Geometrical Exponents of Contour Loops on Random Gaussian Surfaces

Jané Kondev and Christopher L. Henley
Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, New York 14853
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We derive the universal geometrical exponents of contour loops on equilibrium rough surfaces, using analytical scaling arguments (confirmed numerically): the fractal dimension D_f, the distribution of contour lengths, and the probability that two points are connected by a contour. This is sufficient to calculate *exact* critical exponents in certain nontrivial two-dimensional spin models that can be mapped to interface models. The novel scaling relation between D_f and the roughness exponent that we find can be used to analyze scanning tunneling microscopy images of rough metal surfaces.

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The study of random Gaussian surfaces has permeated many different areas of physics, ranging from models of biological membranes and crystalline surfaces to string theory [1]. They have been successfully used as a tool for understanding phase transitions in two-dimensional models that can be mapped to a two-dimensional Coulomb gas [2]. These surfaces are self-affine, and have also been widely used to model growth-roughened metal surfaces [3]. Fluctuations in these disparate systems, be they thermal (membranes and interfaces), quantum (strings), or due to a random driving force (deposited surfaces), are those of a random Gaussian surface, and their strength is governed by the *stiffness* K. In this Letter we show that certain geometrical exponents of random Gaussian surfaces are *independent* of the stiffness: namely, those associated with contour loops. This result leads to an exact calculation of all the critical exponents in certain two-dimensional lattice models, and a novel scaling relation for self-affine surfaces. We also propose the *experimental* measurement of these geometrical exponents in STM studies of rough metal surfaces.

(a) Definitions.—A random Gaussian surface is given by the height function $h(\mathbf{r})$, $\mathbf{r} \in \mathbb{R}^2$. We assume that the height takes its values in $\mathbb{R}^2$ or on a circle. The former is used in models of membranes and rough surfaces [1], and the latter is encountered in the Coulomb gas description of two-dimensional critical lattice models [2], and has been studied widely in conformal field theory [4].

The probability distribution functional of $h(\mathbf{r})$ is given by the Boltzmann factor $e^{-f_\zeta[h]}$, where f_ζ is the Gaussian free energy

$$f_\zeta[h] = \frac{K}{2} \int^{1/a} d^2\mathbf{q}(\mathbf{q}^2)^{1+\zeta} |\tilde{h}(\mathbf{q})|^2 . \quad (1)$$

The constant K is the (dimensionless) stiffness, $\tilde{h}(\mathbf{q})$ is the Fourier transform of the height, ζ is the roughness exponent, and $1/a$ is the large momentum cutoff provided by the lattice spacing a. For random Gaussian surfaces encountered in the study of critical models $\zeta = 0$, while a nonzero roughness ($0 \le \zeta \le 1$) is typical of growth roughened metal surfaces. The above free energy also describes height fluctuations in the Edwards-Wilkinson ($\zeta = 0$) and the Mullins-Herring ($\zeta = 1$) models of nonequilibrium surface growth [5].

Now we consider a contour plot of a random Gaussian surface with a fixed spacing Δ between heights of successive contours. In scanning tunneling microscopy (STM) images of rough metal surfaces Δ is usually the height of a single step on the surface; here we take it to be an arbitrary constant much smaller than the typical (rms) fluctuation of $h(\mathbf{r})$. The contour plot consists of closed nonintersecting lines in the plane that connect points of equal height (Fig. 1). In this way to each random surface configuration we assign a configuration of the *contour ensemble*.

We define a contour correlation function $\mathcal{G}_1(\mathbf{r})$, which measures the probability that two points separated by $\mathbf{r}$ lie on the same contour loop. The contour lines are considered to be of finite width given by the cutoff a. Because of rotational symmetry of the contour ensemble $\mathcal{G}_1(\mathbf{r})$ depends on r only, and for large separations ($r \gg a$)

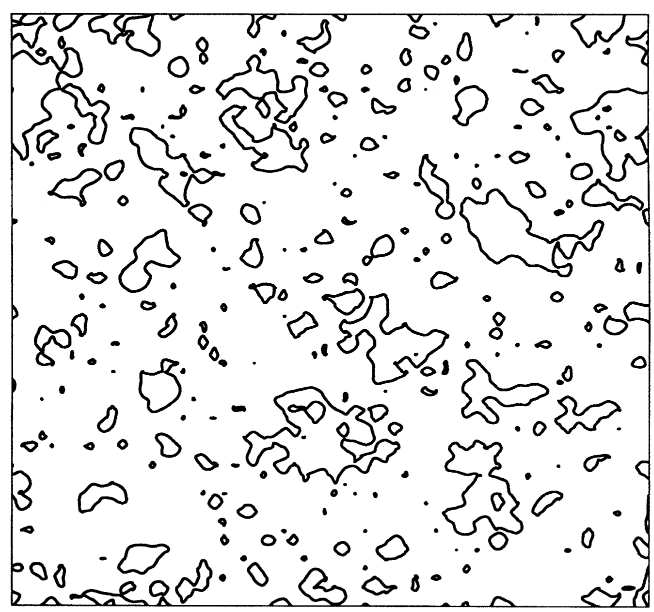

FIG. 1. Contour plot of a $\zeta = 0$ random Gaussian surface.

