sufficient to obtain a quite good description of the wetting phase transition [24].

B. Asymptotic equations

1. Bulk equation

In this section we show how the HRT evolution equations describe the asymptotic regime near phase transitions. The standard bulk HRT with spherical cutoff in the asymptotic critical region is known to give the same evolution equation obtained by the momentum-space RG approach [2,3]. Here we show that the introduction of a cylindrical cutoff does not modify this property of the bulk HRT equation.

In the thermodynamic states close to the bulk critical point, Eq. (13) can be simplified. This regime is characterized by the growth of long-range fluctuations—that is, by the divergence of $\mathcal{F}_{2b}^Q(q=0,\kappa=0)$ for $Q\to 0$—i.e., in the final stages of the evolution. In order to study the critical region we have to extract the singular contribution to the free energy from the evolution equation (13): Only a small neighborhood of the integration domain, close to $q=0$ and $Q\sim 0$, contributes to the singularity. In this domain we can simplify the argument of the logarithm due to the divergence of the pair correlation function for q and κ approaching zero:

$$\frac{\partial}{\partial Q}\left(\frac{\beta\mathcal{A}_b^Q}{V}\right) = \frac{K_{d-1}}{2}Q^{d-2}\int_{-q_0}^{q_0}\frac{dq}{2\pi}\ln[\mathcal{F}_{2b}^Q(Q,q)].$$

Here q_0 is an arbitrary ultraviolet cutoff which is introduced to extract the singular contribution to the integral. Note that this equation does not contain the interatomic potential explicitly and acquires a universal form independent of the specific microscopic interaction. The next step is to choose a form for the bulk pair correlation function. As usual, we adopt an Ornstein-Zernike form for the direct correlation function:

$$\mathcal{C}_{2b}^Q(\kappa,q) = -\frac{1}{\mathcal{F}_{2b}^Q(\kappa,q)} = -b(\kappa^2+q^2) + \frac{\partial^2}{\partial\rho^2}\left(\frac{-\beta\mathcal{A}_b^Q}{V}\right), \qquad (25)$$

where we imposed the sum rule (14) and we assumed that b remains finite also at the critical point. This particular ansatz for the pair correlation function implies that the critical exponent η is zero. We know that in three dimension η is not zero, but its value is small and it is zero to first order in the ϵ expansion [21] so that, in three dimensions, this is a good approximation. Substituting this parametrization in the evolution equation we obtain

$$\frac{\partial}{\partial Q}\left(\frac{-\beta\mathcal{A}_b^Q}{V}\right) = \frac{K_{d-1}}{2}Q^{d-1}\int_{-q_0/Q}^{+q_0/Q}\frac{du}{2\pi} \times\ln\left[Q^2 b(1+u^2) - \frac{\partial^2}{\partial\rho^2}\left(\frac{-\beta\mathcal{A}_b^Q}{V}\right)\right].$$

We can eliminate the explicit dependence on the cutoff Q in the evolution equation by another change of variable:

$$t = -\ln(Q),$$

$$z = (\rho_b - \rho_{bc})\sqrt{\frac{b}{K_{d-1}}}e^{[(2-d)/2]t},$$

$$H_t(z) = -\frac{\beta}{V}(\mathcal{A}_{bc}^Q - \mathcal{A}_b^Q)\frac{e^{dt}}{K_{d-1}},$$

where ρ_{bc} and $\mathcal{A}_{bc}$ are the density and free energy at the critical point. Using these variables the asymptotic evolution equation becomes

$$\frac{\partial H_t(z)}{\partial t} = dH_t(z) + \frac{2-d}{2}zH_t'(z) + \frac{1}{2}\int_{-\infty}^{+\infty}\frac{du}{2\pi}\ln\left[\frac{H''(z)+u^2+1}{H''(0)+u^2+1}\right], \qquad (26)$$

where $H'(z)$ and $H''(z)$ are the first and second derivatives of H with respect to z and we set $q_0/Q\to\infty$ in the $Q\to 0$ limit. The integration can be easily performed and we obtain

$$\frac{\partial H_t(z)}{\partial t} = dH_t(z) + \frac{2-d}{2}zH_t'(z) + \frac{1}{2}[\sqrt{H_t''(z)+1} - \sqrt{H_t''(0)+1}]. \qquad (27)$$

This equation can be analytically investigated in $d=4-\epsilon$ dimensions. The fixed point and the relevant eigenvalues provide the critical exponents to first order in ϵ: $\gamma=1+\epsilon/6$, $\beta=1/2-\epsilon/6$, and $\delta=3+\epsilon$, which coincide with the known exact RG results [21]. As expected, to lowest order in ϵ, the choice of cutoff symmetry does not modify the universal properties close to the bulk critical point within the HRT approach.

2. Surface equation

The surface evolution equation we have obtained, Eq. (16), depends on the form of the density profile through the quantity $\alpha^Q(\kappa)$, Eqs. (17) and (18), if $g^Q(z)$ is taken to represent the spatial derivative of $\rho^Q(z)$. Here and in the following we assume that the shape of $\rho^Q(z)$ is not affected by fluctuations. Fluctuations are assumed to shift rigidly the mean-field density profile by a Q-dependent amount l_Q identified as the distance of the interface from the wall: $\Delta\rho^Q(z) = \Delta\rho f(z - l_Q)$. This assumption can be related to the nonhomogeneity of the spectrum of fluctuations and is customary in most studies of the wetting phenomena [8,10]. From Eq. (6) we see that the fluctuations perpendicular to the interface—i.e., the fluctuations which distort the form of the profile—are only weakly divergent and as a first approximation we can neglect their effect. Note that this assumption is not justified near the bulk critical point, where the interplay between bulk and surface fluctuations does modify also the form of the density profile. Our analysis is therefore valid only away from the bulk critical point. The long-wavelength behavior of the surface correlation function $F_s^Q(\kappa)$ is modeled by an Ornstein-Zernike form

