Ground-state properties of solid-on-solid models with disordered substrates

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We study the glassy *superrough* phase of a class of solid-on-solid models with a disordered substrate in the limit of vanishing temperature by means of *exact* ground states, which we determine with a minimum-cost-flow algorithm. Results for the height-height correlation function are compared with analytical and numerical predictions. The domain-wall energy of a boundary-induced step grows logarithmically with system size, indicating the marginal stability of the ground state, and the *fractal* dimension of the step is estimated. The sensibility of the ground state with respect to infinitesimal variations of the quenched disorder is analyzed. [S0163-1829(97)52112-6]

There has been much interest recently in the properties of crystal surfaces upon disordered substrates,[1–4] in particular the effect of the presence of pinning potentials on surface roughening. Further motivation comes from the close relationship of the corresponding disordered solid-on-solid model to the two-dimensional vortex-free XY model with random fields and to the randomly pinned planar flux array.[5–13] The latter is particularly relevant with respect to the technologically important aspect of flux pinning in high-T_c superconductors.[14]

It has been demonstrated that these systems have a phase transition at a critical temperature from a thermally rough phase into a *superrough* phase at low temperatures. Whereas the existence of this transition is established by now, the qualitative and quantitative features of the glassy low-temperature phase are still debated. Predictions of earlier renormalization-group (RG) calculations[15,6,2,9] turned out to be incompatible with results of extensive numerical simulations.[10,3,11] The subsequent discovery of the relevance of replica-symmetry-breaking (RSB) effects in variational[16] and RG (Refs. 12 and 13) calculations lead to a variety of results, from which those obtained by the variational treatment are again in disagreement with the most recent numerical study.[17,18]

For us the situation seems to be the following: close to the transition the discrimination between various predictions is numerically hard because of its smallness on intermediate length scales. Far from the transition (i.e., deep in the glassy phase at low temperatures) the picture should become much clearer, meaning that the disorder-dominated effects become stronger. The clearest evidence for the latter can be expected for strictly zero temperature, when the roughness is exclusively produced by the substrate alone. However, to reach this limit, Monte Carlo simulations of glassy systems like those we are interested in suffer from notorious equilibration problems.[19] At zero temperature the properties of the system under discussion are completely determined by its minimal energy configuration or ground state. Since, as we show in this paper, it is possible to calculate this state *exactly*, a detailed and reliable picture of the zero-temperature limit of the glassy phase can be obtained.

Thus the aim of the present paper is twofold: first we calculate numerically the zero temperature limit of the height-height correlation function for finite systems and compare the result with various analytical predictions and finite temperature simulations. Second, motivated by the observation of manifestly glassy features (like RSB, slow dynamics, metastable states) in the low-temperature phase, we ask how far concepts developed for finite-dimensional spin glasses can be applied here, and explore the nature of this ground state in much greater detail. We investigate its stability with respect to step excitations, analyze this fractal-boundary-induced domain wall itself, and study the chaotic nature of the ground state by an application of infinitesimal variations of the substrate heights. To our knowledge, these important issues have never been discussed in the present context.

The solid-on-solid (SOS) model we consider here is defined by the Hamiltonian

$$H=\sum_{\langle ij\rangle} f(h_i-h_j), \tag{1}$$

where $\langle ij\rangle$ are nearest-neighbor pairs on a d-dimensional lattice ($d=1$ and 2), and $f(x)$ is an arbitrary convex $[f''(x)\geqslant 0]$ and symmetric $[f(x)=f(-x)]$ function, for instance, $f(x)=x^2$. Each height variable $h_i=d_i+n_i$ is the sum of an integer particle number, which can also be negative, and a substrate offset $d_i\in[0,1[$. For a flat substrate, $d_i=0$ for all sites i, we have the well known SOS model.[20] The disordered substrate is modeled by random offsets $d_i\in[0,1]$.[2] In the present paper we are only interested in uncorrelated disorder, meaning that all offsets are distributed independently. The method we use is, however, applicable to any disorder distribution, in particular to the case of correlated disorder (i.e., $[d_i d_{i+\mathbf{r}}]_{\rm av}=g(\mathbf{r})$, with $g(\mathbf{r})$ an arbitrary function).[4] In what follows, $[\,]_{\rm av}$ denotes the disorder average.

