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Decay of Grooves Cut in a Surface with Singular Orientation when the Neighbouring Orientations are Unstable

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Abstract. — The decay of a grooved profile when the average orientation is singular is treated in the particular case when the orientations close to the singular one are unstable. The system is assumed to exchange atoms with its vapour. The step fluctuations, which allow the profile decay, are treated by a partially exact transfer matrix method. The time \( \tilde{\tau} \) to peel the topmost layer is obtained as a function of the width \( \ell \) of a terrace: \( \tilde{\tau} \propto \ell \exp(\kappa \ell) \), where the constant \( \kappa \) depends on the temperature.

1. Introduction

The smoothing of grooves artificially made in a crystal surface is a classical problem (Blakely [1], Bonzel [2] and Preuss [3]) solved by Mullins [4] in the case of a non-singular orientation. If the final (or average) orientation of the surface is singular, the non-linear problem which arises is controversial. Indeed, it is not clear whether the facets which temporarily arise in experiments are a result of a miscut as claimed by Lançon and Villain [5], or intrinsic properties as claimed by Spohn [6] and Hager et al. [7]. The problem is somewhat simpler if the orientations close to the singular one are unstable, because in that case the topmost layer is peeled without perturbing too much the lower ones. The present work is an investigation of this situation.

At equilibrium, the parts with singular orientations form facets with sharp edges. It is reasonable to assume that the top and the bottom parts of the decaying profile also have facets with sharp edges (Fig. 1). Indeed, the sloping parts of the surface are formed of steps which interact through an attractive interaction (in contrast with the usual case discussed by Bonzel and Preuss [2] and then by Rettori and Villain [8] and then by others).

The exchange of matter (atom per atom) may be either by diffusion on the surface, inside the solid or by exchange with the vapour [4]. The last process, called SALK (surface attachment limited kinetics), is much simpler than the other ones. We shall restrict our attention to this

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case. This process is supposed to apply not only to true evaporation/condensation of a crystal in contact with a vapour phase, but also in the case of surface diffusion on the crystal surface (no exchange with vapour) when exchange of the mobile species (e.g. adatoms) with sources and sinks (e.g. kinks and steps) is so difficult as to be rate limiting. Then the mobile species may be considered to have an uniform chemical potential $\mu$ as if it were a vapour bathing the surface. The exchange of matter between this mobile layer and the sources or sinks is assumed proportional to the difference between $\mu$ and the local chemical potential $\mu + \delta\mu$ determined by surface energy changes resulting from surface displacements. It is not clear whether this limiting case actually exists, but it has been used extensively as a basis for model calculations [9].

In a realistic model of the profile considered here, the two topmost steps should be assumed to fluctuate between their lowest energy positions. The other steps might be assumed to be straight. However, this simplified model is fairly complicated, and we will study a yet simpler model with a single fluctuating step (Fig. 2). The system will be assumed to exchange atoms with its vapour, so that it is sufficient to consider a single ridge.

In Sections 2 and 3, the relaxation mechanism is analyzed and the problem is reduced to the equilibrium statistical mechanics of a single fluctuating line attracted by a fixed line. This problem is a classical one and its thermodynamical properties will be recalled in Section 4. Its dynamical behaviour, however, requires a special analysis which is given in Section 5, where the relaxation time is estimated. In Section 6 the principal results are presented. A dictionary
of the notations used is at the end of the text. The most complicated part of the algebra is contained in the appendices. In Appendix A and B some equilibrium properties are evaluated using the transfer matrix method and in Appendix C, the dynamic problem is treated using an alternative approach: a Fokker-Planck equation is derived and solved approximately, and the typical times involved are estimated.

2. Characteristic Time and Length

If the topmost step is in its ground state (or nearly so) at time $t = 0$ and begins to fluctuate, one has to wait a typical time $t_1$ until it makes junctions with the immobile step (Fig. 3a). After a junction has taken place, both ends of the topmost terrace evaporate and recoil at the velocity $v$, which is only a function of the terrace width $\ell$, and of the line tension $W_1/a$ of the step. If one considers one of the recoiling step loops, it will merge (Fig. 3c) after a time $\tau$ with another loop recoiling at the opposite velocity, which has been created at time $t_2$ (Fig. 3b).

Let $L_1$ be the distance between the points where the junctions at times $t_1$ and $t_2$ have taken place. Let $p_1$ be the probability per unit length and time to have a junction. The time $t_1$
is the time one has to wait before observing a junction in a length of order $L_1$. Therefore, $p_1L_1t_1 \approx 1$. But (assuming $t_2 > t_1$) the time $t_2 - t_1$ is also the time one has to wait before observing a junction in a length of order $L_1$. Therefore $p_1L_1(t_2 - t_1) \approx 1$. Thus:

$$t_1 \approx t_2 \approx t_2 - t_1 \approx \frac{1}{p_1L_1} \quad (2.1)$$

The quantity $(\bar{\tau} - t_1)$ is comprised between $L_1/v$ (if $t_2 = \bar{\tau}$) and $L_1/(2v)$ (if $t_2 = t_1$). Therefore

$$\bar{\tau} - t_1 \approx \frac{L_1}{v} \quad (2.2)$$

The left hand side $\bar{\tau} - t_1$ of this equation is of course larger than $t_2 - t_1$, but cannot be much larger; otherwise, this would imply that the probability of a junction in a length $L_1$ during a time much larger than $t_2 - t_1$ is negligible, and this would be in contradiction with the definition of $p_1$. Therefore, $\bar{\tau} - t_1 \approx t_2 - t_1$. Comparison with (2.1) and (2.2) yields

$$t_1 \approx \frac{L_1}{v} \quad (2.3)$$

Now, (2.2) reads $\bar{\tau} \approx t_1 + L_1/v$ or inserting (2.3) and (2.1):

$$\bar{\tau} \approx \frac{L_1}{v} \approx \frac{1}{p_1L_1} \quad (2.4)$$

Then, it is clear that

$$\bar{\tau} \approx \frac{1}{\sqrt{vp_1}} \quad (2.5)$$

Thus, the time $\bar{\tau}$ necessary to peel the topmost layer will be known if we are able to calculate $v$ and $p_1$. The velocity $v$ is proportional to the difference between the evaporation rate $\sigma$ of the curved step and the evaporation rate $\sigma_0$ of the straight step. This difference is itself proportional to the local excess $\delta\mu$ of the chemical potential. The precise formulae are

$$v = a(\sigma - \sigma_0) = a\sigma_0\beta\delta\mu \quad (2.6)$$

where $a$ is the interatomic distance and $\beta = 1/(k_BT)$. The excess chemical potential is the excess free energy per particle. Since a loop of width $\ell$ and length $vdt$ has an energy $W_1vdt/a$ and contains $\ell vdt/a^2$ particles, it follows $\delta\mu = W_1a/\ell$ and (2.6) reads

$$v \approx a^2\sigma_0\beta\frac{W_1}{\ell} \quad (2.7)$$

3. The Junction Probability $p_1(\ell)$

The junction probability can be evaluated ignoring the non-fluctuating step. In reality when the fluctuating line touches the immobile one, the process becomes irreversible and the two separated parts of the topmost layer begin to recoil. In our calculation we will simply obtain an estimate of the typical time after which the fluctuating line touches the other for the first time.

Consider a part of length $L$ of the fluctuating step. At time $t = 0$, it is supposed to be straight at position $x(y,0) = 0$ for any value of $y$. At time $t$, the maximum value $h(t)$ of $x(y,t)$ will be called the elongation. We want to know the typical time $\tau_1(\ell,L)$ after which
Fig. 4. — Typical excursion (of elongation $h$) of the top of the profile on a length $L$ a) explicitly representing the lower steps and the non fluctuating step and b) ignoring them. A excursion with elongation larger than $\ell$, the size of the terrace, is shown in c). For this configuration we can define the distance $Y$ along which all the points have a position $x \geq \ell$.

$h(t)$ reaches the value $\ell$ for the first time (Fig. 4a). This time should satisfy

$$p_1(\ell)\tau_1(\ell, L) \approx 1$$

(3.1)

Insertion of this equation into (2.5) gives us

$$\tilde{\tau} \approx \sqrt{\frac{L\tau_1(\ell, L)}{v}}$$

(3.2)

The immobile step has no part in the calculation of $\tau_1$. Therefore, it can be ignored. We now consider a single step (Fig. 4b).
Rather than calculating $\tau_1(\ell, L)$, it may be easier to calculate the typical time $\tau_0(\ell)$ during which the elongation $h$ remains larger than $\ell$ if it is larger than $\ell$ at a given time. It turns out that both quantities are related by a simple relation which uses an equilibrium property, namely the probability $p_0^+(L, \ell)$ that the elongation at a particular time is larger than a particular value $\ell$ much larger than the thermal average elongation. Indeed, the periods in which the elongation is larger than $\ell$ have a typical duration $\tau_0(\ell)$ and are separated by a time interval of order $\tau_1(\ell, L)$. Therefore

$$p_0^+(L, \ell) \simeq \frac{\tau_0(\ell)}{\tau_1(\ell, L)} \quad (3.3)$$

The quantity $p_0^+(L, \ell)$ is not easy to calculate exactly. In order to use (in an approximate way) the exact data which are available, we introduce the equilibrium probability $p_2^+(L, Y, h)$ that, on a line of given length $L$, a number $Y/a$ (and no more) of points have a position $x \geq h$. Obviously

$$p_0^+(L, \ell) = \sum_{Y > 0} p_2^+(L, Y, \ell) \quad (3.4)$$

On the other hand, consider a number $\bar{N}$ of replicas of the system (i.e. a line of length $L$) taken from the canonical ensemble with the canonical probability. The number of points of a given ordinate $y$ which have a position $x \geq h$ is $\bar{N}p_0^+(h)$, where

$$p_0^+(h) = \sum_{x \geq h} p(x) \quad (3.5)$$

is the equilibrium probability that for a given $y$, $x(y) \geq h$. The probability $p(h)$ is known exactly as recalled in the next section. The total number of points of the line which have a position $x \geq h$ is obtained by multiplying the number of points of a given ordinate $y$ which have a position $x \geq h$ by the number $L/a$, and therefore it is equal to $(L/a)\bar{N}p_0^+(h)$. On the other hand, the number of points of a given ordinate $y$ which have a position $x \geq h$ can also be written as

$$\bar{N} \sum_{Y > 0} \left( \frac{Y}{a} \right) p_2^+(L, Y, h) \quad (3.6)$$

Equating this to $(L/a)\bar{N}p_0^+(h)$, one obtains

$$\sum_{Y > 0} Y p_2^+(L, Y, h) = Lp_0^+ \quad (3.7)$$

This formula may be exploited in an approximate way if $Y$ is replaced by its average value $\bar{Y}$:

$$\bar{Y} \sum_{Y > 0} p_2^+(L, Y, h) = Lp_0^+ \quad (3.8)$$

Insertion into (3.4) now yields

$$p_0^+(L, h) = \frac{Lp_0^+(h)}{\bar{Y}} \quad (3.9)$$

Now, using (3.2), (3.3) and (3.9) we obtain the basic formula for the peeling time:

$$\tilde{\tau} \simeq \sqrt[\bar{Y}]{\frac{\tau_0(\ell)}{vp_0^+(\ell)}} \quad (3.10)$$

where $v$ is given by (2.7) as pointed out before and $p_0^+(\ell)$ is exactly known. Its value will be recalled in Section 4.

Before estimating $\bar{Y}$ and $\tau_0(\ell)$ we define more precisely our model and recall some well-known equilibrium properties.
4. Equilibrium Properties of a Fluctuating Step

In the previous sections, the problem has been reduced to the statistical mechanics of a line which can fluctuate around a fixed line which attracts it. As will be seen, an "unbinding" transition can occur for this system: the two lines can be bound (localized solution) if the temperature is sufficiently low or, for a fixed temperature, if the attractive potential is sufficiently strong. The first exact theory of binding of two walls in \( d = 2 \) was done by Abraham [10] using the transfer matrix method. Chui and Weeks [11] treated the same problem under a solid-on-solid condition. A different derivation, with an extension to \( d = 3 \) was proposed by Vallade and Lajzerowicz [12].

The problem treated in Appendix A is the study of the fluctuations of a step which has a stiffness \( \gamma \) (defined by (5.1) below) and is bound by an attractive potential \(-W_0\) to a straight line.

We will assume throughout the paper that the distance between kinks along the step, which is of the order of \( \gamma a^2/k_B T \), is large with respect to \( a \), that is to say \( \gamma a \gg k_B T \). This assumption allows one to use equation (A.3c), that is, to consider only transitions of one step away or toward the binding line.

In Appendix A, by using the transfer matrix method, it is shown that the density of probability \( p(x) \) to find a point of the step at a distance \( x \) of the borderline is, for \( x \neq 0 \),

\[
p(x) = |\alpha_0|^2 \exp(-2\kappa x)
\]

where \( \kappa \) is a real number.

Since the integral of the probability is unity, the constant in (4.1) is

\[
|\alpha_0|^2 \simeq 2\kappa
\]

The probability to find a point of the step at a distance larger than \( x \) of the borderline is given by integrating (4.1):

\[
p_0^+(x) \simeq \exp(-2\kappa x)
\]

The width of the topmost layer is assumed to be large with respect to the size of the thermal fluctuations which is of the order of \( 1/\kappa \), then \( \ell \kappa \gg 1 \). Moreover, the continuum limit implies that \( \kappa a \ll 1 \). Thus, the relative order of the length scales is \( \ell \gg 1/\kappa \gg a \).

It might be argued that the assumption \( \kappa a \ll 1 \) is very special, since it will be valid only on a very small range of temperatures. This assumption implies that a fluctuation of large elongation would be relatively easy. If a large value of \( W_0 \) (say \( W_1/2 \)) is chosen, which would be physically reasonable, it could make \( \kappa a \) comparable to unity and would restrict allowed fluctuations to a few times \( a \).

