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Growth Instabilities Induced by Elasticity in a Vicinal Surface

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Abstract. — We study the effect of elasticity on the step-bunching instability in heteroepitaxial growth on a vicinal substrate. Three main effects are taken into account: the Schwoebel barrier and the step-step and the step-adatom elastic interactions. The first one is always stabilizing, the second one generally destabilizing and the last one, stabilizing or not according to the sign of the misfit with the substrate. At very low values of the flux $F$, only the step-step interaction is effective: the stabilization is provided by the broken bond mechanism and the destabilization by the misfit mechanism. At increasing $F$, the stabilization is governed by the Schwoebel effect and only the misfit mechanism needs to be taken into account. A stability phase diagram, taking into account also a possible instability for island nucleation, is drawn in the plane $(F,T) \equiv (\text{flux,temperature})$: a stable region appears, at intermediate values of $F$.

1. Introduction

A non-hydrostatic stress may give rise to morphological instabilities, when applied to a solid with a surface. This is because, when the thickness $h$ of the stressed solid is high enough, the elastic strain energy (proportional to $h$) overcomes the surface tension (independent of $h$) and a plane surface may be no more energetically favoured. It is important to point out that this process is governed by the mass transport, which can be provided by surface diffusion or by a particle reservoir (a gas or a liquid) in contact with the solid.

In the past, starting from the pioneering work of Asaro and Tiller [1], several authors (Grinfeld [2], Srolovitz [3], Nozières [4]) have studied the stability of a plane interface. The main result of a linear analysis is the existence of a critical wavelength $\lambda_0$, beyond which the interface is unstable with respect to a sinusoidal perturbation of arbitrary amplitude (it will be referred to the following as ATG instability). The existence of $\lambda_0$ is due to the capillarity which stabilizes the flat surface with respect to short wavelength deformations. The gravity or the van der Waals interactions may provide a similar stabilization for excitations of long wavelength [4], inducing a threshold $\sigma_c$ in the non-hydrostatic stress $\sigma$ for the rising of the instability. As $\sigma = \sigma_c$, the perturbation of wavevector $k = k_c < 1/\lambda_0$ becomes unstable.

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For the comprehension of the later stages in the evolution of the morphology of the film, a non-linear analysis is necessary. Nozières [4] has performed a non-linear energy calculation, taking the gravity into account. Such a calculation shows that at the bifurcation point \((k = k_c, \sigma = \sigma_c)\), the first non-linearity lowers the free energy (negative sign of the quartic term in the interface displacement), so that the instability is subcritical: the analogous of a first order transition.

Numerical studies have been performed by Yang and Srolovitz [5] and by Kasner and Misbah [6]. They find that, after the above-mentioned instability, there is the formation of deep cracklike grooves which become sharper and sharper as they deepen. According to these authors, this could connect the ATG instability with the fracture process, even if the two phenomena have completely different characters, because in the latter there is no mass transport and the fracture propagates by breaking the chemical bonds.

Experimentally, there are different examples of instabilities driven by the strain energy. Thiel et al and Torii and Balibar [7] have applied an external stress to a \(^4\)He crystal and have shown that above a threshold, grooves form on the surface. In most cases, the stress is due to the presence of a substrate whose lattice constant does not match the adsorbate (heteroepitaxy) In films of pure germanium on silicon, D.J. Eaglesham and M. Cerullo [8] have reported a dislocation-free Stranski-Krastanov layer, with an initially commensurate, layer by layer growth followed by the formation of bubbles. A. Ponchet et al. [9] have observed spatial modulations in strained GaInAsP multilayers, which allow partial elastic relaxations. Also, Béréhar et al. [10] have studied the stress relaxation in single-crystal films of polymerized polydiacetilene, in epitaxy with their monomer substrate. Polymerization is obtained through irradiation with low-energy electrons and induces a uniaxial stress. Above a critical thickness, the authors report a wrinkled surface deformation, but their interpretation as an ATG instability may be questionable, because of the slow diffusion process of such big molecules.

Snyder et al. [11] have stressed the importance of kinetic effects on the instability, by showing how the surface diffusion determines the growth mode of heteroepitaxial strained layers: thus a reduced kinetics in films of \(\text{In}_x\text{Ga}_{1-x}\text{As}\) on GaAs gives rise to highly strained pseudomorphic films.

In an epitaxial film, the relaxation of the misfit strain may also occur via misfit dislocations, which eventually lead towards an incommensurate structure. However, only if the relaxation is total the ATG instability should be forbidden. On the other hand, we can also observe dislocations after the instability. In experiments on strained \(\text{Si}_{1-x}\text{Ge}_x\) layers on Si, Pidduck et al. [12] have observed an initially defect-free Stranski-Krastanov growth, followed by the formation of dislocations; these authors also speculate on a possible subsequent increase in the modulation period.

The instability has a technological interest, too. In fact the growth in strained structure may give rise to the self-organized formation of semiconductor microstructures such as quantum dots and wires. Moisson et al. [13] have shown that the deposition of InAs on GaAs, after a first two-dimensional growth proceeds by the formation of single-crystal, regularly arrayed dots, of quantum size. Similar microstructures have been obtained by Nötzel et al. [14], during the growth of strained InGaAs/AlGaAs multilayers on gallium arsenide substrates.

With regard to the rising of an instability, an important feature is the orientation of the surface. In the case of a non-singular one, a continuum approximation is correct and the classical picture of the ATG instability emerges. On the other hand, in the case of a high symmetry orientation, the surface tension is non-analytic and Tersoff and LeGoues [15] have shown in this case the existence of an activation barrier.

Usually, the instability is studied as a problem of thermodynamical equilibrium. Kinetic effects have been taken into account by Srolovitz [3] and by Spencer et al. [16], but their
approximations make the analysis valid for a non-singular surface, close to the equilibrium. However, Duport et al. [17] have studied the case of a vicinal surface and they have shown that the discrete character of the lattice may be very important, since the adatom-step interaction is otherwise neglected, and that when the adsorbate grows, the surface kinetic may stabilize the growth process via the Schwoebel effect. Also, if neither growth nor evaporation is present, the vicinal surface has a behaviour similar to that of a non-singular surface: an instability appears and no activation barrier is present.

The main result of their paper is to show the existence of a new possible instability in MBE growth; it is an elastic instability other than the ATG instability, since the underlying mechanism is different and it appears or does not appear, according to the sign of the misfit $\delta a$. Let us now describe very briefly the growing process for a vicinal surface and let us explain how such a mechanism works.

A vicinal surface does not grow layer by layer, but through step-flow, with all the steps moving at the same velocity. After an adatom has reached the surface, it diffuses on the terrace until it sticks to a step (see Fig. 1). The growth velocity of each step is therefore determined by the rate of attachment of the adatoms on it and the stability of the step-flow growth (uniform velocity of all the steps) will depend on which ledge the adatoms prefer to stick to. In the presence of a uniform flow, the number of atoms reaching a given terrace is proportional to the terrace area; so, if the sticking to the upper step is favoured, a larger terrace (larger than the neighbouring ones) becomes smaller, and viceversa: the step flow growth is stable. On the contrary, if sticking to the lower step is favoured, a large terrace becomes larger and larger and a step bunching instability arises.

How does the adatom choose the step to stick to? During the diffusion process, it feels the step-adatom interaction: the steps produce an elastic deformation proportional to the misfit $\delta a$, which interacts with the deformation induced by the adatom via the so-called broken bond mechanism, and whose strength is proportional to a force dipole moment $m$. Thus, the resulting interaction may be stabilizing (if the adatom is pushed towards the upper step) or destabilizing (in the opposite case), according to the sign of $m$ and $\delta a$. 

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Fig. 1. — In this Figure, a growing stepped surface is shown: there is a flux $F$ of atoms per second and per lattice site; after the landing of the adatom on the surface, it moves with a diffusion coefficient $D$; close to a step, the adatom has a probability $D'\frac{j^1}{a}$ (or $D'\frac{j^2}{a}$) per unit time to stick to the step from above (below). Analogously, the probabilities of detachment from the step to the upper and lower terrace are $D'\frac{j^1}{a}$ and $D'\frac{j^2}{a}$, respectively. In this Figure, we have also depicted the different types of instability to which a stepped surface may be subjected: step-bunching, island formation, step meandering.
However, as pointed out in [17], the asymmetry in the probabilities of attachment, from above and from below, to a step (Schwoebel effect) is a possible source of stabilization of the growth process.

In reference [17] it was assumed that the sticking of an adatom to a step is an irreversible process. As a consequence, the adatom is not able to reach thermal equilibrium and minimize the step-step interaction, which therefore results to be ineffective. In this paper we will take the step-step interaction into account, and we will be able to interpolate between our previous analysis and the works of Srolovitz [3] and Spencer et al. [16]. As in reference [17] and in the current literature, the thickness of the substrate will be assumed to be infinite.

The paper is organized as follows: in Section 2 we study the possible origins of elastic deformations on a stepped surface and we give the expressions for the adatom-step and step-step interactions. In Section 3 we introduce the Schwoebel effect, while in Section 4 we show the destabilizing character of the step-step interaction. Then, we perform a stability analysis of the step-flow growth: in Section 5 we write the equations of motion for each step, and in Section 6 we linearize and solve them. Only the main formulae will be given, while all the details of the calculation will be deferred to the Appendices. Section 7 is devoted to the study of the limiting case of low flux, this will allow us to compare our results with those of Spencer et al. [16]. Finally in Section 8 we will discuss the hypotheses underlying our stability analysis and in Section 9 we will summarize the main points we have addressed in the paper.

2. Elastic Interaction between Adatom and Steps

The elastic interaction between an adatom (on a high symmetry surface) and the substrate may have two different origins. The first one is a deformation of the surface, because of the different lattice constants of adsorbate and substrate; it is called "misfit mechanism" and occurs only in heteroepitaxy. In the second case, the deformation originates from the dipole of forces which the adatom exerts on the other atoms; it is called "broken bond mechanism" and is effective even in homoepitaxy. Let us focus on the latter mechanism.

It is described in Figure 2a in the case of central, pairwise interactions between nearest and next-nearest neighbours. The adatom exerts forces $f_R$ on the other atoms, the location of which is designated by $R$. At equilibrium the total force is zero, but the dipole tensor

$$m_{\alpha\gamma}a^2 = \sum_R R_\alpha f_R^\gamma$$

has non-zero diagonal elements. If the $x$ and $y$ axes are chosen parallel to the surface, symmetry imposes: $m_{xx} = m_{yy} = m$. Having introduced the atomic area $a^2$, the force dipole moment $m_{\alpha\gamma}$ results in having the dimension of a force divided by a length that, is the dimension of a surface stress.

At a long distance $r$ of an adatom, the components $u_{xx}$, $u_{yy}$ of the strain tensor are proportional [18–20] to \(\frac{(m - m_{zz}\sigma/(1 - \sigma))}{r^3}\), where $\sigma$ is the Poisson coefficient. The part of this expression, which is proportional to $m_{zz}$ is often ignored [18, 21]. Quadrupolar and higher order effects will be neglected.

The broken bond effect is not additive, in that the number of broken bonds of a pair of adatoms is not twice as much as for a single crystal. Accordingly, the stress exerted by a large terrace is localized near the ledge (Fig. 2b), so that the elastic effect of a terrace is that of a distribution of force dipoles along its edge [22].

The second mechanism of elastic interaction is the so-called "misfit mechanism", and it results from the fact that the adatoms would like to have an interatomic distance different
Fig. 2. — We have represented the broken bond mechanism in the case of pairwise interaction between nearest and next-nearest neighbour atoms. a) For an adatom. We have also indicated the moduli of the forces. b) In the case of a terrace, where the forces are localized near the terrace edge. In both cases we have considered only the forces due to the presence of an adatom or a step, not of the surface; in the latter case the forces disappear after surface relaxation.

from that of the substrate. In opposition to the previous one, this effect is additive, i.e. proportional to the size and the thickness of the terrace. However, if the substrate is infinitely deep, the stress exerted by complete layers does not need to be taken into account, since the size of these layers is fixed by the substrate.

On the contrary, if the adsorbate has a modulated surface of variable height $h(x,y)$, it is equivalent to an adsorbate with a plane surface on which the substrate acts as an external surface stress given by (see Appendix A1):

$$\frac{\eta_{\alpha\gamma}}{a} = \frac{\delta a}{a} \frac{E}{1-\sigma} (\delta_{x\alpha} + \delta_{y\gamma}) \delta_{\alpha\gamma} h(x,y)$$

(2)

where $E$ is the Young modulus, $\eta$ has the dimension of a surface stress and $(\frac{\delta a}{a})$ is the relative difference (or misfit) between the lattice constant of the substrate ($a_{s\beta}$) and that of the free adsorbate ($a_{ad}$):

$$\frac{\delta a}{a} = \frac{a_{ad} - a_{s\beta}}{a_{s\beta}}.$$

In the case of heteroepitaxy, addressed in this paper, the misfit mechanism (being additive) dominates the elastic effect of a large terrace (at least far from its edge), while it is ineffective for an isolated adatom, which interacts via the broken bond mechanism. The elastic deformations give rise to an effective interaction between defects: the adatom, through the broken bond effect, feels the deformation produced by the terrace through the misfit mechanism. It is the form of the potential, felt by the adatom, which determines the stabilizing or destabilizing character of such an interaction.
Fig. 3. — At the bottom, a one-dimensional array of straight steps and the labelling used in the text. Above, the potential felt by the adatom because of the interaction with the steps and the Schwoebel barrier: both the cases of a stabilizing (a) and destabilizing (b) step-adatom interaction, are shown.

