On radial stationary solutions to a model of non-equilibrium growth

CARLOS ESCUDERO[1,*], ROBERT HAKL[2,†], IRENEO PERAL[3,‡] and PEDRO J. TORRES[4,§]

[1]*Departamento de Matemáticas & ICMAT (CSIC-UAM-UC3M-UCM),*
Universidad Autónoma de Madrid, E-28049 Madrid, Spain
email: cel@icmat.es
[2]*Institute of Mathematics, AS CR, Žižkova 22, 616 62 Brno, Czech Republic*
[3]*Departamento de Matemáticas, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[4]*Departamento de Matemática Aplicada, Universidad de Granada, E-18071 Granada, Spain*

We present the formal geometric derivation of a non-equilibrium growth model that takes the form of a parabolic partial differential equation. Subsequently, we study its stationary radial solutions by means of variational techniques. Our results depend on the size of a parameter that plays the role of the strength of forcing. For small forcing we prove the existence and multiplicity of solutions to the elliptic problem. We discuss our results in the context of non-equilibrium statistical mechanics.

Key words: non-equilibrium growth; radial solutions; variational methods; boundary value problems

1 Introduction

Epitaxial growth is characterized by the deposition of new material on existing layers of the same material under high vacuum conditions. This technique is used in the semiconductor industry for the growth of thin films [5]. The crystals grown may be composed of a pure chemical element like silicon or germanium, or may either be an alloy like gallium arsenide or indium phosphide. In case of molecular beam epitaxy the deposition takes place at a very slow rate and almost atom by atom. The goal in most situations of thin film growth is growing an ordered crystal structure with flat surface. But in epitaxial growth it is quite usual finding a mounded structure generated along the surface evolution [19]. The actual origin of this mounded structure is to a large extent unknown, although some mechanisms (like energy barriers) have already been proposed. Attempting to perform *ab initio* quantum mechanical calculations in this system is computationally too demanding, which opens the way to the introduction of simplified models. These have been usually developed within the realm of non-equilibrium statistical mechanics, and can be of a discrete probabilistic nature or have the form of a differential equation [5]. Discrete

models usually represent adatoms (the atoms deposited on the surfaces) as occupying lattice sites. They are placed randomly at one such site and then are allowed to move according to some rules that characterize different models. A different modelling possibility is using partial differential equations, which in this field are frequently provided with stochastic forcing terms. In this work we will focus on rigorous and numerical analyses of ordinary differential equations related to models which have been introduced in the context of epitaxial growth. We hope that a systematic mathematical study will contribute to the understanding of this sort of processes, which are relevant both in pure physics and its industrial applications in the long term.

The mathematical description of epitaxial growth uses the function

$$u : \Omega \subset \mathbb{R}^2 \times \mathbb{R}^+ \to \mathbb{R}, \tag{1.1}$$

which describes the height of the growing interface in the spatial point $x \in \Omega \subset \mathbb{R}^2$ at time $t \in \mathbb{R}^+$. Although this theoretical framework can be extended to any spatial dimension N, we will concentrate here on the physical situation, $N = 2$. A basic modelling assumption is of course that u is a univalued function, a fact that holds in a reasonably large number of cases [5]. The macroscopic description of the growing interface is given by a partial differential equation for u, which is usually postulated using phenomenological and symmetry arguments [5, 20]. A prominent example of such a theory is given by the Kardar–Parisi–Zhang equation [17]:

$$u_t = \nu \Delta u + \gamma |\nabla u|^2 + \eta(x, t), \tag{1.2}$$

which has been extensively studied in the physical literature and it is currently being investigated for its interesting mathematical properties [1, 2]. It has been argued however that epitaxial growth processes should be described by some equations coming from a conservation law and, in particular, that the term $|\nabla u|^2$ should not be present in such an equation [5]. To this end, among others, the conservative counterpart of the Kardar–Parisi–Zhang equation was introduced [18, 21, 22]:

$$u_t = -\mu \Delta^2 u + \kappa \Delta |\nabla u|^2 + \zeta(x, t). \tag{1.3}$$

This equation is conservative in the sense that the first moment $\int_\Omega u \, dx$ is constant if the appropriate boundary conditions are used. It can be considered as a higher order counterpart of the Kardar–Parisi–Zhang equation, and it poses as well a number of fundamental mathematical questions [6–8].

In this work, we will focus on a variation of the last equation. Its formal derivation will be presented in the following section. The remainder of this work will be devoted to clarify the analytical properties of the radial stationary solutions to the model under consideration.

2 Formal derivation of the model

Herein, we will adopt a variational formulation of the surface growth equation, which has been postulated as a simple and yet physically relevant way of developing growth models [20]. In order to proceed with our formal derivation, we will assume that the

height function obeys a gradient flow equation with a forcing term

$$u_t = \sqrt{1 + (\nabla u)^2} \left[-\frac{\delta \mathscr{I}(u)}{\delta u} + \xi(x, t) \right]. \tag{2.1}$$

The functional $\mathscr{I}$ denotes a potential that describes the microscopic properties of the interface and, at the macroscopic scale, it is assumed that it can be expressed as a function of the surface mean curvature only [20]

$$\mathscr{I}(u) = \int_\Omega F(H) \sqrt{1 + (\nabla u)^2} \, dx, \tag{2.2}$$

where the presence of the square root terms models growth along the normal to the surface, H denotes the mean curvature and F is an unknown function of H. We will furthermore assume that this function can be expanded in a power series

$$F(H) = K_0 + K_1 H + \frac{K_2}{2} H^2 + \frac{K_3}{6} H^3 + \cdots, \tag{2.3}$$

and subsequently formally apply the small gradient expansion, which assumes $|\nabla u| \ll 1$. This is a classical approximation in this physical context [20] and it is basic in the derivation of the Kardar–Parisi–Zhang equation [17] among others. In the resulting equation, only linear and quadratic terms in the field u and its derivatives are retained, as higher order non-linearities are assumed not to be relevant in the large-scale description of a growing interface [5]. The final result reads

$$u_t = K_0 \Delta u + 2K_1 \det(D^2 u) - K_2 \Delta^2 u - \frac{1}{2} K_3 \Delta (\Delta u)^2 + \xi(x, t), \tag{2.4}$$

which is, as well as (1.3), a conservative equation in the sense that $\int_\Omega u \, dx$ is constant if appropriate boundary conditions are used. We note that powers of the mean curvature higher than the cubic one in expansion (2.3) do not contribute to equation (2.4) as they imply cubic or higher non-linearities of the field u or its derivatives. The terms in equation (2.4) have a clear geometrical meaning. The term proportional to K_0 is the result of the minimization of the zeroth order of the mean curvature, that is, it corresponds to the minimization of the surface area. Its functional form simply reduces to standard diffusion. The term proportional to K_1 comes from the minimization of the mean curvature and actually it is the determinant of the Hessian matrix, which is nothing but the small gradient approximation of the surface Gaussian curvature. So we see that, through the small gradient approximation, *a gradient flow pursuing the minimization of the mean curvature leads to an evolution that favours the growth of the Gaussian curvature.* The term proportional to K_2 comes from the minimization of the squared mean curvature. A functional involving the squared mean curvature is known as Willmore functional and it has its own status within differential geometry [23]. The bilaplacian accompanying K_2 is the corresponding linearized Euler–Lagrange equation of the Willmore functional when looking for flat minimizers, and it has already appeared in the context of mathematical elasticity [16]. Finally, the term proportional to K_3 comes from the minimization of the cubic power of the mean curvature and it involves a non-linear combination of Laplacians

