Vicinal Surfaces and the Calogero-Sutherland Model

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(Received 16 February 1996)

A miscut (vicinal) crystal surface can be regarded as an array of meandering but noncrossing steps. Interactions between the steps are shown to induce a *faceting transition* of the rough surface between a homogeneous Tomonaga-Luttinger liquid state and a low-temperature regime of local step clusters in coexistence with ideal facets. This morphological transition is governed by a hitherto neglected critical line of the well-known *Calogero-Sutherland model*. Its exact solution yields expressions for measurable quantities that compare favorably with recent experiments on Si surfaces. [S0031-9007(96)00702-8]

PACS numbers: 68.35.Rh, 05.30.Fk

Miscutting a crystal at a small angle with respect to one of its symmetry planes produces a *vicinal surface* [1]. It often consists of a regular array of terraces separated by monatomic steps. The steps meander by thermal activation but they do not cross or terminate; their density is determined by the miscut angle. This picture, the well-known *terrace-step-kink model* [2], neglects the formation of islands, voids, and overhangs on the surface, and is hence expected to be valid below the roughening transition of the ideal facet. In the simplest approximation, such steps are modeled as the world lines of *free fermions* moving in one spatial dimension r and imaginary time t, thus taking into account the no-crossing constraint through the Pauli principle [3,4]. While the free fermion model is sometimes a qualitatively satisfactory approximation [5], it has become clear that *interactions* between the steps can induce phase transitions that change the surface morphology drastically [2]. From a theoretical point of view, models of interacting fermions are important realizations of two-dimensional Euclidean field theories, some of which are exactly solvable. For example, steps with short-ranged interactions can be mapped onto the Thirring model and, in the more complex case of reconstructed surfaces, onto the Hubbard model [6] or chiral clock-step models [7].

Interactions between steps are produced by a variety of physical mechanisms [8]. For example, elastic forces lead to a long-ranged mutual *repulsion* that decays as r^{-2} with the step separation r [9]. Short-ranged interactions (including all forces that decay faster than r^{-2}) can be of either sign. Using scanning tunneling microscopy on Cu surfaces, Frohn *et al.* [10] have found evidence for step-step *attractions* that decay over distances of a few lattice spacings. In a beautiful series of x-ray scattering experiments, Song and Mochrie [11] have recently discovered an important manifestation of attractive forces on miscut Si(113) surfaces in equilibrium. At sufficiently high temperatures ($T \gtrsim 1300$ K), a surface of miscut angle θ_0 is a homogeneous ensemble of fermionic steps whose local density $\rho(r,t)$ has the expectation value $\langle \rho(r,t) \rangle = \tan\theta_0 \equiv \rho_0$ and somewhat smaller fluctuations $\langle \rho(r,t)\rho(r',t') \rangle$ than expected for free fermions. As the temperature is lowered, however, the fluctuations increase substantially, until a *faceting transition* occurs at a temperature $T^*(\rho_0) \approx 1200$ K. Below that temperature, the attractive forces cause the steps to cluster locally. Hence the surface splits up into domains of an increased and *temperature-dependent* [12] step density $\langle \rho(r,t) \rangle = \overline{\rho}(T) > \rho_0$ alternating with step-free (113) facets [$\langle \rho(r,t) \rangle = 0$]. A critical temperature $T_c = 1223$ K is identified from the extrapolation $\overline{\rho}(T_c) = 0$.

The idea that short-ranged forces between noncrossing steps may produce a faceting transition goes back to Chui and Weeks [13]. In the mean-field theory of Ref. [2], faceting occurs due to a presumed long-ranged attraction, but the quantitative properties are in conflict with the experimental findings of Ref. [11]. In this Letter, I show that a long-ranged repulsion and a short-ranged attraction can conspire to produce a quite complex temperature dependence of the surface morphology, including a faceting transition in quantitative agreement with these experiments. This gives strong evidence that both kinds of forces are indeed present in the step system. I obtain three temperature regimes characterized by qualitatively different step configurations (see Fig. 1): (a) Well above the critical temperature T_c, the steps are dominated by the no-crossing constraint and the long-ranged repulsion. Hence they are well separated from each other with relatively small fluctuations. Below a crossover temperature $\tilde{T}(\rho_0)$, the short-ranged attraction becomes important. (b) In the critical regime close to T_c, the probability of a

