Surface Science Letters 240 (1990) L591–L598
North-Holland

SURFACE SCIENCE LETTERS

Surface Science Letters

The influence of step–step interactions on step wandering

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Received 9 July 1990; accepted for publication 7 September 1990

We derive relationships between the amount of step wandering and the strength of step–step interactions to aid interpretation of scanning tunneling microscopy images of steps on surfaces. We make contact with well-established results for the statistical mechanics of interfacial wandering. In particular, we use the analogy between a step meandering in a potential and a quantum-mechanical particle moving in a one-dimensional potential well. We also set out an approximate procedure for computing the terrace-width distribution for non-interacting steps using free-fermion techniques, and show using Monte Carlo that the resulting temperature-independent distribution is a good aproximation until remarkably high temperatures.

Recent developments in surface imaging techniques, such as reflection [1] and transmission [2] electron microscopy, low-energy electron microscopy (LEEM) [3], and scanning tunneling microscopy (STM) [4] have made it possible to observe directly the wandering of steps on surfaces. In principle, a statistical analysis of such images (similar in spirit to analysis of field-ion microscopy data [5]) provides a method for determining quantitative values for the energies which determine the step configurations. In particular, a question which has attracted recent attention [6–9] is the importance of the interactions between steps in determining the observed step configurations. In this paper, we present first a qualitative physical description of the relationship between step interactions and experimental observations of step wandering. We then discuss a simple model with analytical solutions which can be used for estimating step interactions without the need for extensive computations. We conclude by presenting an outline of the methods needed for a more accurate analysis, which allow the accuracy of this simple model to be tested. By making contact with well-established results for interfacial wandering, we are able to expand on points made by previous workers [7,8].

Consider a wandering step trapped between two straight steps separated by distance $2l$, with the configuration of the step given by $x(y)$ as in

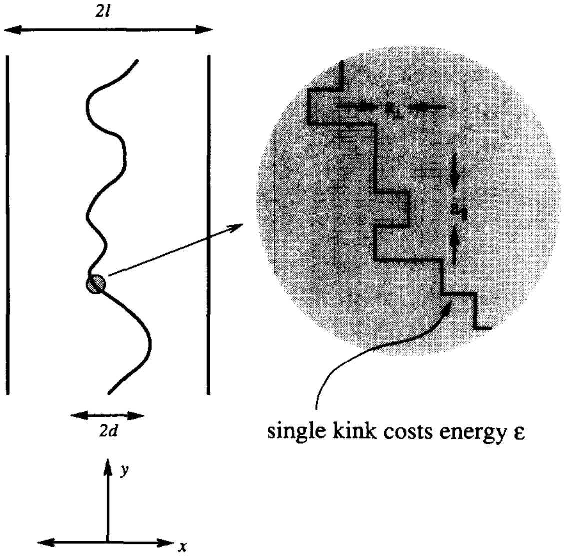

Fig. 1. On the left, a step wandering between two straight steps separated by $2l$ is shown schematically. The interactions due to the straight steps limits the wandering to a width $2d$. On the right, the kink structure in the step edge underlying the wandering is pictured.

fig. 1. This model of step wandering has a long history [10]. It seems to be an especially good model for single-layer height steps on Si(100) misoriented towards the [110] direction, where the wandering due to kinks is observed [11] to be very small on alternate steps. Repulsive interactions will tend to limit the amount of wandering by making closely spaced steps unfavorable. Restricting step fluctuations, however, will cost entropy. Before embarking on a detailed analysis, we first briefly discuss some of the qualitative features predicted by this balance between entropy and energy. We proceed by supposing that the straight steps create a potential per unit step length $V(x, l)$ for the wandering step, and ask how the step wandering depends on temperature, the strength of V, and the energy ϵ required to create a kink. Interactions between steps can arise from elastic strain or from dipole–dipole interactions [12].