of the field. We note that from a more puristic geometrical viewpoint, one would retain only even powers of the mean curvature in expansion (2.3), which would give rise to a symmetric solution to the corresponding simplification of equation (2.4) (i.e. a solution invariant to the transformation $u \to -u$). However, from a physical viewpoint, we are seeking for a solution to a partial differential equation which represents the interface between two different media (solid structure and vacuum in the present case) so this symmetry is not guaranteed a priori, and we need to retain the odd powers of the mean curvature in expansion (2.3).

For our current purposes, we will focus on the associated stationary problem to a simplification of equation (2.4). Such an equation can be obtained employing well-known facts from the theory of non-equilibrium surface growth. We may invoke classical scaling arguments in the physical literature to disregard the last term as a higher order correction which will not be present in the description of the largest scale properties of the evolving surface [5]. This practically reduces to setting $K_3 = 0$ in equation (2.4). In epitaxial growth, one may phenomenologically set $K_0 = 0$, and we will assume so for the rest of this work. The underlying physical reason is that the diffusion proportional to K_0 is triggered by the effect of gravity on adatoms, and this effect is negligible in the case of epitaxial growth [5]. The resulting equation reads

$$u_t = 2K_1 \det(D^2 u) - K_2 \Delta^2 u + \xi(x, t). \tag{2.5}$$

This partial differential equation can be thought of as being an analogue of equation (1.3). Indeed, it has been shown that this equation might constitute a suitable description of epitaxial growth in the same sense as equation (1.3), and it even shows more intuitive geometric properties [11]. So, at the physical level, we can consider equation (2.5) as a higher order conservative counterpart of the Kardar–Parisi–Zhang equation. At the mathematical level, we can consider it as a sort of Gaussian curvature flow [4,9] which is stabilized by means of a higher order viscosity term. Furthermore, this viscosity term, as we have seen, has a clear geometrical meaning. As we explain above, in this work we are concerned with the stationary version of (2.5), which reads

$$\begin{cases} \Delta^2 u = \det \left(D^2 u \right) + \lambda f, & x \in \Omega \subset \mathbb{R}^2, \\ \text{boundary} \quad \text{conditions}, \end{cases} \tag{2.6}$$

after getting rid of the equation constant parameters by means of a trivial re-scaling of field and coordinates. Our last assumption is that the forcing term $f = f(x)$ is time independent. This type of forcing is known in the physical literature as columnar disorder, and it has an actual experimental meaning within the context of non-equilibrium statistical mechanics [14]. The constant λ is a measure of the intensity of the rate at which new particles are deposited, and for physical reasons we assume $\lambda \geqslant 0$ and $f(x) \geqslant 0$. We will devote our efforts to rigorously and numerically clarify the existence and multiplicity of solutions to this elliptic problem when set on a radially symmetric domain.

3 Radial problems

3.1 Dirichlet boundary conditions

We start looking for radially symmetric solutions of boundary-value problem (2.6) with $f = f(r)$, where r is the radial coordinate, and homogeneous Dirichlet boundary conditions.

We set the problem on the unit disc. That is, we look for solutions of the form $u = \tilde{u}(r)$, where

$$r = \sqrt{x_1^2 + x_2^2}.$$

By means of a direct substitution, we find

$$\frac{1}{r}\left\{ r\left[\frac{1}{r}\left(r\tilde{u}' \right)' \right]' \right\}' = \frac{1}{r}\tilde{u}'\tilde{u}'' + \lambda f(r), \tag{3.1}$$

where $' = d/dr$, and the conditions $\tilde{u}'(0) = 0$, $\tilde{u}(1) = 0$, $\tilde{u}'(1) = 0$, and $\lim_{r \to 0} r u'''(r) = 0$; the first condition imposes the existence of an extremum at the origin and the second and third conditions are the actual boundary conditions. The fourth boundary condition is technical and imposes higher regularity at the origin. If this condition were removed, this would open the possibility of constructing functions $u(r)$ whose second derivative had a peak at the origin. This would in turn imply the presence of a measure at the origin when calculating the fourth derivative of such an $u(r)$, so this type of function cannot be considered as an acceptable solution of (3.1) whenever $f(r)$ is a function. Throughout this section, we will assume $f \in L^1([0,1], r\,dr)$, that is f is an absolutely integrable function against measure $r\,dr$ on the unit interval, and we drop the tilde on $\tilde{u}$ in order to simplify the notation.

Now we proceed to prove the existence of at least two solutions to this boundary-value problem. From now on, we will employ the functional space $\mathring{W}^{2,2}([0,1], r\,dr)$, which is the closure of the space of radially symmetric smooth functions compactly supported inside the unit ball of $\mathbb{R}^2$ with the norm of $W^{2,2}([0,1], r\,dr)$. We will look for solutions to our problem within this functional space.

Lemma 3.1 *Differential equation (3.1) subjected to Dirichlet boundary conditions is the Euler–Lagrange equation of functional*

$$\begin{cases} J_\lambda : \mathring{W}^{2,2}([0,1], r\,dr) \to \mathbb{R} \\ \qquad u \qquad \to J_\lambda(u) = \dfrac{1}{2}\displaystyle\int_0^1 \left[\left(u''\right)^2 + \dfrac{\left(u'\right)^2}{r^2} \right] r\,dr \\ \qquad\qquad\qquad\qquad + \dfrac{1}{6}\displaystyle\int_0^1 \left(u'\right)^3 dr - \lambda \displaystyle\int_0^1 f\,u\,r\,dr. \end{cases} \tag{3.2}$$

Proof We consider Euler first variation of functional (3.2):

$$\left. \frac{d}{dt} J_\lambda(u + t\phi) \right|_{t=0} = \tag{3.3}$$

$$= \int_0^1 \left[u''\phi'' + \frac{u'\phi'}{r^2} \right] r\,dr + \frac{1}{2}\int_0^1 \left(u'\right)^2 \phi'\,dr - \lambda \int_0^1 f\,\phi\,r\,dr$$

$$= \int_0^1 \left(\frac{1}{r}\left\{ r\left[\frac{1}{r}\left(r\,u' \right)' \right]' \right\}' - \frac{1}{r}u'\,u'' - \lambda f \right) \phi\,r\,dr,$$

where the last equality is obtained by means of integration by parts and application

of the boundary conditions, and ϕ belongs to $\mathring{W}^{2,2}([0,1], r\,dr)$ but it is otherwise arbitrary. □

The existence and multiplicity of solutions to our boundary-value problem will be obtained by searching critical points of functional (3.2). We start proving a result concerning the geometry of this functional.