The random offsets induce a frustration into the system in the same sense as quenched randomness in the inter-

action strengths does in the context of spin-glass models.[19] The minimum-energy surface (being the set of particle numbers $\{n_i\}$ that minimize the energy function H), is no longer flat ($h_i=$const.), but a highly nontrivial object, and the calculation of this ground state is a complex combinatorial optimization problem. By introducing the height difference variables $x_{ij}=n_i-n_j$ for links on the dual lattice we can reformulate our task as a *minimum cost flow* problem

$$\text{minimize}\sum_{\langle ij\rangle} c_{ij}(x_{ij}), \tag{2}$$

with integer x_{ij} and convex, flow-dependent (i.e., x-dependent) cost functions $c_{ij}(x)=f(x-d_{ij})$, $d_{ij}=d_i-d_j$. For this problem we developed an efficient pseudopolynomial algorithm which is described in much detail in Ref. 21. It is guaranteed to find the *exact* ground state, typically in 15 min on a Sparc 20 workstation for a system with $N=256\times256$ sites. We used fixed boundary conditions (b.c.'s) for the model (because for technical reasons[21] the algorithm works only on a planar graph). We would like to point out that this is the first extensive application of a minimum cost flow algorithm to a problem in theoretical physics to our knowledge.[22]

Much effort, numerically as well analytically, has been devoted to the calculation of the height-height correlation function $C(\mathbf{r},\mathbf{r}')=[(h_{\mathbf{r}}-h_{\mathbf{r}'})^2]_{\text{av}}$ in the case $f(x)=x^2$ close to the transition.[2,3,6–13,15–18] The zero-temperature limit has not been investigated so far and the results we present here are the first reported in the literature,[23] to our knowledge. At high temperatures ($T\gg T_g=2/\pi$) one expects $C(\mathbf{r},\mathbf{r}')=T/2\pi\ln|\mathbf{r}-\mathbf{r}'|$ in an infinite lattice. Because of the natural bending of this logarithmic curve by any boundary conditions this expression should be replaced[17] for finite lattices by $C(\mathbf{r},\mathbf{r}')=T/2\pi P_L(\mathbf{r},\mathbf{r}')$, where for fixed b.c.'s the propagator is given by

$$P_L(\mathbf{r},\mathbf{r}')=\frac{2}{L^2}\sum_{n,m=1}^{L}\frac{[\sin(q_0xn)\sin(q_0ym)-\sin(q_0x'n)\sin(q_0y'm)]^2}{2-\cos q_0n-\cos q_0m}, \tag{3}$$

with $\mathbf{r}=(x,y)$, $\mathbf{r}'=(x',y')$ and $q_0=\pi/(L+1)$. As mentioned above, at low temperatures $T<T_g$ different scenarios are currently under discussion in the literature: a Gaussian scaling, with $C(r)$ linear in $\log(r)$, and a $\log^2(r)$ behavior. In the first case a plot $C(r)$ versus $P_L(r)$ should yield a straight line, in the second case one should be able to fit $C(r)$ to a quadratic polynomial in $P_L(r)$ (see Ref. 17).

We define the site averaged correlation function. $\overline{C(r)}=2/L^2\sum_{x=1}^{L/2}\sum_{y=1}^{L}[(h_{(x,y)}-h_{(x+r,y)})^2]_{\text{av}}$, and also the corresponding site-averaged lattice propagator $\overline{P_L(r)}$, which behaves for $L\to\infty$ and $r\ll L$ like $\overline{P_L(r)}\sim\ln(r)/2\pi$. In Fig. 1 we show $\overline{C(r)}$ versus $\overline{P_L(r)}$ for a system size $L=128$. Obviously one does *not* obtain a straight line, which one would obtain if $\overline{C(r)}\sim a_0+a_1\overline{P_L(r)}$. Thus the Gaussian scaling $\overline{C(r)}\propto\log(r)$ for $r\to\infty$ can definitely be excluded on these length scales.