Before we discuss in detail the form of the fluctuations in step position for this model, we give a qualitative analysis of the expected behavior. Suppose $V(x, l)$ is strong enough that direct collisions between steps never occur, so that the step wanders freely only over a range d, i.e. $|x| \leq d < l$. The free energy cost per unit length of restricting the step to d has the form $kTb^2(T)/a_{\|}d^2$ [13], where the diffusivity, $b^2(T)$, is the local mean square length of each kink perpendicular to the step edge (including unkinked sites in the average, so that perfectly straight steps have $b = 0$), and $a_{\|}$ is defined in fig. 1. This diffusivity, an important quantity in all that follows, is a property of *isolated* steps. Suppose $U(x)$ is the potential between two steps separated by x, per unit length of the steps. The potential felt by the wandering step is then

$$\begin{aligned} V(x, l) &= U(l+x) + U(l-x) \\ &\approx 2U(l) + c(l)x^2, \end{aligned} \tag{1}$$

where in the final form we have expanded about $x = 0$, and $c(l) = U''(l)$. The energy per unit length of the step is roughly the integral of the potential with respect to d, divided by d, or $2U(l) + c(l)d^2/3$. Minimizing the sum of the entropic and energetic contributions to the free energy with respect to d to find the equilibrium value of d gives:

$$d \propto \left(\frac{kTb^2(T)}{c(l)\, a_{\|}} \right)^{1/4}. \tag{2}$$

We will make this relationship more precise below, but first we offer some preliminary comments on the general form of the dependence of step fluctuations on mean step separation l and temperature. For elastic or dipole-induced step–step interactions, $U(x)$ decays as Ax^{-2} [12]. From eq. (1), $c(l)$ then varies as A/l^4. Thus from eq. (2) the width of thermal step fluctuations will be proportional to the average terrace size l, with the proportionality constant depending on A, T and b^2. (Indeed such a proportionality has been observed on Si(111) [9].) On Si(100), because of the anisotropy of the (2×1) reconstruction, $U(x) = B \ln(|x|) + C$, which leads to $c(l) = B/l^2$ [6] and thus $d \sim l^{1/2}$. Hence by studying the l dependence of d, one should be able to deduce the form of the step–step potential. As discussed in more detail below, for steps with net orientation along a high symmetry direction and with kink energy ϵ, one expects at low T that $b^2 \sim \exp(-\epsilon/kT) \sim$ kink density. This prediction that the amount of wandering should increase as the one-fourth power of the kink density could in principle be verified by STM measurements on surfaces with kink densities obtained by quenching from different temperatures.

To be more precise, we can compute the actual probabilities of step fluctuations for the simple model of fig. 1. The coarse-grained free energy functional, or effective Hamiltonian, for a configuration $x(y)$ can be written as [7,14]

$$\begin{aligned} &F(x(y)) \\ &\quad = \int \mathrm{d}y \left[\Sigma_0(T) + \tfrac{1}{2}\tilde{\Sigma}(T) \left(\frac{\mathrm{d}x}{\mathrm{d}y} \right)^2 + V(x(y)) \right], \end{aligned} \tag{3}$$

where $\Sigma_0(T)$ is the free energy per unit length of a step oriented in the average direction (i.e. with normal $\hat{x}$), and $\tilde{\Sigma}(T)$ is the step-edge "stiffness"; both are properties of *isolated* steps. The temperature dependence of $\tilde{\Sigma}$ is discussed in detail in refs. [13–15]. In general one expects:

$$\tilde{\Sigma}(T) = \frac{kTa_{\parallel}}{b^2(T)}, \tag{4}$$

where $a_{\parallel}$ is the lattice constant along the step-edge separating possible sites of kinks. The coarse graining of eq. (3) assumes implicitly that $b \ll a_{\perp}$. What happens when this condition is not satisfied will be discussed at the end of this paper; the assumptions of eq. (3) do not cause serious error until remarkably high temperatures.

