

Unexpected transient effect

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When a grooved periodic profile cut in a crystalline surface relaxes through surface diffusion, flatter parts appear at the top and bottom in the transient state which precedes complete smoothing. This has been attributed to a tendency of successive steps of identical sign to draw closer to one another. This kind of kinetic interaction is a consequence of the finite value of the interatomic distance, and is present even if no interaction between steps is taken into account. We investigate this effect in a very simplified model, namely, a one-dimensional profile with alternating pairs of up and down steps, where no annihilation of steps is allowed. The quantitative effect is partly treated analytically.

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I. INTRODUCTION

The present work is devoted to a paradox which arises in a simplified model suggested by a much more complicated problem. The physical problem of interest is the evolution of a surface which initially consists of waves [1–5] made of parallel steps (Fig. 1) (the surface is below its roughening transition temperature, and a profile can be appropriately described as an alternation of steps and terraces). This evolution should eventually smooth out the surface, and this implies that steps progressively disappear. We are interested in the evolution of the profile before steps disappear [6,7]. Experimentally, there is evidence that flatter parts (“pseudofacets”) initially form at the highest and lowest parts of the profile [3–5]. This may be a result of the surface being miscut [8–10], but some analytic theories do predict such pseudofacets [11,12]. The result of simulations [13–18] is not very clear, but often indicates a tendency to faceting [15–18]. In these simulations, steps of opposite sign are allowed to annihilate, and it turns out that pseudofacets persist until the profile completely flattens. Several theoretical explanations [19–22] have been given for this. Pseudofacet formation would be expected, for instance, if there were an attractive interaction between steps of identical sign. However, attractive interactions are absent in most physical cases and also in the Monte Carlo simulations which show pseudofacet formation. We shall therefore use the same model as in those simulations, and ignore elastic [24], electrostatic [25,26], and other dynamical interactions between steps, except for the fact that they cannot cross because step crossing would generate overhangs in the surface. Actually, not only step crossing, but mere step contact between steps, will be forbidden in the model, so that there is an *infinite contact repulsion*.

In this model, which is the simplest possible one, pseudofacet formation can be explained by a mechanism suggested by Adam *et al.* [23]. In the present work, we investigate this mechanism in a simple case by more analytic methods than those of Adam *et al.* Unfortunately, this work, like that of

Adam *et al.*, is restricted to a “(1+1)-dimensional” model, i.e. when the surface is one dimensional, characterized [Fig. 1(b)] by the positions of its steps. In this model the relaxation is achieved through diffusion: atoms detach from steps, diffuse on terraces, and stick at steps.

An essential point in the theory of Adam *et al.* is that the contact repulsion energy has no effect at the beginning of the evolution. The effect of the contact interaction was investigated mainly at or near equilibrium [27,28]. Then the *free* energy of the step system, as a function of the average distance l between steps, is found to contain an l -dependent term which results from the contact repulsion in the energy. In real, (2+1)-dimensional surfaces, this term is proportional to $1/l^2$ times the total step length [27,28]. This term of the free energy, which results from the contact repulsion energy, is often called “entropic repulsion.” In 1+1 dimension it has another expression but is also present. However, we consider a freshly cut surface, where steps are well separated and do not touch one another. Thus, at the beginning of the evolution, there is no contact interaction in the energy,

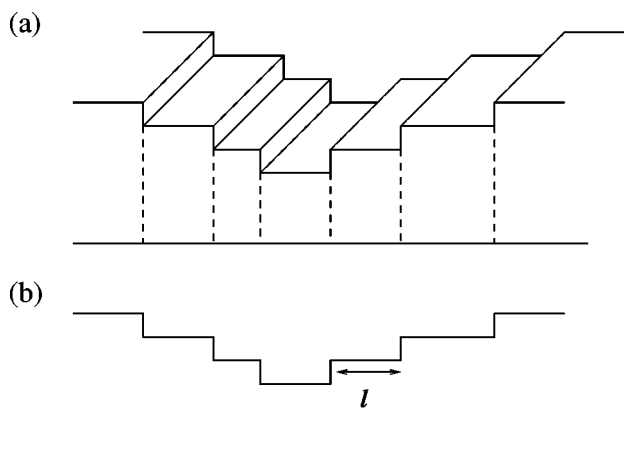


FIG. 1. (a) A groove cut in a surface and (b) its representation as a groove along a one-dimensional profile.

and therefore no entropic repulsion in the free energy.

Since the energy of any allowed configuration of the one-dimensional model does not depend on the distances between steps, one might (erroneously) conclude that the two steps have the same probability to become closer and farther from one another, so that pseudofacets have no reason to appear in our model. As will be seen, this argument would be correct only if steps were point particles, i.e., for a vanishingly small interatomic distance.

As argued by Adam *et al.* [23], the consequence of the nonvanishing interatomic distance a is the following. The minimum allowed amount by which the distance between two steps can change is $2a$, because the change requires the transfer of an atom from the upper (lower) step to the lower (upper) step, so that the distance increases (decreases) by a at both edges. Thus a variation of the distance l between two steps by an amount $2a$ implies the transfer of an atom from one step to the other, and the traveling distance is shorter by an amount $2a$ if the distance becomes shorter ($l \rightarrow l - 2a$) than if it becomes longer ($l \rightarrow l + 2a$). When the distance is shorter, the traveling atom has a lower probability to come back to its starting point, so that the process $l \rightarrow l - 2a$ has a higher probability than the process $l \rightarrow l + 2a$.

