

## TRUNCATED GRADIENT FLOWS OF THE VAN DER WAALS FREE ENERGY

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ABSTRACT. We employ the Padé approximation to derive a set of new partial differential equations, which can be put forward as possible models for phase transitions in solids. We start from a nonlocal free energy functional, we expand in Taylor series the interface part of this energy, and then consider gradient flows for truncations of the resulting expression. We shall discuss here issues related to the existence and uniqueness of solutions of the newly obtained equations, as well as the convergence of the solutions of these equations to the solution of a nonlocal version of the Allen-Cahn equation.

### 1. INTRODUCTION

Solid-solid phase transitions may be well described by suitable gradient flows of the Ginzburg-Landau free energy functional,

$$E_1(u) = \frac{\gamma}{2} \int_{\Omega} |\nabla u|^2 dx + \int_{\Omega} F(u) dx, \quad (1.1)$$

where  $\Omega$  is a bounded domain in  $\mathbb{R}$ ,  $u(x, t)$  is a suitable order parameter and  $\gamma$  is a measure of strength of intermolecular forces. In many situations, the suitable bulk energy  $F(u)$  has a double well structure. Starting from (1.1) and considering the gradient flow with respect to the  $L^2$ -inner product, one obtains the well-known Allen-Cahn equation,

$$u_t = \gamma \Delta u - f(u). \quad (1.2)$$

Here  $f(u) = F'(u)$  is usually a bistable function. This equation has been used in modelling order parameter non-conserving phenomena, such as transitions between variants of a crystalline substance (see, for example, [1, 7, 8, 9, 21]). For order parameter conserving situations, one has to consider a constrained gradient flow. If one uses the gradient with respect to the  $H^{-1}$ -inner product, one obtains:

$$u_t = -\Delta(\gamma \Delta u - f(u)), \quad (1.3)$$

which is the Cahn-Hilliard equation [8, 16]. The equation (1.3) gives a qualitatively faithful description of spinodal decomposition, of the transition from spinodal to metastable behaviour, as well as of critical nuclei.

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The problem with the Ginzburg-Landau approach (apart from the fact that it fails to give a good quantitative fit to the course of coarsening in a number of situations; see [12] for example) is that it is totally phenomenological. Other approaches exist, all of them more or less starting with the Ising model. Examples are the work of Penrose [17] and equations derived from the free energy written down by van der Waals [22] and advocated by Khachaturyan [13] (see equation (1.4) below).

Gradient flows of the van der Waals free energy (in the non-conserving case) have been studied, among others, by [1, 7, 9, 21]. In particular, the paper [9] sets out the general theory of these (integro-differential) equations; [1] gives a careful derivation of the equations directly from the Ising model and describe stationary solutions, while [7, 21] deal mainly with the lack of coarsening and non-compactness of attractors in the case of sufficiently small  $\gamma$  (this is in stark contrast to the Allen-Cahn situation).

For simplicity, we shall take below  $\Omega = \mathbb{R}$ . The van der Waals free energy is then

$$E_2(u) = \frac{\gamma}{4} \int_{\mathbb{R}} \int_{\mathbb{R}} J(|x-y|)(u(y) - u(x))^2 dy dx + \int_{\mathbb{R}} F(u(x)) dx. \quad (1.4)$$

where  $J(\cdot)$  is an  $L^1(\mathbb{R})$  kernel describing intermolecular interactions (for most of the paper we will have to impose additional restrictions on  $J(\cdot)$ ). The  $L^2$  gradient flow of  $E_2$  is

$$u_t = \gamma \int_{\mathbb{R}} J(|x-y|)(u(y) - u(x)) dy - f(u). \quad (1.5)$$

Note that the linear part of equation (1.5) is a bounded operator; for small  $\gamma$  it is a regular perturbation of the kinetic equation

$$u_t = -f(u), \quad (1.6)$$

while the Cahn-Allen equation equation (1.2) is a singular perturbation of (1.6).