Lemma 3.2 *Functional (3.2) admits the following radial (in the Sobolev space) lower bound:*

$$J_\lambda(u) \geqslant g(||u''||_{L^2(\mu)}), \quad where \quad g(x) = \frac{1}{2}x^2 - C_1 x^3 - C_2 \lambda ||f||_{L^1(\mu)} x, \tag{3.4}$$

$C_1, C_2 > 0$ *and μ stands for the radial two-dimensional measure.*

Proof We have the following chain of inequalities:

$$
\begin{aligned}
J_\lambda(u) &\geqslant \frac{1}{2}\int_0^1 (u'')^2 \, r\,dr + \frac{1}{2}\int_0^1 (u')^2 \, dr + \frac{1}{6}\int_0^1 (u')^3 \, dr - \lambda ||f||_{L^1(\mu)} ||u||_{L^\infty(\mu)} \\
&\geqslant \frac{1}{2}\int_0^1 (u'')^2 \, r\,dr + \frac{1}{2}\int_0^1 (u')^2 \, dr + \frac{1}{6}\int_0^1 (u')^3 \, dr - C\lambda ||f||_{L^1(\mu)} \left[\int_0^1 (u')^2 \, dr\right]^{1/2} \\
&\geqslant \frac{1}{2}\int_0^1 (u'')^2 \, r\,dr - C_1 \left[\int_0^1 (u'')^2 \, r\,dr\right]^{3/2} - C_2 \lambda ||f||_{L^1(\mu)} \left[\int_0^1 (u'')^2 \, r\,dr\right]^{1/2} \\
&= \frac{1}{2}||u''||^2_{L^2(\mu)} - C_1 ||u''||^3_{L^2(\mu)} - C_2 \lambda ||f||_{L^1(\mu)} ||u''||_{L^2(\mu)}, \tag{3.5}
\end{aligned}
$$

where we have used that $r \in [0,1]$ together with Hölder inequality in the first inequality, a one-dimensional Sobolev embedding together with the fact that $||u||_{L^\infty(\mu)} \leqslant ||u||_{L^\infty([0,1])}$ in the second inequality, while in the third inequality we have disregarded a non-negative quantity, we have employed two-dimensional Sobolev embeddings and the auxiliary inequalities

$$\int_0^1 (u')^2 \, dr \leqslant \left(\int_0^1 (u')^6 \, r\,dr\right)^{1/3} \left(\int_0^1 \frac{dr}{\sqrt{r}}\right)^{2/3},$$

$$\int_0^1 (u')^3 \, dr \leqslant \left(\int_0^1 |u'|^9 \, r\,dr\right)^{1/3} \left(\int_0^1 \frac{dr}{\sqrt{r}}\right)^{2/3},$$

resulting from the application of Hölder inequality. □

It is clear that for $0 < \lambda < \lambda_c$ small enough, the function $g(x)$ has a negative local minimum and a positive local maximum. It is also clear that there exist $\varphi, \psi \in \mathring{W}^{2,2}([0,1], r\,dr)$ such that the following properties are fulfilled:

$$\text{(a)} \quad \int_0^1 f\,\varphi\, r\,dr > 0,$$

$$\text{(b)} \qquad \int_0^1 (\psi')^3 \, dr < 0.$$

Therefore, we find $J_\lambda(s\varphi) < 0$ for s small enough and $J_\lambda(s\psi) < 0$ for s large enough. Consequently, the geometric requirements of the *mountain pass* theorem are fulfilled [3]. Now we move on to prove the compactness requirements. We start verifying a local Palais–Smale condition for our functional J_λ.

Definition 3.1 *We say* $\{u_n\}_{n\in\mathbb{N}} \subset \mathring{W}^{2,2}([0,1], r\,dr)$ *is a Palais–Smale sequence for* J_λ *at the level L if the following two properties are fulfilled:*

$$\text{(1)} \qquad J_\lambda(u_n) \to L \qquad when \quad n \to \infty,$$

$$\text{(2)} \qquad J_\lambda'(u_n) \to 0 \qquad in \quad \{\mathring{W}^{2,2}([0,1], r\,dr)\}^*.$$

Now we prove the following compactness result for J_λ:

Proposition 3.1 *Every bounded Palais–Smale sequence for* J_λ *at the level L admits a strongly convergent subsequence in* $\mathring{W}^{2,2}([0,1], r\,dr)$.

Proof Since $\{u_n\}_{n\in\mathbb{N}} \subset \mathring{W}^{2,2}([0,1], r\,dr)$ is bounded we find that, up to passing to a subsequence, the following properties hold:

I. $u_n \rightharpoonup u$ weakly in $\mathring{W}^{2,2}([0,1], r\,dr)$,
II. $u_n' \to u'$ strongly in $L^p([0,1], r\,dr)$ for every $1 \leqslant p < \infty$,
III. $u_n \to u$ uniformly in $[0,1]$.

We write the convergence condition $J_\lambda'(u_n) \to 0$ in $\{\mathring{W}^{2,2}([0,1], r\,dr)\}^*$ as follows:

$$\frac{1}{r}\left\{ r\left[\frac{1}{r}\left(ru_n'\right)' \right]' \right\}' = \frac{1}{r} u_n' u_n'' + \lambda f + w_n,$$

$$u_n \in \mathring{W}^{2,2}([0,1], r\,dr), \qquad w_n \to 0 \qquad in \quad \{\mathring{W}^{2,2}([0,1], r\,dr)\}^*,$$

where the w_n's are the error terms. Now we multiply this equation by $u_n - u$ and integrate over the unit interval with the appropriate measure to get

$$\int_0^1 \left[u_n''(u_n'' - u'') + \frac{u_n'(u_n' - u')}{r^2} \right] r \, dr =$$

$$= \int_0^1 u_n' u_n''(u_n - u) \, dr + \lambda \int_0^1 f(u_n - u) r \, dr + \langle w_n, u_n - u \rangle, \qquad (3.6)$$

after integration by parts on the first line. The three summands on the second line converge to zero in the limit $n \to \infty$ by the above listed properties I (the third summand)

and III (the first and second summands). On the other hand, we have

$$\int_0^1 \left[(u_n'' - u'')\frac{u_n'}{r} - (u_n'' - u'')\left(u'' + \frac{u'}{r}\right) - \frac{u_n' - u'}{r}\left(u'' + \frac{u'}{r}\right) + \frac{u_n' - u'}{r}u_n'' \right] r \, dr \to 0 \quad (3.7)$$

as $n \to \infty$ due to convergence property I and the facts

$$\int_0^1 u_n'' u_n' \, dr = \frac{1}{2} (u_n')^2 \big|_0^1 = 0, \qquad \int_0^1 u'' u' \, dr = \frac{1}{2} (u')^2 \big|_0^1 = 0,$$

due to the boundary conditions. Now, if we sum expression (3.7) to the first line of (3.6), we obtain

$$\int_0^1 |\Delta(u_n - u)|^2 r \, dr \to 0 \qquad \text{as} \quad n \to \infty, \tag{3.8}$$

where $\Delta = \partial_{rr} + r^{-1}\partial_r$ is the radial Laplacian, and thus the desired conclusion. $\qquad \square$

Before moving to the main result of this section, we need one last technical lemma. We introduce the cut-off function Υ which is assumed to be non-increasing, smooth and given by $\Upsilon(t) = 1$ if $t \leqslant \ell$ and $\Upsilon(t) = 0$ if $t \geqslant \ell^*$ for two given real numbers $\ell^* > \ell > 0$.

