Discrete Free Energy Functionals for Elastic Materials with Phase Change

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Summary. We discuss two different approaches related to Γ-limits of free energy functionals. The first gives an example of how symmetry breaking may occur on the atomistic level, the second aims at deriving a general analytic theory for elasticity on the lattice scale that does not depend on an explicitly chosen reference system.

1 Introduction

The analysis of the mechanical properties of crystals gives rise to internal energies that are connected to the geometry of the considered crystal and are often linked to properties of the atomistic scale as explained in [CK88] and [JF00]. Applications to this theory include among others fatigue phenomena and fracture mechanics. In the past, various attempts were made to develop a mathematically rigid theory. In particular we want to mention [Bal77], [CLL98], [AO05], [OP99], [FT02] and [Tru96]. Nevertheless, up to now, the relationship between macroscopic and atomistic scale is not completely understood.

Here we contribute to this topic. The text is subdivided into two parts. The first gives a simple example where symmetry breaking occurs in the Γ-limit of a one-dimensional monatomic chain when the interatomic distance vanishes. Effects similar to the one presented in this first part may also show to be relevant for numerical approximation schemes where in certain cases a competition between elastic energy and surface energy leads to wrong numerical solutions, see [Ble06].

The second line of investigation is the use of many-body Hamiltonians of Kac type to describe elastic deformations, phase changes and eventually plastic deformations of a domain $\Omega \subset \mathbb{R}^n$ without postulating a reference configuration on the particle level. It is interesting to compare this ansatz to [AO05], where a theory based on algebraic topology is developed.

One of the aims is to make a connection with the existing theory on linear elastic dislocations, see [TK76], [Mer79], [CC*97], [BC05].

2 Phase transitions with symmetry breaking

2.1 The energy functional

For given length $L > 0$, let $\Omega := (0, L) \subset \mathbb{R}$ be a domain that contains a regular monatomic chain.

We suppose that the undeformed discrete reference configuration of Ω is given by a system of $n+1$ atoms with equal distance located at points $R_i^n \in \mathbb{R}$,

$$R_i^n := ih^n \quad 0 \le i \le n.$$

Here, the setting $h^n := L/n$ defines for given number $n \in \mathbb{N}$ the interatomic distance. The limit $n \to \infty$ corresponds to $h^n \searrow 0$. The superscript n is always used to indicate the dependence on the number of subdivisions.

By $\widehat{R}_i^n$, $0 \le i \le n$ we denote the position of atom i after the deformation. Finally, by u_i^n, $0 \le i \le n$ we denote the two-dimensional displacement vector of atom i, given by the relationship

$$u_i^n = \widehat{R}_i^n - R_i^n, \quad 0 \le i \le n.$$

For given deformations $\{u_i^n\}_{0 \le i \le n}$ we introduce the abbreviations

$$p_i^n := \frac{u_{i+1}^n - u_i^n}{h^n}$$

and for shortness the numbers $s_1 := 1$, $s_2 := 2$ and $s_3 := \frac{1}{2}$.

We will study the behaviour of the following energy functional.

$$W^n(u^n) := \begin{cases} +\infty & \text{if } p_i^n = 0 \text{ for some } i, \\ \sum_{k=1}^3 W_k^n(u^n) & \text{else} \end{cases}$$

where

$$W_1^n(u^n) := \sum_{i=0}^{n-2} (h^n)^{-\alpha} \prod_{k=1}^{3} \Big| s_k - \frac{p_{i+1}^n}{p_i^n} \Big|^2, \qquad W_2^n(u^n) := \sum_{i=0}^{n-3} \Big| 1 - \frac{p_{i+2}^n}{p_i^n} \Big|^2,$$

$$W_3^n(u^n) := h^n \sum_{i=0}^{n-2} \Big[\Big(\frac{p_i^n + p_{i+1}^n}{2} - \alpha_1 \Big)^2 \beta_i^n + \Big(\frac{p_i^n + p_{i+1}^n}{2} - \alpha_2 \Big)^2 \gamma_i^n \Big]$$

and

$$\beta_i^n := \Big[1 - (h^n)^{-\alpha} \Big| 1 - \frac{p_{i+1}^n}{p_i^n} \Big|^2 \Big]_+, \gamma_i^n := \Big[1 - (h^n)^{-\alpha} \Big| 2 - \frac{p_{i+1}^n}{p_i^n} \Big|^2 \Big| \frac{1}{2} - \frac{p_{i+1}^n}{p_i^n} \Big|^2 \Big]_+.$$

Here, $0 < \alpha < 1$ and $[x]_+ = x$ for $x \geq 0$ and $[x]_+ = 0$ for $x < 0$.

