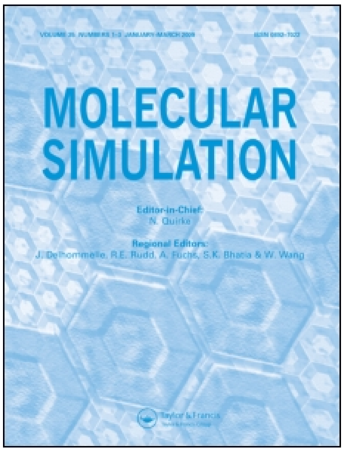

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A Bridge between the Microscopic Interaction Potentials in a Fluid and Effective Long-wavelength Hamiltonians

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A Bridge between the Microscopic Interaction Potentials in a Fluid and Effective Long-wavelength Hamiltonians

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The asymptotic and preasymptotic critical behavior of the three-dimensional Ising universality class, which includes easy axis magnets and fluids, is believed to be described by effective ψ^4 scalar field theory with suitable, non-universal, coupling constants. Universal properties do not depend on the specific values of these coupling constants but this is not so for the non-universal properties. Here we show that the coupling constants dependence on microscopic potentials can be studied using the Hierarchical Reference Theory (HRT), which implements the basic ideas of Wilson momentum renormalization group to microscopic Hamiltonians. We discuss the application of this method to two different microscopic models of intermolecular potential of a simple fluid and to the Ising model. Also the wetting phase transition in a fluid near a wall is described by an effective Hamiltonian. This Hamiltonian contains an effective interfacial potential, which describes the effective interaction of interface with the wall. Here we show how to extend the HRT formalism to inhomogeneous system and how, in such theory, we can extract the interfacial quantities and study their behavior.

Keywords: Microscopic interaction potential; Writing Hierarchical Reference Theory; Effective Hamiltonians; Critical region

INTRODUCTION

In the study of critical phenomena effective Hamiltonians plays a central role. They are used to describe the behavior of systems in the critical region where only long-wavelength fluctuations are relevant and formally obtained by tracing out the short-wavelength fluctuations of the order parameter. We mention two different cases of such effective Hamiltonians. The first is the usual ψ^4 scalar field Hamiltonian:

$$H_\psi = \int d^d\mathbf{r} = \left[\frac{1}{2}(\nabla\psi)^2 + \frac{1}{2}r\psi^2 + u\psi^4\right], \qquad (1)$$

where $\psi(\mathbf{r})$ is the order parameter, d is the dimensionality and r and u are two non-universal coupling constants. This Hamiltonian is used to describe the critical behavior of the three-dimensional Ising universality class to which also the liquid–vapor critical point belongs. Although the universal quantities are independent of the value of $r, u > 0$ and on possible higher order terms neglected in Eq. (1), this is not so for many physically interesting properties, like the critical temperature or the extent of the corrections to scaling. The second Hamiltonian which we consider is used to study the wetting [2,3] critical phenomena such as the drying of a fluid near a hard wall:

$$H_l = \int d^{d-1}\mathbf{r}_\parallel \left[\frac{1}{2}\sigma(\nabla l)^2 + V(l)\right], \qquad (2)$$

where σ is the surface tension and the single valued function $l(\mathbf{r}_\parallel) > 0$ represents the height of the interface. The first term represents the *elastic* free energy of the interface, the second one the direct interaction free energy of interface with the wall. The form of effective interfacial potential $V(l)$ depends on the range of the microscopic interaction potential. In the case of short range potentials it becomes, for large l [2,3,5–7]:

$$V(l) \simeq -W\exp(-ml/\xi) + U\exp(-nl/\xi), \qquad (3)$$

where m, n are two dimensionless constants with $n > m$. The parameter ξ can be identified with