The Asaro-Tiller-Grinfeld instability derives from a step-step interaction due only to the misfit mechanism: therefore the potential is proportional to \((\delta a)^2\) and the instability takes place for any sign of \(\delta a\). On the contrary, the instability which will be addressed in the present paper depends on a step-adatom interaction where both the mechanisms (misfit and broken bond mechanism) come into play; since \(m\) and \(\delta a\) may have identical or different signs, the elastic interaction can be destabilizing (in the former case) or stabilizing (in the latter case).

Now, it is important to evaluate the elastic energy \(U_a(x)\) for an adatom on the \(n'\)th terrace, where \(x\) is defined in Figure 3. This can be done under the assumption [18, 21–23] that adatoms and steps can be represented as force dipoles acting on a plane surface. For straight steps parallel to the \(y\) axis, the only nonvanishing element of the force dipole tensor, which results from the misfit mechanism, is \(\eta_{xx}/a\). Since the elastic interaction energy between two force dipoles is minus the product of one force dipole times the local deformation induced by
the second one, after integration on the plane of the terrace, in the limit \( l \gg a \) we obtain \([20]\)

\[
U_n(x) = \hat{U} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p} + x - \frac{\ell_a}{2}} - \frac{1}{\sum_{p=0}^{k} \ell_{n-p} - x - \frac{\ell_a}{2}} \right)
\]

with

\[
\hat{U} = \frac{2(1 + \sigma)}{\pi(1 - \sigma)} \alpha^2 \delta a ((1 - \sigma)m - \sigma m_{zz})
\]

The term proportional to \( m_{zz} \) had been neglected in reference \([17]\).

In the same approximation, the elastic energy of an atom incorporated into the \( n \)'th step can be seen as the variation of the step-step interaction when an atom is added to the \( n \)'th step, that is to say,

\[
\epsilon_n = \hat{\epsilon} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p}} - \frac{1}{\sum_{p=0}^{k} \ell_{n-1-p}} \right)
\]

with

\[
\hat{\epsilon} = \frac{2E}{\pi} \frac{1 + \sigma}{1 - \sigma} (\alpha \delta a)^2
\]

### 3. The Schwoebel Effect

As originally pointed out by Ehrlich \([24]\), even in a free diffusion process (i.e. without adatom-step interaction) adatoms have no reason to go with the same probability to the lower and to the upper ledge. This effect will be taken into account by introducing two different coefficients: \( D''/a \) is the probability per unit time for an adatom near an upward step to stick to that edge, \( D'/a \) is the same probability for a downward step. Several theoretical studies \([25, 26]\) confirm the existence of an energy barrier in the proximity of the upper ledge of a step (see Fig. 3), that is to say, \( D' < D'' \) and the adatom prefers to go to the upper ledge. Schwoebel \([27]\) was the first to notice that, as a consequence of this, the growth of a parallel array of steps is stabilized (Schwoebel effect).

It will be useful, in the following, to define the quantity \( L = a \left( \frac{D}{D'} + \frac{D'}{D''} \right) \). This length measures the difficulty, for the adatom, to stick to a step. We shall assume that \( \frac{D}{D'} \simeq 1 \) and \( \frac{D'}{D''} \ll 1 \), so that \( L \simeq a \frac{D}{D'} \).

### 4. Elastic Interaction between Steps

In the previous section it has been clarified how the adatom, during its diffusion process, interacts with the steps. Because of this interaction, it goes preferably to the upper or lower ledge according to the sign of \((m - m_{zz}\sigma/(1 - \sigma))\delta a\): the destabilizing case (lower ledge) corresponds to a positive value. When it is near a downward step, the adatom feels the Schwoebel barrier, which reduces its probability of attachment.

In the Introduction, it was said that the ATG instability is a consequence of step-step interaction. Indeed, once the adatom is incorporated, this interaction may come into play, but it is effective only if the adatom can escape from the steps and eventually attach to the other ones in order to reduce the step-step energy. Duport et al. \([17]\) made the assumption that the incorporation of the adatoms at the step was irreversible, so that the ATG instability was not
Fig. 4. — As in Figure 3a, but now also the destabilizing step-step interaction is shown.

included in their treatment. On the contrary, in the present work, atom detachment from steps will be taken into account.

It will first be checked, by a simplified argument taking only interactions between nearest neighbour steps into account, that the step-step interaction (5) destabilizes a regular array of steps, in agreement with the general ATG instability. The exact proof (taking all terraces into account) results from the calculations of the next sections.

If an atom is transferred from the (n+1)'th to the n'th step, the energy variation is

$$\delta E = \epsilon_n - \epsilon_{n+1} = \bar{\epsilon} \left( \frac{2}{\ell_n} - \frac{1}{\ell_{n+1}} - \frac{1}{\ell_{n-1}} \right)$$  \hspace{1cm} (7)$$

The atom transfer is energetically favorable if $\delta E < 0$, i.e. if $\ell_n$ is larger than $\ell_{n+1}$ and $\ell_{n-1}$ (see Fig. 4). Since the transfer lengthens the n'th terrace, wide terraces become even wider. This means that atom exchange between terraces is destabilizing. Even so, the previous argument is valid only if equilibrium can be reached, that is to say if the incorporation of the adatoms at the step is reversible within a reasonable time before new adatoms come from the beam.

The probabilities of detachment of an atom per unit time and per unit length of the step from the n'th step to the upper and lower terrace will be called $D'p_n^+/a$ and $D''p_{n-1}^-/a$, respectively. The quantities $p_n^+$ and $p_n^-$ are close to the equilibrium density of adatoms $p_0$, with a small correction due to elasticity. The probability of detachment $D'p_n^+/a$ is related to the probability of attachment $D'/a$ of an adatom (supposed to be close to the step) by the detailed balance principle. This principle states that the ratio $p_n^+$ of the two probabilities is proportional to the exponential of the difference between the energy of an adatom at the respective positions, divided by $k_B T$. This energy may be written as a quantity independent of elasticity, plus a correction. This correction is equal to (5) for the incorporated atom, and to $U \left( \frac{\ell_n}{2} \right)$ (see Eq. (3)) for the atom close to the step.
Accordingly, we can write:

\[ p_n^+ = p_0 \exp \left\{ -\beta \left[ U \left( \frac{\ell_n}{2} \right) - \epsilon_n \right] \right\} \]  
\[ p_n^- = p_0 \exp \left\{ -\beta \left[ U \left( -\frac{\ell_n}{2} \right) - \epsilon_{n+1} \right] \right\} \]  

with \( 1/\beta = k_B T \).

5. Equations of Motion for the Steps and the Terraces

Let us now investigate the linear stability of a regular array of straight, parallel steps. In our one-dimensional model, each terrace is characterized only by its length \( \ell_n = x_n - x_{n+1} \), whose time dependence is a function of the length of all the terraces:

\[ \frac{d\ell_n}{dt} = F(\{\ell_i\}) \]  

We shall linearize this equation near the stationary solution \( \ell_n = \ell \), corresponding to the step-flow growth.

Within each terrace, we can write a conservation equation for the adatom density \( p_n(x,t) \):

\[ \frac{\partial}{\partial t} p_n(x,t) = -\frac{\partial}{\partial x} J_n(x,t) + F \]  

where \( J_n \) is the current of adatoms and \( F \) is the beam intensity. The evaporation rate has been neglected. It will be assumed that the time variation of \( p_n \) is very slow with respect to the adatom motion, so that the conservation law takes the stationary form

\[ -\frac{\partial}{\partial x} J_n(x,t) + F = 0 \]  

and the time dependence of \( p_n \) and \( J_n \) will be ignored in the following.

The integration of (11) is straightforward

\[ J_n(x) - Fx = A_n \]  

where \( A_n \) is an integration constant, depending on the terrace. If \( F = 0 \), the current is uniform on each terrace, and it is equal to \( A_n \).

The relation between the density \( p_n \) and the current \( J_n \) is provided by the Einstein-Fokker-Planck equation [28]

\[ J_n(x) = -D \left[ \frac{\partial p_n}{\partial x} + \frac{p_n(x)}{k_B T} \frac{\partial U_n}{\partial x} \right] \]  

where \( D \) is the diffusion constant and \( U_n(x) \) is the energy of an adatom on the \( n \)'th terrace, given by (3).

From Equations (12) and (13), the following expression for the adatom density \( p_n(x) \) is found

\[ p_n(x) = p_n \left( -\frac{\ell_n}{2} \right) \exp \left\{ \beta \left[ U_n \left( -\frac{\ell_n}{2} \right) - U_n(x) \right] \right\} \]
\[ - \frac{1}{D} \int_{x_n}^{x} dy (A_n + Fy) \exp \{ \beta [U_n(y) - U_n(x)] \} \]  

(14)
where the middle of each terrace is taken as the origin for the terrace itself.

Now the boundary conditions at \( x = \pm \frac{\ell_n}{2} \) are necessary. They are obtained by writing that the sticking rate is, on the one hand, equal to the absolute value of the current, and on the other hand proportional to the difference between the local adatom density and the step equilibrium adatom density:

\[
J_n \left( \frac{\ell_n}{2} \right) = \frac{D'}{a} \left[ p_n \left( \frac{\ell_n}{2} \right) - p_n^+ \right] \tag{15a}
\]

\[
J_n \left( -\frac{\ell_n}{2} \right) = -\frac{D''}{a} \left[ p_n \left( -\frac{\ell_n}{2} \right) - p_n^- \right] \tag{15b}
\]

Jointly with (12), we have

\[
\frac{D'}{a} \left[ p_n \left( \frac{\ell_n}{2} \right) - p_n^+ \right] = A_n + F\frac{\ell_n}{2} \tag{16a}
\]

\[
\frac{D''}{a} \left[ p_n \left( -\frac{\ell_n}{2} \right) - p_n^- \right] = -A_n + F\frac{\ell_n}{2} \tag{16b}
\]

Finally, to study the stability of the regular array of steps, we need the quantity

\[
\frac{d\ell_n}{dt} = \frac{d}{dt} (x_n - x_{n+1}) \tag{17}
\]

Since it results that

\[
\frac{1}{a^2} \frac{d}{dt} x_n(t) = J_n \left( \frac{\ell_n}{2} \right) - J_{n-1} \left( -\frac{\ell_{n-1}}{2} \right)
\]

\[
\frac{1}{a^2} \frac{d}{dt} x_{n+1}(t) = J_{n+1} \left( \frac{\ell_{n+1}}{2} \right) - J_n \left( -\frac{\ell_n}{2} \right)
\]

with the aid of Equation (12), the required expression is attained

\[
\frac{1}{a^2} \frac{d\ell_n}{dt} = \frac{F}{2} (\ell_{n-1} - \ell_{n+1}) + 2A_n - A_{n+1} - A_{n-1} \tag{18}
\]

6. Linear Stability Analysis of the Step-Flow Growth

In the spirit of a linear stability analysis, we will consider small deviations from the stationary solution \( \ell_n(t) = \ell \), so that we can consider a single Fourier mode:

\[
\ell_n(t) = \ell + \zeta(t) \cos[Kn - \phi(t)] \equiv \ell_n^0 + \delta\ell_n(t) \tag{19}
\]

and we will seek the equation governing the amplitude \( \zeta(t) \).