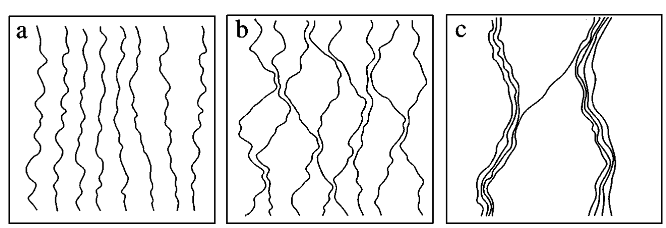

FIG. 1. Typical configurations of noncrossing (fermionic) steps coupled by inverse-square and short-ranged forces. (a) High-temperature regime [$T > \tilde{T}(\rho_0)$]. (b) Critical regime [$\tilde{T}(\rho_0) > T > T^*(\rho_0)$]. (c) Faceted regime [$T < T^*(\rho_0)$].

step being close to one of its neighbors is substantially enhanced. This goes along with increased step fluctuations and a broader distribution of terrace widths. (c) At the temperature $T^*(\rho_0) < T_c$, a first-order faceting transition occurs. Below $T^*(\rho_0)$, the steps form local bundles of density $\overline{\rho}(T) > \rho_0$. On average, the distance between two neighboring bundles is larger than the width of an individual bundle. The fluctuations of these "composite" steps are smaller than those of individual steps.

Specifically, I consider a system of p fermionic lines $r_i(t)$ governed by the effective action

$$S = \frac{1}{T} \int dt \left[\frac{1}{2} \sum_{i=1}^{p} \dot{r}_i^2 + \sum_{i<j} \left[g\,\omega_a(r_{ij}) + h\,\delta_a(r_{ij}) \right] \right], \tag{1}$$

where $\dot{r}_i \equiv dr_i/dt$ and $r_{ij} \equiv r_i - r_j$. The action contains kinetic terms with a line tension normalized to 1, "contact" interactions $\delta_a(r)$ of microscopic range a [14], and an "equal-time" approximation $\omega_a(r) = r^{-2}$ to the elastic interactions for $|r| > a$ [15]. The universal properties can be expressed in terms of the rescaled coupling constants $g_0 \equiv g/T^2$ and $h_0 \equiv h/T^2$. In the limit $\rho_0 a \ll 1$ of small miscut angles, this system can be mapped onto the *Calogero-Sutherland model* [16], an exactly solvable continuum theory well known in the context of the fractional quantum Hall effect and random matrix theory. Its two branches of solutions are labeled by the parameter

$$\lambda^{\pm}(g_0) = \frac{1 \pm \sqrt{1 + 4g_0}}{2}\,. \tag{2}$$

The strong temperature dependence of the surface morphology described above is shown to arise from crossover phenomena between these two branches of solutions. At high temperatures, the surface is governed by the solution $\lambda^+(g/T^2)$. At the critical temperature T_c [implicitly given by $h/T_c^2 = h_0^-(a, g/T_c^2)$, where $h_0^-(a, g_0)$ is a nonuniversal function], the surface scales according to the solution $\lambda^-(g_0^c)$ (as long as $g_0^c \equiv g/T_c^2 < 3/4$; beyond that point, this branch of solutions ceases to exist). The solution $\lambda^-(g_0^c)$ also determines the faceting properties. Hence a number of observables can be predicted in terms of the single nonuniversal parameter g_0^c.

(a) The wave function (5) below yields immediately the step density correlation function $\langle \rho(0,t)\rho(r,t)\rangle \sim \Psi_2^2(r) \sim r^{2\lambda}$ in the limit $|r| \ll \rho_0^{-1}$, where multiparticle effects can be neglected. Two steps at distance r from each other enclose a terrace of width r if no further steps are in between; this condition is also negligible for $r \ll \rho_0^{-1}$. Hence the terrace width distribution, which can be measured by surface scanning techniques, has the same short-distance tail $\sim r^{2\lambda}$ [5]. In the high-temperature regime $[\lambda = \lambda^+(g/T^2) > 1]$, short terraces are rare, while at T_c $[\lambda = \lambda^-(g_0^c) < 0]$, they are abundant.

(b) The surface stiffness γ, defined as the universal prefactor of the height difference correlation function

$$C(r) \equiv \tfrac{1}{2}\,\langle [h(0,t) - h(r,t)]^2 \rangle \simeq \gamma^{-1} \ln|\rho_0 r| + \cdots \tag{3}$$

on scales $|r| \gg \rho_0^{-1}$, shows a characteristic temperature dependence. Its high-temperature asymptotic value is $\gamma = 1/2$. As the temperature is lowered, it first *increases* as $\gamma = \lambda^+(g/T^2)/2 = \lambda^+(g_0^c T_c^2/T^2)/2$, then *decreases* in the critical regime [taking the value $\gamma = -\lambda^-(g_0^c)/2 < 1/4$ at T_c], and again sharply *increases* below $T^*(\rho_0)$ to values $\gamma > 1/2$ for composite steps. Most aspects of this pattern have been observed [11], but the measurements are not yet conclusive in the high-temperature regime.