However, experimentally, for various reasons (e.g. feasibility), we are interested by macro- or at least mesoscopic profiles. The profile width \( \ell \) then must be much larger than \( a \). Therefore, the product \( \kappa a \) should be small, otherwise the product \( \kappa \ell \) will be huge and the relaxation time too (as will be seen later). On the other hand, since \( \kappa \) changes rapidly with \( T \), the temperature range where \( \kappa \ell \) is small is very narrow. In this way the assumption \( \ell \gg 1/\kappa \gg a \) is really physical.

In this connection, in Figure 5 a plot of \( \kappa \) versus \( W_0 \) is presented (obtained by solving Eq. (A.25)), in which \( \kappa \) goes to zero as \( W_0 \) approaches the limiting value given by equation (A.26b) (as an equality). Since \( 1/\kappa \) is the order of the average elongation, this plot gives the reader a feel for the difficulty of a fluctuating step to cross the top terrace.

The transfer matrix method demonstrates the existence of a transition at a certain temperature \( T_C \) at which the constant \( \kappa \) vanishes. Above this temperature, the step prefers to increase
Fig. 5. — $\kappa$ as function of $W_0$, the binding potential. The order of the average elongation of an excursion is $1/\kappa$. The solid curve ($\beta W_1 = 0.5$) may be unreliable because $\exp(-\beta W_1)$ would be too big.

its entropy rather than its potential energy, and thus is not bound to the terrace edge. This transition is called unbinding transition or delocalisation transition. When $T > T_C$, there are no forbidden orientations in the vicinity of the average surface orientation, and this is the case discussed in references [5] to [8]. In the present work, the condition $T < T_C$ is assumed. Then in the continuum limit, which corresponds to $\kappa a \ll 1$, we obtain the relations (see in Appendix A, Eqs. (A.23) and (A.25), which define $\kappa$, and Eq. (A.46))

$$W_0 \ll k_BT\quad(4.4a)$$

$$\exp(\kappa a) \approx \frac{2W_0\gamma a}{(k_BT)^2}\quad(4.4b)$$

The transition temperature is given by the condition $\kappa = 0$ and therefore

$$k_BT_C = \sqrt{2W_0\gamma a}\quad(4.4c)$$

5. Estimate of $\bar{Y}$

Our next task is to calculate $\bar{Y}$ and $\tau_0$. In this section an estimate for $\bar{Y}$ is obtained using a simple and intuitive argument and in Appendix B it is evaluated through a detailed calculation. The evaluation of $\tau_0$ will also be performed in two ways: in Section 6 through a simple argument and in Appendix C.

A simple way to estimate $\bar{Y}$ is through the evaluation, for two limiting cases, of the average quadratic difference $\langle \delta x^2 \rangle_y$ between the horizontal positions of two points of the line separated by a distance $y$. 

If \( y \ll \tilde{Y} \), then \( \langle \delta x^2 \rangle_y \) must be approximately the same as in the absence of an attractive potential, namely
\[
\langle \delta x^2 \rangle_y = \frac{y}{\beta \gamma} \quad (5.1)
\]

On the other hand, if \( y \gg \tilde{Y} \), the attractive potential must be considered, and
\[
\langle \delta x^2 \rangle_y = \int_0^\infty \int_0^\infty (x - x')^2 p_{\text{joint}}(y; x, x') dx dx' \quad (5.2)
\]

where \( p_{\text{joint}}(y; x, x') \) is the joint probability that \( x(0) = x \) and \( x(y) = x' \) simultaneously. It can be written as the sum of an uncorrelated probability and a correction, namely
\[
p_{\text{joint}}(y; x, x') = p(x)p(x') + \delta p(y; x, x') \quad (5.3)
\]

If \( y \gg \tilde{Y} \), the correlation term is negligible and
\[
\langle \delta x^2 \rangle_y = \int_0^\infty \int_0^\infty (x - x')^2 p(x)p(x') dx dx' \quad (5.4)
\]

which can be written as
\[
\langle \delta x^2 \rangle_y = 2 \int_0^\infty x^2 p(x) dx - 2 \left( \int_0^\infty xp(x) dx \right)^2 \quad (5.5)
\]

Using (4.1) and (4.2), this yields
\[
\langle \delta x^2 \rangle_y = \frac{1}{2\kappa^2} \quad (5.6)
\]

\( \tilde{Y} \) can then be defined as the crossover value between the behaviours (5.1) and (5.6), so that
\[
\tilde{Y} = \frac{\beta \gamma}{2\kappa^2} \quad (5.7)
\]

A more elaborated evaluation of \( \tilde{Y} \) is done in detail in Appendix B and the final result is almost the same as the previous one:
\[
\tilde{Y} = 0.45 \frac{\beta \gamma}{\kappa^2} \quad (5.8)
\]

The above result is consistent with the assumption \( \tilde{Y} \gg \frac{\gamma a^2}{k_0 \tilde{Y}} \) in the limit \( \kappa a \ll 1 \), that is to say, this result is valid when \( \tilde{Y} \) is much greater than the vertical distance between kinks, and this occurs for large values of the elongation.

Since \( \tilde{Y} \) is defined as (see Eq. (3.9) for instance) the average length along which the points of the line have positions \( x > h \) for an excursion with elongation larger than \( h \) (where \( h \) is much larger than the thermal average elongation), the fact that \( \tilde{Y} \) does not depend on \( h \) is surprising. In general \( \tilde{Y} \) would depend on \( h \), however the result (5.8) shows that \( \tilde{Y} \) does not depend on \( h \) if the elongation is sufficiently large.

6. The Typical Time \( \tau_0 \)

The last unknown quantity is \( \tau_0(\ell) \). A simple way to estimate this quantity is to consider the recoil of an exceptional excursion of amplitude \( h \).
Let \( \sigma \) be the evaporation probability from the fluctuating curve per site and per second, and let \( \Gamma \rho \) be the adsorption probability from the vapour when this vapour has a density
\[
\rho = \rho_0 \exp(\beta \mu) \tag{6.1}
\]

The quantity \( \mu \) is the vapour chemical potential counted from an appropriate origin. At equilibrium, adsorption and emission mutually compensate and
\[
\sigma = \Gamma \rho_0 \exp(\beta \mu) \tag{6.2}
\]

In reality, an excursion of large amplitude \( h \) is not at equilibrium with the vapour which has a fixed density \( \rho_0 \), so that the adsorption rate per site has a fixed value
\[
\sigma_0 = \Gamma \rho_0 \tag{6.3}
\]

On the contrary, the emission rate per site has a value given by (6.2) as a function of the chemical potential \( \mu(h) \) that the vapour would have if it were in equilibrium with the excursion of amplitude \( h \):
\[
\sigma = \sigma_0 \exp(\beta \mu) \tag{6.4}
\]

This value will be assumed to be uniform on the whole excursion. In this way, the velocity of recoil of the excursion is given by
\[
\frac{\partial h}{\partial t} = \sigma_0 (1 - \exp(\beta \mu)) a \tag{6.5}
\]

Assuming that \( \beta \mu \ll 1 \), one can write
\[
\frac{\partial h}{\partial t} = -\sigma_0 \beta a \tag{6.6}
\]

The chemical potential \( \mu \) can be written as \( (\gamma a^2)/R \), where \( R \) is the radius of curvature of the excursion. The quantity which appear in this expression for \( \mu \) is the line stiffness \( \gamma \) rather than the line tension \( W_1/a \) as in (2.7) because this expression for \( \mu \) is valid for weak slope fluctuations while (2.7) is related to a macroscopic loop. To estimate \( R \) we recall a result from Appendix A, where the typical extension \( \lambda \) of a fluctuation of elongation \( h \) is obtained. One finds that
\[
\lambda(x) = \frac{4 \gamma x}{k_B T \kappa} \tag{6.7}
\]

Assuming the excursion is an arc of circle or parabola of base length \( \lambda \) and amplitude \( h \), one finds \( R = (\beta^2 \gamma^2 h)/\kappa^2 \) multiplied by a constant of order unity. Insertion into (6.6) yields
\[
\frac{\partial h}{\partial t} = -\frac{\sigma_0 \kappa^2 a^3}{16 \beta \gamma h} \tag{6.8}
\]

The fact that \( h > \ell \) at \( t = 0 \) implies that the typical elongation \( \bar{h} \) that exceeds \( \ell \) and \( \ell + \frac{1}{\kappa} \) Therefore, the typical time \( \tau_0 \) necessary for \( \bar{h} \) to become smaller than \( \ell \) is \( 1/(\kappa \left| \frac{\partial h}{\partial t} \right|) \).

Replacing \( \frac{\partial h}{\partial t} \) by its expression (6.8), one obtains that
\[
\tau_0(h) \simeq \frac{\beta \gamma h}{\sigma_0 \kappa^3 a^3} \tag{6.9}
\]
7. Results

In this section, the assumptions and the principal results of the preceding sections are recalled, in order to obtain a final expression for the time $\bar{\tau}$ to peel the topmost layer.

We assumed that the step which fluctuates is bound to the limiting borderline of the topmost layer, that is to say, the step is below the unbinding transition: the wavevector of the bound state is $\kappa$.

The topmost layer is assumed to be large with respect to the size of the thermal fluctuations which is of the order of $1/\kappa$, then $\ell \kappa \gg 1$. Moreover, the continuum limit implies that $\kappa a \ll 1$. In this way the relative order of the length scales is $\ell \gg 1/\kappa \gg a$.

Finally, we have supposed that the typical length between kinks along a step, $\beta \gamma a^2$, is larger than the interatomic distance $a$ and that we are near the unbinding transition in order that the large excursions are not too exceptional. In this way $\gamma a \gg k_B T \gg W_0$.

The quantity we want to calculate is the peeling time of the topmost layer, which is given by (3.10). It is sufficient to insert into that formula the expressions (2.7), (4.3), (5.7) and (6.9) to obtain the final result

$$\bar{\tau} \simeq \ell \frac{\kappa}{\kappa^2 \sigma_0 a^2} \sqrt{\frac{\beta \gamma^2}{2 \kappa a W_1}} \exp(\kappa \ell) \quad (7.1)$$

where $\kappa$ is defined by (4.4b).

All these results refer to the case when the topmost terrace is limited by a fluctuating step and a rigid one. If it is limited by two fluctuating steps, a formula analogous to (3.10) should apply, namely

$$\bar{\tau}_2 \simeq \sqrt{\frac{\tau_0 \bar{Y}}{v \rho_0^+ (\ell)}} \quad (7.2)$$

where $p_{00}^+(h)$ is the probability that, for a given $y$, the distance between both topmost steps is greater than $h$. This probability is given by integrating the probability $p_{00}(h)dh$ that, for a given $y$, the distance between both topmost steps is between $h$ and $h + dh$. Now

$$p_{00}(h) = \int_{q=0}^{h} p(h - q)p(q)\,dq \quad (7.3)$$

or using (4.1) and (4.2):

$$p_{00}(h) = 4\kappa^2 h \exp(-2\kappa h) \quad (7.4)$$

Integration now yields

$$p_{00}^+(\ell) = \int_{\ell}^{\infty} p_{00}(h)\,dh = 4\kappa^2 \int_{\ell}^{\infty} h \exp(-2\kappa h)\,dh = (2\kappa \ell + 1) \exp(-2\kappa \ell) \quad (7.5)$$

Equations (2.7), (5.7) and (6.9), which respectively yield $v$, $\bar{Y}$ and $\tau_0$, are still expected to hold. Inserting these relations and (7.5) into (7.2), one obtains the peeling time of a layer in the case of two fluctuating steps as

$$\bar{\tau}_2 \simeq \frac{1}{2\kappa^3 \sigma_0 a^2} \sqrt{\frac{\beta \gamma^2 \ell}{a W_1}} \exp(\kappa \ell) \quad (7.6)$$
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Notation Dictionary

- $a$: interatomic distance.
- $k_B$: Boltzmann constant.
- $\ell$: terrace width.
- $L$: length of an arbitrary part of the system.
- $L_1$: distance between the points where the junctions at times $t_1$ and $t_2$ have taken place.
- $L(A)$: number of adsorption sites.
- $N$: number of lattice sites in the $x$ direction.
- $p_1$: junction probability per unit length and unit time.
- $p^+(L,Y,h)$: equilibrium probability that, on a line of given length $L$, a number $Y/b$ of points have a position $x \geq h$.
- $p(h)$: equilibrium probability that for a given $y$, $x(y) = h$, independent of $y$.
- $t_1$: time one has to wait before observing a junction in a length of order $L_1$.
- $p^+(h)$: equilibrium probability that for a given $y$, $x(y) \geq h$.
- $p^+(L,\ell)$: equilibrium probability that the elongation at a particular time is larger than a particular value $\ell$ much larger than the thermal average value of $x$.
- $p(y; x, x')$: joint probability that $x(0) = x$ and $x(y) = x'$.
- $p^0_\text{cond}(y, x, x')$: conditional probability that $x(y) = x'$ if $x(0) = x$.
- $p_0(h)$: probability that, for a given $y$, the distance between both topmost steps is $h$.
- $p^0(\ell)$: probability that, for a given $y$, the distance between both topmost steps is greater than $\ell$.
- $P_L(h, t)$: probability that the elongation at time $t$ of a line segment of length $L$ is $h$.
- $T$: temperature.
- $v$: recoil velocity of the topmost terrace.
- $W_0$: attractive potential due to the binding line ($W_0 > 0$).
- $W_1$: step free energy per atom. $W_1/a$ is also the line tension at low temperature ($W_1 > 0$).
- $\bar{Y}(h)$: average value of the length $Y'$, along which the points have positions $x \geq h$ for an excursion of elongation larger than $h$, where $h$ is much larger than the thermal average elongation.
Appendix A

Unbinding Transition in 1+1 Dimensions

We consider (Fig. 3a) a fixed straight wall \( x = 0 \) and a line which is at the position \( x(y) \geq 0 \). The line has a stiffness which maintains it straight at the temperature \( T = 0 \), and it is attracted by the fixed wall due to a potential \( V(x) < 0 \) for \( x = 0 \).

