2 | The Behaviour of Interfaces in Ordered and Disordered Systems

G. Forgacs

Department of Physics, Clarkson University, Potsdam, NY 13676, USA

R. Lipowsky

Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, Postfach 1913, D 5170 Jülich 1, Germany

Th. M. Nieuwenhuizen

Van der Waals-Zeeman Laboratorium, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands

Appendix. Functional renormalization of interface potentials

In this appendix, we will briefly describe functional renormalization methods as applied to interface potentials. First, we perform the partial trace in the partition function over the small–scale fluctuations. One then has to consider a certain expectation value which can be evaluated (i) within a perturbative cumulant expansion, or (ii) by an approximate but non–perturbative approach, originally developed by Wilson in the context of bulk critical phenomena. This approach has been previously reviewed by Lipowsky (1988c, 1990b).

Lipowsky, R. (1988c). *Random Fluctuations and Growth* (ed. H.E. Standley and N. Ostrowsky). Kluwer, Dordrecht.

Lipowsky, R. (1990b). *Fundamental Problems in Statistical Mechanics VII* (ed. H. van Beijeren). North Holland, Amsterdam.

1 Integration over small-scale fluctuations

As discussed in Section 3, the interfacial configurations can be described, on large scales, by a single-valued displacement field, $z = z(x)$. In thermal equilibrium, the statistical weight of the configuration z is given by the Boltzmann factor, $\exp(-\mathcal{H}\{z\})$. For convenience, we absorb the factor $1/T$ into the definition of the effective Hamiltonian $\mathcal{H}$ which has the general form

$$\mathcal{H}\{z\} = \mathcal{H}_0\{z\} + \mathcal{H}_1\{z\} \tag{A.1}$$

with the "free" part

$$\mathcal{H}_0\{z\} \equiv \int_p \tfrac{1}{2}(K/T)p^{2-\eta}|\tilde{z}(p)|^2 \tag{A.2}$$

and the "perturbative" part

$$\mathcal{H}_1\{z\} = \int_x V[z(x)]/T. \tag{A.3}$$

This Hamiltonian implicitly contains a small-scale cutoff, a.

The model defined by (A.1)–(A.3) will now be studied by functional renormalization group (RG) methods. Such a RG method consists of three basic steps. First, the fluctuating field, $z(x)$, is divided up into two parts:

$$z(x) = z_<(x) + z_>(x), \tag{A.4}$$

where $z_<$ represents the small-wavenumber or large-scale fluctuations with $0 < |p| < 1/ab$ and $z_>$ contains the large-wavenumber or small-scale fluctuations with $1/ab < |p| < 1/a$. This division is chosen in such a way that the free part of the Hamiltonian, which is quadratic in z, also separates into two parts:

$$\mathcal{H}_0\{z\} = \mathcal{H}_0\{z_<\} + \mathcal{H}_0\{z_>\}. \tag{A.5}$$

In the second step of the RG, the small-scale fluctuations, $z_>$, are integrated out which gives rise to an effective Hamiltonian, $\mathcal{H}'\{z_<\}$, for the large-scale fluctuations alone:

$$\exp[-\mathcal{H}'\{z_<\}] = \frac{1}{N}\int \mathcal{D}\{z_>\}\exp[-\mathcal{H}\{z_< + z_>\}]. \tag{A.6}$$

where N is a normalization factor. It follows from (A.1) and (A.5) that

$$\mathcal{H}\{z_< + z_>\} = \mathcal{H}_0\{z_<\} + \mathcal{H}_0\{z_>\} + \mathcal{H}_1\{z_< + z_>\}. \tag{A.7}$$

When this expression is inserted into (A.6), one obtains

$$\exp[-\mathscr{H}'\{z_<\}] = \exp[-\mathscr{H}_0\{z_<\}]\langle\exp[-\mathscr{H}_1\{z_< + z_>\}]\rangle.$$
(A.8)

Here and below, the expectation value, $\langle\ldots\rangle$, represents a functional integral over the small-scale fluctuations with the harmonic weight, $\exp[-\mathscr{H}_0\{z_>\}]$.