The quantities \( A_m \) entering equation (18) are obtained starting from equation (14) (see Appendix B), and depend on all the lengths \( \{\ell_n\} \), so that we can define \( A_n^0 \) and \( \delta A_n \) through the relation

\[
A_n(\{\ell_n\}) = A_n(\{\ell\}) + \delta A_n \equiv A_n^0 + \delta A_n \tag{20}
\]

where \( A_n^0 \) is independent of \( n \), and \( \delta A_n \) is a very complicated expression

\[
\delta A_n = \sum_m \frac{\partial A_n}{\partial \ell_m} \delta\ell_m \tag{21}
\]
In all the following treatment, we assume that the elastic energies are very small compared to the thermal energy: \( \frac{U}{a} \ell \ll k_B T = \frac{1}{\beta} \). Within this limit, \( \delta A_n \) takes the form

\[
\delta A_n = -\beta p_0 D \frac{\delta \epsilon_n - \delta \epsilon_{n+1}}{\ell + L} - \frac{F L (L - 2aD/D'\ell)}{2 (\ell + L)^2} \delta \ell_n - \frac{\beta F}{2} \frac{L^2}{(\ell + L)^2} U_0^0 \left( \frac{\ell}{2} \right) \delta \ell
\]

\[
+ \beta F \frac{\int_{-\ell/2}^{\ell/2} y U_n^0(y) dy}{(\ell + L)^2} \delta \ell_n + \beta F \frac{(L - \ell) (L - 2aD/D'\ell)^2}{(\ell + L)^2} U_0^0 \left( \frac{\ell}{2} \right) \delta \ell_n
\]

\[
+ \frac{\beta F \ell}{2} \left[ \frac{aD}{D''} \delta U_n \left( -\frac{\ell}{2} \right) - (L - aD/D') \delta U_n \left( \frac{\ell}{2} \right) \right] - 2\delta \int_{-\ell/2}^{\ell/2} y U_n(y) dy
\]

\[
- \frac{\beta F \ell}{2} \left( 2 \frac{aD}{D''} - L \right) \frac{aD}{D''} \delta U_n \left( -\frac{\ell}{2} \right) + (L - aD/D') \delta U_n \left( \frac{\ell}{2} \right) + \delta \int_{-\ell/2}^{\ell/2} U_n(y) dy
\]

(22)

where \( \delta X \), as in equation (20), is the part of \( X \) proportional to \( \zeta \). The different quantities appearing in (22) are written below and derived in the Appendix:

\[
\delta \int_{-\ell/2}^{\ell/2} y U_n(y) dy = \bar{U} \left\{ \gamma_1 + \frac{1}{2} - \ln \left( \frac{\ell}{a} \right) \right\} \delta \ell_n + \sum_{k=1}^{\infty} \gamma_k [\ell_{n+k} + \ell_{n-k}]
\]

(23)

with

\[
\gamma_p = \sum_{k=p}^{\infty} \left( \frac{1}{2k} + \frac{1}{2(k+1)} - \ln \left( \frac{k+1}{k} \right) \right)
\]

(24)

\[
\delta \int_{-\ell/2}^{\ell/2} U_n(y) dy = \frac{\bar{U}}{\ell} \sum_{k=1}^{\infty} \left( \frac{1}{k+1} - \frac{1}{k} \right) (\delta \ell_{n+k} - \delta \ell_{n-k})
\]

(25)

\[
\delta U_n \left( \frac{\ell}{2} \right) = \frac{\bar{U}}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n-k} - \delta \ell_{n+k-1})
\]

(26a)

\[
\delta U_n \left( -\frac{\ell}{2} \right) = -\frac{\bar{U}}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n+k} - \delta \ell_{n-k+1})
\]

(26b)

with

\[
C_k = \sum_{p=k}^{\infty} \frac{1}{p^2}
\]

(27)

\[
\delta \epsilon_n - \delta \epsilon_{n+1} = -\frac{2F}{\pi} \frac{1 + \sigma}{1 - \sigma} (a \bar{a})^2 \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n+k-1} - \delta \ell_{n-k} - \delta \ell_{n+k} + \delta \ell_{n+1-k})
\]

(28)

\[
U_0^0 \left( \frac{\ell}{2} \right) = -\frac{\bar{U}}{a}
\]

(29)

\[
\int_{-\ell/2}^{\ell/2} y U_n^0(y) dy = 2\ell \bar{U} \left[ 1 - \frac{1}{2} \ln \left( \frac{\ell}{a} \right) - \alpha \right]
\]

(30)
with

$$\alpha = \sum_{k=1}^{\infty} \left[ \left( k + \frac{1}{2} \right) \ln \left( 1 + \frac{1}{k} \right) - 1 \right]$$ (31)

With the previous expressions, the evolution equation (18) for the terraces array, for weak deviations $\delta A_n$ is written as

$$\frac{1}{a^2} \frac{d\ell_n}{dt} = \frac{F}{2} (\delta \ell_{n-1} - \delta \ell_{n+1}) + 2\delta A_n - \delta A_{n+1} - \delta A_{n-1}$$ (32)

Insertion of (23-31) into (22), allows us to put $\delta A_n$ in the form

$$\delta A_n = R\zeta \cos(Kn - \phi) + Q\zeta \sin(Kn - \phi)$$ (33)

where $R$ and $Q$ are $\ell$-dependent. Substituting such an expression into (32) and using the definition (19) of $\delta \ell_n$, we find

$$\frac{1}{a^2} \frac{d\ell_n}{dt} = 4R\zeta \sin^2 \left( \frac{K}{2} \right) \cos(Kn - \phi) + 4Q\zeta \sin^2 \left( \frac{K}{2} \right) \sin(Kn - \phi) + 2F\zeta \sin(K) \sin(Kn - \phi)$$ (34)

By comparison with the equation

$$\frac{1}{a^2} \frac{d\ell_n}{dt} = \frac{d\zeta}{dt} \cos(Kn - \phi) + \zeta \frac{d\phi}{dt} \sin(Kn - \phi)$$ (35)

the following relation is established

$$\frac{1}{a^2} \frac{d\zeta}{dt} = 4R\zeta \sin^2 \left( \frac{K}{2} \right)$$ (36)

where we can identify the relaxation frequency $a^2\Omega(K)$, defined by $\frac{1}{a^2} \frac{d\zeta}{dt} = \Omega(K)\zeta$, as

$$\Omega(K) = 4R(K) \sin^2 \left( \frac{K}{2} \right)$$ (37)

The step-flow growth will become stable if $\Omega(K)$, i.e. $R(K)$, is negative for any value of $K$. Then, the next step is just to calculate $R(K)$, which is done in Appendix E. It is worth noting that the stability condition $R(K) < 0$ can be formally put into the form

$$\text{Re} \left\{ \sum_k \frac{\partial A_n}{\partial \ell_k} e^{iK(n-k)} \right\} < 0$$ (38)

which generalizes the condition \( \frac{dA}{d\ell} < 0 \), found in reference [17].

In Appendix E, $R(K)$ is found to be equal to

$$R(K) = R_0 - R_1 \sum_{k=1}^{\infty} \gamma_k \cos(Kk) + R_2 \sin \left( \frac{K}{2} \right) \sum_{k=1}^{\infty} C_k \sin \left[ K \left( k - \frac{1}{2} \right) \right]$$ (39)
with \( R_0, R_1, R_2 \) given respectively by:

\[
R_0 = -\frac{F}{2} \left( L - \frac{aD}{D''} \right)^2 \frac{1 - \left( \frac{D'}{D''} \right)^2}{(\ell + L)^2} + 2\beta F\bar{U} \frac{(1 - \alpha)\ell}{(\ell + L)^2} + \beta F\bar{U} \frac{L \ln \left( \frac{\ell}{a} \right)}{(\ell + L)^2}
\]

\[
- \beta F\bar{U} \frac{(\gamma + \frac{1}{2})}{\ell + L} + \beta F\bar{U} \frac{\ell L^2 + 2(L - \ell) \left[ L \frac{aD}{D''} - \left( \frac{D'}{D''} \right)^2 \right]}{a(\ell + L)^3}
\]

(40a)

\[
R_1 = 2\beta F\bar{U} \frac{1}{\ell + L}
\]

(40b)

\[
R_2 = \frac{8E}{\pi} \frac{1 + \sigma}{1 - \sigma} (a\delta a)^2 \beta p_0 D \frac{1}{(\ell + L)\ell^2} + 2\beta F\bar{U} \frac{L\ell + 4 \left[ L \frac{aD}{D''} - \left( \frac{D'}{D''} \right)^2 \right]}{\ell(\ell + L)^2}
\]

(40c)

Expression (39) has two extrema for \( K = 0 \) and \( K = \pi \). Analytical expansions for small \( K \) and numerical tests led us to conclude that the first one is a minimum, the second one is a maximum and that no other extremum exists. The stability condition becomes \( R(\pi) < 0 \), that is to say

\[
R(\pi) = R_0 - R_1 \sum_{k=1}^{\infty} (-1)^k \gamma_k + R_2 \sum_{k=1}^{\infty} \frac{1}{(2k - 1)^2} < 0
\]

(41)

After having evaluated the two summations, we obtain the final form (\( \gamma \) is the Euler constant)

\[
R_0 + \frac{1}{2} R_1 \left( \gamma - \ln \frac{\pi}{2} \right) + \frac{\pi^2}{8} R_2 < 0
\]

(42)

Two limiting cases are worthy of mention: the case of terraces very large with respect to \( L \) and the case of weak flux.

Limit \( \ell \gg L \gg a \)

In this limit, equation (42) becomes

\[
\frac{L^2}{2\ell^2} > \beta \bar{U} \frac{1}{\ell} \left( 2\ln 2 + \frac{L \ln \left( \frac{\ell}{a} \right) + \frac{L}{a}}{\ell} \right) + \pi E D \frac{1 + \sigma}{1 - \sigma} (a\delta a)^2 \frac{\beta p_0}{F\ell^3}
\]

(43)

The term on the left derives from the Schoeobel effect, while the terms on the right correspond, the first one, to the step-atom interaction and, the second one, to the step-step interaction. The first one is proportional to \( \bar{U} \) and therefore it may be stabilizing \( (\bar{U} < 0) \) or destabilizing \( (\bar{U} > 0) \), according to the sign of the product \( (m - m_{zz}\sigma)/(1 - \sigma))\delta a \).

The stability condition (12) of reference [17] is only recovered if \( \ell \gg \frac{L^2}{a} \) and if the term of step-step interaction is neglected. If so, (43) is rewritten as

\[
\frac{L^2}{\ell} > \beta 8m a^2 \frac{\delta a(1 + \sigma)}{\pi} \ln 2
\]

(44)

This is the condition found in reference [17], apart from a factor \( 2\ln 2 \) (instead of 2 as claimed in [17]).
Limit of weak flux and large \( L \)

The limit of weak flux will be discussed extensively in the next section, with reference to the paper of Spencer et al. [16]. For the moment, let us observe that the condition of low flux is written as

\[
F \ll \frac{\pi^2 \varepsilon_0 D}{2 \bar{U} \ell^2}
\]

(45)

In this limit, we can retain (see Eq. (E.6)) only the term of step-step interaction independent of \( F \), and the Schwoebel term of zero order in \( \beta \). Then the stability condition takes the form

\[
2\pi E D \frac{1 + \sigma}{1 - \sigma} (a \delta a)^2 \beta p_0 < \frac{F \ell^2 L^2}{\ell + L}
\]

(46)

Indeed, a further condition on step-adatom interaction must be satisfied to obtain (46): \( \beta \bar{U} \ll L^2/(\ell + L) \). Since we have already supposed \( \beta \bar{U} \ll a \), the previous condition is always fulfilled unless \( \ell > L^2/a \), in which case we fall within the limit of large terraces.

It is noteworthy that in the limit of strong Schwoebel effect (\( L \gg \ell \)) we recover the same stability condition (46), because in both cases the step-adatom interaction is negligible.

7. Limit of Low Flux

In this section we want to compare our results with the theory of Spencer, Voorhees and Davis [16] (SVD in the following), which is valid for a nonsingular surface close to equilibrium. Indeed, SVD have assumed a flux so low that only the step-step interaction needs to be taken into account.

In the previous section, we have already said that in this limit only two terms can be retained: the step-step interaction, which is independent of \( F \), and the term coming from the existence of a Schwoebel barrier, which is of zero order in \( \beta \). The stability criterion takes the form (46), but it is not directly comparable with equation (3) of SVD. So, let us go back to our equation (36), which -in the case of low flux- takes the form

\[
\frac{1}{a^2} \frac{d\zeta}{dt} = 4 \zeta \sin^2 \left( \frac{K}{2} \right) \left\{ -\frac{F}{2} \frac{L^2}{(\ell + L)^2} + \frac{4\varepsilon_0 D}{(\ell + L)\ell^2} \sum_{k=1}^\infty C_k \sin \left( \frac{K}{2} \right) \sin \left[ \frac{K(2k-1)}{2} \right] \right\}
\]

(47)

The summation can be done explicitly

\[
\sum_{k=1}^\infty C_k \sin \left( \frac{K}{2} \right) \sin \left[ \frac{K(2k-1)}{2} \right] = \sum_{p=1}^\infty \frac{\sin^2 \left( \frac{Kp}{2} \right)}{p^2} = \frac{\pi K}{4} - \frac{K^2}{8}
\]

(48)

so as to obtain

\[
\frac{1}{a^2} \frac{d\zeta}{dt} = 4 \zeta \sin^2 \left( \frac{K}{2} \right) \left\{ -\frac{F}{2} \frac{L^2}{(\ell + L)^2} + \frac{\varepsilon_0 D}{(\ell + L)\ell^2} \left( \pi K - \frac{K^2}{2} \right) \right\}
\]

(49)

In the approximation \( K \ll 1 \), if we introduce the 'true' wavevector \( k = \frac{K}{\ell} \), the previous relation can be written as

\[
\frac{1}{a^2} \frac{d\zeta}{dt} = k^2 \left\{ -\frac{F}{2} \frac{L^2 \ell^2}{(\ell + L)^2} + \frac{\pi \varepsilon_0 D \ell}{(\ell + L)k} \right\}
\]

(50)
The second term on the right (proportional to $k^3$) corresponds to the term of elastic interaction in equation (3) of SVD, if the hypothesis of equal elastic constants for adsorbate and substrate is done. Actually, the only difference is the presence in our equation (50) of the prefactor $\ell/(\ell + L)$, which takes into account how the step-step interaction is modified by the Schwoebel effect.

