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Functional renormalization description of the roughening transition

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Abstract. We reconsider the problem of the static thermal roughening of an elastic manifold at the critical dimension $d = 2$ in a periodic potential, using a perturbative Functional Renormalization Group approach. Our aim is to describe the effective potential seen by the manifold below the roughening temperature on large length scales. We obtain analytically a flow equation for the potential and surface tension of the manifold, valid for low temperatures. On a length scale L, the renormalized potential is made up of a succession of quasi parabolic wells, matching onto one another in a singular region of width $\sim L^{-6/5}$ for large L. For strong periodic potential, the perturbation theory breaks down, and we argue, based on a variational calculation, that the transition becomes first order. We also obtain numerically the step energy as a function of temperature, and relate our results to the existing experimental data on ^{4}He. Finally, we examine the case of a non local elasticity which is realized physically for the contact line.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 64.60.-i General studies of phase transitions – 68.35.-p Solid surfaces and solid-solid interfaces

1 Introduction

The roughening transition has been studied in great detail, both theoretically and experimentally [1,2]. Direct analogies with the (two dimensional) XY-model or the Coulomb gas furthermore make this problem particularly enticing [3]. More recently, the role of disorder on the roughening transition or on the properties of the XY model, has attracted considerable interest [4–8]. In particular, replica calculations and Functional Renormalization Group (FRG) methods have been applied to this problem, with sometimes conflicting results [9]. In this paper, we wish to reconsider the problem of the roughening transition in the absence of disorder, from a FRG point of view, where the flow is not *a priori* projected onto the first harmonic of the periodic potential. Within a renormalization scheme where only local and second order derivative terms are considered, we establish equations for the evolution of the full periodic potential $V(\varphi)$, and the surface tension γ with the length scale $L = \mathrm{e}^{\ell}$, which we analyze both numerically and analytically, in the low temperature phase. If we start with a sinusoidal periodic potential, the shape of the fixed point potential $V^*(\varphi)$ evolves to a nearly parabolic shape with matching points becoming more and more singular as the length scale increases. The nature of the singularity is investigated in detail close to the fixed point, that is for small values of the rescaled temperature $\overline{T} = \frac{T}{2\pi\gamma\lambda^2}$ where λ is the periodicity of the potential and γ the elastic stiffness. We find that the width $\Delta\varphi$ of the singular region scales as $L^{-3g(\overline{T})/5}$, where $g(\overline{T})$ governs the scaling of the surface stiffness with the length scale according to $\gamma(L) \sim L^{g(\overline{T})}$. The exponent $g(\overline{T})$ tends towards 2 with negative corrections which we calculate, when $\overline{T}$ goes to 0 (*i.e.* for $L \to \infty$).

The paper is organized as follows. In Section 2, we introduce the model: we outline the calculations involved and discuss the differences with the approach of Nozières and Gallet (NG). We then explain in Section 3, by a mean field argument the origin of the singularity that develops during the renormalization flow. In Section 4, we present a scaling form for the singularity of the renormalized potential, valid close to its maxima and for small renormalized temperatures. Using our renormalization group flow, we compute in Section 5 the step energy as a function of temperature. Finally, in Section 6, we look at the case of a contact line in a periodic potential, as a physical realization of a non local elastic stiffness. The various technical points concerning our renormalization scheme and the corresponding calculations are relegated in Appendix A, while we discuss in Appendix B the first order nature of the roughening transition for large values of the bare pinning potential, where the perturbative FRG breaks down.

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2 Model and functional renormalization group

We consider an elastic interface whose height fluctuations are described by a profile $\Phi(x)$, where x is a d-dimensional vector, in the presence of a deterministic periodic potential V. Supposing that the slope of the interface is everywhere small, the energy of the system is:

$$H[\Phi] = \frac{\gamma}{2}\int \mathrm{d}^d x\ (\nabla\Phi(x))^2 + \int \mathrm{d}^d x\ V\left(\frac{\Phi(x)}{\lambda}\right) \qquad (1)$$

where γ is the elastic stiffness and λ the periodicity of the potential. In the absence of periodic potential, the height fluctuations of the surface on a length scale L scale as L^{2-d}. For $d > 2$, the interface is therefore always flat. For the critical dimension $d = 2$, the interface is rough only if the temperature exceeds a certain critical temperature T_R. When the potential V is harmonic, this model is the continuous version of the Sine-Gordon model. NG have studied the statics of this problem using a two-parameter renormalization group scheme, and have written flow equations for $\gamma(L)$ and the amplitude $v_\mathrm{o}(L)$ of the periodic potential. They suppose that during the flow, v_o remains small compared to the *temperature* and neglect all higher harmonics of the potential. Correspondingly, within this procedure, the renormalization scheme ceases to be valid when v_o becomes of the order of the temperature. In the low temperature "flat" phase, this occurs after a finite renormalization since v_o grows with distance. The procedure used in [1] to obtain various physical quantities is then to "interrupt" the renormalisation at a scale L such that $v_\mathrm{o}(L) \sim T$.

In our calculation, we consider a general periodic function with the only constraint that it should be sufficiently smooth (we shall explain this more quantitatively in the following). Since we re-sum the whole perturbation expansion in v_o/T, there is however no constraint on the amplitude of the potential, and the renormalization procedure can in principle be carried on any length scale without interruption. The relevant coupling constant then appears to be v_o/γ rather than v_o/T. During the renormalization flow, we keep track of the whole function $V(\varphi)$ instead of projecting onto the first harmonic, so that we have a more quantitative knowledge of the behaviour of the potential for low temperatures.

Technically, we proceed by considering the partition function:

$$Z = \int \mathrm{d}\Phi(x)\ \mathrm{e}^{-\beta H[\Phi(x)]}. \qquad (2)$$

We perform the renormalization procedure by splitting the field Φ into a slowly-varying and a rapidly-varying part as:

$$\Phi(x) = \Phi^<(x) + \Phi^>(x). \qquad (3)$$

The Fourier modes k of $\Phi^<$ are such that $0 \le |k| \le |\Lambda|/s$, and those of $\Phi^>$, such that $|\Lambda|/s \le |k| \le |\Lambda|$, where $s = \mathrm{e}^{d\ell}$, $|\Lambda|$ being a high momentum cut-off, of the order of $1/a$, where a is the lattice spacing. We integrate over the fast modes in the partition function and retain only the terms that renormalize the gradient term and the potential term. The other terms that are generated are discarded. We give more details on our specific renormalisation scheme in Appendix A, where we establish a set of flow equations for $d = 2$, for the rescaled dimensionless potential $\overline{V} = \frac{V}{\gamma\lambda^2|\Lambda|^2}$ and the dimensionless temperature $\overline{T} = \frac{T}{2\pi\gamma\lambda^2}$. The flow equation for the local potential can be established non ambiguously and reads:

$$\frac{\mathrm{d}\overline{V}}{\mathrm{d}\ell} = (2-g)\overline{V} - \pi\frac{\overline{V}'^2}{(1+\overline{V}'')} + \frac{\overline{T}}{2}\ln(1+\overline{V}''), \qquad (4)$$

where g comes from the renormalization of the surface tension (or the temperature), through $\frac{\mathrm{d}\gamma}{\mathrm{d}\ell} = g\gamma$. The calculation of g is not obvious, and different procedures have been proposed in the literature [1,10], in particular to deal with infrared divergences which appear in the calculation. The particular scheme we use is detailed in Appendix A and compared to the scheme used by NG. While we do not claim that the scheme adopted here is exact, most of the results presented in this paper do not depend crucially on the exact form for g. On the other hand, the numerical values of the bare parameters needed to fit, say, experiments on ^{4}He surfaces do depend on the particular renormalization scheme. Within the scheme used here we find that g is given, in the small $\overline{T}$ limit, by:

$$g = -4\pi\int_0^1 \mathrm{d}\varphi\ \frac{\overline{V}^2(\varphi)\overline{V}'^2(\varphi)}{\left(1+\overline{V}''(\varphi)\right)^5} + \frac{\overline{T}}{4}\int_0^1 \mathrm{d}\varphi\ \frac{\overline{V}^2(\varphi)}{\left(1+\overline{V}(\varphi)\right)^4}\cdot \qquad (5)$$

These equations call for some comments.