It is easier to suppose that \( x \) and \( y \) are discrete variables, \( x/a \) and \( y/a \) being integers, where \( a \) is the interatomic distance. It is also easier to use periodic boundary conditions. The energy is

\[
U(\{x\}, \{y\}) = \sum_{y=0}^{(N-1)a} V_1(x(y)) + \sum_{y=0}^{(N-1)a} V_2(x(y), x(y + a)) \tag{A.1}
\]

where

\[
V_1(x) = -W_0 \delta_{0,x} \tag{A.2}
\]

with \( W_0 > 0 \) the attractive potential and \( V_2 \) corresponds to the stiffness. We can write

\[
V_2(x, x) = 0 \tag{A.3a}
\]

\[
V_2(x, x + a) = V_2(x + a, x) = W_1 > 0 \tag{A.3b}
\]

and for the other values,

\[
V_2(x, x') = \infty \tag{A.3c}
\]

Equation (A.3c) means that \( x(y) - x(y - 1) \) can only have the values 0, \( a \) or \( -a \), otherwise the Boltzmann factor is equal to zero.
A.1. The Partition Function. — The partition function is

\[ Z = \sum_{x_0, x_1, \ldots, x_{N-1}} \exp[-\beta V_1(x_0)] \exp[-\beta V_2(x_0, x_1)] \exp[-\beta V_1(x_1)] \times \exp[-\beta V_2(x_1, x_2)] \ldots \exp[-\beta V_2(x_{N-1}, x_0)] \]  

(A.4)

where \( x_p = x(pa) \). It is useful to introduce the notation

\[ \langle x|\Theta|x' \rangle = \exp \left[ -\frac{\beta}{2} V_1(x) \right] \exp[-\beta V_2(x, x')] \exp \left[ -\frac{\beta}{2} V_1(x') \right] \]  

(A.5)

Now (A.4) can be written

\[ Z = \sum_{x_0, x_1, \ldots, x_{N-1}} \langle x_0|\Theta|x_1 \rangle \langle x_1|\Theta|x_2 \rangle \ldots \langle x_p|\Theta|x_{p+1} \rangle \ldots \langle x_{N-1}|\Theta|x_0 \rangle \]  

(A.6)

The quantity \( \langle x|\Theta|x' \rangle \) can be considered as an element of a real Hermitian matrix \( \Theta \). For the moment we do not give the vectorial meaning to the notation \( |x\rangle \). We will do it later, but now this notation is only a part of the quantity \( \langle x|\Theta|x' \rangle \), which we can call \( \Theta_{xx'} \). Equation (A.6) is written

\[ Z = \text{Tr} \Theta^N \]  

(A.7)

The trace is easy to calculate if the eigenvalues \( \theta_k \) are known. Then

\[ Z = \sum_k \theta_k^N \]  

(A.8)

The interesting case is the limit \( N = \infty \). In this case, by supposing that there is a gap between the greatest eigenvalue \( \theta_0 \) and the others eigenvalues, equation (A.8) is written

\[ Z = \theta_0^N \]  

(A.9)

This expression is not universal, because there is not always a gap, but is quite general. The calculation of the eigenvalues, instead, is specific of each problem.

A.2. Eigenvalues. — An eigenvalue \( \theta \) is defined from the equation

\[ \sum_{x'} \langle x|\Theta|x' \rangle \phi(x') = \theta \phi(x) \]  

(A.10)

where we have omitted the indice \( k \).

From equations (A.5) and (A.3c), equation (A.10) reduces to

\[ \langle x|\Theta|x \rangle \phi(x) + \langle x|\Theta|x + a \rangle \phi(x + a) + \langle x|\Theta|x - a \rangle \phi(x - a) = \theta \phi(x) \]  

(A.11)

For \( x \geq 2a \), from equations (A.5), (A.2) and (A.3), one can written equation (A.11) as

\[ \phi(x) + \epsilon \phi(x + a) + \epsilon \phi(x - a) = \theta \phi(x) \]  

(A.12)

where

\[ \epsilon = \exp(-\beta W_1) \]  

(A.13)

Equation (A.12) obviously has the following solution for \( x \geq a \)

\[ \phi_k(x) = \alpha_k \exp(-kx) \]  

(A.14)
with the eigenvalue
\[
\theta_k = 1 + \varepsilon [\exp(ka) + \exp(-ka)] \tag{A.15}
\]

Since the matrix $\Theta$ is Hermitian, its eigenvalues must be real and then there are three possibilities: i) $k$ is real, ii) $k$ is purely imaginary, iii) the imaginary part of $k$ is equal to $i\pi$. The third possibility yields an eigenvalue (A.15) which is smaller than one and can not be the largest eigenvalue. We will see that $k$ can be or not a real value (and only one). To understand the importance of this fact, let us calculate the distribution of points of the fluctuating line.

A.3. DISTRIBUTION OF THE FLUCTUATING LINE. — The probability $p(x)$ that $x(y)$ has a value $x$ is independent of $y$ and is given by
\[
p(x) = \frac{1}{Z} \sum_{x_1, \ldots, x_{N-1}} \exp[-\beta V_1(x)] \exp[-\beta V_2(x, x_1)] \exp[-\beta V_3(x_1)] \exp[-\beta V_2(x_{N-1}, x)]
\]

where $Z$ is given by equation (A.4). Transforming this equation in the same way as we had transformed equation (A.4), we obtain the following expression, similar to equation (A.6):
\[
p(x) = \frac{1}{Z} \sum_{x_1, \ldots, x_{N-1}} \langle x|\Theta|x_1\rangle \langle x_1|\Theta|x_2\rangle \cdots \langle x_p|\Theta|x_{p+1}\rangle \langle x_{N-1}|\Theta|x \rangle \tag{A.16}
\]

To obtain a compact relation similar to equation (A.7) it is suitable to introduce the vectors $|x\rangle$ and the operators $X$ defined from
\[
\langle x'|x \rangle = \delta_{xx'} \tag{A.17a}
\]
and
\[
\langle x'|X|x \rangle = \delta_{xx'}x \tag{A.17b}
\]

This is a little abstract. For a physicist familiar with quantum physics, it is useful to consider the vectors $|x\rangle$ as representing the states of a particle that moves along the $x$ axis satisfying the equation of Schrödinger (A.10). From equation (A.16) we obtain
\[
p(x) = \frac{1}{Z} \langle x|\Theta^N|x \rangle \tag{A.18}
\]

To utilize this equation, we have to introduce the eigenvectors $|k\rangle$ of $\Theta$. Substituting
\[
\Theta = \sum_k |k\rangle \theta_k \langle k| \tag{A.19}
\]
in equation (A.18), we obtain
\[
p(x) = \frac{1}{Z} \sum_k \theta_k^N \langle x|k\rangle \langle k|x \rangle \tag{A.20a}
\]

If the condition of validity of equation (A.9) is satisfied, equation (A.20a) can be written
\[
p(x) = \frac{1}{Z} \theta_0^N \langle x|0\rangle \langle 0|x \rangle = \langle x|0\rangle \langle 0|x \rangle \tag{A.20b}
\]

where we have used equation (A.9) to write the second equation and we have introduced the eigenvector $|0\rangle$ which corresponds to the greatest eigenvalue $\theta_0$. This eigenvector is given by equation (A.14), where $k$ has a particular value $\kappa$, that is to say,
\[
|0\rangle = \sum_x |x\rangle \phi_0(x) = \alpha_0 D|0\rangle + \alpha_0 \sum_{x \neq 0} |x\rangle \exp(-\kappa x) \tag{A.21}
\]
where $D$ is a constant. Inserting equation (A.21) into equation (A.20b), using equation (A.17b), and supposing $\kappa$ to be real, we obtain, for $x$ different from 0, equation (4.1). If $\kappa$ is positive, the fluctuating line is localized. In this article, this condition is assumed to be fulfilled.

If all the $k$ were imaginary, the general term of equation (A.20a) is independent of $x$. The fluctuating line is delocalized.

A.4. SEARCH FOR A BOUND STATE. — A bound state corresponds to the solution (A.14) with real $k$. Equation (A.14) must also be solution of equation (A.11) for $x = 0$ and $x = a$, that is to say,

\begin{align}
A^2 \phi_0(0) + \epsilon A \phi_0(a) &= \theta \phi_0(0) \quad \text{(A.22a)} \\
\phi_0(a) + \epsilon \phi_0(2a) + \epsilon A \phi_0(0) &= \theta \phi_0(a) \quad \text{(A.22b)}
\end{align}

where

\[ A = \exp(\beta W_0/2) \quad \text{(A.23)} \]

By replacing into equation (A.22) $\phi_0(0)$, $\phi_0(a)$, and $\phi_0(2a)$ calculated from equation (A.21), we find

\begin{align}
A^2 D + \epsilon A \exp(-\kappa a) &= \theta D \quad \text{(A.24a)} \\
AD &= 1 \quad \text{(A.24b)}
\end{align}

Inserting the value for $\theta$ given in equation (A.15), we obtain the following equation of second order in $\exp(\kappa a)$:

\[ A^2 + \epsilon A^2 \exp(-\kappa a) = 1 + \epsilon[\exp(-\kappa a) + \exp(\kappa a)] \]

or

\[ f(e^{\kappa a}) = e^{2k} - \frac{1}{\epsilon}e^{\kappa a} - (A^2 - 1) = 0 \quad \text{(A.25)} \]

The solutions of this equation in $\exp(\kappa a)$ are always real and with opposite sign. The positive solution is the only one which corresponds to a real value of $k$. It corresponds to a localized solution if $\kappa$ is positive, that is to say if $\exp(\kappa a)$ is greater than 1, that is to say if $f(1) < 0$. Then

\[ f(1) = 1 - \left(1 + \frac{1}{\epsilon}\right)(A^2 - 1) < 0 \]

or

\[ A^2 > 1 + \frac{\epsilon}{1 + \epsilon} \quad \text{(A.26a)} \]

or

\[ \exp(\beta W_0) > \frac{1 + 2\exp(-\beta W_1)}{1 + \exp(-\beta W_1)} \quad \text{(A.26b)} \]

We observe that the two lines are bounded if the temperature is sufficiently low or, for a fixed temperature, if the attractive potential is sufficiently strong.
A.5. Joint Probability. — The probability that $x(y') = x$ and simultaneously $x(y'+y) = x'$ is

$$p(y; x, x') = \frac{1}{Z} \sum_{x_1, \ldots, x_N} \exp[-\beta V_1(x)] \exp[-\beta V_2(x, x_1)] \exp[-\beta V_1(x_1)] \exp[-\beta V_2(x, x_1)] \exp[-\beta V_1(x_1)] \exp[-\beta V_2(x_1, x_1)] \exp[-\beta V_1(x_1)] \exp[-\beta V_2(x_1, x_1)]$$

or

$$p(y; x, x') = \frac{1}{Z} \sum_{x_1, \ldots, x_N} \langle x|\Theta|x_1\rangle \langle x_1|\Theta|x_2\rangle \cdots \langle x_{y/a-1}|\Theta|x' \rangle \sum_{x_{y/a+1}, \ldots, x_N} \langle x'|\Theta|x_{y/a+1}\rangle \cdots \langle x_{N-1}|\Theta|x \rangle$$

or

$$p(y; x, x') = \frac{1}{Z} (x|\Theta^{y/a}|x') \langle x'|\Theta^{N-y/a}|x \rangle$$

For $y$ much smaller than the size $Na$ of the system, this expression can be written

$$p(y; x, x') = \sum_k \left( \frac{\theta_k}{\theta_0} \right)^{y/a} \langle x|k|k| \rangle \langle k\rangle \langle k\rangle \langle x'\rangle \langle k\rangle \langle 0\rangle \langle 0\rangle \langle x \rangle \tag{A.27a}$$

or

$$p(y; x, x') = \sum_k \left( \frac{\theta_k}{\theta_0} \right)^{y/a} \langle x|k|\rangle \langle k\rangle \langle x'\rangle \langle k\rangle \langle 0\rangle \langle 0\rangle \langle k\rangle \langle x \rangle \tag{A.27b}$$

An useful check is obtained for $y = 0$, using equations (A.27a), (A.20b) and the relation $\sum_k |k\rangle \langle k| = 1$:

$$p(0; x, x') = \sum_k \langle x|k\rangle \langle k\rangle \langle x'\rangle \langle 0\rangle \langle 0\rangle \langle x \rangle = \delta_{xx'} p(x) \tag{A.28}$$

It is convenient to distinguish between the localized state $|0\rangle$ and the unbound state $|q\rangle$. Equation (A.27) is written

$$p(y; x, x') = p(x)p(x') + \delta p(y; x, x') \tag{A.29}$$

with

$$\delta p(y; x, x') = \sum_{q \neq 0} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \langle x|q\rangle \langle q\rangle \langle x'\rangle \langle 0\rangle \langle 0\rangle \langle x \rangle \tag{A.30}$$

The wave function of the unbounded state is written

$$|q\rangle = D_q \alpha_q |0\rangle + \alpha_q \sum_{x \neq 0} \sin(qx - \gamma_q) |x\rangle \tag{A.31}$$

where $D_q$ and $\gamma_q$ are solutions of the system

$$A^2 D_q + \varepsilon A \sin(qa - \gamma_q) = \theta D_q \tag{A.32a}$$

$$\sin(qa - \gamma_q) + \varepsilon \sin(2qa - \gamma_q) + \varepsilon AD_q = \theta \sin(qa - \gamma_q) \tag{A.32b}$$
or, replacing \( \theta \) by its expression (A.15),

\[
A^2 D_q + \epsilon A \sin(qa - \gamma_q) = [1 + 2\epsilon \cos(qa)] D_q \tag{A.33a}
\]

\[
AD_q = -\sin \gamma_q \tag{A.33b}
\]

Eliminating \( D_q \), we obtain

\[
A^2 + \epsilon A^2 [\cos(qa) - \sin(qa) \cot \gamma_q] = 1 + 2\epsilon \cos(qa) \tag{A.34}
\]

or

\[
\cot \gamma_q = \frac{A^2 - 1 + \epsilon \cos(qa)(A^2 - 2)}{\epsilon A^2 \sin(qa)} \tag{A.35}
\]

We see that \( \gamma_q \) is proportional to \( q \) if \( q \) is small.