The comparison of the stabilizing terms clearly shows their different origin: SVD consider a nonsingular surface and the stabilization is provided by the capillarity, proportional to $k^4$. On the contrary, we consider a stepped surface, whose total area does not change during the growth, and the stabilization derives from the Schwoebel effect, which contributes to equation (50) with a term proportional to $k^2$. While the capillarity stabilizes against fluctuations of short wavelengths, the Schwoebel barrier stabilizes the region of long wavelengths, and the instability arises for

$$\lambda < \lambda_{\text{max}} = \frac{2\pi \beta p_0 D}{FL^2} \left( \frac{\ell + L}{\ell} \right)$$

(51)

However, since our stabilizing term derives from a kinetic mechanism (the Schwoebel effect), it cancels in the limit $F = 0$. To fill the gap between our results and those of SVD, we must reconsider the nature of the step-step interaction: in fact, we have supposed that the interaction of order $1/\ell^2$ between the dipole forces located at the ledges of the steps and coming from the broken bond mechanism, were negligible with respect to the interaction of order $(\ln \ell)$, coming from the misfit mechanism. In other words, we have neglected a stabilizing interaction, which corresponds -for a nonsingular surface- to the capillarity, and which is important at equilibrium ($F = 0$).

In the following, we will remove such a hypothesis and the flux $F$ will be supposed to be so low that the stabilization provided by the Schwoebel effect can be neglected. Then, if in analogy to $m$ we define $f$ as the sum of the dipole forces acting at the edge of the steps and coming from the broken bond mechanism, equation (47) can be written as

$$\frac{1}{a^2} \frac{d\zeta}{dt} = -4 \zeta \sin^2 \left( \frac{K}{2} \right) \frac{\beta p_0 D}{(\ell + L)} (\delta \epsilon^*_n - \delta \epsilon^*_{n+1})$$

(52)

with

$$\delta \epsilon^*_n = \delta \epsilon_n - \frac{4(1 - \sigma^2)(fa^2)^2}{\pi E} \sum_{k=0}^{\infty} \left( \frac{1}{(\sum_{p=0}^{k} \ell_{n+p})^3} - \frac{1}{(\sum_{p=0}^{k} \ell_{n+1-p})^3} \right)$$

$$- \frac{2(1 + \sigma)}{\pi} a^2 f \delta a \sum_{k=0}^{\infty} \left( \frac{1}{(\sum_{p=0}^{k} \ell_{n+p})^2} - \frac{1}{(\sum_{p=0}^{k} \ell_{n+1-p})^2} \right)$$

(53)

By analogy to $\epsilon_n$, $\epsilon^*_n$ is the total variation of the step-step interaction when an adatom is incorporated into the $n$th step. In equation (53), the three quantities on the right correspond to the interaction by misfit mechanism, to the interaction by broken bond mechanism and to the step-step interaction, respectively if both the mechanisms are effective, one for each step.

After a manipulation similar to that performed in Appendices C and E, at order $k^4$, we find

$$\frac{1}{a^2} \frac{d\zeta}{dt} = \zeta k^2 \frac{\beta p_0 D \ell}{(\ell + L)} \left[ \epsilon \left( \pi k - \frac{\ell k^2}{2} \right) - \frac{4(1 - \sigma^2)(fa^2)^2}{\ell \pi E} \frac{\pi^2 k^2}{2} \right.$$  

$$\left. - \frac{4(1 + \sigma)}{\pi} a^2 f \delta a \left( \frac{3}{2} - \ln(k\ell) \right) k^2 \right]$$

(54)

Let us now suppose that one of the two mechanisms prevails, so that the third term is always negligible. In the two opposite limits, we obtain:
Interaction via misfit mechanism: \( \text{Et} \frac{\delta a}{a} \gg f \)

In this limit we simply have equation (47) at \( F = 0 \), and there is instability for all the physical wavelengths \( \lambda > \ell \).

Interaction via broken bond mechanism: \( \text{Et} \frac{\delta a}{a} \ll f \)

In this case, equation (54) becomes:

\[
\frac{1}{a^2} \frac{d\zeta}{dt} = k^2 \beta \rho_0 D \ell \left( \ell + L \right) \left[ \ell \pi \sigma - \frac{4(1 - \sigma^2)(fa^2)^2}{\ell \pi E} \pi^2 k^2 \right]
\]

and an instability arises for \( \lambda > \lambda_{\text{min}}, \) with

\[
\lambda_{\text{min}} = \frac{2}{\pi \ell} \left( \frac{1 - \sigma}{} \right)^2 \left( \frac{\delta a}{a} \right)
\]

So, we have recovered the result of SVD, in the case of a vicinal surface. Their result is valid in the limit of not too large terraces, otherwise the step-step interaction via misfit mechanism cannot be neglected. The validity condition \( \text{Et} \frac{\delta a}{a} \ll f \) corresponds to \( \lambda_{\text{min}} > \ell \), i.e. the stability region corresponds to a physical domain of the spectrum.

8. Discussion

The present section will be mainly devoted to the discussion of the hypotheses underlying our stability analysis. Some of them have already been stated at the beginning of the paper.

First of all, we have supposed (see the Introduction) that there are no misfit dislocations, which is experimentally verified in some systems \([8,12]\). This is correct if the misfit \( (\delta a/a) \) and the thickness \( h \) of the adsorbate are not too large. For the heteroepitaxy of semiconductors (for example Ge\textsubscript{x}Si\textsubscript{1-x}/Si), a misfit \( (\delta a/a) \approx 1\% \) -corresponding to \( x \approx 0.25- \) can be considered as a typical value.

For this value J.C. Bean et al. \([29]\) found a critical thickness \( h_C \approx 100a \). Such results, and the following theoretical interpretation \([30]\) have been criticized because they concern a non equilibrium case \([31]\).

Anyhow, the system we have been discussing is actually out of equilibrium and the mechanical equilibrium theory of Matthews and Blakeslee \([32]\) gives a critical thickness \( h_C \) of the same order for a misfit \( (\delta a/a) \approx 1\% \). We conclude that, for a significant range of values of the thickness \( h \) of the adsorbate, the hypothesis of no misfit dislocations is reasonable.

Moreover, the temperature \( T \) is supposed to be higher than the elastic interactions (see Section 6):

\[
T \gg \frac{\ell}{a} \approx a^2 m(1 + \sigma) \left( \frac{\delta a}{a} \right)
\]

A typical value of the misfit is \( \delta a/a \approx 1\% \); also, in Appendix A2 we give a rough valuation of \( m \) for a triangular lattice: \( a^2 m \approx 0.17 W_{\text{coh}} \) with \( W_{\text{coh}} \approx 35000 \) K. Then, the previous condition is written \( T \gg 60 \) K. Since typical values of \( T \) for MBE growth are around 400-800 K, the above approximation is correct.

In addition to the previous ones, there are some hypotheses concerning other kinds of instabilities which may occur during the growth of a stepped surface.
First of all, a serious limitation of our model is that it is one-dimensional and therefore applies only to straight steps. In reality, steps form meanders because of thermal fluctuations or stochastic fluctuations resulting from diffusion. Worse than that, even if deterministic equations are accepted, which generalize those of Section 5 in the two-dimensional case when elastic effects are neglected, straight steps turn out to be unstable \[33, 34\]. Even worse, a nonlinear study suggests that there is no steady state, but a chaotic state \[35\] unless a sufficiently strong anisotropy stabilizes a steady state \[36\]. However Johnson \textit{et al.} \[37\] have shown that the Schwoebel effect does prevent step-bunching in step-flow growth on a two dimensional surface. Presumably this happens in heteroepitaxy too, when elastic effects are taken into account. Thus, our treatment can be expected to be qualitatively correct, if \(\ell\) represents a local average of the distance between steps at a given time.

Finally, let us discuss the possibility of islands formation on the terraces, which has been disregarded up to now. Generally speaking, this is correct if the flux \(F\) is not too high and the terrace width \(\ell\) not too large, so that the average lifetime of an adatom is short and consequently the probability of island nucleation, low. A rough valuation of such probability and of the consequent instability threshold can be given.

We shall assume a 'minimal model' for the island formation: an adatom diffuses on the terrace until it sticks to a step or it encounters another adatom, forming a stable pair which can neither decay nor diffuse. The addressing quantity is the diffusion length \(\ell_D\), that is to say, the average distance travelled by the adatom in the absence of steps, before the creation of a stable pair. In this minimal model, \(\ell_D\) equals the average distance between nucleation centers and the average size of the islands just before their coalescence. We shall assume that the step-flow growth is stable against island formation if \(\ell < \ell_D\) \[37\]. The order of magnitude of \(\ell_D\) \[38, 39\] is

\[
\ell_D \simeq \left(\frac{a^2D}{F}\right)^{1/6}
\]

and the stability condition is easily found to be: \(F < Da^2/\ell^6\).

In Figure 5 we show the regions of stability in the plane \((F,T)\), at fixed \(\ell\). We can observe that at a given temperature the step-flow growth is destabilized by step-bunching at low flux and by island formation at high flux. At high temperatures no stability domain is predicted. However, our hypothesis that a pair of adatoms is stable is not correct at high temperatures: actually, this is correct only at low temperatures while during the growth of \(T\) a stable nucleation center is made of three, four or more adatoms. This fact makes island nucleation more difficult, lifts up the upper curve and stabilizes the step-flow growth.

Quantitatively, this means that \(\ell_D\) is no longer \(\ell_D \propto F^{-1/6}\). The correct exponent is now given \[39\] by \(\gamma = i^*/(2i^* + 4)\) where \((i^* + 1)\) is the number of adatoms forming a stable nucleation center: \(so,\ \gamma = 1/6\) for \(i^* = 1\) (the dimer is stable) and \(\gamma = 1/4\) for \(i^* = 2\) (the trimer is stable). Unfortunately, the proportionality constant does not depend only on \(D\), but also on all the average lifetimes \((\tau_2, \tau_3, \ldots, \tau_n)\) of the unstable nucleation centers.

Another comment on the validity of the previous calculation is appropriate. The stability condition derives from a comparison between a diffusion length \(\ell_D\), valid for a high symmetry surface, and the terrace length of a stepped surface. If there is no Schwoebel effect, this is correct because when the adatom feels the step, it is automatically incorporated. Instead, in the presence of a Schwoebel barrier the adatom can be reflected, so that the time \(\tau\) necessary to be incorporated increases and the probability of forming a stable pair increases as well. In the former case (no Schwoebel effect), \(\tau\) is the time necessary to reach the nearest step, that is to say (see Fig. 3) \(\tau \approx (l/2 - |x|)^2/D\) and if we average over \(x\) we find \(\bar{\tau} \approx l^2/12\). In the latter case, if we consider the limit of an infinite Schwoebel barrier, the adatoms can be
Fig. 5. — Stability phase diagram for a stepped surface with \( l = 30a \) and a misfit \( \delta a/a = 1\% \). The values of \( D, p_0, L, m, E \) are given in the text. A step-bunching instability arises in the region below the full line and an instability for island nucleation in the region above the dashed line.

incorporated only at the upper ledge and \( \tau \) is smaller than \((l/2 + x)^2/D\), so that \( \tau < l^2/3 \). We conclude that the presence of a Schwoebel barrier does not modify qualitatively Figure 5. A more quantitative analysis of the stability against island nucleation will be the object of future work.

9. Conclusions

We have studied the elasticity-driven step-bunching instability of a vicinal surface. The surface has been modeled as a one-dimensional array of straight steps; the growth occurs via step-flow, i.e. through sticking of the adatoms to the steps.

The step-flow growth is stable if the adatom prefers to stick to the upper ledge. Which ledge is indeed the favoured one depends on kinetic and thermodynamical effects, the latter being effective only if adatoms are allowed to detach from steps after incorporation, so that equilibrium can be attained. Kinetics effects are the Schwoebel effect and the step-adatom interaction: the first one is stabilizing, while the second one may be stabilizing or not, according to the sign of the misfit \( \delta a/a \). This fact gives rise to a new possible instability in MBE, which has been discussed in reference [17]. Here we have also taken into account thermodynamical effects - that is to say the step-step interaction- and we have generalized the step-adatom interaction, previously restricted to nearest neighbours: the latter extension has no important consequence on the stability condition.