– The relevant perturbative parameter appears to be $\overline{V}$, rather than V/T. In the limit $\overline{V} \ll 1$, and in the case where the potential is purely harmonic (*i.e.* $V(\varphi) = v_\mathrm{o}\cos(2\pi\varphi)$), the RG equations read:

$$\frac{\mathrm{d}u_\mathrm{o}}{\mathrm{d}\ell} = \left(2 - \frac{\pi T}{\gamma\lambda^2}\right)u_\mathrm{o}$$
$$\frac{\mathrm{d}\gamma}{\mathrm{d}\ell} = 2\pi^4\left(\frac{2\pi T}{\gamma\lambda^2}\right)\frac{u_\mathrm{o}^2}{\gamma^2\lambda^4} \qquad (6)$$

where $u_\mathrm{o} = v_\mathrm{o}/|\Lambda|^2$. The first equation is trivial and identical to the one in NG, and immediately leads to the value of the roughening transition temperature: $T_\mathrm{R} = 2\gamma_\infty\lambda^2/\pi$, where γ_∞ is the renormalized value of γ. The second is close to, but different from the one obtained in the particular renormalization scheme used by NG: near the critical temperature T_R, the coefficient between parenthesis is equal to 4 in our case and to 0.4 according to NG. As mentioned above and discussed in Appendix A, this comes from the different

treatment of the gradient terms in both approaches, in particular how the infrared divergences which appear in the calculation are handled. The expression (5) is actually expected to be valid only for $\overline{T} \to 0$.

– The renormalization of the surface tension, as measured by g, is *positive* for small $\overline{V}$ and, as shown in Section 4, must tend towards $g = 2$ for $\overline{T} \to 0$. One can check that, as has been pointed out by NG, if the initial potential is parabolic (*i.e.* $V(\phi) = v_0\phi^2$), then the coefficient g vanishes identically, and there is no renormalization of the surface tension. This is indeed expected since in this (quadratic) case, all modes are decoupled.
– The flow equations only make sense if $\overline{V}'' > -1$. We have checked numerically that if this condition is satisfied at the beginning, it prevails throughout the flow. On the other hand, if the initial potential is so steep that this condition is violated, the perturbative calculation is meaningless. This comes from the fact that metastable states, where the surface zig-zags between nearby minima of the potential, appear at the smallest length scales. In this respect, it is useful to note that the last term of the flow equation on $\overline{V}$ comes from the integration of the Gaussian fluctuations of the fast field around the slow field. The condition $\overline{V}'' > -1$ is a stability condition for these fast modes. If the unrenormalized potential is harmonic (*i.e.* $V(\varphi) = v_\mathrm{o}\cos(2\pi\varphi)$), and the unrenormalized surface tension given by γ_o, then this condition reads $\frac{v_\mathrm{o}}{\gamma}\left(\frac{2\pi}{\lambda|\Lambda|}\right)^2 < 1$, which simplifies to $\frac{v_\mathrm{o}}{\gamma} < 1$ in the case where $\lambda = a$. If the initial value of the potential is too large, one actually expects the transition to become first order. In our calculation, this is associated with an instability of the fast modes. A variational calculation presented in Appendix B indeed predicts the transition to become first order when $\frac{v_\mathrm{o}}{\gamma} \geq 1$ (but see the discussion in [12,1]).
– Wegner and Houghton have derived a formal equation for the renormalization of a Hamiltonian with a gradient square term and an arbitrary (not necessarily periodic) potential term $V(\phi)$ [11]. Our equation is nothing but a particular projection of Wegner and Houghton's general equation, retaining the local potential term and the gradient square term. As mentioned above, the treatment of the gradient square term is somewhat ambiguous. On the other hand, the extraction of the potential term is rather straightforward and we believe that equation (4) for $\overline{V}$ is exact. The important term in this equation is the second term, proportional to $\overline{V}'^2$, and independent of temperature. This term leads to the appearance of singularities in the flow equation: up to second order in $\overline{V}$, this equation is close to the Burgers' equation (see below) for which it is well known that shocks develop in time. The fact that this term survives even in the zero temperature limit is at first sight strange, since one could argue that for $T = 0^+$, there are no longer any thermal fluctuations, and thus no renormalization. This argument is not correct because we are computing a *partition function*, thereby implicitly assuming that the infinite time limit is taken *before* the zero temperature limit. Such a non trivial renormalization has also been found in the context of pinned manifolds [13,14], and can be understood very simply using a mean-field approximation, which we detail in the next section.

3 Mean field analysis and effective potential

In this section, we show on a simplified mean field version of the model how the new non linear term V'^2 (which survives in the $T = 0$ limit) arises in the flow equation of the potential. Using a discrete formulation of the problem and replacing the local elasticity modeled by the surface tension term by a coupling to all neighbours, we can rewrite the energy as:

$$H_\mathrm{mf}(\{\Phi\}_i, \overline{\Phi}) = \frac{\gamma}{2a}\sum_i^N (\Phi_i - \overline{\Phi})^2 + a\sum_i^N V(\Phi_i) \qquad (7)$$

where $\overline{\Phi}$ is the center of mass of the system, a the lattice spacing and $L = Na$. Implementing the constraint $\overline{\Phi} = 1/N\sum\Phi_i$ by means of a Lagrange multiplier in the partition function, we have:

$$Z[\overline{\Phi}] = \int \mathrm{d}\eta \int \prod_i \mathrm{d}\Phi_i \; \mathrm{e}^{-\beta H_\mathrm{mf}(\{\Phi\}_i,\overline{\Phi}) - \eta\left(N\overline{\Phi} - \sum_i \Phi_i\right)} \qquad (8)$$

which can also be expressed as:

$$Z[\overline{\Phi}] = \int \mathrm{d}\eta \; \mathrm{e}^{N\log z(\overline{\Phi} + \eta a/\beta\gamma) + N\frac{\eta^2 a}{2\beta\gamma}} \qquad (9)$$

where

$$z(\Psi) = \int \mathrm{d}\Phi \; \mathrm{e}^{-\frac{\beta\gamma}{2a}(\Psi-\Phi)^2 - \beta a V(\Phi)} = z\left(\overline{\Phi} + \frac{\eta a}{\beta\gamma}\right). \qquad (10)$$

We are left with a simpler problem since we now have a one-body problem. We introduce the auxiliary partition function $z_R(\Psi, \tau)$ defined as:

$$z_\mathrm{R}(\Psi, \tau) = \sqrt{\frac{\beta\gamma}{2\pi a\tau}} \int \mathrm{d}\Phi \; \mathrm{e}^{-\frac{\beta\gamma}{2a}\frac{(\Psi-\Phi)^2}{\tau} - \beta a V(\Phi)}. \qquad (11)$$

Up to a multiplicative constant, one has $z(\Psi) = z_\mathrm{R}(\Psi, \tau = 1)$, where $z_\mathrm{R}(\Psi, \tau)$ verifies the diffusion equation:

$$\frac{\partial z_\mathrm{R}}{\partial \tau} = \frac{a}{2\beta\gamma}\frac{\partial^2 z_\mathrm{R}}{\partial \Psi^2} \qquad (12)$$

with an initial condition given by:

$$z_\mathrm{R}(\Psi, \tau = 0) = \mathrm{e}^{-\beta a V(\Psi)}. \qquad (13)$$

Defining now the effective pinning potential $V_{\rm R}$ as:

$$aV_{\rm R}(\Psi,\tau) = -T\log z_{\rm R}(\Psi,\tau) \tag{14}$$

we can then easily show that $V_{\rm R}$ is the Hopf-Cole solution of the non linear Burgers' equation [14]:

$$\frac{\partial V_{\rm R}}{\partial(\tau a)} = \frac{T}{2\gamma}\frac{\partial^2 V_{\rm R}}{\partial\Psi^2} - \frac{a}{2\gamma}\left(\frac{\partial V_{\rm R}}{\partial\Psi}\right)^2 \tag{15}$$

where the temperature independent non linear term $V_{\rm R}^2$ indeed appears. It is known from results on the Burgers' equation, that, with "time" τ, the effective potential $V_{\rm R}$ develops shocks, smoothed out at finite temperature, between which it has a parabolic shape. The appearance of singularities is due to the non linear term in the partial differential equation, *which indeed survives in the limit* $T = 0$.

It is interesting to see how this "toy" renormalization group captures some important features of the full scheme, such as the one shown above for a non disordered potential. These singularities (shocks) which appear can be interpreted as the sign that a finite external force must be applied to the pinned object to drive it at a small non zero velocity [15].

4 Analysis of the low temperature effective potential

4.1 Scaling ansatz for $\overline{V}(\phi)$

In this section, we go back to the model introduced in Section 2 and analyze the nature of $\overline{V}$ close to the low temperature fixed point, that is for small values of the rescaled temperature $\overline{T}$. Since $g > 0$ in the low temperature phase, this corresponds to the large scale structure of the renormalized potential for all temperatures $T < T_{\rm R}$.

Expanding $\overline{V}$ around one of its minima $\varphi = \varphi^*$ as $\overline{V}(\varphi) = \overline{V}_{\rm m} + \frac{1}{2}\kappa(\varphi-\varphi^*)^2$ where $\kappa > 0$, and replacing $\overline{V}$ in the flow equation (4), we have

$$\begin{aligned}\frac{{\rm d}\overline{V}_{\rm m}}{{\rm d}\ell} &= (2-g)\overline{V}_{\rm m} + \frac{\overline{T}}{2}\ln(1+\kappa)\\ \frac{{\rm d}\kappa}{{\rm d}\ell} &= (2-g)\kappa - 2\pi\frac{\kappa^2}{1+\kappa}\cdot\end{aligned} \tag{16}$$

One can actually check that a parabolic shape for $\overline{V}$ is exactly preserved by the renormalization flow. However, since the potential has to be periodic, these parabolas should match periodically around each maximum. The region of the maximum is therefore expected to be singular in the limit $\overline{T}$.