The step edge stiffness could be determined directly by measuring b from atomic resolution STM images of an "isolated" step. One can also estimate b from an STM or LEEM image of an isolated step without requiring atomic resolution by using

$$\left\langle (x(0) - x(y))^2 \right\rangle = \frac{b^2}{a_{\parallel}} y. \tag{5}$$

Alternatively, given a model which specifies the energies of kinks of various lengths, b (and hence $\tilde{\Sigma}(T)$) can be straightforwardly calculated. For example, if the only allowed kinks have length $a_{\perp}$ and cost energy ϵ, as illustrated in fig. 1, then b can be estimated from

$$\begin{aligned} b^2 &= \left\langle (x(y + a_{\parallel}) - x(y))^2 \right\rangle \\ &= \frac{2a_{\perp}^2 \exp(-\epsilon/kT)}{1 + 2\exp(-\epsilon/kT)}. \end{aligned} \tag{6}$$

(Note b vanishes, and hence $\tilde{\Sigma}$ diverges, as T becomes small.) Generalizations to more complicated step geometries and kink Hamiltonians are easily made.

Expectation values for the position of the step can be conveniently obtained by transcribing the statistical mechanical problem given by eq. (3) into one of one-dimensional quantum mechanics [15–17], using, for example, the methods of ref. [18]. In this transcription the probability of a step passing through x at y and x' at y' is

$$\begin{aligned} &P(x, x'; y, y') \\ &\quad = \sum_s \exp[(E_0 - E_s) | y' - y |] \\ &\qquad \times \psi_0^*(x) \psi_0(x') \psi_s^*(x') \psi_s(x), \end{aligned} \tag{7}$$

where ψ_s are the eigenstates of Schrödinger's equation:

$$-\frac{b^2}{2a_{\parallel}} \frac{\mathrm{d}^2\psi_s}{\mathrm{d}x^2} + \frac{V}{kT}\psi_s = E_s\psi_s, \tag{8}$$

and $s = 0$ denotes the ground state. In this context, the "mass" of a step segment is proportional to b^{-2}, i.e. step stiffness translates to the inertia of massive particles, and the y-axis corresponds to imaginary time. The probability of a step to pass through x, for any y, is just

$$P(x) = \int_{-\infty}^{\infty} \mathrm{d}x' P(x, x'; y, y') = | \psi_0(x) |^2. \tag{9}$$

For the simple harmonic oscillator potential of eq. (1), we find the familiar Gaussian ground-state wavefunction, yielding a step distribution function

$$P(x) = \frac{1}{w\sqrt{2\pi}} \exp\left(-\frac{x^2}{2w^2} \right), \tag{10}$$

with the width of the Gaussian given by

$$w(T, l) = \left(\frac{kTb^2(T)}{8c(l)a_{\parallel}} \right)^{1/4}. \tag{11}$$

This expression has the same form anticipated by eq. (2), and provides the relationship between coarse-scale deviations and mciroscopic fluctuations. Notice that values of x a few times w are extremely rare: the repulsions act effectively as exclusions, as observed explicitly on vicinal Si(111) in ref. [9], and implicitly on vicinal Si(100) in refs. [4,7], for example.

From the discussion above, it is clear that the step distribution function will narrow with increasingly repulsive interactions. To find the limit of the distribution function when the interaction becomes very weak, we consider the high temperature limit of eqs. (10) and (11). As the temperature increases, b (and hence w) increases. When w becomes comparable to l, the harmonic-well approximation should break down. At sufficiently high T, the only important interaction is the non-crossing condition for the steps, i.e. the steps do not interact except that they cannot cross. In this case $V(x, l)$ becomes an infinite square-well potential of width $2l$. The wavefunctions are well-known, and

$$P(x)=\frac{1}{l}\cos^2\left(\frac{\pi x}{2l}\right), \quad |x| \le l. \tag{12}$$