Of course, all steps should be taken into account, and the effect disappears for a regular array of equidistant steps (an equilibrium configuration), but is present for a periodic profile, as demonstrated by Monte Carlo simulations [23]: if diffusion kinetics is used, a blunting of the profile is observed in the transient state (this does not happen with evaporation-condensation kinetics). Thus, in a realistic model, the effect leads to pseudo-facet formation. How? If successive steps of the same sign attract each other, the maximal slope of a periodic profile increases, and consequently the top and bottom flatten. This provides a qualitative explanation of pseudofacets. All quantitative calculations were, until now, simulations.

The simulation performed by Adam *et al.* [23] does not provide much insight into how the effect leads to pseudofacet formation. The present paper is an attempt to provide this insight, at the cost of realism. Realism and insight in the present case are incompatible. Here we give an analytic calculation in an oversimplified toy model.

II. A TOY MODEL

The features of our model aim at a simplification of the algebra. They are as follows.

- (i) The model is $1 + 1$ dimensional.
- (ii) The profile is constituted by alternating *pairs* of down steps and *pairs* of up steps (Fig. 2). A pair is the smallest possible group which gives rise to the phenomenon of interest, namely, the distance between steps of identical sign decreases at short times, implying an increase of the distance between steps of opposite sign, and the formation of pseudofacets.
- (iii) The only allowed process is the exchange of atoms between two consecutive steps of identical sign. Exchange between steps of opposite sign is forbidden. This is not expected to be important, since it does not modify the distance

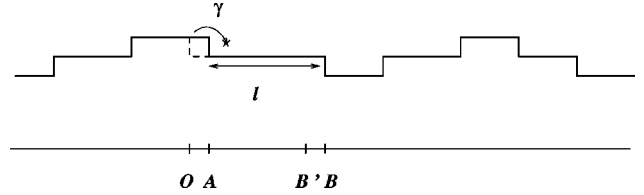


FIG. 2. The one-dimensional profile on a two-dimensional crystal when the height is just two layers. The scheme of the detachment of an atom from a step is also shown.

between steps of opposite sign and does not modify the *average* distance between steps of identical sign. Creation of new terraces between two steps is also forbidden.

(iv) The interaction between any pair of steps of identical sign and the neighboring steps is treated in a mean field approximation, just forbidding the distance l between both steps to be larger than an upper bound Na , where N is a constant integer. Moreover, overhangs are forbidden, so that $l \geq 0$. Actually the value 0 will also be forbidden, so that

$$a \leq l \leq Na. \quad (1)$$

The integer N is determined by the condition that, at infinite time, the average value $\langle l(\infty) \rangle$ of l is equal to

$$\langle l(\infty) \rangle = \frac{N+1}{2} a, \quad (2)$$

since all values consistent with Eq. (1) have the same probability.

(v) Step annihilation is forbidden. This condition simplifies the calculation, and also makes the paradox more striking. Suppose indeed that, initially, all distances between steps have the same value l_0 . At infinite time, in a model subject to condition (v), the average value of the distance between steps should also be l_0 , since all states have the same probability. However, it will be shown that the distance $\langle l(t) \rangle$ between steps of identical sign initially decreases before it reaches a minimum and increases toward the value $\langle l(\infty) \rangle = l_0$.

The above defined toy model reduces to a system of *independent pairs of steps* of identical sign. The problem is simply to calculate the probability $P(l; t)$ that, at time t , the distance between both steps of a particular pair is equal to l .

Let two consecutive steps of identical sign be at distance l at a particular time. We now calculate the probability per unit time $\alpha^+(l)$ that the distance increases by the minimum allowed amount, which is $2a$. This probability can be written as

$$\alpha^+(l) = \gamma p_0(l), \quad (3)$$

where (i) γ is the probability per unit time that an atom initially in O (Fig. 2) detaches from the upper step and comes to the point A defined by $OA = a$; and (ii) $p_0(l)$ is the probability that this atom initially at A , sticks to the lower step at position B defined by $AB = l$ (the lattice is assumed simple

cubic) without returning to O . The latter quantity was calculated by Adam *et al.*, but the result is rederived below for the sake of completeness.

To reach the distance $AB=l$, the atom first has to reach the distance $AB'=l-a$. This is done with probability $p_0(l-a)$. Then, if the atom is in B' , its probability to reach B is equal to 1 minus the probability to go back to O , which is $p_0(l)$ because $OB'=l$. Thus

$$p_0(l) = p_0(l-a)[1 - p_0(l)]$$

or

$$p_0(l) = \frac{p_0(l-a)}{p_0(l-a) + 1}. \quad (4)$$

It is easily checked that the formula

$$p_0(l) = \frac{a}{l+a} \quad (5)$$

solves Eq. (4). Since it can fit any initial condition, it is the general solution. The correct initial condition is

$$p_0(0) = 1, \quad (6)$$

which is fitted by $b=a$. Thus

$$p_0(l) = \frac{a}{l+a}, \quad (7)$$

so that Eq. (3) yields

$$\alpha^+(l) = \frac{\gamma a}{l+a}. \quad (8)$$

The probability per unit time $\alpha^-(l)$ that the distance decreases by $2a$ can be calculated in an analogous way. In this case, the atom has to detach from the lower step, which it does in the time unit with a probability γ which is assumed to be the same as before. After detachment, the atom is now on the step edge, and must only diffuse by a distance $l-2a$ to stick to the upper step. Thus Eq. (8) is to be replaced by