In order to investigate the nature of singularity of the renormalized periodic potential for small but non zero $\overline{T}$, we make a scaling ansatz on $\overline{V}''$ for small φ. As mentioned above, the value $\overline{V}''(0) = -1$ is special and corresponds to the appearance of small scale instabilities. Now since we expect a singularity to develop as $\overline{T}$ goes to 0, it is plausible (and indeed self-consistent) that $\overline{V}''(0)$ tends towards -1. As $\overline{T}$ goes to 0, we thus make the scaling ansatz:

$$\overline{V}''(\varphi) = -1 + \overline{T}^{\delta}\mathcal{F}'\left(\frac{\varphi}{\overline{T}^{\alpha}}\right) \tag{17}$$

where $\mathcal{F}'(0) > 0$. This means that the width of the singular region shrinks as $\Delta\varphi \sim \overline{T}^{\alpha}$, while the difference between the maximum value of $\overline{V}''$ and -1 goes to zero as $\overline{T}^{\delta}$.

Integrating the previous equation in the scaling region leads to:

$$\overline{V}'(\varphi) = -\varphi + \overline{T}^{\delta+\alpha}\mathcal{F}\left(\frac{\varphi}{\overline{T}^{\alpha}}\right) \tag{18}$$

with $\mathcal{F}(0) = 0$ to ensure that $\varphi = 0$ is a maximum of $\overline{V}$. Integrating once more the above equation, one finds:

$$\overline{V}(\varphi) = \overline{V}_{\rm M} - \frac{\varphi^2}{2} + \overline{T}^{\delta+2\alpha}\mathcal{G}\left(\frac{\varphi}{\overline{T}^{\alpha}}\right) \tag{19}$$

with $\mathcal{G}' = \mathcal{F}$. Replacing this last equation in the flow equation for $\overline{V}$, we obtain:

$$\frac{{\rm d}\overline{V}_{\rm M}}{{\rm d}\ell} = (2-g)\overline{V}_{\rm M} + \frac{\delta\overline{T}}{2}\log\overline{T}. \tag{20}$$

4.2 g tends towards 2 for small $\overline{T}$

Suppose that equations (16) have a fixed point as $\overline{T}$ goes to zero, and that close to the fixed point all the terms have the same order of magnitude. This leads to the relation $\kappa \propto 1/\ell$. Supposing moreover that the parabolic solution extends almost over a whole period and that the correction brought about by the rounding off of the singularity around the maxima of the potential is small, we also have

$$(\overline{V}_{\rm M} - \overline{V}_{\rm m}) \propto \frac{\kappa}{2}\cdot \tag{21}$$

Now, subtracting equation (20) from equation (16), we find in the limit $\overline{T} \to 0$:

$$\frac{\rm d}{{\rm d}\ell}(\overline{V}_{\rm M} - \overline{V}_{\rm m}) = (2-g)(\overline{V}_{\rm M} - \overline{V}_{\rm m}) + \frac{\delta}{2}\overline{T}\log\overline{T} \tag{22}$$

which is consistent with $(\overline{V}_{\rm M} - \overline{V}_{\rm m})$ and

$$(2-g) \simeq \frac{1}{\ell} \simeq \frac{1}{\log\overline{T}}\cdot \tag{23}$$

The result that $g \to 2$ is independent of the way we calculate g, the correction to the surface tension, and compatible with our numerical integration of the flow equations. In particular, it shows that at zero temperature, the renormalized potential diverges as $(L/a)^2$, where L is the size of the system.

4.3 Shape of the matching region

We can deduce an equation satisfied by $\mathcal{F}'$, by using the above ansatz in the following flow equation for $\overline{V}'$:

$$\frac{\mathrm{d}\overline{V}'}{\mathrm{d}\ell} = (2-g-2\pi)\overline{V}' + 2\pi\frac{\overline{V}'}{1+\overline{V}'} + \pi\overline{V}'^2\frac{\overline{V}'''}{(1+\overline{V}'')^2} + \frac{\overline{T}}{2}\frac{\overline{V}'''}{1+\overline{V}''}\,. \tag{24}$$

Close to the fixed point, we again suppose that to leading order in $\overline{T}$, $\frac{\mathrm{d}\overline{V}'}{\mathrm{d}\ell}=0$ in the above equation. Plugging in the ansatz for $\overline{V}'$ and $\overline{V}''$, and considering the leading term in $\overline{T}$, we get to lowest order in $\overline{T}$:

$$-\frac{2\pi u}{\mathcal{F}'(u)}\,\overline{T}^{\alpha-\delta} + \frac{\pi u^2\mathcal{F}''(u)}{\mathcal{F}'^2(u)}\,\overline{T}^{\alpha-\delta} + \frac{\mathcal{F}''(u)}{2\mathcal{F}'(u)}\,\overline{T}^{1-\alpha} = 0. \tag{25}$$

We can show that necessarily $\alpha-\delta = 1-\alpha$. Indeed, if $1-\alpha<\alpha-\delta$, $\mathcal{F}''$ would be equal to zero while if $1-\alpha>\alpha-\delta$, $\mathcal{F}'(0)$ would be equal to zero, both alternatives being thus impossible. Hence, equation (25) can be rewritten as

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}u}\log\mathcal{F}' - \pi\frac{\mathrm{d}}{\mathrm{d}u}\left(\frac{u^2}{\mathcal{F}'}\right) = 0 \tag{26}$$

which yields after integration:

$$\mathcal{F}'(u)\log\left(\frac{\mathcal{F}'(u)}{\mathcal{F}'(0)}\right) = 2\pi u^2. \tag{27}$$

This equation fully determines the shape of the renormalized potential in the matching region, by integrating twice $\mathcal{F}'(u)$.
At this stage, we can note that the exponent relation

$$2\alpha-\delta = 1 \tag{28}$$

is again independent of the scheme used to calculate of g (see Appendix A).

In the rest of this section, we calculate the exponents α and γ. Using the fact that $g(\overline{T}\to 0)=2$, we also obtain the numerical value of $\mathcal{F}'(0)$. These results now somewhat depend on the precise renormalization scheme we use to calculate the correction g to the surface tension (see Appendix A).

Replacing the derivatives of $\overline{V}$ by their expressions in terms of $\mathcal{F}'$ and $\mathcal{F}''$, in equation (5), and changing variables from φ to $u=\frac{\varphi}{\overline{T}^{\alpha}}$, we get to lowest order in $\overline{T}$:

$$g(\overline{T}) \simeq -\overline{T}^{\alpha-3\delta}\,8\pi\int_0^\infty \mathrm{d}u\; u^2\frac{\mathcal{F}''^2(u)}{\mathcal{F}'^5(u)} + \overline{T}^{1-\alpha-2\delta}\,\frac{1}{2}\int_0^\infty \mathrm{d}u\;\frac{\mathcal{F}''^2(u)}{\mathcal{F}'^4(u)}\,. \tag{29}$$

From the exponent relation $2\alpha-\delta=1$ derived previously, and the fact that $g(\overline{T}\to 0)$ is finite, we have another exponent relation $\alpha=3\delta$, which turns out to be identical to $1-\alpha-2\delta=0$. Therefore, both terms in g contribute equally in the limit $\overline{T}\to 0$. From the above exponent relations, we obtain $\alpha=3/5$ and $\delta=1/5$. The width of the singular region thus decreases as $\overline{T}^{3/5}\propto L^{6/5}$ for $L\to\infty$.

Defining a new variable x as

$$x = \frac{\mathrm{e}\mathcal{F}'(u)}{\mathcal{F}'(0)}, \tag{30}$$

we can furthermore express $g(\overline{T}\to 0)$ as:

$$g(0) = \frac{2}{\pi^2}\left(\frac{2\pi\mathrm{e}}{\mathcal{F}'(0)}\right)^{5/2}\left\{-\int_{\mathrm{e}}^\infty \mathrm{d}x\;\frac{(x\log(x/\mathrm{e}))^{3/2}}{x^5\log(x)} + \int_{\mathrm{e}}^\infty \mathrm{d}x\;\frac{(x\log(x/\mathrm{e}))^{1/2}}{x^4\log(x)}\right\}. \tag{31}$$

Hence, using the fact that $g(\overline{T}\to 0)=2$, we finally find the constant $\mathcal{F}'(0)\simeq 0.904$.

