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Super-roughening: A new phase transition on the surfaces of crystals with quenched bulk disorder

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We present and study a model for surface fluctuations and equilibrium crystal shapes in solids with quenched bulk translational disorder but infinitely long-ranged orientational order. Strictly speaking, such surfaces have no sharp surface phase transition. However, for reasonable values of the bulk correlation length ξ_B ($\xi_B \gtrsim 30$ Å should be sufficient), an experimentally sharp "super-roughening" transition occurs at a temperature T_{SR}. This transition separates a high-temperature "rough" phase of the surface from a low-temperature "super-rough" phase that, counterintuitively, is even rougher. Specifically, the root-mean-square equilibrium vertical fluctuation in the position of the interface $\overline{\langle h^2 \rangle}^{1/2}$ diverge like $\sqrt{\ln L}$ as the length L of the surface $\rightarrow \infty$ for $T > T_{\mathrm{SR}}$ (just as in ordered solids for T greater than the roughening temperature T_R), while $\overline{\langle h^2 \rangle}^{1/2} \propto \ln L$ for $T < T_{\mathrm{SR}}$. This causes the correlation function $C(q_z;\mathbf{x}) \equiv \langle e^{iq_z[h(\mathbf{x})-h(0)]} \rangle$ measured in surface-sensitive scattering experiments (e.g., anti-Bragg x-ray scattering) to go from algebraic decay $C(q_z;\mathbf{x}) \propto |\mathbf{x}|^{-\eta(q_z)}$ in the rough phase to short-ranged order $C(q_z;\mathbf{x}) \propto |\mathbf{x}|^{-\bar{\eta}(q_z)\ln(|\mathbf{x}|)}$ in the super-rough phase. The functional dependence of $\eta(q_z)$ on q_z differs from that for fluctuating surfaces of both bulk ordered solids (above T_R) and liquids. We identify an experimentally measurable correlation length ξ_{SR} that diverges as $T \rightarrow T_{\mathrm{SR}}^-$ as $\exp[A T_{\mathrm{SR}}^2/(T_{\mathrm{SR}}-T)^2]$, where A is a constant of order $\ln^{-4}|\xi_B/a|$ and a is a lattice constant. The equilibrium crystal shapes do not have facets in either the rough or the super-rough phase. At low temperatures in the super-rough phase, however, nearly flat regions appear, with a radius of curvature scaling like $(\xi_B)^{-1}$.

I. INTRODUCTION

After many years of intensive theoretical[1] study a fairly clear and complete understanding of the roughening transition on the surface of crystals has emerged[2] and has begun to be tested experimentally.[3] All of the theoretical work to date[1,4] has been based on a highly idealized model that assumes that translational correlations in the bulk crystal are infinitely long ranged. We shall refer to this idealization as the bulk-ordered crystal. But real crystals typically have only finite ranged translational correlations due to the presence of quenched defects of various types (e.g., pinned dislocation lines). So, we will consider the question of what effect this type of disorder has upon the roughening transition.

In particular, we focus on crystals with infinitely long-ranged orientational order but only a finite correlation length ξ_B for translational order.[5] This would describe, e.g., single crystals with a random tangle of dislocation lines quenched in,[6] but with no grain boundaries (i.e., no sample mosaic). In samples with a small mosaic, our results will apply up to a length scale comparable to the size of a single mosaic grain. Our main results are as follows: (1) Quenched disorder destroys both the low-temperature smooth phase[1] and the conventional roughening transition. However, these are replaced by a new phase transition at a nonzero temperature T_{SR} and a new low-temperature phase, which we call the *super-rough* phase. (2) As its name implies, the crystal surface is actually rougher in the low-temperature superrough phase than in the high-temperature rough phase. (3) The additional roughness of the superrough phase can be observed experimentally using, e.g., x-ray diffraction;[3] such experiments could thereby provide an unambiguous signature of the super-roughening transition. In addition, these measurements would also observe clear quantitative and qualitative effects of the bulk disorder on the correlation functions of the rough phase at $T > T_{\mathrm{SR}}$ as well. (4) Surprisingly, the superroughening transition has virtually no effect on macroscopic properties like the crystal shape and the Wulff plot.[1] (5) For large ξ_B, the superrough transition temperature T_{SR} is near the ordinary roughening transition temperature T_R of a bulk-ordered crystal of the same material.

Let us elaborate on these results in more detail.

(1) The super-rough phase owes its existence to the presence of *quenched* disorder[7] in the bulk solid. It is important to realize that the properties of the system would be totally different if the disorder were *annealed* (i.e., equilibrium); in this case the system would simply be a (bond orientationally ordered) liquid and there would be no surface phase transition. The super-roughening transition is not a "true" (i.e., infinitely sharp in the thermodynamic limit) phase transition either, but its rounding would only be detectable on length scales larger than $L_c \equiv \xi_B e^{\alpha \xi_B / a}$, where a is a lattice constant and α is a constant of order 1. The length scale L_c can be enormous even for fairly short (and easily experimentally accessible) ξ_B: e.g., $\xi_B = 100$ Å, $a = 4$ Å, and $\alpha = 1$ gives $L_c \approx 720$ m.

For length scales $L > L_c$, the behavior of the surface crosses over to that of an interference pinned by random bond impurities[8] at all temperatures, with no surface phase transition. Knowledge of this length scale enables us to identify a criterion for the optimal value of ξ_B at which to study super roughening experimentally. Since ξ_B can presumably be "tuned" (roughly) by varying the sample preparation, such a criterion could prove useful. The optimal value of ξ_B is that which maximizes the number of decades of length scale (over which our theory is applicable) that can be probed by whatever experimental technique is being employed. The lower limit of this range is ξ_B, since, for shorter length scales the bulk looks ordered and surface fluctuations should be accurately described by conventional roughening theory. The upper limit is the smaller of L_c and the maximum length scale $L_{\max}$ probed by the particular experimental technique being used (e.g., in high-resolution synchrotron x-ray scattering, $L_{\max}$ is set by the instrumental wave-vector resolution and is typically $\sim 1-10$ μm).

Since L_c goes down with decreasing ξ_B, the goal of optimizing the experimental window clearly involves a competition between making L_c large and ξ_B small. Since there is nothing to be gained by taking $L_c > L_{\max}$, the optimum is simply given by that value of ξ_B that makes $L_c = L_{\max}$, namely,

$$\xi_B \exp(\alpha\xi_B/a) = L_{\max} .$$

For synchrotron x-ray experiments, taking $L_{\max} = 1\mu$, $a = 4$ Å, and $\alpha = 1$, this condition gives $\xi_B = 24$ Å, and hence a factor of roughly 400 in length scale over which super roughening could be observed. Thus the theory we present here should be eminently testable; indeed, the biggest practical obstacle may be the manufacturing of sufficiently dirty crystals (to reach the optimal value of ξ_B) without destroying the bond orientational order required for the theory to be valid.

(2) The (rms) height fluctuations $\overline{\langle h^2(\mathbf{r})\rangle}^{1/2}$ [where $h(\mathbf{r})$ denotes deviations from the average height of the interface at a point $\mathbf{r}$ on the surface, $\langle\ \rangle$ denote a thermal average, and the bar denotes an average over the quenched disorder], are given by

$$\overline{\langle h^2(\mathbf{r})\rangle}^{1/2} = W_S(T)\ln(L/a), \quad T < T_{\rm SR} \tag{1.1}$$

in the super-rough phase, and by

$$\overline{\langle h^2(\mathbf{r})\rangle}^{1/2} = W_R(T)\sqrt{\ln(L/a)} , \quad T > T_{\rm SR} \tag{1.2}$$

in the rough phase, where L is the linear extent of the surface, and $W_S(T)$ and $W_R(T)$ are functions of the degree of disorder as well as temperature. The results (1.1) and (1.2) apply asymptotically in the limit $L_c \gg L \gg \xi_B$. Note that in that limit (1.1) is larger than (1.2) regardless of the values of W_R and W_S; this means, as claimed, that at *any* temperature in the super-rough phase the fluctuations are larger than at *any* temperature in the rough phase.

For $L \gg L_c$, the two phases become identical, with the width $\overline{\langle h^2\rangle}^{1/2}$ scaling as in the random-bond interface problem[8]; i.e., $\overline{\langle h^2\rangle}^{1/2} = W_{\rm RB}(L/L_c)^{\zeta}$, with[8,9] $\zeta \cong 0.5$, and $W_{\rm RB}$ a constant chosen to match Eqs. (1.1) or (1.2) at $L = L_c$ (whichever is appropriate at the temperature in question).

The counterintuitive result that the low-temperature phase is rougher than the high-temperature phase may be understood by the following heuristic argument (which is confirmed by the detailed quantitative calculations we will present later): At high temperatures (i.e., in the rough phase) thermal fluctuations kick the surface out of any "potential wells" (a concept we will make more precise later when we define our model) that disorder in the bulk may cause. Therefore, in the rough phase, the (long-wavelength) fluctuations of the surface largely ignore the bulk; thus at these high temperatures it makes little difference what state the bulk is in. As a result, surfaces of bulk-ordered crystals, bulk-disordered crystals, and liquids will all have rms height fluctuations with the same functional dependence on L, namely, (1.2).

At sufficiently low temperatures, on the other hand, the surface becomes "locked" to the bulk. In the pure problem, such locking smooths the surface. In the bulk-disordered case, though, locking to the bulk causes the surface to meander (or fluctuate) *more* since the favorable bulk lattice planes (that the surface attempts to follow) are themselves disordered. This leads to the larger fluctuations given by (1.1).

Unlike the pure problem,[1] $W_R(T)$ in (1.2) takes on a nonuniversal value at $T = T_{\rm SR}$; however, this value is bounded below

$$W_R(T_{\rm SR}) > \frac{\sqrt{2}}{G_0} , \tag{1.3}$$

where G_0 is the smallest nonzero reciprocal lattice vector of the bulk normal to the crystal face under discussion. By contrast, the value $W_R(T_R)$ at the pure roughening transition is universally[1] $W_R(T_R) = 2/G_0$.

(3) The (long-wavelength) fluctuations of the surface should be directly observable by surface-sensitive scattering experiments using either x rays or atomic beams.[3] Such experiments are exponentially sensitive to fluctuations in h since they measure

$$C(q_z;\mathbf{x}) \equiv \overline{\langle e^{iq_z[h(\mathbf{x})-h(0)]}\rangle} .$$

As in the bulk-ordered problem,[1] in the rough phase of bulk-disordered crystals this correlation function is expected to decay algebraically with distance:

$$C(q_z;\mathbf{x}) = I(q_z)|\mathbf{x}|^{-\eta(q_z)}, \quad T > T_{\rm SR} , \tag{1.4}$$

while in the super-rough phase we predict an asymptotic decay faster than any power:

$$C(q_z;\mathbf{x}) = \begin{cases} I(q_z)|\mathbf{x}|^{-\eta(q_z)}, & |\mathbf{x}| < \xi_{\rm SR} \\ I(q_z)|\mathbf{x}|^{-\overline{\eta}(q_z)\ln|\mathbf{x}|}, & |\mathbf{x}| > \xi_{\rm SR} . \end{cases} \tag{1.5}$$

Here $I(q_z)$, $\eta(q_z)$, and $\overline{\eta}(q_z)$ are functions of both temperature and the degree of disorder. Equation (1.4) has the same form as it would in the rough phase of the surface of a bulk-ordered crystal. However, these two phases are not identical; the exponent $\eta(q_z)$ has a different functional dependence (on q_z) in the two phases, as shown explicitly in (3.20) and (3.21) (see also Fig. 1). We are unable to calculate $\bar{\eta}(q_z)$.

The crossover in (1.5) defines a correlation length in the super-rough phase, ξ_{SR}. This correlation length diverges as $T \to T_{\mathrm{SR}}^{-}$ as

$$\xi_{\mathrm{SR}}(T)=\xi_B \exp\left[\frac{A}{(T_{\mathrm{SR}}-T)^2/T_{\mathrm{SR}}^2}\right] , \tag{1.6}$$

where the constant

$$A=O((T_R-T_{\mathrm{SR}})^2/T_{\mathrm{SR}}^2)=O(\ln^{-4}(\xi_B/a)) .$$

The power-law form in (1.4) implies that, in the rough phase, the surface x-ray structure factor

$$S(\mathbf{q}_\perp,q_z)\equiv \int d^2r\, C(q_z;\mathbf{x})e^{i\mathbf{q}_\perp\cdot\mathbf{x}}$$

diverges as $|\mathbf{q}_\perp|\to 0$ for $\eta(q_z)<2$ [which is always satisfied as $q_z\to 0$, see Eq. (3.21)]. In contrast, (1.5) indicates that, in the super-rough phase, $S(\mathbf{q}_\perp,q_z)$ is always finite in the limit $|\mathbf{q}_\perp|\to 0$; this difference provides a clear and unambiguous experimental signature of the super-roughening transition.

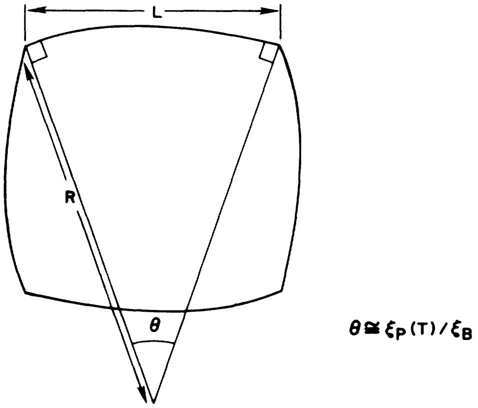

FIG. 2. The equilibrium shape of a bulk-disordered crystal for fairly large ξ_B/a at temperatures T well below T_{SR}. The surface contains a number of slightly curved regions that we call pseudofacets (e.g., the segment of length L in this figure). When $\xi_P(T)$ gets $\gg a$, these pseudofacets start to shrink according to Eq. (2.3), and are connected to each other by regions whose radii of curvature are $O(L)$. We have chosen to show the crystal shape without these (as it would be at low temperatures) for reasons of clarity.