$$\alpha^-(l) = \gamma p_0(l-2a) = \frac{\gamma a}{l-a}. \quad (9)$$

The above argument assumes the same detachment probability per unit time upward and downward, i.e., no Schwoebel effect [29,30]. It is easy to take the Schwoebel effect into account. If the detachment probability from O to A is unchanged, a detached atom in A again has the probability $p_0(l-a) = a/l$ to reach B' . The probability that, having reached B' , it reaches B , is $p_{down}(l) = p_1(l) + p_2(l)$, where $p_1(l) = q$ is the probability to go down and stick at once, and $p_2(l)$ is the probability to go first away from the step (by the distance a), then to come back to B' , and eventually to stick in B . The probability to go first away from the step is $(1-q)$; the probability to come back to B' is $(1-a/l)$, because the probability *not* to come back is a/l as given by Eq.

(7), and the probability to go down to B after coming back to B' is $p_{down}(l)$. Thus $p_{down}(l) = q + (1-q)(1-a/l)p_{down}(l)$ or $p_{down}(l) = [1 + (a/l)(1-q)/q]^{-1}$, and the probability that a detached atom in A sticks in B is

$$p_0(l) = \frac{a}{l} p_{down}(l) = \frac{a}{l+a(1-q)/q}. \quad (10)$$

In the absence of the Schwoebel effect, $q=1/2$, and Eq. (10) coincides with Eq. (7).

Since there is no interaction between steps, all allowed configurations have the same energy and the same probability. The detailed balance principle implies

$$\alpha^+(l-2a) = \alpha^-(l). \quad (11)$$

As noted by Adam *et al.* [23], relations (8) and (9) satisfy this requirement. Relation (9) can even be deduced from Eq. (8) and the detailed balance principle.

III. PARADOX

According to Eqs. (8) and (9), the probability that the distance between steps of identical sign becomes shorter is larger than the probability that it becomes longer. Therefore, if one starts from a given initial step distance $l(0)$, the average distance $\langle l(t) \rangle$ between steps of identical sign must initially decrease at short times t .

This occurs even if the initial value $l(0)$ is smaller than or equal to the equilibrium value $\langle l(\infty) \rangle$ given by Eq. (2). If $l(0) \ll \langle l(\infty) \rangle$, then $\langle l(t) \rangle$ has an initial decrease followed by a minimum and an increase until the value given by Eq. (2) is eventually reached.

This unexpected minimum is a paradox. It simulates the pseudofaceting observed in simulations on more realistic systems. The advantage of the present toy model is to simplify its analysis, since the paradox is characterized by the function $\langle l(t) \rangle$ which can be compared with the value given by Eq. (2) at infinite time. Moreover, there is a hope to calculate this function analytically. This is the task of the next sections.

IV. MASTER EQUATION

Since $2a$ is the minimum amount by which the distance l between two steps of identical sign can change, the probability $\tilde{P}(l,t)$ that the distance is l at time t satisfies the master equation

$$\begin{aligned} \frac{d}{dt} \tilde{P}(l,t) = & \alpha^+(l-2a) \tilde{P}(l-2a,t) \\ & + \alpha^-(l+2a) \tilde{P}(l+2a,t) \\ & - [\alpha^+(l) + \alpha^-(l)] \tilde{P}(l,t). \end{aligned} \quad (12)$$

In order to avoid uninteresting complications, it will be assumed that the initial distance $l(0)$ is an even number of times the atomic distance a , so that $l/a = 2n$ is an even integer at any time, and the probability $\tilde{P}(l,t) = \tilde{P}(2na,t) = P(n,t) = P_n(t)$ vanishes if n is not an integer. It follows

that $(N+1)$ has to be replaced by $(N+2)$ in Eq. (2), but this modification is unimportant for large N . Master equation (12) now reads

$$\frac{d}{dt}P_n(t) = \alpha_{n-1}(P_{n-1} - P_n) + \alpha_n(P_{n+1} - P_n),$$

$$n = 2, 3, \dots, \frac{N}{2} - 1, \quad (13)$$

where N is assumed to be even, the detailed balance relation (11) has been used and the notation

$$\alpha_n = \alpha^+(2na) = \frac{\gamma}{2n + \zeta}, \quad n = 1, 2, \dots, \frac{N}{2} - 1 \quad (14)$$

has been introduced. The parameter ζ is equal to 1 in the absence of any Schwoebel effect.

For $n=1$, condition (1) imposes that Eq. (13) is replaced by

$$\frac{d}{dt}P_1(t) = \alpha_1(P_2 - P_1), \quad (15)$$

which can be considered a particular case of Eq. (13) if one defines

$$\alpha_0 = 0. \quad (16)$$

For $n=N/2$, the definition of the model implies $\alpha_n=0$, so that Eq. (13) is replaced by

$$\frac{d}{dt}P_{N/2}(t) = \alpha_{N/2-1}(P_{N/2-1} - P_{N/2}). \quad (17)$$

Master equations (13), (15), and (17) are linear, and their solution can be expanded along normal modes, i.e.,

$$P_n(t) = \sum_k \gamma_k \phi_n^{(k)} e^{-\omega_k t}, \quad (18)$$

where $\phi_n^{(k)}$ and $-\omega_k$ designate the eigenvectors and eigenvalues of the ‘‘master matrix,’’ i.e.,

$$\alpha_{n-1}(\phi_{n-1}^{(k)} - \phi_n^{(k)}) + \alpha_n(\phi_{n+1}^{(k)} - \phi_n^{(k)}) = -\omega_k \phi_n^{(k)},$$

$$n = 1, 2, 3, \dots, N/2. \quad (19)$$

The eigenvalues ω_k can be arranged so that ω_k is an increasing function of the integer k .