5 Step energy as a function of temperature

From physical considerations we know that below the roughening temperature, the interface grows by forming terraces. An important quantity governing the kinetics of growth is therefore the step energy. The width ξ of a step and its energy per unit length β_S can be obtained by comparing the elastic energy and the potential energy of a profile $\Phi(x)$ which changes by one period over the length ξ. Requiring that these two energies are of the same order of magnitude leads to: $\gamma/\xi^2 \sim v_\mathrm{o}$ where v_o is the amplitude of the periodic potential, or $\xi\sim\sqrt{\gamma/v_\mathrm{o}}$, and a step energy which scales as $\beta_S\propto\sqrt{v_\mathrm{o}\gamma}$.

Since a step profile include Fourier modes such that $\xi^{-1}<k<|\Lambda|$, it is natural to use in the above equations the values of γ and v_o calculated for the length $L=a\mathrm{e}^\ell=\xi$. Since $\xi(L)\sim L/\sqrt{\overline{v}_\mathrm{o}(L)}$, one sees that this corresponds to stopping the renormalization procedure when $\overline{v}_\mathrm{o}(L)\sim 1$, and not when $v_\mathrm{o}(L)\sim T$, as assumed in [1].

We have integrated numerically the RG flow, starting from $\gamma=1$ and from harmonic potentials of various amplitudes $v_\mathrm{o}\ll 1$, and stopping for an arbitrary value $\overline{v}$, chosen here to be $\overline{v}_\mathrm{c}=0.4$[1]. The resulting step energy as a function of temperature is plotted in Figure 1. For T close to T_R, one finds that ξ diverges as $\mathrm{e}^{1/\sqrt{T_\mathrm{R}-T}}$, as it should since our RG flow essentially boils down to the standard one, up to a numerical prefactor [1]. For small temperatures, however, we find that β_S tends to a finite value with a linear slope in temperature. This slope is seen to decrease as the initial amplitude of the potential $\overline{v}_\mathrm{o}$ increases. For $\overline{v}_\mathrm{o}=0.01$, β_S decreases by $\sim 30\%$ when T increases from 0 to 0.25 T_R. This decrease falls to $\sim 10\%$

[1] Other values of $\overline{v}_\mathrm{c}$ would not change the qualitative features reported below, provided $\overline{v}_\mathrm{c}$ is not too large.

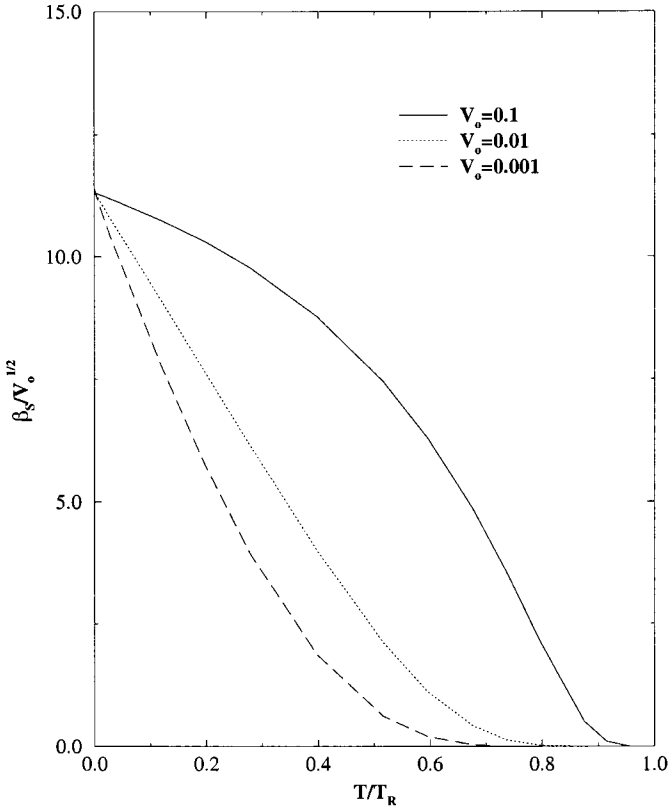

Fig. 1. $\beta_S/\sqrt{\overline{v}_\mathrm{o}}$ as a function of the rescaled temperature for three different values of the bare periodic potential $\overline{v}_\mathrm{o}$, with $\gamma_\mathrm{o} = 1$.

for $\overline{v}_\mathrm{o} = 0.1$. Again, the above results are only weakly affected by the renormalisation scheme chosen for the surface tension. This comes from the fact that for $v_\mathrm{o} \ll 1$, g remains quite small until the last steps of the renormalisation procedure.

Experiments on ^{4}He, on the other hand, have established that the step energy does only depend very weakly on temperature at small temperature, by not more than 5% when the temperatures varies from 0.05 T_R to 0.25 T_R [2]. This suggests that the initial amplitude of the potential is of the same order as γ_o: in this case, the width of the step is of order a, and the bare parameters are not renormalized except possibly very close to T_R. The conclusion that experiments must be in the regime $\overline{v}_\mathrm{o} \sim 1$ is somewhat in contradiction with the estimate $\overline{v}_\mathrm{o} \sim 0.05$ obtained in [2], although the difference might be due to rather large numerical factors. Another possibility is that the low temperature measurements of the step energy are affected by residual impurities [16].

6 Case of the contact line

In this section, we repeat the previous analysis for the case of a contact line on a periodic substrate [17,18]. The roughness of a contact line on a disordered substrate, at zero temperature, has been studied analytically and compared with the experimental predictions for the case of super-fluid helium on a disordered cesium substrate, where the disorder arises from randomly distributed wettable heterogeneities which are oxidized areas of the substrate [19,20]. A physical realization of the theoretical situation we consider here could be achieved by preparing a substrate with equally spaced oxidized lines which would act as periodic pinning grooves. In this case the critical dimension is $d = 1$. We denote by Φ the position of the line with respect to a mean position. The energy of the system is the sum of an elastic term and a potential term given by:

$$H[\Phi] = \frac{\gamma}{2} \int \frac{\mathrm{d}k}{2\pi} |k| |\Phi(k)|^2 + \int_0^L \mathrm{d}x \; V(\Phi(x)) \qquad (32)$$

where L is the length of the substrate and γ the stiffness.

The renormalization procedure is carried as before except that the propagator is now given by $G(k) = \frac{1}{\beta\gamma|k|}$. Moreover the renormalization of the stiffness now only comes from the scale change leading to the much simpler flow equation for γ:

$$\frac{\mathrm{d}\gamma}{\mathrm{d}\ell} = \gamma. \qquad (33)$$

Defining as before the rescaled parameters $\overline{V}$ and $\overline{T}$ with $\overline{V} = \frac{V}{\gamma\lambda^2|\Lambda|}$ and $\overline{T} = \frac{2T}{\gamma\lambda^2}$, the flow equations for $\overline{V}$ and $\overline{T}$ read:

$$\frac{\mathrm{d}\overline{V}}{\mathrm{d}\ell} = \overline{V} - \frac{\overline{V}'^2}{1+\overline{V}''} + \frac{\overline{T}}{2}\log(1+\overline{V}'') \qquad (34)$$

and

$$\frac{\mathrm{d}\overline{T}}{\mathrm{d}\ell} = -\overline{T}. \qquad (35)$$

During the flow, $\overline{T}$ flows to zero and the renormalized rescaled potential $\overline{V}$ develops shocks between which it has a parabolic shape. We characterize the singularities that develop around the maxima of $\overline{V}$ by the following scaling ansatz:

$$1 + \overline{V}''(\varphi) = T^\delta \mathrm{e}^{-\frac{A}{T}} \mathcal{F}'\left(\frac{\varphi}{T^\alpha \mathrm{e}^{-\frac{B}{T}}}\right) \qquad (36)$$

where $\mathcal{F}'(0) > 0$ and $\mathcal{F}(0) = 0$. Putting $u = \frac{\varphi}{\overline{T}^\alpha \mathrm{e}^{-\frac{B}{T}}}$, this implies that for $u \sim 1$,

$$\overline{V}'(u) = -\overline{T}^\alpha \mathrm{e}^{-\frac{B}{T}} u + \overline{T}^{\delta+\alpha} \mathrm{e}^{-\frac{A+B}{T}} \mathcal{F}(u) \qquad (37)$$

and

$$\overline{V}(u) = \overline{V}_\mathrm{M} - \overline{T}^{2\alpha} \mathrm{e}^{-\frac{2B}{T}} \frac{u^2}{2} + \overline{T}^{\delta+2\alpha} \mathrm{e}^{-\frac{A+2B}{T}} \mathcal{G}(u) \qquad (38)$$

with $\mathcal{G}' = \mathcal{F}$. Inserting the previous expressions into the flow equation $\overline{V}'$:

$$\frac{\mathrm{d}\overline{V}'}{\mathrm{d}\ell} = -\overline{V}' + 2\overline{V}'\frac{\overline{V}''}{1+\overline{V}'} + \overline{V}'^2 \frac{\overline{V}'''}{(1+\overline{V}'')^2} + \frac{\overline{T}}{2}\frac{\overline{V}'''}{1+\overline{V}''} \qquad (39)$$

and supposing that $\frac{\mathrm{d}\overline{V}'}{\mathrm{d}\ell} = 0$, to leading order as $\overline{T}$ goes to zero, we have to leading order in $\overline{T}$:

$$-\frac{2u}{\mathcal{F}'(u)}\,\overline{T}^{\alpha-\delta}\mathrm{e}^{\frac{A-B}{\overline{T}}} + \frac{u^2\mathcal{F}''(u)}{\mathcal{F}'^2(u)}\overline{T}^{\alpha-\delta}\mathrm{e}^{\frac{A-B}{\overline{T}}} + \frac{\mathcal{F}''(u)}{2\mathcal{F}'(u)}\,\overline{T}^{1-\alpha}\mathrm{e}^{\frac{B}{\overline{T}}} = 0. \quad (40)$$