In heteroepitaxy, it is generally correct to restrict the step-step interaction to the misfit mechanism: the latter is destabilizing and it prevails on the other possible destabilizing terms (the step-adatom interaction) within the limits of strong Schwoebel effect \((L \gg \ell)\) or weak flux. However, if \( F \) is too low or even zero, the stabilization provided by the Schwoebel barrier is no longer effective and the step-step interaction via broken bond mechanism must be invoked; such an interaction can be considered, for a stepped surface, the analogous to the surface energy (capillarity).
If stability with respect to island nucleation is considered, we find that at a given temperature, the step-flow growth is destabilized by step-bunching at low flux and by island formation at high flux, while it is stable at intermediate values.

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Appendix A

Proof of Equation (2)

Let us consider an adsorbate, grown on a substrate with the same elastic constants.

The elastic free energy in the substrate can be written as

$$ F_{\text{sub}} = \frac{1}{2} \int_{V_{\text{sub}}} \sum_{\alpha \beta \gamma \xi} \Omega_{\alpha \beta}^\gamma_\xi [\epsilon_{\alpha \beta}(r)] \epsilon_{\gamma \xi}(r) $$

(A.1)

where the integral is on the volume of the substrate, $(\alpha, \beta, \gamma, \xi)$ are the coordinates $x, y, z$, the quantity $\epsilon(r)$ is the strain tensor at point $r$ and $\Omega$ is the elastic tensor. In the case of an isotropic solid, it is given by [40]:

$$ \Omega_{\alpha \beta}^\gamma_\xi = \mu (\delta_{\alpha \gamma} \delta_{\beta \xi} + \delta_{\alpha \xi} \delta_{\beta \gamma}) + \lambda \delta_{\alpha \beta} \delta_{\gamma \xi} $$

(A.2)

where $\lambda$ and $\mu$ are the Lamé coefficients.

The substrate will be assumed to be infinite in the $-z$ direction. Therefore, the strain vanishes for very large values of $-z$. Thus it is natural to count the strain from an origin such that the substrate strain is zero. The substrate actually introduces a strain $b$ into the adsorbate. However, the strain in the adsorbate will be counted from such an origin that it is zero if the adsorbate is in registry with the substrate. Then the free energy in the adsorbate film is

$$ F_{\text{ad}} = \frac{1}{2} \int_{V_{\text{ad}}} \sum_{\alpha \beta \gamma \xi} \Omega_{\alpha \beta}^\gamma_\xi [\epsilon_{\alpha \beta}(r)] \epsilon_{\gamma \xi}(r) + b_{\alpha \beta}] [\epsilon_{\gamma \xi}(r) + b_{\gamma \xi}] $$

(A.3)

where $V_{\text{ad}}$ is the volume of the adsorbate. In the absence of any interaction with the substrate, the adsorbate strain (with respect to the substrate) would take the value $\epsilon = -b$ which minimizes (A.3).

Assuming that the axes $x$ and $y$ parallel to the surface are equivalent, the components $b_{\alpha \beta}$ along these axes are obviously

$$ b_{xx} = b_{yy} = -\frac{\delta a}{a} $$

(A.4a)

The other nonvanishing component of the tensor $b$ is easily deduced from elasticity theory, namely (for an isotropic solid)

$$ b_{zz} = \frac{2\lambda}{\lambda + 2\mu} \frac{\delta a}{a} = \frac{2\sigma}{1 - \sigma} \frac{\delta a}{a} $$

(A.4b)

where $\sigma = \frac{\lambda}{2(\lambda + \mu)}$ is the Poisson coefficient.
For a fixed number \( N_{\text{ad}} \) of adsorbed atoms, the term of second order in \( b \), in (A.3), which is proportional to \( N_{\text{ad}} \), is a constant and will be omitted. Formula (A.3) can therefore be written as

\[
F_{\text{ad}} = \frac{1}{2} \int_{V_{\text{ad}}} d^3 r \sum_{\alpha\beta\gamma} \Omega_{\alpha\beta}^{\gamma} \epsilon_{\alpha\beta}(r) \epsilon_{\gamma}(r) \quad \text{(A.5)}
\]

where

\[
\tilde{\eta}_{\alpha\beta} = - \sum_{\gamma} \Omega_{\alpha\beta}^{\gamma} b_{\gamma} \quad \text{(A.6)}
\]

plays the role of an external volume stress. The stress tensor \( \tilde{\eta}_{\alpha\beta} \) is independent of the surface shape, and therefore its symmetry properties may be derived assuming a plane surface. Since relaxation is free in the \( z \) direction, the components \( \tilde{\eta}_{\alpha z} \) are zero at equilibrium. On the other hand, symmetry implies \( \tilde{\eta}_{xy} = 0 \) and \( \tilde{\eta}_{xx} = \tilde{\eta}_{yy} \). In particular, for an isotropic solid, from (A.6) and (A.4a-A.4b) we obtain

\[
\frac{\tilde{\eta}_{\alpha\gamma}}{a} = \frac{\delta a}{a} \frac{E}{1 - \sigma} (\delta_{x\alpha} + \delta_{y\gamma}) \delta_{\alpha\gamma} \quad \text{(A.7)}
\]

For an infinitely thick substrate, the average strain on the adsorbate perpendicular to \( z \) vanishes. Therefore, the contribution of the completely filled layers to the second integral at the right hand side of (A.5) vanishes too. The integral can thus be limited to the incompletely filled layers.

\( \epsilon_{\alpha,\beta}(x, y, z) \) may be assumed to be independent of \( z \) in the incompletely filled layers, so the second volume integral in (A.5) reduces to a surface integral, where the number \( h(x, y) \) of incompletely filled layers has to be introduced. If we define the external surface stress

\[
\eta_{\alpha,\gamma} = \tilde{\eta}_{\alpha,\gamma} h(x, y), \quad \text{(A.8)}
\]

equation (2) is recovered.

**Value of the Dipole Moment \( m \)**

Let us calculate \( m \) for a triangular lattice (bidimensional model). We shall assume that the adatom interacts with the surface through pair interactions \( V(r) \) with its nearest \( (nn) \) and next-nearest \( (nnn) \) neighbours (see Fig. 2).

In the bulk, the condition of minimum energy is written as

\[
\frac{d}{dr_1} [N V(r_1) + N V(r_2)] = 0 \quad \text{(A.9)}
\]

where \( N = 6 \) is the number of \( (nn) \) and \( (nnn) \), and \( r_1, r_2 = \sqrt{3} r_1 \) are the distances between \( (nn) \) and \( (nnn) \).

So, the relation between \( f_1(nn) \)-force and \( f_2(nnn) \)-force is

\[
f_1 = \sqrt{3} f_2 \quad \text{(A.10)}
\]

At the surface, a relaxation phenomenon occurs: the interatomic distances and the forces \( (f'_1, f'_2) \) are modified. We shall assume, for the moment, that the distances are not changed, so the equilibrium condition for the adatom is written as

\[
\sqrt{3} f'_1 + 2 f'_2 = 0 \quad \text{(A.11)}
\]
Now, because of its simplicity, a Lennard-Jones interaction will be assumed:

$$V(r) = V_0 \left[ \left( \frac{r_0}{r} \right)^{12} - \left( \frac{r_0}{r} \right)^6 \right]$$  \hspace{1cm} (A.12)

but the resulting value for the dipole moment is expected to be typical also for other, some realistic potentials.

If the \textit{nnn}-force is supposed to be unchanged at the surface

$$f'_2 = f_2,$$  \hspace{1cm} (A.13)

the following relation between \(f'_1\) and \(f_1\) can be established

$$f'_1 = \frac{2}{3} f_1$$  \hspace{1cm} (A.14)

Accordingly, the diagonal elements of the dipole tensor (1) are easily calculated:

$$m_{xx} = \frac{1}{a} \left( \frac{f'_1}{2} - \frac{3\sqrt{3}}{2} f'_2 \right) = -\frac{7}{2\sqrt{3}} \frac{f_2}{a}$$  \hspace{1cm} (A.15a)

$$m_{zz} = -\frac{1\sqrt{3}}{a} \frac{f'_2}{2} = -\frac{3}{2} \frac{f_2}{a}$$  \hspace{1cm} (A.15b)

The interatomic distance \(a\) results nearly equal to \(a \simeq 2^{1/6} r_0\), and the force \(f_2\) can be determined

$$f_2 = \frac{dV}{dr} \bigg|_{\sqrt{3}a} \simeq \frac{\sqrt{3} V_0}{27a}.$$  \hspace{1cm} (A.16)

Since the cohesion energy per atom \(W_{coh}\) nearly equals \(\frac{N}{2} |V(a)|\), it results

$$a^2 |m_{xx}| = \frac{a}{2\sqrt{3}} f_1 \simeq \frac{7}{54} V_0 \simeq 0.17 W_{coh}$$  \hspace{1cm} (A.17a)

$$a^2 |m_{zz}| = \frac{a\sqrt{3}}{2} f_2 \simeq \frac{V_0}{18} \simeq 0.07 W_{coh}$$  \hspace{1cm} (A.17b)

If the distance between the adatom and the substrate is allowed to change and a numerical calculation is performed, the above results are nearly unmodified. Also, a calculation on a tridimensional \textit{bcc} lattice gives values of the same order of magnitude: \(a^2 |m_{xx}| \simeq 0.16 W_{coh}\) and \(a^2 |m_{zz}| \simeq 0.24 W_{coh}\).

Appendix B

In the following Appendix we will show the details of the calculation in order to obtain the equations discussed in Section 6. The organization of the Appendices is the following: in Appendix B we obtain the general expression for \(\delta A_n\) (Eq. (22)); in Appendix C we calculate explicitly the different quantities appearing in \(\delta A_n\), while Appendix D is devoted to the calculation of some summations; finally, in Appendix E we give \(R(K)\) (Eq. (39)) and the stability condition in the different limits.

Let us start deriving \(A_n\) from equation (14), by evaluating the adatom density \(p_n(x)\) for \(x = \frac{\ell_n}{2}\) and then eliminating \(p_n\left(\frac{\ell_n}{2}\right)\) and \(p_n\left(-\frac{\ell_n}{2}\right)\) by means of (16a) and (16b). The
The result is:

\[
A_n = \frac{F \ell_n \left[ \frac{D'}{D''} e^{\beta U_n(-t_2)} - e^{\beta U_n(t_2)} \right] + \frac{D'}{aD} \left[ p_n e^{\beta U_n(-t_2)} - p_n e^{\beta U_n(t_2)} \right] - \frac{D'}{aD} \int_{-t_2}^{t_2} ye^{\beta U_n(y)} dy}{e^{\beta U_n(t_2)} + \frac{D'}{D''} e^{\beta U_n(-t_2)} + \frac{D'}{aD} \int_{-t_2}^{t_2} e^{\beta U_n(y)} dy}
\]

and after substitution of \( p_n \) through equations (8), we have

\[
A_n = \frac{F \ell_n \left[ \frac{D'}{D''} e^{\beta U_n(-t_2)} - e^{\beta U_n(t_2)} \right] + \frac{D'}{aD} \left[ e^{\beta \epsilon_{n+1}} - e^{\beta \epsilon_n} \right] - \frac{D'}{aD} \int_{-t_2}^{t_2} ye^{\beta U_n(y)} dy}{e^{\beta U_n(t_2)} + \frac{D'}{D''} e^{\beta U_n(-t_2)} + \frac{D'}{aD} \int_{-t_2}^{t_2} e^{\beta U_n(y)} dy}
\]

(B.1)

In the hypothesis that the elastic energies are much smaller than \( k_B T = \frac{1}{\beta} \), at the first order in \( \beta \) we obtain:

\[
A_n = \frac{\frac{F \ell_n}{2} \left( \frac{D'}{D''} - 1 \right) + \frac{\beta F \ell_n}{2} \left[ \frac{D'}{D''} U_n(-\frac{\ell_n}{2}) - U_n(\frac{\ell_n}{2}) \right]}{\ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''}} - \frac{-\beta \frac{D'}{aD} p_0(\epsilon_n - \epsilon_{n+1}) - \frac{\beta D'}{aD} \int_{-t_2}^{t_2} yU_n(y) dy}{\ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''}}
\]

\[
- \frac{\frac{\beta F \ell_n}{2} \left( \frac{D'}{D''} - 1 \right) \left[ \frac{D'}{D''} U_n(-\frac{\ell_n}{2}) + U_n(\frac{\ell_n}{2}) + \frac{D'}{aD} \int_{-t_2}^{t_2} U_n(y) dy \right]}{\left( \ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''} \right)^2}
\]

(B.2)