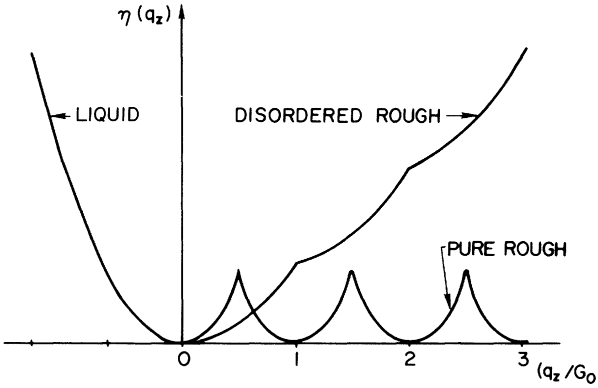

FIG. 1. Plot of the dependence of $\eta(q_z)$ on q_z at fixed temperature for liquids, bulk-ordered solids, and quenched bulk-disordered solids. The dependence is strictly parabolic for all q_z in a liquid, while in a bulk-ordered solid it consists of a periodic sequence of parabolic segments, with period G_0, where G_0 is the smallest reciprocal lattice vector of the crystal orthogonal to the surface. This periodicity reflects the underlying periodicity of the crystal lattice. In our system, the quenched bulk-disordered solid, $\eta(q_z)$ is no longer periodic, but still consists of parabolic segments joined by cusps which now occur at q_z's that are integral multiples of G_0.

(4) Unlike the rich behavior of the correlation functions, the equilibrium crystal shape in the presence of quenched bulk disorder shows no signature of the super-roughening transition. In both the rough and the super-rough phases, there are no flat facets on the surface; the surface has a nonzero radius of curvature everywhere (see Fig. 2). However, there is an interesting crossover behavior in systems with a long bulk correlation length: At low temperature in the super-rough phase, there are large nearly flat regions on the surface that we call pseudofacets. A quantitative characterization of what we mean by "nearly flat" is the radius of curvature R of these regions: As the bulk correlation length ξ_B goes to infinity (i.e., as the bulk becomes less disordered), this diverges as

$$R=L\xi_B/a , \tag{1.7}$$

where L is of order the crystal size. With increasing temperature, this radius of curvature shrinks according to

$$R=L\frac{\xi_P}{\xi_P(T)} , \tag{1.8}$$

where $\xi_P(T)$ is a correlation length associated with the *pure* problem, which diverges at the *pure* roughening transition temperature $T_R > T_{\mathrm{SR}}$ as[1]

$$\xi_P(T)=\xi_0\exp[B/(T/T_R-1)^{1/2}] , \tag{1.9}$$

where $\xi_0=O(a)$ and $B=O(1)$.

While the radius of curvature of the pseudofacet is decreasing, its linear extent l_F is shrinking as well, according to the same law followed by a *facet* in the *pure* roughening problem[1]

$$l_F=L\frac{a}{\xi_P(t)} . \tag{1.10}$$

Of course, (1.8) only applies when $R \gg L$; once $\xi_P(T)=O(\xi_B)$, $R\sim L$ and the pseudofacet ceases to be well defined. Thus, from the point of view of the equilibrium crystal shape the effect of the bulk disorder would appear to be simply to round the sharp roughening transition, in much the same way as a uniform magnetic field rounds the ferromagnetic-paramagnetic transition. However, as we have seen, the correlation functions still define a sharp super-roughening transition at $T_{\mathrm{SR}} \lesssim T_R$; there is no signature of this transition in the equilibrium crystal

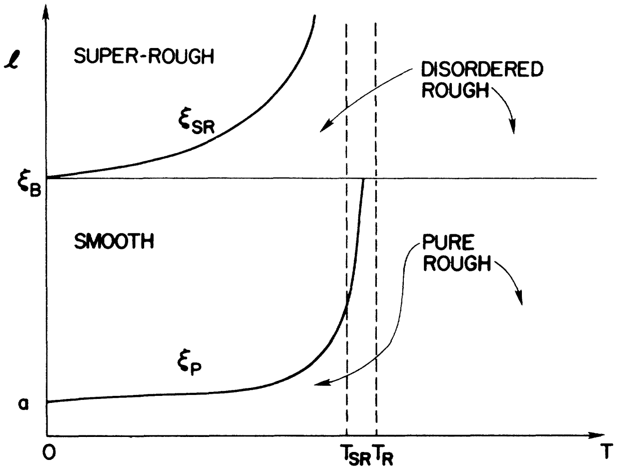

FIG. 3. The various regimes of length and temperature exhibiting qualitatively different surface correlation functions.

shape, however.

The temperature-dependent length scales ξ_{SR} and ξ_P and the temperature-independent length scale ξ_B break the length scale l and temperature T plane up into a number of regions of different behavior of $C(q_z;\mathbf{x})$, as illustrated in Fig. 3. For $|\mathbf{x}|\equiv l<\xi_B$, the bulk looks ordered; hence we have conventional roughening behavior on the surface, with the length scale ξ_P separating pure rough behavior [defined by Eq. (1.4) with $\eta(q_z)$ given by its pure form, Eq. (3.20)] from smooth behavior [$C(q_z;\mathbf{x})\to \text{const}\neq 0$ as $|\mathbf{x}|\to\infty$]. $\xi_P(T)$ is infinite for $T>T_R$, so we see pure rough behavior all the way up to ξ_B at these temperatures. For length scales $>\xi_B$, we see the super-rough behavior described in Eq. (1.5), with ξ_{SR} characterizing the crossover from rough to super-rough behavior.

(5) At the super-roughening transition temperature T_{SR}, $\xi_P(T)\sim\xi_B$ (this is another result of our theory); this implies that $T_{SR}\simeq T_R$ if $\xi_B\gg a$; specifically,

$$T_{SR}=T_R\left[1-\frac{g}{\ln^2(\xi_B/a)}\right] \tag{1.11}$$

with g a constant of order 1. Hence the temperature window over which we can see all four behaviors of $C(q_z;\mathbf{x})$ (pure rough, smooth, disordered rough, and super rough) with increasing l is quite small (see Fig. 3).

The remainder of this paper is organized as follows: In Sec. II we present and motivate our model. We also apply the replica technique to handle the quenched bulk disorder, derive the connection between replicated and physical correlation functions, and develop renormalization-group recursion relations for this problem. In Sec. III we use this machinery to derive the results quoted earlier; in Sec. IV we discuss the crossovers between pure and bulk-disordered behavior. Appendix A treats the rounding of the super-roughening transition, while in Appendix B we calculate the exponent $\eta(q_z)$ in the bulk-disordered rough phase.

II. THE MODEL

In this section we motivate a model Hamiltonian that should describe long-wavelength surface fluctuations on a solid with quenched bulk disorder. We also develop a replicated form of the partition function of the surface, which enables us to perform quenched averages over the bulk-disorder systematically. Using this formalism, we calculate the experimentally measurable correlation functions, and present the renormalization-group recursion relations.

A. Formulation

We wish to consider solids that have long-ranged orientational order but no true long-ranged translational order. The bulk correlation length, ξ_B, which measures the range of translational correlations is, however, taken to be much larger than the lattice spacing a. A single crystal threaded by a quenched random arrangement of dislocation lines would be an example of such a solid. Of interest are the interfacial fluctuations of a surface orthogonal to an axis of bond-orientational order in the bulk (i.e., a surface that would have been parallel on average to a crystal plane had the bulk been ordered).

The disorder in the bulk is described conveniently in terms of the density deviation from its mean value ρ_0, $\delta\rho(\mathbf{R})\equiv\rho(\mathbf{R})-\rho_0$, which is assumed to take the form

$$\delta\rho(\mathbf{R})=\mathrm{Re}\sum_{\mu}\rho_\mu e^{i\mathbf{G}_\mu\cdot\mathbf{R}}e^{i\phi_\mu(\mathbf{R})} . \tag{2.1}$$

Here $\mathbf{G}_\mu$ are reciprocal lattice vectors of the *ordered* solid. The functions $\eta_\mu(\mathbf{R})\equiv e^{i\phi_\mu(\mathbf{R})}$ describe the translational disorder and are taken, for simplicity, to satisfy (complex) Gaussian statistics with range ξ_B:

$$\begin{aligned}&\overline{\eta_\mu(\mathbf{R})}=0 ,\\ &\overline{\eta_\mu^*(\mathbf{R})\eta_{\mu'}(\mathbf{R}')}=f\left[\left|\frac{\mathbf{R}-\mathbf{R}'}{\xi_B}\right|\right]\delta_{\mu\mu'} ,\end{aligned} \tag{2.2}$$

where $f(\mathbf{x})$ is assumed to decay exponentially when its dimensionless argument $\mathbf{x}$ satisfies $|\mathbf{x}|\gtrsim 1$, and the bar denotes an average over disorder. Note that the correlation function $f(\mathbf{R}/\xi_B)$ is assumed to be a function only of the ratio $\mathbf{R}/\xi_B$; furthermore, we will assume it is analytic at $\mathbf{R}=0$. These assumptions, benign though they seem, are both violated by the real-space correlation function that leads to a conventional Lorentzian line shape, namely, $e^{-R/\xi_B}/R$, as well as by the scaling form $R^{-(d-2+\eta)}f(R/\xi_B)$ taken by correlations near second-order phase transitions. Nonetheless, it can be shown that both assumptions are true for any reasonable model of quenched, as opposed to equilibrium, disorder. We will discuss this point further in Appendix A. It should be pointed out that we need not assume that $f(\mathbf{R}/\xi_B)$ is isotropic in $\mathbf{R}$; indeed in Appendix A we will use the separable form

$$f(\mathbf{R}/\xi_B)=g(|\mathbf{x}|/\xi_B)h(z/\xi_B) ,$$

where $\mathbf{R}\equiv(\mathbf{x},z)$, to analyze the rounding of the super-roughening transition.

The assumptions embodied in (2.2) imply that the solid described in (2.1) has long-ranged orientational order, yet translational order which falls off with the bulk correlation length, $\overline{\delta\rho(\mathbf{R})\delta\rho(\mathbf{0})}\sim \exp(-R/\xi_B)$. To motivate an interfacial Hamiltonian, imagine cleaving the solid along a (single-valued) surface σ, specified by the function $z=h(\mathbf{x})$, whose average orientation coincides with a symmetry axis (i.e., $\hat{z}$) of the bond-oriented solid. Here $\mathbf{x}$ denotes coordinates in the average (i.e., $h=0$) plane of the surface. Symmetry allows in the surface free energy a term proportional to an integral of the (local) bulk density over the surface σ:

$$E_\sigma=\bar{K}\int d\sigma[\rho_0+\delta\rho(\mathbf{x},z=h(x,y))] \ . \qquad (2.3)$$

Such a term will therefore always be present. Upon reexpressing the surface element as $d\sigma=(1+(\nabla h)^2)^{1/2}d^2x$, and expanding to leading order in ∇h and $\delta\rho$, one arrives at a surface Hamiltonian of the form

$$\beta H=\int d^2x[\tfrac{1}{2}K'(\nabla h)^2+V\delta\rho(\mathbf{x},z=h(\mathbf{x}))] \ . \qquad (2.4)$$

In the following, we study the statistical surface fluctuations of $h(\mathbf{x})$ in the presence of the *quenched* disorder present in $\delta\rho$. This procedure is legitimate provided the surface fluctuations *do not* anneal away the bulk disorder. However, we will show that statistical excursions of the interfacial "height" will typically be small, so only the top surface layers can be annealed at all; thus the surface should still "feel" the effects of the quenched bulk disorder from below.

In the absence of the second term in (2.4), the interfacial width due to thermal fluctuations increases very slowly with the system size L,

$$\langle h^2\rangle^{1/2}\sim\left[\frac{1}{K'}\ln\left[\frac{L}{a}\right]\right]^{1/2} , \qquad (2.5)$$

where $a=2\pi/G_0$ is a crystal lattice constant. Note that K' has the dimensions of inverse length squared; we will see shortly that for temperatures $T\lesssim T_{\mathrm{SR}}$, $K'\gtrsim a^{-2}$. Thus in this temperature range $\langle h^2\rangle\sim a\sqrt{\ln(L/a)}$, which can be quite small (e.g., for $L=1$ mm and $a=4$ Å, $\langle h^2\rangle^{1/2}=15$ Å). One might naively expect that as long as these fluctuations are considerably smaller than the bulk correlation length, i.e., that of

$$\langle h^2\rangle^{1/2}\ll\xi_B \ , \qquad (2.6)$$

then we can neglect, in the Hamiltonian (2.4), the dependence of the disorder at the surface on the surface height h, i.e., that we can make the simplifying approximation

$$\phi_\mu(x,y,h)\cong\phi_\mu(x,y,h=0) \ .$$

This approximation, as we shall see in a moment, leads to the prediction of a thermodynamically sharp superroughening transition. In Appendix A, we will show that keeping the dependence of ϕ_μ on h leads to a broadened or rounded transition that is no longer a true thermodynamic transition. It also leads to a crossover to the behavior of a random-bond interface[8,9] for $L>L_c$. Furthermore, we will demonstrate that the condition that this rounding be experimentally unobservable is somewhat stricter than (2.5) and (2.6) would imply. In fact, the actual condition is

$$\xi_B\gg a\ln(L/\xi_B) \ , \qquad (2.7)$$

where L is the largest length scale probed by the experiment in question (e.g., 10 μm in very-high-resolution x-ray measurements), which should be contrasted with the weaker condition $\xi_B\gg a\sqrt{\ln(L/a)}$ implied by (2.5) and (2.6). The condition (2.7) is nonetheless still easily satisfied; for $L=1$ μm and $a=4$ Å, (2.7) becomes $\xi_B\gg 24$ Å, as mentioned in the Introduction. It should be fairly easy to produce samples with ξ_B this large. Measurements on length scales L that violate (2.7) will be described by the theory of interfaces in random-bond systems,[8,9] as discussed in the Introduction.

Under the assumption (2.7) we can ignore, in the Hamiltonian (2.4), the dependence of the *disorder* on the surface height h: $\phi_\mu(x,y,h)\simeq\phi_\mu(x,y)$. Then (2.4) can be simply expressed as

$$\beta H=\int d^2x\{\tfrac{1}{2}K'(\nabla h)^2+V\rho_1\cos[G_0h(\mathbf{x})+\phi_z(\mathbf{x})]\} \ , \qquad (2.8)$$

where we have kept only the Bragg peak $\mu=1$ corresponding to the smallest $\mathbf{G}$ orthogonal to the surface, and $G_0\equiv|\mathbf{G}_1|$. The terms involving other $\mathbf{G}$'s can be shown to be irrelevant.