This expression was derived in ref. [10] for steps using slightly different methods. Thus in the limit of no energetic interactions, the step distribution function becomes independent of T. (This independence arises because $P(x)$ is an *average* over y, and thus does not depend on the amount of step wandering. Ultimately, the temperature independence comes from the assumptions of eq. (3): in the absence of energetic step interactions, changes in temperature correspond merely to changes in the scale of the y-axis. The breakdown of these assumptions causes a small temperature dependence discussed below.) Thus, large temperature dependences of $P(x)$ only occur when *energetic* step interactions are important in determining the distribution of step positions. It is possible to invent potentials which show the crossover from eq. (10) to eq. (12) analytically [19]. We emphasize that even with no energetic interactions, the distributions are small at small separations due to the "entropic repulsion" between steps. To deduce interactions between steps, one must observe more than a peaked distribution; one must see differences from eq. (12), or its generalization discussed below. Information about fluctuations transverse to the step edge can be obtained using eq. (7) along with knowledge of the excited states of the potential. The correlations in x as one moves along the step are

$$\langle x(0)x(y)\rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \int_{-\infty}^{\infty} \mathrm{d}x''\, x'x'' P(x', x''; 0, y). \tag{13}$$

For the harmonic oscillator potential, only the $s=1$ state in eq. (7) contributes because of the orthonormality of Hermite polynomials. By explicit substitution of the simple harmonic wavefunctions into eq. (13), it is straightforward to show that

$$\langle x(0)x(y)\rangle = w^2 \exp(-y/\xi), \tag{14}$$

with the correlation length ξ given by

$$\xi(T, l)=\left(\frac{kTa_{\|}}{2b^2(T)c(l)}\right)^{1/2}. \tag{15}$$

Eq. (14) is similar to eq. (23) of ref. [7]. (The two differences are the temperature dependence of ξ and numerical factors in w.)

Kochanski [8] argues, from equipartition, that $c(l)w^2$ is proportional to kT/ξ, and indeed uses this proportionality to define ξ. Combining the correlation length of eq. (15) and the probability distribution of eq. (10), we explicitly verify this result; eliminating b^2 from these equations yields

$$w^2(T)c(l)=\frac{kT}{4\xi(T, l)}. \tag{16}$$

The large correlation length found numerically be Kochanski is related to the vanishing of b at low T [13–15]. Eq. (16) provides a way of estimating c without directly determining b: If one measures ξ and w, one can use eq. (16) to solve for c (a procedure adopted in ref. [7], with a version of eq. (14)).

For the case of noninteracting steps, the correlation length can be similarly found to be

$$\xi(T, l)=\frac{8a_{\|}}{2\pi^2}\left(\frac{l}{b(T)}\right)^2. \tag{17}$$

This equation provides an interpretation of ξ: from eq. (5), one expects the average distance between step collisions along the step to be proportional to $(l/b)^2$, which is proportional to ξ. For interacting steps, the role of l is replaced by w; from eqs. (10) and (15):

$$\xi(T, l)=2a_{\|}\left(\frac{w}{b(T)}\right)^2. \tag{18}$$

Thus decreasing w decreases ξ by increasing the number of effective collisions between steps.

In all of the above, the neighboring steps of the wandering step act as rigid, straight walls. On real surfaces, all steps wander simultaneously. However, following ref. [15], we expect that the dependence given by eqs. (10)–(18) of the $P(x)$ and ξ on temperature, interaction strengths, and angle of misorientation will be qualitatively correct. Before transcending the fixed-wall approximation, we show that the equations derived for the fixed wall case give a convenient method of *estimating* step interactions: we consider vicinal Si(100), on which steps alternate between two types, one wandering much more freely than the other. Swartzentruber et al. [20] have determined the kink Hamiltonian for the more freely wandering steps: from their results we estimate $b = 11$ Å. Alerhand et al. [6] propose that elastic step–step interactions of the form $U(x) = B \ln(x)$ exist between these types of steps, with $B \approx 3$ meV/Å. This value can be checked by comparison with STM results for Si(100) steps separated by ~ 250 Å presented in ref. [20]. Using eq. (1), $c(l) = B/l^2 \approx 4.8 \times 10^{-5}$ meV/Å^3 for $l = 250$ Å. Using these values of c and b in eqs. (11) and (15) with $T = 900$ K [20], yields the prediction $w = 50$ Å and $\xi = 160$ Å. Casual analysis of the STM image in ref. [20] yields results not obviously inconsistent with these values. The reverse calculation, in which existing STM data [6,7] is analyzed to determine B, could be used to put experimental limits on the true value of B.