The other parameters are determined: \( D_q \), from equation (A.33b); \( \alpha_q \), from the normalization condition. In short, for an infinite system in the \( x \) direction, all values of \( q \) are allowed. However, it may be preferable to assume a large but finite size \( L = Na \), so that \( q \) takes discrete values which, as usual, are the integer multiples of \( 2\pi / L \). Then, the normalization condition takes the form

\[
|\alpha_q|^2 \left[ \sum_x \sin^2(qx - \gamma_q) + \frac{\sin^2 \gamma_q}{A^2} \right] = 1 \tag{A.36a}
\]

which, for large \( L \), reduces to

\[
|\alpha_q|^2 \simeq \frac{2}{N} \tag{A.36b}
\]

By using (A.30) and (A.31) we obtain

\[
\delta p(y; x, x') = |\alpha_0|^2 \sum_q |\alpha_q|^2 \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \sin(qx - \gamma_q) \sin(qx' - \gamma_q) \exp[-\kappa(x + x')] \]

\[
= |\alpha_0|^2 \sum_q |\alpha_q|^2 \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \cos[q(x - x')] \exp[-\kappa(x + x')] \]

\[
-|\alpha_0|^2 \sum_q |\alpha_q|^2 \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \cos[q(x + x') - 2\gamma_q] \exp[-\kappa(x + x')] \tag{A.37a}
\]

or, substituting the expression (A.15) for \( \theta \)

\[
\delta p(y; x, x') = |\alpha_0|^2 \sum_q |\alpha_q|^2 \left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \cos[q(x - x')] \exp[-\kappa(x + x')] \tag{A.37b}
\]

\[
-|\alpha_0|^2 \sum_q |\alpha_q|^2 \left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \cos[q(x + x') - 2\gamma_q] \exp[-\kappa(x + x')] \]

It is pretty hard, from this formula, to recover (A.28) for \( y = 0 \). As a matter of fact, formula (A.37b) is not very convenient for small \( y \). However, if \( y \) is large enough, the quantity

\[
\left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a}
\]
is concentrated in the vicinity of \( q = 0 \). A caveat is that the summand in (A.36a) vanishes for \( q = 0 \), so that one should be careful. For \( qa \ll 1 \) and \( \epsilon \ll 1 \),

\[
\left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} = \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon} \right)^{y/a}
\]

\[
= \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \left( 1 - \frac{4\epsilon \sin^2(qa/2)}{1 + 2\epsilon} \right)^{y/a}
\]

\[
\approx \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \left( 1 - \frac{\epsilon (qa)^2}{1 + 2\epsilon} \right)^{y/a}
\]

\[
\approx \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \exp \left[ -\frac{\epsilon y}{1 + 2\epsilon} qa^2 \right]
\]

The above result is valid only for small values of \( qa \), then insertion into (A.37b) gives a good estimate of \( \delta p(y; x', x) \) if the small values of \( qa \) are the ones which mainly contribute to the summation, that is to say, if \( \epsilon y \gg a \). Under this assumption,

\[
\delta p(y; x, x') \approx |\alpha_0|^2 \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a}
\]

\[
\times \left\{ \sum_q |\alpha_q|^2 \exp \left[ -\frac{\epsilon y}{1 + 2\epsilon} qa^2 \right] \cos[q(x - x')] \exp[-\kappa(x + x')] \right\}
\]

The sum may be replaced by an integral from \(-\pi/a\) to \(\pi/a\), which may be extended to \(-\infty\) to \(\infty\) if \( y \) is not too small. On the other hand, it will be seen below (Eq. (A.44)) that the argument of the Gaussian is equal to \(-k_B T y q^2 / \gamma\). Using (A.37), one obtains

\[
\delta p(y; x, x') \approx \frac{|\alpha_0|^2}{2\pi} \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a}
\]

\[
\times \left\{ \int_{-\infty}^{\infty} dq \exp \left[ -\frac{k_B T y q^2}{2\gamma} \right] \cos[q(x - x')] \exp[-\kappa(x + x')] \right\}
\]

\[
- \int_{-\infty}^{\infty} dq \exp \left[ -\frac{k_B T y q^2}{2\gamma} \right] \cos[q(x + x') - 2\gamma] \exp[-\kappa(x + x')] \right\}
\]

(A.38)

The first integral has the great merit that it does contain \( \gamma_q \). The second integral may be expected to be much smaller than the first one since the integrand oscillates rapidly. A careful calculation confirms this for large enough values of \( y \). The first integral is readily calculated and under the assumption that \( k_B T y / \gamma a^2 \gg 1 \) one obtains

\[
\delta p(y; x, x') \approx \frac{|\alpha_0|^2}{2\pi} \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \sqrt{\frac{\gamma}{k_B T y}} \exp \left[ -\frac{\gamma(x' - x)^2}{2k_B T y} - \kappa(x + x') \right]
\]

(A.39)

One can easily deduce the conditional probability

\[
p_{\text{cond}}(y; x', x) = p(x') + \delta p_{\text{cond}}(y; x', x)
\]
that \( x(y) \) has the value \( x' \) if \( x(0) \) has the value \( x \). Dividing (A.39) by (4.1), one obtains

\[
\delta p_{\text{cond}}(y; x, x') \simeq \frac{a}{2\pi} \left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \sqrt{\frac{\gamma}{k_B T y}} \exp \left[ -\frac{\gamma(x' - x)^2}{2k_B T y} \right] \exp[-\kappa(x' - x)]
\]

This formula is somewhat less cumbersome in the limit \( \kappa a \ll 1 \) (see (A.44) below). In this limit one can write

\[
\left( \frac{1 + 2\epsilon}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \simeq \exp \left( -\frac{k_B T \kappa^2 y}{2\gamma} \right)
\]

and

\[
\delta p_{\text{cond}}(y; x, x') \simeq \frac{a}{2\pi} \sqrt{\frac{\gamma}{k_B T y}} \exp \left\{ - \left[ \frac{k_B T \kappa^2 y}{2\gamma} + \frac{\gamma(x' - x)^2}{2k_B T y} + \kappa(x' - x) \right] \right\}
\]

(A.40)

This formula may be used to determine what will be called the extension of a fluctuation of elongation \( x \), i.e., the vertical distance after which the line has lost the memory and come back to its thermal position. The extension \( \lambda(x) \) may be obtained by setting \( x' = x \) in (A.40). If \( y \) is small, the expression (A.40) is much larger than the equilibrium value \( p(x) \) given by (4.1). If \( y \) is large, it is much smaller than \( p(x') \). The extension \( \lambda(x) \) is defined by \( \delta p_{\text{cond}}(\lambda; x, x) = p(x) \). Neglecting prefactors, one obtains from (4.1) and (A.40) the expression (6.7) for \( \lambda(x) \).

Since \( \lambda \gg \beta \gamma a^2 \) by hypothesis, replacing \( \lambda \) by its expression (6.7) one obtains \( x/k \gg a^2 \), which is consistent with our previous consideration of large excursions \( x \gg a \).

A.6. CONTINUUM LIMIT. — It is easier to obtain the quantities of interest in the continuum limit (for example, this was already done when sums were replaced by integrals in this Appendix). Since all the elementary transitions of the fluctuating step have the size of the interatomic distance \( a \) (because they are due to emission or absorption of atoms), the appropriate condition to attain the continuum limit is, instead of \( a \) goes to zero, to consider \( \kappa \ll 1/a \). In this case, the observable quantities must tend to a fixed limit. One of these quantities is \( \kappa \), defined by equation (A.25). Another is the average quadratic difference between the horizontal positions of two points of the line separated by a vertical distance \( L \)

\[
\langle \delta x^2 \rangle_L = \langle [x(L) - x(0)]^2 \rangle
\]

(A.41)

It is sufficient to calculate this quantity without attractive potential. The line is analogous to the trajectory of a one-dimensional random walker which makes \( L \) steps of amplitude \( a \) and \(-a\) with probability \( \frac{1}{(1+2\epsilon)} \), \( \frac{\epsilon}{(1+2\epsilon)} \) and \( \frac{\epsilon}{(1+2\epsilon)} \) respectively. Then

\[
\langle \delta x^2 \rangle_L = \frac{L}{a} a^2 = \frac{2\epsilon}{1 + 2\epsilon}
\]

(A.42)

On the other hand, in the continuum limit one can write that

\[
\frac{1}{L} \langle \delta x^2 \rangle_L = \frac{k_B T}{\gamma}
\]

(A.43)

In this expression, \( \gamma \) is the stiffness. In the continuum limit, we then have

\[
\frac{2\epsilon}{1 + 2\epsilon} = \frac{k_B T}{\gamma a}
\]

(A.44)
In order to obtain an expression in the continuum limit for the quantity $\kappa$ defined by equation (A.25), one can write from equation (A.25) that

$$A^2 - 1 = \frac{\epsilon e^{2\kappa a}}{\epsilon + e^{\kappa a}}$$

(A.45)

By using equation (A.23) and under the assumptions $\kappa a \ll 1$ and $\gamma a \gg k_B T$, equation (A.45) yields

$$\exp(\beta W_0) - 1 \simeq \frac{e^{\kappa a}}{2\beta \gamma a} \ll 1$$

(A.46)

From (A.46) results that $\beta W_0 \ll 1$ and then equation (4.4b) is obtained. Equation (4.4b) can be alternatively written as

$$\kappa a \simeq 2\beta^2 W_0 \gamma a - 1$$

(A.47)

Another result, which comes from the continuum limit analysis and will be useful in Appendix C, is the value of $|\alpha_0|^2$. Using (4.1), (A.24b) and the normalisation condition, we have

$$|\alpha_0|^{-2} \simeq \frac{a}{A^2} + \frac{1}{2\kappa}$$

(A.48)

then, when $\kappa a \ll 1$, equation (4.2) is obtained.

Appendix B

Calculation of $\tilde{Y}$

The quantity $\tilde{Y}$ can be evaluated using the conditional probability $p_{\text{cond}}^0(y, x, x')$ that $x(y) = x'$ if $x(0) = x$. Weighted integration on $x \geq h$ yields the conditional probability $p_{\text{cond}}^{+0}(y, h, x')$ that $x(y) = x'$ if $x(0) > h$. An approximate evaluation of $\tilde{Y}$ is given by the condition

$$p_{\text{cond}}^{++}(\tilde{Y}, h, h) = \int_{-\infty}^{\infty} p_{\text{cond}}^{+0}(\tilde{Y}, h, x')dx' = \frac{1}{2}$$

(B.1)

This formula determines in principle, $\tilde{Y}(h)$ and therefore $p_{L}^0(L, h)$ through the approximate formula (3.9).

The conditional probability is related by the following formula to the joint probability $p(y; x, x')$ that $x(0) = x$ and $x(y) = x'$:

$$p_{\text{cond}}^{++}(\tilde{Y}, h, h') = \frac{a^{-1}}{p(x)dx} \int_{h}^{\infty} dx \int_{h'}^{\infty} dx' p(y; x, x')$$

(B.2)

The numerator $a^{-1}$ arises from the replacement of sums by integrals. Substituting $p(y; x, x')$ by $p(x)p(x') + \delta p(y; x, x')$ as in Appendix A, one obtains

$$p_{\text{cond}}^{++}(\tilde{Y}, h, h') = a^{-1} \int_{h'}^{\infty} p(x')dx' + \frac{a^{-1}}{p(x)dx} \int_{h}^{\infty} dx \int_{h'}^{\infty} dx' \delta p(y; x, x')$$

(B.3)

The integrands are calculated in Appendix A and their values are given by equation (4.1) and

$$\delta p(y; x, x') = \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \sin(qx - \gamma_q) \sin(qx' - \gamma_q) \exp[-\kappa(x + x')]$$

(B.4)
where $|\alpha_0|^2$ and $\kappa$ are positive constants. $N$ is the number of lattice sites in the $x$ direction (replaced by infinity in the following),

$$\tan \gamma_q = \frac{A^2 \sin(qa)}{2 \cosh(\kappa a) - 2 \cos(qa) + A^2 [\cos(qa) - \exp(-\kappa a)]}$$  \hspace{1cm} (B.5)

$$\theta_0 = 1 + 2 \epsilon \cosh(\kappa a)$$  \hspace{1cm} (B.6a)

and

$$\theta_q = 1 + 2 \epsilon \cos(qa)$$  \hspace{1cm} (B.6b)

From (4.1) and (B.4), the integrals in (B.3) are seen to be

$$\int_{h}^{\infty} p(x)dx = |\alpha_0|^2 \frac{\exp(-2\kappa h)}{2\kappa}$$  \hspace{1cm} (B.7)

and

$$\int_{h}^{\infty} dx \int_{h'}^{\infty} dx' \delta p(y; x, x') = \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \left( \frac{\theta_0}{\theta_q} \right)^{x/a} \times \int_{h}^{\infty} dx \sin(qx - \gamma_q) \int_{h'}^{\infty} dx' \sin(qx' - \gamma_q) \exp[-\kappa(x + x')]$$

In order to use (B.1) we only need the case $h = h'$:

$$\int_{h}^{\infty} dx \int_{h'}^{\infty} dx' \delta p(y; x, x') =$$

$$= \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \left[ \int_{h}^{\infty} dx \Im[\exp(iqx - i\gamma_q - \kappa x)] \right]^2$$

$$= \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \left[ \frac{\exp(iqh - i\gamma_q - \kappa h)}{\kappa - iq} \right]^2$$

$$= \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \exp(-2\kappa h) \left[ \frac{\exp(iqh - i\gamma_q)}{\kappa - iq} \right]^2$$

$$= \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \exp(-2\kappa h) \left[ \frac{\kappa \sin(qh - \gamma_q) + q \cos(qh - \gamma_q)}{\kappa^2 + q^2} \right]^2$$

Defining

$$\tan \phi_q = \frac{q}{\kappa}$$  \hspace{1cm} (B.9)

one finally obtains

$$\int_{h}^{\infty} dx \int_{h'}^{\infty} dx' \delta p(y; x, x') = \frac{2|\alpha_0|^2}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \exp(-2\kappa h) \frac{\exp(-2\kappa h)}{\kappa^2 + q^2} \sin^2(q \phi_q - \gamma_q)$$  \hspace{1cm} (B.10)