$$F_s^Q(\kappa) = \left[-(\Delta\rho)^2 \left(\frac{\partial^2 \beta\sigma^Q}{\partial(\beta\mu)^2} \right)^{-1} + b_s\kappa^2 \right]^{-1}, \tag{28}$$

where b_s is a nonuniversal constant that tends to a finite limit at the wetting transition and we have used the exact sum rule (24):

$$\frac{\partial^2(-\beta\sigma^Q)}{\partial(\beta\mu)^2} = (\Delta\rho)^2 F_s^Q(\kappa = 0), \tag{29}$$

where $\Delta\rho = \int dz g^Q(z) = (\rho_\alpha - \rho_\beta)$ is the difference between the bulk density of the two phases across the interface. Because we assume to be away from bulk critical point, this quantity is regular at wetting transition. The assumptions we made on the density profile and on the surface correlation function are similar to those underlying the usual RG group treatment of the wetting transition [1,8–10]. Note that for wetting phenomena the critical exponent η is known to be zero [1,5] but the Ornstein-Zernike form for the surface correlation function is strictly accurate only in the interfacial region [18,19].

Away from the bulk critical point, the asymptotic form of the evolution equation for the surface free energy then becomes

$$\frac{\partial(-\beta\sigma^Q)}{\partial Q} = \frac{K_{d-1}}{2} Q^{d-2} \ln\left(\left[\frac{\partial^2(-\beta\sigma^Q)}{\partial(\beta\mu)^2} \right]^{-1} + b_s' Q^2 \right), \tag{30}$$

where $b_s' = b_s(\Delta\rho)^2$ and we have disregarded nonsingular terms. Notice that Eq. (30) does not depend on the specific shape of the density profile. The asymptotic evolution equation (30) is in fact fully equivalent to the nonperturbative "functional" RG approach [9,10]. To prove this remarkable correspondence, we introduce the surface free energy $a^Q(\Gamma)$ by Legendre transform of $\sigma^Q(\mu)$:

$$a^Q(\Gamma) = \sigma^Q(\mu^Q) + \mu^Q\Gamma. \tag{31}$$

Here Γ is the adsorption (23) and then μ^Q is such that

$$\mu^Q = \frac{\partial a^Q(\Gamma)}{\partial\Gamma}. \tag{32}$$

The asymptotic evolution equation of $a^Q(\Gamma)$ follows straightforwardly from the evolution equation of σ^Q, Eq. (30), and from the properties of the Legendre transform

$$\frac{\partial(-\beta a^Q)}{\partial Q} = \frac{K_{d-1}}{2} Q^{d-2} \ln\left(-\frac{\partial^2(-\beta a^Q)}{\partial\Gamma^2} + b_s Q^2 \right). \tag{33}$$

By means of the change of variables,

$$t = -\ln(Q),$$

$$l = \Gamma\left(\frac{b_s'}{K_{d-1}}\right)^{1/2} e^{[(d-3)/2]t},$$

$$V_t(l) = \frac{\beta e^{(d-1)t}}{K_{d-1}} a^Q,$$

we obtain the known RG equation [5,8–10]

$$\frac{dV_t(l)}{dt} = (d-1)V_t(l) + \frac{1}{2}(3-d)\frac{\partial V_t(l)}{\partial l} + \frac{1}{2}\ln\left[\frac{\partial^2 V_t(l)}{\partial l^2} + 1\right], \tag{34}$$

where $V_t(l)$ is the effective interfacial potential in the RG approach. From this formal equivalence, we can identify the renormalized effective interaction $V_t(l)$ as the surface Helmholtz free energy a^Q and the height of the interface l as a measure of the absorption Γ. The initial (i.e., bare) form of $V_t(l)$ is then given by the value of $a^Q(\Gamma)$ at a suitable matching cutoff $Q = Q_0 \ll 1$. The appropriate value should include the effects of short-wavelength fluctuations (i.e., of fluctuations at $Q > Q_0$) but a rough estimate is obtained starting from the mean-field free energy. It is possible to show that, in the sharp-kink approximation [1] for the density profile of a continuous system, the initial form of our $V_t(l)$ is given by Eq. (2)—i.e., the same used in the effective capillary-wave Hamiltonian.

III. LATTICE GAS COMPLETE WETTING

A. Mean field

In this section we consider the wetting transition in a semi-infinite lattice gas model with nearest-neighbor interaction in contact with an unstructured wall. The interaction between the wall and lattice gas is described by an external potential u_i, where the subscript $i \geq 1$ labels layers of the lattice gas: we consider a planar geometry with an external potential translationally uniform in directions parallel to the wall. It is convenient to introduce an interlayer interactions v_{ij} which collects all inter-atomic nearest-neighbor interactions of the particles belonging to the ith and jth layers, which are assumed to be nearest neighbors. Note that there is also a contribution v_{ii} which describes the interaction of particles within the same layer. We shall discuss in the following only the particular model for which the external potential acts only on the first layer and is attractive:

$$u_i = u\delta_{i,1}$$

and

$$v_{ij} = \begin{cases} v, & i,j \text{ nearest-neighbors layers}, \\ 4v, & i = j, \\ 0, & \text{otherwise}, \end{cases}$$

with $u,v<0$. In the mean-field approximation, the free energy A_{mf} of the system reads

$$\frac{-\beta A_{mf}}{S} = -\frac{\beta A_R}{S} + \frac{1}{2}\sum_{i,j} \rho_i \rho_j \phi_{ij}, \tag{35}$$

where ρ_i is the density of the i layer, $\phi_{ij}=-\beta v_{ij}$, and S is the area of the layers. The reference system is a hard-core lattice gas:

$$\frac{-\beta A_R}{S} = -\sum_i [(1-\rho_i)\ln(1-\rho_i) + \rho_i \ln(\rho_i)]. \tag{36}$$