This model is illustrated pictorially in Fig. 4(a). For

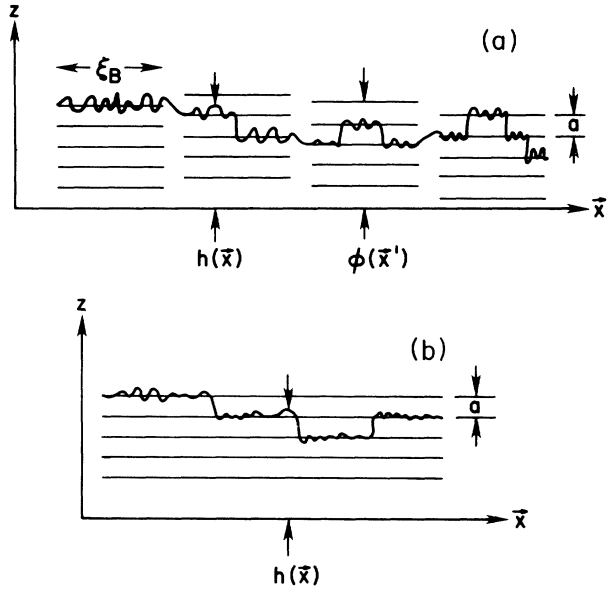

FIG. 4. Pictorial representation of our model. $\phi(\mathbf{x})$ represents the quenched random displacements of the bulk lattice planes along their normal $\hat{z}$ while $h(\mathbf{x})$ is the height along $\hat{z}$ of the surface. $\phi(\mathbf{x})$ is coherent (or, equivalently, the lattice planes are unbroken) over distances of order the bulk correlation length ξ_B. (b) Depiction of the conventional roughening model for bulk-ordered crystals. It is basically the same as (a) except that the bulk translational correlation length ξ_B is infinite; i.e., the bulk planes are unbroken over the entire sample.

purposes of comparison, Fig. 4(b) provides a similar depiction of the standard model for the roughening of bulk ordered crystals. It can be shown, using the renormalization-group arguments that we will present later, that any other terms one might consider adding to this Hamiltonian are "irrelevant" in the renormalization-group sense. This means that the long-distance behavior of an arbitrary complicated model consistent with the symmetries of the system can be reproduced exactly by (2.8) for a suitable "renormalizable" choice of the constants K' and V.

This Hamiltonian is identical to the standard model for the pure roughening problem[1] except for the presence of the quenched random field ϕ.

It should be emphasized that (2.8) has a discrete symmetry, $h(\mathbf{x})\rightarrow h(\mathbf{x})+ma$ for integers m, which is *not* shared by the original Hamiltonian (2.4). Since the inequality in (2.7) is easily satisfied, though, this should not matter in practice. It does mean, however, that the rough–super-rough transition present in (2.8) and described later, would be "rounded" in terms of the full model (2.4). This is discussed in more detail in Appendix A.

The statistical surface fluctuations described by (2.8) can be analyzed by considering the partition function

$$Z\{\phi\}=\int Dh\, e^{-\beta H\{h,\phi\}}\ . \tag{2.9}$$

Surface thermodynamic properties follow then from the ensemble averaged free energy,

$$\bar{F}=-k_BT\overline{\ln Z}\ , \tag{2.10}$$

where the bar denotes an average over the quenched random variable ϕ.

This partition function is identical[10] to that of a two-dimensional (2D) XY model without vortices in a random field.[11,12] The model with vortices was studied in Refs. 11 and 12; the latter also studied the Gaussian (vortex free) limit. The analogy we are using is that the free energy for the angle field θ in the XY model is almost the same as that for the height variable h in our model. The analogy breaks down, however, precisely in the fact that the XY model allows real vortices (as opposed to the "dummy" vortices that arise from the dual transformations on the cosine term), whereas the interface model does not. A "real" vortex in the XY model is a configuration of spins in which, as one moves around the vortex, θ increases from 0 to 2π. This is a low-energy configuration in the XY model because $\theta=2\pi$ is indistinguishable from $\theta=0$ (both correspond to an XY spin pointing in the same direction). In the interface model, such a configuration of h would have a step along the discontinuity from $h=0$ to $2\pi/G$, this step costs a large energy E (i.e., E is linear in the system size) and hence such fluctuations are irrelevant to the interface problem. Thus, our problem is equivalent to the one studied in Refs. 11 and 12 *only* if we ignore the "real" vortices in the XY model.

We will use the replica approach, recursion relations, and some of their correlation functions of Ref. 12 to derive our results. Our results for the $h-h$ correlation function in the super-rough phase, for

$$C(q_z;\mathbf{x})\equiv\langle \overline{e^{iq_z[h(\mathbf{x})-h(0)]}}\rangle$$

in both phases, and for the crystal shapes, while founded upon the results of Ref. 12, are new. The same is true of our arguments in Appendix A concerning the rounding of the transition.

B. Replicas

The quenched average in Eq. (2.10) is evaluated using the replica procedure.[13] The important identities that we use are

$$\bar{F}=-k_BT\lim_{n\rightarrow 0}\frac{\overline{Z}^{\,n}-1}{n} \tag{2.11}$$

and

$$\overline{Z}^{\,n}=\int\left[\prod_{\alpha=1}^{n}Dh_\alpha\right]\exp\left[-\sum_{\alpha'=1}^{n}\beta H\{h_{\alpha'},\phi\}\right]\ . \tag{2.12}$$

Performing the quenched average over ϕ will now couple the previously uncoupled replicas h_α. This average can be done perturbatively in the strength V of the $\cos(G_0h_\alpha-\phi)$ term in (2.8), yielding

$$\begin{aligned}\overline{\exp\left[\sum_{\alpha=1}^{n}\beta H\{h_\alpha,\phi\}\right]}&=\overline{\exp\left[-\int d^2x\left[\tfrac{1}{2}K\sum_{\alpha=1}^{n}|\nabla h_\alpha(\mathbf{x})|^2-V\rho_1\sum_{\alpha=1}^{n}\cos[G_0h_\alpha(\mathbf{x})-\phi(\mathbf{x})]\right]\right]}\\&=\left[-\frac{K}{2}\int d^2x\sum_{\alpha=1}^{n}|\nabla h_\alpha(\mathbf{x})|^2\right]\\&\quad\times\left[1-V\rho_1\sum_{\alpha=1}^{n}\int d^2x\,\overline{\cos[G_0h_\alpha(\mathbf{x})-\phi(\mathbf{x})]}\right.\\&\quad\left.+\tfrac{1}{2}(V\rho_1)^2\int d^2x\,d^2x'\sum_{\alpha,\beta=1}^{n}\overline{\cos[G_0h_\alpha(\mathbf{x})-\phi(\mathbf{x})]\cos[G_0h_\beta(\mathbf{x}')-\phi(\mathbf{x}')]}+O(V^3\rho_1^3)\right]\ .\end{aligned} \tag{2.13}$$

The quenched averages appearing in this expression may now be evaluated with the help of Eq. (2.2):

$$\begin{aligned}&\overline{\cos[G_0h_\alpha(\mathbf{x})-\phi(\mathbf{x})]}=0\ ,\\&\overline{\cos[G_0h_\alpha(\mathbf{x})-\phi(\mathbf{x})]\cos[G_0h_\beta(\mathbf{x}')-\phi(\mathbf{x}')]}=\tfrac{1}{2}\cos\{G_0[h_\alpha(\mathbf{x})-h_\beta(\mathbf{x}')]\}f((\mathbf{x}-\mathbf{x}')/\xi_B)\ .\end{aligned}\tag{2.14}$$

Using these in (2.13) and reexponentiating (i.e., writing $1+x\approx e^x$ for small x) we obtain

$$\overline{Z}^{\,\overline{n}}=\int\prod_{\alpha=1}^{n}Dh_\alpha e^{-\beta H\{h_\alpha\}}\ ,\tag{2.15a}$$

where

$$\beta H\{h_\alpha\}=\tfrac{1}{2}K\int d^2x\sum_{\alpha=1}^{n}|\nabla h_\alpha(\mathbf{x})|^2-\tfrac{1}{2}(V\rho_1)^2\int d^2x d^2x'\sum_{\alpha,\beta=1}^{n}\cos\{G_0[h_\alpha(\mathbf{x})-h_\beta(\mathbf{x}')]\}f((\mathbf{x}-\mathbf{x}')/\xi_B)\ .\tag{2.15b}$$

(The dummy index β should not be confused with $\beta\equiv 1/k_BT$, as the distinction should always be clear from context.)

Now we can exploit the fact that $f(\mathbf{x}/\xi_B)$ is short ranged (i.e., falls off exponentially for $|\mathbf{x}|\gtrsim\xi_B$) to gradient expand the cosine term. We thereby obtain our final replicated Hamiltonian:

$$\begin{aligned}\beta H=&\tfrac{1}{2}\int d^2x\sum_{\alpha\beta}K_{\alpha\beta}\nabla h_\alpha\cdot\nabla h_\beta\\&-u\sum_{\alpha,\beta}\int d^2x\cos\{G_0[h_\alpha(x)-h_\beta(x)]\}\ ,\end{aligned}\tag{2.16}$$

where $u=A_f(\xi_BV\rho_1)^2$ and $A_f\equiv\frac{1}{2}\int d^2x\,f(\mathbf{x})$ is a constant of order unity. An implicit "short" distance cutoff, of order ξ_B, is understood in (2.16). The stiffness matrix $K_{\alpha\beta}$ is

$$K_{\alpha\beta}\equiv K\delta_{\alpha\beta}+(K-\tilde{K})(1-\delta_{\alpha\beta})\tag{2.17}$$

with

$$\tilde{K}=K=K'+\tfrac{1}{2}B_f\xi_B^4(V\rho_1G_0)^2\ .$$

Here $B_f\equiv\int d^2y|\mathbf{y}|^2f(\mathbf{y})$ is another constant of order unity. We have written this matrix with K and $\tilde{K}$ different in anticipation of their becoming different under renormalization, even though they start out equal.

C. Gaussian correlation functions

Before presenting the recursion relations for this model, it is first instructive (and will later prove useful) to calculate the spatially Fourier transformed thermal and annealed averaged height-height correlation functions $\overline{\langle|h(\mathbf{q})|^2\rangle}$ when $u=0$. Using very similar manipulations to those just presented for the partition function, we can show that

$$\overline{\langle|h(\mathbf{q})|^2\rangle}=\lim_{n\to 0}\langle h_\alpha(\mathbf{q})h_\alpha(-\mathbf{q})\rangle\ ,\tag{2.18}$$

where we are *not* applying the Einstein summation convention (i.e., α is not summed over in this equation), and $\langle h_\alpha(\mathbf{q})h_\alpha(-\mathbf{q})\rangle$ denotes a thermal average of $|h_\alpha(\mathbf{q})|^2$ over the distribution embodied in the partition function Eq. (2.8). When $u=0$ this distribution is both Gaussian and local in $\mathbf{q}$ space; thus the desired average can be taken just by inverting the matrix $K_{\alpha\beta}$ in (2.16). This inverse can easily be calculated by assuming that $K_{\alpha\beta}^{-1}$ has the same form as $K_{\alpha\beta}$ [i.e., $K_{\alpha\beta}^{-1}=A\delta_{\alpha\beta}+B(1-\delta_{\alpha\beta})$] and verifying this form by solving $K_{\alpha\beta}^{-1}K_{\beta\gamma}=\delta_{\alpha\gamma}$ (the definition of the inverse) for A and B. The result is[12]

$$\langle h_\alpha(\mathbf{q})h_\beta(-\mathbf{q})\rangle=\frac{1}{\tilde{K}q^2}\left[\delta_{\alpha\beta}+\frac{\tilde{K}-K}{nK-(n-1)\tilde{K}}\right]\ ,\tag{2.19}$$

which when inserted into (2.18) yields

$$\overline{\langle|h(\mathbf{q})|^2\rangle}=\frac{1}{\tilde{K}q^2}\left[2-\frac{K}{\tilde{K}}\right]\ .\tag{2.20}$$

As we shall see in the following, after renormalization $K<\tilde{K}$; therefore,

$$(\overline{\langle|h(q)|^2\rangle})>\frac{1}{\tilde{K}q^2}>0\ .$$

The last inequality is reassuring.

D. Recursion relations

The renormalization-group recursion relations are[12]

$$\frac{d\tilde{K}}{dl}=0\ ,\tag{2.21a}$$

$$\frac{dK}{dl}=-A_K\frac{G_0^2}{\Lambda^4}u^2\ ,\tag{2.21b}$$

$$\frac{du}{dl}=\left[2-\frac{G_0^2}{2\pi\tilde{K}}\right]u-\frac{A_u}{\Lambda^2}u^2\ ,\tag{2.21c}$$

where A_K and A_u are dimensionless, nonuniversal constants of order unity and Λ is an ultraviolet cutoff of order ξ_B^{-1}. The precise value of Λ used in these recursion relations is unimportant, since, as we shall soon see, it drops out of all physically observable results.