Moreover, although a fit like $\overline{C(r)}\sim a_0+a_1\overline{P_L(r)}+a_2\overline{P_L(r)}^2$ works fine at first sight, there is still a significant bending in the plot of $\overline{C(r)}/\overline{P_L(r)}$ versus $\overline{P_L(r)}$ shown in the inset of Fig. 1, indicating the possible presence of even higher-order terms. The fit parameters $a_1=0.21$ and $a_2=0.57$ are compatible with a linear zero-temperature extrapolation of the finite T results of Ref. 17. The existence of a $\log^2$ term is compatible with earlier[6,1,2,9] replica symmetric RG calculations and with the most recent one involving RSB.[12,13] Note that the RG prediction for the coefficient is[9] $a_2/2\pi=2/\pi^2\tau^2+\mathcal{O}(\tau^3)$, where τ is the distance from the critical point. Since $\tau=1$ in our case ($T=0$), it is hard to compare the numerical value of the coefficient. Neglecting the higher order corrections one obtains $a_2/2\pi=2/\pi^2\approx0.20$, which is twice as large as our estimate.

We also studied the correlation function for different convex cost functions $f(x)=|x|^n$ with varying n. We observed that with increasing power n for smaller distances, large height differences $|x_{ij}|>1$ are suppressed due to their larger costs. At larger distances, however, the roughness increases systematically with n, expressed in monotonically increasing fit values for the coefficient of the $\log^2$ term. This is due to the *decreased* costs for small height differences ($x_{ij}=\pm1$).

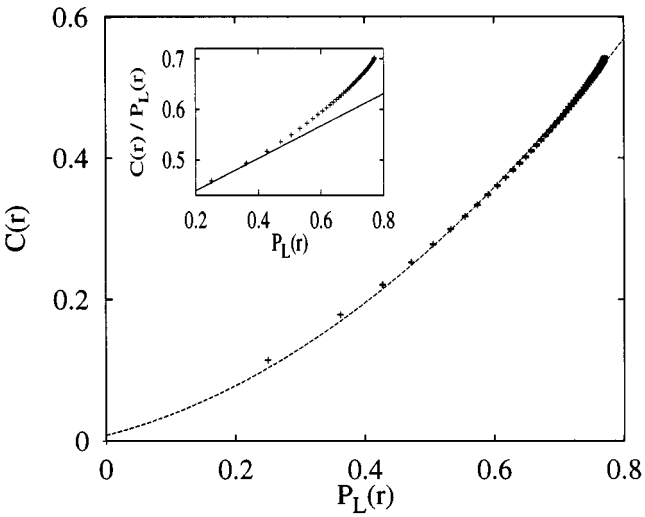

FIG. 1. The site averaged correlation function $\overline{C(r)}$ versus the lattice propagator $\overline{P_L(r)}$ for $L=128$ and averaged over 2000 samples. The broken line is a least square fit to $\overline{C(r)}=0.008+0.21\overline{P_L(r)}+0.57\overline{P_L(r)}^2$. The inset shows $\overline{C(r)}/\overline{P_L(r)}$ versus $\overline{P_L(r)}$, and the straight line indicates the amount of curvature of the data.