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it falls off as a power law (as will be shown below),

$$\mathcal{G}_1(r) \sim \frac{1}{r^{2x_1}} . \quad (2)$$

In many critical models on the lattice that renormalize to a Coulomb gas, the exponent x_1 appears as the scaling dimension of a "magnetic" type operator [2].

The fractal dimension D_f is the exponent which relates the length s of a contour to its radius R,

$$s \sim R^{D_f}, \quad (3)$$

where R is defined as the radius of the smallest disk that contains the contour, and s is measured with a ruler of length a. We assume that contours are self-similar, in which case D_f also governs the dependence of s on the ruler length a. The fractal dimension characterizes the shapes of the perimeters of islands one sees in STM images of growth-roughened metal surfaces; a particularly nice example is provided by a recent study of Ag growth on Ag(111) [6].

The distribution of contour lengths $P(s)$ measures the probability that a contour which passes through a fixed point in the plane has a length s, and is given by a power law (as will be shown below),

$$P(s) \sim s^{-(\tau-1)} . \quad (4)$$

(b) Scaling relations.—The fluctuations of a random Gaussian surface are invariant under the rescaling,

$$h(\mathbf{r}) \to c^{-\zeta}\, h(c\mathbf{r}) , \quad (5)$$

where $c > 1$ is an arbitrary constant. This invariance is expressed by the fact that the free energy f_ζ is a fixed point of a momentum-shell renormalization group that consists of integrating out the "fast" Fourier components of the height $\{\tilde{h}(\mathbf{q}) : 1/ca < |\mathbf{q}| < 1/a\}$, followed by a rescaling of $\mathbf{r}$ and h as given by Eq. (5), which restores the cutoff a to its original value.

If we parametrize a contour as $\mathbf{l}(s)$, where s is the arc length as measured by a ruler of length a, then after the rescaling given by Eq. (5) it is mapped to

$$\mathbf{l}(s) \to c^{-1}\mathbf{l}(c^{D_f}s) . \quad (6)$$

In using Eq. (6), we must assume that the contours of the height function obtained by coarse graining a given realization of $h(\mathbf{r})$ are essentially the same as the coarse-grained version of the contours of $h(\mathbf{r})$. This scaling property of the contour ensemble justifies the power law dependence of $\mathcal{G}_1(r)$ on r and $P(s)$ on s, in Eqs. (2) and (4), respectively, and it leads to the conclusion that x_1 is *independent* of K. This is to be expected since contour loops are insensitive to the amplitude of height fluctuations, which is controlled by the stiffness. Also note that Eqs. (5) and (6) are valid for any self-affine surface, not just a Gaussian one.

The fractal dimension D_f and the exponent τ can be related to the exponent x_1 by the following simple scaling argument, similar to the one given by Saleur and Duplantier [7]. First, consider the ensemble mean $\chi(R)$ of the length of that portion of the contour passing through the origin $\mathbf{0}$ which lies within a radius R from $\mathbf{0}$. This is proportional to the following integral:

$$\chi(R) \sim \int_0^R \mathcal{G}_1(\mathbf{r})\, d^2\mathbf{r} . \quad (7)$$

On the other hand, using the distribution of contour lengths Eq. (4), we can estimate $\chi(R)$ as

$$\chi(R) \sim \int_0^\infty \min(s, R^{D_f}) P(s)\, ds . \quad (8)$$

The factor s is used for contours whose radius is less than R; for contours whose radius is greater than R, the portion within a distance R from the origin has length $\sim R^{D_f}$. Equating the right-hand sides of Eqs. (7) and (8) we find the scaling relation

$$D_f(3 - \tau) = 2 - 2x_1 . \quad (9)$$

Second, the average number of contours per unit area $n(R)$, with a radius comparable to R, scales with R as

$$n(R) \sim R^{-2+\zeta} . \quad (10)$$

To come to this conclusion first apply the rescaling Eq. (5) to each configuration of $h(\mathbf{r})$, and then consider its action on the contour ensemble. Consider the *total* number of contours in a box of side R and of radius comparable to it, $R^2 n(R)$. Since the contours are mapped one-to-one in Eq. (6), we can identify this with the number of new contours in a box of side R/c and of comparable radius, $(R/c)^2 n'(R/c) = R^2 n(R)$. The new contour ensemble has a rescaled contour interval $\Delta' = c^{-\zeta}\Delta$, but otherwise it has the same probability weighting as the original one, so $n'(R) = c^{\zeta} n(R)$. Combining these two equations yields Eq. (10).