Lemma 3.3 *The functional defined as*

$$J_\lambda^0(u) = \frac{1}{2} \int_0^1 \left[(u'')^2 + \frac{(u')^2}{r^2} \right] r \, dr + \frac{1}{6} \int_0^1 (u')^3 \, \Upsilon\left(||\Delta u||_2\right) dr - \lambda \int_0^1 f \, u \, r \, dr, \tag{3.9}$$

fulfils the following properties for suitable values of ℓ, ℓ^* and λ:

i. *If $||\Delta u||_2 < \ell$ then $J_\lambda^0 = J_\lambda$.*
ii. *If $J_\lambda^0 < 0$ then $||\Delta u||_2 < \ell$.*
iii. *If $\mathfrak{m} = \inf_{u \in \dot{W}^{2,2}([0,1], r\, dr)} J_\lambda^0(u)$ then J_λ verifies a local Palais–Smale condition at the level $\mathfrak{m}$.*

Proof Property *i* is obvious. For $\lambda_c > 0$ small enough, the lower radial bound g of J_λ attains a maximum at a positive level of 'energy' for $0 < \lambda < \lambda_c$. We denote as x_0 the smaller root of $g(x)$ and as x_m the location of the maximum. Now we choose $\ell = x_0$ and $\ell^* = x_m$. Functional J_λ^0 admits the following radial lower bound:

$$J_\lambda^0(u) \geqslant h(||u''||_{L^2(\mu)}), \quad \text{where} \quad h(x) = \frac{1}{2} x^2 - C_1 x^3 \, \Upsilon(x) - C_2 \, \lambda \, ||f||_{L^1(\mu)} \, x,$$

where C_1 and C_2 are the same constants as in Lemma 3.2. So this functional is bounded from below and positive for $x > x_0$. Thus, property *ii* is fulfilled.

Property *iii* follows from the fact that all Palais–Smale sequences of minimizers of this functional are bounded since $\mathfrak{m} < 0$ together with an application of Proposition 3.1. $\qquad \square$

Now we state the main result of this section.

Theorem 3.1 *There exists a positive real number λ_c such that for $0 < \lambda < \lambda_c$ Dirichlet problem (3.1) has at least two solutions.*

Proof The functional J_λ is well defined in $\mathring{W}^{2,2}([0,1], r\,dr)$ as the Sobolev inequalities immediately reveal. One of the key points of our proof is the application of Ekeland's version of the mountain pass theorem. Our functional fulfils the regularity required to this end, that is, continuity, Gateaux differentiability and weak−∗ continuity of its derivative. We will prove the existence of two solutions to our boundary-value problem by finding two critical points of functional J_λ, one of them is a negative local minimum and another is a positive mountain pass critical point.

We start proving the existence of the local minimum at a negative level of 'energy'. Our proof will be based on the arguments in [13] for solving problems with concave–convex semi-linear non-linearities. For $\lambda_c > 0$ small enough, the lower radial estimate g attains a maximum at a positive level of 'energy' for $0 < \lambda < \lambda_c$. In the proof of Lemma 3.3, we have shown that functional J_λ^0 is bounded from below and positive for $x > x_0$. Accordingly, $\mathfrak{m}$ is a negative critical value of J_λ^0, and thus of J_λ, from where we conclude the existence of a local minimum.

Next, we move to prove the existence of a positive mountain pass critical point. We have already proved the existence of a negative local minimum, which will be denoted as $u^{(0)}$ from now on. We know $J_\lambda(u^{(0)}) < 0$ and we know that there exists $u^{(2)}$ with $\left|\left|[u^{(2)}]''\right|\right|_{L^2(\mu)}$ large enough such that $J_\lambda(u^{(2)}) < J_\lambda(u^{(0)})$. We introduce the set of paths in the Banach space

$$\Theta = \{\theta \in \mathscr{C}([0,1], \mathring{W}^{2,2}([0,1], r\,dr)) | \ \theta(0) = u^{(0)}, \ \theta(1) = u^{(2)}\}.$$

We introduce as well the value

$$\wp = \inf_{\theta \in \Theta} \max_{s \in [0,1]} J_\lambda[\theta(s)],$$

and apply Ekeland's variational principle [10] to prove the existence of a Palais–Smale sequence at it. This means there exists a sequence $\{u_n\}_{n \in \mathbb{N}} \subset \mathring{W}^{2,2}([0,1], r\,dr)$, such that $J_\lambda(u_n) \to \wp$ as $n \to \infty$ and $J'_\lambda(u_n) \to 0$ in $\{\mathring{W}^{2,2}([0,1], r\,dr)\}^*$.

We must now prove that this Palais–Smale sequence is bounded. For $u \in \mathring{W}^{2,2}([0,1], r\,dr)$, the following equality holds:

$$-\int_0^1 u' u'' u\,dr = -\frac{1}{2}(u')^2 u \Big|_0^1 + \frac{1}{2} \int_0^1 (u')^3\,dr = \frac{1}{2} \int_0^1 (u')^3\,dr.$$

We select $\{u_n\}_{n \in \mathbb{N}} \subset \mathring{W}^{2,2}([0,1], r\,dr)$ Palais–Smale sequence for J_λ at level $\wp$ and denote $\langle z_n, u_n \rangle = \langle J'_\lambda(u_n), u_n \rangle$ to find

$$
\begin{aligned}
\wp + o(1) &= J_\lambda(u_n) - \frac{1}{3}\langle J'_\lambda(u_n), u_n \rangle + \frac{1}{3}\langle z_n, u_n \rangle \\
&\geq \frac{1}{6} \int_0^1 \left[(u_n'')^2 + \frac{(u_n')^2}{r^2} \right] r\,dr - \frac{2}{3} C_2\, \lambda\, ||f||_{L^1(\mu)}\, ||u_n''||_{L^2(\mu)} + \frac{1}{3}\langle z_n, u_n \rangle \\
&\geq C\, ||u_n''||_{L^2(\mu)},
\end{aligned}
$$

for a suitable positive constant C, large enough n and small enough λ. In consequence, the sequence is bounded in $\mathring{W}^{2,2}([0,1], r\, dr)$.