Note that $\tilde{K}$ is unrenormalized; this is true to all orders[12] and has important physical consequences for the crystal shapes. This result can be demonstrated as follows: We can rewrite (2.16) as

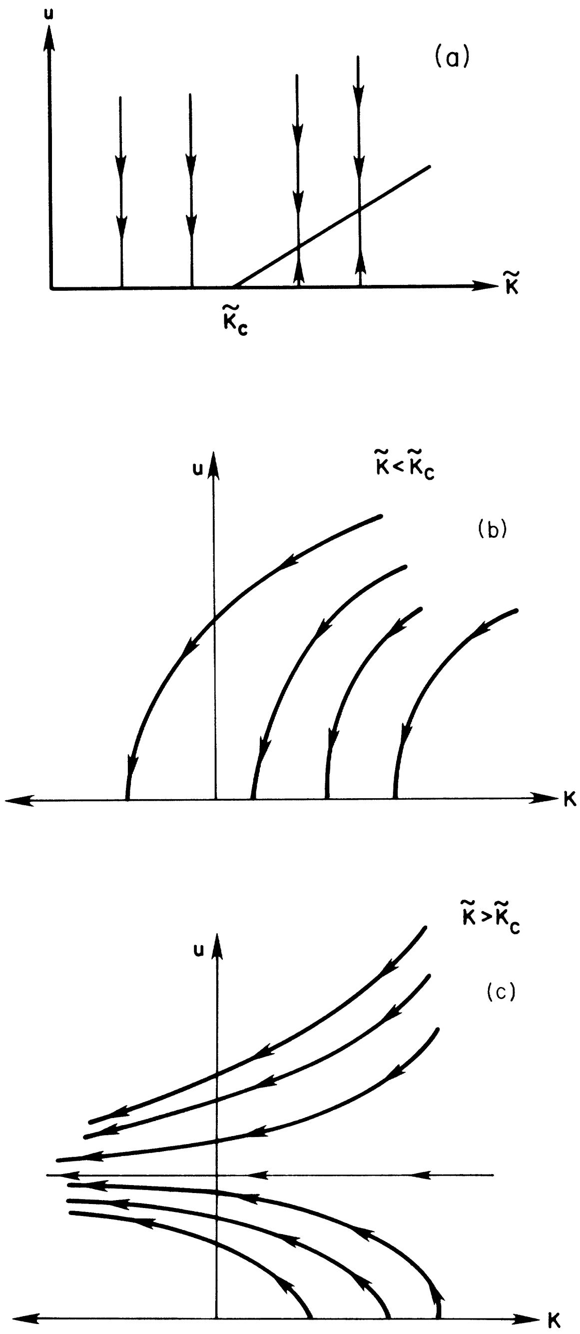

FIG. 5. (a) The renormalization-group flows in the $y-\tilde{K}$ plane implied by the recursion relations (2.21). Because $\tilde{K}$ is unrenormalized, the flows in this plane are all along vertical lines. For $\tilde{K}<\tilde{K}_c$ (which corresponds to high temperatures), u flows to zero (i.e., is irrelevant) and the surface is rough. For $\tilde{K}>\tilde{K}_c$, u flows to a nonzero value $u_*(\tilde{K})$; and the surface is super rough. The super-roughening transition therefore occurs when $\tilde{K}$ passes through $\tilde{K}_c$; that is $\tilde{K}(T_{\mathrm{SR}})=\tilde{K}_c$. Note that $u_*(\tilde{K})$ is linear in $\tilde{K}-\tilde{K}_c$ for $\tilde{K}\gtrsim\tilde{K}_c$. (b) The renormalization group flows in the $u-K$ plane at fixed constant $\tilde{K}<\tilde{K}_c$. Note that any initial u flows to zero, and K flows to a (nonuniversal) fixed point value. This corresponds to the rough phase. (c) Flows in the $u-K$ plane for $\tilde{K}>\tilde{K}_c$. Now u flows to a nonzero value u_* and K flows to $-\infty$ as a result. This behavior of K makes the surface superrough.

$$\beta H=\frac{1}{2}\int d^2x\left[K_1\sum_{\alpha=1}^{n}|\nabla h_\alpha|^2+K_2\sum_{\alpha\neq\beta}|\nabla(h_\alpha-h_\beta)|^2-u\sum_{\alpha\neq\beta}\cos[G_0(h_\alpha-h_\beta)]\right], \tag{2.22}$$

where, for $n=0$, $K_1=\tilde{K}$ and $K_2=\frac{1}{2}(\tilde{K}-K)$. Clearly, the u term in (2.22) is invariant under the transformation $h_\alpha(\mathbf{x})\rightarrow h_\alpha(\mathbf{x})+g(\mathbf{x})$ for all α. Thus, under the action of the renormalization group, it can only generate terms that preserve this symmetry. The term $K_1\sum_{\alpha=1}^{n}|\nabla h_\alpha|^2$ clearly does *not* have this symmetry; therefore it is *not* renormalized by u. Since u is the only anharmonicity in this model, there is nothing else in the Hamiltonian to renormalize K_1 either. Hence, K_1 and therefore $\tilde{K}$ for $n=0$ suffers no renormalization.

The renormalization-group flows predicted by the recursion relations (2.21) are depicted in Fig. 5. Their physical implications will be discussed in the next section.

III. RESULTS FOR $|\mathbf{x}|>\xi_B$

In this section we use the results of Sec. II to derive experimentally observable properties of the super-roughening transition. The first of these is the fact that the transition exists. This can be seen from (2.21c), since for $\tilde{K}<G_0^2/4\pi$ the random potential u flows to zero under renormalization and is thus irrelevant at long length scales, whereas for $\tilde{K}>G_0^2/4\pi$ it is relevant (a small u will grow). Thus

$$K=\tilde{K}_c\equiv\frac{G_0^2}{4\pi} \tag{3.1}$$

marks a phase boundary between two qualitatively different types of long distance behavior. Since $\tilde{K}$ decreases with increasing temperature, the phase in which u is irrelevant is the high-temperature (rough) phase, while the u relevant (super-rough) phase occurs at low temperature.

In Sec. III A, we will show that this transition can be unambiguously identified by experimental measurements of the appropriate height-height correlation function. We also demonstrate that even the correlations of the rough phase differ from those of the surface of a bulk-ordered crystal. In Sec. III B, we show that, surprisingly, the equilibrium crystal shapes are totally unaffected by the super-roughening transition, with neither the rough nor the super-rough phase having flat facets.

A. Non-Gaussian correlation functions

The long-distance properties that distinguish between these two phases are manifest in the interfacial correlation functions. Specifically, consider the ensemble averaged height-height correlation function, $\langle|h(q)|^2\rangle$. When $u=0$ this is given by (2.20). Since u flows to 0 for $l\rightarrow\infty$ in the rough phase, (2.20) will hold on large length scales, with K replaced by its $l\rightarrow\infty$ value K_∞. Although K_∞ is not necessarily positive in this phase, it will have a *finite* value since $u(l)$ vanishes sufficiently fast (exponentially) as $l \to \infty$ [see Fig. 5(b)]. Moreover, since the renormalization of $K(l)$ is always negative, K_∞ is always bounded above by $\tilde{K}$.

The actual mean-square fluctuation in the height of a surface, with linear dimension L, can be obtained by summing (2.20) over $\mathbf{q}$ with an infrared cutoff proportional to L^{-1} (and ultraviolet cutoff ξ_B^{-1})):

$$\overline{\langle h^2(\mathbf{r})\rangle} = \frac{1}{\tilde{K}}\left[2-\frac{K_\infty}{K}\right]\int\frac{d^2q}{(2\pi)^2}\frac{1}{q^2} = \frac{1}{2\pi\tilde{K}}\left[2-\frac{K_\infty}{\tilde{K}}\right]\ln\left[\frac{L}{\xi_B}\right] . \tag{3.2}$$

Since $\tilde{K} < G_0^2/4\pi$ in the rough phase, and $K_\infty < \tilde{K}$ always, the coefficient of the logarithm in (3.2) can be bounded from below:

$$\frac{\overline{\langle h^2\rangle}}{\ln(L/\xi_B)} > \frac{2}{G_0^2} , \tag{3.3}$$

which is the result quoted in the Introduction. Note, however, that although $\tilde{K}$ is universal at the super-roughening transition ($\tilde{K}_c = G_0^2/4\pi$), K_∞ is not [its value depending on the initial strength $u(l=0)$ of the random potential.] Thus the coefficient of the logarithm in (3.3) is not universal[12] at the super-roughening transition, unlike the analogous coefficient at the roughening transition in the pure problem.

In the super-rough phase, $\tilde{K} > G_0^2/4\pi$, and a sufficiently small initial u will grow under renormalization. It will not grow without bound, however; eventually it approaches a nonzero fixed point value at large l that can be obtained near the transition by equating the right-hand side of (2.21c) to zero [see Fig. 5(c)]:

$$u(l\to\infty) \equiv u_* = D\left[2-\frac{G_0^2}{2\pi\tilde{K}}\right] \tag{3.4}$$

with a universal constant $D \equiv \Lambda^2/A_u$. Notice that u_* vanishes linearly with temperature as T_{SR} is approached from below (assuming, as one usually does in critical phenomena, that the parameters of our model—in this case $\tilde{K}$—are smooth and analytic functions of temperature near the transition), i.e.,

$$u_*(l) = u_0 t, \quad t \equiv (T_{\mathrm{SR}}-T)/T_{\mathrm{SR}} , \tag{3.5a}$$

with

$$u_0 = -T_{\mathrm{SR}}\frac{d}{dT}\left[\frac{DG_0^2}{2\pi\tilde{K}}\right]\Bigg|_{T=T_{\mathrm{SR}}} = -\frac{2}{A_u}\frac{d\ln\tilde{K}}{d\ln T}\Bigg|_{T=T_{\mathrm{SR}}}\Lambda^2 , \tag{3.5b}$$

where we have used the fact that $\tilde{K}(T_{\mathrm{SR}}) = G_0^2/4\pi$. We will see later that

$$[d\ln\tilde{K}/d\ln T]|_{T=T_{\mathrm{SR}}}$$

is large when $\xi_B \gg a$; u_0 is consequently large as well. Equation (3.5) provides the basis for most of our predictions of the temperature dependence of critical phenomena near the super-roughening transition.

Since $u_* \neq 0$ in the superrough phase, (2.21b) indicates that $K(l\to\infty)$ is driven to $-\infty$. More specifically,

$$K(l) = K_a(l) - u_*^2 A_K \frac{G_0^2}{\Lambda^4} l \tag{3.6a}$$

with

$$K_a(l) \equiv K(l=0) - A_K\frac{G_0^2}{\Lambda^4}\int_0^l dl'[u^2(l') - u_*^2] . \tag{3.6b}$$

Since the integrand in (3.6b) vanishes exponentially fast as $l\to\infty$ for $u_* \neq 0$, $K_a(l)$ asymptotes to a finite constant, $K_a \equiv K_a(\infty)$. One may also verify from the recursion relations that $K_a(\infty)$ is finite even *at* T_{SR}, where $u_* = 0$.

What does this imply for the long-wavelength interfacial correlation functions in the super-rough phase? To answer this, consider applying the same renormalization-group techniques used in the preceding section on the partition function to the height-height correlation function. Specifically, by employing the rescaling of $h(q)$ and q we have

$$\Gamma(g,\tilde{K},K(0),u) = \overline{\langle h(\mathbf{q})h(-\mathbf{q})\rangle} = \langle h_\alpha(\mathbf{q})h_\alpha(-\mathbf{q})\rangle = e^{2l}\Gamma(e^l q,\tilde{K},K(l),u(l)) . \tag{3.7}$$

This relation can be used to calculate $\Gamma(\mathbf{q})$ by choosing l such that $e^l q = \xi_B^{-1}$, the ultraviolet cutoff. At this point, the long length scale ($>\xi_B$) fluctuations should no longer be important so that $\Gamma(e^l\mathbf{q},u)$ on the right-hand side of (3.7) should be analytic in u. Moreover, in the asymptotic $q\to 0$ limit, $e^l \to \infty$ so that $u(l)$ approaches its fixed point value u_*. Thus, close to the transition where u_* is small, one may safely replace u_* on the right side of (3.7) by zero and evaluate using the Gaussian result (2.20). This gives

$$\Gamma(q,\tilde{K},K(0),u) = \frac{e^{2l}}{\tilde{K}}\left[2-\frac{K(l)}{\tilde{K}}\right]\frac{1}{e^{2l}q^2} = \frac{1}{\tilde{K}}\left[2-\frac{K_a(\infty)}{\tilde{K}}\right]\frac{1}{q^2} - \frac{u_*^2}{\tilde{K}^2 q^2}A_K\frac{G_0^2}{\Lambda^4}\ln(q\xi_B) , \tag{3.8}$$

where in the last step we have used (3.6a) for $K(l)$ and the condition $e^l q = \xi_B^{-1}$ to solve for l as a function of q. The last term clearly dominates as $q\to 0$. Evaluating $\langle h^2(r)\rangle$ as before, and keeping only this dominant last term, we now find

$$\overline{\langle h^2(\mathbf{r})\rangle} = -\frac{u_*^2}{\tilde{K}^2}\int\frac{d^2q}{(2\pi)^2}\frac{1}{q^2}\ln(q\xi_B) = \frac{u_*^2}{2\pi\tilde{K}^2}A_K\frac{G_0^2}{\Lambda^4}\ln^2\left[\frac{L}{\xi_B}\right] , \tag{3.9}$$

for a system with linear dimension L. Although this result was derived only for small u_* (near the transition), we expect the $(\ln L)^2$ dependence on L to be valid for asymptotically large L throughout the entire super-rough phase. For T near $T_{\rm SR}$, we can use Eq. (3.5) to estimate the value of the coefficient of $[\ln(L/\xi_B)]^2$ in this expression. We find

$$A_K \frac{u_*^2 G_0^2}{\tilde{K}^2 \Lambda^4} = A_K \frac{u_0^2 t^2 G_0^2}{\tilde{K}^2 \Lambda^4} = t^2 \frac{16 A_K}{A_u^2} \left[\left. \frac{d \ln \tilde{K}}{d \ln T} \right|_{T=T_{\rm SR}} \right]^2 a^2 , \qquad (3.10)$$

where we have again used the fact that $\tilde{K}(T_{\rm SR}) = G_0^2/4\pi$ and $G_0 = 2\pi/a$. Recalling that A_K and A_u are $O(1)$, we see that this coefficient is of order $a^2 t^2$ times a dimensionless factor of order $\{[d \ln\tilde{K}/d \ln T]|_{T=T_{\rm SR}}\}^{1/2}$. We will see later that this factor is of order $\ln^{-4}(\xi_B/a)$, and hence large when $\xi_B \gg a$. Note that Λ has dropped out of this expression for the correlation function in Eq. (3.9), in keeping with our earlier claim that all observable quantities are independent of it.

Notice that in the super-rough phase the interfacial width increases more rapidly with the system size L than in the rough phase (3.2). Physically, the super-rough phase corresponds to glassy phase where the interface has become "pinned" to the disorder felt from the bulk. The interface exhibits large excursions in order to take advantage of favorable regions of disorder.