Let us assume, for a moment, that we had performed this functional integral and thus had explicitly evaluated the expectation value $\langle\exp[-\mathscr{H}_1\{z_< + z_>\}]\rangle$. In order to iterate the RG transformation, we would like to write the new Hamiltonian $\mathscr{H}'\{z_<\}$ as

$$\mathscr{H}'\{z_<\} = \mathscr{H}_0'\{z_<\} + \mathscr{H}_1'\{z_<\},$$
(A.9)

with

$$\mathscr{H}_0'\{z_<\} = \int_p \tfrac{1}{2}(K'/T)p^{2-\eta}|\tilde{z}_<(p)|^2$$
(A.10)

and

$$\mathscr{H}_1'\{z_<\} = \int_x V'[z_<(x)]/T.$$
(A.11)

i.e. we would like to parametrize the new Hamiltonian $\mathscr{H}'\{z_<\}$ in the same way as the original Hamiltonian, $\mathscr{H}\{z\}$ (see (A.1)–(A.3)). *A priori*, it is not clear that such a parametrization of $\mathscr{H}'\{z_<\}$ is indeed possible. In fact, the new Hamiltonian $\mathscr{H}'\{z_<\}$ as obtained from (A.8) will, *in general*, not have the form given by (A.9)–(A.11): the integration over the small-scale fluctuations typically generates new terms in $\mathscr{H}'\{z_<\}$ which have not been present in the original Hamiltonian $\mathscr{H}\{z\}$. However, one can often argue that these new terms are *irrelevant* as far as the critical behaviour is concerned. One may then employ additional approximation schemes in order to ensure that the form of the Hamiltonian is not changed under the RG. Two such schemes will be described further below.

In the final step of the RG, the spatial coordinate, x, and the fluctuating field, z, are rescaled according to

$$x \to x' \equiv x/b \quad \text{and} \quad z_> \to z(x') \equiv z_<(x = bx')/b^\zeta$$
(A.12)

where $b > 1$ is an arbitrary rescaling factor. This transformation changes the small-scale cutoff from its new value, ba, back to its original value, a.

If the new Hamiltonian can be brought into the form as given by (A.9)–(A.11), one may obtain the renormalized interface potential, $V^{(1)}(z)$, from

$$\int_{x'} V^{(1)}[z(x')] \equiv \int_x V'[z_<(x)] = \int_{x'} b^{d-1}V'(b^\zeta z(x'))$$

which implies

$$V^{(1)}[z(x')] = b^{d-1} V'[b^\zeta z(x')].$$ (A.13)

2 Cumulant expansion and linear renormalization of interface potential

What remains to be done is to actually calculate the expectation value $\langle \exp[-\mathcal{H}_1\{z_< + z_>\}]\rangle$ in the expression (A.8) which defines the new Hamiltonian $\mathcal{H}'$. In this subsection, we will *assume* that the interface potential, V, and thus the perturbation $\mathcal{H}_1$ as given by (A.3) are *small* in some sense. One may then perform an expansion in powers of V or $\mathcal{H}_1$. This leads to the cumulant expansion of $\langle \exp[-\mathcal{H}_1]\rangle$ as given by

$$\langle \exp[-\mathcal{H}_1]\rangle = \exp\left[\sum \frac{1}{n!}\langle(-\mathcal{H}_1)^n\rangle_c\right] \approx \exp[-\langle\mathcal{H}_1\rangle + \tfrac{1}{2}\langle\mathcal{H}_1\mathcal{H}_1\rangle_c]$$

(A.14)

where the subscript c stands for cumulant (i.e. $\langle\mathcal{H}_1\mathcal{H}_1\rangle_c \equiv \langle\mathcal{H}_1\mathcal{H}_1\rangle - \langle\mathcal{H}_1\rangle^2$, etc.). It then follows from (A.8) that the new Hamiltonian has the form

$$\mathcal{H}'\{z_<\} \approx \mathcal{H}_0\{z_<\} + \langle\mathcal{H}_1\{z_< + z_>\}\rangle$$ (A.15)

up to *first order* in $\mathcal{H}_1$. Obviously, this expression has the desired form (A.9)–(A.11) with the new free part

$$\mathcal{H}_0'\{z_<\} = \mathcal{H}_0\{z_<\} = \int_p \tfrac{1}{2}(K/T)p^{2-\eta}|\tilde{z}_<(p)|^2$$ (A.16)

and the new perturbative part

$$\mathcal{H}_1'\{z_<\} = \langle\mathcal{H}_1\{z_< + z_>\}\rangle.$$ (A.17)