We can now calculate the variation \( \delta A_n \), resulting from a small sinusoidal deformation of the regular array of steps (see Eqs. (19-21)). The result is the following:

\[
\delta A_n = -\frac{\beta p_0 \frac{D'}{aD} (\delta \epsilon_n - \delta \epsilon_{n+1})}{\ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''}}
\]

\[
+ \frac{\frac{F}{2} \left( \frac{D'}{D''} - 1 \right) + \frac{\beta F}{2} \delta \left[ \frac{D'}{D''} U_n(-\frac{\ell_n}{2}) - U_n(\frac{\ell_n}{2}) \right]}{\ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''}} \delta \ell_n
\]

\[
- \frac{\frac{F}{2} \left( \frac{D'}{D''} - 1 \right) + \frac{\beta F}{2} \left[ \frac{D'}{D''} U_n(-\frac{\ell_n}{2}) + U_n(\frac{\ell_n}{2}) + \frac{D'}{aD} \int_{-t_2}^{t_2} U_n(y) dy \right]}{\left( \ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''} \right)^2} \delta \ell_n
\]

\[
+ \frac{\beta F}{2} \left[ \frac{D'}{D''} \delta U_n(-\frac{\ell_n}{2}) - \delta U_n(\frac{\ell_n}{2}) \right] - \frac{\beta F \frac{D'}{D''} \delta \int_{-t_2}^{t_2} yU_n(y) dy}{\ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''}}
\]

\[
- \frac{\beta F}{2} \left[ \frac{D'}{D''} \delta U_n(-\frac{\ell_n}{2}) + \delta U_n(\frac{\ell_n}{2}) + \frac{D'}{aD} \delta \int_{-t_2}^{t_2} U_n(y) dy \right] \delta \ell_n
\]

\[
- \frac{\beta F}{2} \left[ \frac{D'}{D''} - 1 \right] \left[ \frac{D'}{D''} \delta U_n(-\frac{\ell_n}{2}) + \delta U_n(\frac{\ell_n}{2}) + \frac{D'}{aD} \delta \int_{-t_2}^{t_2} U_n(y) dy \right]
\]

\[
\left( \ell_n \frac{D'}{aD} + 1 + \frac{D'}{D''} \right)^2
\]
The first term is the only one taken into account by Srolovitz [3] and by Spencer et al. [16]. The next two terms are finite at $\beta = 0$ for a finite Schwoebel effect, stabilizing the growth at high temperatures. Among the last terms, only a few have been considered by Duport et al. [17].

Using the parity of the function $U_n^0(x) = -U_n^0(-x)$, introducing the quantity $L$ defined in Section 3 and after a rearrangement of the different terms, equation (22) is found

$$
\delta A_n = -\beta_0 D_0 \frac{\delta \epsilon_n - \delta \epsilon_{n+1}}{L + L} - F \frac{L}{2} \left( \frac{L - \frac{a_0}{D_0}}{(L + L)^2} \right) \delta \epsilon_n - \frac{\beta F}{2} \frac{L^2}{(L + L)^2} U_n^0 \left( \frac{\ell}{2} \right) \delta \epsilon_n
$$

$$
+ \frac{\beta F}{L + L} \left( \frac{\ell}{a_0 D_0} \right) \delta U_n \left( \frac{\ell}{2} \right) \delta \epsilon_n
$$

$$
+ \frac{\beta F L}{2} \left( \frac{a_0 D_0}{D_0} \delta U_n \left( \frac{\ell}{2} \right) - \left( L - \frac{a_0}{D_0} \right) \delta U_n \left( \frac{\ell}{2} \right) \right) - \delta \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} U_n(y) dy
$$

$$
- \frac{\beta F L}{2} \left( \frac{2}{a_0 D_0} \delta U_n \left( \frac{\ell}{2} \right) + \left( L - \frac{a_0}{D_0} \right) \delta U_n \left( \frac{\ell}{2} \right) + \delta \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} U_n(y) dy \right) \delta \epsilon_n
$$

\[ \text{(B.4)} \]

Appendix C

Computation of the Integrals Involving $yU$ and $U$

The potential $U_n(x)$ (see Eq. (3)) has been defined as:

$$
U_n(x) = \bar{U} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p} + x - \frac{\epsilon_n}{2}} - \frac{1}{\sum_{p=0}^{k} \ell_{n+p} - x + \frac{\epsilon_n}{2}} \right)
$$

\[ \text{(3)} \]

It follows that

$$
\int_{-\frac{\ell}{2} - \eta}^{\frac{\ell}{2} - \eta} yU_n(y) dy = \bar{U} \left( 2I_0 + \sum_{k=1}^{\infty} (I_k + I_{-k}) \right)
$$

\[ \text{(C.1)} \]

where a cut-off $\eta$ has been introduced. We put $\eta = \alpha$ in $I_0$ and $\eta = 0$ otherwise, that is to say

$$
I_k = \int_{-\frac{\ell}{2} - y}^{\frac{\ell}{2} - y} \sum_{p=0}^{k} \ell_{n+p} - \frac{\epsilon_n}{2} + y
$$

$$
= \int_{-\frac{\ell}{2} - y}^{\frac{\ell}{2} - y} \sum_{p=0}^{k} \ell_{n+p} + \frac{\epsilon_n}{2} - y
$$

for $k \neq 0$ and

$$
I_0 = \int_{-\frac{\ell}{2} - \eta}^{\frac{\ell}{2} - \eta} \sum_{p=0}^{k} \ell_{n+p} - \frac{\epsilon_n}{2} + y
$$

$$
= \int_{-\frac{\ell}{2} - \eta}^{\frac{\ell}{2} - \eta} \sum_{p=0}^{k} \ell_{n+p} + \frac{\epsilon_n}{2} - y
$$

All the integrals have the general form

$$
\int_{-\frac{\ell}{2} - \eta}^{\frac{\ell}{2} - \eta} y dy = \ell_n - y_0 \ln \frac{y_0 + \frac{\ell_n}{2}}{y_0 - \frac{\ell_n}{2} + \eta}
$$
For \( y_0 = \frac{\ell_n}{2} \) and \( \eta = a \) we obtain
\[
I_0 = \ell_n - \frac{\ell_n}{2} \ln \left( \frac{\ell_n}{a} \right)
\]
while for \( y_0 = \sum_{p=0}^{k} \ell_{n+p} - \frac{\ell_n}{2} \) and \( \eta = 0 \) we have
\[
I_k = \ell_n - \left( \sum_{p=0}^{k} \ell_{n+p} - \frac{\ell_n}{2} \right) \ln \left( \frac{\sum_{p=0}^{k} \ell_{n+p}}{\sum_{p=1}^{k} \ell_{n+p}} \right)
\]
The linearized variations are given by
\[
\delta I_0 = \frac{\delta \ell_n}{2} - \frac{\delta \ell_n}{2} \ln \left( \frac{\ell}{a} \right) \tag{C.2a}
\]
and, for \( k \neq 0 \)
\[
\delta I_k = \delta \ell_n - \left( \sum_{p=0}^{k} \delta \ell_{n+p} - \frac{\delta \ell_n}{2} \right) \ln \left( \frac{k+1}{k} \right) - \left( k + \frac{1}{2} \right) \left( \sum_{p=0}^{k} \frac{\delta \ell_{n+p}}{k+1} - \sum_{p=1}^{k} \frac{\delta \ell_{n+p}}{k} \right)
= \left( \frac{1}{2(k+1)} - \frac{1}{2} \ln \frac{k+1}{k} \right) \delta \ell_n + \sum_{p=1}^{k} \delta \ell_{n+p} \left( \frac{1}{2k} + \frac{1}{2(k+1)} - \ln \frac{k+1}{k} \right) \tag{C.2b}
\]
Using the explicit expressions of \( \delta I_k \) we derive
\[
\frac{1}{\bar{U}} \delta \int_{t^{\frac{1}{2}} - \eta}^{t^\frac{1}{2} - \eta} y U_n(y) dy = \left( 2\delta I_0 + \sum_{k=1}^{\infty} (\delta I_k + \delta I_{-k}) \right)
= \delta \ell_n - \delta \ell_n \ln \left( \frac{\ell}{a} \right) + \sum_{k=1}^{\infty} \left( \frac{1}{k+1} - \ln \frac{k+1}{k} \right) \delta \ell_n
+ \sum_{k=1}^{\infty} \left[ \sum_{l=1}^{k} (\delta \ell_{n+l} + \delta \ell_{n-l}) \right] \left( \frac{1}{2k} + \frac{1}{2(k+1)} - \ln \frac{k+1}{k} \right) \tag{C.3}
\]
Defining the quantity
\[
\gamma_p = \sum_{k=p}^{\infty} \left( \frac{1}{2k} + \frac{1}{2(k+1)} - \ln \frac{k+1}{k} \right) \tag{24}
\]
we can finally write
\[
\delta \int_{t^{\frac{1}{2}} - \eta}^{t^\frac{1}{2} - \eta} y U_n(y) dy = \bar{U} \left\{ \gamma_1 + \frac{1}{2} - \ln \left( \frac{\ell}{a} \right) \right\} \delta \ell_n + \sum_{k=1}^{\infty} \gamma_k [\delta \ell_{n+k} + \delta \ell_{n-k}] \tag{23}
\]
Let us now proceed with calculating the integral of \( U \).
\[
\int_{t^{\frac{1}{2}} - \eta}^{t^\frac{1}{2} - \eta} U_n(y) dy = \bar{U} \sum_{k=0}^{\infty} \int_{t^{\frac{1}{2}} - \eta}^{t^\frac{1}{2} - \eta} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p} + y - \frac{\ell_n}{2}} - \frac{1}{\sum_{p=1}^{k} \ell_{n-p} - y - \frac{\ell_n}{2}} \right) dy
\]
Since the $k = 0$ term does not contribute (the corresponding integrand is an odd function) and for the other the cut-off $\eta$ can be omitted, the integral takes the form

$$
\int_{-\frac{\ell n}{2} - \eta}^{\frac{\ell n}{2} - \eta} U_n(y) dy = \bar{U} \sum_{k=1}^{\infty} \int_{-\frac{\ell n}{2}}^{\frac{\ell n}{2}} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p} + y - \ell n \over 2} - \frac{1}{\sum_{p=0}^{k} \ell_{n+p} - y - \ell n \over 2} \right) dy
$$

$$
= \bar{U} \sum_{k=1}^{\infty} \left( \ln \frac{\sum_{p=0}^{k} \ell_{n+p}}{\sum_{p=1}^{k} \ell_{n+p}} - \ln \frac{\sum_{p=0}^{k} \ell_{n+p}}{\sum_{p=1}^{k} \ell_{n+p}} \right)
$$

and its variation can be written

$$
\delta \int_{-\frac{\ell n}{2} - \eta}^{\frac{\ell n}{2} - \eta} U_n(y) dy = \bar{U} \sum_{k=1}^{\infty} \left( \frac{\sum_{p=0}^{k} \delta \ell_{n+p}}{(k+1)\ell} - \frac{\sum_{p=1}^{k} \delta \ell_{n+p}}{k \ell} - \frac{\sum_{p=0}^{k} \delta \ell_{n+p}}{(k+1)\ell} + \frac{\sum_{p=1}^{k} \delta \ell_{n+p}}{k \ell} \right)
$$

At the end, we have

$$
\delta \int_{-\frac{\ell n}{2} - \eta}^{\frac{\ell n}{2} - \eta} U_n(y) dy = \bar{U} \sum_{k=1}^{\infty} \left( \frac{1}{k + 1} - \frac{1}{k} \right) (\delta \ell_{n+k} - \delta \ell_{n-k})
$$

(25)

**Computation of $U$ on the Steps**

From the definition (3) it follows that

$$
U_n\left(\frac{\ell n}{2} - \eta\right) = \bar{U} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p} + \eta} - \frac{1}{\sum_{p=1}^{k} \ell_{n+p} + \eta} \right)
$$

(C.4)

and

$$
U_n\left(-\frac{\ell n}{2} + \eta\right) = \bar{U} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=1}^{k} \ell_{n+p} + \eta} - \frac{1}{\sum_{p=0}^{k} \ell_{n+p} - \eta} \right)
$$

(C.5)

For an array of terraces of equal length, we have

$$
U_n^0\left(\frac{\ell}{2}\right) = -U_n^0\left(-\frac{\ell}{2}\right) = \bar{U} \left( \sum_{k=1}^{\infty} \frac{1}{(k+1)\ell} - \sum_{k=1}^{\infty} \frac{1}{k \ell} + \frac{1}{\ell} - \frac{1}{a} \right)
$$

$$
= -\frac{\bar{U}}{a}
$$

(29)

In equation (C.4), we can omit $\eta$ because in the only term ($k = 0$) where the cutoff enters, it appears as a constant and therefore it is needless for the variation. Thus we obtain

$$
\delta U_n\left(\frac{\ell n}{2}\right) = -\bar{U} \frac{\delta \ell n}{\ell^2} - \bar{U} \sum_{k=1}^{\infty} \left( \frac{\sum_{p=0}^{k} \delta \ell_{n+p}}{(k+1)^2 \ell^2} - \frac{\sum_{p=1}^{k} \delta \ell_{n-p}}{k^2 \ell^2} \right)
$$

