Vicinal Surfaces, Fractional Statistics, and Universality

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We propose that the phases of all vicinal surfaces can be characterized by four fixed lines, in the renormalization group sense, in a three-dimensional space of coupling constants. The observed configurations of several Si surfaces are consistent with this picture. One of these fixed lines also describes one-dimensional quantum particles with fractional exclusion statistics. The featureless steps of a vicinal surface can therefore be thought of as a realization of fractional-statistics particles, possibly with additional short-range interactions.

A crystal surface cut at a small angle to a symmetry direction is called a vicinal surface [1]. Such a miscut surface consists of terraces of the symmetry plane, separated by monatomic steps running across the sample in a preferred direction dictated by the cut. The density of the steps (number of steps per unit transverse length), ρ, is related to the miscut angle θ ($\rho \sim \tan\theta$). In thermal equilibrium, the configuration of the surface is determined by the steps and their interactions. Vicinal surfaces constitute a special class of objects in low dimensional statistical mechanics and are useful as substrates in many technological and experimental situations. An understanding of the phases and phase transitions of vicinal surfaces is therefore important.

Various types of behaviors of vicinal surfaces are known. For example, it is known that vicinal Si(111) surfaces have single steps or triplets [2] but never pairs, while pairs of steps are seen on Si(001) [3]. An unusual phenomenon occurs in the case of Si(113) where a uniform-step-density phase, on cooling, phase separates into a flat surface and a phase with a large angle (i.e., a high density of steps) [4,5]. In other words, a small-angle vicinal Si(113) surface becomes thermodynamically unstable. The coexistence curve, on the temperature-versus-miscut-angle orientational phase diagram, ends at a tricritical point with the shape [4] given by an exponent $\beta = 0.42$–0.54. A variant of the phase diagram has also been reported in Ref. [4(b)]. Is there a natural way of characterizing this zoo of vicinal surfaces?

In this paper our aim is to develop a long-distance, universal behavior for vicinal surfaces, where microscopic details such as the specific material, the lattice structure, surface reconstruction if any, etc., do not play a direct role. This is best done in a continuum approach [6–8]. The steps are treated as fluctuating elastic strings (directed polymers), and all the effects of the surface go into the elastic energies of the steps and their effective interactions. Therefore, our approach is valid for any vicinal surface that can be characterized by featureless, wandering steps.

A major interaction of the steps is known from theory [6,9] and experiments [10] to be $|\mathbf{r}_i(z) - \mathbf{r}_j(z)|^{-2}$, where z is the special direction of the steps and $\mathbf{r}_i$ is the transverse d-dimensional coordinate of a point at z along the length of the ith step. (Our interest is, of course, at $d = 1$.) This long-range interaction is generally repulsive, originating from the elastic effects of the terraces, although, for metals, dipoles or quenched impurities on the steps can produce an attractive r^{-2} potential [6]. A theoretical explanation [7] of the observed tricriticality [4] requires an additional attractive short-range interaction. The continuum description of Ref. [7] is justified *a posteriori* by the existence of a renormalization group fixed point with a diverging length scale (see also Refs. [8,11]).

In an effective Hamiltonian for the steps, the interaction need not be restricted to just pairwise-additive potentials, and, in a renormalization-group (RG) approach, one should include allowed marginal operators. We keep the three-body short-range interaction since it is marginal at $d = 1$ (see below) [7,12]. All m-step interactions are irrelevant for $m > 3$ at $d = 1$. The Hamiltonian is

$$
H = \sum_i \int_0^N dz\, \frac{\kappa_i}{2}\, \dot{\mathbf{r}}_i^2(z)
$$
$$
+ \sum_{i>j} \int_0^N dz \left[v_2 \delta_\Lambda[\mathbf{r}_{ij}(z)] + \frac{g}{r_{ij}^2(z)} \right]
$$
$$
+ v_3 \sum_{i>j>k} \int_0^N dz\, \delta_\Lambda[\mathbf{r}_{ij}(z)]\delta_\Lambda[\mathbf{r}_{jk}(z)], \quad (1)
$$