A correlation length in the super-rough phase, $\xi_{\rm SR}$, can be defined by considering the correlation function

$$G(\mathbf{x}) \equiv \langle [h(\mathbf{x}) - h(0)]^2 \rangle ,$$

which is related to $\Gamma(\mathbf{q})$ by

$$G(\mathbf{x}) = \int \frac{d^2 q}{(2\pi)^2} (1 - e^{i\mathbf{q}\cdot\mathbf{x}}) \Gamma(\mathbf{q}) . \qquad (3.11)$$

Inserting $\Gamma(\mathbf{q})$ for the super-rough phase (3.8) one finds

$$G(\mathbf{x}) = \frac{1}{2\pi\tilde{K}} \left[2 - \frac{K_a}{\tilde{K}} \right] \ln(|\mathbf{x}|/\xi_B) + \frac{u^{*2}}{\tilde{K}^2} A_K \frac{G_0^2}{\Lambda^4} \left[\ln \left[\frac{|\mathbf{x}|}{\xi_B} \right] \right]^2 . \qquad (3.12)$$

The value of $|\mathbf{x}|$ at which the $[\ln(|\mathbf{x}|/\xi_B)]^2$ term in (3.12) becomes comparable to the first term gives us a natural definition for $\xi_{\rm SR}(T)$. One thereby obtains

$$\xi_{\rm SR}(T) = \xi_B \exp \left[\frac{\tilde{K}}{2\pi} \left[2 - \frac{K_a}{\tilde{K}} \right] \Big/ u_*^2 \right] \propto \exp(A/t^2) . \qquad (3.13)$$

Here we have used expression (3.6) for the asymptotic behavior of $u_*(t)$ near the transition temperature $T_{\rm SR}$. The last proportionality in (3.13) holds near $T_{\rm SR}$, and the dimensionless constant

$$A = \left[\frac{\tilde{K}}{2\pi} \left[2 - \frac{K_0}{\tilde{K}} \right] \Big/ \left[A_K \frac{G_0^2}{\Lambda^4} u_0^2 \right] \right] \Bigg|_{T=T_{\rm SR}} = \frac{A_u^2}{32\pi A_K} \left[2 - \frac{K_a}{\tilde{K}} \right] \Big/ \left[\left. \frac{d \ln \tilde{K}}{d \ln T} \right|_{T=T_{\rm SR}} \right]^2 . \qquad (3.14)$$

Note that since $u_0 \propto \Lambda^2$, (3.14) is also independent of Λ. We will show later that $A = O(\ln^{-4}(\xi_B/a))$. Experimentally, $\xi_{\rm SR}$ is significant because for $|\mathbf{x}| < \xi_{\rm SR}$ the experimentally observable surface correlation function still decays algebraically, while for $r > \xi_{\rm SR}$ it decays far more rapidly (see the following).

The changeover from $\langle h^2 \rangle^{1/2} \propto \sqrt{(\ln L)}$ to $\langle h^2 \rangle^{1/2} \propto (\ln L)$ is the signature of the super-roughening transition. At first glance, this might seem a rather unspectacular change; in a 10 cm sample with $\xi_B = 100$ Å, the ratio of the height fluctuations in the super-rough phase to those in the rough phase is $[\ln(L/\xi_B)]^{1/2} \sim 4$. Fortunately, the most direct experimental probe of these fluctuations, namely, surface scattering, is exponentially sensitive to height fluctuations, and hence this changeover should be quite easy to observe experimentally.

More specifically, surface-sensitive scattering experiments,[3] using either x rays, atomic beams, or neutrons, measure the structure factor:

$$S(\mathbf{q}_\perp, q_z) = \int d^2 x \langle e^{i q_z [h(\mathbf{x}) - h(0)]} \rangle e^{i \mathbf{q}_\perp \cdot \mathbf{x}} , \qquad (3.15)$$

where $\mathbf{q}_\perp$ and q_z denote components of the scattering wave vector along and orthogonal to the surface, respectively. Thus we are interested in the correlation function

$$C(q_z; \mathbf{x}) \equiv \langle e^{i q_z [h(\mathbf{x}) - h(0)]} \rangle . \qquad (3.16)$$

This can be calculated as follows.

In the super-rough phase the large $|\mathbf{x}|$ asymptotics of C can be extracted (for small q_z) by expanding the exponential in Eq. (3.16) to quadratic order and then reexponentiating,

$$C \sim \exp[-\tfrac{1}{2} q_z^2 \langle (\Delta h)^2 \rangle] .$$

Using the result of Sec. III B one finds then that C decays faster than any power $C \sim (|\mathbf{x}|^{-\eta(q_z) \ln|\mathbf{x}|})$, implying that $S(\mathbf{q}_\perp, q_z)$ is *finite* and *analytic* at $\mathbf{q}_\perp = 0$. In contrast, in the rough phase, since the interfacial width grows logarithmically, one expects power-law behavior

$$C(q_z; \mathbf{x}) \sim |\mathbf{x}|^{-\eta(q_z)}, \quad |\mathbf{x}| \to \infty \qquad (3.17)$$

with an exponent $\eta(q_z)$.

For a fluid interface, described for example by (2.6) with $V \equiv 0$, $\eta(q_z)$ depends quadratically on q_z. For a crystal interface, however, $\eta(q_z)$ will reflect the periodicity of the bulk density. Consider, for example, a rough interface of an *ordered* crystal, described by (2.8) with $\phi_z \equiv 0$. In the solid-on-solid solid limit one expects

$$C_{\mathrm{ord}}(q_z;\mathbf{x})=\left[\frac{K}{\ln(|\mathbf{x}/a|)}\right]^{1/2}\times\sum_{n=-\infty}^{\infty}e^{iq_z na}\exp\left[-\frac{\pi K n^2a^2}{\ln(|\mathbf{x}/a|)}\right], \tag{3.18}$$

where the second exponential accounts for logarithmic surface fluctuations (the $\sqrt{K/\ln|\mathbf{x}/a|}$ prefactor is the normalization) and the *sum* over integers n accounts for the discreteness of the underlying lattice (or height variable). Performing the sum in (3.18) (using the Poisson summation formula) yields,

$$C_{\mathrm{ord}}(q_z;\mathbf{x})=\sum_{m=-\infty}^{\infty}\left|\frac{\mathbf{x}}{a}\right|^{-(q_z-G_0m)^2/4\pi K}, \tag{3.19}$$

where we have used $G_0=2\pi/a$. The dominant term in this sum at large $|\mathbf{x}|$ is clearly the one with the smallest value of $(q_z-G_0m)^2$. This is readily seen to be the term with $m=[q_z/G_0+\frac{1}{2}]$, where $[x]$ is the largest integer $<x$. Therefore, the asymptotic form of $C_{\mathrm{ord}}(q_z;\mathbf{x})$ is algebraic, with the exponent $\eta_{\mathrm{ord}}(q_z)$ taking a "scalloped" periodic form:[1,14]

$$\eta_{\mathrm{ord}}(q_z)=\frac{1}{4\pi K}\left[q_z-G_0\left[\tfrac{1}{2}+\frac{q_z}{G_0}\right]\right]^2;\ q_z>0\ . \tag{3.20}$$

Here the square brackets denote the integer part. Equation (3.20) is plotted in Fig. 1.

When the crystal is *disordered,* $\eta(q_z)$ must be computed from (2.8) or the replicated form (2.16). Provided the interface is in the rough phase, where u flows to zero at long distances, the correlation function C can be evaluated as an expansion in powers of u [from (2.16)]. Each successive even power of u (i.e., u^{2m}) proves to dominate $C(q_z;\mathbf{x})$ [and thereby $\eta(q_z)$] in the interval $m<(q_z/G_0)<m+1$. The general form for $\eta(q_z)$ is calculated in Appendix B. We find

$$\eta(q_z)=\frac{G_0^2}{4\pi\tilde{K}}\left\{(2-K/\tilde{K})\left[\frac{q_z}{G_0}\right]^2+\left[\frac{q_z}{G_0}\right]\left[1+\left[\frac{q_z}{G_0}\right]-2\frac{q_z}{G_0}\right]\right\},\ \ q_z>0\ , \tag{3.21}$$

where once again the square brackets denote the integer part. This curve is sketched in Fig. 1. Not surprisingly, the exponent (3.21) lies between the parabolic fluid exponent and the exponent for the ordered crystal (3.20). The atomic discreteness of the ordered crystal interface is still evident in the exponent for the disordered solid's surface.

B. Crystal shapes

For a crystal with true long-range order, the conventional smooth to rough interfacial transition manifests itself in the equilibrium crystal shape, or equivalently the Wulff plot (see Fig. 6). A smooth interface corresponds to a cusp in the Wulff plot and a crystal facet. In the rough phase the angle-dependent surface tension $\gamma(\theta)$ is analytic even for $\theta=0$, $(\gamma(\theta)=\gamma_0+\frac{1}{2}\gamma_0''\theta^2)$, which corresponds to a crystal symmetry axis.

One might ask whether the rough to super-rough transition, for a *disordered* solid, is also manifest in the Wulff plot (or angular-dependent surface tension). Below is a brief argument that this is in fact not the case; $\gamma(\theta)$ *always* varies quadratically for small θ, in both the rough and the super-rough phase, with a coefficient that varies smoothly at the transition.

The angular dependence of the surface tension can be extracted by evaluating the free energy from (2.10) with appropriate boundary conditions

$$h(x=L,y)=h(x=0,y)+\theta L\ . \tag{3.22}$$

Equation (3.22) imposes an interfacial tilt, by an angle θ, away from the crystal symmetry axis. For an interface of size $L\times L$ (in the x-y plane) one then has

$$\gamma(\theta)=F_L(\theta)/(L^2\sec\theta),\ \ L\to\infty\ .$$

When the system is replicated, as in (2.8), the boundary condition (3.22) applies to *each* of the n interfaces $\{h_\alpha\}$. This fact enables one to relate $F(\theta)$ trivially to $F(\theta=0)$. Specifically, for each configuration h_α of the tilted inter-

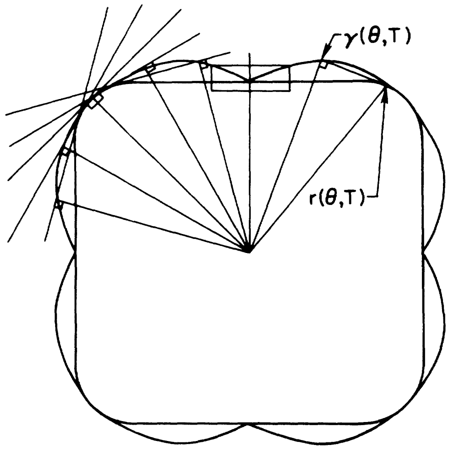

FIG. 6. The Wulff construction for determining the equilibrium crystal shape $r(\theta,T)$ given the direction dependent surface tension $\gamma(\theta,T)$. The construction consists of drawing a radius from the origin to each point on a polar plot (actually a three-dimensional surface, through which this figure is a two-dimensional slice) of $\gamma(\theta,T)$. One then draws the planes [which in this 2(d) figure are, of course, lines] orthogonal to each of these radius vectors. The resultant infinite set of planes fills all of the space except for a hole in the middle whose shape is the equilibrium shape of the crystal. Cusps in the polar plot of $V(\theta,T)$ are readily seen via this construction to lead to flat facets in the equilibrium crystal shape.

face satisfying the boundary condition (3.22), define an "untilted" configuration by $\tilde{h}_\alpha = h_\alpha - (\theta x/L)$. The terms in H that depend only on $h_\alpha - h_\beta$ are unaffected by this change of variable, since all of the replicas change in the same way. The replicated Hamiltonian (2.16) can therefore be simply written in terms of $\tilde{h}_\alpha$ as

$$\beta H(\{h_\alpha\}) = \beta H(\{\tilde{h}_\alpha\}) + \frac{n}{2}\tilde{K}\theta^2 L^2 \ . \tag{3.23}$$

The change of variables ($h \rightarrow \tilde{h}$) can also be performed in the functional integral for the partition function. Since $\tilde{h}_\alpha$ satisfies the appropriate boundary condition for an untilted interface ($\theta = 0$), one thereby obtains, quite generally,

$$F(\theta) = F(0) + \tfrac{1}{2}\tilde{K}\theta^2 L^2 \ . \tag{3.24}$$

Note that the result (3.24) is *independent* of the strength of the disorder u. Moreover, it applies to *both* the rough and super-rough phases. Thus, in contrast to the conventional smooth to rough transition for an ordered crystal, the rough/super-rough transition has no effect on either the Wulff plot or the crystal shape.

The preceding conclusion might seem a bit surprising, particularly in view of the fact that the interfacial height-height correlation functions evaluated in Sec. III A, *do* differ in the rough and super-rough phases. To see that this is *not* inconsistent with (3.24), it is instructive to rederive (3.23) for small θ, using only $\theta = 0$ interfacial correlation functions. To this end, imagine applying an external "tilt" field μ to the interface Hamiltonian (2.6), $H \rightarrow H + (\mu/L)\int d^2x\, \partial_x h$. The *mean* tilt angle θ follow from the free energy per area, $f(\mu)$ as

$$\theta = \overline{\langle \partial_x h \rangle} = -\frac{\partial f}{\partial \mu}(\mu = 0) \ . \tag{3.25}$$

Since the angular-dependent surface tension $\gamma(\theta)$ is the Legendre transformation of f, $\gamma(\theta) = f + \theta\mu$, the curvature γ_0'' is equal to $-(\partial^2 f/\partial\mu^2)^{-1}$, evaluated at $\mu = 0$. Thus γ_0'' can be expressed in terms of a *connected* interfacial correlation function for the untilted interface, namely.

$$\gamma_0'' = L^{-2}\int d^2x\, d^2x' [\overline{\langle \partial_x h(x)\partial_x h(x')\rangle} - \overline{\langle \partial_x h(x)\rangle\langle \partial_x h(x')\rangle}] \ . \tag{3.26}$$

After replicating, Fourier transforming, and performing an ensemble average one has

$$(\gamma_0'')^{-1} = \frac{1}{(2\pi)^2}\lim_{q\rightarrow 0} q^2[\langle |h_\alpha(q)|^2\rangle - \langle h_\alpha(q)h_\beta(-q)\rangle] \ , \tag{3.27}$$

where the brackets now refer to an average with respect to the replicated Hamiltonian (2.16) and $\beta \neq \alpha$ is understood.