On the other hand, the number density $n(R)$ can also be calculated from the distribution of loop lengths as

$$n(R) \sim \int_{R^{D_f}}^\infty \tilde{P}(s)\, ds, \quad (11)$$

where $\tilde{P}(s) \sim P(s)/s$ is the probability for a randomly chosen loop to have a length s [as opposed to $P(s)$ for loops going through a fixed point]. Equating Eqs. (10) and (11) leads to the second scaling relation

$$D_f\,(\tau - 1) = 2 - \zeta . \quad (12)$$

The scaling relations Eqs. (9) and (12) for $\zeta = 0$ have been recently derived by Cardy [8] for Wilson loops in the complex $O(n)$ model.

Finally, from the scaling relations Eqs. (9) and (12), we find for the fractal dimension D_f and the exponent τ,

$$D_f = 2 - x_1 - \zeta/2 , \qquad \tau - 1 = \frac{2 - \zeta}{2 - x_1 - \zeta/2} . \quad (13)$$

The first scaling relation is reminiscent of the relation

$$D = 2 - \zeta \quad (14)$$

due to Mandelbrot [9]. The important difference is that this relation gives the fractal dimension D of the *level set* of a random Gaussian surface, and *not* the fractal dimension of a single contour loop. Moreover, Eq. (14) can be easily derived within our framework: Instead of the contour correlation function the correlation function that measures the probability that two points have the same height needs to be considered. It can be shown that this probability is governed by the exponent ζ ($x_1 = \zeta/2$), which leads to Mandelbrot's result, after having made use of the scaling relation Eq. (13).

Now we turn our attention to the contour correlation exponent x_1. It has been calculated *exactly* in the case $\zeta = 0$, from the mapping of the four-state Potts model to a solid-on-solid model [7], $x_1 = 1/2$. We suspect that the value of x_1 in the $\zeta = 0$ ensemble can be calculated using a renormalization group based on the rescaling Eqs. (5) and (6), but we find that this is a nontrivial problem.

We argue that the result $x_1 = 1/2$ is *universal*, independent of ζ. The fractal dimension D_f of a contour loop must satisfy $D \geq D_f \geq 1$, since it is a subset of the level set and has topological dimension one. From this and Eq. (14) we conclude that for $\zeta = 1$ the fractal dimension of a contour loop is $D_f = 1$, which in turn leads to $x_1 = 1/2$ from Eq. (13). Now we *conjecture* that x_1 is a monotonic function of ζ ($0 \leq \zeta \leq 1$) from which we conclude that the exponent x_1 must be constant. The formula for D_f that follows from Eq. (13) differs from the one proposed by Isichenko [10] [$D_f = (10 - 3\zeta)/7$], which was derived from an approximate "multiscale" analysis.

(c) Simulation results.—In order to check the above calculations we have done numerical simulations of a random Gaussian surface for $\zeta = 0$. We generate a large number of surface configurations by doing a fast Fourier transform of $\tilde{h}(\mathbf{q})$ which is sampled from the Boltzmann distribution with a free energy given by the Gaussian model. This model is a discrete version of f_0 defined on the square lattice. For each generated surface we measure the length s and radius R for a contour loop passing through a point picked at random; the contour is a walk on the dual lattice that cuts those bonds of the square lattice that have vertices with heights lying above and below the contour height. The data from 5000 surfaces are plotted on a logarithmic scale in Fig. 2. From a least-squares fit of the data by a line we find $D_f = 1.49 \pm 0.01$ and $\tau - 1 = 1.35 \pm 0.03$, both in agreement with Eq. (13) for $\zeta = 0$ and $x_1 = 1/2$.

For the remainder of this Letter we discuss the relevance of these results for calculating exact exponents in two-dimensional critical lattice models and for experiments on rough metal surfaces.

(d) Critical models.—The fluctuations in many two-dimensional models are well described by f_0, which is equivalent by a duality to the vacuum phase of the two-dimensional Coulomb gas [2]. Here we consider a slightly more general case of a height function with d components which describes a two-dimensional interface in $d + 2$ dimensions; all the results derived for $d = 1$ carry over. Two critical lattice models that we have studied are the $n = 2$ fully packed loop (FPL) model on the honeycomb lattice [11] and the four-coloring model on the square lattice [12].