where $\dot{\mathbf{r}}_i(z) = \partial\mathbf{r}_i/\partial z$, κ_i is the elastic constant of the ith step, each of length $N(\to \infty)$, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and g, v_2, and v_3 are, respectively, the long-range two-body, the short-range two-body, and the short-range three-body coupling constants. The short-range interactions are taken as contact interactions, and power counting shows that this is sufficient [13]. There is a short-distance cutoff (reminiscent of the lattice) so that, in Fourier modes, $\delta_\Lambda(\mathbf{q}) = 1$, for $|q| < \Lambda$, and 0, otherwise. For the

tricritical point, one takes [7,8] $v_2 = v_{20}(T - T_t)$ but, for generality, we consider both positive and negative values of all three parameters (g, v_2, v_3). The partition function is then given by the summation of the Boltzmann factor over all possible configurations with free end points. Two special cases of Eq. (1) ($v_3 = 0$, and g = 0) were considered in Ref. [7] in connection with the tricritical point seen in Si(113). The physical picture used is that of phase separating polymers with the critical point of the coexistence curve coinciding with the binding-unbinding critical point of two steps (zero density). It was shown in Refs. [7,8] that $\beta = 0.5$ occurs for $g = 3/4$.

The resemblance of Eq. (1) with the Calogero-Sutherland model [14,15] is apparent, and we shall discuss some issues related to this. The Hamiltonian ($\hbar = 1$) describes a set of interacting quantum particles which can be chosen as bosons. The thermodynamic properties of the quantum system can be obtained from Eq. (1) with N as the inverse temperature. In the limit of infinite lengths of the steps, the properties of the vicinal surface are given by the ground state of the corresponding quantum problem [6].

The main contents of the paper are the following: (i) We show that, for the $v_3 = 0$ case, at $g = 3/4$ the continuous transition goes over to a first-order transition [15,16]. This requires a study of reunion exponents [17,18] for the steps with the long-range interaction. The change in the order of the transition is then connected to the observed behavior of Si(113). (ii) We obtain a fixed-point (or, rather, a fixed-line) description for the above Hamiltonian, and, from the nature of the fixed points, we argue that the observed features of various Si vicinal surfaces are described by these fixed points. We then conjecture that *all vicinal surfaces are described by these fixed lines (and the flows) in a three-dimensional parameter space*. (iii) It is quite common to use a quantum description where the steps are treated as fermions, but we conclude, from the equivalence with the Calogero-Sutherland model on the $v_3 = 0$ fixed line, that the steps should rather be treated as *one-dimensional fractional-exclusion-statistics particles with only short-range interactions*.

As far as the RG flows of the various parameters are concerned, one may just restrict oneself to two or three steps ("vertex functions"). For a many-step system, one also needs the chemical potential μ, but its flow is determined by dimensional analysis [12,15,19]. In the momentum-shell renormalization-group approach, short-wavelength fluctuations are integrated out in a thin shell $(\Lambda/b, \Lambda)$ in Fourier space, and the effect is absorbed by redefining the parameters. The system is then rescaled to its original state, whereby the cutoff goes back to Λ. (We choose $\Lambda = 1$.) The change of the parameters with distance in the long-distance limit is then recovered from the RG flow equations. The spatial rescaling factor is anisotropic, $r \rightarrow br$, $z \rightarrow b^\zeta z$, and the choice $\zeta = 2$ keeps the elastic constant invariant [19]. For simplicity, we choose $\kappa_i = 1$, for all i.

Since the RG transformation is analytic, the long-range term does not get renormalized. That there is no renormalization of g turns out to be rather natural when we discuss the quantum problem. We just quote the well-known recursion relations in terms of the dimensionless variable [15] $u_2 = L^{2-d} K_d v_2 + g/(d - 2)$, where $K_d = 2\pi^{d/2}/[\Gamma(d/2)(2\pi)^d]$, and L is an arbitrary length scale in the transverse direction ($b = 1 + \delta L/L$). Restricting ourselves to $d = 1$, the flow equations are [12,15,19]

