Lattice deformations and elastic energy functionals in d dimensions - a variational and functional analytic approach

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Introduction

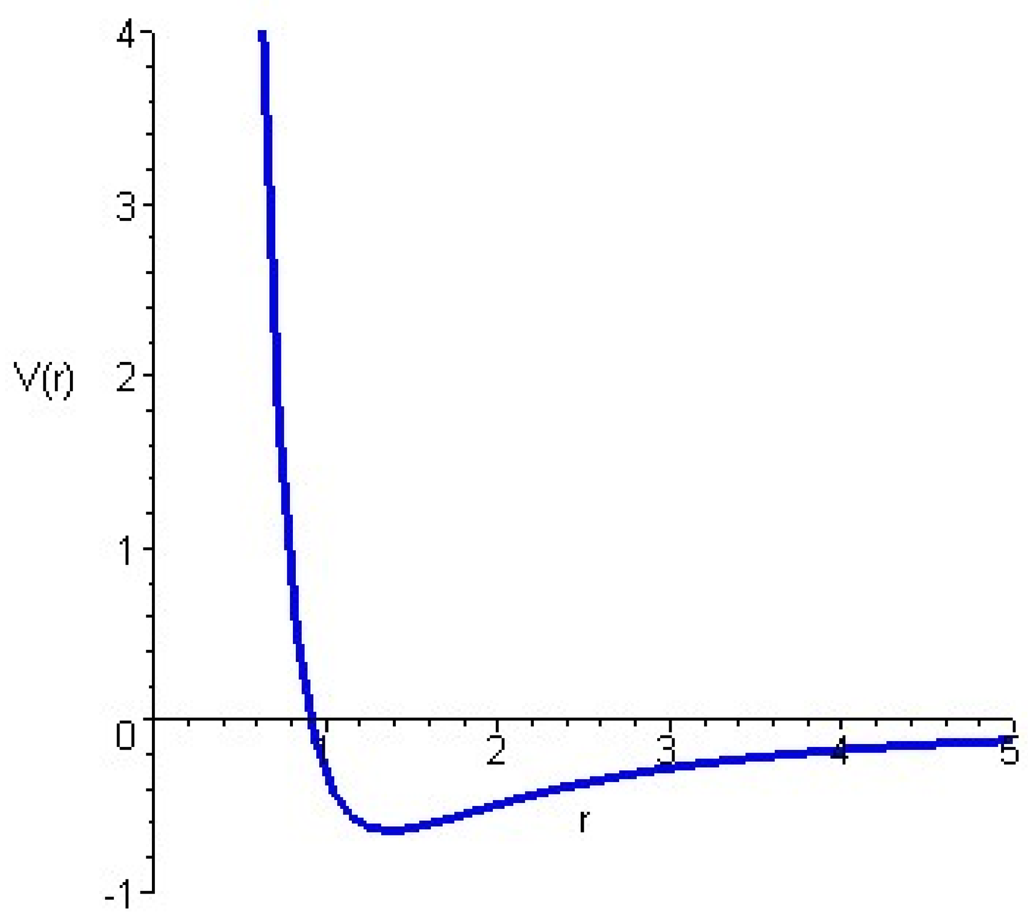
My thesis [4] makes a contribution to the fundamental and widely open question on how, on which length- and timescales, and with which accuracy detailed, fully atomistic models of crystalline solids can be approximated by (classical or noclassical) continuum models of linear elasticity, finite elasticity, dislocations, plasticity, or fracture.

Specifically, in [4] I am interested in putting the standard atomistic energy functionals for crystalline solids into a rigorous mathematical framework. My main result is a precise mathematical way in which to isolate the 'elastic' part of the total energy from the 'binding' part of the total energy. The former consists of the total interaction energy of the atoms minus their total interaction energy in an (undeformed, crystalline, equilibrium) reference configuration. To define it mathematically for general localized deformations requires performing a careful limit process, since in an infinite crystal both contributions are infinite even though their difference, the elastic energy of interest, is finite.