To go beyond the approximation of a single wandering step, we appeal to results of *many-body* quantum mechanics in one-dimension [12,21], i.e. by associating *every* step with a quantum mechanical particle. To insure that steps do not cross through each other (which would give rise to presumably unphysical overhangs), it is sufficient that these particles be [spinless] fermions, i.e. they obey the Pauli exclusion principle. From knowledge of the correlation functions of non-interacting fermions in one dimension, we shall compute the terrace-width distribution functions $P(x)$ of steps which have no energetic interactions. This calculation serves as a starting point in deducing interactions between steps, and also to check the importance of some of the assumptions made in the preceding analysis.

The pair correlation function for fermions separated by distance $x = ma_\perp$ can be written as

$$g_0(m) = \langle \Omega | a^\dagger(0) a(0) a^\dagger(m) a(m) | \Omega \rangle, \qquad (19)$$

where $a^\dagger(m)$ and $a(m)$ are creation and destruction operators, respectively, at position $x = ma_\perp$, and $|\Omega\rangle$ is the many-particle ground state. For non-interacting fermions, $g_0(m)$ can be easily calculated [21,22]:

$$g_0(m) = \rho^2 - \frac{\sin^2(\rho \pi m)}{(\pi m)^2}. \qquad (20)$$

Here ρ is the inverse of the mean separation between the fermions, l, which is the average surface slope in the stepped-surface analogy. The probability of finding steps separated a distance l, regardless of whether there are other steps between 0 and $ma_\perp$ is given directly by $g_0(m)$. Knowledge of $g_0(m)$ is *not*, however, sufficient to compute the terrace width distribution function. We must determine multiparticle correlation functions:

$$\begin{aligned} g(m) = \langle \Omega | a^\dagger(0) a(0) &\left[1 - a^\dagger(1) a(1)\right] \cdots \\ &\times \left[1 - a^\dagger(m-1) a(m-1)\right] \\ &\times a^\dagger(m) a(m) | \Omega \rangle, \end{aligned} \qquad (21)$$

i.e. the correlation function for the case of *no* fermions between 0 and $x = ma_\perp$. Using the particle–hole symmetry of free fermions, we can rewrite this expression as

$$\begin{aligned} g(m) = \langle \Omega | &\left[1 - a^\dagger(0) a(0)\right] a^\dagger(1) a(1) \cdots \\ &\times a^\dagger(m-1) a(m-1) \\ &\times \left[1 - a^\dagger(m) a(m)\right] | \Omega \rangle. \end{aligned} \qquad (22)$$

Expanding the right hand side, we then find

$$g(m) = G(m+1) - 2G(m) + G(m-1), \qquad (23)$$

where $G(m)$ is the correlation function for m consecutive fermions. Following standard procedures, $G(m)$ can be easily computed, at least numerically as the determinant of a $m \times m$ [Toeplitz] matrix T_{ij} given by

$$T_{ij} = \begin{cases} (1-\rho), & \text{if } i = j, \\ \dfrac{\sin[\pi(1-\rho)(i-j)]}{\pi(i-j)}, & \text{otherwise.} \end{cases} \qquad (24)$$

The distribution function $P(x)$ is actually a conditional probability, viz. the probability that, given a step at position 0, the next occurs at x. Thus, $P(x = ma_\perp) = g(m)/\rho = lg(m)$, since ρ is the chance of finding a step at any position. Fig. 2 shows terrace width distribution (scaled to the