Formally, one can derive the Ginzburg-Landau functional from the van der Waals one by performing a gradient expansion and retaining only the leading term. Trying to retain more than the leading term is, however, fraught with difficulties: as we show below in Section 2, retaining an even number of terms leads to an ill-posed problem, and even in the case of an odd number of terms (considered, e.g. in [2, 3]), it is not clear how semiflows generated by high order parabolic equations are supposed to approximate the flow generated by equation (1.5).

In this paper, motivated by the work of Rosenau [18] and of Slemrod [20], we show that if instead of polynomial approximations we use Padé approximants, we recover a family of equations that, in addition to being in some aspects easier to handle than the original integro-differential equation (1.5), also have the desired well-posedness and convergence properties.

We start by going through the usual gradient expansion scheme, following [3]. Then we derive our new equations based on Padé approximants, we discuss the well-posedness and we prove a convergence property of the solutions to the newly obtained equations.

## 2. TRUNCATION SCHEME

We aim to derive the truncated gradient flows of (1.4) by expanding in Taylor series the term  $(u(y) - u(x))$ , and then truncate to some order the new expression.

Since we are expanding the interface part of the free energy, we shall omit the bulk energy part in the computations below. Thus, consider

$$L(u) = \frac{\gamma}{4} \int_{\mathbb{R}} \int_{\mathbb{R}} J(|x-y|)(u(y) - u(x))^2 dy dx.$$

Below we shall use the notation  $D^k u$  for the  $k$ -th derivative of  $u$ . Setting  $x = \eta + \xi$  and  $y = \xi - \eta$ , we have formally:

$$\begin{aligned} L(u) &= \frac{\gamma}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} J(2|\eta|)[u(\xi - \eta) - u(\xi + \eta)]^2 d\eta d\xi \\ &= 2\gamma \int_{\mathbb{R}} \int_{\mathbb{R}} J(2|\eta|) \left[ \sum_{k=1}^{\infty} \frac{\eta^{2k-1}}{(2k-1)!} D^{2k-1} u(\xi) \right]^2 d\xi d\eta \\ &= 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^{\infty} \frac{\eta^{2k}}{(2k)!} \left[ \int_{\mathbb{R}} \sum_{i=1}^k C_{2k}^{2i-1} D^{2i-1} u(\xi) D^{2k-2i+1} u(\xi) d\xi \right] d\eta, \end{aligned} \quad (2.1)$$

where  $C_{2k}^{2i-1}$  is defined by

$$C_{2k}^{2i-1} = \frac{(2k)!}{(2i-1)!(2k-2i+1)!}, \quad k = 1, 2, \dots; \quad i = 1, 2, \dots, k.$$

We now truncate to the  $n$ th-order the last expression of  $L(u)$  and write

$$L_n(u) = 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^n \frac{\eta^{2k}}{(2k)!} \left[ \int_{\mathbb{R}} \sum_{i=1}^k C_{2k}^{2i-1} D^{2i-1} u(\xi) D^{2k-2i+1} u(\xi) d\xi \right] d\eta.$$

Again, proceeding formally, we compute the  $L^2$ -gradient flow of the truncated free energy  $E_n(u)$ , where