$$L\frac{du_2}{dL} = u_2 - u_2^2 + g, \qquad L\frac{dg}{dL} = 0,$$

$$\text{and} \quad L\frac{d\mu}{dL} = 2\mu. \tag{2}$$

The flow equation for u_2 has two fixed points $u_{s,u}^* = \{1 \pm [1 + 4g]^{1/2}\}/2$, s,u denoting, respectively, the stable and unstable fixed points [Fig. 1(a)]. The unstable fixed point describes the binding-unbinding transition of two steps. The critical point has a length-scale exponent $\nu_\perp = 1/\sqrt{1 + 4g}$. For a many-step system, this unstable fixed point corresponds to the tricritical point mentioned earlier, provided the fixed point describes a critical behavior. Since the density ρ vanishes at this tricritical point, the assumption of a single length scale then tells us that ρ^{-1} should diverge as the length scale. Therefore, $\beta = \nu_\perp$. For $\beta = 1/2$, as for Si(113), one would require $g = 3/4$ as obtained in Ref. [7].

We now show that $g = 3/4$ is indeed a special point. Let us consider the free energy [17] of two steps. Configurations of the steps are of the type shown in Fig. 1(e). The bubblelike contributions [region B in Fig. 1(e)] represent the steps in the high-temperature phase described by the stable fixed point. It is shown in Ref. [17] (we, therefore, skip the details) that the nature of the singularity of the free energy is determined by the decay of the partition function of the bubble of length N, $Z_R(N) \sim N^{-\psi}$, where ψ is the reunion exponent [18]. If $1 < \psi \le 2$, then the transition is continuous, while for $2 < \psi$ it is first order, but with a weak singularity and a diverging length scale [20].

The reunion exponent ψ determines the behavior of the partition function of two steps starting at the origin and reuniting anywhere in space [17,18]. We need the exponent in the high-temperature phase characterized by the stable fixed point. The zeroth- and the first-order diagrams for the reunion partition function Z_R are shown in Figs. 1(f) and 1(g). These contributions require renormalization of the partition function itself, over and above the renormalization of the parameters. This extra renormalization yields a nontrivial ψ different from the Gaussian value $\psi = d/2$ in d dimensions. In the limit $N \rightarrow \infty$, the loop contributions lead to the recursion relation for $Z_R(N)$ as $LdZ_R/dL = -2(d/2 + u_2)Z_R$, so that, at $d = 1$ at the stable fixed point $u_2^* = u_s$, we get $\psi = 1 + (1 + 4g)^{1/2}/2$. This is an exact result from which we recover the vicious walker exponent [17] $\psi = 3/2$ for $g = 0$. (The details and generalizations to arbitrary number of steps will be discussed elsewhere.) We see that
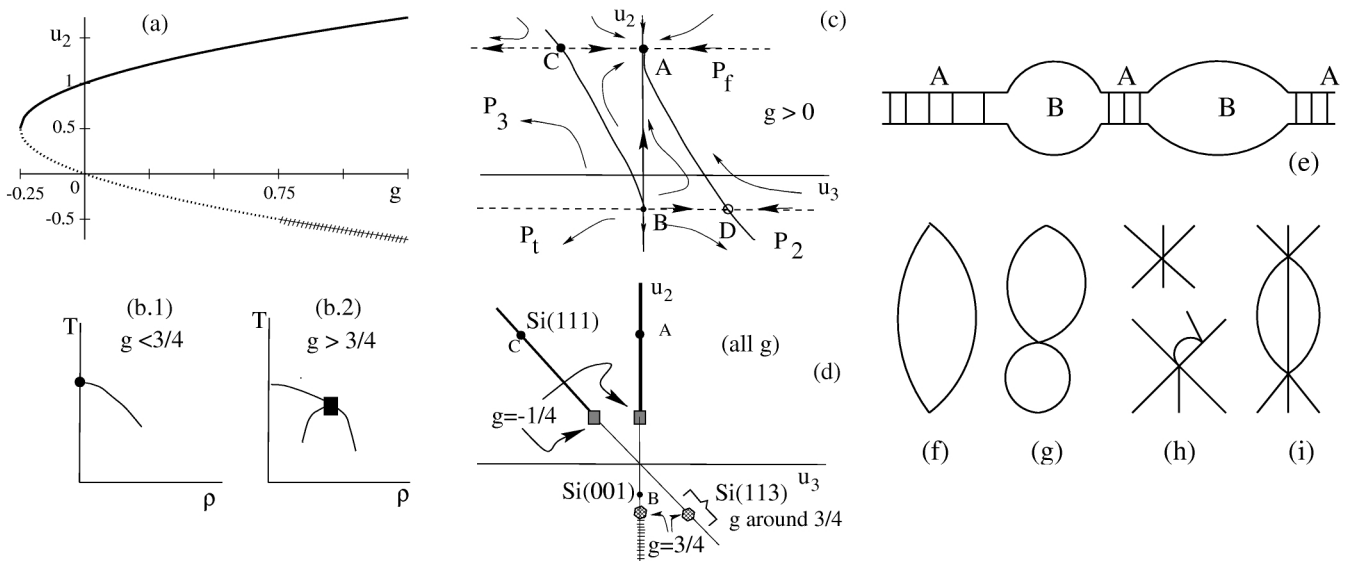
FIG. 1.　(a) Renormalization-group fixed lines for $v_3 = 0$. These are stable (thick line), unstable critical (dotted), and unstable first order (hatched).　(b) A schematic orientational phase diagram in the T vs ρ plane for $u_2 \leq 0$. For $g \leq 3/4$, there is a tricritical point (b.1) with $\beta \approx 0.5$. For $g > 3/4$, a low-density first-order line connects the $\rho = 0$ transition to the coexistence curve either at the $\rho \neq 0$ critical point of the latter or at an off-critical point (b.2).　(c) The fixed points in the (u_2, u_3) plane for a $g > 0$. Arrows indicate the RG flows. The phases are P_f (uniformly stepped, fractional-statistics-like), P_3 (a phase with 3-steps bunching but no pairs), P_2 (pairs of steps but no triplets), and P_t (all possible bunches).　(d) The fixed lines on a $u_2 - u_3$ plane as $g (\geq -1/4)$ is varied. Si surfaces showing similar behavior are indicated (not necessarily having same g). Different types of lines represent different behaviors as noted in (a) and (c).　(e) A typical configuration of two steps consisting of sequences of bound (A) and unbound (B) fragments of various lengths.　(f, g): A zeroth-order and a first-order reunion diagrams of two steps.　(h) and (i) show the first- and second-order diagrams for v_3 renormalization.