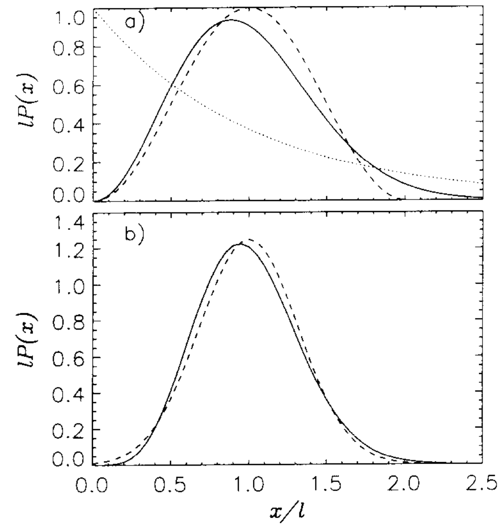

Fig. 2. (a) Scaled terrace width distributions for many non-interacting wandering steps (solid line) compared with the case of non-interacting straight steps (dotted line). The scaled distribution $lP(x/l)$ is insensitive to l [23]. The approximation of eq. (12) for a single wandering step is also shown (dashed line). (b) Scaled terrace width distribution for steps interacting through a repulsive A/x^2 potential (solid line) with $A\tilde{\Sigma} = 2(kT)^2$, compared to the approximation of eqs. (10) and (11) (dashed line).

average terrace separation) calculated numerically from the above equations in the continuum limit of l large. (On the scale of the figure, this limit turns out to describe any l accurately [23].) It is peaked near (but slightly below) the mean terrace width [23]. Contrasted with this distribution is the exponential distribution expected for a sequence of straight, non-interacting steps, and the result of eq. (12) for a single wandering step. (We have shifted the origin of x by l to make the comparison.) As with the wandering step trapped between two straight steps, the absence of closely-spaced steps is symptomatic of entropic repulsions between steps, and must be considered in deducing step–step interactions. The approximate form of eq. (12) is likely to be experimentally indistinguishable from exact many-step results in many cases.

The free-fermion prediction of $P(x)$ of fig. 2 for *non-interacting* steps is temperature independent – again a consequence of the assumption of the Hamiltonian of eq. (3). To ascertain the temperature range of the validity of this approximation, we have performed Monte Carlo simulations [24] of the terrace–step–kink model directly (see fig. 3 for sample Monte Carlo configurations). In the particular model used [24], kinks of size $\pm na_\perp$ cost energy $n\epsilon$, and the average terrace length l is $8a_\perp$. Fig. 4 shows the calculated $P(x)$ at a variety of temperatures (being careful to chose system sizes greater than ξ). As discussed above, one expects eq. (3) and thus the above expression for