$$E_n(u) = L_n(u) + \int_{\mathbb{R}} F(u(x)) dx.$$

We have

$$\begin{aligned} \left\langle \frac{\delta E_n(u)}{\delta u}, v \right\rangle &= \frac{d}{d\theta} E_n(u + \theta v)|_{\theta=0} \\ &= 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^n \frac{\eta^{2k}}{(2k)!} \left\{ \sum_{i=1}^k C_{2k}^{2i-1} \int_{\mathbb{R}} [D^{2i-1} u(\xi) D^{2k-2i+1} v(\xi) \right. \\ &\quad \left. + D^{2i-1} v(\xi) D^{2k-2i+1} u(\xi)] d\xi \right\} d\eta + \int_{\mathbb{R}} f(u(\xi)) v(\xi) d\xi \\ &= 2\gamma \int_{\mathbb{R}} J(2|\eta|) \sum_{k=1}^n \frac{\eta^{2k}}{(2k)!} \left\{ \sum_{i=1}^k C_{2k}^{2i-1} \int_{\mathbb{R}} [(-1)^{2k-2i+1} D^{2k} u(\xi) \right. \\ &\quad \left. + (-1)^{2i-1} D^{2k} u(\xi)] v(\xi) d\xi \right\} d\eta + \int_{\mathbb{R}} f(u(\xi)) v(\xi) d\xi \\ &= -\gamma \int_{\mathbb{R}} \left\{ \sum_{k=1}^n \left[ \frac{2^{2k+1}}{(2k)!} \int_{\mathbb{R}} J(2|\eta|) \eta^{2k} d\eta \right] D^{2k} u(\xi) - f(u(\xi)) \right\} v(\xi) d\xi \\ &= -\gamma \int_{\mathbb{R}} \left\{ \sum_{k=1}^n \rho_{2k} D^{2k} u(\xi) - f(u(\xi)) \right\} v(\xi) d\xi, \quad \text{for all } v \in L^2(\Omega), \end{aligned} \quad (2.2)$$

where  $\langle \cdot, \cdot \rangle$  is the  $L^2$  inner product and  $\rho_{2k}$  is the non-negative quantity

$$\rho_{2k} = \frac{2^{2k+1}}{(2k)!} \int_{\mathbb{R}} J(2|\eta|)\eta^{2k} d\eta = \frac{1}{(2k)!} \int_{\mathbb{R}} J(|z|)z^{2k} dz, \quad k = 1, 2, \dots \quad (2.3)$$

Note that in (2.2) we used integration by parts, and homogeneous boundary conditions for the derivatives of  $u$  of any order. For the infinite series to be at least formally defined we must assume that all the moments  $\rho_{2k}$  of  $J(\cdot)$  are finite. Thus, the  $L^2$ -gradient flow derived using  $E_n$  is

$$\frac{\partial u}{\partial t}(x, t) = \gamma \sum_{k=1}^n \rho_{2k} D^{2k} u(x, t) - f(u(x, t)), \quad x \in \mathbb{R}. \quad (2.4)$$

Note that we can also derive formally the  $L^2$ -gradient flow of the expanded free energy (2.1). This is

$$\frac{\partial u}{\partial t} = \gamma \sum_{k=1}^{\infty} \rho_{2k} D^{2k} u - f(u), \quad (2.5)$$

which can be written in the form

$$\frac{\partial u}{\partial t} = \gamma \int_{\mathbb{R}} J(|z|) \cosh(zD)(u) dz - f(u), \quad x \in \mathbb{R},$$

which is reminiscent of equations derived in [19]. By  $\cosh(zD)$  we have defined the differential operator

$$\cosh(zD)(u) = \frac{1}{(2k)!} \sum_{k=1}^{\infty} z^{2k} D^{2k} u.$$

The symbol of this operator is then

$$\cos(z\xi) = \frac{1}{(2k)!} \sum_{k=1}^{\infty} (-1)^k z^{2k} \xi^{2k}.$$

As a remark, we note that an easier (but also formal) way of obtaining equation (2.5) is to observe that the symbol of the integral operator  $A$ , such that

$$Au(x) = \int_{\mathbb{R}} J(|x-y|)(u(y) - u(x))dy,$$

is given by

$$\mathcal{S}(A)(k) = \int_{\mathbb{R}} J(w)(\cos(kw) - 1)dw, \quad (2.6)$$

then one can expand  $(\cos(kw) - 1)$  in Taylor series and integrate term by term the resulting expression. Let us now define the operator  $\tilde{A}_n u = \sum_{k=1}^n \rho_{2k} D^{2k} u$ , and for each  $n \in \mathbb{N}$  consider the following initial value problem in  $H^{2n}(\mathbb{R})$ :

$$\begin{aligned} u_t &= \gamma \tilde{A}_n u - f(u), \quad (x, t) \in \mathbb{R} \times (0, \infty), \\ u(0) &= u_0. \end{aligned} \quad (2.7)$$

Well-posedness of these problems is not obvious. If  $J(\cdot) \geq 0$  and  $n$  is an even number, these problems are not well-posed in positive time. Clearly, if  $n$  is an odd number the problems (2.7) for  $n$  are not well-posed in negative time (various aspects of (2.7) for  $n$  odd have been considered in [2, 3]). This is to be expected, as we are trying to approximate the flow generated by a bounded operator by parabolic

semiflows. If the usual assumption of nonnegativity of  $J(\cdot)$  (which in certain cases does not have any physical basis) is not imposed, taking polynomial truncations becomes even more contentious. We note that the limit as  $n \rightarrow \infty$  of (2.7) has been considered by Dubinskii [6].