The concept behind this ansatz is the following. A minimiser of W_1^n either fulfils $p_{i+1}^n \simeq p_i^n$ which specifies one lattice order that is in the sequel referred to as Phase 1, or $p_{i+1}^n \simeq 2p_i^n$ resp. $p_{i+1}^n \simeq \frac{1}{2}p_i^n$ which characterises Phase 2.

W_2^n represents a surface energy. It counts(and limits) the number of transitions between the two phases, as within a phase one asymptotically has $p_{i+2}^n = p_i^n$. Finally, W_3^n represents an elastic energy. We will show below that β_i^n converges in $L^1(\Omega)$ to the indicator function of Phase 1 and γ_i^n to the indicator function of Phase 2 as $n \to \infty$; α_k is the elastic constant to Phase k.

The functional W_1^n represents the electrostatic energy due to interatomic potentials that force the atoms to positions of a certain given lattice order.

For the analysis we extend the discrete deformation values $\{u_i^n\}_i$, to piecewise linear functions u^n in $L^2(\Omega) \cap \mathcal{A}^n$, where $\mathcal{A}^n$ denotes the space of piecewise linear functions, see [BDG99].

2.2 Identification of the Γ-limit for W^n

Now we can state the main result. It characterises the Γ-limit of W^n as n tends to infinity. Let $\chi_1 := \chi$, $\chi_2 := 1 - \chi$. For $u \in H^{1,2}(\Omega)$, $\chi \in BV(\overline{\Omega}, \{0,1\})$ set

$$E(u,\chi) := \frac{1}{4}\int_\Omega |\nabla\chi| + \sum_{k=1}^{2}\int_\Omega \chi_k\ (u' - \alpha_k)^2.$$

Additionally we introduce $W : L^2(\Omega) \to \mathbb{R}$ by

$$W(u) := \begin{cases} \inf_{\chi\in BV(\overline{\Omega},\{0,1\})} E(u,\chi) \text{ if } u \in H^{1,2}(\Omega) \text{ is strictly monotone,} \\ +\infty \text{ else.} \end{cases}$$

Theorem 2.1 (Characterisation of the Γ-limit of W^n).
The following statements are valid:
(i) The boundedness of the energy functional $W^n(u^n)$ implies the boundedness of $\left(\int_\Omega |(u^n)'|^2\right)_n$ uniformly in n.
(ii) W is the Γ-limit of W^n as $n \to \infty$ with respect to convergence in $L^2(\Omega)$.

Proof of (i):
Step 1: Construction of the characteristic function χ:
By C we denote various positive constants that may change from line to line.

Let $(u^n) \subset L^2(\Omega)$ be a sequence with $W^n(u^n) \leq C$. We set

$$d_k^i := \left|\frac{p_{i+1}^n}{p_i^n} - s_k\right|, \quad k_0^i := \operatorname{argmin}\Big\{k \mapsto d_k^i \mid 1 \leq k \leq 3\Big\}.$$

The boundedness of $W_1^n(u^n)$ implies

$$\sum_{i=0}^{n-1}(h^n)^{-\alpha}\prod_{k=1}^{3}\left(s_k-\frac{p_{i+1}^n}{p_i^n}\right)^2\le C.$$