The height-height correlation function evaluated in Sec. II B also depends directly on the average $\langle |h_\alpha(q)|^2\rangle$. As noted there, the singular small q dependence of $\langle |h_\alpha(q)|^2\rangle$ differs in the rough ($1/q^2$) and super-rough ($\ln q/q^2$) phases. However, in the *connected* correlation function (3.27) this difference cancels out between the two terms. Indeed, upon evaluating (3.27) using H from (2.16) with $u = 0$, one finds that the K dependence of the two terms cancels, yielding simply $\gamma_0'' = \tilde{K}$. Since $\tilde{K}$ is unrenormalized, this reduces to the trivial result (3.24). Thus, all the differences between the rough and super-rough phases, manifest separately in the two contributing terms in (3.27), cancel one another exactly in the "connected" combination. This is closely analogous to the relation between the magnetic susceptibilities and structure factors in random field magnets,[15,16] and reconfirms our earlier statement that the crystal shapes are unaffected by the super-roughening transition.

IV. CROSSOVERS

In the preceding sections we have discussed the behavior of the surface only for length scales L large compared to the bulk correlation length ξ_B. In this section, we consider the crossover between this behavior and the bulk-ordered behavior which prevails for $L < \xi_B$, and the consequences of this crossover for the correlation functions, the Wulff plot, and the equilibrium crystal shape.

We begin by summarizing the behavior of the bulk-ordered crystal as obtained from the standard theory of roughening.[1] This theory predicts that below the roughening temperature T_R (which we will show in a moment is very nearly equal to but always slightly greater tan T_{SR}), the correlation function $C(q_z;\mathbf{x})$ is given by

$$C(q_z;\mathbf{x}) \equiv \langle e^{iq_x[h(\mathbf{x}) - h(\mathbf{0})]}\rangle \sim \begin{cases} |\mathbf{x}|^{-\eta_P(q_z)}, & |\mathbf{x}| < \xi_P \\ C_\infty(q_z) \ , & |\mathbf{x}| > \xi_P \ , \end{cases} \tag{4.1}$$

where the correlation length ξ_P diverges at the roughening temperature T_R as

$$\xi_P \sim \exp[B/\sqrt{(T_R - T)/T_R}] \tag{4.2}$$

and $C_\infty \eta_p(q_z)(q_z)$ vanishes like $(\xi_P)^{-\eta_P(q_z)}$, as can readily be seen by matching at $|\mathbf{x}| = \xi_P$. [In Eq. (4.2) B is a dimensionless constant of order unity.] In all of these expressions, $\eta_P(q_z)$ is the exponent for algebraic decay for the bulk ordered surface given in Eq. (3.20). The constant behavior of C at large $|\mathbf{x}|$ is the signature of the asymptotic flatness of the surface; hence we will refer to it as the smooth behavior. For $T > T_R$, ξ_P is infinite, and the algebraic behavior described above persists out to the bulk correlation length ξ_B. This behavior is summarized in Fig. 3, which shows the different regimes of behavior of the correlation function $C(q_z;\mathbf{x})$ at different temperatures.

We will now show that the roughening temperature T_R is close to but always slightly larger than the super-roughening temperature T_{SR}. The bulk-ordered problem is described by a Hamiltonian of the form Eq. (2.16), but of course with the random field $\phi = 0$. Both K and u renormalize in this model; in the smooth phase, K and u both renormalize to infinity, while in the rough phase u renormalizes to zero while K renormalizes to a finite value (the smooth and rough phases are in this renormalization-group sense precisely analogous to the super-rough and rough phases, respectively, of the bulk-disordered problem). Of course, the bulk-ordered recursion relations cease to hold and are superseded by the bulk-disordered recursion relations given in Eq. (2.21), once we have renormalized out to ξ_B (which occurs after a renormalization-group time $l^*=\ln[\xi_B/a)]$. The renormalized elastic constants $K_{\text{pure}}(l^*)$ and $V_{\text{pure}}(l^*)$ derived from the bulk-*ordered* recursion relations then enter as *initial* conditions on $\tilde{K}$, K, and u in the bulk-*disordered* recursion relations; in particular,

$$\tilde{K}(l^*)=K_{\text{pure}}(l^*), l^*\equiv\ln(\xi_B/a) \ . \tag{4.3}$$

Our expression below Eq. (2.17) for $\tilde{K}$ in terms of K, V, and ξ_B may be thought of as a lowest order in V form of this more general result. $\tilde{K}$ does not renormalize any further once we are beyond l^* (since we are then at length scales greater than ξ_B, where, as we showed earlier, $\tilde{K}$ does not renormalize), so its value for all length scales larger than ξ_B is determined by (4.3). The pure correlation length ξ_P separates those length scales ($|\mathbf{x}|<\xi_P$) on which the bulk-ordered problem[1] is *smooth* from those on which it is *rough;* this implies that for length scales

$$|\mathbf{x}|\gg\xi_P,\ K_{\text{pure}}[l=\ln(|\mathbf{x}|/a)]$$

has renormalized to very large values (specifically,

$$K_{\text{pure}}(l)\gg K_c^{\text{pure}}=\tfrac{1}{2}\tilde{K}_c=\frac{G_0^2}{8\pi} \ , \tag{4.4}$$

which implies that $K_{\text{pure}}(l)\gg G_0^2$) while for

$$|\mathbf{x}|<\xi_P, K_{\text{pure}}(l=\ln(|\mathbf{x}|/a))$$

remains of order G_0^2. Thus

$$l_{\text{smooth}}\equiv\ln\frac{\xi_P(T)}{a} \ , \tag{4.5}$$

is the renormalization-group time that separates large $K_{\text{pure}}(l)$ from $K_{\text{pure}}(l)\sim O(G_0^2)$. Therefore, at those temperatures where $l_{\text{smooth}}\ll l^*$ as defined in (4.3), $K_{\text{pure}}(l^*)$, and hence, using (4.2), $\tilde{K}(l^*)$, will be driven to very large values. (Specifically $\gg G_0^2$.) We will therefore be in the super-rough phase. We can only reach sufficiently small values of $K_{\text{pure}}(l^*)$ and hence $\tilde{K}(l\to\infty)$ to have a super-roughening transition (which occurs at $\tilde{K}=G_0^2/4\pi$) by making $l_{\text{smooth}}\sim l^*$, which implies, using (4.3) and (4.5), that $\xi_P(T_{\text{SR}})\sim\xi_B$. This, in turn, implies, using (4.2), that

$$T_{\text{SR}}=T_R\left\{1-g\Big/\left[\ln\left[\frac{\xi_B}{a}\right]\right]^2\right\} \ , \tag{4.6}$$

where $g\equiv B^2$ is of order unity. This shows that the super-roughening transition in a bulk disordered crystal with correlation length $\xi_B\gg a$ will occur at a temperature T_{SR} quite close to the temperature T_R at which the roughening transition would occur in a bulk-ordered crystal of the same material.

We can also use this result to estimate $d\tilde{K}/dT|_{T_{\text{SR}}}$, which we need, via Eqs. (3.13) and (3.14), to calculate the temperature dependence of ξ_{SR} near T_{SR}. Since $\tilde{K}$ must change from its value $\tilde{K}_c=G_0^2/4\pi$ at T_{SR} to the value $K_c^{\text{pure}}=G_0^2/8\pi$ at T_R, its derivative in this temperature range is of order

$$\left.\frac{d\tilde{K}}{dT}\right|_{T_{\text{SR}}}=\frac{K_c^{\text{pure}}-\tilde{K}_c(T_{\text{SR}})}{T_R-T_{\text{SR}}}=-\frac{\ln^2(\xi_B/a)}{gT_{\text{SR}}}\frac{G_0^2}{4\pi} \ . \tag{4.7}$$

Inserting this into Eq. (3.14) for A shows that

$$A=\frac{1}{32\pi^2}\frac{(2-K_a)}{\tilde{K}}\frac{g^2A_u^2}{A_K}\ln^{-4}\left[\frac{\xi_B}{a}\right] \ . \tag{4.8}$$

All of the factors in this expression are of order unity except for $\ln^{-4}(\xi_B/a)$, which is $\ll 1$ for $\xi_B\gg a$. Thus, $A=O(\ln^{-4}(\xi_B/a))$, as claimed in the introduction.

Although, as we showed in Sec. III, the Wulff plot and the equilibrium crystal shape are unaffected by the super-roughening transition, both are affected by the (nearly sharp) *roughening* transition when $\xi_B\gg a$.

We can understand this by noting that when the crystal is cut at an angle θ, the equilibrium configuration of the surface is a set of steps of height a separated by a mean distance a/θ (see Fig. 7). For $T<T_R$, the Wulff plot will show three distinct regimes: In region 1 (see Fig. 8), the tilt angle θ is greater than a/ξ_P, which means that characteristic features of the surface (i.e., steps) are separated by less than ξ_P. As just discussed, at this length scale the crystal should exhibit bulk-ordered rough behavior; this means that the Wulff plot should go like a parabola $\sigma(\theta)\approx K'\theta^2$, where K' is the elastic constant in Eq. (2.8) and σ is the surface energy. For $a/\xi_B<\theta<a/\xi_P$ (i.e., for length scales between ξ_P and ξ_B), the surface looks smooth, meaning that the Wulff plot becomes linear (region 2 in Fig. 8). It must join smoothly to the parabola in region 1, which means that the slope of this straight line is $(a/\xi_P)K$. Finally, in region 3 where $\theta<a/\xi_B$, the surface is disorder-dominated rough (or superrough; it does not matter), so the Wulff plot is again parabolic; to join smoothly to the straight line in region 2, $\sigma\approx(\xi_B/\xi_P)\theta^2$.

When $\xi_B\gg\xi_P$ (i.e., at low temperature), the curvature in region 3 is very high. This leads, via the Wulff construction, to a crystal shape which has nearly the appearance of a normal faceted crystal. At sufficiently high temperatures the crystal will also contain rounded regions with radius of curvature of order L coming from regions I and II of the Wulff plot. We have not shown such regions in Fig. 2 for clarity. Figure 2 shows this crystal shape for a hypothetical square crystal. The crystal also contains "pseudofacets" which come from region 3 of the

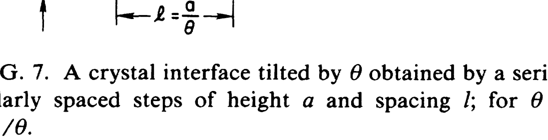

FIG. 7. A crystal interface tilted by θ obtained by a series of regularly spaced steps of height a and spacing l; for $\theta\ll 1$, $l=a/\theta$.

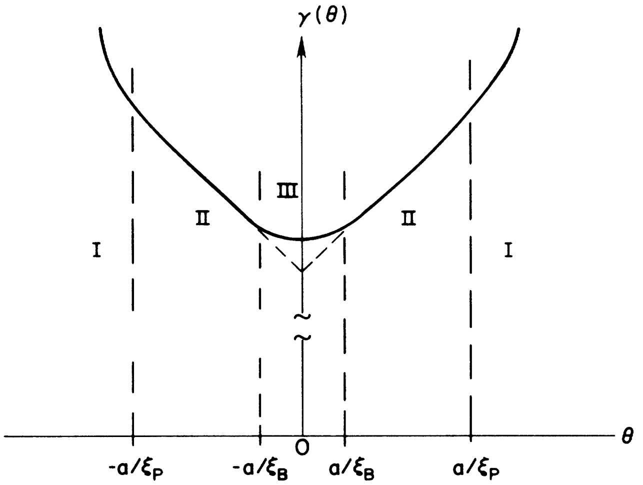

FIG. 8. A magnified view of the Wulff plot for small θ in a bulk-disordered crystal below $T_{\rm SR}$, showing the curved regions at $\theta \gg a/\xi_P$, the straight (cuspy) region $a/\xi_p \gg \theta \gg a/\xi_B$, and the (sharply but not infinitely) curved region $\theta \ll a/\xi_B$.

Wulff plot. The radius of curvature here is very large: $R=(\xi_B/\xi_P)L$. This makes sense, since in a perfect crystal $\xi_B \rightarrow \infty$ and there are perfectly flat facets with infinite radius of curvature. As the temperature increases and ξ_P, begins to approach ξ_B, two things happen to the crystal shape: curved regions appear and grow because the slope in region 2 of Fig. 8 is decreasing, and the pseudofacets shrink and become more curved. When T gets near T_R, the curvature of the pseudofacet and of the curved region gradually become equal and the two parts of the crystal surface merge. The curvature at this point should be near the universal value which occurs in ordinary pure roughening. However, there is no real phase transition in the crystal shape; all the changes described here occur continuously.

ACKNOWLEDGMENTS

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APPENDIX A

In this Appendix we will discuss the rounding of the super-roughening transition due to the dependence of $\phi(\mathbf{R})$ on h in Eq. (2.4) and show that while in principle this is an important effect, in practical experiments the rounding should be unobservable.

For the sake of simplicity in the later calculations, we will begin by assuming that the phase correlation function in Eq. (2.2) has the separable form

$$f(\mathbf{R}/\xi_B)=g_\perp(\mathbf{x}/\xi_B)g_z(z/\xi_B)\ , \tag{A1}$$

where $\mathbf{x}$, as before, denotes the two components of $\mathbf{R}$ in the mean plane of the surface, while z denotes the direction orthogonal to the surface. We do not believe that this simplifying assumption restricts the generality of our results. We will also assume that g_z decays exponentially for $z \gtrsim \xi_B$, and furthermore, that it is analytic near $z=0$. This last assumption, and the assumption that the correlation functions depend *only* on the ratio $\mathbf{R}/\xi_B$, innocuous though they appear, are both violated by many of the standard forms usually assumed in fitting the x-ray peak shapes of disordered systems. For example, a Lorentzian peak implies

$$\langle e^{i[\phi(\mathbf{R})-\phi(0)]}\rangle \propto e^{-|\mathbf{R}/\xi_B|}/|\mathbf{R}|\ ,$$

which is neither analytic as $|\mathbf{R}|\rightarrow 0$ nor a function only of the ratio $\mathbf{R}/\xi_B$. In critical phenomena, one more generally observes correlations of the form $|\mathbf{R}|^{2-d+\eta}g(|\mathbf{R}|/\xi_B)$, which likewise violate both our assumptions.