It is well known that in the mean-field approximation the bulk critical temperature is $k_B T_c/|v|=3/2$. For $T<T_c$ there are two stable phases α and β, which coexist for $\mu_0=-3|v|$. This value of the chemical potential at coexistence is not modified by fluctuations due to the particle-hole symmetry of the model, which also leads to a relationship between the bulk densities of the two coexisting phases: $\rho_\alpha=1-\rho_\beta$. The mean-field density profile is related to the external potential by thermodynamics:

$$\gamma_i = -\frac{\partial}{\partial \rho_i}\left(\frac{\beta A_{mf}}{S}\right) = \ln\left[\frac{\rho_i}{1-\rho_i}\right] - \sum_j \rho_j \phi_{ij}, \tag{37}$$

where $\gamma_i=\beta(\mu-u_i)$. This is a nonlinear equation for the density profile which can be conveniently written as

$$\rho_i = \frac{e^{x_i}}{1+e^{x_i}}, \tag{38}$$

where

$$x_i = \gamma_i + \sum_j \rho_j \phi_{ji}.$$

On general grounds, for nearest-neighbor interactions there are two possible scenarios depending on the value of u/v [26], named the strong substrate regime $(u/v>1)$ and the intermediate substrate regime $(1/2<u/v<1)$. There is also another regime for $0<u/v<1/2$, the weak substrate regime, but its properties follow from those of the intermediate regime due to the symmetry of the Ising model: they describe the same phenomena of the intermediate regime but on "the other side" of the coexistence line [26]; i.e., in one case the bulk density is ρ_α in the other case is ρ_β. In Figs. 1 and 2 we sketch the phase diagrams in the strong and intermediate regimes, respectively. For $u/v>1$ an infinite sequence of transitions occurs, corresponding to condensation of successive monolayers. The critical temperatures of these layer transitions approach, for high-oder multilayers, a well-defined temperature T_R, the roughening temperature. At a temperature below T_R isotherms for the adsorption Γ show an infinite sequence of sharp steps as $\mu \to \mu_0$. Between T_R and T_c the steps are rounded but Γ still diverges, approaching coexistence. Instead for $u/v<1$ the layer transitions no longer extend to the $T=0$ axis but now meet the coexistence axis below a characteristic wetting temperature T_W. Notice that the phase diagrams of the intermediate and strong substrate regimes are similar for $T>T_W$.

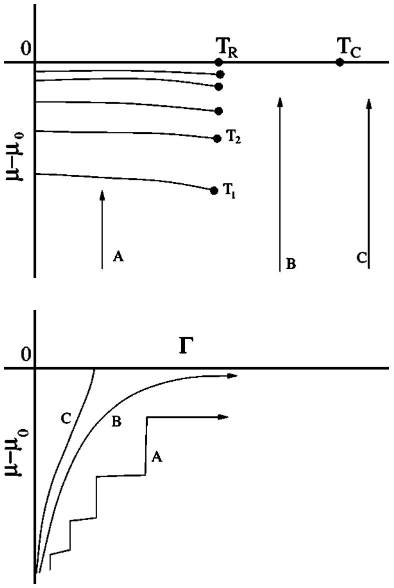

FIG. 1. Typical surface phase diagram with representative gas-phase adsorption isotherms for strong substrate regime $(u/v>1)$. Here μ is in units v and Γ is in units of lattice spacing.

Mean-field theory fails to describe the roughening transition and it incorrectly predicts $T_R=T_c$ [27]. Therefore, at the mean-field level there is no smooth wetting transition but only a sequence of layer transitions; nevertheless, it is interesting to note that in the intermediate regime for high temperatures the behavior of $\Gamma(\mu)$ at fixed T is very similar to that of a smooth wetting transition. We numerical solve the nonlinear mean-field density profile equation (38), with stan-

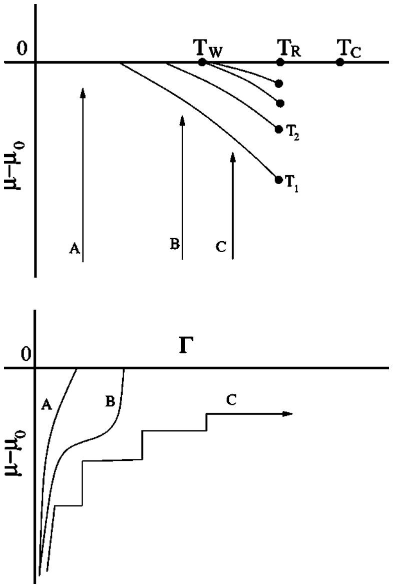

FIG. 2. Typical surface phase diagram with representative gas-phase adsorption isotherms for intermediate substrate regime $1/2<u/v<1$. Here μ is in units v and Γ is in units of lattice spacing.