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the bulk correlation length. To build such an effective interfacial Hamiltonian we must trace out the bulk degrees of freedom. It is important to note that the use of such an effective surface Hamiltonian can be justified only when bulk fluctuations are small *i.e.* far for bulk critical point [4]. These two Hamiltonians are known to describe the critical phenomena, but the missing ingredient is still the link between them and the specific microscopic model appropriate for a given physical system. Hierarchical Reference Theory (HRT) [8,9] provides a systematic way to derive an effective Hamiltonian from a given microscopic model. This theory, which implements the basic ideas of Wilson momentum space renormalization group (RG) to microscopic Hamiltonians, allows us to derive an exact hierarchy of differential equations describing the evolution of the free energy and of 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 by imposing an approximation for the pair correlation function. With this closure, usually of the Ornstein-Zernike (OZ) form, the HRT has genuine non-classical critical behavior but the critical exponents are only approximate and in particular the correlation exponent η is zero. As a consequence the HRT theory describes, with good accuracy, fluid in regions not asymptotically close to critical point. A possibility is to use HRT to treat fluctuations not over all length scales but to use it to trace out fluctuations up to a certain wave vector cut-off, and then switch to a description based on an effective Hamiltonian in which the non-universal coupling constants have been determined by HRT, at least for the three-dimensional Ising universally class. Also in the case of wetting the HRT can help us to understand the microscopic origin of the effective interfacial potential.

This work is organized as follows: in the "Homogeneous Theory" Section we give a brief summary of bulk HRT formalism together with the discussion of the method we use to extract from HRT the coupling constants of the effective Hamiltonian. The application of this method to three different cases is also reported. In the "Theory for Inhomogeneous States" Section, we show how HRT can be extended to inhomogeneous system and how we can extract the effective interfacial potential. In the "Conclusion" Section, we briefly summarize the most relevant results.

HOMOGENEOUS THEORY [1]

Bulk HRT Theory

Here we consider a system of point-like particles interacting via a two body potential. The starting point in the derivation of HRT equations is the separation of the inter-atomic potential $v(r)$ in two parts:

$$v(\mathbf{r}) = \mathrm{v}_{\mathrm{R}}(\mathbf{r}) + \mathrm{w}(\mathbf{r}), \tag{4}$$

where $v_{\mathrm{R}}(\mathbf{r})$ is the short-range repulsive part of $v(\mathbf{r})$. The thermodynamic and structural properties of the system with interaction $v_{\mathrm{R}}(\mathbf{r})$, the "reference system", are assumed known, at least numerically. Instead $w(\mathbf{r})$ is an attractive term, which triggers the liquid–vapor phase transition. Using this separation and performing a Legendre transformation on grand canonical partition function, a formal diagrammatic expansion for the Helmholtz free energy can be written to all orders in perturbation theory. We implement the basic ideas of Wilson's RG approach [10] within such a formal perturbative expansion to study how the thermodynamic quantities evolve due to the inclusion of fluctuations. This can be done by introducing a sequence of intermediate potentials characterized by an infrared spherical sharp cut-off in Fourier space:

$$w^{Q}(\mathbf{k}) = \begin{cases} w(\mathbf{k}) & k \geq Q, \\ 0 & k < Q \end{cases} \tag{5}$$

and studying models interacting via $v^{Q}(\mathbf{r}) = v_{\mathrm{R}}(\mathbf{r}) + w^{Q}(\mathbf{r})$ hereafter referred to as *Q-systems*. For $Q = \infty$, we reduce to the reference system while for $Q = 0$ the full interaction is recovered. We can construct exact differential equations for studying how the Helmholtz free energy and the correlation functions change when we introduce additional fluctuations by decreasing Q. In fact fluctuations with $k < Q$ are strongly suppressed in the Q-system. Since the Helmholtz free energy has a singular contribution due to the mean field terms, it is convenient to introduce a modified free energy $\mathscr{A}^{Q}$ which is continuous in Q also for $Q \to 0$. The first equation of the hierarchy thus obtained is the evolution equation for $\mathscr{A}^{Q}$

$$\frac{\partial}{\partial Q}\left(\frac{-\beta\mathscr{A}^{Q}}{V}\right) = \frac{1}{2}\int_{k=Q} \frac{d\Omega_k}{(2\pi)^3} \ln\left[1 + F_2^{Q}(\mathbf{k})\phi(\mathbf{k})\right], \tag{6}$$