Since $\mathcal{F}'(0) > 0$, we obtain a non trivial solution only if

$$2\alpha - \delta = 1 \quad \text{and} \quad A - B = B \quad (41)$$

and $\mathcal{F}'$ is again solution of equation (27). We can obtain the values of the parameters A and B by considering separately the singular part and the regular part of the renormalized rescaled potential $\overline{V}$ close to the fixed point. We expand $\overline{V}$ around one of its minima φ^* as:

$$\overline{V}(\varphi) = \overline{V}_{\mathrm{m}} + \frac{\kappa}{2}(\varphi - \varphi^*)^2 \quad (42)$$

and plug the resulting expression in the flow equation for $\overline{V}$. This yields:

$$\frac{\mathrm{d}V_{\mathrm{m}}}{\mathrm{d}\ell} = V_{\mathrm{m}} + \frac{\overline{T}}{2}\log(1+\kappa)$$
$$\frac{\mathrm{d}\kappa}{\mathrm{d}\ell} = \kappa - \frac{2\kappa^2}{1+\kappa}\,. \quad (43)$$

We note that the fixed point value for κ is now finite as $\overline{T}$ goes to zero and is given by $\kappa^* = 1$. Similarly the flow equation for $\overline{V}(0) = \overline{V}_{\mathrm{M}}$ is:

$$\frac{\mathrm{d}\overline{V}_{\mathrm{M}}}{\mathrm{d}\ell} = \overline{V}_{\mathrm{M}} + \frac{\overline{T}}{2}\log\left(T^{\delta}\,\mathrm{e}^{-\frac{A}{\overline{T}}}\mathcal{F}'(0)\right). \quad (44)$$

Combining equations (43) and (44), the flow equation for the amplitude of $\overline{V}$ is given to leading order as $\overline{T} \to 0$ by:

$$\frac{\mathrm{d}}{\mathrm{d}\ell}(\overline{V}_{\mathrm{M}} - \overline{V}_{\mathrm{m}}) = (\overline{V}_{\mathrm{M}} - \overline{V}_{\mathrm{m}}) - \frac{A}{2}\,. \quad (45)$$

Now, we expect that the singularity brings but a small correction to the parabolic part of the rescaled potential $\overline{V}$, so that at the fixed point the amplitude of $\overline{V}$ is given by $\frac{\kappa^*}{2}$, leading to $A = 1$. The value of the exponents α and δ would require the analysis of sub dominant terms. The conclusion of this section is that in the case of the contact line, the width of the singular region of the renormalized potential decreases exponentially with length scale: the potential quickly becomes a succession of matched parabolas.

7 Conclusion

In this paper, we studied the problem of the thermal roughening transition using a FRG formalism. We have shown that below the roughening temperature, the periodic potential on large length scales cannot be described by its lowest harmonic, but rather evolves towards a "scalloped" shape with singularities (shocks) generated by the non-linear renormalization flow. We expect that this result is more generally valid, and also holds in the case of a disordered pinning potential [13,14]. By performing a resummation of our perturbation expansion, our results are in principle valid in the strong coupling regime, where the coupling constant is proportional to V/γ (rather than V/T). Correspondingly, when calculating physical quantities, we claim that the renormalization procedure should be interrupted not when $V(L) \sim T$ (as advocated in NG), but rather when L reaches the size of the objects under investigation (for example the width of the steps). By comparing the numerical integration of the FRG flow with the experimental determination of the low-temperature step energy of liquid ^{4}He, and in particular its temperature dependence, we have concluded that the surface of ^{4}He crystals are such that the bare coupling to the lattice is of the same order of magnitude as the bare surface tension.

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Appendix A: Derivation of the flow equations

In this Appendix, we sketch the procedure to obtain the flow equations (4). We consider the partition function

$$Z = \int \mathrm{d}[\Phi]\ \mathrm{e}^{-\beta\mathcal{H}(\Phi(x))} \quad (46)$$

where $\mathcal{H}$ is the Hamiltonian given by (1). We split the field Φ into a fast moving and a slow moving component and average over the fast moving part. We can rewrite the partition function, up to a multiplicative constant, as:

$$Z = \int \mathrm{d}[\Phi^<]\ \mathrm{e}^{-\beta\int_< \frac{\mathrm{d}^d k}{(2\pi)^d}|k|^2|\Phi^<(k)|^2} \times \left\langle \mathrm{e}^{-\beta\int \mathrm{d}^d x\ V(\frac{\Phi(x)}{\lambda})}\right\rangle_{\mathrm{o}} \quad (47)$$

where $\langle ...\rangle_{\mathrm{o}}$ represents the thermal average with respect to the Gaussian weight:

$$\mathrm{e}^{-\beta\int_> \frac{\mathrm{d}^d k}{(2\pi)^d}|k|^2|\Phi^>(k)|^2}. \quad (48)$$

In the rest of this section we denote $\frac{\mathrm{d}^d k}{(2\pi)^d}$ by $\tilde{\mathrm{d}}k$.

Renormalization of the periodic potential V

We look for contributions to the potential V resulting from the above averaging, which are of the same form as the terms present in the Hamiltonian before starting the renormalization procedure and which are of order $\mathrm{d}\ell$.

These terms are represented by connected graphs and are all obtained by expanding the potential term with respect to $\Phi^>$ up to second order. There are only two ways of obtaining such graphs of order $\mathrm{d}\ell$:

- By contracting p two-legged terms $-\frac{\beta}{2}\int \mathrm{d}^d x\ (\frac{\Phi^>(x)}{\lambda})^2 V''(\frac{\Phi^<(x)}{\lambda})$ with $1 \leq p \leq \infty$. We must calculate:

$$\frac{1}{p!}\left(-\frac{\beta}{2\lambda^2}\right)^p \int \prod_{j=1}^{p} \mathrm{d}^d x_j\ V''\left(\frac{\Phi^<(x_j)}{\lambda}\right) \times \int \prod_{j=1}^{p} \tilde{\mathrm{d}}k_j \tilde{\mathrm{d}}k'_j \mathrm{e}^{\mathrm{i}(k_1+k'_1)x_1 \ldots \mathrm{i}(k_p+k'_p)x_p} \times \left\langle \Phi^>(k_1)...\Phi^>(k'_p)\right\rangle_{\mathrm{o}} \quad (49)$$

which gives after averaging over the fast modes:

$$\frac{(-1)^p}{2p}\left(\frac{1}{\gamma\lambda^2}\right)^p \int \prod_{j=1}^{p} \mathrm{d}^d x_j V''\left(\frac{\Phi^<(x_j)}{\lambda}\right) \times \int \prod_{j=1}^{p} \tilde{\mathrm{d}}k_j \frac{\mathrm{e}^{\mathrm{i}k_1(x_1-x_2)+\ldots \mathrm{i}k_p(x_p-x_1)}}{|k_1|^2...|k_p|^2}\cdot \quad (50)$$

In the above expression, the space dependence of V'' is slowly varying, and since the integral is dominated by the region where the x_j's are close to one another, we can with little error, treat these terms as approximately equal to $V''\left(\frac{\Phi^<(x_1)}{\lambda}\right)$. After integrating over the rest of the x_j's and summing up over p, we are left with:

$$-\beta \mathrm{d}\ell\ \frac{K_d|\Lambda|^d T}{2}\int \mathrm{d}^d x\ \log\left(1+\frac{V''}{\gamma\lambda^2|\Lambda|^2}\right). \quad (51)$$