We know, by Proposition 3.1, that J_λ satisfy a local Palais–Smale condition at the level $\wp$, so we have $J_\lambda(u^{(1)}) = \lim_{n\to\infty} J_\lambda(u_n) = \wp > 0$. Also, $u^{(1)}$ is a mountain pass critical point, and in consequence $J'_\lambda(u^{(1)}) = 0$, so our differential equation is fulfilled in $\mathring{W}^{2,2}([0,1], r\, dr)$. □

3.2 Navier boundary conditions

In this section, we consider again problem (3.1) on the unit interval but this time subjected to Navier boundary conditions. In the radial setting, these conditions translate to $u(1) = 0$ and $u''(1) + u'(1) = 0$, and we also assume the extremum condition $u'(0) = 0$ at the origin for symmetry reasons. We again assume $f \in L^1([0,1], r\, dr)$.

As in the previous section, we prove the existence of at least two solutions to this boundary-value problem. Our functional framework will be given by the space $\hat{W}^{2,2}([0,1], r\, dr)$, which we define as the intersection $\mathring{W}^{2,2}([0,1], r\, dr) \cap \mathring{W}^{1,2}([0,1], r\, dr)$. We will look for solutions to our problem belonging to this functional space and which fulfil the boundary condition $u''(1) + u'(1) = 0$. Note that, in principle, it is not clear how this condition is fulfilled, because the second derivatives are just square integrable. However, if we consider the linear problem

$$\Delta^2 u = f,$$

$$u = 0, \quad \Delta u = 0,$$

in $\Omega \in \mathbb{R}^2$ open, bounded and provided with a smooth boundary, we find $u \in W^{3,p}(\Omega) \, \forall \, 1 \leqslant p < 2$ for $f \in L^1(\Omega)$. Consequently, $u \in W^{3-1/p,p}(\partial\Omega)$, and we can interpret this boundary condition in the sense of traces.

In this case, the solutions to the differential equation correspond to critical points of a slightly different functional.

Lemma 3.4 *Differential equation (3.1) subjected to Navier boundary conditions is the Euler–Lagrange equation of functional*

$$\begin{cases} I_\lambda : \hat{W}^{2,2}([0,1], r\, dr) \to \mathbb{R} \\ \qquad u \qquad \to I_\lambda(u) = \frac{1}{2}\int_0^1 \left(u'' + \frac{u'}{r}\right)^2 r\, dr + \frac{1}{6}\int_0^1 (u')^3 \, dr - \lambda \int_0^1 f\, u\, r\, dr. \end{cases}$$
(3.10)

Proof We consider Euler first variation of functional (3.10):

$$\left.\frac{d}{dt} I_\lambda(u + t\phi)\right|_{t=0} =$$

$$= \int_0^1 \left(u'' + \frac{u'}{r}\right)\left(\phi'' + \frac{\phi'}{r}\right) r\, dr + \frac{1}{2}\int_0^1 (u')^2 \phi'\, dr - \lambda \int_0^1 f\, \phi\, r\, dr$$

$$= \int_0^1 \left(\frac{1}{r}\left\{r\left[\frac{1}{r}(r\,u')'\right]'\right\}' - \frac{1}{r}u'\,u'' - \lambda f\right)\phi\, r\, dr,$$
(3.11)

where the last equality is obtained by means of integration by parts and application of the boundary conditions, and ϕ belongs to $\hat{W}^{2,2}([0,1], r\,dr)$ but it is otherwise arbitrary.

$\square$

Now we prove a result concerning the geometry of I_λ. First, we note that both J_λ and I_λ are well defined in $W^{2,2}([0,1], r\,dr)$, the space of all functions $u : [0,1] \longrightarrow \mathbb{R}$ whose second derivative (u'') and first derivative normalized by the independent variable (u'/r) are square integrable on the unit interval against measure $r\,dr$, as can be seen by means of a direct application of the Sobolev inequalities.

Lemma 3.5 *Let $u \in W^{2,2}([0,1], r\,dr)$. Then $I_\lambda(u) \geqslant J_\lambda(u)$.*

Proof We want to prove

$$I_\lambda(u) \geqslant \frac{1}{2} \int_0^1 \left[(u'')^2 + \frac{(u')^2}{r^2} \right] r\,dr + \frac{1}{6} \int_0^1 (u')^3 \, dr - \lambda \int_0^1 f\,u\,r\,dr. \qquad (3.12)$$

This follows from

$$\int_0^1 \left(u'' + \frac{u'}{r} \right)^2 r\,dr = \int_0^1 \left[(u'')^2 + \frac{(u')^2}{r^2} + 2u''\frac{u'}{r} \right] r\,dr, \qquad (3.13)$$

and

$$\int_0^1 \left(u''\frac{u'}{r} \right) r\,dr = \int_0^1 u''\,u'\,dr = \frac{1}{2} (u')^2 \Big|_0^1 \geqslant 0, \qquad (3.14)$$

because $u'(0) = 0$.

$\square$

Remark 3.1 *Note that this result implies that the geometry of I_λ corresponds to the same mountain pass shape of J_λ.*

In the following, we will prove the existence of at least two solutions in this case too. The proofs run in parallel to those of the previous section, so we will simply adapt the arguments and write exclusively those parts in which the differences are explicit.

Proposition 3.2 *Every bounded Palais–Smale sequence for I_λ at the level L admits a strongly convergent subsequence in $\hat{W}^{2,2}([0,1], r\,dr)$.*

Proof Since $\{u_n\}_{n\in\mathbb{N}} \subset \hat{W}^{2,2}([0,1], r\,dr)$ is bounded we find that, up to passing to a subsequence, the following properties hold:

I. $u_n \rightharpoonup u$ weakly in $\hat{W}^{2,2}([0,1], r\,dr)$,

II. $u_n' \to u'$ strongly in $L^p([0,1], r\,dr)$ for every $1 \leqslant p < \infty$,

III. $u_n \to u$ uniformly in $[0,1]$.

We write the convergence condition $I'_\lambda(u_n) \to 0$ in $\{\hat{W}^{2,2}([0,1], r\,dr)\}^*$ as follows:

$$\frac{1}{r}\left\{ r\left[\frac{1}{r}\left(ru'_n\right)'\right]'\right\}' = \frac{1}{r}u'_n u''_n + \lambda f + w_n,$$

$$u_n \in \hat{W}^{2,2}([0,1], r\,dr), \quad w_n \to 0 \quad \text{in} \quad \{\hat{W}^{2,2}([0,1], r\,dr)\}^*,$$

where the w_n's are the error terms. Now we multiply this equation by $u_n - u$ and integrate over the unit interval with the appropriate measure to get

$$\int_0^1 \left\{ \left(u''_n + \frac{u'_n}{r}\right)\left[(u_n - u)'' + \frac{(u_n - u)'}{r}\right]\right\} r\,dr$$

$$= \int_0^1 u'_n u''_n (u_n - u)\,dr + \lambda \int_0^1 f(u_n - u) r\,dr + \langle w_n, u_n - u\rangle, \qquad (3.15)$$

after integration by parts on the first line. The three summands on the second line converge to zero in the limit $n \to \infty$ by the above listed properties I (the third summand) and III (the first and second summands). On the other hand, we have

$$\int_0^1 \left\{ \left(u'' + \frac{u'}{r}\right)\left[(u_n - u)'' + \frac{(u_n - u)'}{r}\right]\right\} r\,dr \to 0 \qquad (3.16)$$

as $n \to \infty$ due to convergence property I.