Nonetheless, we believe that in the case of quenched disorder, both assumptions are correct. We will return to this point at the end of this Appendix. For now, we will explore the implications of Eq. (A1) for the super-roughening transition.

We proceed, as earlier, by replicating the partition function and performing the quenched averages over disorder perturbatively in V. Everything goes through as before up to the point of evaluating the quenched averages. These now become [cf. Eq. (2.14)]

$$\overline{\cos[G_0 h_\alpha(\mathbf{x})+\phi(\mathbf{x},h_\alpha)]}=0 \tag{A2}$$

$$\overline{\cos[G_0 h_\alpha(\mathbf{x})+\phi(\mathbf{x},h_\alpha(\mathbf{x}))]\cos[G_0 h_\beta(\mathbf{x}')+\phi(\mathbf{x}',h_\beta(x'))]}$$
$$=\tfrac{1}{2}\cos\{G_0[h_\alpha(\mathbf{x})-h_\beta(\mathbf{x}')]\}g_\perp(\mathbf{x}-\mathbf{x}'/\xi_B)g_z([h_\alpha(x)-h_\beta(x')]/\xi_B) \tag{A3}$$

Upon reexponentiating and gradient expanding, these lead to the replicated Hamiltonian:

$$H=\int d^2x \left[\tfrac{1}{2}K_{\alpha\beta}\sum_{\alpha,\beta=1}^{n} \nabla h_\alpha(\mathbf{x})\cdot\nabla h_\beta(\mathbf{x}) - u\sum_{\alpha\neq\beta} V(h_\alpha(\mathbf{x})-h_\beta(\mathbf{x})) \right]\ , \tag{A4}$$

where

$$V(y)=\cos(G_0 y)g_z(y/\xi_B)\ . \tag{A4$'$}$$

We now proceed by Fourier transforming $V(y)$ as a function of its argument y. The Hamiltonian (A4) can be rewritten:

$$H=\int d^2x\left[\tfrac{1}{2}K_{\alpha\beta}\sum_{\alpha,\beta=1}^{n}(\nabla h_\alpha\cdot\nabla h_\beta)-u\int_{-\infty}^{\infty}\frac{dG}{2\pi}\widetilde{V}(G)\times\sum_{\alpha\neq\beta}\cos\{G[h_\alpha(\mathbf{x})-h_\beta(\mathbf{x})]\}\right], \tag{A5}$$

where

$$\widetilde{V}(G)\equiv\int_{-\infty}^{\infty}\cos(Gy)V(y)dy$$

is the Fourier transform of $V(y)$.

The $\widetilde{V}$ term in this expression is now readily recognized as just a linear superposition of (an infinite number of) terms of the form in Eq. (2.16), with G_0 just replaced, for each of the Fourier components $\widetilde{V}(G)$, by the appropriate G. Because it is such a linear superposition, the recursion relations to linear order for each $\widetilde{V}(G)$ are precisely the same as those for u found earlier [cf. Eq. (2.21)] except for the replacement $G_0 \to G$ and $u \to \widetilde{V}(G)$. Thus we have

$$\frac{d\widetilde{V}(G)}{dl}=\left[2-\frac{G^2}{2\pi\widetilde{K}}\right]\widetilde{V}(G)\ . \tag{A6}$$

This recursion relation can be instructively rewritten by Fourier transforming back to real space, giving a partial differential equation recursion relation for $V(y,l)$

$$\frac{\partial V(y,l)}{\partial l}=\left[2+\frac{1}{2\pi\widetilde{K}}\frac{\partial^2}{\partial y^2}\right]V(y,l)\ . \tag{A7}$$

Writing $V(y,l)=e^{2l}U(y,l)$ we obtain a diffusion equation for U,

$$\frac{\partial U}{\partial l}(y,l)=\frac{1}{2\pi\widetilde{K}}\frac{\partial^2 U}{\partial y^2} \tag{A8}$$

with the renormalization-group "time" l playing (appropriately) the role of time. We can easily solve this equation using Green functions and the initial condition

$$U(y,l=0)=V(y,l=0)=\cos(G_0y)g_z(y/\xi_B)\ .$$

Doing so and using our expression for V in terms of U gives an expression for $V(y,l)$,

$$V(y,l)=\left[\frac{\widetilde{K}}{2l}\right]^{1/2}e^{2l}\int_{-\infty}^{\infty}dx\, e^{-\pi\widetilde{K}(x-y)^2/2l}\times\cos(G_0x)g_z\left[\frac{x}{\xi_B}\right]. \tag{A9}$$

A good measure of the effect of the renormalized potential on the height fluctuations (and hence on all the other features of this problem) is the renormalized mass

$$M(l)\equiv-\left.\frac{\partial^2 V}{\partial y^2}\right|_{y=0}, \tag{A10}$$

which combined with (A9) yields

$$M(l)=-\left[\frac{\widetilde{K}l}{2}\right]^{1/2}e^{2l}\int_{-\infty}^{\infty}dx\cos(G_0x)g_z\left[\frac{x}{\xi_B}\right]\times e^{-\pi\widetilde{K}x^2/2l}\frac{\pi\widetilde{K}}{l}\times\left[\frac{\pi\widetilde{K}}{l}x^2-1\right]. \tag{A11}$$

Now we proceed by expanding $g_z(x/\xi_B)$ in powers of its argument, and asymptotically evaluating (A11) in the limit $(G_0\xi_B)\gg G_0^2l/\widetilde{K}\gg 1$. We obtain

$$M(l)=G_0^2\exp\left[\left[2-\frac{G_0^2}{2\pi\widetilde{K}}\right]l\right]\times\left[1-\frac{1}{2}\left[\frac{lG_0}{\pi\widetilde{K}\xi_B}\right]^2\left.\frac{dg_z^2(t)}{dt^2}\right|_{t=0}+O\left[\left[\frac{lG_0^2}{\widetilde{K}\xi_BG_0}\right]^4,\ \frac{lG_0^2}{\widetilde{K}(\xi_BG_0)^2}\right]\right] \tag{A12}$$

The lowest-order term in this expression (i.e., the 1) is the only one we would have gotten using the approximation we have made throughout this paper of neglecting the dependence of the random phase ϕ on h.

Clearly this approximation breaks down once the second-order term is comparable to the first. Since by our assumption of analyticity, $d^2g(t)/dt^2|_{t=0}$ is of order 1, this will occur when $lG_0/\pi\widetilde{K}\xi_B\sim O(1)$, or $l\sim\pi\widetilde{K}\xi_B/G_0$. Converting this to a length scale via the relation $L=\xi_Be^l$ (the prefactor is ξ_B because our starting Hamiltonian (A4) had an implicit ultraviolet cutoff of ξ_B because of the gradient expansion) yields

$$L_c=\xi_Be^{\alpha(\xi_B/a)}, \tag{A13}$$

where $a\sim\widetilde{K}a^2$ is of order 1 (in the temperature regime of interest where $\widetilde{K}\sim G_0^2/4\pi\sim\pi/a^2$). This is, of course, the result quoted in the introduction.

We now return to the question of whether or not the ϕ correlation functions should depend only on the ratio $\mathbf{R}/\xi_B$, and if so, whether or not this dependence is analytic. In critical phenomena, we are familiar with correlation functions of the form

$$C(\mathbf{R})=R^{2-d+\eta}g(R/\xi)\ ,$$

which are clearly *not* functions of $\mathbf{R}/\xi$ alone. However, the origin of this form is clear: the factor $R^{2-d+\eta}$ is the scaling behavior of the correlation function at the critical point, where $\xi=\infty$; ξ defines the length scale at which this scaling behavior starts to break down. An analogous form for the correlation function of a crystal with quenched bulk disorder would be

$$C(R)=|\mathbf{R}|^{2-d+\eta}g(\mathbf{R}/\xi_B)\ ;$$

with again, the factor $R^{2-d+\eta}$ representing the decay of order when $\xi_B=\infty$ there is, by definition, no quenched disorder in the solid (in contrast to the critical phenomena case, where, even at the critical point, there are still large fluctuations—namely, the critical fluctuations—leading to decorrelation); ergo, we have a perfect ordered crystal in this limit. The correlation function, therefore, must not decay when $\xi_B=\infty$; hence $\eta=d-2$ and $C(\mathbf{R})=g(\mathbf{R}/\xi_B)$, as we assumed here.

In renormalization-group jargon, the correlation length ξ in critical phenomena is associated with flows away from a finite temperature, disordered fixed point, characterizing the system at T_c, where $C(R)$ already decays to zero as $|\mathbf{R}|\to\infty$; while in the quenched disorder problem, ξ_B is associated with flows away from an ordered, $T=0$ fixed point characterizing the pure, ordered crystal, in which $C(\mathbf{R}\to\infty)$ is finite, reflecting the presence of long-ranged order.

This argument is supported by an analytic calculation[17] of $C(\mathbf{R})$ for a simple model of a tangled quenched random array of dislocations. This calculation also finds an analytic $C(\mathbf{R}/\xi_B)$ near $R=0$.

APPENDIX B

In this Appendix, we compute the exponent $\eta(q_z)$ for the algebraic decay of the experimentally measurable correlation function

$$C(q_z,\mathbf{x}\equiv\overline{\langle\exp\{iq_z[h(\mathbf{x})-h(\mathbf{0})]\}\rangle}\propto\left|\frac{\mathbf{x}}{a}\right|^{-\eta(q_z)} .$$

We begin by writing in terms of the replica fields h_γ:

$$C(q_z,\mathbf{x})=\langle\exp\{iq_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]\}\rangle , \tag{B1}$$

where the average is over the Hamiltonian (2.16) in the usual $n\to0$ limit. We proceed by evaluating this average perturbatively in u. This leads to

$$\begin{aligned}C(q_z,\mathbf{x})&=\left\langle\exp\left[iq_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]+u\sum_{\alpha\neq\beta}\int d^2x_1\cos\{G_0[h_\alpha(\mathbf{x}_1)-h_\beta(\mathbf{x}_1)]\}\right]\right\rangle_G\\&=\sum_{m=0}^{\infty}\frac{u^m}{m!}\int\left[\prod_{i=1}^{m}dx_i\right]\sum_{\{\alpha_i\neq\beta_i\}}\left\langle\exp\{iq_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]\}\prod_{j=1}^{m}\cos\{G_0[h_{\alpha_j}(\mathbf{x}_j)-h_{\beta_j}(\mathbf{x}_j)]\}\right\rangle_G ,\end{aligned}\tag{B2}$$

where $\sum_{\{\alpha_i\neq\beta_i\}}$ is a sum over all n possible values (remember $n\to0$ at the end) of each α_i and β_i, with i running from 1 to m, and α_i and β_i not equal, and where $\langle\ \rangle_G$ denotes an average over the Gaussian ensemble defined by the Hamiltonian (2.16) with $u=0$.

We will first go explicitly through the first few terms in the expansion to identify those terms in the sum on $\{\alpha,\beta\}$ and regions of integration over $\mathbf{x}_i$ which dominate each term in perturbation theory. These low-order terms establish a pattern which permits us to write down the dominant terms at arbitrary order. We evaluate these terms, and we finally identify which order, for a given q_z, dominates at large $|\mathbf{x}|$; this will give us our final result for $\eta(q_z)$. We have verified that this approach, when applied to the pure (bulk-ordered) roughening problem, recovers the result, Eq. (3.20), derived by other means.

Consider first the zeroth-order term

$$C_0(q_z,\mathbf{x})=\langle e^{iq_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]}\rangle_G . \tag{B3}$$

Using the fact that for a variable with a Gaussian distribution $\langle e^x\rangle=e^{1/2\langle x^2\rangle}$,

$$C_0(q_z,\mathbf{x})=\exp\{-\tfrac{1}{2}q_z^2\langle[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]^2\rangle_G . \tag{B4}$$

The Gaussian average in the exponential is now readily evaluated using Eq. (2.19) and some straightforward Fourier transform manipulations. We find

$$C_0(q_z,\mathbf{x})=A_0\left|\frac{\mathbf{x}}{a}\right|^{-\eta_0(q_z)} ,\quad |\mathbf{x}|\to\infty , \tag{B5}$$

with

$$\eta_0(q_z)=\frac{q_z^2}{2\pi\widetilde{K}}\left[2-\frac{K}{\widetilde{K}}\right] . \tag{B6}$$

Here $a=2\pi/G_0$ is a lattice constant, and the constant A_0 is a dimensionless "fudge factor" of order unity that takes into account fluctuations on short length scales (large q) which are not accurately described by Eq. (2.19).

The first-order term

$$C_1(q_z,\mathbf{x})=\sum_{\alpha\neq\beta}\int d^2x'\langle e^{iq_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]}\times\cos\{G_0[h_\alpha(\mathbf{x}')-h_\beta(\mathbf{x})]\}\rangle_G \tag{B7}$$

vanishes in the thermodynamic ($L\to\infty$) limit, for all $\mathbf{x}$. To see this, we rewrite the cosine using $\cos x=(e^{ix}+e^{-ix})/2$ and again use the fact that for a Gaussian ensemble $\langle e^x\rangle=e^{1/2\langle x^2\rangle}$. This yields

$$\begin{aligned}C_1(q_z,\mathbf{x})=\sum_{\alpha\neq\beta}\int d^2x'\exp(-\tfrac{1}{2}\langle\{q_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]\\-G_0[h_\alpha(\mathbf{x}')-h_\beta(\mathbf{x}')]\}^2\rangle_G)\\+(G_0\to-G_0)\end{aligned}\tag{B8}$$

Consider for the moment just the piece of the argument of the exponential proportional to the G_0^2. This piece is also proportional to

$$C_{\alpha\beta}=\langle h_\alpha^2(\mathbf{x}')\rangle_G+\langle h_\beta^2(\mathbf{x}')\rangle_G-2\langle h_\alpha(\mathbf{x}')h_\beta(\mathbf{x}')\rangle_G .$$

Using Eq. (2.19) and Fourier transforming back to real space yields

$$C_{\alpha\beta}=\frac{1}{\pi\tilde{K}}\ln\left(\frac{L}{a}\right)\left[2-\frac{K}{\tilde{K}}-\left(1-\frac{K}{\tilde{K}}\right)\right]$$

$$=\frac{\ln(L/a)}{\pi\tilde{K}}\to\infty$$

as $L\to\infty$, where L is the linear extent of the surface. Thus the argument of the exponential in Eq. (B8) has a piece proportional to G_0^2 which goes to $-\infty$ in the thermodynamic limit. This *cannot* be cancelled (for arbitrary a_z) by any of the other terms arising from the expansion of the exponent in Eq. (B8), since those terms have a different dependence on G_0. After exponentiating, the power-law dependence on L given by the preceding equation is sufficiently strong to make this term vanish in the thermodynamic limit.