- By contracting 2 one-legged terms $-\beta\int \mathrm{d}^d x\ (\frac{\Phi^>(x)}{\lambda})V'(\frac{\Phi^<(x)}{\lambda})$ with p two-legged terms $-\frac{\beta}{2}\int \mathrm{d}^d x\ \left(\frac{\Phi^>(x)}{\lambda}\right)^2 V''\left(\frac{\Phi^<(x)}{\lambda}\right)$ with $0 \leq p \leq \infty$. To illustrate our method, we begin with $p=0$. Expressing the fast modes in Fourier space, we have in discrete space:

$$\frac{1}{2!}\beta^2\left(\frac{1}{\lambda^2}\right)\left(\frac{a}{L}\right)^{2d}\sum_x\sum_y V'\left(\frac{\Phi^<(x)}{\lambda}\right) V'\left(\frac{\Phi^<(y)}{\lambda}\right)\sum_k\sum_{k'}\mathrm{e}^{\mathrm{i}kx+\mathrm{i}k'y}\left\langle \Phi^>(k)\Phi^>(k')\right\rangle_{\mathrm{o}} \quad (52)$$

which gives after averaging over the fast modes:

$$\frac{\beta}{2}\left(\frac{1}{\gamma\lambda^2}\right)a^{2d}\sum_x\sum_y V'\left(\frac{\Phi^<(x)}{\lambda}\right) \times V'\left(\frac{\Phi^<(y)}{\lambda}\right)\frac{1}{L}\sum_k \frac{\mathrm{e}^{\mathrm{i}k(x-y)}}{|k|^2}\cdot \quad (53)$$

In the above expression, the main contribution comes from the part $x=y$, while the part with $x\neq y$ averages to zero for slowly varying $\Phi^<$. Using the fact that $|\Lambda| = \frac{2\pi}{a}$, the result is:

$$\beta \mathrm{d}\ell \frac{K_d(2\pi)^d}{2}\int \mathrm{d}^d x\ \frac{\overline{V}'^2(\Phi^<(x)/\lambda)}{\gamma\lambda^2|\Lambda|^2}\cdot \quad (54)$$

Proceeding in a similar way for $1\leq p\leq\infty$, we have

$$\beta^2\left(\frac{-\beta}{2}\right)^p\frac{1}{(p+1)!}\frac{(p+1)(p+2)}{2}\left(\frac{1}{\lambda^2}\right)^{p+1}\left(\frac{a}{L}\right)^{(p+2)d} \times \sum_{x,y,x_1\ldots x_p} V'\left(\frac{\Phi^<(x)}{\lambda}\right)V'\left(\frac{\Phi^<(y)}{\lambda}\right) \times V''\left(\frac{\Phi^<(x_1)}{\lambda}\right)...V''\left(\frac{\Phi^<(x_p)}{\lambda}\right) \times \sum_{k,k',k_1\ldots k'_p} \mathrm{e}^{\mathrm{i}kx+\mathrm{i}k'y+\mathrm{i}(k_1+k'_1)x_1+\ldots+\mathrm{i}(k_p+k'_p)x_p} \times \left\langle \Phi^>(k)\Phi^>(k')\Phi^>(k_1)...\Phi^>(k'_p)\right\rangle_{\mathrm{o}} \quad (55)$$

which yields after retaining the $x=y$ part and averaging over the fast modes:

$$\frac{\beta}{2}(-1)^p a^d\left(\frac{1}{\lambda^2}\right)^{p+1}\int\prod_{j=1}^{p}\mathrm{d}^d x_j \mathrm{d}^d x V'^2(\Phi^<(x)) \times \prod_{j=1}^{p} V''(\Phi^<(x_j))\int\prod_{j=1}^{p}\tilde{d}k_j\tilde{d}k \times \frac{\mathrm{e}^{\mathrm{i}k(x-x_1)+\mathrm{i}k_1(x_1-x_2)\ldots+\mathrm{i}k_p(x_p-x)}}{|k|^2|k_1|^2...|k_p|^2}\cdot \quad (56)$$

Treating the above expression as equation (50) we are left with:

$$\beta \mathrm{d}\ell\ (-1)^p\frac{K_d(2\pi)^d}{2}\int \mathrm{d}^d x\ \left(\frac{V''(\Phi^<(x)/\lambda)}{\gamma\lambda^2|\Lambda|^2}\right)^p. \quad (57)$$

Summing up over p, we finally obtain:

$$\beta \mathrm{d}\ell\ \frac{K_d(2\pi)^d}{2}\int \mathrm{d}^d x\ \frac{V'^2(\Phi^<(x)/\lambda)}{\gamma\lambda^2|\Lambda|^2} \times\left(1+\frac{V''(\Phi^<(x)/\lambda)}{\gamma\lambda^2|\Lambda|^2}\right). \quad (58)$$

Taking into account the rescaling of the potential term, and supposing we are in the flat phase so that Φ and λ are not rescaled, we obtain for $d=2$:

$$\frac{\mathrm{d}V}{\mathrm{d}\ell} = 2V - \pi\ \frac{\left(\frac{V'^2}{\gamma\lambda^2|\Lambda|^2}\right)}{1+\left(\frac{V''}{\gamma\lambda^2|\Lambda|^2}\right)} + \frac{T}{4\pi\gamma}\log\left(1+\frac{V''}{\gamma\lambda^2|\Lambda|^2}\right). \quad (59)$$

This flow equation can be rewritten in terms of the rescaled parameters $\overline{V} = \frac{V}{\gamma\lambda^2|\Lambda|^2}$ and $\overline{T} = \frac{T}{2\pi\gamma\lambda^2}$. Putting $g = \frac{1}{\gamma}\frac{\mathrm{d}\gamma}{\mathrm{d}\ell}$, we have:

$$\frac{\mathrm{d}\overline{V}}{\mathrm{d}\ell} = (2-g)\overline{V} - \pi\frac{\overline{V}'^2}{(1+\overline{V}'')} + \frac{\overline{T}}{2}\log(1+\overline{V}''). \quad (60)$$

This result is nothing but a projection onto a purely local potential of the general renormalisation flow of Wegner and Houghton [11].

Renormalization of the surface tension γ

We establish in this section a particular renormalisation scheme for the elastic constant γ, valid in the limit when $\overline{T} \to 0$. The contributions to the gradient term are obtained from equations (50) and (56).

- Consider first the contribution due to equation (56). Here, $x = y$ plays a special role. It is thus natural to expand V'' around this particular point as:

$$V''\left(\frac{\Phi^>(x_j)}{\lambda}\right) = V''\left(\frac{\Phi^>(x)}{\lambda}\right) + \frac{1}{\lambda}(x_j - x)\nabla\Phi^>(x)V'''\left(\frac{\Phi^>(x)}{\lambda}\right). \quad (61)$$

The contribution of equation (56) to the gradient term is given by:

$$\begin{aligned}&\frac{\beta\gamma}{2}a^d(-1)^p\left(\frac{1}{\gamma\lambda^2}\right)^{p+2}\sum_{n<m}\int\prod_{j=1}^{p}\mathrm{d}^d\tilde{x}_j\mathrm{d}^d x\\ &\times(\tilde{x}_n\nabla\Phi(x))(\tilde{x}_m\nabla\Phi(x))V'^2\left(\frac{\Phi^<(x)}{\lambda}\right)\\ &\times V''^{p-2}\left(\frac{\Phi^<(x)}{\lambda}\right)V'''^2\left(\frac{\Phi^<(x)}{\lambda}\right)\\ &\times\int\prod_{j=1}^{p}\tilde{d}k_j\tilde{d}k\ \frac{\mathrm{e}^{\mathrm{i}k\tilde{x}_1+\mathrm{i}k_1(\tilde{x}_1-\tilde{x}_2)\ldots+\mathrm{i}k_p\tilde{x}_p}}{|k|^2|k_1|^2\ldots|k_p|^2}\cdot\end{aligned} \quad (62)$$

After integrating over $\tilde{x}_i$ for $i \neq m, n$, we are left with:

$$\begin{aligned}&\frac{\beta\gamma}{2}a^d(-1)^p\frac{1}{\gamma^{p+2}}\sum_{n<m}\int\mathrm{d}^d x\mathrm{d}^d\tilde{x}_m\mathrm{d}^d\tilde{x}_n\sum_{\nu=1}^{N}\tilde{x}_m^\nu\tilde{x}_n^\nu(\nabla\Phi(x))_\nu^2\\ &\times V'^2\left(\frac{\Phi^<(x)}{\lambda}\right)V''^{p-2}\left(\frac{\Phi^<(x)}{\lambda}\right)V'''^2\left(\frac{\Phi^<(x)}{\lambda}\right)\\ &\times\int\tilde{\mathrm{d}}k\tilde{\mathrm{d}}k'\tilde{\mathrm{d}}k''\ \frac{\mathrm{e}^{-\mathrm{i}k\tilde{x}_n+\mathrm{i}k''\tilde{x}_m+\mathrm{i}k'(\tilde{x}_n-\tilde{x}_m)}}{(|k|^2)^n(|k'|^2)^{m-n}(|k''|^2)^{p+1-m}}\cdot\end{aligned} \quad (63)$$

