Equilibria configurations for epitaxial crystal growth with adatoms

Riccardo Cristoferi
Joint work with Marco Caroccia and Laurent Dietrich

Carnegie Mellon University

BIRS Workshop
Topics in the Calculus of Variations: Recent Advances and New Trends

May 21, 2018

Outline of the talk

- Surface evolution

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- Surface evolution
- A model with adatoms

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- The big plan

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- What we have done/are doing

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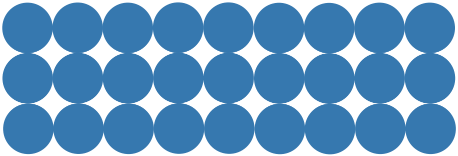
- A model with adatoms
- The big plan
- What we have done/are doing
- Future plans

Epitaxial growth



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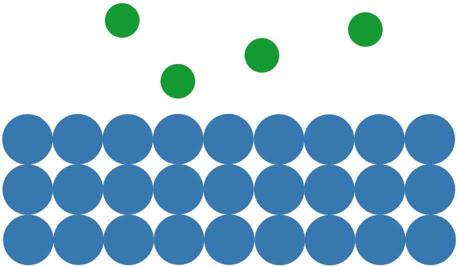

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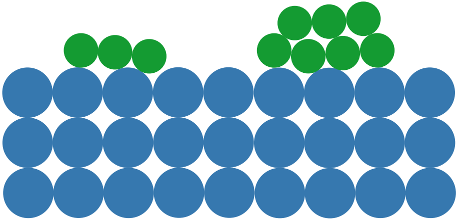

Epitaxial growth - Surface evolution

According to the *Einstein-Nernst law*, the surfaces $\{E_t\}_{t\geq 0}$ evolve following the volume preserving equation

$$\rho V = D\Delta_{\partial E_t}\mu \qquad \text{on } \partial E_t\,,$$

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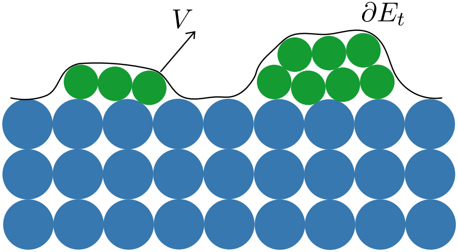

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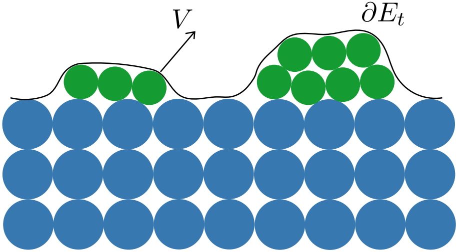

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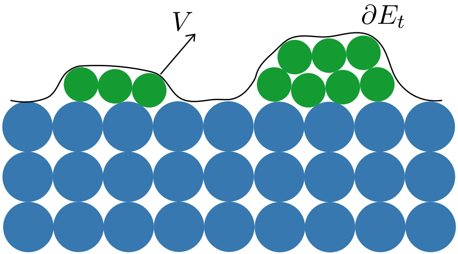

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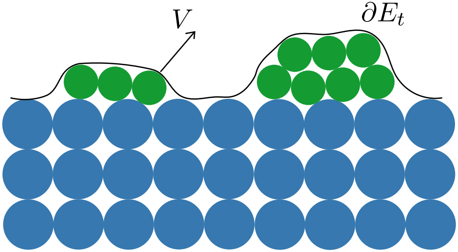

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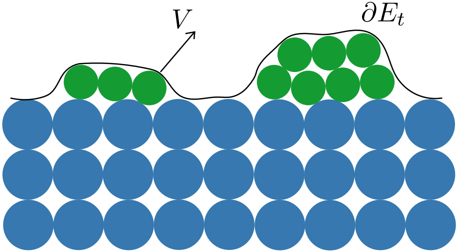

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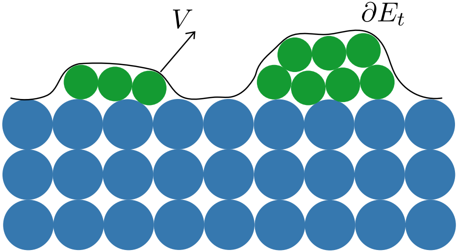

Adatoms

On the surface:

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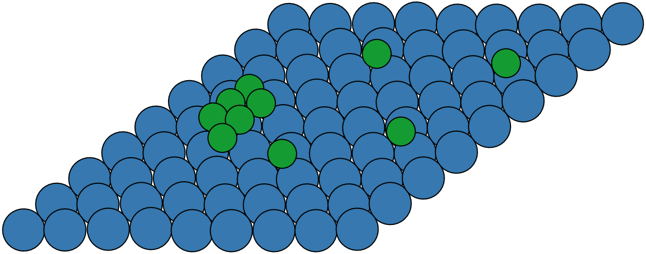
On the surface: Atoms