(c) In the faceted regime, the line bundles are of density $\overline{\rho}(T) \sim (T_c - T)^{1/[1-2\lambda^-(g_0^c)]}$, which agrees with the measured density $\overline{\rho}(T) \sim (T_c - T)^{0.42\pm0.10}$ [11] if $g_0^c \approx 3/4$.

(d) The differences $\tilde{T}(\rho_0) - T_c$ and $T_c - T^*(\rho_0)$ (i.e., the size of the critical regime) scale as $\rho_0^{1-2\lambda^-(g_0^c)}$. This is also consistent with the data for $g_0^c \approx 3/4$.

The solutions of the Calogero-Sutherland model labeled by $0 < \lambda < \infty$ are known to describe a line of Tomonaga-Luttinger liquid critical points [17] that contains the self-dual point $\lambda = 2$, the free fermion point $\lambda = 1$, and the Kosterlitz-Thouless point $\lambda = 1/2$. Notice, however, that for repulsive long-ranged forces ($g > 0$) the root $\lambda^-(g_0^c)$ is negative. Solutions of the Calogero-Sutherland model with $\lambda < 0$ have not been discussed before as they were deemed unphysical. The solutions labeled by $0 > \lambda > -1/2$ form a new line of Tomonaga-Luttinger liquid critical points; faceting on vicinal surfaces seems to be their first realization. This line is the analytic continuation of the line $0 < \lambda < \infty$ beyond the free boson point $\lambda = 0$ (see Fig. 2), and it terminates at its Kosterlitz-Thouless point $\lambda = -1/2$. There is another closely related physical manifestation of the solutions $\lambda^-(g_0^c)$ in the particular case $p = 2$, where the action (1) is a model for two interfaces in a two-dimensional system in the so-called intermediate fluctuation regime [18]. In

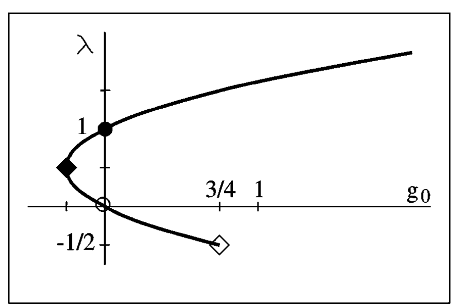

FIG. 2. The two branches $\lambda^+(g_0)$ and $\lambda^-(g_0)$ of the Calogero-Sutherland model. On vicinal surfaces, they govern the high-temperature regime and the faceting transition, respectively. The solutions $0 < \lambda < \infty$ and $0 > \lambda > -1/2$ form two distinct lines of Luttinger liquid critical points. Special points are $\lambda = 1$ (free fermions), $\lambda = 0$ (nonrelativistic free bosons), and $\lambda = \pm 1/2$ (Kosterlitz-Thouless points).

these systems, the well-known line of *wetting* critical points [18,19] turns out to correspond to that branch of solutions. The wetting transition at $T = T_c$ is of second order for $\lambda > -1/2$, but of first order for $\lambda \leq -1/2$ [18,19]. One may speculate that the faceting described here turns into a similar first-order transition at $T = T_c$ for $\lambda^-(g_0^c) \leq -1/2$.

To derive these results, it is convenient to regard the ensemble of steps as a many-body quantum system. The Hamiltonian of this system,

$$H = -\frac{1}{2}\int dr\, \psi^\dagger(r,t)\partial_r^2\psi(r,t) + g_0\Omega_a(t) + h_0\Phi_a(t)\,, \tag{4}$$

acts on p-particle states; its form is determined by the action (1). ψ and $\psi^\dagger$ are anticommuting fields; $\Omega_a(t) \equiv \int dr dr' \rho(r,t)\omega_a(r-r')\rho(r',t)$ and $\Phi_a(t) \equiv \int dr dr' \rho(r,t)\delta_a(r-r')\rho(r',t)$ are the long- and short-ranged interactions written in terms of the density operator $\rho(r,t) \equiv \psi^\dagger(r,t)\psi(r,t)$. In a system of finite width L with periodic boundary conditions and the periodic potential $\omega_a(r) = (\pi^2/L^2)\sin^{-2}(\pi r/L)$ (for $a < r < L - a$), the two-particle ground state takes the exact form [16] $\Psi_2(r_{12}) = \sin^\lambda(\pi r_{12}/L)$ for $a < r_{12} < L - a$, with λ given by Eq. (2). Matching this wave function with the fermionic boundary condition $\Psi_2(0) = \Psi_2(L) = 0$ [20] requires a contact potential of fixed strength $h_0 = h_0^\pm(a, g_0)$. In the limit $a \to 0$, the p-particle ground state is the simple product