In the following, we will approximate the flow generated by (1.5) by taking operator Padé approximants of (2.7).

Let  $\mathcal{S}(\tilde{A}_{2n})$  be the symbol of the operator  $\tilde{A}_{2n}$  (a polynomial of degree  $4n$ ). If  $q_{2n}/r_{2n}$  is the  $[2n/2n]$  Padé approximant of  $\mathcal{S}(\tilde{A}_{2n})$ , (where  $p_{2n}, q_{2n}$  are polynomials of degree  $2n$ ), then we consider the differential operators  $R_n$  and  $Q_n$  of order  $2n$ , such that their symbols are  $q_{2n}$  and  $r_{2n}$ , respectively. In this way, the truncation to degree  $2n$  of the symbol of  $\tilde{A}_{2n}R_n$  is the symbol of  $Q_n$ . For each  $n \in \mathbb{N}$  we define the operator

$$A_n = Q_n R_n^{-1} \quad (2.8)$$

acting on  $L^2(\mathbb{R})$ , which is a  $[2n/2n]$  Padé-type approximant of the operator

$$\tilde{A}_\infty = \sum_{k=1}^{\infty} \rho_{2k} D^{2k} u.$$

Instead of (2.7), we shall consider now the problem,

$$\begin{aligned} u_t &= \gamma A_n u - f(u), \quad (x, t) \in \mathbb{R} \times (0, \infty), \\ u(0) &= u_0. \end{aligned} \quad (2.9)$$

Note the nice commutativity property:  $R_n Q_n = Q_n R_n$  on smooth enough functions (usual property of differential operators with constant coefficients). Thus, we can rewrite the equation

$$u_t + f(u) = Q_n R_n^{-1} u$$

as

$$R_n(u_t + f(u)) = Q_n u.$$

When  $n = 1$ , problem (2.9) turns out to be the initial value problem

$$\left( \rho_2 I - \rho_4 \frac{\partial^2}{\partial x^2} \right) (u_t + f(u)) = \gamma \rho_2^2 \frac{\partial^2 u}{\partial x^2}, \quad x \in \mathbb{R}, \quad (2.10)$$

where  $I$  is the identity operator.

The Cahn-Hilliard equation and the viscous diffusion equation [14] can easily be derived from the conserved order parameter version of equation (1.5), which is (see [21]):

$$u_t = \gamma \int_{\mathbb{R}} J(|x - y|) (Au(x, t) - Au(y, t) - f(u(x, t)) + f(u(y, t))) dx dy. \quad (2.11)$$

After the change of variables and expanding in Taylor series, one obtains

$$u_t = -\gamma \tilde{A}_\infty \circ \tilde{A}_\infty u + \tilde{A}_\infty f(u) \quad (2.12)$$

Truncating at the first order term and scaling time, one obtains the Cahn-Hilliard equation in the scalar form,

$$u_t = \frac{\partial^2}{\partial x^2} \left( f(u) - \gamma \rho_2 \frac{\partial^2 u}{\partial x^2} \right).$$

Setting  $\gamma = 0$  in (2.12) and taking the  $[2/2]$  Padé approximant leads to

$$\left( \rho_2 I - \rho_4 \frac{\partial^2}{\partial x^2} \right) u_t = \gamma \rho_2^2 \frac{\partial^2}{\partial x^2} f(u),$$

which was analyzed in [14] in an  $L^\infty(\mathbb{R})$  setting.