where $\phi = -\beta w$. $\mathscr{F}_2^{Q}$ is a two body correlation function in the momentum space and its evolution in Q involves the three and the four particle correlation functions. This gives rise to a hierarchy of differential equations but we can truncate it at the first equation (6) if we use an approximation for the two point correlation function. The approximation that we use belongs to the class of the "Ornstein-Zernike" closures, *i.e.* a form for $\mathscr{F}_2^{Q}(\mathbf{k})$ which is analytic in $\mathbf{k}$ for $\mathbf{k} \to 0$. In this limit, it reads

$$\mathscr{C}_2^{Q}(\mathbf{k}) = -\left(\mathscr{F}_2^{Q}(\mathbf{k})\right)^{-1} = -\frac{\partial^2}{\partial\rho^2}\left(\frac{-\beta\mathscr{A}^{Q}}{V}\right) + bk^2, \tag{7}$$

where the first term of the r.h.s. embodies the compressibility sum rule and b is a non-universal constant that is finite also near the phase transition. With a closure of this general form, the evolution equation for free energy (6) takes the following universal form, independent from details of the microscopic interaction:

$$\frac{\partial H_t(z)}{\partial t} = dH_t(z) + \frac{2-d}{2} z H_t'(z) + \frac{1}{2}\ln\left[\frac{H_t''(z)+1}{H_t''(0)+1}\right] \quad (8)$$

when we are in the critical region and Q is sufficiently small. Here the prime indicates the derivate with respect to z and

$$Q = e^{-t}, \quad (9)$$

$$z = (\rho - \rho_c)\left(\frac{K_d}{b}\right)^{1/2} Q^{-(2-d)/2}, \quad (10)$$

$$H_t(z) = -\frac{1}{K_d} Q^{-d}\left(\frac{-\beta\mathscr{A}^Q}{V} - \frac{-\beta\mathscr{A}^Q}{V}\bigg|_{\rho_c}\right) \quad (11)$$

with for $d = 3$ $K_\mathrm{d} = (2\pi^2)^{-1}$, ρ_c is the critical density. Equation (8) is formally identical to the Wegner–Hougton RG equation in the local potential approximation (LPA) [11] applied to an effective Hamiltonian of the type:

$$H = \int\left[\frac{1}{2}(\nabla\psi(x))^2 + v_2\psi^2(x) + \sum_{m=3}^{\infty} v_m\psi^m(x)\right] d^d x. \quad (12)$$

We can use this formal equivalence to identify, in long-wavelength regime, the expansion coefficients of the local potential V in the effective Hamiltonian with the derivatives of HRT free energy evaluated at a given cut-off wave vector Q_0:

$$v_m = \frac{1}{m!}\frac{Q_0^{m/2-3}}{b^{m/2}}\frac{\partial^m}{\partial\rho^m}\left(\frac{\beta\mathscr{A}^Q}{V}\right)_{\rho=\rho_\mathrm{c}}\bigg|_{Q=Q_0}. \quad (13)$$

In this way we can calculate, for different microscopic models, the values of the coupling constants in the long-wavelength effective Hamiltonian. If Q_0 is sufficiently small, higher order terms in ψ can be neglected in Eq. (12) and we finally obtain an effective ψ^4 Hamiltonian which may be studied by means of accurate renormalization group equations [12], known to provide reliable results for universal quantities. We can also study the effects of the terms beyond the ψ^4 term in the effective Hamiltonian. The precise value of the cut-off at which we switch from HRT to the effective Hamiltonian is somehow arbitrary, but internal consistency of the method requires that the physical quantities should not depend on the choice of the matching point, in a physically acceptable range.