The coefficient of $\phi_{n-1}^{(k)}$ in the equation of system (19) whose right hand side is $-\omega_k \phi_n^{(k)}$, and that of $\phi_n^{(k)}$ in the equation whose right hand side is $-\omega_k \phi_{n-1}^{(k)}$, are both equal to the real quantity α_{n-1} . In other words, the ‘‘master matrix’’ is Hermitian. This hermiticity, which is a result of the detailed balance relations (11), implies that the eigenvalues $-\omega_k$ are real. It is easy to see that there is a solution of Eq. (13) independent of time,

$$P_n(\infty) = \gamma_0 \phi_n^{(0)} = 2/N, \quad (20)$$

which must be the long time limit of $P_n(t)$. Since this is a nonzero, finite limit, all values ω_k must be positive except one: $\omega_0=0$.

We tried to solve the problem analytically, in analogy with the familiar case $\alpha_n = \alpha_1$, independent of n . This case corresponds to the diffusion of a particle, when $\phi_n^{(k)}$ designates the Fourier components of the probability P_n . When α_n depends on n through Eq. (14), the calculation is much more complicated. We only treated the ‘‘continuum limit’’ in which $P(n,t)$ and $\phi_n^{(k)}$ can be considered as continuous functions of n and the right hand sides of Eqs. (13), (15), and (17) can be replaced by the first term of their Taylor expansion. This is correct, as will be seen, if $N \gg 1$ and if the quantities $\gamma_k e^{-\omega_k t}$ are small for large ω_k . The result of the calculation, which is given in the Appendixes, is that the average distance between steps at time t is $\langle l(t) \rangle = 2a \langle n(t) \rangle$, where

$$\frac{\langle l(t) \rangle}{a} = 2 \langle n(t) \rangle$$

$$= \frac{N}{2} - \sum_{k=1}^{N/2-1} \frac{4(2n_0 + \zeta) J_{-2/3}[z_k(n_0)] \int_{z_k(1)}^{z_k(N/2)} dz J_{1/3}(z)}{3v_k^2 [J_{-2/3}(v_k)]^2}$$

$$\times \exp\left(-\frac{9v_k^2}{(N+\zeta)^3} \gamma t\right), \quad (21)$$

where n_0 is the initial value of $n = l/(2a)$, and v_k and $z_k(n)$ are defined by

$$v_k = \frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2} (N + \zeta)^{3/2} \quad (22)$$

and

$$z_k(n) = \frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2n + \zeta)^{3/2}. \quad (23)$$

Equation (21) is in fact very complicated because the eigenvalues ω_k , defined by Eq. (19), are difficult to calculate.

In the continuum limit, i.e., for small ω_k (or k) the eigenvalues ω_k are given by

$$J_{1/3}(v_k) = J_{1/3} \left[\frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2} (N + \zeta)^{3/2} \right] = 0. \quad (24)$$

Using the approximation

$$J_\nu(z) = \sqrt{\frac{2}{\pi z}} \sin\left(z + \frac{\pi}{4} - \frac{\nu\pi}{2}\right), \quad (25)$$

valid for large z , Eq. (24) yields for k not too small,

$$\frac{1}{3} v_k = \lambda_k (N + \zeta)^{3/2} = \left(\frac{\omega_k}{\gamma} \right)^{1/2} (N + \zeta)^{3/2} = k\pi - \frac{\pi}{12}. \quad (26)$$

According to this equation, the highest eigenfrequency, which corresponds to $k=N/2$, is proportional to $1/N$ and

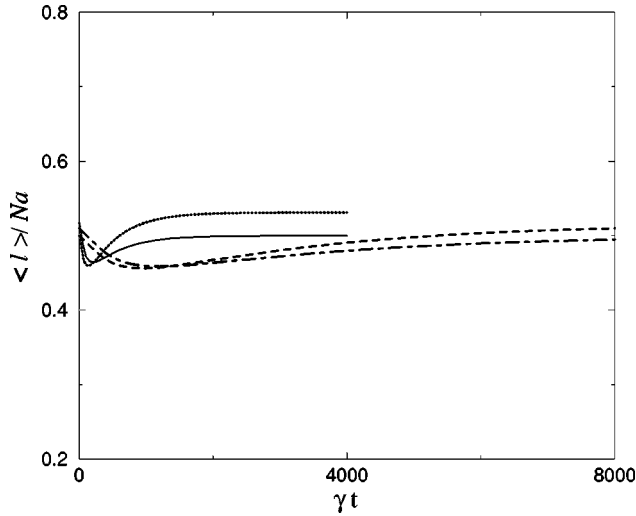


FIG. 3. Reduced average distance $\langle l(t) \rangle / (Na)$ between steps of identical sign at a scaled time γt when the initial distance between steps is $Na/2$. Full curve: as deduced from Eq. (21) for $N=32$. Dash-dotted curve: as deduced from Eq. (21) for $N=60$. Dotted curve: numerical solution of the master equation for $N=32$. Dashed curve: numerical solution of the master equation for $N=60$.

vanishes for large N . This result is probably incorrect. The highest frequencies are of the order of γ , since this is the order of magnitude of the largest coefficients α_n . However, most of these coefficients are of the order of γ/N , in agreement with Eq. (26). Note that formulas (24)–(26) hold only for small ω_k as stated above.