Therefore there exists a constant $C>0$ such that

$$\sup_i d^i_{k_0^i}\le C(h^n)^{\alpha/2}. \tag{2.1}$$

For n large enough we can thus define an indicator function χ^n to Phase 1 by

$$\chi^n(x):=\begin{cases} 0 & \text{if } x\in[ih^n,(i+1)h^n),\ i\le n-2,\ k_0^i\ne 1,\\ 1 & \text{if } x\in[ih^n,(i+1)h^n),\ i\le n-2,\ k_0^i=1,\\ \chi^n(L-2h^n) & \text{if } x\in[L-h^n,L].\end{cases}$$

Next we show that $\chi^n\in BV(\overline{\Omega};\{0,1\})$, i.e.

$$\int_\Omega|\nabla\chi^n|\le C. \tag{2.2}$$

This follows from the boundedness of $W_2^n(u^n)$. Since for large n

$$\frac{p_{i+1}^n}{p_i^n}=s_k+o(1)\quad\text{for some } k\in\{1,2,3\},$$

we see that if $\chi^n(x)$ jumps in $x=(i+1)h^n$ between 0 and 1, then

$$\left(1-\frac{p_{i+2}^n}{p_i^n}\right)^2\ge\frac14+o(1)$$

which shows $W_2^n(u^n)\ge\left(\frac14+o(1)\right)\int_\Omega|\nabla\chi^n|$ and proves (2.2). Here we adapted the Landau notation and denote by $o(1)$ terms that tend to 0 as $n\to\infty$. With (2.2), well-known compactness results imply the existence of a subsequence (again denoted by) χ^n and a $\chi\in BV(\overline{\Omega},\{0,1\})$ such that $\chi^n\to\chi$ in $L^1(\Omega)$.

Step 2: Convergence of β^n, γ^n in $L^1(\Omega)$:

We extend the discrete quantities $\{\beta_i^n\}_i$, $\{\gamma_i^n\}_i$ to piecewise constant functions in $L^1(\Omega)$ by the definition

$$\beta^n(x):=\begin{cases}\beta_i^n & \text{if } x\in[ih^n,(i+1)h^n) \text{ and } i\le n-2,\\ 0 & \text{if } x\in[L-h^n,L].\end{cases}$$

In the same manner, the extension γ^n of $\{\gamma_i^n\}_i$ is defined.

Straightforward computations show

$$\beta^n\to\chi,\quad \gamma^n\to(1-\chi)\quad\text{in } L^1(\Omega)\text{ for } n\to\infty, \tag{2.3}$$

where the function $\chi \in BV(\overline{\Omega}, \{0,1\})$ is the limit of χ^n found in Step 1.

Step 3: Boundedness of $\int\limits_\Omega |(u^n)'|^2$ uniformly in n:

We choose constants $a \in \mathbb{R}^+$, $b \in \mathbb{R}$ such that

$$\min\{(x-\alpha_1)^2, (x-\alpha_2)^2\} \geq ax^2 - b.$$

Due to the boundedness of $W_3^n(u^n)$ we thus find that there exist constants C_1, $C_2 > 0$ such that

$$C_1 \geq (h^n)^2 C_2 \sum_{i=0}^{n-2} \left(\frac{p_{i+1}^n + p_i^n}{2}\right)^2 (\beta_i^n + \gamma_i^n).$$

Since $p_{i+1}^n = s_k p_i^n + o(1)$ for a $k \in \{1,2,3\}$ and large n we find that

$$\left(\frac{p_{i+1}^n + p_i^n}{2}\right)^2 \geq \left(1 + \frac{1}{2} + o(1)\right)\left(\frac{p_i^n}{2}\right)^2.$$

The term $\left(\beta_i^n + \gamma_i^n\right)$ can for large n be estimated from below by a constant. So we find the existence of a constant $C > 0$ with

$$C \geq (h^n)^2 \sum_{i=0}^{n-2} \left(\frac{p_i^n}{2}\right)^2. \tag{2.4}$$

Due to the estimate $(p_{n-1}^n)^2 \leq (2+o(1))p_{n-2}^n$ the sum in (2.4) can be extended to $i = n-1$ and the estimate still holds.