Results

We have applied this method to three different systems: the three-dimensional Ising model and a fluid model with two different intermolecular potentials. We study the values of the coefficients calculated with Eq. (13) as a function of Q. For the Ising model we consider the first three even terms v_2, v_4 and v_6 because the odd terms vanish by symmetry. In the case of fluid systems we consider also the effects of the first odd terms, *i.e.* v_3 and v_5. We also study the reduced temperature dependence of susceptibility and correlation length and order parameter as obtained by integrating Dohm's RG equations. The first case we consider is the Ising model. In this case the v_6 term as function of Q has a minimum so one can think to fix at this point the value of Q_0 where we switch from HRT to an effective ψ^4 Hamiltonian, in order to minimize the effect of v_6 term. Nonetheless we empirically find that the results obtained for physical quantities show very little dependence on the matching value in the region $0.5 < Q_0 < 1.25$ and so we choose to fix at each temperature the matching value to $Q_0 = 1.0$, in order to obtain a unified criterium even for other models which do not display a minimum in the v_6 coefficient. For the Ising model we can use the accurate results of series expansion [13] to check our results. We see that HRT results are in good agreement with series expansions if the reduced temperature is not too small. Conversely, below a reduced temperature of about 10^{-2}, HRT predictions deviate from the correct result but at this temperature the results from the Dohm equations are already rather accurate (see Fig. 1). The second case we consider is a fluid with Lennard–Jones pair potential. At $Q_0\sigma = 1$ we switch from HRT to effective Hamiltonian. Here the v_5 term differs from

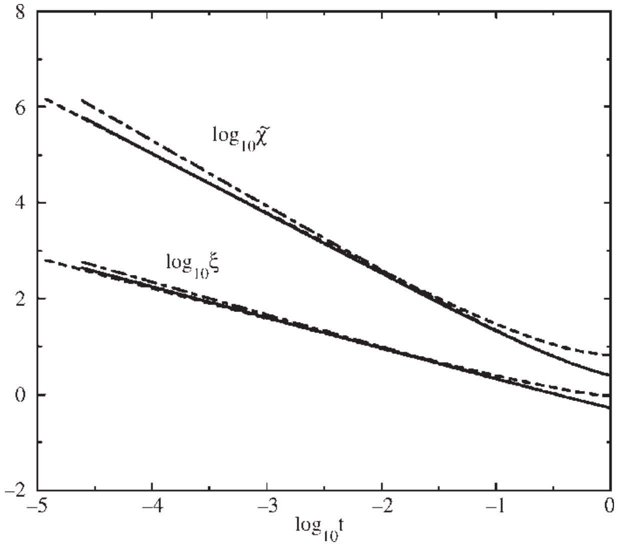

FIGURE 1 The reduced susceptibility (in units of ideal gas susceptibility) and correlation length (in units of lattice spacing) for the Ising model above T_c. Solid line Fisher Burford approximation: dot-dashed line, HRT results: and the dashed line, Dohm equations with HRT initial conditions.

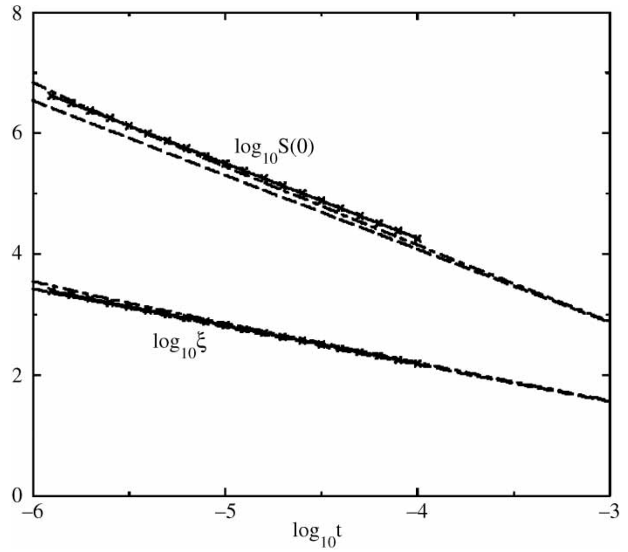

FIGURE 2 The reduced isothermal compressibility $S(0)$ (in units of ideal gas compressibility) and correlation length (in units of σ) for LJ potential above T_c. Solid line, experimental data for Kr in the asymptotic region; dot-dashed line, HRT results; the dashed line, Dohm equations.