Approximation (24) is obviously good for long times, when Eq. (18) is dominated by small values of ω_k . However, even for short times, formulas (21)–(24) are in good agreement with the numerical solution of Eq. (13), for the discrete model, as shown by Fig. 3. This figure shows that, even when the initial distance between steps coincides with the equilibrium value, a minimum width is attained in the transient state before the long time limit is reached. It is worth mentioning that for long times the numerical solution of the master equation and the results deduced from Eq. (21) do not converge exactly to the same value: the numerical solution goes to $1/2 + 1/N$, and the results of Eq. (21) (for the continuum limit, where $N \gg 1$) go to $1/2$.

A comment is appropriate about the summation on k in Eq. (21). In principle, the “master matrix” has only N eigenvalues ω_k (only $N/2$ if odd values of l/a are discarded), while Eq. (24) has an infinity of solutions. For large N the number of eigenvalues tends to infinity, and this discrepancy is not essential.

The results of calculations based on formulas (21) and (24) are given on Fig. 4. The first $N/2$ values of ω_k have been used in the summation on k in Eq. (21). We have checked that the results do not change appreciably if N eigenvalues are used (if odd values of l/a are not discarded). The roots v_k of the Bessel functions have been found using MATHEMATICA, and the other variables which depend on N , γ , n_0 etc. been calculated as functions of v_k . The time evolution of the reduced average distance $\langle l(t) \rangle / (Na)$ between steps of identical sign is shown for $N=32$ and 60 , for several

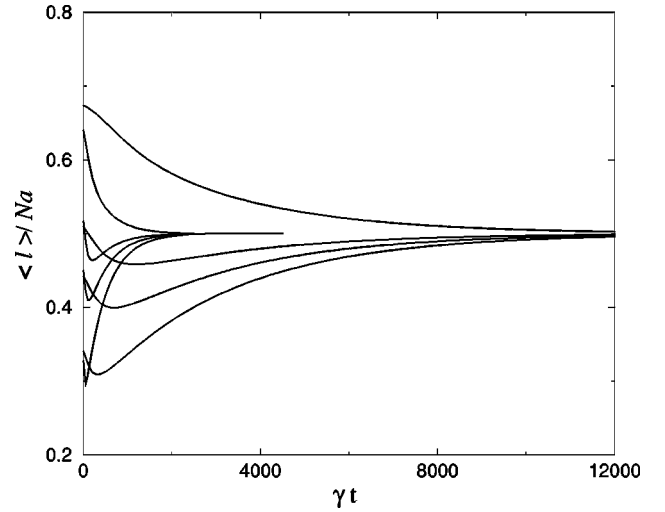


FIG. 4. Reduced average distance $\langle l(t) \rangle / (Na)$ between steps of identical sign at time t , as deduced from Eq. (21) for various values of the initial distance between steps. The maximum distance is $N=60$.

initial conditions. The surface is prepared in such a way that the steps do not touch each other. Thus there is no entropic repulsion at the beginning (far from equilibrium). After some time entropic repulsion sets in. Our model, in which step annihilation is forbidden, shows this clearly through the minimum of the distance between identical steps. Thus the attractive interaction does not survive this entropic repulsion after a certain time. For sufficiently long times all curves go to the equilibrium value $1/2$. Obviously for smaller values of γ , this happens later in time.

For $N=60$ the transient effect persists for longer times than for $N=32$. This indicates that, for greater N , the effect could be more important, since there is more time available for the smaller width to become stable, if for instance, annihilation of steps is allowed, and if this new factor could trap the system into a metastable state. To verify this hypothesis, which is motivated by what is seen in simulations, a more realistic model for the periodic profile has to be used, in order to take into account the connection between steps of opposite sign, and to allow the annihilation of these steps when they become too close.

In the physical case, when there are many steps of the same sign in the sloping parts of the profile rather than just two steps, the effect will not vanish, as would be the case for a regular array of steps of the same sign. The effect will survive due to the presence of steps of opposite sign at the hills and valleys of the profile (where the effect does not exist). What has been observed in the simulation of Adam *et al.* [23], with a $(1+1)$ -dimensional, otherwise realistic, model, is that the distance between steps of identical sign decreases, so that the sloping parts become steeper. Of course, fluctuations of the distance between steps have been observed, but no step pairing, in contrast with the observation made by Kandel and Weeks [32] in a very different context (crystal growth).

Very recently, Israeli and Kandel [22] considered what happens in the evolution of a one-dimensional profile if an

attractive interaction between steps of opposite sign exists (this could be an elastic interaction or an effective attraction simulating the effect of step fluctuations). The entropic repulsion between identical neighbor steps was also considered. Israeli and Kandel found, in a scaling scenario, that pseudofacets form at the top and bottom of the profile in the transient state, and that the step density is smaller near its extrema, due to the faster annihilation process. Without that attractive interaction they found that the profile evolves with cusps replacing the pseudofacets. Here the atomic distance is taken into account, and pseudofacets can *also* appear in the absence of a real attractive interaction.