The first quantity on the right hand side is exactly the $k = 0$ term of the summation, so that we can rewrite

$$
\delta U_n\left(\frac{\ell n}{2}\right) = -\bar{U} \sum_{k=1}^{\infty} \left( \frac{\sum_{p=0}^{k-1} \delta \ell_{n+p}}{k^2 \ell^2} - \frac{\sum_{p=1}^{k} \delta \ell_{n-p}}{k^2 \ell^2} \right)
$$
Introducing the quantities
\[ C_k = \sum_{p=k}^{\infty} \frac{1}{p^2} \] (27)
the previous relation becomes
\[ \delta U_n \left( \frac{\ell_n}{2} \right) = \frac{\bar{U}}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n-k} - \delta \ell_{n+k-1}) \] (26a)

A similar calculation for equation (C.5) produces
\[ \delta U_n \left( -\frac{\ell_n}{2} \right) = -\frac{\bar{U}}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n+k} - \delta \ell_{n-k+1}) \] (26b)

**Computation of \( \delta \epsilon_n - \delta \epsilon_{n+1} \)**

Starting from equation (5)
\[ \epsilon_n = \bar{\epsilon} \sum_{k=0}^{\infty} \left( \frac{1}{\sum_{p=0}^{k} \ell_{n+p}} - \frac{1}{\sum_{p=0}^{k} \ell_{n-1-p}} \right) \] (5)
we find
\[ \delta \epsilon_n = -\bar{\epsilon} \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n+k-1} - \delta \ell_{n-k}) \]
and therefore
\[ \delta \epsilon_n - \delta \epsilon_{n+1} = -\bar{\epsilon} \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n+k-1} - \delta \ell_{n-k} - \delta \ell_{n+k} + \delta \ell_{n+1-k}) \] (28)

**Integrals Involving \( U \): Uniform Case**

From the definition (3) of \( U \), we immediately recover that
\[ \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} U_n^{0}(y) dy = 0 \] (3)
On the other hand
\[ \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} y U_n^{0}(y) dy = \bar{U} \sum_{q=0}^{\infty} \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} \left( \frac{y}{y + \frac{\ell}{2} + q\ell} - \frac{y}{\frac{\ell}{2} + q\ell - y} \right) dy \]
\[ = \bar{U} \sum_{q=0}^{\infty} \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} \left( 2 - \frac{\frac{\ell}{2} + q\ell}{y + \frac{\ell}{2} + q\ell} - \frac{\frac{\ell}{2} + q\ell}{\frac{\ell}{2} + q\ell - y} \right) dy \]
\[ = \bar{U} \left\{ 2\ell - \ell \ln \frac{\ell}{a} + \sum_{q=1}^{\infty} \left[ 2\ell - 2\left( \frac{\ell}{2} + q\ell \right) \ln \frac{q+1}{q} \right] \right\} \]
and finally

\[ \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} y U_n^0(y) dy = 2\ell \ell \left[ 1 - \frac{1}{2} \ln \left( \frac{\ell}{a} \right) - \alpha \right] \]

where

\[ \alpha = \sum_{k=1}^{\infty} \left( k + \frac{1}{2} \right) \ln \left( 1 + \frac{1}{k} \right) - 1 \]

The value of \( \alpha \) will be given in the following paragraph (Eq. (D.9)), but it is already possible to check the convergence of the summation, since for \( k \gg 1 \),

\[ 1 - \left( k + \frac{1}{2} \right) \ln \left( 1 + \frac{1}{k} \right) \simeq -\frac{1}{12k^2} \]

**Appendix D**

**Calculation of \( \gamma_p \) and \( \alpha \)**

\( \gamma_p \) has been defined in equation (24) as

\[ \gamma_p = \sum_{k=p}^{\infty} \left( \frac{1}{2k} + \frac{1}{2(k+1)} - \ln \frac{k+1}{k} \right) = -\lim_{s \to \infty} \left( \ln \frac{s+1}{p} - \sum_{q=p}^{s} \frac{1}{q} + \frac{1}{2p} - \frac{1}{2(s+1)} \right) \]

The connection with the Euler constant \( \gamma \) is apparent, in that

\[ \gamma_1 = \gamma - \frac{1}{2} = 0.07721 \]  
\[ \gamma_2 = \gamma_1 - \ln 2 + \frac{1}{2} + \frac{1}{4} = 0.02035 \]

and so on.

We are interested in the behaviour of \( \gamma_p \) for large \( p \). Let us define the function \( R(p, s) \) such that

\[ \gamma_p = -\lim_{s \to \infty} R(p, s) \]

Then,

\[ R = \ln \frac{s+1}{p} - \sum_{q=p}^{s} \frac{1}{q} + \frac{1}{2q} - \frac{1}{2s+2} = \int_{p}^{s+1} \frac{dx}{x} - \sum_{q=p}^{s} \frac{1}{q} + \frac{1}{2p} - \frac{1}{2s+2} \]

\[ = \sum_{q=p+1}^{s} \left( \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dx}{q + x} - \int_{0}^{\frac{1}{2}} \frac{dx}{p + x} + \int_{-\frac{1}{2}}^{0} \frac{dx}{s + 1 + x} + \frac{1}{2p} - \frac{1}{2s+2} \right) \]

We can develop the integrands for small \( \left( \frac{x}{p} \right) \) and \( \left( \frac{x}{s} \right) \)

\[ R \simeq \sum_{q=p+1}^{s} \int_{-\frac{1}{2}}^{\frac{1}{2}} \left( \frac{1}{q} - \frac{x}{q^2} + \frac{x^2}{q^3} \right) dx - \sum_{q=p+1}^{s} \frac{1}{q} + \int_{0}^{\frac{1}{2}} \left( \frac{1}{q} - \frac{x}{q^2} + \frac{x^2}{q^3} \right) dx \]

\[ + \int_{-\frac{1}{2}}^{0} \left( \frac{1}{s} - \frac{x}{s^2} + \frac{x^2}{s^3} \right) dx - \frac{1}{2p} - \frac{1}{2s+2} \]
\[ R \approx \sum_{q=p+1}^{s} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{x^2}{q^3} \, dx + \int_{0}^{1} \left( -\frac{x}{q^2} - \frac{x^2}{q^3} \right) \, dx + \int_{-\frac{1}{2}}^{0} \left( -\frac{x}{s^2} + \frac{x^2}{s^3} \right) \, dx + \frac{1}{2s} - \frac{1}{2s+2} \]

\[ R \approx \sum_{q=p+1}^{s} \frac{1}{24q^3} - \frac{1}{8q^2} + \frac{1}{8s^2} + \frac{1}{2s^2} \approx \int_{p}^{s} \frac{dp}{24q^3} - \frac{1}{8q^2} + \frac{1}{8s^2} + \frac{1}{2s^2} \]

Finally, we find

\[ \gamma_p \approx \frac{5}{48p^2} \quad (D.4) \]

Let us now evaluate the summation \( \sum_{p=1}^{\infty} \gamma_p \)

\[
\sum_{p=1}^{\infty} \gamma_p = \sum_{p=1}^{\infty} \sum_{q=p}^{\infty} \left( \frac{1}{2(q+1)} + \frac{1}{2q} - \ln \frac{q+1}{q} \right) \\
= \lim_{s \to \infty} \sum_{q=1}^{s} \sum_{p=1}^{q} \left( \frac{1}{2(q+1)} + \frac{1}{2q} - \ln \frac{q+1}{q} \right)
\]

which can be rewritten, by interchanging \( p \) and \( q \):

\[
\sum_{p=1}^{\infty} \gamma_p = \lim_{s \to \infty} \sum_{q=1}^{s} \sum_{p=1}^{q} \left( \frac{1}{2(q+1)} + \frac{1}{2q} - \ln \frac{q+1}{q} \right) \\
= \lim_{s \to \infty} \sum_{q=1}^{s} \left( 1 - \frac{1}{2(q+1)} - q \ln \frac{q+1}{q} \right) \\
= \lim_{s \to \infty} \left( s - \sum_{q=1}^{s} \frac{1}{2(q+1)} - \sum_{q=1}^{s} \ln \left( \frac{q+1}{q} \right) \right) \\
= \lim_{s \to \infty} \left( s - \frac{1}{2} \sum_{q=1}^{s} \frac{1}{q+1} - \sum_{q=1}^{s} \ln \left( \frac{q+1}{q} \right) \right) \\
= \lim_{s \to \infty} \left( s - \frac{1}{2} \sum_{q=1}^{s} \frac{1}{q+1} - \sum_{q=1}^{s} \ln \left( \frac{q+1}{q} \right) \right) \\
(D.5a)
\]

If we rewrite the last term on the right as the logarithm of a product, we easily obtain

\[
\sum_{p=1}^{\infty} \gamma_p = \lim_{s \to \infty} \left( s - \frac{1}{2} \sum_{q=1}^{s} \frac{1}{q+1} - \ln \left( \frac{(s+1)^2}{s!} \right) \right)
\]

If the Stirling formula is used

\[ s! = \Gamma(s+1) \simeq (s+1)^{s+\frac{1}{2}} e^{-s} - \sqrt{2\pi}, \quad (D.6) \]

we have

\[
\sum_{p=1}^{\infty} \gamma_p = \lim_{s \to \infty} \left\{ s - \frac{1}{2} \sum_{q=1}^{s} \frac{1}{q+1} - \ln \left( \frac{(s+1)^{-\frac{1}{2}}}{e^{-s} - \sqrt{2\pi}} \right) \right\} \\
= \lim_{s \to \infty} \left( \frac{1}{2} \ln(s+1) - \frac{1}{2} \sum_{q=1}^{s} \frac{1}{q+1} - \frac{1}{2} \ln(2\pi) \right) \\
= \frac{1}{2} \left[ \ln(2\pi) - \gamma_1 - \frac{3}{2} \right] \quad (D.7a)
\]

or equivalently

\[
\sum_{p=1}^{\infty} \gamma_p + \frac{1}{2} \gamma_1 = \ln(\sqrt{2\pi}) - \frac{3}{4} = 0.169 \quad (D.7b)
\]
The coefficient $\alpha$ can now be deduced from (D.5a), since
\[
\lim_{s \to \infty} \sum_{q=1}^{s} \left(1 - q \ln \frac{q + 1}{q}\right) = \sum_{p=1}^{\infty} \gamma_p + \lim_{s \to \infty} \sum_{q=1}^{s} \frac{1}{2(q+1)}
\]
Then the summation (31) becomes
\[
\alpha = \lim_{s \to \infty} \sum_{q=1}^{s} \left[ \left(q + \frac{1}{2}\right) \ln \frac{q + 1}{q} - 1 \right] = \lim_{s \to \infty} \sum_{q=1}^{s} \left[ \frac{1}{2} \ln \frac{q + 1}{q} - \frac{1}{2(q+1)} \right] - \sum_{p=1}^{\infty} \gamma_p
\]
and from (D.1) for $p = 1$
\[
\alpha = \frac{1}{4} - \frac{1}{2} \gamma_1 - \sum_{p=1}^{\infty} \gamma_p \quad (D.8)
\]
Finally
\[
\alpha = 1 - \frac{1}{2} \ln(2\pi) = \ln \frac{e}{\sqrt{2\pi}} = 0.0811 \quad (D.9)
\]
and
\[
\frac{1}{2} \gamma_1 + \sum_{p=1}^{\infty} \gamma_p = \frac{1}{4} - \alpha \quad (D.10)
\]

Appendix E

We have seen in equation (37) that the interesting quantity, in order to establish if the growth is stable or unstable, is given by $R(K)$, defined in equation (33) as the part of $\delta A_n$ in phase with the shift $\delta \ell_n$.