$\psi = 2$ for $g = 3/4$. This then establishes [16,17] that the transition is first order for $g > 3/4$.

In the case of a first-order two-step phase transition, this may not be the critical point of the phase-coexistence line of a many-step system. In such a case, a phase diagram of the type shown in Fig. 1(b.2) is plausible, where a first-order line continues from the zero-density transition point, ending on the coexistence curve [hidden region in Fig. 1(b.2), see figure caption]. The first-order line represents a tranition from a uniform phase of single steps to a uniform phase of pairs, and, at the tranition, there will be diverging fluctuations in the mean spacing between the members of the pairs (for $3 > \psi > 2$). In recent experiments on Si(113) such a phase diagram has been observed [4] for certain azimuthal angles of the miscut direction, though the low-density line is yet to be detected.

Let us now consider the effect of the three-body interaction [12,13,21]. Even though v_3 is marginal (dimensionless at $d = 1$), there are contributions in v_3 renormalization, from both v_2 and g (i.e., u_2) via the reunion exponent of three steps. Note that v_3 does not affect u_2 or g. Taking into account the first nontrivial contribution [Figs. 1(h) and 1(i)], the recursion relation for $u_3 = L^{1-d} v_3$ is ($d = 1$)

$$L \frac{du_3}{dL} = -3u_2 u_3 - Au_3^2, \qquad (3)$$

where the numerical value of the constant $A > 0$ is not crucial. The fixed points [Fig. 1(c)] are $u_3^* = 0$ and $u_3^* = -3u_2/A$. The stability of the $u_3^* = 0$ fixed point depends on the sign of u_2^*. At $u_2^* = u_s^*$ (fixed point A), a small u_3 is

irrelevant, but the new fixed point C, $u_3^* = -3u_s/A < 0$, is unstable. In contrast, at $u_2^* = u_u^*$ (fixed point B), with $g > 0$, u_3 is relevant, and $u_3^* = (3|u_u|)/A > 0$ is stable. The flows for any $g > 0$ are shown in Fig. 1(c).