### 3. WELL-POSEDNESS AND CONVERGENCE

Clearly, for each  $n \in \mathbb{N}$ , the operator  $A_n$  defined by (2.8) is a linear operator, since both  $Q_n$  and  $R_n$  are linear and the inverse of a linear operator is linear. Since the symbol of  $A$  (equation (2.6)) is a bounded function from  $\mathbb{R}$  into  $\mathbb{R}$ , so are the symbols of  $A_n$ ,  $n \in \mathbb{N}$ . Therefore, by applying the Plancherel formula in the form

$$\|A_n u\|_2 = \|\widehat{A_n u}\|_2 = \|\mathcal{S}(A_n)\widehat{u}\|_2,$$

where  $\widehat{u}$  is the Fourier transform of  $u \in L^2(\mathbb{R})$ , we see that  $A_n$  are bounded operators in  $L^2(\mathbb{R})$ . Furthermore, it is not hard to show that if  $J(\cdot) \geq 0$  the symbol of  $A_n$  is negative for each  $n$ .

We now restrict ourselves to the space  $\{u \in L^2(\mathbb{R}); \text{supp } u = \Omega\}$ , where  $\Omega$  is a bounded domain in  $\mathbb{R}$ , and for each  $n \in \mathbb{N}$  we study the following initial-value problem

$$\begin{aligned} u_t &= \gamma A_n u - f(u), & (x, t) \in \Omega \times (0, \infty), \\ u(0) &= u_0. \end{aligned} \tag{3.1}$$

We would like to prove that this problem generates a flow on a forward-invariant subset of  $L^2(\Omega)$ , which contains all the steady state patterns. Here we are guided by the function-theoretic setting in [10]. Let

$$Z = L^2(\Omega) \cap \{|u(x)| \leq 1 \text{ a.e. in } \Omega\}. \tag{3.2}$$

Then by Theorem 2.16 of Hoh [11], which builds on the work of Corrège, the negativity of symbols of  $A_n$  implies that  $Z$  is forward-invariant under the flow generated by (3.1); for (1.5) this result has been proved in [9] and used extensively in [7].

We make the following assumptions:

- (A1)  $J(\cdot) \geq 0$ ;  $J \in L^1(\mathbb{R})$  and there exists  $\alpha > 0$  such that  $\int_{\mathbb{R}} J(x)e^{\alpha|x|} dx < \infty$ ;
- (A2) the function  $f : Z \rightarrow Z$  is locally Lipschitz continuous.

Note that (A1) assures that all the coefficients  $\rho_{2k}$ ,  $k \in \mathbb{N}$ , are defined and positive, and that the operator  $A_n$  is defined for each  $n \in \mathbb{N}$ .

For a fixed  $n \in \mathbb{N}$ , we say that a function  $u : [0, T) \rightarrow L^2(\Omega)$  is a (*classical*) solution of (3.1) on  $[0, T)$  if  $u$  is continuous on  $[0, T)$ , continuously differentiable on  $(0, T)$ , and (3.1) is satisfied on  $[0, T)$ . We have:

**Theorem 3.1.** *Suppose that the hypotheses (A1) and (A2) are satisfied. Then for each  $u_0 \in Z$ ,  $n \in \mathbb{N}$ , the initial-value problem (3.1) has a unique global solution  $u_n \in C([0, \infty) \times Z)$ . Moreover, for each  $n \in \mathbb{N}$  the mapping  $u_0 \rightarrow u_n$  is continuous in  $L^2(\Omega)$ .*

*Proof.* The theory of Lipschitz perturbations of linear evolution equations (see Pazy [15]) assures the existence and uniqueness of a local solution  $u_{n_0}(x, t, u_0)$ , defined on a maximal interval of existence  $[0, \tau^{n_0})$  (with  $\tau^{n_0}$  depending on  $\|u_0\|_2$ ), and also the continuity of  $u_{n_0}$  with respect to the initial condition. Moreover, if  $\tau^{n_0} < \infty$ , then  $\lim_{t \nearrow \tau^{n_0}} \|u(t)\|_2 = \infty$ , which is not possible by the forward invariance of  $Z$ .  $\square$

For each  $n \in \mathbb{N}$ , we denote by  $\{T_n(t) : Z \rightarrow Z, t \geq 0\}$  the continuous semigroup of bounded nonlinear operators

$$T_n(t)u_0 = u_n(t; u_0), \quad t \geq 0.$$

Also, let  $\{T(t) : Z \rightarrow Z, t \geq 0\}$  be the continuous semigroup of bounded nonlinear operators generated by (1.5).