Setting and problem

Consider

- the unbounded cubic lattice $\mathcal{L} := \mathbb{Z}^d$ $(d \in \mathbb{N})$
- a smooth and sufficiently rapidly decreasing interatomic pair potential function $V : \mathbb{R}^+ \to \mathbb{R}$ describing an interaction of the atoms (the following figure shows a "typical" potential function)



- an outer force $f : \mathcal{L} \to \mathbb{R}^d$ the atoms are exposed to
- the energy functional $E_{B_R} : \{y : \mathcal{L} \to \mathbb{R}^d | y \text{ injective}\} \to \mathbb{R}$,

$$E_{B_R}(y) := \frac{1}{2} \sum_{\substack{x, x' \in \mathcal{L} \cap B_R \\ x \neq x'}} V(|y(x) - y(x')|) - \sum_{x \in \mathcal{L} \cap B_R} f(x) y(x),$$

  in which B_R denotes the open $\|.\|_\infty$-ball with radius $R > 0$
- the associated energy functional $\Delta_R : \{y : \mathcal{L} \to \mathbb{R}^d | y \text{ injective}\} \to \mathbb{R}$,

$$\Delta_R(y) := E_{B_R}(y) - E_{B_R}(y_0),$$

  in which $y_0 : \mathcal{L} \to \mathbb{R}^d$ is the identity.

Which conditions on injective displacements $y : \mathcal{L} \to \mathbb{R}^d$ guarantee the existence of the limit $\lim_{R\to\infty} \Delta_R(y)$? This question is the main problem examined in [4]. It is inspired by [2] and [1].

Main results

(1) If $y : \mathcal{L} \to \mathbb{R}^d$ is injective, if $y - y_0$ is summable and if f is bounded, then $\lim_{R\to\infty} \Delta_R(y)$ does exist.

(2) If $d = 1$, if $y : \mathcal{L} \to \mathbb{R}^d$ is injective and if $y - y_0$ and f are square summable, then $\lim_{R\to\infty} \Delta_R(y)$ does exist.

(3) If $d > 1$ and if f is square summable, then V can be chosen such that there exists an injective $y : \mathcal{L} \to \mathbb{R}^d$ such that $y - y_0$ is square summable and $\lim_{R\to\infty} \Delta_R(y)$ does *not* exist.

(4) The unexpected difference between (2) and (3), i.e., the surprising dependence on the dimension, is solely of geometric origin and cannot be overcome by strengthening the assumptions on the decay of V.