Substituting (B.7) and (B.10) in (B.3) one obtains

$$p_{\text{cond}}^{++}(y; h, h) = |\alpha_0|^2 \frac{\exp(-2\kappa h)}{2\kappa a} + \frac{a^{-1}}{N} \sum_{q} \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \frac{4\kappa}{\kappa^2 + q^2} \sin^2(q \phi_q - \gamma_q)$$  \hspace{1cm} (B.11)
In particular, for \( y = 0 \)

\[
1 = |\alpha_0|^2 \frac{\exp(-2\kappa h)}{2\kappa a} + \frac{a^{-1}}{N} \sum_q \frac{4\kappa}{\kappa^2 + q^2} \sin^2(qh + \phi_q - \gamma_q) \tag{B.12}
\]

Subtracting the last two equations yields

\[
p_{\text{cond}}^{++}(y; h, h) = 1 - \frac{a^{-1}}{N} \sum_q \left[ 1 - \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \right] \frac{4\kappa}{\kappa^2 + q^2} \sin^2(qh + \phi_q - \gamma_q) \tag{B.13}
\]

It will now be assumed that

\[
\kappa h \gg 1 \tag{B.14}
\]

In that case, the square of the sinus in (B.13) may be replaced by its average value 1/2 and (B.13) reads

\[
p_{\text{cond}}^{++}(y; h, h) = 1 - \frac{a^{-1}}{N} \sum_q \left[ 1 - \left( \frac{\theta_q}{\theta_0} \right)^{y/a} \right] \frac{2\kappa}{\kappa^2 + q^2}
\]

We now replace the sum by an integral, thus introducing a factor \( aN/(2\pi) \), and use (B.6). We obtain

\[
p_{\text{cond}}^{++}(y; h, h) = 1 - \frac{1}{\pi} \int_{-\pi/a}^{\pi/a} \left[ 1 - \left( \frac{1 + 2\epsilon \cos(qa)}{1 + 2\epsilon \cosh(\kappa a)} \right)^{y/a} \right] \frac{\kappa dq}{\kappa^2 + q^2}
\]

In the limit \( \kappa a \ll 1 \) and \( \epsilon \ll 1 \), that is to say (as explained in Sect. 3 and in Appendix A), when the step stiffness \( \gamma a \) is large with respect to the thermal energy \( k_B T \), the above formula reads

\[
p_{\text{cond}}^{++}(y; h, h) = 1 - \frac{1}{\pi} \int_{-\pi/a}^{\pi/a} \left[ 1 - \exp \left[ \frac{2\epsilon y}{a} \cos(qa) - \frac{2\epsilon y}{a} \cosh(\kappa a) \right] \right] \frac{\kappa dq}{\kappa^2 + q^2}
\]

Moreover we assume that \( \epsilon y \gg a \), then only the values of \( q \) which are small with respect to \( 1/a \) contribute to the integral. In this way an estimate for \( p_{\text{cond}}^{++}(y; h, h) \) is

\[
p_{\text{cond}}^{++}(y; h, h) \simeq 1 - \frac{1}{\pi} \int_{-\infty}^{\infty} \left[ 1 - \exp \left[ -\frac{\epsilon y a^2}{a} \right] \right] \frac{\kappa dq}{\kappa^2 + q^2}
\]

The contribution of the first term between brackets is easily integrated and cancels the first term of the right hand side. Replacing \( \epsilon \) by its value \( k_B T/(2\gamma a) \) valid in the limit \( k_B T \ll \gamma a \) as seen in appendix A, one obtains

\[
p_{\text{cond}}^{++}(y; h, h) = \frac{1}{\pi} \int_{-\infty}^{\infty} \exp \left[ -\frac{k_B T y}{2\gamma} \left( \kappa^2 + q^2 \right) \right] \frac{\kappa dq}{\kappa^2 + q^2}
\]

Introducing the variable \( u = q/\kappa \), formula (B.1) reads

\[
\frac{1}{\pi} \int_{-\infty}^{\infty} \exp \left[ -\frac{k_B T y}{2\gamma} (1 + u^2) \right] \frac{du}{1 + u^2} = \frac{1}{2}
\]
This last equation can be expressed as

$$\text{Erf} \left( \sqrt{\frac{k_B T \gamma \kappa^2}{2 \gamma}} \right) = \frac{1}{2}$$

The numerical solution is easy and gives us equation (5.8). This result is consistent with the assumption $\gamma \gg \frac{\gamma_0^2}{k_B T}$ in the limit $\kappa \ll 1$.

The probability $p_0^+(L, h)$ (which will be useful in Appendix C) can now be obtained, by inserting (5.8) into (3.9) and by using (4.1):

$$p_0^+(L, h) \simeq \frac{\kappa L |\alpha_0|^2}{\beta \gamma} \exp (-2\kappa h) \quad (B.15)$$

Appendix C

Calculation of $\tau_0$

C.1. BASIC EQUATIONS FOR DYNAMICS. — Another way to estimate the time $\tau_0(\ell)$ is to derive a Fokker-Planck equation for the coarse grained probability. Such an equation should yield $\tau_0(\ell)$: it is sufficient to solve the Fokker-Planck equation for states with elongation larger than $\ell$.

In all cases, assuming SALK, the transition probability has to be evaluated as a function of the adsorption rate of atoms from the vapour by steps.

The next task is to write the Fokker-Planck equation for the probability $P_L(h, t)$ that the elongation at time $t$ of a line segment of length $L$ is $h$. The general form of the Fokker-Planck equation is

$$\frac{\partial}{\partial h} P_L(h, t) = \frac{\partial}{\partial h} \left\{ \frac{\partial}{\partial h} [A_L(h)P_L(h, t)] + B_L(h)P_L(h, t) \right\} \quad (C.1)$$

The functions $A_L(h)$ and $B_L(h)$ which are appropriate for the problem of interest here have now to be determined. A relation between the two functions can be obtained as follows. If $P_L(h, t)$ is replaced in (C.1) by the equilibrium probability $P_L(h, \infty)$, the left hand side should vanish, and therefore the quantity between brackets in the right hand side should be constant. This constant must actually vanish because it represents a current of probability. It follows that

$$\frac{\partial}{\partial h} [A_L(h)P_L(h, \infty)] + B_L(h)P_L(h, \infty) = 0 \quad (C.2)$$

or

$$B_L(h) = -\frac{dA_L(h)}{dh} - A_L(h) \frac{\partial}{\partial h} [\ln P_L(h, \infty)] \quad (C.3)$$

The probability $P_L(h, \infty)$ is the opposite of the derivative of the quantity $p_0^+(L, h)$ which is approximately given by (B.15), then

$$\frac{\partial}{\partial h} [\ln P_L(h, \infty)] = -2\kappa \quad (C.4)$$

and equation (C.3) can be rewritten

$$B_L(h) = 2\kappa A_L(h) - \frac{d}{dh} A_L(h) \quad (C.5)$$
Instead of writing directly the Fokker-Planck equation for $P_L(h,t)$, we shall introduce a new variable $A$, defined as the area of the excursion responsible for the elongation $h$. Assuming that the excursion is an arc of parabola with amplitude $h$ and basis $\lambda(h)$, one finds

$$A = \frac{2}{3} \lambda(h) h$$  \hspace{1cm} (*6*)

It is shown in Appendix A (formula (6.7)) that

$$\lambda(h) = Qh$$  \hspace{1cm} (*7*)

with

$$Q = \frac{4 \beta \gamma}{\kappa}$$  \hspace{1cm} (*8*)

It follows that $A$ is proportional to $h^2$:

$$A = \frac{2}{3} Q h^2$$  \hspace{1cm} (*9*)

Recall that the evaporation rate from the fluctuating curve per site is given by

$$\sigma = \sigma_0 \exp(\beta \mu)$$  \hspace{1cm} (*10*)

where $\sigma_0$ is the adsorption rate per site and $\mu(h)$ is the chemical potential that the vapour would have if it were in equilibrium with the excursion of amplitude $h$.

This value will be assumed to be uniform on the whole excursion. The evolution of the probability $\bar{p}(A,t)$ that $A$ has a particular value is determined by the following facts: i) On each adsorption site there is a probability $\sigma_0$ to adsorb an atom from the vapour, and therefore to increase the area $A$ by a quantity $a^2$ equal to the atomic area. ii) On each adsorption site there is a probability $\sigma$ to evaporate an atom into the vapour, and therefore to decrease the area $A$ by a quantity $a^2$. iii) The number of adsorption sites, $L(A)$ is approximately equal to the length of the excursion divided by the atomic distance $a$:

$$L(A) \approx \frac{2}{a} \sqrt{h^2 + \left( \frac{\lambda(h)}{4} \right)^2}$$  \hspace{1cm} (*11*)

since $1/Q \ll 1$. The resulting evolution equation is

$$\frac{\partial}{\partial t} \bar{p}(A,t) = \sigma_0 L(A-a^2) \bar{p}(A-a^2,t) - \sigma_0 L(A) \bar{p}(A,t) + \sigma (A+a^2) L(A+a^2) \bar{p}(A+a^2,t) - \sigma(A) L(A) \bar{p}(A,t)$$  \hspace{1cm} (*12*)

Replacing the right hand side of (*12) by its Taylor expansion yields

$$\frac{\partial}{\partial t} \bar{p}(A,t) = -\sigma_0 a^2 \frac{\partial}{\partial A} \left[ L(A) \bar{p}(A,t) \right] + a^2 \frac{\partial}{\partial A} \left[ \sigma(A) L(A) \bar{p}(A,t) \right]$$

$$+ \frac{\sigma_0 a^4}{2} \frac{\partial^2}{\partial A^2} \left[ L(A) \bar{p}(A,t) \right] + a^4 \frac{\partial^2}{\partial A^2} \left[ \sigma(A) L(A) \bar{p}(A,t) \right]$$  \hspace{1cm} (*13*)

This is the Fokker-Planck equation for $\bar{p}(A,t)$. It is easy to deduce the Fokker-Planck equation for $P_L(h,t)$. Indeed $\bar{p}(A,t)$ and $P_L(h,t)$ are densities of probability and the probability that $A$ is in a given interval $dA$ should be the same in terms of the variable $A$, and of the variable $h$:

$$\bar{p}(A,t) dA = P_L(h,t) dh$$  \hspace{1cm} (*14*)
Substituting the relation
\[ dA = \frac{4}{3} Qdh \delta h \simeq Qdh \] (C.15)
deduced from (C.9), one obtains
\[ P_L(h, t) = Qh \delta(A, t) \] (C.16)
Insertion into (C.13) yields
\[ \frac{\partial}{\partial t} P_L(h, t) = \frac{\sigma_0 a^2}{Q} \frac{\partial}{\partial h} \left\{ \left[ \exp(\beta \mu) - 1 \right] \frac{L(h) P_L(h, t)}{h} \right\} \]
\[ + \frac{\sigma_0 a^4}{2Q^2} \frac{\partial^2}{\partial h^2} \left\{ \left[ \exp(\beta \mu) + 1 \right] \frac{L(h) P_L(h, t)}{h} \right\} \] (C.17)
where, as seen from (C.7) and (C.11):
\[ L(h) \simeq \frac{2h}{a} \sqrt{1 + \left( \frac{Q}{4} \right)^2} \] (C.18)
Formula (C.17) is easily cast into the desired Fokker-Planck equation:
\[ \frac{\partial}{\partial t} P_L(h, t) = \frac{\sigma_0 a^2}{Q} \frac{\partial}{\partial h} \left\{ \left[ \exp(\beta \mu) - 1 \right] \frac{L(h) P_L(h, t)}{h} \right\} \]
\[ + \frac{\sigma_0 a^4}{2Q^2} \frac{\partial^2}{\partial h^2} \left\{ \left[ \exp(\beta \mu) + 1 \right] \frac{L(h) P_L(h, t)}{h^2} \right\} + \frac{\sigma_0 a^4}{2Q^2} \frac{\partial}{\partial h} \left\{ \left[ \exp(\beta \mu) + 1 \right] \frac{L(h) P_L(h, t)}{h^3} \right\} \] (C.19)
or using (C.18):
\[ \frac{\partial}{\partial t} P_L(h, t) = \frac{\sigma_0 a^3}{Q^2} \sqrt{1 + \left( \frac{Q}{4} \right)^2} \frac{\partial^2}{\partial h^2} \left\{ \left[ \exp(\beta \mu) + 1 \right] \frac{P_L(h, t)}{h} \right\} \]
\[ + \frac{\sigma_0 a}{Q} \sqrt{1 + \left( \frac{Q}{4} \right)^2} \frac{\partial}{\partial h} \left\{ \left[ \exp(\beta \mu) - 1 \right] P_L(h, t) + \frac{\exp(\beta \mu) + 1}{2Q} a^2 \frac{P_L(h, t)}{h^2} \right\} \] (C.20)
Comparing with (C.1), one sees that
\[ A_L(h) = \frac{\sigma_0 a^3}{Q^2 h} \sqrt{1 + \left( \frac{Q}{4} \right)^2} \left[ \exp(\beta \mu) + 1 \right] \] (C.21)
or, using (C.8):
\[ A_L(h) = \frac{\sigma_0 a^3 \kappa}{8\beta \gamma h} \sqrt{1 + \left( \frac{\kappa}{\beta \gamma} \right)^2} \left[ \exp(\beta \mu) + 1 \right] \] (C.22)
Comparison between (C.1) and (C.20) yields
\[ B_L(h) = \sigma_0 a \sqrt{1 + \left( \frac{\kappa}{\beta \gamma} \right)^2} \left\{ \left[ \exp(\beta \mu) - 1 \right] + \frac{\exp(\beta \mu) + 1}{8\beta \gamma h^2} \kappa a^2 \right\} \] (C.23)
Substituting $A_L(h)$ and $B_L(h)$ by their expression, (C.5) reads

$$\exp(\beta \mu) - 1 = \frac{a^2 \kappa}{8 \beta \gamma h} \left\{ 2 \kappa \left[ \exp(\beta \mu) + 1 \right] - \frac{d}{dh} \left[ \exp(\beta \mu) + 1 \right] \right\}$$  \hspace{1cm} (C.24)

If we assume that $\kappa h \gg 1$ and $\beta \mu \ll 1$, the second term of the right hand side is negligible as can be checked self-consistently a posteriori, and equation (C.24) yields

$$\beta \mu \simeq \frac{a^2 \kappa^2}{2 \beta \gamma h}$$  \hspace{1cm} (C.25)

It is easy to check the second assumption i) by definition, $\kappa$ is smaller than $1/a$. ii) $\kappa h \gg 1$ implies by using i) that $h/a \gg 1$. iii) $\beta \gamma a^2$ is at least of the same order of magnitude as $a$, because this length is the typical distance between kinks along the step. Then by using i), ii) and iii), it is easy to see that

$$\beta \mu \ll 1$$

Finally, under the assumption that $\kappa h \gg 1$, and by substituting (C.25) in (C.22) and (C.23), the expressions of $A_L(h)$ and $B_L(h)$ at the relevant order are

$$A_L(h) = \frac{\Omega}{h}$$  \hspace{1cm} (C.26a)

$$B_L(h) = \frac{\Omega}{h} \left( 2 \kappa + \frac{1}{h} \right)$$  \hspace{1cm} (C.26b)

where

$$\Omega = \frac{\sigma_0 a^3 \kappa}{4 \beta \gamma} \sqrt{1 + \left( \frac{\kappa}{\beta \gamma} \right)^2} \simeq \frac{\sigma_0 a^3 \kappa}{4 \beta \gamma}$$  \hspace{1cm} (C.26c)

since $\left( \frac{\kappa}{\beta \gamma} \right)^2$ is negligible compared to unity.