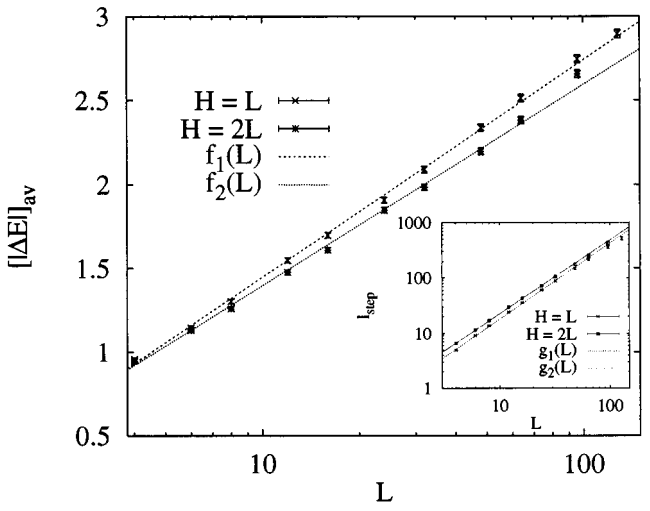

FIG. 2. The averaged step energy $[|\Delta E|]_{\rm av}$ as a function of system size L, averaged over 10^4 samples. It is $f_1(L)=0.15+0.56\ \ln(L)$ and $f_2(L)=0.19+0.52\ \ln(L)$, see Eq. (4). The inset shows the step length $\mathcal{L}_{\rm step}$ as a function of system size. Here it is $g_1(L)=0.77L^{1.37}$ and $g_2(L)=1.04L^{1.33}$; see Eq. (5). The boxes are data for an $L\times 2L$ geometry, the crosses for $L\times L$. Note that for larger H the step energy is slightly smaller and the step length slightly larger, since the step has more space to optimize its configuration.

Moreover, we conclude that the coefficient for the $\log^2$ term is a non-universal number at zero temperature because of its significant dependence on the actual shape of the cost function $f(x)$.

An intriguing question concerns the stability of the ground state with respect to thermal fluctuations. To attack this problem we take over the concept of domain-wall renormalization that is well known in the context of random spin systems:[24–26] we ask how much energy a step (or domain wall) of height 1 in a system of linear size L would cost. If this energy is an increasing function of the size L, it indicates the stability of the ground state even at finite temperatures (disregarding other, more complicated excitations). The step is induced by appropriate boundary conditions: we fix the lower boundary to zero ($h_{(x,0)}=0$), and the upper boundary to 1 ($h_{(x,L+1)}=1$). At the left and right boundaries we enforce $h_{(0,y)}=h_{(L+1,y)}=\theta(y-L/2)$, with $\theta(x)=0$ for $x<0$ and $\theta(x)=1$ for $x\geqslant 0$. This procedure induces a straight step ($h_{(x,y)}=0$ for $y<L/2$, $h_{(x,y)}=1$ for $y\geqslant L/2$) in the pure case ($d_i=0$), which costs an energy $\Delta E=L$ (implying that the flat surface is stable at finite temperatures in this case). In addition to quadratic geometries we also varied the height (i.e., the distance between the upper and lower boundaries) and considered rectangular geometries with $L\times H$ sites.

We calculated the ground state first for $h_i=0$ on the whole boundary, and then for the step inducing boundaries described above [we choose $f(x)=x^2$ from now on]. In Fig. 2 we show the averaged step energy as a function of system size. The data are nicely fitted by a logarithmic L dependence

$$[|\Delta E|]_{\rm av}\sim a+b\ \ln L \quad \text{with} \quad b=0.52\pm 0.02. \tag{4}$$

At first sight the tempting conclusion of this observation would be that there exists a *low-temperature phase with long-range order*, with an order parameter given by the overlap of the system with its ground state (note that the boundaries are fixed so that this definition is unambiguous). However, due to the strong chaotic rearrangement of the state upon temperature changes, which we discuss below, most probably this quasi-long-range order is destroyed at finite temperatures. We think that this result merits a further investigation, e.g., via simulations.

An inspection of the geometrical shape of the step that is induced by the boundary condition described above reveals that it is *fractal*, crossing the whole sample. Therefore we varied H to ensure that the limitation in the y direction does not influence the quantitative results we obtain. We calculated the averaged length of the step as a function of system size, which is depicted in the inset of Fig. 2, and obtain a good fit to be given by

$$\mathcal{L}_{\rm step}\propto L^{d_{\rm step}} \quad \text{with} \quad d_{\rm step}=1.35\pm 0.02, \tag{5}$$

where $d_{\rm step}$ is the fractal dimension[27] of the step. To our knowledge, this is the first estimate of such an exponent in the present context, which we expect to be universal, as we checked for various forms for $f(x)$.