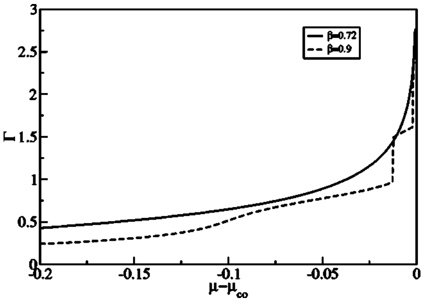

FIG. 3. Two absorption isotherm in the mean-field approximation for $\beta = v/k_bT = 0.72$ and $\beta = 0.9$ ($\beta_c = 2/3$) and $u/v = 0.95$. We see that for low temperature the layer transitions are evident, but for high temperature the isotherm is smooth. μ is in units v and Γ is in units of lattice spacing.

dard technique [28], in the intermediate regime $u/v = 0.95$ at different temperatures and we calculate the adsorption

$$\Gamma = \sum_i (\rho_i - \rho_b),$$

where ρ_b is the bulk density obtained by

$$\beta\mu = \ln\left[\frac{\rho_b}{1-\rho_b}\right] - 6\rho_b\phi.$$

At low temperature, as previously discussed, we see a sequence of layer transitions while at high temperature the layer transitions are still present but are shifted very near the coexistence line. As a consequence, the $\Gamma(\mu)$ isotherm, shown in Fig. 3, is smooth and looks very similar to what is expected in the wetting regime: The divergence close to the coexistence line is well represented by $\Gamma(\mu) \simeq A \ln(\mu - \mu_{co})$ as in wetting. A fit of the data points gives a value $A \simeq 0.45$ in a wide range of temperatures (see Fig. 4).

If we suppose that the capillary-wave effective Hamiltonian describes the critical behavior of wetting phenomena, we can use our data on the critical amplitude A to estimate the wetting parameter ω:

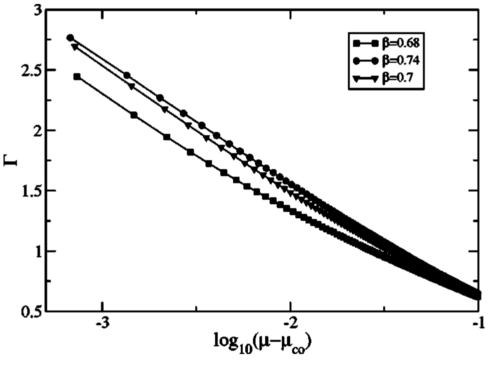

FIG. 4. The logarithm plot of the adsorption isotherm in mean-field approximation for $\beta = v/k_bT = 0.74$, $\beta = 0.70$, $\beta = 0.68$, and $u/v = 0.95$. We see that in the asymptotic region the three adsorption isotherms are well approximated by straight lines. μ is in units of v and Γ is in units of lattice spacing.

$$\left(1 + \frac{\omega}{2}\right) = \frac{A}{\Delta\rho\xi_b}, \tag{39}$$

where $\Delta\rho$ is the difference between the bulk density of the two phases across the interface and we use $l \simeq \Gamma(\Delta\rho)^{-1}$. Near coexistence $\Delta\rho = 1 - 2\rho_b$ due to the particle-hole symmetry of the system. The *true* correlation length ξ_b [13] can be obtained from the Ornstein-Zernike form of the bulk correlation we have adopted in this investigation:

$$\cosh(\xi_b^{-1}) = 1 + \frac{1}{2}(\xi_b^*)^{-2}, \tag{40}$$

$$(\xi_b^*)^2 = \frac{\rho_b(1-\rho_b)\beta}{1 - 6\beta\rho_b(1-\rho_b)}, \tag{41}$$

where ξ_b^* is the second-moment correlation length, analytically obtained by expanding to the second order the Fourier transform of the direct correlation function. By substituting into Eq. (39) our numerical result for the critical amplitude A, we obtain $\omega_{mf} \simeq 0$ as expected in the mean-field approximation.

We can also evaluate the mean-field surface susceptibility χ_s defined as

$$\chi_s = \frac{\partial\Gamma}{\partial\mu} = \sum_i \left(\frac{\partial\rho_i}{\partial\mu} - \frac{\partial\rho_b}{\partial\mu}\right).$$

To obtain χ_s in the mean field, we differentiate the density profile equation (37) with respect to the chemical potential:

$$\beta = \frac{\partial\rho_i/\partial\mu}{\rho_i(1-\rho_i)} - 4\beta\frac{\partial\rho_i}{\partial\mu} - \beta\frac{\partial\rho_{i+1}}{\partial\mu} - \beta\frac{\partial\rho_{i-1}}{\partial\mu}.$$

This is a tridiagonal set of linear equations in $\partial\rho_i/\partial\mu$ that can be numerically solved. This route gives more accurate results than the direct numerical differentiation of the adsorption. Close to coexistence, the surface susceptibility diverges as $\chi_s \simeq A/\Delta\mu$.

B. HRT surface equation

After having discussed the mean-field approximation, which defines the initial condition of the HRT equation, we are ready to tackle the numerical solution of the HRT surface equation. In this first application of the HRT approach to inhomogeneous systems we are mainly interested in surface fluctuations in a temperature range not too close to the bulk critical point. In such a regime, the dependence of the surface evolution equation (22) on bulk quantities via the definition (17) can be neglected. Therefore, as first step, we have chosen to adopt a local density approximation for $\alpha^Q(\kappa)$, Eq. (18):

$$\alpha^Q(\kappa) = \int \frac{dq}{2\pi}|g^Q(q)|^2\phi(q,\kappa). \tag{42}$$

In Appendix A we show how the evolution equation for the surface tension, Eq. (16), constructed for a continuum system, must be modified to be applied to a lattice system [2,29]. The evolution equation for the surface tension of the lattice gas in three dimensions is given by

$$\frac{\partial(-\beta\sigma^Q)}{\partial Q} = \frac{1}{2}D_2(Q)\ln[1 + F_s(Q)\alpha(Q)], \qquad (43)$$

with $Q \in [-1:1]$ and $D_2(Q)$ is the two-dimensional density of states (see Appendix A).