If one inserts (A.3) and (A.11) into the latter expression, one immediately finds the new potential:

$$V'(z_<) = \langle V(z_< + z_>)\rangle = \left\langle \exp\left[z_>\frac{\partial}{\partial z_<}\right]\right\rangle V(z_<).$$ (A.18)

The last expectation value is easily calculated since $z_>$ has a Gaussian distribution. One then obtains

$$V'(z_<) = \exp[\tfrac{1}{2}\langle z_>^2\rangle \partial^2/\partial z_<^2] V(z_<).$$ (A.19)

For a "hard" spherical cutoff, the roughness $\langle z_>^2\rangle$ of the small-scale fluctuations is given by the momentum shell integral

$$\langle z_>^2\rangle = \frac{T}{K}\int_{1/ba}^{1/a} \mathrm{d}^{d-1}p/(2\pi)^{d-1}p^{2-\eta} \equiv \tilde{a}_\perp^2.$$ (A.20a)

The length scale $\tilde{a}_\perp$ depends on the rescaling factor b. It is convenient to introduce another b-independent scale, $a_\perp$, defined by

$$a_\perp^2 \equiv \tilde{a}_\perp^2 \, 2\zeta/(b^{2\zeta} - 1) = c_{\mathrm{d}}(T/K)a^{2\zeta} \qquad \text{(A.20b)}$$

with the dimensionless coefficient $c_{\mathrm{d}} \equiv 2/(4\pi)^{d-1}\Gamma[(d-1)/2]$. One then has $\tilde{a}_\perp^2 \approx a_\perp^2 \, \Delta s$ in the limit of small $\Delta s \equiv b - 1$, which will be discussed at the end of this appendix.

It now follows from the rescaling transformation (A.13) that the interface potential, $V^{(0)}(z) \equiv V(z)$, is renormalized according to

$$V^{(0)}(z) \to V^{(1)}(z) = \mathscr{L}[V^{(0)}(z)] \qquad \text{(A.21)}$$

with

$$\mathscr{L}[V(z)] \equiv b^{d-1}\exp[\tfrac{1}{2}\tilde{a}_\perp^2 \, \partial^2/\partial y^2]V(y)|_{y=b^\zeta z}. \qquad \text{(A.22)}$$

This differential operator can be expressed in terms of the integral

$$\mathscr{L}[V(z)] = b^{d-1}\int_{-\infty}^{\infty}\frac{\mathrm{d}z'}{\sqrt{2\pi}\,\tilde{a}_\perp}\exp\left[-\tfrac{1}{2}(b^\zeta z - z')^2/\tilde{a}_\perp^2\right]V(z')$$

$$= b^{d-1}\int_{-\infty}^{\infty}\frac{\mathrm{d}z'}{\sqrt{2\pi}\,\tilde{a}_\perp}\exp\left[-\tfrac{1}{2}(z'/\tilde{a}_\perp)^2\right]V(b^\zeta z - z'). \quad \text{(A.23)}$$

The latter form for the linear RG is intuitively appealing since it represents an averaging or coarse graining of the potential $V(z')$ over the scale $\tilde{a}_\perp$, i.e. over the roughness of the small-scale fluctuations.

3   Nonlinear renormalization of interface potential

We will now describe a nonperturbative RG method which has been developed by Wilson (1971) in the context of bulk critical phenomena. More recently, this approach has been extended to interfacial phenomena by Lipowsky and Fisher (1986b, 1987). In this approach, the expectation value $\langle \exp[-\mathscr{H}_1\{z_< + z_>\}]\rangle$ is directly calculated with the help of several approximations.