$$\Psi_p(r_1,\dots,r_p) = \prod_{i<j}\Psi_2(r_{ij}) \tag{5}$$

with energy $E_p = \lambda^2\pi^2 p(p^2-1)/3L^2$, provided $\lambda > -1/2$ [otherwise the wave function (5) is not normalizable]. An integrable continuum model emerges, known as the Calogero-Sutherland model [16]. The free energy density $f_p = E_p/L$ has a well-defined thermodynamic limit $f(\rho_0) = \lim_{p\to\infty} f_p$ at fixed density $\rho_0 = p/L$, which encodes the bulk properties of the step system.

For a given value $-1/4 < g_0 < 3/4$, the Hamiltonian (4) defines two different continuum theories, corresponding to the branches $\lambda^\pm(g_0)$ in Eq. (2). The stability of these solutions in the thermodynamic parameter space (g_0, h_0) can be studied perturbatively, using the methods of Refs. [21–23] (where more details can be found). The expansion of the dimensionless free energy $F_p \equiv L^3 f_p$ about the branch point $\lambda^\pm = 1/2$ has the form

$$F_p(g_0', h_0') - F_p(0,0) = \frac{(-1)^{M+N}}{M!N!}\sum_{M+N\geq 1} F_{M,N}\, g_0'^M h_0'^N$$

with $g_0' \equiv g_0 + 1/4$, $h_0' \equiv h_0 - h_0^-(a, -1/4)$, and

$$F_{M,N} = \rho_0^{-2}\int \prod_{i=2}^{M+N} dt_i \left\langle \prod_{i=1}^{M}\Omega_a(t_i)\prod_{i=M+1}^{M+N}\Phi_a(t_i)\right\rangle .$$

The brackets $\langle\cdots\rangle$ denote connected expectation values in the unperturbed p-particle ground state (5) at $\lambda = 1/2$. In the limit $a \to 0$, the coefficients $F_{M,N}$ develop logarithmic singularities. With an appropriate normalization of the operators Φ_a and Ω_a, one finds at the lowest orders

$$F_{1,0} = \rho_0^{-2}\langle\Omega_a\rangle = s\rho_0^{-2}\langle\Phi_a\rangle + O(s^0)\,,$$

$$F_{0,2} = \rho_0^{-2}\int dt\,\langle\Phi_a(0)\Phi_a(t)\rangle = 2s\rho_0^{-2}\langle\Phi_a\rangle + O(s^0)\,,$$

and hence

$$F_p(g_0', h_0') - F_p(0,0) = -\rho_0^{-2}\langle\Phi_a\rangle[h_0' + s(g_0' - h_0'^2)] + O(s^0, g_0'^2, g_0'h_0', h_0'^3)\,,$$

where $s \equiv -\ln(\rho_0 a)$. Up to this order, the singularities can be absorbed into the renormalized coupling constant $h_R \equiv h_0'(1 - sh_R) + sg_0' + \cdots$, while no renormalization is needed for g_0. This leads to the parabolic flow equations

$$\frac{d}{ds}g_0 = 0\,, \quad \frac{d}{ds}h_R = \frac{1}{4} + g_0 - h_R^2\,, \tag{6}$$

which are independent of p. They have first been obtained by functional renormalization group methods for $p = 2$ [19] and have been derived for arbitrary p in Refs. [24,25]. It is possible to check that $F_{1,0}$ and $F_{0,2}$ contain the only primitive singularities of the perturbation series. The renormalization group equations (6) are thus exact to all orders in a minimal subtraction scheme.

There are two lines of fixed points, $h_R^\pm = \pm\sqrt{1+4g_0}/2$. The renormalization group eigenvalue of temperature variations (or variations of h_R),

$$y^\pm(g_0) = \frac{1}{2}\frac{\partial}{\partial h_R}\bigg|_{h_R^\pm(g_0)}\left(\frac{dh_R}{ds}\right) = \mp\frac{\sqrt{1+4g_0}}{2}\,, \tag{7}$$

also governs the scaling of the contact operator Φ_a, e.g., $\langle\Phi_a\rangle^\pm(g_0) \sim \rho_0^{2[1-y^\pm(g_0)]}$. This is precisely the scaling of $\langle\Psi_p|\Phi_a|\Psi_p\rangle$ obtained from the exact solution (5) with λ given by (2). The two lines of fixed points $h_R^\pm(g_0)$ can thus be identified with the two branches of solutions $\lambda^\pm(g_0)$ of the Calogero-Sutherland model.