C.2. EXPLOITATION OF THE FOKKER-PLANCK EQUATION. — From (C.1) one can derive an equation for the average value

$$\bar{h}(t) = \int_0^\infty h P_L(h,t) dh$$  \hspace{1cm} (C.27)

For the sake of simplicity, it will be assumed that the integrand has no singularity. As a matter of fact, the model studied in appendix A has a singularity at $x = 0$, but extension to this case would be easy.

Multiplying equation (C.1) by $h$ and integrating, one obtains indeed

$$\frac{d}{dt} \bar{h}(t) = \int_0^\infty h \frac{\partial^2}{\partial h^2} [A_L(h) P_L(h,t)] dh + \int_0^\infty h \frac{\partial}{\partial h} [B_L(h) P_L(h,t)] dh$$  \hspace{1cm} (C.28)

Integrating by parts and assuming $P_L(\infty, t) = 0$, one obtains

$$\frac{d}{dt} \bar{h}(t) = -B_L(\bar{h}) + A_L(0) P_L(0, t)$$  \hspace{1cm} (C.29)

where $B_L(\bar{h})$ is

$$B_L(\bar{h}) = \int_0^\infty B_L(h) P_L(h,t) dh$$  \hspace{1cm} (C.30)
Fig. 6. — a) Probability \( \frac{p_0(L; x)}{\int_{h_0}^{\infty} p_0(L; x''')dx''' \} \) that the elongation of a line segment of length \( L \) is \( x \) at \( t = 0 \), normalized under the condition \( x > h_0 \). b) Time dependent conditional probability \( P_L(x'; x, t) \) that the elongation is \( x \) at time \( t \) if it was \( x' \) at time \( t = 0 \).

A particular case of interest is when, for \( t = 0 \), the probability satisfies \( P_L(h, 0) = 0 \) for \( h < h_0 \) where \( h_0 \) is some large value (Fig. 6). Then, if for sufficiently short times \( t \) the probability \( P_L(0, t) \) is negligible, equation (C.30) reads

\[
\frac{d}{dt} \bar{h}(t) = -B_L(\bar{h})
\]  

(C.31)

In the last equation, \( B_L(\bar{h}) \) may be approximated by \( B_L(\bar{\bar{h}}) \). By inserting equation (C.26b) into equation (C.31), neglecting the term proportional to \( 1/\bar{h}^2 \) and then integrating, one obtains

\[
\bar{h}(t)^2 = \bar{h}(0)^2 - 4\kappa\Omega t
\]  

(C.32)
One can also derive an equation for the second moment of the distribution $P_L(h, t)$ defined by

$$\overline{h^2}(t) = \int_0^\infty h^2 P_L(h, t) \, dh \quad (C.33)$$

Following an analogous procedure as above, multiplying equation (C.1) by $h^2$ and integrating, one obtains

$$\frac{d}{dt} \overline{h^2}(t) = \int_0^\infty h^2 \frac{\partial^2}{\partial h^2} [A_L(h) P_L(h, t)] \, dh + \int_0^\infty h^2 \frac{\partial}{\partial h} [B_L(h) P_L(h, t)] \, dh \quad (C.34)$$

Again, integrating by parts, using the property $A_L(\infty) = 0$, and assuming $P_L(0, t) = 0$, one obtains

$$\frac{d}{dt} \overline{h^2}(t) = 2A_L(h) - 2\bar{h}B_L(h) \quad (C.35)$$

where $A_L(\bar{h})$ is given by an analogous expression as the one for $\bar{B}_L(h)$ (C.30). We can approximate equation (C.35) by

$$\frac{d}{dt} \overline{h^2}(t) = 2A_L(\bar{h}) - 2\bar{h}B_L(h) \quad (C.36)$$

and then, using equation (C.31), this relation becomes

$$\frac{d}{dt} \overline{h^2}(t) = \frac{d}{dt} \bar{h}(t)^2 + 2A_L(\bar{h}) \quad (C.37)$$

Integrating this expression one obtains

$$\overline{h^2}(t) - \bar{h}(t)^2 = \bar{h}^2(0) - \bar{h}(0)^2 + 2A_L(\bar{h}) \quad (C.38)$$

Now, by writing the coefficients of the Fokker-Planck equation as $A_L(h) = \Omega/h$ and $B_L(h) = 2\kappa\Omega/\bar{h}$ and considering an initial configuration of elongation $x'$, one obtains from equation (C.32) that the average $u_1 = \bar{h}$ is written

$$\bar{h}(t) = \sqrt{x'^2 - 4\kappa\Omega t} \quad (C.39)$$

and that the variance $\sigma^2 = \overline{h^2}(t) - \bar{h}(t)^2$ is written

$$\sigma^2 = \frac{2\Omega}{\bar{h}(t)} t = \frac{2\Omega}{\sqrt{x'^2 - 4\kappa\Omega t}} t \quad (C.40)$$

By supposing that the distribution $P_L(h, t)$ is a Gaussian, it can be written as

$$P_L(x, t) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp \left[ -\frac{(x-u_1)^2}{2\sigma^2} \right] \quad (C.41)$$

As can be seen through the relations already obtained for the first and second moments (Eqs. (C.39) and (C.40)), $P_L(x, t)$ does not depend explicitly on $L$. This must be a consequence of considering that there is only one exceptional excursion (of elongation $x$ much larger than the thermal fluctuation) along a line segment of length $L$, that is to say, $L$ is not too large.
Now, using equations (C.39) and (C.40), one can write equation (C.41), which is in fact an expression for the conditional probability \( P_L(x(0) = x'; x, t) \) (since it was considered that \( P_L(x, t = 0) = \delta(x - x') \)), as

\[
P_L(x(0) = x'; x, t) = \left( \frac{4\pi\Omega}{\sqrt{x'^2 - 4\kappa\Omega t}} \right)^{-1/2} \exp \left[ -\frac{(x - \sqrt{x'^2 - 4\kappa\Omega t})^2}{4\Omega} \frac{\sqrt{x'^2 - 4\kappa\Omega t}}{t} \right] \quad (C.42)
\]

Remind that an assumption about short times was already done. In this way equation (C.42) is valid for sufficiently short times such that \( t \ll \frac{\tau^2}{4\kappa^2 \Omega} \) (see Eq. C.39).

From equation (C.42) we want to obtain the conditional probability \( P_L^{++}(h_0; t) \) which is the probability that the elongation at a particular time \( t \) is larger than \( h_0 \) if it was larger than \( h_0 \) at the time \( t = 0 \). The purpose here is to find \( \tau_0(h_0) \) which is the typical time during which an elongation remains larger than \( h_0 \) if it was larger than \( h_0 \) at \( t = 0 \). The time \( \tau_0 \) will be determined by the condition \( P_L^{++}(h_0; \tau_0) = 1/2 \). The conditional probability can be written as

\[
P_L^{++}(h_0; t) = \int_{h_0}^{\infty} dx \int_{h_0}^{\infty} dx' \frac{p_0(L; x')}{\int_{h_0}^{\infty} dx'' p_0(L; x'')} P_L(x'; x, t) \quad (C.43)
\]

where the appropriated weight in the integrand is the probability that the elongation in a given instant \( t = 0 \) was \( x' \), normalized under the condition \( x' > h_0 \) (see Fig. 5a).

Using equation (B.15) and equation (C.41) the expression (C.43) for the conditional probability becomes

\[
P_L^{++}(h_0; t) = \int_{h_0}^{\infty} \frac{2\kappa \exp[-2\kappa(x' - h_0)]}{\sqrt{2\pi\sigma^2}} \int_{h_0}^{\infty} \frac{dx}{\sqrt{2\pi\sigma^2}} \exp \left[ -\frac{(x - u_1)^2}{2\sigma^2} \right] \quad (C.44)
\]

where \( u_1 \) and \( \sigma^2 \) are given by (C.39) and (C.40).

In order to develop equation (C.44) it is easier to work with the appropriated dimensionless variables, \( X' = x'\sqrt{\kappa}/h_0, X = x\sqrt{\kappa}/h_0, s = \sqrt{\kappa h_0} \) and \( t' = t/\tau \) where \( \tau = \frac{h_0}{4\kappa^2 \Omega} \). Equation (C.44) can then be written

\[
P_L^{++}(h_0; t) = \frac{2s^{3/2}}{\sqrt{\pi}} \int_s^{\infty} \exp[-2s(X' - s)] dX' \quad (C.45)
\]

For sufficiently short times, that is to say, \( t' \ll X'^2, t' \ll X^2 \), equation (C.45) can be approximated by

\[
P_L^{++}(h_0; t) \approx \frac{2s^{3/2}}{\sqrt{\pi}} \int_s^{\infty} \exp[-2s(X' - s)] \left( \frac{X'}{t'} \right)^{1/2} dX' \quad (C.46)
\]

Integrating in the variable \( X \), one obtains

\[
P_L^{++}(h_0; t) \approx s \int_s^{\infty} \exp[-2s(X' - s)] \left\{ 1 - \text{Erf} \left[ \left( \frac{sX'}{t'} \right)^{1/2} \left( s - X' + \frac{t'}{2X'} \right) \right] \right\} dX' \quad (C.47)
\]
that can be written as

\[ P_{L}^{++}(h_0; t) \simeq \frac{1}{2} \left\{ 1 - 2s \int_{s}^{\infty} \exp[-2s(X' - s)] \text{Erf} \left[ \left( \frac{sX'}{t'} \right)^{1/2} \left( s - X' + \frac{t'}{2X'} \right) \right] \right\} dX' \]  

(C.48)

Performing the variable transformation \( \eta = x' - s \) and under the condition \( \eta \ll s \), which is equivalent to the condition \( h_0 \kappa \gg 1 \), one can write

\[ P_{L}^{++}(h_0; t) \simeq \frac{1}{2} \left\{ 1 - 2s \int_{0}^{\infty} \exp(-2\eta) \text{Erf} \left[ \left( \frac{s^2}{t'} \right)^{1/2} \left( \frac{t'}{2s} - \eta \right) \right] \right\} d\eta \]  

(C.49)

Through another change of variables, \( \rho = 2a\eta \), equation (5.25) can be written

\[ P_{L}^{++}(h_0; t) \simeq \frac{1}{2} \left\{ 1 - \int_{0}^{\infty} \exp(-\rho) \text{Erf} \left( \frac{t' - \rho}{2t'^{1/2}} \right) \right\} d\rho \]  

(C.50)

To find the typical time \( \tau_0 \) one must impose that \( P_{L}^{++}(h_0, \tau_0) = 1/2 \). This implies that \( t'_0 = \tau_0/\tau \) will be given by the solution of

\[ \int_{0}^{\infty} \exp(-\rho) \text{Erf} \left( \frac{t'_0 - \rho}{2t'^{1/2}} \right) d\rho = 0 \]  

(C.51)

The numerical solution of this equation is \( t'_0 \simeq 0.91 \), which yields, if we substitute \( h_0 \) by \( \ell \)

\[ \tau_0(\ell) \simeq 0.91 \frac{\ell}{4\kappa^2\Omega} \]  

(C.52)

Replacing \( \Omega \) by its expression (C.26c),

\[ \tau_0(\ell) \simeq 0.91 \frac{\beta \gamma \ell}{\kappa^3 a^3 \sigma_0} \]  

(C.53)

References

The Imaginary Part of Rock Jointing

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Abstract. — The distribution of joint spacings in a granitic massive in Saudi Arabia is found to be well-described by a power-law with characteristic exponent \( \mu \approx 0.5 \). We compare the cumulative and density distributions and show how to correct the cumulative distribution for bias due to the finite sampling size. The exponent \( \mu \) is close to those obtained for size distribution in fragmentation processes. We study simple models of fragmentation/jointing processes, which predict that the power law distribution must be decorated by a log-periodic modulation if the fragmentation involves a preferred ratio (even approximately so, i.e. with disorder) corresponding to an approximate discrete scale invariance. We corroborate this prediction by carrying out a more detailed analysis of the density distribution and find at least 6 log-periodic oscillations. This implies that the exponent \( \mu \) possesses an imaginary part, embodying the existence of an average discrete scaling structure with preferred fragmentation ratio close to \( 1/2 \). The confidence level of this result is found better than 97% from synthetic tests.

1. Introduction, Geological Setting and Data Presentation

Jointing is certainly the most ubiquitous form of brittle fracture affecting rocks. Joints are usually defined as discontinuities across which no significant displacement occurs, which differentiate them from faults. Moreover, they are considered in general as mode I ruptures, i.e. “crack opening” [1,2] (for a different point of view, see [3]) whereas faults correspond to modes II or III (shear ruptures) [4].