Now, if we subtract expression (3.16) from the first line of (3.15), we obtain

$$\int_0^1 |\Delta(u_n - u)|^2\, r\,dr \to 0 \qquad \text{as} \quad n \to \infty, \qquad (3.17)$$

where $\Delta = \partial_{rr} + r^{-1}\partial_r$ is the radial Laplacian, and thus the desired conclusion. $\qquad \square$

Theorem 3.2 *There exist a positive real number λ_c such that for $0 < \lambda < \lambda_c$ the Navier problem for (3.1) has at least two solutions.*

Proof The functional I_λ is well defined in $\hat{W}^{2,2}([0,1], r\,dr)$ as the Sobolev inequalities immediately reveal. As in the previous section, we will prove the existence of two solutions to our boundary-value problem by finding two critical points of the functional I_λ, one of them is a negative local minimum and another is a positive mountain pass critical point. The proof of the existence of the minimum is identical in both cases, so it will not be reproduced herein.

Therefore, we concentrate in proving the existence of the positive mountain pass critical point. We employ the same minimax technique as in the previous section and the existence of a Palais–Smale sequence $\{u_n\}_{n\in\mathbb{N}} \subset \hat{W}^{2,2}([0,1], r\,dr)$ such that $J_\lambda(u_n) \to \wp$ and $J'_\lambda(u_n) \to 0$ as $n \to \infty$ in $\{\hat{W}^{2,2}([0,1], r\,dr)\}^*$, where $\wp$ is the critical mountain pass level.

We must now prove that this Palais–Smale sequence is bounded. For $u \in \hat{W}^{2,2}([0,1], r\,dr)$, the following equality holds:

$$-\int_0^1 u'\, u''\, u\, dr = -\frac{1}{2}(u')^2\, u \Big|_0^1 + \frac{1}{2}\int_0^1 (u')^3\, dr = \frac{1}{2}\int_0^1 (u')^3\, dr.$$

We select $\{u_n\}_{n\in\mathbb{N}} \subset \hat{W}^{2,2}([0,1], r\,dr)$ Palais–Smale sequence for I_λ at the level $\wp$ and denote $\langle z_n, u_n \rangle = \langle I'_\lambda(u_n), u_n \rangle$ to find

$$
\begin{aligned}
\wp + o(1) &= I_\lambda(u_n) - \frac{1}{3}\langle I'_\lambda(u_n), u_n \rangle + \frac{1}{3}\langle z_n, u_n \rangle \\
&\geq \frac{1}{6}\int_0^1 \left(u''_n + \frac{u'_n}{r} \right)^2 r\, dr - \frac{2}{3} C_2\, \lambda\, \|f\|_{L^1(\mu)}\, \|u''_n\|_{L^2(\mu)} + \frac{1}{3}\langle z_n, u_n \rangle \\
&\geq C\, \|u''_n\|_{L^2(\mu)},
\end{aligned}
$$

for a suitable positive constant C, large enough n and small enough λ. In consequence, the sequence is bounded in $\hat{W}^{2,2}([0,1], r\,dr)$.

We know, by Proposition 3.2, that I_λ satisfies a local Palais–Smale condition at the level $\wp$, so we have $I_\lambda(u_*) = \lim_{n\to\infty} I_\lambda(u_n) = \wp > 0$. Also, u_* is a mountain pass critical point, so $I'_\lambda(u_*) = 0$, and our differential equation is fulfilled in $\hat{W}^{2,2}([0,1], r\,dr)$. $\qquad\square$

4 Numerical results

So far we have proved the existence of at least two solutions to both Dirichlet and Navier problems. In this section, we will clarify the nature of these solutions by means of numerically solving the boundary-value problems employing a shooting method. Our first step will be to transform differential equation (3.1) into a form more suitable for the numerical treatment. To this end and from now on, we will assume $f(r) \equiv 1$.

Integrating once equation (3.1) against measure $r\,dr$ and using boundary condition $\lim_{r\to 0} r u'''(r) = 0$ yields

$$r\left[\frac{1}{r}\left(r\tilde{u}' \right)' \right]' = \frac{1}{2}(\tilde{u}')^2 + \frac{1}{2}\lambda r^2. \tag{4.1}$$

By changing variables $w = r u'$, we find the equation

$$w'' - \frac{1}{r} w' = \frac{1}{2}\frac{w^2}{r^2} + \frac{1}{2}\lambda r^2. \tag{4.2}$$

We have performed some numerical simulations with the final-value problem for this ordinary differential equation using a fourth-order Runge–Kutta method. We have employed the final conditions $w(1) = 0$ and $w'(1)$ arbitrary, which correspond to Dirichlet boundary conditions, to check how big λ could be in order to have solutions. We have solved this problem for $r \in [0,1]$ and looked for solutions such that $\lim_{\epsilon\to 0^+} w(\epsilon)/\epsilon = 0$, which corresponds to the extremum condition $u' = 0$ for the original differential equation. The results of the simulations are represented in Figure 1. One observes that for $\lambda = 0$ there are one trivial and one non-trivial solutions. For $0 < \lambda < \lambda_c$, there are two non-trivial solutions that approach each other for increasing λ. In particular, the smaller of these
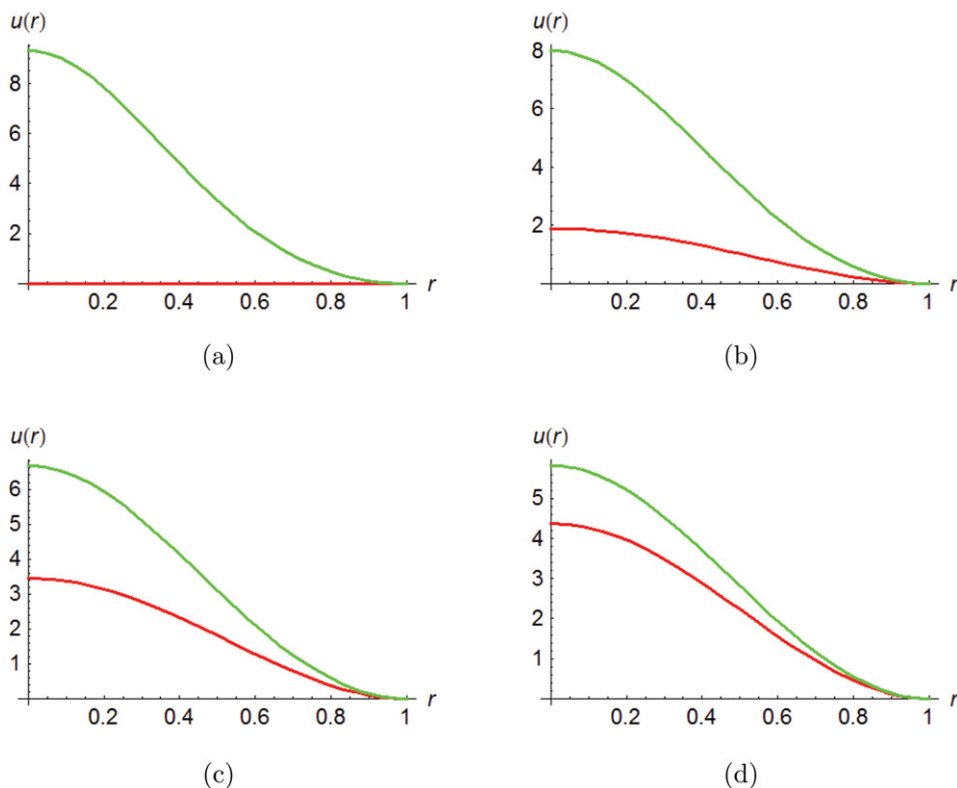
FIGURE 1. (Colour online) Radial solutions corresponding to Dirichlet boundary conditions calculated as explained in the text. Red (lower) line: minimum solution. Green (upper) line: mountain pass solution. Panel (a): $\lambda = 0$; panel (b): $\lambda = 100$; panel (c): $\lambda = 150$; panel (d): $\lambda = 165$.