Using the fact that $\mathrm{i}x^\nu\mathrm{e}^{\mathrm{i}kx} = \frac{\partial}{\partial k^\nu}\mathrm{e}^{\mathrm{i}kx}$, and an integration by parts, the above expression reads :

$$\begin{aligned}&\frac{\beta\gamma}{2}a^d\frac{(-1)^p}{\gamma^{p+2}}\sum_{n<m}\int\mathrm{d}^d x(\nabla\Phi^<(x))_\nu^2V'^2\\ &\times\left(\frac{\Phi^<(x)}{\lambda}\right)V'''^2\left(\frac{\Phi^<(x)}{\lambda}\right)V''^{p-2}\left(\frac{\Phi^<(x)}{\lambda}\right)\\ &\times\int\mathrm{d}^d\tilde{x}_n\mathrm{d}^d\tilde{x}_m\int\tilde{\mathrm{d}}k'\frac{\mathrm{e}^{\mathrm{i}k'(\tilde{x}_n-\tilde{x}_m)}}{(|k'|^2)^{m-n}}\\ &\times\left[\int_{B_\nu}\frac{1}{(|k|^2)^n}\mathrm{e}^{-\mathrm{i}k\tilde{x}_n}+2n\int\tilde{\mathrm{d}}k\frac{k^\nu}{(|k|^2)^{n+1}}\mathrm{e}^{-\mathrm{i}k\tilde{x}_n}\right]\\ &\times\left[\int_{B_\nu}\frac{1}{(|k|^2)^{p+1-m}}\mathrm{e}^{-\mathrm{i}k''\tilde{x}_m}+2(p+1-m)\right.\\ &\left.\times\int\tilde{\mathrm{d}}k''\frac{k^\nu}{(|k''|^2)^{p+2-m}}\mathrm{e}^{-\mathrm{i}k''\tilde{x}_m}\right].\end{aligned} \quad (64)$$

The integral $\int_{B_\nu}$ involves an integral over the boundary of k_ν with the constraint that the vector k is in the shell, and the usual "volume" integration over the k_μ's for $\mu \neq \nu$. In order to complete the calculation, we have to evaluate the three different terms which come from the expansion of the terms within brackets.
The contribution from the product of the two volume terms gives in terms of the rescaled variables, after integrating over $\tilde{x}_n$ and $\tilde{x}_m$ and summing up over p:

$$\frac{\beta\gamma}{2}\frac{4K_d(2\pi)^d}{d}\mathrm{d}\ell\frac{(-1)^p}{\gamma^{p+2}}\int(\nabla\Phi^<(x))_\nu^2\times\frac{\overline{V}'^2\left(\frac{\Phi^<(x)}{\lambda}\right)\overline{V}'''^2\left(\frac{\Phi^<(x)}{\lambda}\right)}{\left(1+\overline{V}''\left(\frac{\Phi^<(x)}{\lambda}\right)\right)^5}\cdot \quad (65)$$

Since we are looking for the contribution to the gradient term, only the projection of the periodic function $\frac{\overline{V}'^2\overline{V}'''^2}{(1+\overline{V}'')^5}$ on the zeroth harmonic counts. The contribution to the elastic constant, for $d = 2$ is thus:

$$-\gamma\mathrm{d}\ell\ \frac{4}{d}K_d(2\pi)^d\int_0^1\mathrm{d}\varphi\ \frac{\overline{V}'^2(\varphi)\overline{V}'''^2(\varphi)}{\left(1+\overline{V}''(\varphi)\right)^5}\cdot \quad (66)$$

The next term that one should consider is the product of a boundary term and a volume term. This term however does not contribute for symmetry reasons. Finally the last contribution is, after having integrated over $\tilde{x}_n$ and $\tilde{x}_m$:

$$(-1)^p\frac{\beta\gamma}{2}\int\mathrm{d}^x\ \frac{V'^2V'''^2V''^{p-2}}{\gamma^{p+2}}\times\int_{B_\nu(k)}\frac{1}{(|k|^2)^{p+1}}\int_{B_\nu(k'')}\delta^d(k-k''). \quad (67)$$

This last integral is in principle divergent, since it is proportional to $\delta(0)$. However, this infrared divergence

is removed if the points x_i's are constrained to lie in a region a size ξ, where ξ is the correlation length. This is, in essence, the regularisation proposed by NG – see below. Up to a numerical factor, this amounts to replacing $\delta(0)$ by ξ/a. One can then easily convince oneself that the integral term is proportional to $\frac{1}{(|\Lambda|^2)^{p+2}}$ multiplied by a constant linear in p. After summing over p, we thus have an overall contribution to γ due to this boundary term which has the same structure as before, but with a smaller power for the $(1+\overline{V}'')$ term in the denominator. Using the low temperature scaling of the singularity presented in Section 4, we can see that the boundary contribution is subleading when $\overline{T}$ goes to zero, where ξ/a remains finite. This term however becomes important for $T \to T_{\rm R}$, and a more careful analysis would be needed in this region.

- Consider now equation (50). In order to obtain a term of the form $(\nabla\Phi^{>}(x))^2$, we have to expand two V'' terms. We proceed as follows: if we choose to expand $V''(\Phi^{<}(x_n)/\lambda)$ and $V''(\Phi^{<}(x_m)/\lambda)$ with $m<n$, we perform the expansion with respect to $(x_m+x_n)/2$. The V'' terms thus give:

$$-\frac{1}{4}\left(\left(\frac{x_n-x_m}{\lambda}\right)\nabla\Phi^{<}\left(\frac{x_n+x_m}{2}\right)\right)^2 \times V'''^2\left(\Phi\left(\frac{x_n+x_m}{2\lambda}\right)\right)V''^{p-2}\left(\Phi\left(\frac{x_n+x_m}{2\lambda}\right)\right). \tag{68}$$

Integrating over x_j for $j\neq m,n$, we get:

$$-\frac{\beta\gamma}{2}\frac{(-1)^p}{p}\frac{T}{\gamma}\left(\frac{1}{\gamma\lambda^2}\right)^p \times\sum_{m<n}\int \mathrm{d}^d x_m \mathrm{d}^d x_n\left(\nabla\Phi^{<}\left(\frac{x_n+x_m}{2}\right)\right)_\nu^2 \times V'''^2\left(\Phi\left(\frac{x_n+x_m}{2}\right)\right)V''^{p-2}\left(\Phi\left(\frac{x_n+x_m}{2}\right)\right) \times\int \tilde{\mathrm{d}}k\tilde{\mathrm{d}}k'\ (x_m-x_n)_\nu^2\ \frac{\mathrm{e}^{\mathrm{i}(k-k')(x_m-x_n)}}{(|k|^2)^{p-n+m}(|k'|^2)^{n-m}}\,. \tag{69}$$

Writing $(x_m-x_n)_\nu^2\mathrm{e}^{\mathrm{i}(k-k')(x_m-x_n)}=\frac{\partial}{\partial k_\nu}\frac{\partial}{\partial k'_\nu}\mathrm{e}^{\mathrm{i}(k-k')(x_m-x_n)}$, and performing the rest of the calculation as described above, we find that the main contribution to the elastic term in terms of the rescaled parameters $\overline{V}$ and $\overline{T}$, in the limit $\overline{T}\to 0$, is given by

$$\gamma\mathrm{d}\ell\ \frac{\overline{T}}{2d}\int_0^1 \mathrm{d}\varphi\ \frac{\overline{V}'''^2(\varphi)}{\left(1+\overline{V}''(\varphi)\right)^4} \tag{70}$$

finally leading, for $d=2$, to the renormalization of γ given in the main text. As above, the boundary term gives rise to sub-leading corrections in the low temperature limit. Note that if we had chosen another expansion scheme to obtain the contribution to the gradient term, for instance if we had expanded the terms with respect to the centre of mass of $x_1, x_2, ..., x_p$, we would have obtained a somewhat different expression for g. This would only affect the precise value of the exponents α and δ obtained in the text, but not the qualitative features of the solution.