Understanding the spatial organization of joints in rocks is of prime importance, as it controls the meso-scale permeability within reservoirs. More fundamentally, joints can be considered as potential nucleation sites for faults [5–8]. Most of the previous work on jointing dealt with rupture in sedimentary rocks [1,9,10]. In such media, the spatial distribution of a given directional joint set is often found homogeneous and reveals the existence of a well-defined characteristic scale. Moreover, when only one joint set is present, this scale is often found

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equal, or proportional, to the thickness of the mechanical bed in which joints develop [1,10,11] (see also [12–15] for some different points of view). We have to note, however, that this scale seems also to be controlled by the lithology, which determines the physical and mechanical properties of rock [1,9]. In crystalline rocks, it is commonly observed that the joint distribution is much more heterogeneous [1,16].

The aim of this paper is to provide a quantitative description of joint organization in a granite massive belonging to the western Arabian plate basement. We present here new results on the spacing distribution between parallel joints pertaining to the same set. This analysis complements that of [17–19] on the 2D spatial organization of joints and faults affecting the sedimentary cover of Saudi Arabia at different scales (from 1 cm to 100 km), using multifractal distributions, anisotropic wavelet analysis, and geostatistics. In such a sedimentary medium (consisting mainly of sandstone rock) the geometrical multifractal analysis qualified jointing as homogeneous, in other words, joint networks are not fractal or multifractal. In the present paper, we focus on joints affecting the crystalline basement to show that, on the contrary, the joint spacing distribution in granitic rock describes a highly heterogeneous, self-similar process. Self-similarity could lie in the rate process of jointing, as we shall show.

The study area is located in the western Arabian plate, at the oriental edge of the outcropping basement (the geographical location being approximately N26°E43°). At large scale (controlled by faulting processes), only two major tectonic directions appear: N110-directed strike-slip faults, constituting the Najd fault system created during the panafriacan orogeny, and N140 normal faults, created during the Miocene extension phase that induced the Red Sea opening. The studied granitic massive outcrops have a disk-like shape with an average diameter of 12 km. This massive is affected by two sets of fractures trending respectively N30 and N110. The origin of both sets will be discussed in a later paper, but field arguments suggest that the N110 set was the first to appear in time. Some detailed field observations did not reveal any shear displacement for this set. The N30E trending set is characterized by very few fractures, that will not be analyzed here. Joints pertaining to the main N110-trending set are perfectly linear and parallel to each other, their lengths being over several hundreds of meters, that we will now consider as infinite. As we have no means to infer their extent at depth, we will consider this parameter as equal, or at least proportional, to the length. To quantify their arrangement, it is thus enough to carry out and study a N20-trending 1D-profile, along which all intersections with joints were mapped. The data set used in the present work (Fig. 1) consists in a 630.33 meter long profile with $N_s + 1 = 484$ joints. The $N_s$ spacings between consecutive joints range from $s_{\text{min}} = 9 \text{ mm}$ up to $s_{\text{max}} = 123.1 \text{ m}$, thus covering more than four decades. We note that a multifractal analysis of this set (corresponding to a multi-point correlation analysis), using improved tools described in [17,18,20], qualifies it as scale invariant (to be published). We now turn our attention to the distribution of joint spacings, corresponding to the one-point correlation.

2. Power Law Analysis

2.1. Cumulative Distribution. — A standard method to study the spacing distribution is to compute the cumulative distribution, namely the number of spacings larger than a given length $s$, which is represented in Figure 2, in double-logarithmic scales and with a uniform logarithmic sampling with 500 points. For small spacings, the plot seems linear, which is the signature of a power law, followed by a roll-off for larger spacings. One could argue that this roll-off is the signature of a finite typical length above which the distribution is no more self-similar. Instead, we argue for another explanation, according to which the roll-off is simply the consequence of the finite size of our data set and stems from the influence of the largest
values in the set. To see this, let us assume that the density distribution of spacings is a power law:

\[ P(s) ds \sim s^{-(1+\mu)} ds. \]  

(1)

Now, since there is obviously a largest value \( s_{\text{max}} \) in the data set, the observed cumulative distribution reads:

\[ N(l > s) \sim \int_s^{s_{\text{max}}} P(l) dl \sim s^{-\mu} - s_{\text{max}}^{-\mu}. \]  

(2)

It is the presence of the correction term \(-s_{\text{max}}^{-\mu}\) on the r.h.s. of equation (2) which induces a roll-off in the log-log plot of Figure 2. To check this, we fit the data of Figure 2 with this expression (2) (excluding the points for which \( N(l > s) = 1 \), which determine the largest spacing), taking \( \mu \) and \( s_{\text{max}} \) as free parameters. All our fits are done with a standard simulated annealing procedure [21]. We thus get \( \mu \approx 0.47 \) and \( s_{\text{max}} \approx 110.1 \). Note the good agreement with the actual value \( s_{\text{max}} = 123.1 \) m (the second largest spacing value being about 58 m), confirming our hypothesis. In fact, it is possible to get a complete theoretical description of this roll-off, using the rank-ordering method [22, 23]. Extreme probability theory allows one to obtain the maximum likelihood expression of the \( n \)-th largest value \( s_n \), which for a power law distribution (1) reads

\[ s_n = \left[ \frac{(\mu N_s + 1)}{\mu n + 1} \right]^{1/\mu}, \]  

(3)

where \( N_s = 483 \) is the number of spacings. The typical deviation \( \Delta s \) of the \( n \)-th rank around the maximum likelihood expression \( s_n \) verifies \( \Delta s_n/s_n = 1/\sqrt{n} \) [23]. We assume in this expression that equation (1) is normalized to unity and \( s \) to \( s_{\text{min}} \). By definition, \( N(l > s) = n \) where \( n \) is such that \( s_n \geq s \). By inverting equation (3), this yields exactly equation (2). Note that expression (3) simplifies into a pure power law \( s_n \sim n^{-1/\mu} \) for large \( N_s \) and \( \mu \) not too small. This is a valid approximation for \( \mu \) say of order or larger than 1. In our case, \( \mu \) is a bit smaller (\( \approx 1/2 \)) and the \(-s_{\text{max}}^{-\mu}\) correction is not negligible. In sum, roll-off or bends in cumulative distributions may be intrinsic effects of power law distributions for small exponents. This is to be contrasted with the interpretation in terms of a breakdown or a change of scaling that has been proposed in the analysis of cumulative distribution of large earthquakes [24].
Fig. 2. — Cumulative distribution of spacings. The data set is plotted using a continuous line, whereas the fitting curve given by equation (2) is represented by a dashed-line. The fitting procedure with equation (2) does not take account of the points for which $N(S > s) < 2$.

2.2. DENSITY DISTRIBUTION. — A direct check of the pure power law (1) is given by the analysis of the density distribution. In principle, it is not biased by any roll-off due to the interplay between finite size and the cumulative construction. In general however, it is not used much because it suffers from much larger fluctuations, and from the arbitrariness of the binning size. If one is careful enough, unbiased statistics can nevertheless be extracted with good precision. To this end, we transform each spacing value $s_k$ into its logarithmic $\lambda_k = \log_{10} s_k$. We then consider the following distribution $\Lambda$:

$$\Lambda(\lambda) = \sum_{k=1}^{N_s} \delta(\lambda - \lambda_k)$$

where $N_s$ is the total number of spacings (here $N_s = 483$), and $\delta(x)$ is the Dirac distribution. The $\Lambda$ distribution is then filtered by convoluting it with a square window of size $2w$. We thus obtain the number of logarithmic spacing data between $\lambda - w$ and $\lambda + w$. To get the correct smoothed density distribution $h(\lambda)$ normalized to unity, we divide it by $N_s$ and by the window interval (in linear scale) $10^{\lambda+w} - 10^{\lambda-w}$. We use 500 sampling points and those intervals for which the smoothed density vanishes are discarded. We tested several values for the smoothing window size ($2w = 0.1, 0.15, 0.2, 0.5$ and 1) and fitted each curve with a law of the form:

$$\log_{10} h(\lambda) = A - (1 + \mu)\lambda$$

Both values of $A$ and $\mu$ did not vary significantly from fit to fit, $\mu$ being found equal to $0.45 \pm 0.05$, in good agreement with the value determined from the cumulative distribution. $A$ is found equal to $1.30 \pm 0.05$. Figure 3 shows the data and its fit by equation (5) for $2w = 0.15$. 
3. Models of Fragmentation Predicting Power Law Distributions

3.1. PHYSICAL MECHANISMS. — How can we rationalize these results? Several mechanisms are available to explain the formation of joints [1,25,26]. They generally assume that both the maximum and intermediate stress axis (σ₁ and σ₂) are contained within the joint plane, being thus normal to the least one (σ₃). If σ₃ is compressive, joints will propagate when the fluid pressure will exceed it. However, boundary tensile stresses can also take place during flexure of strata, erosion and uplift. Thus, this kind of scenario implies that joints propagate in an overall effective tensile state of stress. However, this case generally leads to stress screening around joints, which prevent a too close proximity between two fractures, thus providing a possible explanation for the typical spacing observed in sedimentary layers [27]. This does not seem to be the case here, as the spacing distribution is a power law valid over the whole sampling interval. We can also consider that joints are mainly due to a high compressive maximum stress, whose axis is contained within the plane of jointing. In this case, joint propagation is due to some local tensile stress developing at their tips. This imposes no condition on the minimum spacing value. It is also worth noting that such a high stress would prevent joints from deviating from their original plane while approaching another one [28–30], which is the case here, as joint traces can be considered as “infinitely” long and perfectly straight lines. Moreover, as no fracture branching was observed in the field, we can suspect that the growth process was quasi-static. This boundary condition is very similar to a compressive continuous fragmentation process. In this analogy, a fragment is an unbroken domain bordered
by two joints. We should note here that this process, very close to uniaxial splitting commonly observed in low confinement stress rock mechanics experiments, can be achieved due to high fluid pressure, even if this does not create by itself local tensile stresses [2].

Now, let’s compute $M(r)$, the cumulative mass of fragments of linear dimension less than $r$. In our case, as joints are considered as almost infinite either in the direction perpendicular to the profile or in the vertical direction, the typical linear dimension of a fragment is the spacing between two joints. Moreover, in this picture, the mass of fragments will be linearly dependent of the distance between their two bordering joints. Thus we have:

$$M(r) \sim \int_0^r sP(s)ds$$

that is $M(r) \sim r^{1/2}$. Interestingly enough, many experimental observations (see [31]) report such scaling laws for $M(r)$ with exponents between 0.5 and 1.

### 3.2. Multiplicative Model of Fragmentation

Let us consider the following toy model of fragmentation. We start from an initially unbroken granite massive (bordered by two initial joints) and assume that the rate of fragmentation is $p$ per unit of time: the probability that a fragment breaks into two pieces (i.e. a joint appears somewhere in the middle between the two bordering joints) is $p$ per unit time. When this occurs, the initial fragment of size $L$ is broken into two pieces of size $xL$ and $(1-x)L$ with $0 < x < 1$. If $x$ is a random variable, then, as long as there exists a sharp cut-off $0 < x_{\text{min}} \leq x$, the distribution of fragments is that of a product of random variables of finite size, namely a log-normal distribution. At this step, we can note that such a model could also be applied to jointing in sedimentary layers, which often display log-normal spacing distribution [10,11]. Within this simple model, there are essentially two strategies for obtaining power laws. The first one is to assume that there is a non-vanishing probability of getting arbitrarily small $x$’s, for instance with a probability $P(x) \sim x^{-\nu}$. A given fragment after $t$ time steps has a length given by $l = x_1 \cdots x_t$ where $x_1, \ldots, x_t$ is a realization of the process. Taking the logarithm, we obtain a sum of random variables $\log l = \log x_1 + \cdots + \log x_t$, in which the $X_i = \log x_i$ are distributed exponentially according to the distribution $\nu e^{-\nu |X|}$. As a consequence of the central limit theorem, this sum is again distributed according to a Gaussian (hence the log-normal when re-exponentiating); however, for a finite sequence of fragmentation steps, the central limit theorem does not apply to the extreme tail of the distribution for large fragments. In this region, the distribution is governed by the initial distribution [32]. More precisely, for the exponential distribution $\nu e^{-\nu |X|}$, the distribution of the sum of $t$ terms is the Gamma distribution $\nu^t |X| t^{-1} e^{-\nu |X|}$ [33] which converges to the Gaussian distribution except far in the tail $|X| > |X^*| \sim t(\log t)^{1/2}$ (where $|X^*|$ is estimated by comparing the exact form of theGamma distribution with the asymptotic Gaussian expression) for which the distribution of $l$ is $P(l) \sim \nu^t |l|^{t-1} l^{-\nu} \approx t^{-(1+\mu)}$. We thus recover the relation $\mu = \nu - 1$ previously found using a detailed mathematical analysis [34]. Note that a power law scaling is obtained in this argument in the large fragments part of the distribution. However, our observed power law holds down to 1 cm, which is the typical size of mineral grains and which we believe to be the smallest fragments one can produce in this case. What we observe here is probably the small size limit of the distribution and the preceding model should not apply to our geological situation.

Consider the alternative extreme situation where the fragment ratio’s $x_i$ are all equal to a constant factor $x$. For the sake of pedagogy, let us take the simplest case $x = 1/2$ and assume a large population of initial domains. Each domain can follow a different and independent fragmentation scenario. For the sake of simplicity, when a rupture occurs in a domain, we assume that all the fragments are ruptured in two pieces. In addition, in a given discrete
history of fragmentation steps, all ruptures are supposed to occur in the first few time steps, followed by a quiescent phase. It follows that, in all the domains taken together, the fraction of fragments of size $s$ such that $2^{-(n-1)} < s < 2^{-(n+1)}$ is $P(s) = 2^n (1 - p)^t s^{-n}$. The quantity $(1 - p)^t n^{-1} p^n$ is the probability for having a domain with $n$ rupture events and the first term $2^n$ accounts for the number of fragments of size $2^{-n}$. Noting $s = 2^{-n}$, we find $P(s) \sim s^{-\mu}$ with $\mu = \frac{\log \frac{1-\mu}{2}}{\log 2}$. From the relation $P(s) = \int_{s/2}^{2s} p(s) ds$ where $p(s)$ is the fragment density distribution, we obtain $p(s) \sim s^{-(1+\mu)}$. The value $\mu \approx 1/2$ corresponds to a fragmentation rate $p \approx 0.26$. Complications do not change the qualitative properties of this model. We now exploit. For instance, we could have assumed a random occurrence of the rupture events during the time $t$; this would have introduced a very slowly varying $\log(\log(s))$ term in the exponent $\mu$.