According to the discussion in Sec. II A, the factor $g^Q(q)$ in Eq. (42) is related to the Fourier transform of the first derivative of the density profile. This definition, however, cannot be stricltly carried over to lattice models where the density profile is defined only on lattice sites. Instead, we parametrized $g^Q(z)$ in terms of a rigidly shifted mean-field density profile,

$$g^Q(z) = \rho_Q'(x) = \rho_{mf}'(z - l_Q), \qquad (44)$$

where l_Q is the (unknown) Q-dependent position of the interface and $\rho_{mf}(z)$ is an analytic interpolation of the mean field ρ_i obtained by fitting the discrete density profile with a suitable continuum density profile:

$$\rho_{mf}(z) = \frac{1}{2}\left[(a + b) + (a - b)\mathrm{erf}\left(\frac{z}{\xi_\perp}\right)\right]. \qquad (45)$$

This form does adequately represent the actual density profile by taking a equal to the bulk density and b to the contact density ρ_1. The width $\xi_\perp$ of the interface is only weakly dependent on the thermodynamic state and diverges logarithmically at wetting. As a first approximation we set $\xi_\perp$ independent of μ. Instead, the position of the interface l_Q does depend on the state and will be strongly renormalized by fluctuations. In fact, l_Q is easily related to the adsorption Γ_Q, via the parametrization (44):

$$\Gamma_Q = \frac{\partial(-\beta\sigma^Q)}{\partial\beta\mu} = \int_0^\infty dz[\rho_{mf}(z - l_Q) - \rho_b] \simeq \frac{l_Q}{2}(\rho_1 - \rho_b). \qquad (46)$$

Note that, due to the parametrization (44), the value of l_Q drops out of the definition of $\alpha^Q(\kappa)$, Eq. (42), which then becomes Q independent (see Appendix B). We parametrized the surface correlation function by an OZ form,

$$F_s^Q(\kappa) = \frac{\rho_b(1 - \rho_b)}{\left|\int dz\rho_Q'(z)\right|^2[1 - \lambda_Q\alpha^Q(\kappa)]}, \qquad (47)$$

in terms of the unkown parameter λ_Q. When this expression is substituted into Eq. (15) we get

$$\Delta F^Q(z_1,z_2,\kappa) = \tilde{g}^Q(z_1)\tilde{g}^Q(z_2)\frac{\rho_b(1 - \rho_b)}{1 - \lambda_Q\alpha^Q(\kappa)}, \qquad (48)$$

where $\tilde{g}^Q(z) = \rho'^Q(z)/|\int dz'\rho'^Q(z')|$. The first term of Eq. (48) can be interpreted as a normalized function which constrains the range of the correlation function to the interface—i.e., where $\rho_Q'(z)$ does not vanish. The factor $\rho_b(1-\rho_b)$ guarantees the correct $\rho_b \to 0$ limit preserving the symmetry of the model. The chosen form of ΔF^Q, Eq. (48), reproduces the momentum dependence of the known random-phase approximation [23] in which $\alpha^Q(\kappa)$ plays the role of an effective interaction potential on the interface. The yet unknown parameter λ_Q is determined via the surface compressibility sum rule (24), valid for each Q system. By use of the parametrization (47) in the sum rule (24) we obtain the explicit relationship between λ_Q and the thermodynamics:

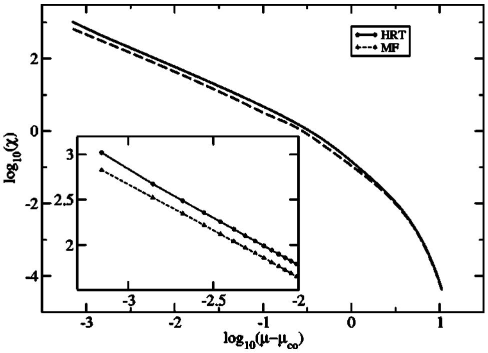

FIG. 5. The double-logarithm plot of χ_s isotherm for $\beta = v/k_bT = 0.72$ and $u/v = 0.95$. We see that the effect of fluctuation is a renormalization of the critical adsorption amplitude.

$$\frac{\partial^2(-\beta\sigma^Q)}{\partial(\beta\mu)^2} = \left|\int dz\rho_Q'(z)\right|^2 F_s(\kappa = 0) = \frac{\rho_b(1 - \rho_b)}{1 - \lambda_Q\alpha^Q(\kappa = 0)}. \qquad (49)$$

Substituting the approximation of $F_s^Q(\kappa)$ in the evolution equation (43) we obtain a closed nonlinear partial differential equation for the surface free energy $\sigma^Q(\mu)$ at fixed temperature. The initial condition for this equation is given by the mean-field theory. The boundary conditions are given at coexistence—i.e., $\mu = \mu_{co}$ where we assume that the surface susceptibility diverges (wetting) and at $\mu \to -\infty$ which corresponds to vanishing bulk density. The equation is written in quasilinear form by a suitable change of variable shown in Appendix B. The evolution equation is then solved by a predictor-corrector algorithm [30].