The NG scheme

Before ending this section, we briefly discuss the Nozières and Gallet's approach and show how it differs from ours. Following NG, we can express the Hamiltonian formally as:

$$H(\overline{\Phi},\delta\Phi)=\frac{\gamma}{2}\int\frac{\mathrm{d}^2k}{(2\pi)^2}\frac{|k|^2}{f(k/|\Lambda|)} \times\left[|\overline{\Phi}(k)|^2(1-\Psi(k))+|\delta\Phi(k)|^2\Psi(k)\right] +\int\mathrm{d}^2x\ V\left(\frac{2\pi}{\lambda}\left(\overline{\Phi}(x)+\delta\Phi(x)\right)\right) \tag{71}$$

where $\overline{\Phi}$ and $\delta\Phi$ are independent statistical variables verifying $\langle\overline{\Phi}_k^2\rangle=\frac{T}{\gamma|k|^2}(1-\Psi)f$ and $\langle\delta\Phi_k^2\rangle=\frac{T}{\gamma|k|^2}\Psi f$, and f the form factor, which depends on the cut-off procedure. Since V is periodic, it can be expressed in terms of its Fourier series, $V(u)=v\sum_{n=1}^{\infty}a_n\cos nu$. To lowest order in perturbation expansion, one has to calculate the 2nd cumulant, which is nothing but the connected part of $\frac{1}{2}\langle V^2\rangle$. Using a Taylor expansion of the cosine, and the fact that the correlator $\langle\delta\Phi(x)\delta\Phi(y)\rangle=\frac{T}{2\pi\gamma}\delta g(x-y)$, where $\delta g(u)=\frac{T}{\gamma}\int\frac{\mathrm{d}^2k}{(2\pi)^d}\frac{1}{|k|^2}\Psi(k)f(k)\ \mathrm{e}^{\mathrm{i}k(x-y)}$, the second cumulant reads:

$$\beta^2v^2\int\mathrm{d}^2x\mathrm{d}^2y\sum_{n,m=1}^{\infty}a_na_m\exp\left(-\frac{\pi T}{\gamma\lambda^2}\delta g(0)\right) \times\left\{\cos\frac{2\pi}{\lambda}(n\overline{\Phi}_x-m\overline{\Phi}_y)\left[\exp\left(-\frac{\pi T}{\gamma\lambda^2}2mn\ \delta g(x-y)\right)-1\right] +\cos\frac{2\pi}{\lambda}(n\overline{\Phi}_x+m\overline{\Phi}_y)\left[\exp\left(-\frac{\pi T}{\gamma\lambda^2}2mn\ \delta g(x-y)\right)+1\right]\right\}. \tag{72}$$

At this stage, if we consider only the lowest harmonics, we should discard the term $\cos\frac{2\pi}{\lambda}(n\overline{\Phi}_x+m\overline{\Phi}_y)$ and retain only the terms $n=m$ in the rest. This is the procedure followed by NG. They then average over the $\overline{\Phi}$ terms so that the final result is:

$$\beta^2v^2\int\ \mathrm{d}^2x\mathrm{d}^2y\sum_{n=1}^{\infty}a_n^2\mathrm{e}^{-\frac{\pi T}{\gamma\lambda^2}\delta g(0)} \times\left(\mathrm{e}^{\frac{\pi T}{\gamma\lambda^2}2n^2\delta g(x-y)}-1\right)\left\langle\cos\frac{2\pi n}{\lambda}(\overline{\Phi}(x)-\overline{\Phi}(y))\right\rangle. \tag{73}$$

Still following NG, we should consider $\overline{\Phi}$ as the sum of an equilibrium part $\overline{\Phi}_{\rm eq}$ and an imposed perturbation ζ. Within this scheme, the average in the previous

expression is:

$$\left\langle \cos\frac{2\pi n}{\lambda}(\overline{\Phi}(x)-\overline{\Phi}(y))\right\rangle_{\rm eq}\left[1-\frac{2\pi^2n^2}{\lambda^2}(\zeta(x)-\zeta(y))^2\right]. \tag{74}$$

The extra factor coming from the average over $\overline{\Phi}_{\rm eq}$ basically acts as a cut-off for distances $x-y$ greater than the correlation length ξ, and leads to a finite renormalisation of γ.

Now, another way of preceding is to keep all terms in expression (72), and expand the exponential in δg. To fix ideas, to first order in δg, the contribution coming from the terms within curly brackets is:

$$-2mn\frac{\pi T}{\gamma\lambda^2}\delta g(x-y)2\sin n\overline{\Phi}_x\sin m\overline{\Phi}_y. \tag{75}$$

The overall contribution due to this term is nothing but $\left(\int {\rm d}^dx V'\right)^2$, which appears in Wegner and Houghton's paper [11]. Within the projection scheme used in the present paper, this term therefore contributes to the renormalisation of the potential term, but not of the surface tension.

Appendix B: The strong coupling limit: A variational calculation

A very simple Gaussian variational calculation of the roughening transition has been proposed by Saito [12], (see also [5]). Here, we show that this method suggests that the roughening transition becomes first order in the strong coupling limit, where the perturbative FRG breaks down.

The variational Hamiltonian is taken to be:

$$\mathcal{H}_{\rm o}=\frac{1}{2}\int {\rm d}^2s\ {\rm d}^2s'\ (\Phi(s)-\Phi_{\rm o})g^{-1}(s-s')(\Phi(s')-\Phi_{\rm o}) \tag{76}$$

from which one can compute a variational free energy, which reads:

$$\frac{\mathcal{F}_{\rm var}}{L^2}=-\frac{1}{2\beta}\int\frac{{\rm d}^2k}{(2\pi)^2}\ \ln\left(\frac{2\pi g(k)}{\beta a^4}\right) + \frac{\gamma}{2\beta}\int\frac{{\rm d}^2k}{(2\pi)^2}\ |k|^2g(k)+v\cos(2\pi\Phi_{\rm o}/\lambda)\ {\rm e}^{-2\pi^2G/\lambda^2}. \tag{77}$$

Here, G is defined as:

$$G=\left\langle\Phi^2(x)\right\rangle_{\rm o}=\frac{1}{\beta}\int\frac{{\rm d}^2k}{(2\pi)^2}\ \tilde{g}(k). \tag{78}$$

The optimal set of parameters $\Phi_{\rm o}$ and $g(k)$ are determined from: $\partial\mathcal{F}_{\rm var}/\partial g(k)=0$ and $\partial\mathcal{F}_{\rm var}/\partial\Phi_{\rm o}=0$. The second equation leads to $\sin(2\pi\Phi_{\rm o}/\lambda)=0$; we choose $\Phi_{\rm o}$ such that the free-energy is minimum, that is, for example $\Phi_{\rm o}=\lambda/2$. From the second equation one finds:

$$\tilde{g}(k)=\frac{1}{\gamma|k|^2+v\left(\frac{2\pi}{\lambda}\right)^2\exp(-2\pi^2G/\lambda^2)}\cdot \tag{79}$$

The width of the interface G then satisfies the following self-consistent equation:

$$\frac{2\pi^2G}{\lambda^2}=\overline{T}\ \ln\left(\frac{\overline{v}+\exp(2\pi^2G/\lambda^2)}{\overline{v}+\left(\frac{a}{L}\right)^2\exp(2\pi^2G/\lambda^2)}\right) \tag{80}$$

where $\overline{v}=\frac{v}{\gamma}\left(\frac{a}{\lambda}\right)^2$ and $\overline{T}=\frac{\pi T}{2\gamma\lambda^2}$. This equation has different types of solutions, depending on the fact that G remains finite or diverges in the limit $L\to\infty$.

• G diverges with L

If G diverges when $L\to\infty$, then necessarily $\overline{v}\ll(a/L)^2\exp(2\pi^2G/\lambda^2)$. In this case, one then finds $G=(T/2\pi\gamma)\ln(L/a)$. Since $(a/L)^2\exp(2\pi^2G/\lambda^2)=(L/a)^{2(\overline{T}-1)}$, the starting hypothesis is only consistent in the high temperature phase $\overline{T}>1$. Hence, for $\overline{T}<1$, *i.e.* for T less than the roughening transition $T_{\rm R}=2\gamma\lambda^2/\pi$, the width of the interface G is finite (flat phase). The variational method thus leads to the exact perturbative transition temperature.

• G is finite

When G is finite, the equation (80) can be written, in the large L limit, in terms of $Q=\exp(2\pi^2G/\lambda^2)$:

$$\ln Q=\overline{T}\ln\left(1+\frac{Q}{\overline{v}}\right). \tag{81}$$

For $\overline{T}<1$, there always exists a solution for Q greater than 1, and therefore a finite G. For $\overline{T}=1$, a finite solution for G only exists if $\overline{v}>1$. In the case $\overline{T}>1$, one can notice that a solution to equation (81) corresponds to a zero of the function:

$$f(Q)=\ln Q-\overline{T}\ln\left(1+\frac{Q}{\overline{v}}\right). \tag{82}$$

This function is concave and has a maximum at $Q^*=\overline{v}/(\overline{T}-1)$. For $\overline{v}<\overline{T}-1$, there is therefore no solution. On the contrary, for $\overline{v}>\overline{T}-1$, f has two zeroes Q_1^* and Q_2^* such that $1<Q_1^*<Q^*<Q_2^*$. The true solution is the one which minimizes the free-energy. After a little algebra, one finds that for $\overline{T}>1$, G is infinite when $\overline{v}<\overline{v}_{\rm c}(\overline{T})$ and finite as soon as $\overline{v}\geq\overline{v}_{\rm c}(\overline{T})$, where $\overline{v}_{\rm c}(\overline{T})=\exp\overline{T}\ln\overline{T}-(\overline{T}-1)\ln(\overline{T}-1)$. The transition is therefore first order. Conversely, for fixed $\overline{v}>1$ the transition temperature depends continuously on $\overline{v}$ and is greater than $T_{\rm R}$, where as for $\overline{v}>1$, the transition always occurs at $T_{\rm R}$ and is second order. Note that $\overline{v}=1$ is precisely the point where perturbation theory breaks down, because of a short wavelength instability.

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