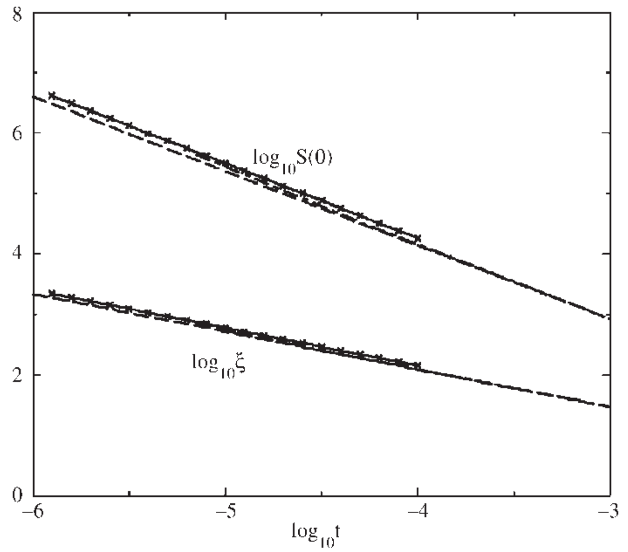

FIGURE 3 The reduced isothermal compressibility $S(0)$ (in units of ideal gas compressibility) and correlation length (in units of σ) for Aziz Axilrod-Teller potential above T_c. Solid line, experimental data for Kr in the asymptotic region; dot-dashed line, HRT results; the dashed line, Dohm equations. The agreement for the compressibility is quite better than that obtained for LJ fluid: conversely results for correlation length are just a little worse.

zero (v_3 is zero at the critical point) but we disregard the odd terms because their inclusion would require a generalization of the RG equations. Even in this case the results show no significant dependence on the values of Q_0 in the range $0.5 < Q_0\sigma < 1.25$. We compare our results with experimental data in Kr [14]. Our estimate for correlation length and order parameter are in good agreement with experimental data but the results for compressibility are not very good (see Fig. 2). A possible origin of the discrepancies encountered is the fact that the LJ potential does not describe very well the true intermolecular interaction. To check this possibility we use a more accurate potential: a realistic form proposed by Aziz for the two-body interaction and the Axilrod-Teller term for a three-body interaction which we include in the reference system. This potential is believed to describe accurately the properties of rare gases [15]. The agreement with experimental results improves for the compressibility, but the correlation length is less accurate than in the former case (see Fig. 3). As a source of inaccuracy in the case of a fluid two possibilities can be considered. The first is that the long-wavelength density fluctuations in a realistic fluid model are only approximately described by a ψ^4 theory *i.e.* the higher order even terms and the odds terms, that are different from zero in this case, cannot be neglected also in critical region. Indeed the coefficients of the ψ^6 term, for fluid models, is significantly larger than in the Ising case. The second possibility concerns the intermolecular potentials, which may describe the true interaction between the fluid particles in the critical region only approximatively.

THEORY FOR INHOMOGENEOUS STATES

Here we show how the HRT formalism can be generalized to inhomogeneous systems and in particular we study the wetting transition. We consider a vapor–liquid interface near a hard wall. Off coexistence there is a microscopic vapor film of thickness l. When the chemical potential μ tends to the coexistence value μ_0 the thickness l diverges for $T > T_W$, the wetting temperature. This phenomenon is called complete drying and is totally equivalent to complete wetting [2,3]. In wetting phenomena the correlation length parallel to the surface $\xi_{\|}$ and the correlation length perpendicular to the surface $\xi_{\perp}$ diverge and are related by [2,3,7]:

$$\xi_{\perp} \simeq \xi_{\|}^{(3-d)/2} \quad d \leq 3. \tag{14}$$

This relationship suggests that the fluctuations perpendicular to the wall diverge much more slowly than the fluctuations parallel to the wall. Therefore, we consider the same expansion for Helmholtz free energy that we used for homogeneous systems, but now we define a sharp *cylindrical* cut-off:

$$w^{Q}(k,q) = \begin{cases} w(k,q) & k \geq Q \\ 0 & k < Q \end{cases}, \tag{15}$$

where κ is the component of the wave vector parallel to the surface. Next we separate the bulk quantities from the surface contributions:

$$\mathscr{A}^Q = \mathscr{A}_b^Q + \Delta\mathscr{A}^Q, \tag{16}$$

$$\rho(\mathbf{r}) = \rho_b + \Delta\rho(\mathbf{r}), \tag{17}$$

$$F_2^Q(\mathbf{r}_1, \mathbf{r}_2) = F_{2b}^Q(|\mathbf{r}_1 - \mathbf{r}_2|) + \Delta F_2^Q(\mathbf{r}_1, \mathbf{r}_2) \tag{18}$$

and so on for all correlation functions. This procedure may be carried out in the diagrammatic expansion of the total Helmholtz free energy. Following what we have done for the bulk case we can calculate the evolution equations for the bulk and surface free energies.