APPENDIX A: EIGENVECTORS IN TERMS OF BESSEL FUNCTIONS

The probability $\bar{P}(l, t) = \bar{P}(2na, t) = P_n(t) = P_n(t)$, that the distance between two steps at time t is l , satisfies the master equation (13). The quantity to be calculated is $\langle l \rangle_t = \langle 2na \rangle_t$. Then

$$\frac{\langle l \rangle_t}{a} = \sum_{n=1}^{N/2} 2nP_n(t). \quad (\text{A1})$$

It will be assumed that $P_n(t)$ do not change very much when n varies by 1. This is clearly reasonable for large values of n , so a necessary condition for this ‘‘continuous approximation’’ to be valid is that N must be large.

In this ‘‘continuum limit,’’ Eq. (13) reads

$$\frac{\partial}{\partial t} P(x, t) = \frac{\partial}{\partial x} \left[\alpha(x) \frac{\partial P(x, t)}{\partial x} \right], \quad (\text{A2})$$

where x varies continuously between 1 and $N/2$, and

$$\alpha(x) = \alpha^+(2xa) = \frac{\gamma}{2x + \zeta}. \quad (\text{A3})$$

In the continuum limit, expression (A1) reads

$$\frac{\langle l \rangle_t}{a} = 2 \int_1^{N/2} x P(x, t) dx, \quad (\text{A4})$$

while expansion (18) becomes

$$P(x, t) = \sum_k \gamma_k \phi_k(x) e^{-\omega_k t}, \quad (\text{A5})$$

where $\phi_k(x)$ and ω_k are defined by

$$\frac{d}{dx} \left[\alpha(x) \frac{d}{dx} \phi_k(x) \right] = -\omega_k \phi_k(x) \quad (1 < x < N/2) \quad (\text{A6})$$

and the boundary conditions

$$\alpha_1 \frac{d}{dx} \phi_k(1) = -\omega_k \phi_k(1) \quad (\text{A7})$$

and

$$\alpha_{N/2-1} \frac{d}{dx} \phi_k(N/2-1) = \omega_k \phi_k(N/2-1). \quad (\text{A8})$$

Relations (A6), (A7), and (A8), respectively, correspond to Eqs. (13), (15), and (17) in the continuum limit.

Introducing the function

$$\tilde{\Xi} = \alpha(x) \phi_k(x), \quad (\text{A9})$$

one can write Eq. (A6) as

$$\frac{d^2}{dx^2} \tilde{\Xi} + \frac{2}{\gamma} \alpha(x) \frac{d}{dx} \tilde{\Xi} + \frac{2}{\gamma} \alpha'(x) \tilde{\Xi} + \omega_k \alpha^{-1}(x) \tilde{\Xi} = 0, \quad (\text{A10})$$

where use has been made of definition (A3), which implies

$$\alpha'(x) = \frac{d\alpha(x)}{dx} = -\frac{2}{\gamma} \alpha^2(x). \quad (\text{A11})$$

Introducing the variable $z_k(x)$ defined by Eq. (23) and defining $\Xi(z_k(x)) = \tilde{\Xi}(x)$, formula (A10) can be written as

$$z^2 \frac{d^2}{dz^2} \Xi(z) + z \frac{d}{dz} \Xi(z) + (z^2 - \nu^2) \Xi(z) = 0, \quad (\text{A12})$$

where $\nu = 2/3$ and $z = z_k$. This equation is a Bessel equation, and its general solution is

$$\begin{aligned} \phi_k(x) = & a_k \frac{\omega_k}{2\gamma} (2x + \zeta) J_{-2/3}[\lambda_k (2x + \zeta)^{3/2}] \\ & - d_k \frac{\omega_k}{2\gamma} (2x + \zeta) J_{2/3}[\lambda_k (2x + \zeta)^{3/2}], \end{aligned} \quad (\text{A13})$$

where

$$\lambda_k = \frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2}. \quad (\text{A14})$$

The derivative of Eq. (A13) can easily be calculated because $J'_\nu(u) = dJ_\nu(u)/du$ satisfies the relation

$$u J'_\nu(u) = \nu J_\nu(u) - u J_{\nu+1}(u) = -\nu J_\nu(u) + u J_{\nu-1}(u), \quad (\text{A15})$$

which implies, for any λ and r , that

$$\frac{d}{du} [u^{\nu r} J_\nu(\lambda u^r)] = \lambda r u^{\nu r-1+r} J_{\nu-1}(\lambda u^r) \quad (\text{A16})$$

and

$$\frac{d}{du} [u^{\nu r} J_{-\nu}(\lambda u^r)] = -r \lambda u^{\nu r-1+r} J_{-\nu+1}(\lambda u^r). \quad (\text{A17})$$

Using Eqs. (A16) and (A17), with $\nu r = 1$ and $u = 2x + \zeta$, the derivative of Eq. (A13) is found to be

$$\begin{aligned} \frac{d}{dx} \phi_k(x) &= -\frac{1}{2} a_k \left(\frac{\omega_k}{\gamma} \right)^{3/2} (2x + \zeta)^{3/2} J_{1/3}[\lambda_k(2x + \zeta)^{3/2}] \\ &\quad - \frac{1}{2} d_k \left(\frac{\omega_k}{\gamma} \right)^{3/2} (2x + \zeta)^{3/2} J_{-1/3}[\lambda_k(2x + \zeta)^{3/2}]. \end{aligned} \quad (\text{A18})$$