In order to shed further light on the possibly glassy features of the low-temperature phase of our system, we study what became known under the notion of *chaos* in spin glasses.[28,11] For the latter, one observes that infinitesimal variations of temperature or interaction strengths decorrelate the state of the system over a distance that is called the overlap length.[28,11] Here we study the same scenario by infinitesimal (random) perturbations of the offsets of the sample, and comparing the resulting changes in the ground-state configuration. To be concrete we define offsets by $d_i'=d_i+\varepsilon_i$, with $\varepsilon_i\in[-\delta/2,+\delta/2]$ and $\delta\ll 1$, and given the unperturbed and perturbed ground-state heights h_i and h_i', respectively; we are interested in the accumulated height difference

$$\chi_L(\delta)=\sum_i\ [(h_i-h_i')^2]_{\rm av}. \tag{6}$$

To obtain an idea about the scaling behavior of this quantity, let us consider the one-dimensional case first, for which the ground state (with free right boundary condition) can be constructed iteratively. The iteration $h_{i+1}=H(h_i,d_{i+1}-d_i)$ leads asymptotically to a random walk: $[(h_{i+r}-h_i)^2]_{\rm av}\sim r$, with a slightly modified short-distance behavior. The same holds for the random variable h_i-h_i' (with the site index i as ''time''), but its amplitude is reduced by factor δ. Thus in one dimension we expect $\chi_L^{(1d)}(\delta)\sim\delta^2 L$, which we also verified numerically. Note that δ is the inverse length scale beyond which h_i-h_i' becomes typically different from zero if $h_0=h_0'=0$.

Motivated by this observation, we hypothesize the following scaling form for χ_L:

$$\chi_L(\delta)/\delta^{\eta}\sim g(L), \tag{7}$$

with $\eta=2$ in one dimension and $g(L)$ an arbitrary function. In Fig. 3 we show a scaling plot of the data we obtained from

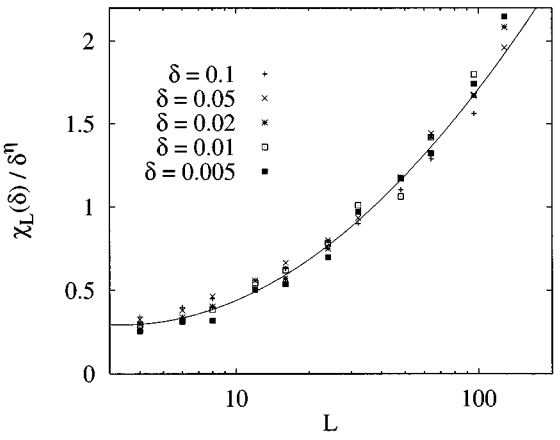

FIG. 3. Scaling plot of χ_L^{2d} as defined in (6) for various values for the perturbation amplitude δ, averaged over 10^4 samples. The best data collapse is obtained for $\eta=0.91$. The full line represents the scaling function involving a dominant $\log^2 L$ term.

our ground-state calculation. The data collapse is acceptable for $\eta=0.91\pm0.05$. One should interpret $1/\delta^\eta$ as the characteristic length scale over which the two ground states decorrelate in analogy to the overlap length in the context of spin glasses.[26,28]

To summarize, our numerical investigation of the zero-temperature limit of the glassy phase in SOS models on disordered substrates revealed the following picture: (1) There *is* a dominant $\log^2(r)$ contribution in the height-height correlation function as predicted by RG calculations. However, we find also indications of the existence of higher nonlinearities in $\log(r)$. (2) Different forms for the microscopic interactions yield qualitatively similar but quantitatively different results for, e.g., the coefficient of the $\log^2$ term (at $T=0$). (3) The step excitation energy increases logarithmically with the system size, indicating a marginal stability of the ground state against thermal fluctuations. (4) The boundary-induced step itself is fractal with a fractal dimension of $d_f\approx1.35$. (5) The concept of the chaos known from spin glasses also applies here, and the chaos exponent for the overlap length is close to 1.

As a future perspective we would like to remark that with our minimum cost flow algorithm it is possible to attack efficiently a large variety of combinatorial optimization problems occurring for disordered and frustrated systems in statistical and solid state physics, in particular those involving ''real'' flows like ensembles of flux lines[14] in lattice models.[29]

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