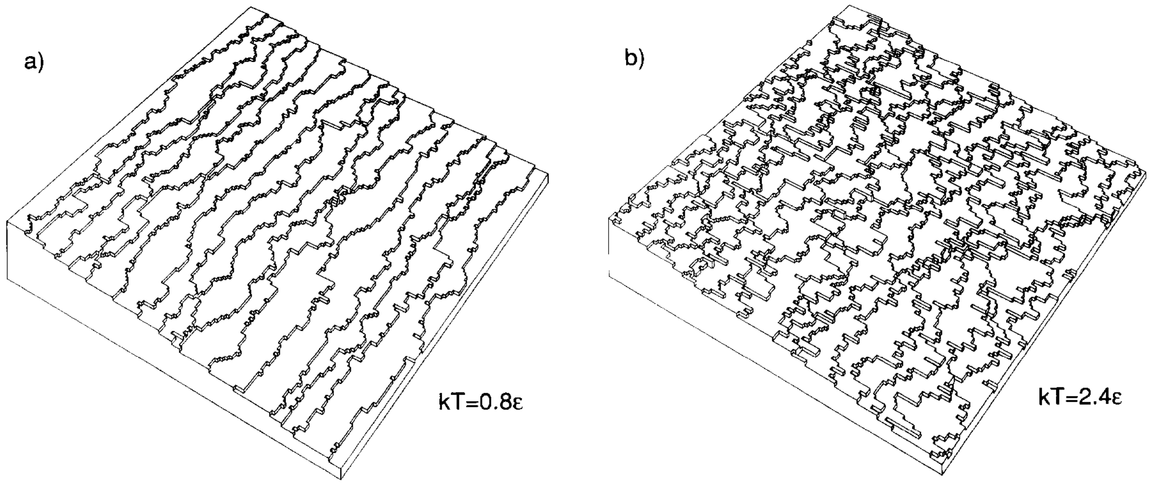

Fig. 3. Sample Monte Carlo configurations for TSK model at temperatures equal to (a) $0.8\epsilon/k$ and (b) $2.4\epsilon/k$. In both cases the average terrace width l is $8a_\perp$.

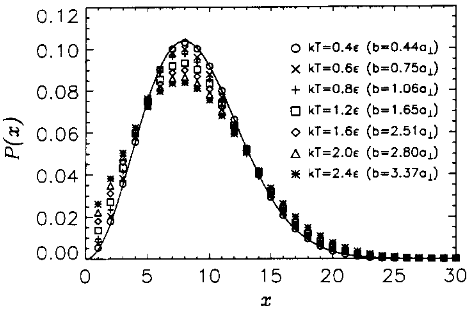

Fig. 4. $P(x)$ for the temperatures corresponding to the temperatures of fig. 3, and several intermediate temperatures (points), compared with the free-fermion prediction of fig. 2. The step position x is measured in units of $a_{\perp}$. The free-fermion approximation is good until the temperature is considerably above the kink energy (i.e., even when b becomes large).

$P(x)$ to be valid only when b is small. However, fig. 4 shows that the low temperature result is valid at surprisingly high temperatures: at $kT = 0.4\epsilon$ ($b = 0.44 a_{\perp}$) the free fermion approximation is excellent. Even at $kT = 2.4\epsilon$ ($b = 3.4 a_{\perp}$), it is qualitatively correct. These Monte Carlo simulations also verify the dependence of ξ [25] on $b(T)$ and l anticipated by eq. (17) [24].

As pointed out by Sutherland [26], one can readily compute correlation functions for fermions interacting with A/x^2 potentials, for special values of A, using the results of Dyson [27]. From these correlation functions we have computed the terrace-width distribution function for the case $A\tilde{\Sigma} = 2(kT)^2$, as shown in fig. 2b. This calculation allows the assumptions leading to eqs. (10) and (11) to be tested: the dashed line in fig. 2b shows that eq. (10), with w computed using the appropriate value of $c(l)$, is an excellent approximation! More details of this calculation are presented in another publication [23]. We point out again that this distribution for interacting steps will in general be temperature dependent. (Indeed, at low enough temperatures the repulsive interactions can force the steps to have long-range order below a roughening temperature [28]. The impact of this transition on the terrace-width distributions should be minor: the remarkably weak singularity in the energy, i.e. local correlations, at a Kosterlitz–Thouless-like transition would be extremely difficult to detect experimentally.)

Finally, we note that in all the above we have assumed thermal equilibrium. This assumption is far from obviously true in any particular situation. Indeed, manifestly non-equilibrium features are observed in refs. [1,2], for example. Analysis of such structures would require a different theory [29].

This work was supported by the NSF under grant DMR-8802986. We thank Jill Goldberg, Dr. Béla Joós, and Dr. X.-S. Wang for many helpful discussions.

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[23] The detailed form of $P(x)$ is discussed by: B. Joós, T.L. Einstein and N.C. Bartelt, submitted.
[24] N.C. Bartelt and T.L. Einstein, in preparation. In the model used, steps are allowed to touch, and thereby form double steps, but overhangs are not allowed. The Monte Carlo simulations were performed on 192×192 lattices with 24 steps. 10^6 Monte Carlo steps per site were used in calculating the averages presented in fig. 4.
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