Figure 1(c) shows that for certain combinations of $g > 0, u_2$, and u_3, the steps in the high-temperature phase behave similar to the $u_3 = 0$ case (region P_f), but for sufficiently large $u_3 < 0$ there will be triplets of steps but never pairs (phase P_3). The transition will be first order but with singularities determined by the g-dependent fixed point C of Fig. 1(c). We like to associate Si(111) vicinal surfaces [2] with this fixed point and the associated flow, because of similar behavior. For fixed points B and D, there could be pairings of steps, induced by a variation in u_2. Such pairings are seen [3], e.g., in Si(001). A many-step system will show a tricritical behavior at these fixed points, as, e.g., in Si(113). These two fixed points B and D of Figs. 1(c) and 1(d) have the same thermodynamic exponents but they differ in the three-step correlation functions. Moreover, if u_2 is a temperaturelike axis, then the temperature deviation is not the proper scaling variable at D. Taking this as a reason for the large range [4] in the observed exponent β, we may associate Si(113) with the fixed point D with g around 3/4 and Si(001) with fixed point B. There is, in fact, no requirement that the long-range interaction should be exactly at $g = 3/4$ for Si(113). Unfortunately, no systematic studies are available for the dependence of g on the various miscut parameters. In case g depends on the azimuthal angle

even slightly, it is possible that for certain azimuthal angles $g > 3/4$ and for these cases, one would see a phase diagram of type Fig. 1(b.2), while, for cases with $g < 3/4$, one would see type Fig. 1(b.1).

We now make a conjecture that all vicinal surfaces are described by the RG flows and the fixed lines we obtained in the three-dimensional parameter space. Other higher-order short-range interactions are irrelevant. All universal properties are determined by the fixed lines, and it is the long-range parameter g that determines the universality class.

Let us now go back to Eq. (1) as a quantum-mechanical problem. With $\nu_3 = 0$, the connection of this Hamiltonian with the Calogero-Sutherland model [14] has been noted in the past [8,15]. The quantum problem is described by the stable fixed line and the negative-g part of the unstable line in Fig. 1(a). Furthermore, the Calogero-Sutherland model describes [22] a gas of noninteracting particles obeying Haldane-Wu fractional exclusion statistics [23]. The long-range $1/r^2$ potential is best thought of as a statistical interaction, with g determining the statistics of the particles. We have established this directly in our approach by a computation of the quantum second virial coefficient along the fixed lines of Fig. 1(a), since the second virial coefficient was shown, from general considerations, by Murthy and Shankar [22] to determine the statistics uniquely. We wish to discuss this technical issue elsewhere. Suffice it to say here that the nonrenormalization of g in our RG approach is a direct manifestation of the fact that the statistics of the particles is independent of length scale and, *hence, a renormalization-group invariant*. This correspondence therefore tells us that the steps on vicinal surfaces are an analog realization of one-dimensional fractional-statistics particles. Though fermions are extensively used to study the equilibrium properties of steps, the latter are better represented by fractional-statistics particles with only short-range interactions.

Our main results have already been summarized. It would be interesting to study the case of unequal elastic constants of the steps, and the regions not describable by any fixed point, where other details of the surface, such as lattice periodicity, may be important [11]. We end with the suggestions that (i) attempts be made to determine accurately the long-range (or statistics) parameter g and its dependence on the miscut features, as, e.g., azimuthal angle, for various surfaces and materials, (ii) measurements be done for three-step correlations, and (iii) the thermodynamic behavior of a finite number of steps be studied even if in finite geometries (by putting barriers). Most interesting would be the special case of $g = -1/4$ which, in the surface context, is the point of coalescence of the stable uniform-density-phase fixed point and the unstable critical point, and, in the quantum context, is the semion, exactly halfway between boson and fermion. Can one find such a surface of a metal?

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