In Fig. 5 we show the logarithm of the susceptibility versus the logarithm of $\mu - \mu_{co}$. Notice that the value of χ_s at the last point of the grid depends on the mesh spacing as can be seen in Fig. 6. For this reason this value is not considered in

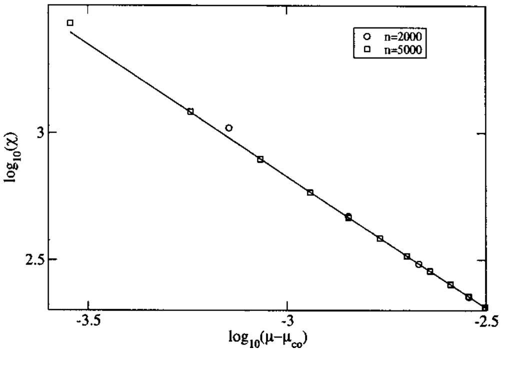

FIG. 6. The double-logarithmic plot of the χ_s isotherm for $\beta = v/k_bT = 0.70$ and $u/v = 0.95$ for two different numbers of mesh points. We see that the number of mesh points—i.e., the grid spacing—affects the value of χ_s at the last point of the grid. The line is only a guide to the eye.

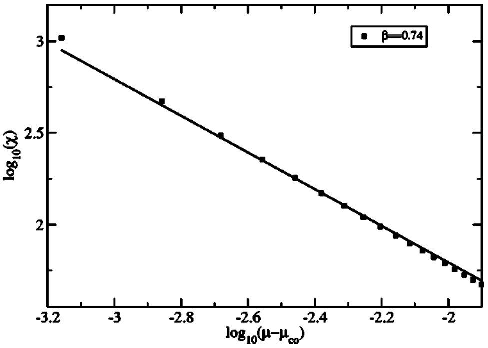

FIG. 7. The double-logarithm plot of the χ_s isotherm for $\beta = v/k_bT = 0.72$ and $u/v = 0.95$ in the asymptotic region. The line is $\ln(\chi_s) = -\ln(\mu-\mu_{co}) + \ln A$, with $A = 0.62$.

the following analysis. In the asymptotic region, close to the coexistence curve, $\ln(\chi_s)$ displays a linear behavior. We fit our data with a linear relation: $\ln(\chi_s) \simeq a \ln(\mu-\mu_{co}) + b$ and we obtain $a = -1.040 \pm 0.001$. This value is compatible with a logarithmic divergence of the adsorption; i.e., the inclusion of fluctuations does not modify divergence of the adsorption, so, as predicted by RG approach, the critical exponent for complete wetting remain mean-field-like even when we introduce the fluctuations. The main effect of fluctuations in the asymptotic region is rather a renormalization of the amplitude A; see Fig. 5. To estimate the value of the amplitude we fit the HRT, results with $\ln(\chi_s) = \ln(A/\Delta\mu) = -\ln(\mu-\mu_{co}) + \ln A$; see Fig. 7. We obtain $A \simeq 0.62$ which is larger than the lattice mean-field result $A \simeq 0.45$. In Fig. 8 we plot the surface susceptibility for two different temperatures. The fluctuations introduce a weak dependence of the critical amplitude on the temperature, which is absent in the mean-field results.

Using Eq. (39) and our numerical result for A, we obtain $\omega_{HRT} \simeq 0.6$ which is smaller than the RG estimation for the Ising model $\omega \simeq 0.8$ [12] and larger than the value $\omega \simeq 0.3$ obtained from simulation results on critical exponents for critical wetting [16]. However, our numerical estimate is obtained at higher temperature: $T \simeq 0.92 T_c$. The deficiencies of the mean-field approximation prevents us from studying a wide range of temperatures and so it is also difficult to extract from our results how ω depends on temperature. However, our data seem to imply an increasing of the wetting parameter for $T \to T_c$ (see Fig. 8).

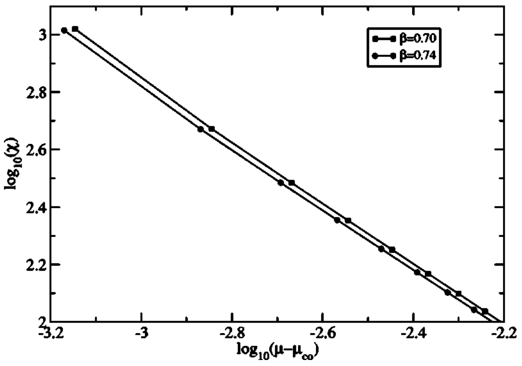

FIG. 8. The double-logarithm plot of the χ_s isotherm for $\beta = v/k_bT = 0.70$ and $\beta = 0.74$; $u/v = 0.95$. We see that the effects of temperature on the critical amplitude are small. The lines are only a guide to the eye.