The sum $\sum_i (p_i^n)^2$ is directly related to $\int_\Omega |(u^n)'|^2$ where u^n is the piecewise affine linear extension of $\{u_i^n\}_i$. With (2.4) extended to $i = n-1$ this yields

$$\sup_n \int\limits_\Omega |(u^n)'|^2 = \sup_n\ h^n \sum_{i=0}^{n-1} (p_i^n)^2 \leq C. \tag{2.5}$$

Proof of (ii):

Step 4: Lower semicontinuity of W^n:

We have to show: for every sequence $(u^n)_{n\in\mathbb{N}}$ with $u^n \to u$ in $L^2(\Omega)$ there exists a subsequence $(u^{n_k})_{k\in\mathbb{N}}$ with

$$W(u) \leq \liminf_{k\to\infty} W^{n_k}(u^{n_k}).$$

For unbounded $W^n(u^n)$ there is nothing to show. So let $W^n(u^n) \leq C$ for all n. From (2.5) follows u^n, $u \in H^{1,2}(\Omega)$ for all $n \in \mathbb{N}$. Because of the reflexivity of the Hilbert space $H^{1,2}(\Omega)$ we know that there exists a subsequence (again denoted by) u^n such that $u^n \rightharpoonup u$, in $H^{1,2}(\Omega)$ for $n \to \infty$. From Step 2 we know that $\chi^n \to \chi$, $\beta^n \to \chi$, $\gamma^n \to 1-\chi$ in $L^1(\Omega)$ for $n \to \infty$. Because of $\frac{p_{i+1}^n}{p_i^n} \geq \frac{1}{2} + o(1)$, for $n \geq n_0$ we find that u^n is monotone for large n.

Now we estimate $W^n(u^n)$ from below. We claim

$$\liminf_{n\to\infty} W^n(u^n) \geq E(u,\chi) \geq W(u). \tag{2.6}$$

With the help of Theorem 3.4, p.74 in [Dac89], the proof of (2.6) is straightforward, estimating every component of $W^n(u^n)$ separately.

Step 5: Existence of a "recovery sequence":

We have to find a sequence $(u^n) \subset L^2(\Omega)$ converging to u in $L^2(\Omega)$ with

$$W(u) \geq \limsup_{n\to\infty} W^n(u^n).$$

If $W(u) = +\infty$, there is nothing to show. Due to the monotonicity properties of u demonstrated above we know that the functional $\chi \mapsto E(u,\chi)$ is bounded from below in the BV-norm. Using the compactness properties of $BV(\Omega)$ and the coercivity of E, it is clear that $E(u,\cdot)$ attains its minimum, i.e. $W(u) = E(u,\chi)$ for some $\chi \in BV(\overline{\Omega},\{0,1\})$.

Next we show that for piecewise affine, strictly monotone u there exists a sequence u^n with $u^n \to u$ and $W^n(u^n) \to E(u,\chi)$. We start with special cases, then generalise.

Case 1: $u' \equiv a_1 > 0$, $\chi \equiv \text{const}$ in Ω:

(a) $\chi \equiv 1$ in Ω: We simply set $u^n := u$ for all n.

(b) $\chi \equiv 0$ in Ω: For $x > 0$ choose u^n such that p_i^n is alternating between $\frac{2}{3}a_1$ and $\frac{4}{3}a_1$. Furthermore u^n satisfies $u^n(x=0) = u(x=0)$.

Case 2: $u' \equiv a_1 > 0$, $\chi \equiv 1$ for $0 \leq x \leq \frac{L}{2}$, $\chi \equiv 0$ for $x > \frac{L}{2}$.

The treatment of this case is more difficult. It is not possible to directly combine the two ansatz functions for u^n of Case 1 because for one index i this would mean $p_i^n = a_1 h^n$ and either $p_{i+1}^n = \frac{2}{3}a_1 h^n$ or $p_{i+1}^n = \frac{4}{3}a_1 h^n$, leading to $\lim_{n\to\infty} W_1^n(u^n) = \infty$.