3.3. Complex Exponents

3.3.1. Multiplicative Model of Fragmentation. — The simple model outlined above has an interesting prediction, namely that fragment sizes come in powers of $1/2$ (more generally in powers of $x$, $1 - x$ and their combination). Using small binning intervals as done in the present analysis then amounts to counting the fragments with a scale mesh much finer than the scaling ratio $1/2$. Thus, when we increase the magnification continuously from say $y = 2^{-p}$ to $y = 2^{-(p+1)}$, the cumulative number of fragments $N(y)$ jumps by a factor $\frac{1-2p}{2p}$ at $y = 2^{-p}$, but then remains unchanged until $y = 2^{-(p+1)}$, at which point they jump again by an additional factor $\frac{1-2p}{2p}$ and so on. For $2^{-p} < y < 2^{-(p+1)}$, $N(y)$ does not change while $y$ decreases, so the measured exponent $\mu(y) = \frac{\log N(y)}{\log y}$ decreases. The exponent $\mu = \frac{\log \frac{1-2p}{2p}}{\log 2}$ is obtained only when $y$ is a negative power of two. For continuous values of $y$ one has

$$N(y) = N_1(y) y^{-\mu} P \left( \frac{\log y}{\log 2} \right),$$

(6)

where $P$ is a function of period unity. Now, since $P$ is a periodic function, we can expand it as a Fourier series

$$P \left( \frac{\log y}{\log 2} \right) = \sum_{n=-\infty}^{\infty} c_n \exp \left( 2n \pi i \frac{\log y}{\log 2} \right).$$

Plugging this expansion back into equation (6), it appears that $\mu$ is replaced by an infinity of complex values

$$\mu_n = \mu + n i \frac{2\pi}{\log 2}. \quad (7)$$

We thus expect log-periodic modulation (given by Eq.(6)) on top of the power law seen in Figure 3, corresponding mathematically to a complex exponent $\mu$ given by equation (7). It turns out that this prediction remains robust when the scaling factor is not constant but exhibits fluctuations that are not too large [35].

3.3.2. Scaling Model of Cheng and Redner. — The presence of complex exponents for fragmentation can be shown explicitly using the scaling theory of [34]. In a nutshell, their approach is to write down a linear integro-differential coupled equation for the time evolution of fragment populations. The fragment distribution $p(l)$ is characterized by the moments $m_\alpha = \int_0^\infty t^\alpha p(l) dl$. Note that calculating a moment corresponds to taking the Mellin transform of $p(l)$. This implies that if we know $m_\alpha$, we shall be able to retrieve $p(l)$ by taking the inverse Mellin transform.
The equations of evolution for the fragment population then transforms into the following recurrence equation for the moments: \(m_{\alpha+\beta} = \omega \frac{1}{L_{\alpha-1}} m_{\alpha}\), where \(\beta\) is the exponent describing the overall rate of breakup (assumed to be proportional to \(l^\beta\)), \(\omega\) is a normalizing constant and \(L_\alpha = \int_0^1 x^\alpha b(x)dx\), where \(b(x)\) is the probability that the fragment ratio be \(x\). From the factor \(\frac{1}{L_{\alpha-1}}\), if there is a value \(\alpha^*\) such that \(L_{\alpha^*} = 1\), then all moments with \(\alpha > \alpha^*\) will become infinite. Provided reasonable analytical conditions hold, it follows that the value \(\alpha^*\) is a pole of \(m_\alpha\). Taking the inverse Mellin transform of \(m_\alpha\) then allows us to get \(p(l)\) and, using the existence of the pole at \(\alpha^*\), this immediately leads us to predict that \(p(l) \sim l^{-(1+\beta+\alpha^*)}\).

One can check that for a large variety of \(b(x)\), there are solutions of \(L_{\alpha^*} = 1\) with complex exponents \(\alpha^*\). With equations (6) and (7), this signals the existence of log-periodic corrections to a pure power law behaviour, which have been overlooked until now in this model.

Complex critical exponents and complex fractal dimensions and their associated log-periodic oscillations have recently been found in irreversible rupture and growth processes [36–38]. Furthermore, it has been suggested [35] that complex exponents are rather common, and generically should be looked for in any model whose critical properties are described by a non-unitary field theory. These include models with non-local properties such as percolation, polymers and their generalizations, models of irreversible growth processes such as rupture, DLA, and models with quenched disorder like spin-glasses. The existence of complex exponents for fragmentation processes has been overlooked until now but, in view of the other examples available [36–38] and of the theoretical framework [35], their existence is rather natural. The main interest in measuring complex exponents is that the imaginary part gives direct access to the preferred scale ratio that describes the self-similarity of the system. For fragmentation processes, this is very important because this scale ratio is nothing but the preferred fragmentation ratio (when it exists) defining the (approximately discrete) fragmentation cascade.

3.3.3. Evidence in the Joint Data. — We now examine if such a prediction is born out in our data. The difference between the density distribution data and fit is shown in Figure 4. We notice some systematic oscillatory-like deviations which do not resemble a Gaussian noise. The oscillatory-like deviations are observed only for small \(w\)’s while, for larger values of the smoothing window \(2w > 0.2\), the residues are noise-like since small wavelength oscillations are washed out in the smoothing procedure. To test for the reality of this oscillations, we have fitted the data of Figure 3 by

\[
\log_{10} h(\lambda) = A' - (1 + \mu')\lambda + \log_{10} \left(1 + B \cos\left(\frac{2\pi \lambda}{T} + \phi\right)\right) \\
\]

(8)

This form corresponds to the first two terms in the Fourier series expansion of (6). It consists in a linear trend (the power law seen in log-log), to which a periodic component is added, with period \(T\) and phase \(\phi\) (in the variable \(\lambda = \log_{10} s\)). The fit performed for \(\lambda > 0.3\) using simulated annealing for \(2w = 0.15\) yields \(A' = -1.33, \mu' = 0.41, B = 0.34, T = 0.35, \phi = 0\). A fit using the whole data set gave \(A' = -1.26, \mu' = 0.41, \alpha' = 0.45, B = 0.18, T = 0.35, \phi = 0\). Except for \(B\), both solution sets are very similar. For \(2w = 0.2\), the results are essentially the same, except that \(\phi = -0.68\). The discrepancy between the phases is due to the bump in the data that appears in the \([-0.3; 0]\) range. The difference observed between the values of \(B\) is explained by the fact that oscillations seem to be of smaller amplitude in the range \([0; 0.01]\). The residual of the data fitted by a pure power law, i.e. the difference between the density distribution and the best simple power law fit, is indicated in Figure 4 by a dashed line. The oscillatory part of equation (8) with \(B = 0.34, T = 0.35\) and \(\phi = 0\) is indicated by a continuous line. The oscillations of the sine curve are numbered from 1 to 12, their maximum and minimum being indicated by subscript \(u\) (up) or \(d\) (down). We acknowledge the fact that the agreement
is not perfect, but this seems mainly due to the fact that observed fluctuations are sometimes slightly shifted from their predicted location. However, this is expected for two reasons: i) we use only the first oscillatory term of the full Fourier series of \( P \left( \frac{\log y}{\log 2} \right) \) in equations (6) and ii) we fit a single realization bound to exhibit statistical fluctuations (see for instance the discussion of the nature of fluctuations and the statistical signature of log-periodic oscillations in the presence of noise for DLA [38]). Nevertheless, at least 6 oscillations of the data curve can be explained by the log-periodic correction. Two others are perhaps observable at very small scale \( (\log_{10}(s) < -1.3) \), but the finite accuracy of spacing measurement (typically few millimeters) certainly pollute the data. Concerning the central part of the curve, one can note that oscillation 7 is far from fitting the data. It seems that this part of the signal corresponds to either a phase reversal, or to a larger wavelength, giving locally \( T \approx 0.5 \), that is a fragmentation ratio of about 3. This could result from additional relevant fragmentation ratios, as has been found for instance in DLA [38].

To check this last point, we performed the one-dimensional wavelet transform of the data signal shown in Figure 4. We will not detail the wavelet transform concept here, as it can be found in many textbooks (for example see [39]). In a nutshell, the wavelet transform consists in convolving a given signal with filters called wavelets, such as to extract the local periodic content of a signal. At each point and for each local frequency, the resulting convolution product is called the wavelet coefficient. Many wavelets can be used, the one we chose being the Morlet wavelet given by the analytical expression:

\[
g(t) = \exp(-t^2/2) \cdot \exp(2\pi it)
\]  

(9)
Fig. 5. — Wavelet coefficient modulus map obtained for data of Figure 4. The horizontal axis stands for position $\lambda$ along the signal, whereas the vertical one stands for the scale $\sigma$ of the wavelet. Level curves are drawn together with their associated values. Long wavelengths maxima occur ($\sigma \approx 1.5$) corresponding to a fragmentation ratio around $32$, as well as another narrow band of high coefficients at shorter wavelengths ($\sigma$ between $0.25$ and $0.5$) corresponding to a preferred fragmentation ratio of around $2$.

This last wavelet defines the mother wavelet. The signal is filtered with the so-called daughter wavelets, $g(t/\sigma)/\sqrt{\sigma}$, where $\sigma$ is the scale parameter corresponding to a local wavelength. The wavelet transform of the signal can then be represented by a map of the modulus of the wavelet coefficients in the $(t, \sigma)$ space. At any given location $t$, the value of $\sigma$ which maximizes the wavelet coefficient is the main wavelength of the signal at this precise location. Figure 5 shows such a map (drawn with level curves). Here $t$ plays the role of $\lambda = \log_{10}(s)$ (i.e. the position along the signal), where $s$ is the spacing size. In our analysis, values of $\sigma$ were allowed to vary between $0.025$ and $2.5$ by steps of $0.025$. Figure 5 reveals that a long wavelength mode exists all along the signal, with $\sigma \approx 1.5$ corresponding to a preferred fragmentation ratio around $32$. As this would imply the existence of only $3$ oscillations throughout the signal, it should be barely significant. For smaller wavelengths, one can note the existence of $2$ distinct behaviours: at the extremities of the signal (say, $\log_{10}(s)$ lying between $-1.5$ and $-0.5$ on one hand and between $0.5$ and $2$ on the other hand, to neglect small scale data that could be polluted by noise), the value of the dominating wavelength $\sigma$ is around $0.25 - 0.3$. For the central part of the signal ($\log_{10}(s)$ comprised between $-0.5$ and $0.5$) the dominating wavelength jumps to $0.5$. This simple computation thus shows that all along the signal the significant dominant wavelength is comprised within a narrow range, $[0.25; 0.5]$, providing a rescaling factor in the range $[1.8; 3.2]$. However, more than $70\%$ of the signal is characterized by a wavelength corresponding to a preferred fragmentation ratio $\lambda \approx 2$. It should be noted here that the log-periodic interpretation of the data is strengthened by the fact that not only the
wavelength of the data shown in Figure 4 is the same in the intervals $[-1.5 : -0.5]$ and $[0.5 : 2]$, but also the phase is correct (this can be easily checked in Fig. 4). This seems to rule out the possibility that the log-periodic oscillations could be just due to chance. The properties of the distribution in the range $[-0.5 : 0.5]$, however, still remain to be explained.

Of course, we are aware that there are presumably other sorts of fits with as many parameters that would work. Our attitude is that it is surely irrational to infer the validity of a description based on one fit, but if it works for many fits (and if there is a reasonable theory for it), it should have some truth to it. As a test, we observe that the value of $T$ we find is very close to the ones that have been found for other problems. The value $T \approx 0.35$ corresponds to a preferred fragmentation ratio $x = 10^{-T} \approx 1/2.2$ close to $1/2$. Remarkably enough, this scaling factor $\approx 2$ has been found in a variety of related problems of rupture [35-37] and growth processes [38] and can also be derived analytically from the analysis of competition between quasi-static crack or branch growth (in preparation).

To check further that the log-periodic structures and especially the value $x \approx 1/2.2$ are not the result of chance, we performed several synthetic tests. These tests consist in generating artificial spacing sets of 483 elements, using a simple power law distribution with a real exponent $\mu = 0.47$. Then, the same fitting procedure as before with equation (8) is used to determine if fluctuations due to the small size of the data-set could generate spurious complex exponents. We indeed observe that we can fit the fluctuations around the average power law by an apparent log-periodic oscillatory behaviour. However, the values for $T$ are always larger than 0.35: among 100 synthetic data sets, only 3 gave a value $T$ lower than 0.4, thus indicating that the level of confidence of our finding for the log-periodic oscillations is about 97%. All taken together, we thus think the value $T = 0.35$ is a genuine property of the fragment size distribution.

4. Conclusion

We have presented a particularly clean data set of rock jointing exhibiting a power law distribution of spacings between joints. Cumulative and density distributions have been used and compared to get a better precision on the exponent. We have interpreted this data within the picture of fragmentation in which two neighboring joints define an effective 1D fragment. We have shown how to rationalize the observed power law distribution. A simple multiplicative model on the one hand and a scaling model of fragmentation on the other have been found to predict the existence of log-periodic corrections to the simple power law distribution for the distribution of fragment sizes. We have checked their existence for the geological data set at a confidence level of 97% using synthetic tests. The log-periodic structure defines a preferred scaling ratio between fragments close to 2, which is also found in other systems. Taken together with other previously reported evidence on other data on rupture, earthquakes and growth processes, the new result provided by our present analysis of rock joints suggests a very coherent picture, namely that complex critical exponents are a general phenomenon in irreversible self-organizing systems and particularly in rupture and growth phenomena [35]. More theoretical work is needed to explain the $\mu$ and $T$ values.

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References