solutions corresponds to a minimum of the 'energy' functional and the larger solution corresponds to a mountain pass critical point. In all the calculated cases, the minimum solution is strictly smaller than the mountain pass solution for all $0 \leqslant r < 1$. For $\lambda > \lambda_c$, no more solutions were numerically found. The critical value of λ was numerically estimated to be $\lambda_c \approx 169$, and it is achieved when both critical points merge. These numerical experiments suggest that no solutions exist for large enough λ.

Now, we move back to differential equation (3.1) but this time subjected to homogeneous Navier boundary conditions. We start as above, with the equation

$$w'' - \frac{1}{r} w' = \frac{1}{2} \frac{w^2}{r^2} + \frac{1}{2} \lambda r^2, \tag{4.3}$$

and $w(1) = w'(1)$ arbitrary, what corresponds to homogeneous Navier boundary conditions.

Also, in this case we have employed a fourth-order Runge–Kutta method. The results of the numerical experiments are plotted in Figure 2. They run in parallel to the results of the Dirichlet case. We have considered the Navier problem again for $r \in [0, 1]$ and have searched for solutions such that $\lim_{\epsilon \to 0^+} w(\epsilon)/\epsilon = 0$, which corresponds to the extremum condition $u' = 0$ for the original differential equation. Using this shooting method, we
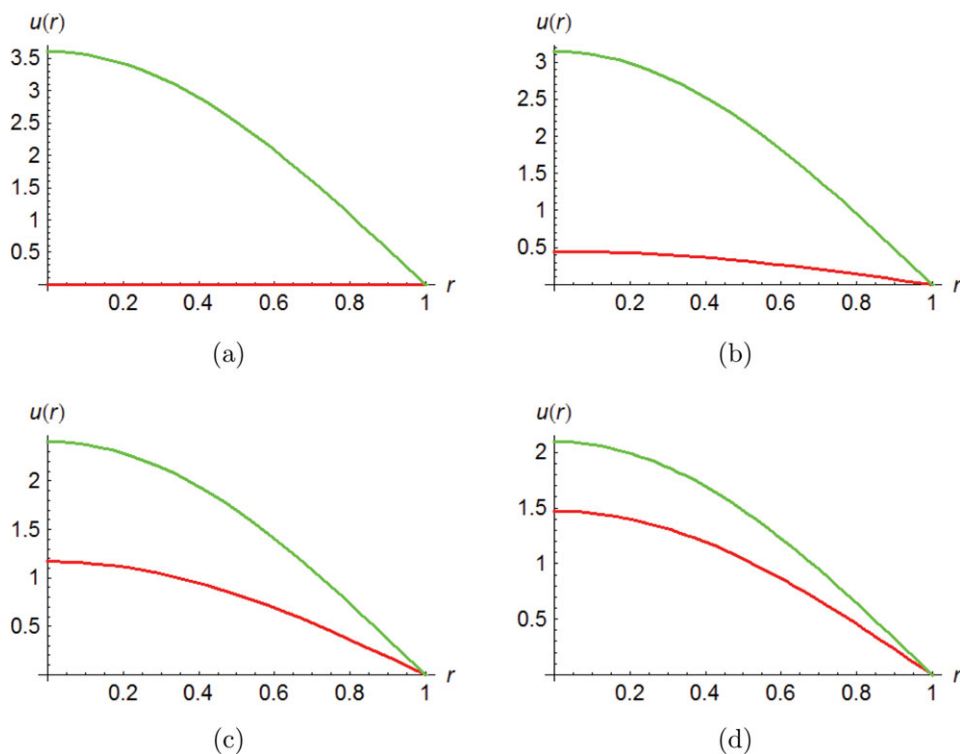
FIGURE 2. (Colour online) Radial solutions corresponding to Navier boundary conditions calculated as explained in the text. Red (lower) line: minimum solution. Green (upper) line: mountain pass solution. Panel (a): $\lambda = 0$; panel (b): $\lambda = 5$; panel (c): $\lambda = 10$; panel (d): $\lambda = 11$.

have found two different solutions which fulfil these requirements. One observes that for $\lambda = 0$ there are one trivial and one non-trivial solutions. For $0 < \lambda < \lambda_c$, there are two non-trivial solutions that approach each other for increasing λ. For $\lambda > \lambda_c$, no more solutions were numerically found. The critical value of λ was numerically estimated to be $\lambda_c \approx 11.34$. Again, the smaller solution corresponds to a minimum of the 'energy' functional and the larger solution corresponds to a mountain pass critical point. In all cases, the minimum solution is strictly smaller than the mountain pass solution for all $0 \leqslant r < 1$.