Therefore we have to introduce a transition layer of width $(h^n)^s$ between the two phases, where $s > 0$ is a small constant to be chosen later. We define

$$\varphi^n(x) := \begin{cases} a_1 & \text{for } 0 \leq x \leq \frac{L}{2}, \\ a_1 + \frac{a_1}{3}(h^n)^{-s}(x - \frac{L}{2}) & \text{for } \frac{L}{2} < x \leq \frac{L}{2} + (h^n)^s, \\ \frac{4}{3}a_1 & \text{for } \frac{L}{2} + (h^n)^s < x \leq L. \end{cases}$$

We set u^n such that $u^n(x=0) = u(x=0)$ and

$$p_i^n := \begin{cases} \varphi^n(ih^n) & \text{for } ih^n \leq \frac{L}{2}, \\ \frac{1}{2}\varphi^n(ih^n),\ \varphi^n(ih^n) \text{ alternating} & \text{for } ih^n > \frac{L}{2}. \end{cases}$$

With this construction, the proof of convergence to 0 of the p_i^n-terms in W_1^n is straightforward. Hence $W_1^n(u^n) \to 0$ as $n \to \infty$.

For the estimation of the functional $W_2^n(u^n)$ we have

$$\Big|1 - \frac{p_{i+2}^n}{p_i^n}\Big|^2 = \Big|1 - \frac{1}{2}\frac{\varphi^n((i+2)h^n)}{\varphi^n(ih^n)}\Big|^2 = \Big|\frac{1}{2} - \frac{1}{2}\ \frac{\varphi^n(ih^n) - \varphi^n((i+2)h^n)}{\varphi^n(ih^n)}\Big|^2.$$

For $I := \frac{\varphi^n(ih^n) - \varphi^n((i+2)h^n)}{\varphi^n(ih^n)}$ simple computations yield

$$I = \begin{cases} 0 & \text{if } (ih^n > \frac{L}{2}) \text{ or } ((i+1)h^n \leq \frac{L}{2}) \\ & \text{or } (\frac{L}{2} < ih^n \leq \frac{L}{2} + (h^n)^s \text{ and } (i+2)h^n > \frac{L}{2} + (h^n)^s), \\ -s_k(h^n)^{1-s} & \text{if } (ih^n > \frac{L}{2} \text{ and } (i+2)h^n \leq \frac{L}{2} + (h^n)^s) \\ & \text{or } (ih^n \leq \frac{L}{2} \text{ and } \frac{L}{2} < (i+1)h^n \leq \frac{L}{2} + (h^n)^s). \end{cases}$$

and for $0 < s < 1$ the convergence of $W_2^n(u^n)$ to $\frac{1}{4}$ can be assured.

For the estimation of $W_3^n(u^n)$, it is clear that outside the strip of width $(h^n)^s$ the summands in $W_3^n(u^n)$ equal $(h^n)^s\big[\chi(a_1-\alpha_1)^2 + (1-\chi)(a_1-\alpha_2)^2\big]$. Inside the strip, we have approximately $(h^n)^{s-1}$ summands, where each summand is of the form $(h^n)C$. Thus, the part inside the strip tends to 0 for $n \to \infty$ as long as $s > 0$.

Case 3: General $\chi \in BV(\overline{\Omega};\{0,1\})$ and piecewise affine, monotone and continuous u: The construction of u^n can be done by iteratively applying the construction given in Case 2.

Case 4: General monotone $u \in H^{1,2}(\Omega)$:

Let u be a generic monotone function in $H^{1,2}(\Omega)$ and let $\{u^n\}$ be a sequence in $\mathcal{A}^n$ such that $u^n \to u$ in $H^{1,2}(\Omega)$. For every n we can apply Case 3 to find a sequence $\{w_l^n\}_l$ such that $w_l^n \to u^n$ in $L^2(\Omega)$ as $n \to \infty$ and $\limsup_l W^l(w_l^n) \leq W(u^n)$. Then we have

$$\limsup_{n\to\infty} \limsup_{l\to\infty} W^l(w_l^n) \leq \limsup_{n\to\infty} W(u^n) = W(u), \tag{2.7}$$

where (2.7) holds because of the strong convergence of u^n to u in $H^{1,2}(\Omega)$. By diagonalisation, we find a sequence $\tilde{u}^n := w_{l(n)}^n$ such that $\tilde{u}^n \to u$ in $L^2(\Omega)$ and $\limsup_{n\to\infty} W^n(\tilde{u}^n) \leq W(u,v)$. $\square$