IV. CONCLUSIONS

In this work we have presented an extension of the HRT approach [2] to inhomogeneous systems and we applied the formalism to the wetting transition in the three-dimensional (3D) Ising model in planar geometry. The approach presented here is, to our knowledge, the first *microscopic* theory able to describe capillary wave fluctuations at the level of the renormalization group approach. Its use is not restricted to the study of wetting but more generally to the study of fluctuations effects in nonhomogeneous systems. Differently from the standard bulk HRT, we introduce a cylindrical cutoff to take into account the anisotropic spectrum of the fluctuations in such a reduced symmetry. We obtain a hierarchy of evolution equations for the bulk properties which reproduces the known RG approach close to the bulk critical point together with an additional hierarchy of differential equations for the surface free energy and the interfacial correlations. This further hierarchy generally depends on bulk correlation functions. In order to close the hierarchy at the lowest level—i.e., keeping only the free energy equations—we analyzed a simple Ornstein-Zernike ansatz for both the bulk and interfacial correlations. Within this approximation, the resulting bulk critical exponents turn out to be exact to first order in $\epsilon = 4-d$ and the surface free energy equation is equivalent to the known functional RG approach applied to the effective capillary-wave Hamiltonian [8–10]. To study the effects of fluctuations also in the nonasymptotic region we investigated by the HRT approach the complete wetting transition in a lattice gas model with nearest-neighbor interactions (i.e., for the Ising model). In order to simplify the analysis we introduced a further decoupling approximation which disregards the effects of bulk fluctuations on surface quantities. The numerical results show an interesting renormalization of the critical adsorption amplitude which can be related to a renormalization of the wetting parameter. The HRT value of the wetting parameter is $\omega \simeq 0.6$ which is smaller the the field-theoretical estimate for this model [12] but it is greater than simulation results for critical exponents of the critical wetting transition [16] at lower temperature. This can probably related to the increase of wetting parameter for $T \to T_c$. Notwithstanding the crudeness of some approximation we introduced, the results for critical and noncritical quantities compare quite favorably with available simulation data. Clearly there is room for improvement within the class of OZ closures of the HRT hierarchy. In particular it would be interesting to allow for a renormalization of the transverse correlation length $\xi_\perp$ which we kept constant. The extension of this approach to different systems, like off-lattice fluids or the Ising model in parallel-plate geometry, looks also promising.

ACKNOWLEDGMENT

We thank R. Evans for helpful suggestions.

APPENDIX A

Consider a lattice system with nearest-neighbor interaction

$$v_{ij}=\begin{cases} v, i, j, & \text{nearest-neighbors site}, \\ 0, & \text{otherwise}. \end{cases} .$$

The Fourier transform of the dimensionless interparticle potential is

$$\phi(q,\kappa)=4w\beta[\gamma_2(\kappa)+\cos(q)],$$

where $w=-v>0$ and

$$\gamma_d(\kappa)=\frac{1}{d}\sum_{i=1}^{d}\cos(k_i).$$

The Brillouin zone is defined by $-\pi<k_i\leqslant\pi$ and we choose the cylindrical of the form [2,29]

$$\phi^Q(q,\kappa)=\begin{cases} \phi(\kappa,q), & \gamma_2(\kappa)\leqslant Q, \\ 0, & \gamma_2(\kappa)>Q, \end{cases}$$

with $Q\in[-1,1]$. The evolution equation for the surface tension of the lattice gas in three dimensions then becomes

$$\frac{\partial(-\beta\sigma^Q)}{\partial Q}=\frac{1}{2}D_2(Q)\ln[1+F_s(Q)\alpha(Q)], \tag{A1}$$

where $\alpha(Q)$ is the value of $\alpha^Q(\kappa)$ evaluated at $\gamma_2(\kappa)=Q$ and $D_2(Q)$ is the two-dimensional density of states:

$$D_2(Q)=\int\frac{d^2\kappa}{(2\pi)^2}\delta(Q-\gamma_2(\kappa))=\frac{2}{\pi^2}K(\sqrt{1-Q^2}),$$

where $K(x)$ is complete elliptic integral of the first kind.

APPENDIX B

In this appendix we provide some detail on the algebraic manipulations on Eq. (43) necessary for implementing an efficient numerical algorithm. As a first step we give the explicit form for the effective surface potential obtained by substituting the parametrization discussed in the text for the function $g^Q(z)$, Eq. (14), into the definition of $\alpha^Q(\kappa)$, Eq. (42). By use of the mean-field density profile (45), $g^Q(z)$ is just a Gaussian function and $\alpha^Q(\kappa)$ is independent of l_Q:

$$\begin{aligned}\alpha^Q(\kappa)&\simeq\frac{(\rho_b-\rho_1)^2}{2\pi}\int_{-\pi}^{\pi}dq e^{-q^2\xi_\perp^2/2}\phi(\kappa,q)\\&=\frac{(\rho_b-\rho_1)^2}{2\pi}\int_{-\pi}^{\pi}dq e^{-q^2\xi_\perp^2/2}2\beta w[(d-1)\gamma(\kappa)+\cos(q)]\\&=\frac{\beta w(\rho_1-\rho_b)^2[(d-1)I_1\gamma(\kappa)+I_2]}{\pi},\end{aligned}\tag{B1}$$

where

$$I_1=\int_{-\pi}^{\pi}dq e^{-q^2\xi_\perp^2/2},$$

$$I_2=\int_{-\pi}^{\pi}dq e^{-q^2\xi_\perp^2/2}\cos(q).$$

Now we introduce the shorthand notation $f_r=\rho_b(1-\rho_b)$ and $b_Q=-\beta\sigma^Q$. The surface susceptibility of the Q-system is easily expressed in terms of b''_Q:

$$b''_Q=\beta^2\frac{\partial^2(-\beta\sigma_Q)}{\partial(\beta\mu)^2}=\beta^2\frac{\partial\Gamma}{\partial\beta\mu}=\beta\chi_s,$$

while the parameter λ_Q is given by Eq. (49). The evolution equation (43) is written in quasilinear form by introducing the new variable v_Q defined by

$$v_Q=\ln[1+P(Q)],$$

where

$$\begin{aligned}P(Q)&=F_s(Q)\alpha(Q)\\&=\frac{b''_Q(\rho_b-\rho_1)^{-2}f_r\alpha_0\alpha(Q)}{b''_Q(\alpha_0-\alpha(Q))+f_r\beta^2\alpha(Q)}\\&=\frac{b''_Q f_r r(Q)}{b''_Q m(Q)+f_r\beta^2\tilde{\alpha}(Q)}\end{aligned}$$

and

$$v_Q=f_r\tilde{\alpha}(Q)+\tilde{\alpha}^2(Q)u_Q,$$

where $\tilde{\alpha}(Q)=\alpha^Q(Q)(\rho_b-\rho_1)^{-2}$. By differentiating twice the evolution equation (43) with respect to the chemical potential and substituting the definition of v_Q we get

$$\frac{\partial b''_Q}{\partial Q}=\frac{1}{2}D_2(Q)\frac{\partial^2 v_Q}{\partial\mu^2}.$$