Sketch of proof

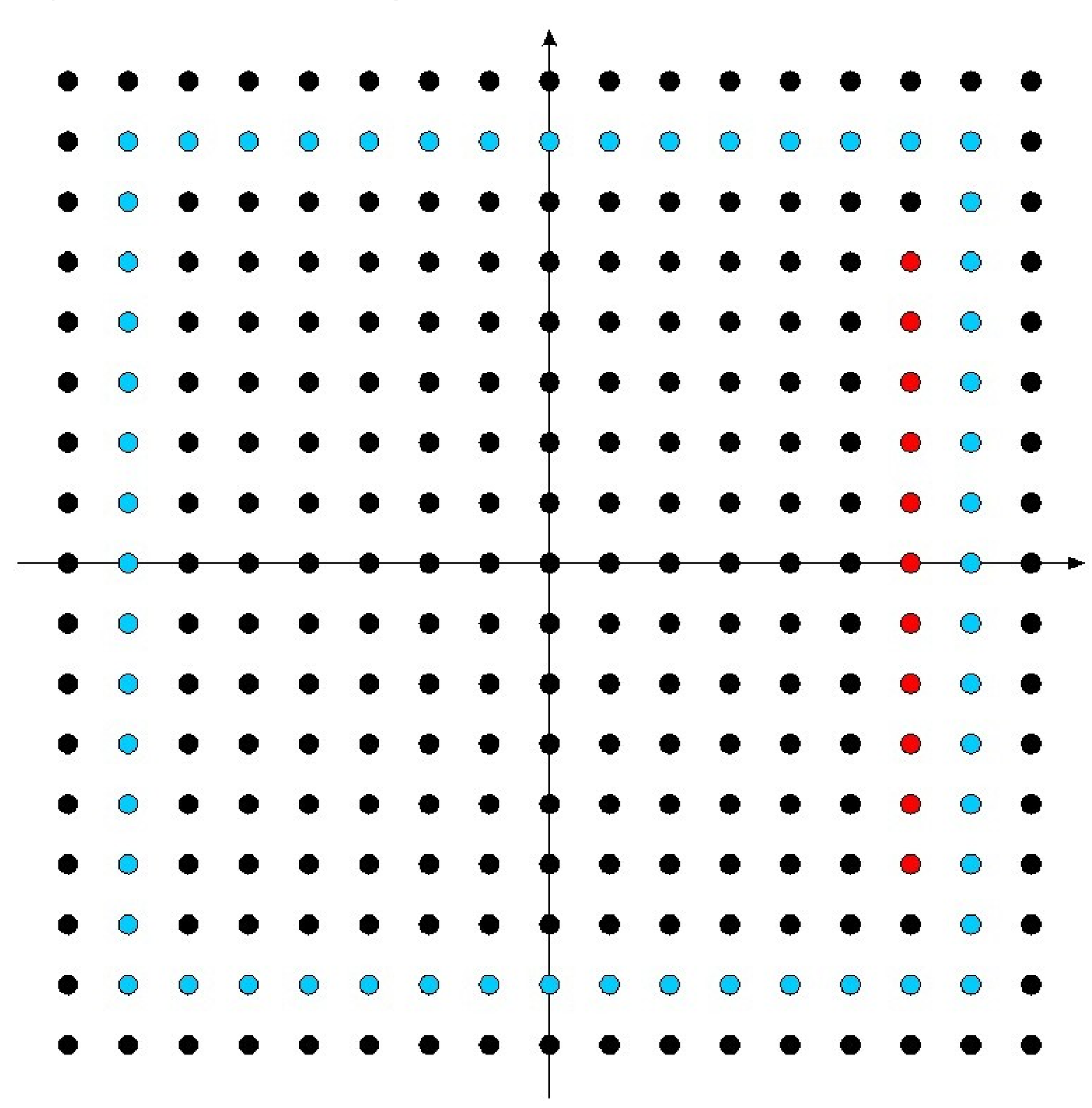
- The proof relies on a mixture of classical calculus, functional analysis and geometry in $\mathbb{R}^d$.
- The problem can be simplified by switching over to a linear approximation via Taylor's theorem, which is developed in [3] for a similar setting. The quadratic error terms can be estimated by a long, yet elementary calculation.
- The proof of (1) is a consequence of this approximation.
- The proof of (2) and (3), however, is more complicated and consists - after a further application of an idea presented in [3] - of the following two steps:

  Step 1: Define for each $k \in \mathbb{N}$ an auxiliary function $w_k : \mathcal{L} \to \mathbb{R}^d$,

$$w_k(x) := \begin{cases} \sum_{\substack{x' \in \mathcal{L} \cap B_k \\ x' \neq x}} V'(|x - x'|) \frac{x - x'}{|x - x'|}, & \text{if } x \in B_k \\ 0, & \text{else.} \end{cases}$$

  The Banach-Steinhaus theorem establishes a connection between the assertions and the $\|.\|_2$-boundedness of $(w_k)_{k\in\mathbb{N}}$.

  Step 2: Reduce the problem of proving or disproving the $\|.\|_2$-boundedness of $(w_k)_{k\in\mathbb{N}}$ to a simple geometric fact: Assume that in the figure below, the blue atoms are those on ∂B_k and the red ones are those on ∂B_{k-1}, with only the first coordinate equal to $k-1$. Then the number of the red atoms is invariant with respect to k if and only if $d = 1$.



- Since in detail the proof of (3) makes use of special potential functions satisfying $V\big|_{[\sqrt{2},\infty)} = 0$ ("short-range potentials"), (4) is quite evident.

Open challenges

The next step will be to study conditions under which minimizers exist. Specifically, I will pursue the following program.

- I would like to clarify the conditions under which atomistic minimizers of elastic energy exist, and study their basic properties.
- In principle, the set-up I am studying allows the physically important possibility that the reference deformation y_0 is not the identity, but corresponds to the presence of defects. The simplest examples would be a single edge- or screw-dislocation. I would like to extend my results to this case, establishing in particular the existence of atomistically energy minimizing configurations with defects.

In the longer run I would also begin to address the question of rigorous passage to continuum limits in various interesting scaling regimes, via Γ-convergence.

References

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[2] Friesecke, G., Theil, F. (2002): Validity and failure of the Cauchy-Born hypothesis in a two-dimensional mass-spring lattice, J. Nonl. Sci. 12 No. 5, 445-478.

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