Inserting Eqs. (A13), (A3), and (A18) into Eqs. (A7) and (A8), one obtains

$$\begin{aligned} &a_k J_{1/3}[\lambda_k(2 + \zeta)^{3/2}] + d_k J_{-1/3}[\lambda_k(2 + \zeta)^{3/2}] \\ &= a_k \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2 + \zeta)^{1/2} J_{-2/3}[\lambda_k(2 + \zeta)^{3/2}] \\ &\quad - d_k \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2 + \zeta)^{1/2} J_{2/3}[\lambda_k(2 + \zeta)^{3/2}] \end{aligned} \quad (\text{A19})$$

and

$$\begin{aligned} &a_k J_{1/3}(v_k) + d_k J_{-1/3}(v_k) \\ &= -(N + \zeta)^{1/2} a_k \left(\frac{\omega_k}{\gamma} \right)^{1/2} J_{-2/3}(v_k) \\ &\quad + (N + \zeta)^{1/2} d_k \left(\frac{\omega_k}{\gamma} \right)^{1/2} J_{2/3}(v_k). \end{aligned} \quad (\text{A20})$$

In Eq. (A20), N has been assumed large ($N \gg \zeta$).

APPENDIX B: APPROXIMATIONS FOR SMALL EIGENVALUES

If ω_k is small, $J_{1/3}$ and $J_{2/3}$ are small in Eq. (A19). It follows that

$$d_k/a_k \approx \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2 + \zeta)^{1/2} \frac{J_{-2/3}[\lambda_k(2 + \zeta)^{3/2}]}{J_{-1/3}[\lambda_k(2 + \zeta)^{3/2}]} \quad (\text{B1})$$

Since $J_\nu(u) \approx u^\nu$ for small u , it follows that $d_k/a_k \ll 1$. Thus, Eq. (A13) reduces to

$$\phi_k(x) = a_k \frac{\omega_k}{2\gamma} (2x + \zeta) J_{-2/3} \left[\frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2x + \zeta)^{3/2} \right]. \quad (\text{B2})$$

Neglecting d_k , Eq. (A20) reduces to

$$J_{1/3}(v_k) = -\frac{3v_k}{N + \zeta} J_{-2/3}(v_k). \quad (\text{B3})$$

Assuming

$$\frac{v_k}{N + \zeta} \ll 1, \quad (\text{B4})$$

Eq. (B3) reduces to $J_{1/3}(v_k) = 0$, which is Eq. (24). It follows from Eq. (26) that condition (B4) is equivalent to

$$\frac{k}{N + \zeta} \ll 1. \quad (\text{B5})$$

APPENDIX C: ORTHOGONALITY OF THE EIGENVECTORS

The functions ϕ_k were defined in Sec. IV as eigenvectors of a Hermitian matrix, and therefore must be orthogonal. The orthogonality relation can be written for large N as

$$\int_1^{N/2} \phi_{k'}(x) \phi_k(x) dx = \delta_{k'k}. \quad (\text{C1})$$

In particular, the orthogonality between $\phi_0(x)$ and $\phi_k(x)$ implies

$$\int_1^{N/2} \phi_k(x) dx = 0. \quad (\text{C2})$$

It is of interest to check that formula (B2), valid for small ω_k , satisfies these orthogonality relations. Using Eqs. (A16) and (B2), relation (C2) reduces to

$$(N + \zeta)^{1/2} J_{1/3}[\lambda_k(N + \zeta)^{3/2}] = (2 + \zeta)^{1/2} J_{1/3}[\lambda_k(2 + \zeta)^{3/2}]. \quad (\text{C3})$$

The left-hand side of Eq. (C3) vanishes because of condition (24), and the right hand side is small for small ω_k . Thus relation (C2) is approximately satisfied.

Relation (C1) reads

$$\begin{aligned} &a_k a_{k'} \left(\frac{9}{2} \lambda_k \lambda_{k'} \right)^2 \int_1^{N/2} dx (2x + \zeta)^2 \\ &\quad \times J_{-2/3}[\lambda_k(2x + \zeta)^{3/2}] J_{-2/3}[\lambda_{k'}(2x + \zeta)^{3/2}] = \delta_{k'k}, \end{aligned} \quad (\text{C4})$$

which can alternatively be written as

$$\begin{aligned} &\frac{27}{4} (N + \zeta)^3 a_k a_{k'} (\lambda_k \lambda_{k'})^2 \\ &\quad \times \int_0^1 r dr J_{-2/3}(rv_k) J_{-2/3}(rv_{k'}) = \delta_{k,k'}, \end{aligned} \quad (\text{C5})$$

where $r = [(2x + \zeta)/(N + \zeta)]^{3/2}$ and $N \gg \zeta = 1$, while v_k is defined by Eq. (22), which, together with Eq. (24) and (A15), implies

$$2J_{-2/3}(v_k) + 3v_k J'_{-2/3}(v_k) = 0. \quad (\text{C6})$$

The Bessel function has the property [31] that, if v_k and $v_{k'}$ are solutions of Eq. (C6), they satisfy the relation

$$\int_0^1 r dr J_{-2/3}(rv_k) J_{-2/3}(rv_{k'}) = \frac{1}{2} [J_{-2/3}(v_k)]^2 \delta_{k,k'}. \quad (\text{C7})$$