Inverting $v=v(b''_Q)$ we find

$$b''_Q=-\frac{\beta^2 f_r\tilde{\alpha}(Q)[e^v-1]}{[\tilde{\alpha}_0-\tilde{\alpha}(Q)][e^v-1]-f_r\tilde{\alpha}_0\tilde{\alpha}(Q)}.$$

Differentiating this relation with respect to Q we obtain

$$\begin{aligned}\frac{\partial b''_Q}{\partial Q}&=-\frac{\partial}{\partial Q}\left(\frac{\beta^2 f_r\tilde{\alpha}(Q)[e^{v_Q}-1]}{[\tilde{\alpha}_0-\tilde{\alpha}(Q)][e^{v_Q}-1]-f_r\tilde{\alpha}_0\tilde{\alpha}(Q)}\right)\\&=\frac{\beta^2 f_r^2\tilde{\alpha}(Q)^2\tilde{\alpha}_0\dot{v}_Q e^{v_Q}-\beta^2 f_r\dot{\tilde{\alpha}}\tilde{\alpha}_0[e^{v_Q}-1]^2}{\{m(q)[e^{v_Q}-1]-f_r r\}^2},\end{aligned}\tag{B2}$$

where $\dot{v}_Q=\partial v_Q/\partial Q$ and $v''=\partial^2 v_Q/\partial\mu^2$. We now introduce the notation

$$\begin{aligned}r(Q)&=\tilde{\alpha}_0\tilde{\alpha}(Q)\\&=\left(\frac{\beta}{\pi}\right)^2[(d-1)^2 I_1^2 Q+I_1 I_2(d-1)(1+Q)+I_2^2],\end{aligned}$$

$$m(Q)=\tilde{\alpha}_0-\tilde{\alpha}(Q)=\frac{\beta}{\pi}(d-1)I_1(1-Q),$$

which give $\dot{r}=\tilde{\alpha}_0\dot{\tilde{\alpha}}$ and $\dot{m}=-\dot{\tilde{\alpha}}$. By solving the algebraic Eq. (B2) for $\dot{v}_Q$ we obtain

$$\dot{v}_Q = \frac{\dot{\tilde{\alpha}}}{f_r\tilde{\alpha}^2(Q)}[e^{v_Q}-1]^2 e^{-v_Q} + \frac{D_2(Q)e^{-v_Q}}{2\beta^2 f_r^2\tilde{\alpha}^2(Q)\tilde{\alpha}_0} \times\{m(Q)[e^{v_Q}-1]-f_r r\}^2 v_Q'', \tag{B3}$$

which is the evolution equation for v_Q. Finally, by a further change of variable, we introduce u_Q by

$$f_r\tilde{\alpha}(Q)+\tilde{\alpha}(Q)^2 u_Q = \ln[1+F_s(Q)\alpha(Q)]. \tag{B4}$$

Switching from the chemical potential to the fugacity $z = e^{\beta(\mu-\mu_{co})}$ we express the derivatives of v_Q in terms of u_Q:

$$\dot{v}_Q = f_r\dot{\tilde{\alpha}} + 2\tilde{\alpha}\dot{\tilde{\alpha}}u_Q + \tilde{\alpha}^2\dot{u}_Q,$$

$$\begin{aligned} v_Q'' &= \tilde{\alpha}f_r'' + \tilde{\alpha}^2 u_Q'' \\ &= \tilde{\alpha}\beta^2\left[z\frac{\partial f_r}{\partial z} + z^2\frac{\partial^2 f_r}{\partial z^2}\right] + \tilde{\alpha}^2\beta^2\left[z\frac{\partial u_Q}{\partial z} + z^2\frac{\partial^2 u_Q}{\partial z^2}\right]. \end{aligned}$$

Substituting these expressions into the evolution equation for v_Q, Eq. (B3), we obtain the quasilinear equation satisfied by u_Q:

$$\frac{\partial u_Q}{\partial Q} = L_1 + L_2 + M\frac{\partial^2 u}{\partial z^2}, \tag{B5}$$

with

$$L_1 = \frac{1}{\tilde{\alpha}^2}\left[\frac{\dot{\tilde{\alpha}}}{f_r\tilde{\alpha}^2}(e^{v_Q}-1)^2 e^{-v_Q} - f_r\dot{\tilde{\alpha}} - 2\tilde{\alpha}\dot{\tilde{\alpha}}u_Q\right], \tag{B6}$$

$$L_2 = \frac{D_2(Q)e^{-v_Q}}{2\beta^2\tilde{\alpha}^4(Q)f_r^2\tilde{\alpha}_0}\{m(Q)[e^{v_Q}-1]-f_r r\}^2 \times\left(\tilde{\alpha}\beta^2\left[z\frac{\partial f_r}{\partial z} + z^2\frac{\partial^2 f_r}{\partial z^2}\right] + \tilde{\alpha}^2\beta^2 z\frac{\partial u_Q}{\partial z}\right), \tag{B7}$$

$$M = \frac{D_2(Q)e^{-v_Q}}{2\beta^2\tilde{\alpha}^2(Q)f_r^2\tilde{\alpha}_0}\{m(Q)[e^{v_Q}-1]-f_r r\}^2\beta^2 z^2. \tag{B8}$$

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