We would like now to show that solutions to (3.1) with  $u(x, 0)$  given, converge in the  $L^2(\Omega)$ -norm to solutions to (1.5) with the same initial data, as  $n \rightarrow \infty$ . In order to prove this, we will use the following lemma:

**Lemma 3.2.** *If  $X$  is a Banach space and the sequence  $\{w_n, n \in \mathbb{N}\} \subset C([0, T]; X)$  converges to  $w$  in the sense of the norm of  $C([0, T]; X)$ , then*

$$\lim_{n \rightarrow \infty} \int_0^T w_n(r) dr = \int_0^T w(r) dr, \text{ in the } X \text{ norm.} \quad (3.3)$$

For a proof of the above lemma, see [4, Theorem 3.3]. We can now prove the following approximation result:

**Theorem 3.3.** *For every  $u_0 \in Z$  and each  $t > 0$ , we have that*

$$\|u_n(t; u_0) - u(t; u_0)\|_2 \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (3.4)$$

*Proof.* Denote by  $\{S(t); t \geq 0\}$  and  $\{S_n(t); t \geq 0\}$  the linear continuous semigroups generated by the linear continuous operators  $A$  and  $A_n$  ( $n \in \mathbb{N}$ ), respectively. Since these semigroups are bounded, we can find some positive constants  $M$  and  $M_n$  ( $n \in \mathbb{N}$ ) so that  $\|S(t)\|_2 \leq M$  and  $\|S_n(t)\|_2 \leq M_n$  ( $n \in \mathbb{N}$ ). If we let  $g(u) = -f(u)$ , then the solutions of (1.5) and, respectively, (3.1) can be written in the form

$$\begin{aligned} u(t; u_0) &= S(t)u_0 + \int_0^t S(t-s)g(u(s)) ds, \quad t \geq 0; \\ u_n(t; u_0) &= S_n(t)u_0 + \int_0^t S_n(t-s)g(u_n(s)) ds, \quad t \geq 0, n \in \mathbb{N}. \end{aligned}$$

The function  $g$  is locally Lipschitz-continuous on  $Z$ , hence for every positive constant  $c$  there is a constant  $L_c > 0$  such that

$$\|g(u) - g(v)\|_2 \leq L_c \|u - v\|_2$$

holds for all  $u, v \in Z$  with  $\|u\|_2 \leq c$ ,  $\|v\|_2 \leq c$ . Since  $T$  and  $T_n, n \in \mathbb{N}$ , are bounded semigroups in  $Z$ , we can choose  $c$  to be the common  $L^2$ -upper bound, and thus for all  $t > 0$ , we have

$$\begin{aligned} &\|u_n(t) - u(t)\|_2 \\ &\leq \|S_n(t)u_0 - S(t)u_0\|_2 + \int_0^t \|S_n(t-s)g(u_n(s)) - S(t-s)g(u(s))\|_2 ds \\ &\leq \|[S_n(t) - S(t)]u_0\|_2 + \int_0^t \|[S_n(t-s) - S(t-s)]g(u(s))\|_2 ds \\ &\quad + \int_0^t \|S_n(t-s)g(u_n(s)) - S_n(t-s)g(u(s))\|_2 ds \\ &\leq \|[S_n(t) - S(t)]u_0\|_2 + \int_0^t \|[S_n(t-s) - S(t-s)]g(u(s))\|_2 ds \\ &\quad + M_n L_c \int_0^t \|u_n(s) - u(s)\|_2 ds, \end{aligned}$$

for all  $n \in \mathbb{N}$ . We can rewrite the last inequality as

$$\begin{aligned} & \frac{d}{dt} \left\{ e^{-M_n L_\omega T} \int_0^t \|u_n(s) - u(s)\| ds \right\} \\ & \leq e^{-M_n L_\omega T} \left\{ \| [S_n(t) - S(t)] u_0 \|_2 + \int_0^t \| [S_n(t-s) - S(t-s)] g(u(s)) \|_2 ds \right\}, \end{aligned}$$

for all  $n \in \mathbb{N}$ . Then, using the above Lemma, the convergence (3.4) is proved if for all  $h \in L^2(\Omega)$  we have

$$\|S_n(t)h - S(t)h\|_2 \rightarrow 0, \quad \text{as } n \rightarrow \infty. \quad (3.5)$$