3 An atomistic model for phase transitions of elastically stressed solids

In this section we present work planned for the last year of support within the priority program. We start with the following Hamiltonian that has been proposed by S. Luckhaus,

$$H(\{x_i\}_{i\in I}) := \int_\Omega \psi(x, \{x_i\}_{i\in I})dx,$$

with

$$\psi(x, \{x_i\}_{i\in I}) = \inf_{A,\tau,\alpha} \Big[\sum_{i\in I} \psi\Big(\frac{x - x_i}{\lambda}\Big) W_\alpha(Ax_i + \tau) + F(A)\Big]. \tag{3.1}$$

Here, I is a finite index set, $\{x_i\}_{i\in I}$ denotes the positions of the atoms, W_α is a periodic, non-negative potential whose zeros are on the unstrained lattice Λ_α corresponding to phase α; F plays the role of an elastic energy, and ψ is a cutoff function, $\lambda \in \mathbb{R}^+$ a scaling parameter. For a spatial point $x \in \Omega$, the infimum in (3.1) is taken with respect to deformations $A = A_x \in \mathrm{GL}(n)$, translations $\tau = \tau_x \in \mathbb{R}^n$ and phase α.

In a suitable way, W_α can be interpreted as a mean field Hamiltonian that is acting on the 'one-particle density'.

This Hamiltonian gives a reasonable description for states which have a lower and upper density close to that of a sheared lattice. One way to incorporate this restriction on the level of the Hamiltonian itself could be to define

$$\tilde{\psi}(x,\{x_i\}_{i\in I}) = \inf_{A,\tau,\alpha}\Big(\sum_{i\in I}\psi\Big(\frac{x-x_i}{\lambda}\Big)W_\alpha(Ax_i+\tau)+F(A) + \int_\Omega \psi\Big(\frac{x-y}{\lambda}\Big)\Big[\delta - W_\alpha(Ay+\tau) - \sum_{i\in I}\varphi(y-x_i)\Big]_+ dy\Big)$$

and to set

$$\tilde{h}(\{x_i\}_{i\in I}) := \int_\Omega \tilde{\psi}(x,\{x_i\}_{i\in I}) + \sum_{i\neq j}\varphi(x_i - x_j).$$

In the last line, φ may have compact support or can be a hard core potential, the positive part $[z]_+$ of z is $[z]_+ := z$ for $z \geq 0$ and $[z]_+ := 0$ for $z < 0$.

If λ is large it makes sense to speak of the open connected sets where

$$\tilde{\psi}(x,\{x_i\}_{i\in I}) < o(\lambda^n)$$

as the domains of one elastic phase.

For x in these phase domains we conjecture that the minimal A_x, τ_x, α_x satisfy that (A_x,τ_x) is unique modulo the affine isotropy group of the lattice, and α_x is constant in each domain.

A precise (and hopefully not too restrictive) estimate when this is the case is currently work in progress.

If one assumes the uniqueness of A_x, τ_x and the constancy of α_x in a simply connected subdomain $\tilde{\Omega}$, then one may construct an elastic deformation Φ such that the projection of $\Phi^{-1}(x)$ is τ_x and such that $\nabla(\Phi^{-1})x$ has a projection close to A_x.

Without assuming simple connectedness of $\tilde{\Omega}$ there may be an obstruction to the existence of Φ. Topologically speaking this obstruction is a homomorphism

$$B : \pi_1(\tilde{\Omega}) \to \Lambda_\alpha$$

from the group of affine mappings into the lattice corresponding to phase α. If the linear component is the identity, B coincides with the Burgers vector.

Since the functional – in terms of A – is automatically invariant under the lattice group, it does not make sense to investigate energy minimisers. It is well-known that energy minima do not sustain shear, [FT89].

So, the question is to characterise metastable states. This is completely open at this time.

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