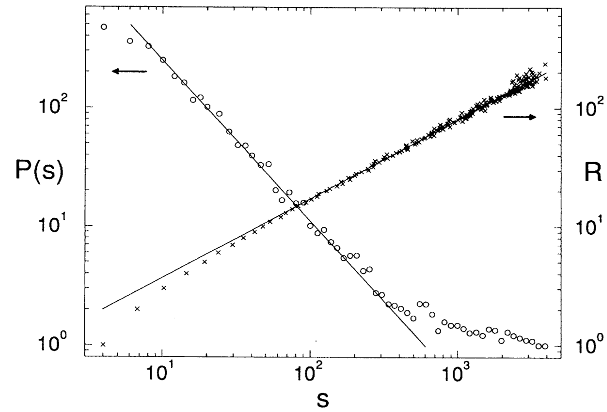

FIG. 2. The radius R ($\times$) as a function of the length s of a contour, and the distribution of contour lengths $P(s)$ ($\circ$) in the Gaussian model. $P(s)$ is the total number of loops of length s, binned in intervals of $0.1s$ at each s. The lines are best fits for $10 < R < 100$ and $10 < s < 300$, respectively. Note that scaling breaks down for small contours due to the cutoff provided by the lattice spacing, and for large contours due to the system size (128×128).

It has been recently shown [13] that the $n = 2$ FPL model is equivalent to the three-coloring model on the honeycomb lattice, which has been exactly solved by Baxter [14]. The three-coloring model can be mapped onto a $\zeta = 0$ random Gaussian surface with two height components ($d = 2$). Contour loops correspond to loops of alternating color, and the contour correlation function exponent can be calculated from Baxter's exact solution to give $x_1 = 1/2$ [13]. This result has also been confirmed numerically [11], and is in agreement with a recent Bethe ansatz solution of the FPL model [15]. Moreover, the distribution of loop lengths for loops of alternating color has been investigated numerically [16], and the exponent in Eq. (4), was found to be 1.34 ± 0.02, in good agreement with the exact result $\tau - 1 = 4/3$ from Eq. (13).

The four-coloring model on the square lattice can be mapped onto a $\zeta = 0$ random Gaussian surface with three height components ($d = 3$) [17]. Contour loops correspond to loops of alternating color, and recent simulations of this model [17] have found $x_1 = 0.497 \pm 0.004$, $D_f = 1.501 \pm 0.003$, and $\tau - 1 = 1.30 \pm 0.03$, all in excellent agreement with our analytical results.

In the above-mentioned models, we have identified the exponent x_1 with the scaling dimension of a particular "magnetic" charge $\mathbf{b}_1$ of the Coulomb gas [13,17], $2x_1 = K/2\pi\, \mathbf{b}_1^2$. From this we have calculated the stiffness K, and consequently all the critical exponents. In the

$n = 2$ FPL model, for which an exact solution exists, we recover the exponents found previously, while in the case of the four-coloring model we find exponents that are in agreement with the conjecture put forward by Read [12] that this model is in the universality class of the $SU(4)_{k=1}$ Wess-Zumino-Witten model.

Finally, we remark that contour exponents analogous to x_1, τ, and D_f may also be defined for spin models (e.g., Potts models [7]) with noninteger conformal charge, but in those cases $x_1 \neq 1/2$, which can be ascribed to the presence of a background charge in the Coulomb gas [7].

(e) Rough metal surfaces.—Rough metal surfaces obtained under different nonequilibrium growth conditions are often found to have the same scaling property Eq. (5) as random Gaussian surfaces. From STM measurements of these surfaces the height can be extracted and the fractal dimension of contour loops determined. Using the scaling relationship Eq. (13), and the value of the exponent $x_1 = 1/2$, the roughness exponent ζ can be calculated and compared to the values predicted by different models of surface growth.

Measurements of this kind have been carried out recently on gold deposits by Gómez-Rodríguez, Baró, and Salvarezza [18]. From STM images of deposits grown in the fast and slow regimes they determine the fractal dimension to be $D_f \approx 1.5$ and $D_f \approx 1.3$, respectively. We calculate the roughness in these two regimes to be $\zeta \approx 0$ and $\zeta \approx 0.4$. The first is expected for Edwards-Wilkinson type of growth, while the second is in good agreement with the Kardar-Parisi-Zhang equation [3].

Recently STM images of *equilibrium* metal surfaces above the roughening transition have also been obtained [19]. The thermal height fluctuations of these surfaces are described by f_0 [20]. We propose that the fractal dimension of contours can be extracted from the data and compared to $D_f = 3/2$, which is what we expect for $\zeta = 0$ roughness.

In conclusion, we have calculated the geometric exponents related to the contour correlation function, the fractal dimension, and the distribution of contour lengths, for contour loops on random Gaussian surfaces. These results can be used for calculating critical exponents in certain two-dimensional models with integer conformal charge, and they lead to a novel scaling relation for self-affine surfaces that can be used for extracting the roughness exponent from STM images of rough surfaces.

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Note added.—Avellaneda *et al.* [21] have found numerically $D_f = 1.28 \pm 0.015$ for a $\zeta = 0.5$ surface, which is close to the predicted value $D_f = 1.25$, from Eq. (13). We are grateful to M. B. Isichenko for bringing this result to our attention.

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