By definition, the expectation value $\langle \exp[-\mathscr{H}_1\{z_< + z_>\}]\rangle$ represents a functional integral over the small-scale fluctuations as given by

$$\langle \exp[-\mathscr{H}_1\{z_< + z_>\}]\rangle = \int \mathscr{D}\{z_>\}\exp[-\mathscr{H}_0\{z_>\} - \mathscr{H}_1\{z_< + z_>\}].$$

$$\text{(A.24)}$$

Now, these small-scale fluctuations, $z_>(x)$, are expanded in a complete set of suitably chosen eigenfunctions or wave packets $W_i(x)$ (Wilson, 1971):

$$z_>(x) = \sum_i z_>^i \sqrt{\Omega} W_i(x). \qquad (A.25)$$

The prefactor $\sqrt{\Omega}$ is included for convenience: it ensures that the components $z_>^i$ have the same dimension as $z_>$, as will become clear further below.

These wave packets are taken to be localized both in momentum and in real space. They are localized in momentum space in the sense that their Fourier modes are restricted to the momentum shell $1/ba < |\mathbf{p}| < 1/a$. Furthermore, the wave packet W_i is also assumed to be localized within a real space cell labelled by i. The volume of this cell cannot be made arbitrarily small, however, because of the assumed localization in momentum space. Indeed, the smallest value of this volume, which will be denoted by Ω, satisfies the "uncertainty relation"

$$\Omega \times \int_{1/ba}^{1/a} d^{d-1}p = (2\pi)^{d-1}. \qquad (A.26)$$

If the expansion as given by (A.25) is used in (A.24), the functional integral becomes a multidimensional integral over the components $z_>^i$:

$$\int \mathscr{D}\{z_>\} \ldots = \int \prod_i dz_>^i \ldots \qquad (A.27)$$

where constant normalization factors have been ignored. In addition, one obtains

$$\mathscr{H}_0\{z_>\} = \sum_i \sum_j \tfrac{1}{2} z_>^i K_{ij} z_>^j \qquad (A.28)$$

with

$$K_{ij} \equiv (K\Omega/T) \int_p p^{2-\eta} \tilde{W}_i(p) \tilde{W}_j(-p). \qquad (A.29)$$

and

$$\mathscr{H}_1\{z_< + z_>\} = \sum_i \int_{x_i} V\left[z_<(x) + \sum_j z_>^j \sqrt{\Omega} W_j(x) \right] \Big/ T \qquad (A.30)$$

where the x_i-integration in the last expression extends over the real space cell i.

Now, some bold approximations will be used in order to simplify the form of the effective Hamiltonian as given by (A.28)–(A.30). First of all, off-diagonal elements of K_{ij} are ignored and K_{ij} is approximated by

$$K_{ij} \simeq \delta_{ij}/l_\perp^2 \qquad (A.31)$$

where δ_{ij} is the usual Kronecker symbol and $l_\perp$ represents a length scale to be specified below. For $\eta = 0$, this truncation corresponds to the assumption that wave packets belonging to different real space cells have essentially no overlap. The same assumption also leads to the estimate

$$\mathcal{H}_1\{z_< + z_>\} \simeq \sum_i \int_{x_i} V[z_< + z^i_> \sqrt{\Omega} W_i]/T \qquad \text{(A.32)}$$

since the only contribution from the j-summation in (A.30) then comes from the term with $j = i$.

In addition, the large-scale fluctuations, $z_<$, are taken to be essentially constant within each real space cell. The value of $z_<$ within cell i will be denoted by $z^i_<$. This implies that the wave packet $W_i(x)$ must be orthogonal to a constant. The latter requirement can be satisified by the simple ansatz $W_i(x) \simeq 1/\sqrt{\Omega}$ for half of the real space cell, and $W_i(x) \simeq -1/\sqrt{\Omega}$ for the other half of this cell. If the latter form is inserted into (A.32), one obtains

$$\mathcal{H}_1\{z_< + z_>\} \simeq \sum_i G'(z^i_<, z^i_>) \qquad \text{(A.33)}$$

with

$$G'(x, y) \equiv \tfrac{1}{2}[V(x + y) + V(x - y)]/\tilde{v}. \qquad \text{(A.34)}$$

The potential scale $\tilde{v}$ is defined by

$$\tilde{v} \equiv T/\Omega \qquad \text{(A.35a)}$$

where Ω is given by (A.26) and thus depends explicitly on the rescaling factor b. It is again convenient to define a b-independent scale by

$$v \equiv \tilde{v}(d - 1)/(1 - b^{(1-d)}) = c_d T/a^{d-1} \qquad \text{(A.35b)}$$

where $c_d = 2/(4\pi)^{d-1} \Gamma[(d - 1)/2]$ as in (A.20b). One then has $\tilde{v} \approx v \Delta s$ in the infinitesimal rescaling limit with small $\Delta s = b - 1$.