We begin with the bulk free energy. Due to the cylindrical cut-off the exact evolution equation now becomes:

$$\frac{\partial}{\partial Q}\left(\frac{\beta\mathscr{A}_b^Q}{V}\right) = \frac{1}{2}K'_{d-1}Q^{d-2} \times \int \frac{dq}{2\pi}\log(1 + \mathscr{F}_{2b}^Q(q,Q)\phi(q,Q)), \tag{19}$$

where $K'_2 = 1/(2\pi^2)$. Introducing the same O-Z closure that we used in the case of the spherical cut-off and with the same change of variables we obtain the universal evolution equation for the critical region:

$$\frac{\partial H_t(z)}{\partial t} = dH_t(z) + \frac{2-d}{2}zH'_t(z) + \frac{1}{2}\left[\sqrt{H''_t(z)+1} - \sqrt{H''_t(0)+1}\right]. \tag{20}$$

It can be shown that this equation leads to the same critical behavior of Eq. (8) to first order in $\epsilon = 4 - d$.

To derive the evolution equation for the surface terms, we assume that $\Delta\mathscr{F}_2^Q$ has the following structure:

$$\Delta\mathscr{F}_2^Q(q_1, q_2, k) = g(q_1)g(q_2)F_s^Q(k), \tag{21}$$

where $g(z) = \rho'(z)$ and we have taken the wall perpendicular to z axis. This form has been extensively adopted in studies of interfacial phenomena [16,17]. With this assumption it is possible to obtain an explicit evolution equation for the surface free energy, which in three dimensions, reads:

$$\frac{\partial}{\partial Q}\left(\frac{\beta\Delta\mathscr{A}^Q}{S}\right) = \frac{K'_2}{2}Q\log\left(1 + F_s^Q(Q)\alpha^Q(Q)\right) \tag{22}$$

where α^Q is:

$$\alpha^Q(k) = \int\frac{dq}{(2\pi)}g(q)\frac{\phi(k,q)}{1+\phi(k,q)\mathscr{F}_{2b}^Q(k,q)}g(-q). \tag{23}$$

We see that the evolution equations for bulk and surface free energy are coupled through this term. It is important to note that Eq. (22) is built starting from an expansion of the free energy at constant density profile *i.e.* every Q-systems has the same $\rho(\mathbf{r})$. In the case of wetting or drying we want to study how the density profile is changed introducing fluctuations with fixed external potential. In order to allow the change in $\rho(\mathbf{r})$ when fluctuations are introduced, it is convenient to perform a Legendre transform an the total free energy $\mathscr{A}^Q$. In this way, it is possible to obtain the evolution equations at fixed activity, *i.e.* keeping fixed the quantity $\gamma(z) = \beta[\mu - W(z)]$, where $W(z)$ is the microscopic interaction between the wall and the molecules of the fluid. We first define the (modified) grand free energy by

$$-\beta\omega^Q = -\beta\mathscr{A}^Q + \int d^3\mathbf{r}\,\rho^Q(z)\gamma(z). \tag{24}$$

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:

$$\rho^Q(z) = -\frac{\delta\beta\omega^Q}{\delta\gamma(z)}. \tag{25}$$

For $Q \to \infty \mathscr{A}^Q$ reduces to the mean field free energy and $\rho^Q(z)$ approaches the density profile in mean field approximation. From the properties of the Legendre transform we obtain:

$$\left(\frac{\partial - \beta\omega^Q}{\partial Q}\right)_\gamma = \left(\frac{\partial - \beta\mathscr{A}^Q}{\partial Q}\right)_\rho \tag{26}$$

so the evolution equation for the grand potential free energy formally coincides with that of the Helmholtz free energy. Therefore, the surface free energy (or surface tension $\sigma^Q = \Delta\omega^Q/S$) obeys the evolution equation:

$$\frac{\partial(\beta\sigma^Q)}{\partial Q} = \frac{1}{2}K_2 Q\log\left(1 + F_s^Q(Q)\alpha^Q(Q)\right). \tag{27}$$