5 Conclusions and outlook

We have analysed a differential equation appearing in the physical theory of epitaxial growth. We have started formally introducing the corresponding partial differential equation and then we have focused on radial solutions to its stationary counterpart. The resulting equation has been posed in the unit disc in the plane subjected to two different sets of boundary conditions. We have proved the existence of at least two solutions to both boundary-value problems for small enough data. In each problem, we have observed both solutions numerically and identified one of them with the local minimum of our 'energy' functional and another with a mountain pass critical point. Due to the

qualitatively similar results in both cases, the following assertions, and in particular the conjectures, refer to both boundary-value problems. Our numerical simulations revealed that the solutions are ordered in the sense that the one corresponding to the minimum lies strictly below (except for the boundary point $r = 1$) the one corresponding to the mountain pass critical point. We found that the mountain pass solution is nontrivial for $0 \leqslant \lambda < \lambda_c$ and the minimum solution is nontrivial for $0 < \lambda < \lambda_c$ and trivial for $\lambda = 0$. We also proved non-existence of solutions for large values of this parameter and found rigorous bounds for the size of the data separating existence from non-existence, but the proofs will be reported elsewhere [12].

We conjecture that the solution corresponding to the minimum is dynamically stable: if we considered the full evolution problem we would find that this solution is locally stable for it. We also conjecture that the mountain pass solution is dynamically unstable. We have numerically observed both solutions become closer for λ approaching the critical value separating existence from non-existence, so we conjecture that the transition from existence to non-existence as we vary the parameter λ is a saddle-node bifurcation for the corresponding evolution problem. We finally conjecture that there exists a unique solution, that is dynamically unstable, for the critical value of λ, precisely the one that corresponds to the bifurcation threshold.

On the physical side, our results can be interpreted within the theory of non-equilibrium potentials [24]. The evolution problems correspond to gradient flows pursuing the minimization of our 'energy' functionals, which play the role of non-equilibrium potentials. If both forcing term and initial condition are small, the system will evolve towards the equilibrium state. If the forcing were stochastic the equilibrium state would become meta-stable. For a large forcing term, there are no equilibrium states, so the system will keep on evolving forever in a genuine non-equilibrium fashion. In the theory of non-equilibrium growth, in which the forcing is normally assumed stochastic, it is known that these features affect both morphology and dynamics of the evolving interface [5]. In the case of existence of a local minimum, this would imply in turn the existence of transient behaviour, as found in different models of epitaxial growth [15]. Non-existence of this state would mean that the asymptotic state is rapidly achieved. Residence times could be estimated with the help of the theory of non-equilibrium potentials [24]. Our results constitute a first step towards the understanding of these phenomena, although more work is needed in order to get their full understanding.

References

[1] ABDELLAOUI, B., DALL'AGLIO, A. & PERAL, I. (2006) Some remarks on elliptic problems with critical growth in the gradient. *J. Differ. Equ.* **222**, 21–62.

[2] ABDELLAOUI, B., DALL'AGLIO, A. & PERAL, I. (2008) Regularity and nonuniqueness results for parabolic problems arising in some physical models, having natural growth in the gradient. *J. Math. Pure Appl.* **90**, 242–269.

[3] AMBROSETTI, A. & RABINOWITZ, P. H. (1973) Dual variational methods in critical point theory and applications. *J. Funct. Anal.* **14**, 349–381.

[4] ANDREWS, B. (1999) Gauss curvature flow: The fate of the rolling stones. *Invent. Math.* **138**, 151–161.

[5] BARABÁSI, A.-L. & STANLEY, H. E. (1995) *Fractal Concepts in Surface Growth*, Cambridge University Press, Cambridge, UK.

[6] BLÖMKER, D., FLANDOLI, F. & ROMITO, M. (2009) Markovianity and ergodicity for a surface growth PDE. *Ann. Probab.* **37**, 275–313.

[7] BLÖMKER, D. & ROMITO, M. (2009) Regularity and blow-up in a surface growth model. *Dyn. Partial Differ. Equ.* **6**, 227–252.

[8] BLÖMKER, D. & ROMITO, M. (2012) Local existence and uniqueness in the largest critical space for a surface growth model, *Nonlinear Differ. Equ. Appl. (NoDEA)*, **19**, 365–381

[9] CHOW, B. (1991) On Harnack's inequality and entropy for the Gaussian curvature flow. *Comm. Pure Appl. Math.* **44**, 469–483.

[10] EKELAND, I. (1974) On the variational principle. *J. Math. Anal. Appl.* **47**, 324–353.

[11] ESCUDERO, C. (2008) Geometric principles of surface growth. *Phys. Rev. Lett.* **101**, 196102.

[12] ESCUDERO, C., HAKL, R., PERAL, I. & TORRES, P. J. preprint. Existence and nonexistence results for a singular boundary value problem arising in the theory of epitaxial growth (2012). URL: http://www.ugr.es/~ecuadif/files/strong_singular_2part.pdf

[13] GARCÍA AZORERO, J. & PERAL, I. (1991) Multiplicity of solutions for elliptics problems with critical exponents or with a non-symmetric term. *Trans. Am. Math. Soc.* **323**, 877–895.

[14] HALPIN-HEALY, T. & ZHANG, Y.-C. (1995) Kinetic roughening, stochastic growth, directed polymers & all that. *Phys. Rep.* **254**, 215–415.

[15] HASELWANDTER, C. A. & VVEDENSKY, D. D. (2007) Multiscale theory of fluctuating interfaces: Renormalization of atomistic models. *Phys. Rev. Lett.* **98**, 046102.

[16] HORNUNG, P. (2011) Euler–Lagrange equation and regularity for flat minimizers of the Willmore functional. *Comm. Pure Appl. Math.* **64**, 367–441.

[17] KARDAR, M., PARISI, G. & ZHANG, Y.-C. (1986) Dynamic scaling of growing interfaces. *Phys. Rev. Lett.* **56**, 889–892.

[18] LAI, Z.-W. & DAS SARMA, S. (1991) Kinetic growth with surface relaxation: Continuum versus atomistic models. *Phys. Rev. Lett.* **66**, 2348–2351.

[19] LENGEL, G., PHANEUF, R. J., WILLIAMS, E. D., DAS SARMA, S., BEARD, W. & JOHNSON, F. G. (1999) Nonuniversality in mound formation during semiconductor growth. *Phys. Rev.* B **60**, R8469–R8472.

[20] MARSILI, M., MARITAN, A., TOIGO, F. & BANAVAR, J. R. (1996) Stochastic growth equations and reparametrization invariance. *Rev. Mod. Phys.* **68**, 963–983.

[21] SUN, T., GUO, H. & GRANT, M. (1989) Dynamics of driven interfaces with a conservation law. *Phys. Rev.* A **40**, R6763–R6766.

[22] VILLAIN, J. (1991) Continuum models of crystal growth from atomic beams with and without desorption. *J. Phys. I* (France) **1**, 19–42.

[23] WILLMORE, T. J. (1992) A survey on Willmore immersions. In: F. Dillen & L. Verstraelen (editors), *Geometry and Topology of Submanifolds, IV (Proceedings of the Conference on Differential Geometry and Vision, Leuven, Belgium, 1991)*, World Scientific, Hackensack, NJ, pp. 11–16.

[24] WIO, H. S. & DEZA, R. R. (2007) Aspects of stochastic resonance in reaction-diffusion systems: The nonequilibrium-potential approach. *Eur. Phys. J. Spec. Top.* **146**, 111–126.