If the approximations for $\mathcal{H}_0\{z_>\}$ and $\mathcal{H}_1\{z_< + z_>\}$ as given by (A.28), (A.31) and (A.33) are inserted into (A.24), one obtains

$$\langle \exp[-\mathcal{H}_1\{z_< + z_>\}] \rangle \simeq \prod_i \int dz^i_> \exp[-\tfrac{1}{2}(z^i_>/l_\perp)^2 - G'(z^i_<, z^i_>)].$$
$$\text{(A.36)}$$

In this way, the functional integral over the small-scale fluctuations has been reduced to a product of one-dimensional integrals over the components $z^i_>$.

The approximation as in (A.36) will now be used in (A.8) in order to define the new Hamiltonian $\mathcal{H}'\{z_<\}$. Inspection of the resulting expression

reveals that the new Hamiltonian can again be written as $\mathcal{H}'\{z_<\} = \mathcal{H}_0'\{z_<\} + \mathcal{H}_1'\{z_<\}$ such that the free part of the Hamiltonian is not renormalized, i.e. $\mathcal{H}_0'\{z_<\} = \mathcal{H}_0\{z_<\}$, while the other part, $\mathcal{H}_1'\{z_<\}$, is obtained from

$$\exp[\mathcal{H}_1'\{z_<\}] = \langle \exp[-\mathcal{H}_1\{z_< + z_>\}] \rangle. \qquad (A.37)$$

The assumption that the large-scale fluctuations, $z_<$, are essentially constant with $z_< \simeq z^i_<$ in real space cell i then implies that

$$\mathcal{H}_1'\{z_<\} = \int_x V'[z_<(x)]/T \simeq \sum_i V'(z_{<i})/\tilde{v} \qquad (A.38)$$

with $\tilde{v} = T/\Omega$ as in (A.35a). Finally, it follows from (A.35)–(A.38) together with the rescaling transformation (A.13), that the initial potential $V^{(0)}(z) \equiv V(z)$ is renormalized according to

$$V^{(1)}(z) = \mathcal{R}[V^{(0)}(z)] \qquad (A.39)$$

with

$$\mathcal{R}[V(z)] \equiv -\tilde{v}b^{d-1} \ln\left\{ \int_{-\infty}^{\infty} \frac{dz'}{\sqrt{2\pi l_\perp}} \exp[-\tfrac{1}{2}(z'/l_\perp)^2 - G(z, z')] \right\}, \qquad (A.40)$$

where the potential enters through

$$G(z, z') \equiv [V(b^\zeta z - z') + V(b^\zeta z + z')]/2\tilde{v}. \qquad (A.41)$$

So far, the length scale $l_\perp$ has not been specified. Its value can be uniquely determined, however, if one requires that the nonlinear recursion relation as given by (A.39)–(A.41) embodies the linear RG as in (A.23) (Lipowsky and Fisher, 1986a, 1987). Indeed, if one compares the linearized recursion as obtained from (A.40) with (A.23), one finds

$$l_\perp = \tilde{a}_\perp = [\langle z_>^2 \rangle]^{1/2} \qquad (A.42)$$

where the latter length scale is given by (A.20).

In the infinitesimal rescaling limit, $b \approx 1 + \Delta s$ with small Δs, the nonlinear recursion relation (A.39)–(A.42) leads to a relatively simple flow equation. If one takes the b dependence of the scale factors $\tilde{v}(b)$ and $\tilde{a}_\perp(b)$ into account, a straightforward calculation leads to the nonlinear flow equation (3.147) where the potential scale v and the length scale $a_\perp$ are defined by (A.35) and (A.20), respectively.