At the fixed points $\lambda^-(g_0^c)$, temperature variations are a relevant perturbation. (For $p = 2$, these fixed points govern the wetting transition at T_c [19].) Above T_c, Eq. (6) yields a crossover to the stable branch of solutions $\lambda^+(g_0)$. Below T_c, the renormalized coupling h_R tends to $-\infty$ under the flow (6), indicating an instability of the step ensemble with respect to the formation of local bundles. The scaling form of the free energy density, $f(\rho_0) \sim \rho_0^3 + (T - T_c)\rho_0^{3-2y^-(g_0^c)}$, determines the singular density dependence of the crossover temperature and of the phase boundary, $\tilde{T}(\rho_0) - T_c \sim T_c - T^*(\rho_0) \sim \rho_0^{2y^-(g_0^c)}$, as well as the characteristic line density $\overline{\rho}(T) \sim (T_c - T)^{1/2y^-(g_0^c)}$ in the faceted regime. On average, a line bundle consists of

$n \approx 20$ lines [11,26] and has a width $n/\overline{\rho}(T)$. Two neighboring bundles at a typical distance n/ρ_0 have an exponentially small overlap $\sim\exp[-\overline{\rho}(T)/\rho_0]$; they can thus be approximated as stable composite steps with nearly step-free facets in between.

From the above discussion, it is clear that the integrability of this system is tied to scale invariance at distances $a \ll r \ll \rho_0^{-1}$. Along the crossover between the critical and the high-temperature regimes, the two-particle wave function does not have the simple power-law asymptotics $\Psi_2(r) \sim |r|^\lambda$ as in (5), and, consequently, the product ansatz (5) breaks down. What happens to scale invariance at distances $r \gg \rho_0^{-1}$? It has been shown that any solution of the Calogero-Sutherland model with $\lambda > 0$ describes a Tomonaga-Luttinger liquid: It belongs to the universality class of the Gaussian model with action $S_G = (\gamma/4\pi)\int[\nabla h(\mathbf{r})]^2 d^2\mathbf{r}$ and stiffness $\gamma = \lambda/2$ [17]. Here $\mathbf{r} \equiv (r, v_F t)$, where $v_F = 2\pi\lambda\rho_0$ is the Fermi velocity, and $h(\mathbf{r})$ is a coarse-grained surface height variable. Using the Bethe ansatz, one finds the low-lying finite-size excitations $\Delta E_{e,m} = 2\pi v_F x_{e,m}/L$ in terms of the scaling dimensions $x_{e,m} = (e^2\gamma + m^2/\gamma)/2$ of the vertex operators $\mathcal{O}_{e,m}$ $(e, m \in \mathbb{Z})$ [17]. It is then easy to show that any solution with $\lambda < 0$ is also a Tomonaga-Luttinger liquid with $\gamma = -\lambda/2$, since the transformation $\lambda \to -\lambda$ acts as the symmetry $\mathcal{O}_{e,m} \to \mathcal{O}_{e,-m}$ on the Gaussian operator algebra. Thus conformal field theories with central charge $c = 1$ govern the steps at T_c *and* at high temperatures—and thus along the entire crossover by virtue of the c theorem [27]. It follows that the system is a Tomonaga-Luttinger liquid for all $T > T_c$ [28]. This property extends to the entire critical regime, where γ can be written in scaling form, $\gamma(T, \rho_0) = \Gamma[(T - T_c)\rho_0^{-2y^-(g_0^c)}]$ [29]. Below $T^*(\rho_0)$, one expects an effective action similar to (1) for the composite steps; the system is then still a Tomonaga-Luttinger liquid.

In summary, the Calogero-Sutherland model has been applied to interacting steps on vicinal surfaces. The thermodynamic complexity of this system arises from the interplay of the two branches of integrable solutions. It will be of interest whether this mechanism also plays a role in other realizations of the Calogero-Sutherland model.

I thank J. L. Cardy, V. Korepin, R. Lipowsky, S. M. Mochrie, and M. Zirnbauer for useful discussions. In particular, I am grateful to S. M. Bhattacharjee for his contribution at the initial stage of this work.

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