By the Trotter approximation theorem [15], in order to have (3.5) it suffices to prove the following convergence in the  $L^2(\Omega)$  norm, for the corresponding resolvents:

$$\text{For every } h \in L^2(\Omega) \text{ and some } \lambda > 0, R(\lambda, A_n)h \rightarrow R(\lambda, A)h \text{ as } n \rightarrow \infty, \quad (3.6)$$

where  $R(\lambda, A) = (\lambda I - A)^{-1}$  and  $R(\lambda, A_n) = (\lambda I - A_n)^{-1}$ ,  $n \in \mathbb{N}$ . Since  $A$  and  $A_n$  ( $n \in \mathbb{N}$ ) are infinitesimal generators of the uniformly continuous semigroups  $\{S(t), t \geq 0\}$  and, respectively,  $\{S_n(t), t \geq 0\}$  ( $n \in \mathbb{N}$ ), then the resolvent sets  $\rho(A)$  and  $\rho(A_n)$  ( $n \in \mathbb{N}$ ) contain  $(0, \infty)$  and

$$\|R(\lambda, A)\|_2 \leq M/\lambda, \|R(\lambda, A_n)\|_2 \leq M_n/\lambda \quad \text{for } \lambda > 0, n = 1, 2, \dots$$

We have then

$$\begin{aligned} \|R(\lambda, A_n)h - R(\lambda, A)h\|_2 &= \|R(\lambda, A_n)\{(\lambda I - A) - (\lambda I - A_n)\}R(\lambda, A)h\|_2 \\ &= \|R(\lambda, A_n)[A_n - A]R(\lambda, A)h\|_2 \\ &\leq \frac{M_n}{\lambda} \| [A_n - A]R(\lambda, A)h \|_2, \quad (\lambda > 0) \end{aligned} \quad (3.7)$$

for all  $h \in L^2(\Omega)$ . On the other side, for each  $n \in \mathbb{N}$  the symbol  $\mathcal{S}(A_n)$  is the  $[2n/2n]$  Padé approximant of  $\mathcal{S}(A)$ . This fact and the Plancherel formula implies

$$\begin{aligned} \|(A_n - A)\xi\|_2 &= \|\mathcal{F}[(A_n - A)\xi]\|_2 \\ &= \|[\mathcal{S}(A_n) - \mathcal{S}(A)]\mathcal{F}\xi\|_2 \\ &\leq \|\mathcal{S}(A_n) - \mathcal{S}(A)\|_2 \|\xi\|_2 \rightarrow 0, \end{aligned} \quad (3.8)$$

as  $n \rightarrow \infty$  for all  $\xi \in L^2(\mathbb{R})$ , where  $\mathcal{F}\xi$  denotes the Fourier transform. Now (3.8) and (3.7) imply (3.6), and this completes the proof.  $\square$

**3.1. Conclusion.** By expanding the nonlocal term in the expression of the free energy (1.4) in Taylor series and truncating the result, one ends up with equations which are not always well-posed, the well-posedness depending on the order of truncation and the direction of time chosen. It is not clear whether the solutions to the unbounded flows can in any sense approximate the solution to the bounded flow given by (1.5). In this paper we proposed a set of new equations, which can be put forward as possible models for phase transitions in solids. (Our method of proof relies on having  $J(\cdot) \geq 0$ , which is a reasonable assumption to make in this context.) By using Padé approximation, we approximated the flow generated by (1.5) by some bounded flows. The new equations have the advantage of being well-posed for all orders of the Padé approximation.



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