Let us call $(\delta A_n)_{a,b,c,...}$ the different terms of $\delta A_n$ and $R_{a,b,c,...}$ the corresponding quantities in $R(K)$. Then, the second term in (22) gives immediately the contribution
\[
R_b = -\frac{F}{2} \frac{L}{\ell + L} \frac{(L - 2aD)}{(D\ell)} \quad (E.1a)
\]
The first term in (22), which is equal to
\[(\delta A_n)_a = -\beta pD \frac{\delta \epsilon_n - \delta \epsilon_{n+1}}{\ell + L}\]
using the equation (28) becomes
\[
(\delta A_n)_a = \epsilon \beta pD \frac{1}{\ell + L} \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k \left( \delta \ell_{n+k-1} - \delta \ell_{n-k} - \delta \ell_{n+k} + \delta \ell_{n+1-k} \right)
\]
and $R$ will gain the quantity
\[
R_a = \frac{\epsilon \beta pD}{\ell + L} \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k \left( 2 \cos(K(k-1)) - 2 \cos(Kk) \right)
= 4 \epsilon \beta pD \sin \left( \frac{\ell k}{2} \right) \frac{1}{\ell^2} \sum_{k=1}^{\infty} C_k \sin \left( \frac{K(2k-1)}{2} \right) \quad (E.1b)
\]
Let us now consider the terms in $\delta A_n$ which depend on the integral of $yU(y)$:

$$
(\delta A_n)_d = \beta F \frac{\int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} yU_n^0(y)dy}{(\ell + L)^2} \delta \ell_n - \beta F \frac{\delta \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} yU_n(y)dy}{\ell + L}
$$
or, using equations (23) and (30)

$$
(\delta A_n)_d = 2\bar{U}\beta F \frac{1 - \frac{1}{2} \ln \left( \frac{x}{a} \right) - \alpha}{(\ell + L)^2} \delta \ell_n
$$

$$
- \bar{U} \beta F \left[ \gamma_1 + \frac{1}{2} - \ln \left( \frac{x}{a} \right) \right] \delta \ell_n + \sum_{k=1}^{\infty} \gamma_k (\delta \ell_{n+k} + \delta \ell_{n-k})
$$

which can be rewritten as

$$
(\delta A_n)_d = \bar{U} \beta F \left[ \frac{2\ell(1 - \alpha)}{(\ell + L)^2} \delta \ell_n + \frac{L \ln \left( \frac{x}{a} \right)}{(\ell + L)^2} \delta \ell_n - \frac{(\gamma_1 + \frac{1}{2}) \delta \ell_n}{\ell + L} - \frac{\sum_{k=1}^{\infty} \gamma_k (\delta \ell_{n+k} + \delta \ell_{n-k})}{\ell + L} \right]
$$

(E.1c)

The corresponding quantity $R_d$ results

$$
R_d = \bar{U} \beta F \left[ \frac{2\ell(1 - \alpha)}{(\ell + L)^2} \delta \ell_n + \frac{L \ln \left( \frac{x}{a} \right)}{(\ell + L)^2} \delta \ell_n - \frac{(\gamma_1 + \frac{1}{2}) \delta \ell_n}{\ell + L} - \frac{2 \sum_{k=1}^{\infty} \gamma_k \cos(Kk)}{\ell + L} \right]
$$

(E.1d)

Let us now turn to the term in (22) involving the integral of $U(y)$

$$
(\delta A_n)_e = -\beta F\ell \left( \frac{2aD}{D''} - L \right) \frac{\delta \int_{-\frac{\ell}{2}}^{\frac{\ell}{2}} U_n(y)dy}{(\ell + L)^2}
$$

If equation (25) is used, $(\delta A_n)_e$ becomes

$$
(\delta A_n)_e = -\beta F \left( \frac{2aD}{D''} - L \right) \bar{U} \sum_{k=1}^{\infty} \left( \frac{1}{k+1} - \frac{1}{k} \right) (\delta \ell_{n+k} - \delta \ell_{n-k})
$$

Since $(\delta \ell_{n+k} - \delta \ell_{n-k}) \propto \sin(Kn - \phi)$, the corresponding contribution to $R$ is zero

$$
R_e = 0.
$$

(E.1e)

The other terms in (22) can be rewritten in the form:

$$
(\delta A_n)_e = -\beta F \left( \frac{L^2}{(\ell + L)^2} U_n^0 \left( \frac{\ell}{2} \right) \delta \ell_n + \frac{\beta F}{2} \left( L - \ell \right) \frac{(L - 2\frac{D\alpha}{D''})^2}{(\ell + L)^3} U_n^0 \left( \frac{\ell}{2} \right) \delta \ell_n
$$

$$
- \beta F \ell \frac{aD \delta U_n \left( \frac{\ell}{2} \right)}{2 D'} \frac{\delta \ell_n}{\ell + L} - \beta F \ell \left( \frac{aD}{D''} \right)^2 \frac{D'}{D''} \left( D' - 1 \right) \frac{\delta U_n \left( \frac{\ell}{2} \right)}{(\ell + L)^2}
$$

$$
- \beta F \ell \frac{aD \delta U_n \left( -\frac{\ell}{2} \right)}{2 D''} \frac{\delta \ell_n}{\ell + L} + \beta F \ell \left( \frac{aD}{D''} \right)^2 \frac{D''}{D'} \left( D'' - 1 \right) \frac{\delta U_n \left( -\frac{\ell}{2} \right)}{(\ell + L)^2}
$$
which can be manipulated using (26a,26b,29) up to obtain

\[
(\delta A_n)_c = \beta F \frac{\bar{U}}{a} \left\{ \ell L^2 + 2(L - \ell) \left[ L \frac{\partial P}{\partial t} - \left( \frac{\partial P}{\partial x} \right)^2 \right] (\ell + L)^3 \right. \\
- \frac{aD\ell \ell + \frac{2aP}{D} \ell}{2D'(\ell + L)^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n-k} - \delta \ell_{n+k-1}) \\
+ \frac{aD\ell \ell + \frac{2aP}{D} \ell}{2D''(\ell + L)^2} \sum_{k=1}^{\infty} C_k (\delta \ell_{n-k+1} - \delta \ell_{n+k}) \left\} 
\]

The insertion of (19) gives for \((\delta A_n)_c\):

\[
(\delta A_n)_c = \beta F \frac{\bar{U}}{a} \left\{ \ell L^2 + 2(L - \ell) \left[ L \frac{\partial P}{\partial t} - \left( \frac{\partial P}{\partial x} \right)^2 \right] \frac{\zeta \cos(Kn - \phi)}{(\ell + L)^3} \right. \\
- \frac{aD\ell \ell + \frac{2aP}{D} \ell}{D'(\ell + L)^2} \sum_{k=1}^{\infty} C_k \sin \left[ K \left( n - \frac{1}{2} \right) - \phi \right] \sin K \left( k - \frac{1}{2} \right) \\
+ \frac{aD\ell \ell + \frac{2aP}{D} \ell}{D''(\ell + L)^2} \sum_{k=1}^{\infty} C_k \sin \left[ K \left( n + \frac{1}{2} \right) - \phi \right] \sin K \left( k - \frac{1}{2} \right) \left\} 
\]

and for \(R_c\)

\[
R_c = \beta F \frac{\bar{U}}{a} \left\{ \ell L^2 + 2(L - \ell) \left[ L \frac{\partial P}{\partial t} - \left( \frac{\partial P}{\partial x} \right)^2 \right] \frac{\zeta \cos(Kn - \phi)}{(\ell + L)^3} \right. \\
+ \frac{L\ell + 4 \left[ L \frac{\partial P}{\partial t} - \left( \frac{\partial P}{\partial x} \right)^2 \right]}{\ell(\ell + L)^2} \sum_{k=1}^{\infty} C_k \sin \left( \frac{K}{2} \right) \sin K \left( k - \frac{1}{2} \right) \left\} 
\]

(E.1f)

All the contributions \(R_{a_1}, \ldots, R_{a_n}\) can be summed up and the result put in the form:

\[
R(K) = R_0 - R_1 \sum_{k=1}^{\infty} \gamma_k \cos(Kk) + R_2 \sin \left( \frac{K}{2} \right) \sum_{k=1}^{\infty} C_k \sin \left[ K \left( k - \frac{1}{2} \right) \right] 
\]

(39)

where \(R_0, R_1, R_2\) have already been given in equations (40).

The two double sums in (39) can be simplified by the following procedure. Let us consider the quantity

\[
S_k = \sum_{p=k}^{\infty} f(p)
\]

where, in our case \(f(p) = \frac{1}{p^2}\) for \(S_k = C_k\) and \(f(p) = \frac{1}{2p^2} + \frac{1}{2(p+1)} - \ln \frac{p+1}{p}\) for \(S_k = \gamma_k\).

Then, we have to calculate the real and imaginary parts of \(F(K)\):

\[
F(K) = \sum_{k=1}^{\infty} S_k e^{i(Kk - \psi)}
\]
\[\sum_{k=1}^{\infty} \sum_{p=k}^{\infty} f(p) e^{i(Kk - \psi)} = \sum_{p=1}^{\infty} f(p) \sum_{k=1}^{p} e^{i(Kk - \psi)} = \sum_{p=1}^{\infty} f(p) \frac{\sin \left( \frac{Kp}{2} \right)}{\sin \left( \frac{K}{2} \right)} e^{i[(p+1)\frac{\phi}{2} - \psi]}\]

For example, for \(S_k = C_k\) and \(\phi = \frac{K}{2}\) we obtain

\[\sum_{k=1}^{\infty} C_k \sin \left( Kk - \frac{K}{2} \right) = \sum_{p=1}^{\infty} \frac{\sin^2 \left( \frac{Kp}{2} \right)}{p^2} \]

which is equation (E.2)

and equation (39) can be rewritten as

\[R(K) = R_0 - R_1 \sum_{k=1}^{\infty} \gamma_k \cos(Kk) + R_2 \sum_{p=1}^{\infty} \frac{\sin^2 \left( \frac{Kp}{2} \right)}{p^2} \]

(E.3)

As mentioned below (40), the stability condition is given by \(R(\pi) < 0\)

\[R(\pi) = R_0 - R_1 \sum_{k=1}^{\infty} (-1)^k \gamma_k + R_2 \sum_{k=1}^{\infty} \frac{1}{(2k-1)^2} < 0 \]

(41)

The second sum is equal to \(\frac{\pi^2}{8}\) [41]. For the first one, some manipulations are necessary:

\[
\sum_{k=1}^{\infty} (-1)^k \gamma_k = -\sum_{p=1}^{\infty} f(p) \sin^2 \left( \frac{p\pi}{2} \right) = -\sum_{p=1}^{\infty} f(2p-1) = \\
= \lim_{s \to \infty} \left[ \ln \left( \frac{2 \cdot 4 \cdot 6 \cdot 8 \cdot \ldots \cdot (2s)}{1 \cdot 3 \cdot 5 \cdot 7 \cdot \ldots \cdot (2s-1)} \right) - \frac{1}{2} \sum_{r=1}^{2s} \frac{1}{r} \right] \\
= \lim_{s \to \infty} \left[ \ln \left( \frac{(2s)!}{(2s)!} \right) - \frac{1}{2} \sum_{r=1}^{2s} \frac{1}{r} \right] = \lim_{s \to \infty} \left[ \ln \left( \frac{(2s)!}{(2s)!} \right) - \frac{1}{2} \ln(2s) \right] - \frac{\gamma}{2} \\
= \frac{1}{2} \ln \left( \frac{\pi}{2} - \gamma \right) = -0.0628
\]

(E.4)

The stability condition (41) can be written as

\[R_0 + \frac{1}{2} R_1 \left( \gamma - \ln \frac{\pi}{2} \right) + \frac{\pi^2}{8} R_2 < 0, \]

(42)

that is to say

\[-\frac{F}{2} \left( \frac{L - aD}{D'} \right)^2 \frac{1 - \left( \frac{D'}{D''} \right)^2}{(\ell + L)^2} + 2\beta F U \ell \frac{1 - \alpha}{(\ell + L)^2} + \beta F U L \left( \frac{\ell}{\alpha} \right) \left( \frac{\ell}{\alpha} + L \right)^2 \]
$\frac{\beta F U}{a(\ell + L)^3} \left[ L \frac{\partial D}{\partial L} - \left( \frac{\partial D}{\partial \sigma} \right)^2 \right] - \frac{\beta F U}{\ell} \ln \frac{\pi}{2} + \pi E D \frac{1 + \sigma}{1 - \sigma} (a \delta \alpha)^2 \frac{1}{\ell^2} \frac{\beta \rho_0}{\ell + L} + \pi^2 \beta F U \frac{L}{\ell(\ell + L)^2} < 0 \quad (E.5)$

If both $\ell, L \gg \frac{aD}{D''}$ the previous formula becomes

$-\frac{F}{2} \frac{L^2}{(\ell + L)^2} + 2\beta F U \frac{1 - \alpha}{(\ell + L)^2} + \beta F U \frac{L \ln \frac{\xi}{a}}{(\ell + L)^2} + \beta F U \frac{\ell L^2}{a(\ell + L)^3}$

$-\beta F U \frac{1}{\ell + L} \ln \frac{\pi}{2} + \pi E D \frac{1 + \sigma}{1 - \sigma} (a \delta \alpha)^2 \frac{1}{\ell^2} \frac{\beta \rho_0}{\ell + L} + \pi^2 \beta F U \frac{L}{8 (\ell + L)^2} < 0 \quad (E.6)$

In the limit $\ell \gg L$, (E.6) reads

$-\frac{F}{2} \frac{L^2}{\ell^2} + 2\beta F U \frac{1 - \alpha}{\ell} + \beta F U \frac{L \ln \frac{\xi}{a}}{\ell^2} + \beta F U \frac{L^2}{a\ell^2}$

$-\beta F U \frac{1}{\ell} \ln \frac{\pi}{2} + \pi E D \frac{1 + \sigma}{1 - \sigma} (a \delta \alpha)^2 \frac{1}{\ell^2} \frac{\beta \rho_0}{\ell + L} + \pi^2 \beta F U \frac{L}{8 \ell^2} < 0 \quad (E.7)$

Since the last term is negligible with respect to the first one, and it results $2(1 - \alpha) - \ln \frac{\pi}{2} = 2 \ln 2$, equation (43) is recovered.

References