Consider now the second-order term

$$C_2(\mathbf{x})=\sum_{\alpha\neq\beta,\alpha'\neq\beta'}\int d^2x'd^2x''\exp(-\tfrac{1}{2}\langle\{q_z[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]+G_0[h_\alpha(\mathbf{x}')-h_\beta(\mathbf{x}')+h_{\alpha'}(\mathbf{x}'')-h_{\beta'}(\mathbf{x}'')]\}^2\rangle_G) \tag{B9}$$

$+3$ other sign permutations.

In light of our experience with the first-order term, a natural first step in evaluating this term seems to be to identify those terms proportional to $G_0^2\ln(L/a)$ in the argument of the exponential. For the explicitly displayed term in (B9), we find that $G_0^2\ln(L/a)$ has coefficient

$$c_2=-2(\delta_{\alpha\alpha'}+\delta_{\beta\beta'}-\delta_{\alpha\beta'}-\delta_{\beta\alpha'})-4\ . \tag{B10}$$

c_2 is nonpositive definite, and can only vanish when $\alpha=\beta'$ and $\beta=\alpha'$. Only for this choice of indices can the second-order term Eq. (B9) *not* vanish. Once we have made this choice, we can rewrite the coefficient of G_0^2 in the exponential as

$$\langle[h_\alpha(\mathbf{x}')-h_\alpha(\mathbf{x}'')+h_\beta(\mathbf{x}'')-h_\beta(\mathbf{x}')]^2\rangle$$
$$=(2/\pi\tilde{K})\ln[|(\mathbf{x}'-\mathbf{x}'')/a|]$$

where we have again used Eq. (2.19) and Fourier transformed back to real space. We have also used the fact that $\alpha\neq\beta$. This term gives the integrand in (B9) an overall multiplicative factor of

$$\left|\frac{\mathbf{x}'-\mathbf{x}''}{a}\right|^{-G_0^2/\pi\tilde{K}}\ . \tag{B11}$$

The exponent $G_0^2/\pi\tilde{K}$ is >4 in the rough regime $\tilde{K}<G_0^2/4\pi$; hence the integral in (B9) (over the difference $\mathbf{x}-\mathbf{x}''$) converges in the infrared. This factor makes the integral tend to be dominated by points with $\mathbf{x}'$ close to $\mathbf{x}''$. Now consider the cross term proportional to q_zG_0 in the argument of the exponential in (B9). By the same manipulations as before, we now find that this leads to a multiplicative factor of

$$\left(\frac{|\mathbf{x}-\mathbf{x}'||\mathbf{x}''|}{|\mathbf{x}'||\mathbf{x}-\mathbf{x}''|}\right)^{(q_zG_0/\pi\tilde{K})(\delta_{\alpha\gamma}-\delta_{\beta\gamma})}\ . \tag{B12}$$

This is the only term that connects the dummy points $\mathbf{x}'$ and $\mathbf{x}''$ to the two points $\mathbf{0}$ and $\mathbf{x}$ that we are trying to calculate. Those terms in the sum on α and β with neither α nor $\beta=\gamma$, therefore, clearly cannot change the dependence of $C(q_z,\mathbf{x})$ on $\mathbf{x}$ from its zeroth-order form, since for those terms the exponent in (B12) vanishes and the dependence on $\mathbf{x}$ comes exclusively from the $\{q_2[h_\gamma(\mathbf{x})-h_\gamma(\mathbf{0})]\}^2$ term in the exponent in (B9), which is precisely the factor that determined the zeroth-order dependence on $\mathbf{x}$. So clearly any different dependence on $\mathbf{x}$ comes from those terms in the sum on α and β with either $\alpha=\gamma$ or $\beta=\gamma$ (but not both, since $\alpha\neq\beta$). For $\beta=\gamma$, the factor (B12) is largest when $\mathbf{x}''$ is near $\mathbf{0}$ and $\mathbf{x}'$ is near $\mathbf{x}$. For $q_zG_0/\pi\tilde{K}>2$, the integrals over $\mathbf{x}'$ and $\mathbf{x}''$ converge near these regions; this condition is always satisfied for $q_z>G_0$ in the rough regime. For smaller q_z, the integral over $\mathbf{x}'$ and $\mathbf{x}''$ is dominated by those regions far from $\mathbf{x}$ and $\mathbf{0}$. As discussed before, when this happens this term has the same functional dependence on $|\mathbf{x}|$ as the zeroth-order term.

Returning to the case $q_zG_0/\pi\tilde{K}>2$, performing the convergent integrals over $\mathbf{x}'$ and $\mathbf{x}''$ amounts, for large $|\mathbf{x}|$, to absorbing the numerical values of these integrals into an overall multiplicative constant and replacing $\mathbf{x}'$ with $\mathbf{0}$ and $\mathbf{x}''$ with $\mathbf{x}$ in (B9). This yields

$$C_2(q_z,\mathbf{x})=c'\left|\frac{\mathbf{x}}{a}\right|^{-\eta_2}\ , \tag{B13}$$

where

$$\eta_2=\frac{G_0^2}{2\pi\tilde{K}}\left[\left(2-\frac{K}{\tilde{K}}\right)\left(\frac{q_z}{G_0}\right)^2-\frac{2q_z}{G_0}+2\right] \tag{B14}$$

and we have ignored all of the aforementioned terms that have the same dependence on $\mathbf{x}$ as the zeroth-order term.

Note that $\eta_2<\eta_0$ when $q_z>G_0$: thus in that regime of $q_zC_2(q_z,\mathbf{x})\gg C_0(q_z,\mathbf{x})$ as $|\mathbf{x}|\to\infty$. This means that once q_z grows beyond G_0, the asymptotic exponent of algebraic decay $\eta(q_z)$ of the full $C(q_z,\mathbf{x})$ changes abruptly from $\eta_0(q_z)$ to $\eta_2(q_z)$. There is no actual discontinuity in $\eta(q_z)$, since $\eta_2(G_0)=\eta_0(G_0)$; its slope $d\eta(q_z)/dq_z$ is discontinuous, however. We shall now show that such a changeover happens every time q_z passes an integral multiple of G_0: at $q_z=mG_0$, $\eta(q_z)$ goes from being equal to η_{2m-2} to η_{2m}, where η_{2m} is the exponent of algebraic decay of the largest term at $2m$'th order in perturbation theory.

The same type of analysis of the next few even terms in perturbation theory shows that a few simple rules determine which terms in the sums over the dummy indices $\{\alpha_i,\beta_i\}$ and which regions of integration over the dummy variables $\mathbf{x}_i$ dominate. These rules are in exact correspondence with the second-order case just presented: (1) All of the indices must be equal to other indices in pairs; otherwise the term vanishes in the thermodynamic limit $L \to \infty$, or it makes a contribution which vanishes at large $\mathbf{x}$ (i.e., has larger η). (2) For each i, one of the indices must be $=\gamma$. (3) For each equal pair of indices, the integral over the dummy position variables $\{\mathbf{x}_i\}$ is dominated by the regime in which one of them is equal to $\mathbf{x}$, and the other to zero. The integrals around these regions converge for $q_z G_0/\pi\tilde{K} > 2$; so, for large $\mathbf{x}$, we can, up to an overall multiplicative factor, simply replace each $\mathbf{x}_i$ by either $\mathbf{x}$ or $\mathbf{0}$.

Using these rules, we can rewrite the general $2m$'th order term as

$$C_{2m} = A_{2m} \sum_{p=1}^{m} \sum_{\{\beta_p\}} \exp\left[-\tfrac{1}{2} \left\langle \left[(q_z - mG_0)[h_\gamma(\mathbf{x}) - h_\gamma(\mathbf{0})] + G_0 \sum_{p=1}^{m} [h_{\beta_p}(\mathbf{x}) - h_{\beta_p}(\mathbf{0})] \right]^2 \right\rangle_G \right] , \tag{B15}$$

where A_{2m} is a constant. Evaluating the average in the exponential as before yields

$$C_{2m} = A_{2m} \sum_{\{\beta_p\}} \left| \frac{\mathbf{x}}{a} \right|^{-\eta_{2m}(\{\beta_p\})} \tag{B16}$$

with

$$\begin{aligned} \eta_{2m}(\{\beta_p\}) = \frac{1}{2\pi\tilde{K}} \Bigg[& (q_z - mG_0)^2 \left[2 - \frac{K}{\tilde{K}} \right] + 2(q_z - mG_0) mG_0 \left[1 - \frac{K}{\tilde{K}} \right] \\ & + mG_0^2 \left[2 - \frac{K}{\tilde{K}} \right] + G_0^2 [m^2 - m - n_e] \left[1 - \frac{K}{\tilde{K}} \right] + n_e \left[2 - \frac{K}{\tilde{K}} \right] G_0^2 \Bigg] . \end{aligned} \tag{B17}$$

Here $n_e(\{\beta_p\})$ is the number of pairs of β's that are equal to each order. Reorganizing this rather messy expression gives

$$\eta_{2m}(\{\beta_p\}) = \frac{G_0^2}{2\pi\tilde{K}} \left[\left[\frac{q_z}{G_0} \right]^2 \left[2 - \frac{K}{\tilde{K}} \right] + m \left[1 - \frac{2q_z}{G_0} \right] + m^2 + n_e \right] . \tag{B18}$$

Clearly, at large $|\mathbf{x}|$, the dominant term in the sum over $\{\beta_p\}$ in (B16) is that with the *smallest* $\eta_{2m}(\{\beta_p\})$; inspection of (B18) makes it clear that this is the term with all of the β's different; $n_e = 0$. Keeping only this term at each order, and summing all the C_{2m}'s, we obtain an expression for $C(q_z, \mathbf{x})$:

$$C(q_z, \mathbf{x}) = \sum_{m=0}^{\infty} A_{2m} \left[\left| \frac{\mathbf{x}}{a} \right| \right]^{-\eta(m, q_z)} \tag{B19}$$

with

$$\eta(m, q_z) = \frac{G_0^2}{2\pi\tilde{K}} \left[\left[\frac{q_z}{G_0} \right]^2 \left[2 - \frac{K}{\tilde{K}} \right] + m^2 + m \left[1 - \frac{2q_z}{G_0} \right] \right] \tag{B20}$$

Note that this agrees with Eq. (B14) for $m = 1$.

The sum in (B19) is also dominated, at large $\mathbf{x}$, by the term with the smallest $\eta(m)$. Minimizing (B20) over all integer m gives $m = [q_z/G_0]$, where $[y]$ is the largest integer $< y$. Inserting this into (B20) and keeping only the corresponding term in (B19) gives Eq. (3.21) for $\eta(q_z)$.

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[1] See, e.g., S. T. Chui and J. D. Weeks, Phys. Rev. B **14**, 4978 (1976); J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, *ibid.* **16**, 1217 (1977). For a more recent discussion see C. Rottmann and M. Wortis, *ibid.* **29**, 328 (1984); and H. van Beijeren and I. Nolden, in *Structure and Dynamics of Surfaces II*, edited by W. Schommers and P. von Blanckenhagen (Springer, Berlin, 1987).

[2] Doubts about this picture have been raised by F. S. Rys, Phys.

Rev. Lett. **56**, 624 (1986).

[3] See, e.g., E. H. Conrad *et al.*, J. Chem. Phys. **84**, 1015 (1986); **85**, 4756(E) (1986); J. Lapujoulade, J. Perreau, and A. Karra, Surf. Sci. **129**, 59 (1983); F. Fabre, D. Gorse, J. Lapujoulade, and B. Salanon, Europhys. Lett. **3**, 737 (1987); G. A. Held, J. L. Jordan-Sweet, P. M. Horn, A. Mak, and R. J. Birgeneau, Phys. Rev. Lett. **59**, 2075 (1987).

[4] This includes all work except for the work of T. L. Ho, J. A. Jaszczak, Y. H. Li, and W. F. Saam, Phys. Rev. Lett. **59**, 1116 (1987). They treat a different mechanism (namely, bond-orientational order) for faceting, which leads to very different behavior from that we find here.

[5] An *equilibrium* phase of this type would be a three-dimensional analog of the 2D hexatic [B. I. Halperin and D. R. Nelson, Phys. Rev. Lett. **41**, 121 (1978); **41**, 519(E) (1978); D. R. Nelson and B. I. Halperin, Phys. Rev. B **19**, 2457 (1979)]. Since crystals with *quenched* bulk translational disorder have this property by definition.

[6] The analogous statement in two dimensions was proven in M. Rubinstein and D. R. Nelson, Phys. Rev. B **26**, 6254 (1982).

[7] The distinction between quenched and annealed disorder is discussed in, e.g., S. K. Ma, *Modern Theory of Critical Phenomena* (Benjamin, Reading, MA, 1976), Chap. 10.

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[10] Except that we allow a finite range ξ_B for correlations of ϕ, whereas in the random field problem one usually takes $\xi_B = 0$. This difference is unimportant in the long-wavelength limit.

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[14] See, e.g., the first of Ref. 3.

[15] E. Pytte, Imry, and D. Mukamel, Phys. Rev. Lett. **46**, 1173 (1981).

[16] We are grateful to E. Pytte for pointing out the similar cancellation that occurs in this problem, knowledge of which helped us immeasurably in producing the derivation presented here.

[17] J. Toner (unpublished).