In order to relate this microscopic theory to the usual effective Hamiltonian approach based on Eq. (3) we make an assumption on the form of the density profile $\rho^Q(z)$. We assume that the system presents a *rigid* interface at a certain distance l from the wall and that fluctuations only change the value of l without modifying the structure of the interface, *i.e.* $\Delta\rho^Q(z) = \Delta\rho f(z - l^Q)$. We also assume the following O-Z form for the surface correlation function $F_s^Q(\kappa)$:

$$F_s^Q(k) = \left(-\frac{\partial^2\beta\sigma^Q}{\partial(\beta\mu)^2} + bk^2\right)^{-1}, \tag{28}$$

where b is a non-universal constant that is finite also near the critical point and we have used the exact sum rule:

$$\frac{\partial^2(-\beta\sigma^Q)}{\partial(\beta\mu)^2} = F_s^Q(k = 0). \tag{29}$$

The assumption we made on the density profile and on the correlation function is similar to the one underling the RG group approach of [5–7] based on the effective interfacial potential.

Away from the bulk critical point the asymptotic, *i.e.* $Q \to 0$, form of the evolution equation for the surface tension becomes:

$$\frac{\partial(-\beta\sigma^Q)}{\partial Q} = \frac{K_2}{2} Q \log\left(\left(\frac{\partial^2(-\beta\sigma^Q)}{\partial(\beta\mu)^2}\right)^{-1} + bQ^2\right) \quad (30)$$

which does not depend on the specific form of the density profile. The asymptotic evolution equation (30) is in fact equivalent to the known RG theory. We first introduce $a^Q(\Gamma)$, where Γ is the absorption [18], as the Legendre transform of the surface tension:

$$a^Q(\Gamma) = \sigma^Q(\mu^Q) + \mu^Q\Gamma \quad (31)$$

and μ^Q is such that

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

Using the evolution equation of σ^Q and the properties of the Legendre transform we calculate the asymptotic evolution equation of $a^Q(\Gamma)$:

$$\frac{\partial(-\beta a^Q)}{\partial Q} = \frac{K_2}{2} Q \log\left(-\frac{\partial^2(-\beta a^Q)}{\partial \Gamma^2} + bQ^2\right). \quad (33)$$

Making the following change of variables:

$$t = -\log(Q), \quad (34)$$

$$l = \Gamma\left(\frac{b}{K_2}\right)^{1/2}, \quad (35)$$

$$V_t(l) = \beta a^Q(\Gamma)\frac{e^{-2t}}{K_2} \quad (36)$$

we obtain the same equation of the RG approach:

$$\frac{\partial V_t(l)}{\partial t} = 2V_t(l) + \frac{1}{2}\log[V_t''(l) + 1], \quad (37)$$

where $V_t(l)$ is the effective interfacial potential in the RG approach. Therefore, we may identify the renormalized effective interaction $V(l)$ 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 given by the value of $a^Q(\Gamma)$ at a suitable matching cut-off $Q = Q_0 \ll 1$. The appropriate value should contain 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.

CONCLUSION

In the homogeneous case, we have seen how the HRT theory can be used to obtain an effective Hamiltonian for the long-wavelength fluctuations of the order parameter from the microscopic interaction potential. We have used a O-Z closure for the two-body correlation function, which provides accurate results for lattice systems. In the continuous case, a more careful treatment of odd operators is required.

In the inhomogeneous case, we have shown that under a few assumptions on the form of the density profile and correlation functions the HRT formalism reproduces, in the asymptotic regime, the RG approach to wetting of Refs. [5–7]. Furthermore, HRT provides a microscopic interpretation of the effective Hamiltonian at the basis of the RG formalism. It will be possible, upon implementing a numerical solution for the non-asymptotic equation of surface tension, to also study non-critical region. It is important to note that HRT can be used, in principle, to also study wetting transition near the bulk critical point where it is questionable whether a description of wetting by means of an effective interfacial Hamiltonian remains valid, due to the interplay of bulk and surface fluctuations.

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