For $k \neq k'$, Eq. (C5) follows from Eq. (C7). For $k = k'$, insertion of Eq. (C7) into Eq. (C5) yields

$$a_k = \frac{3^{1/2}}{2^{1/2}(\frac{3}{2}\lambda_k)^2(N+\zeta)^{3/2}|J_{-2/3}(v_k)|} \quad (\text{C8})$$

Using expansion (A5), Eq. (A4) can be written as

$$\frac{\langle l \rangle_t}{a} = 2 \sum_{k=0}^{N/2-1} \gamma_k e^{-\omega_k t} \int_1^{N/2} x \phi_k(x) dx. \quad (\text{C9})$$

Since all terms vanish at infinite time except the term $k=0$ which must go to Eq. (2), i.e., to $N/2$ if N is large, Eq. (C9) reads

$$\frac{\langle l \rangle_t}{a} = \frac{N}{2} + \sum_{k=1}^{N/2-1} \gamma_k e^{-\omega_k t} \int_1^{N/2} 2x \phi_k(x) dx. \quad (\text{C10})$$

Now by using Eqs. (C2) and (B2) the integral in expression (C10) above becomes

$$\begin{aligned} \int_1^{N/2} 2x \phi_k(x) dx &= \frac{\omega_k}{2\gamma} \int_1^{N/2} (2x+\zeta)^2 a_k \\ &\times J_{-2/3} \left[\frac{1}{3} \left(\frac{\omega_k}{\gamma} \right)^{1/2} (2x+\zeta)^{3/2} \right] dx. \end{aligned} \quad (\text{C11})$$

Using definition (23) to change variables, one obtains

$$\int_1^{N/2} 2x \phi_k(x) dx = a_k \frac{3}{2} \int_{z(x=1)}^{z(x=N/2)} z J_{-2/3}(z) dz, \quad (\text{C12})$$

which can be written, using Eq. (A16), with $r=\lambda=1$ and $\nu=1/3$, as

$$\int_1^{N/2} 2x \phi_k(x) dx = \frac{3}{2} a_k \int_{z(x=1)}^{z(x=N/2)} dz z^{2/3} \frac{d}{dz} [z^{1/3} J_{1/3}(z)]. \quad (\text{C13})$$

If this is integrated by parts, it becomes

$$\begin{aligned} \int_1^{N/2} 2x \phi_k(x) dx &= \frac{3}{2} a_k \left[z_k(N/2) J_{1/3}[z_k(N/2)] \right. \\ &\quad \left. - z_k(1) J_{1/3}[z_k(1)] \right. \\ &\quad \left. - \frac{2}{3} \int_{\lambda_k(2+\zeta)^{3/2}}^{\lambda_k(N+\zeta)^{3/2}} dz J_{1/3}(z) \right]. \end{aligned} \quad (\text{C14})$$

The first term between brackets vanishes because of Eq. (24). The second term is small. Thus

$$\int_1^{N/2} 2x \phi_k(x) dx = -a_k \int_{\lambda_k(2+\zeta)^{3/2}}^{v_k} dz J_{1/3}(z). \quad (\text{C15})$$

Then, from Eq. (C10),

$$\frac{\langle l(t) \rangle}{a} = \frac{N}{2} - \sum_{k=1}^{N/2-1} a_k \gamma_k e^{-\omega_k t} \int_{\lambda_k(2+\zeta)^{3/2}}^{v_k} dz J_{1/3}(z). \quad (\text{C16})$$

Knowing $P(x,0)$, the coefficients γ_k can be obtained by using Eq. (A5) and the orthogonality condition; then,

$$\gamma_k = \int_1^{N/2} dx \phi_k P(x,0). \quad (\text{C17})$$

If the initial condition is $P(x,t=0) = \delta(x-x_0)$, the coefficients γ_k are given by

$$\gamma_k = \phi_k(x_0) = a_k \frac{\omega_k}{2\gamma} (2x_0+\zeta) J_{-2/3}[\lambda_k(2x_0+\zeta)^{3/2}], \quad (\text{C18})$$

where Eq. (B2) has been used.

Insertion of Eqs. (C8) and (C18) into Eq. (C16) yields

$$\begin{aligned} \frac{\langle l(t) \rangle}{a} &= \frac{N}{2} - \sum_{k=1}^{N/2-1} \frac{\omega_k}{2\gamma} (2x_0+\zeta) \\ &\times J_{-2/3}[\lambda_k(2x_0+\zeta)^{3/2}] a_k^2 e^{-\omega_k t} \int_{\lambda_k(2+\zeta)^{3/2}}^{v_k} dz J_{1/3}(z) \end{aligned}$$

or

$$\begin{aligned} \frac{\langle l(t) \rangle}{a} &= \frac{N}{2} - \sum_{k=1}^{N/2-1} 4(2x_0+\zeta) \frac{J_{-2/3}[\lambda_k(2x_0+\zeta)^{3/2}]}{3v_k^2 [J_{-2/3}(v_k)]^2} e^{-\omega_k t} \\ &\times \int_{\lambda_k(2+\zeta)^{3/2}}^{v_k} dz J_{1/3}(z), \end{aligned} \quad (\text{C19})$$

which reduces to Eq. (21).

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