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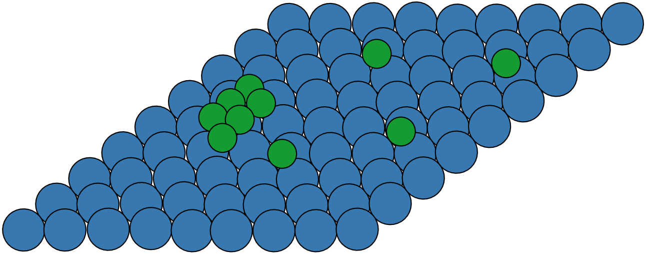
On the surface: Atoms and Adatoms = Adsorbed atoms



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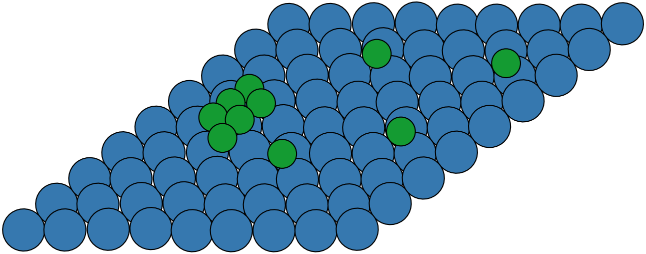

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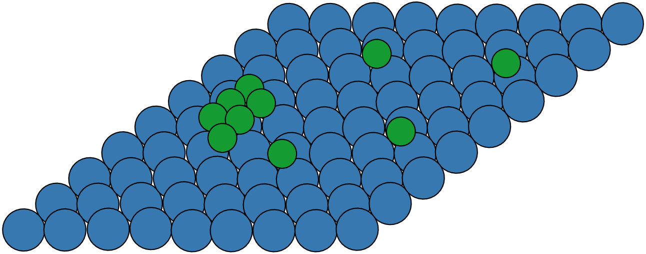

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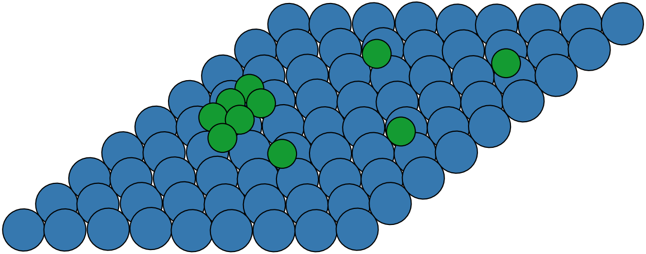
- important in models for solid-vapor interfaces
- effect of regularizing the unstable parabolic equations for surface evolution



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Eliot Fried and Morton E. Gurtin,
A unified treatment of evolving interfaces accounting for small deformations and atomic transport with emphasis on grain-boundaries and epitaxy,
Advances in applied mechanics, 40 (2004), pp. 1-177

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- the kinetic term bV: originates from the constitutive equation $F = bV$, where F is a dissipative force associated with the attachment of vapor atoms on the solid surface.

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$$\begin{cases} \partial_t u + (\rho + uH_{\partial E_t})V = D\Delta_{\partial E_t}[\psi'(u)] & \text{on } \partial E_t, \\ bV + \psi H_{\partial E_t} - (\rho + uH_{\partial E_t})\psi'(u) = 0 & \text{on } \partial E_t, \end{cases}$$

To do:

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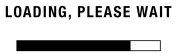
- consider an approximation of $\mathcal{F}$ via a diffuse interface energy $\mathcal{F}_\varepsilon$ 

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Previous works

Martin Burger,
Surface diffusion including adatoms,
Commun. Math. Sci., 4 (2006), pp. 1-51

Andreas Rätz, Axel Voigt,
A diffuse-interface approximation for surface diffusion including adatoms
Nonlinearity, 20 (2007), pp. 177-192

Christina Stöcker, Axel Voigt,
A level set approach to anisotropic surface evolution with free adatoms,
SIAM Journal on Applied Mathematics, 69 (2008), pp. 64-80

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We define the energy functional

$$\mathcal{F}(E, u) := \int_{\partial^* E} \psi(u)\, \mathrm{d}\mathcal{H}^{N-1}\,,$$

where $E \subset \mathbb{R}^N$ is a set of finite perimeter and $u \in L^1(\partial^* E; \mathbb{R}_+)$.

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- E is the *solid*
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- prototype of ψ is $\psi(s) := 1 + s^2/2$ (suggested by Fried and Gurtin)

The minimum problem

Definition

Given $E \subset \mathbb{R}^N$ is a set of finite perimeter and $u \in L^1(\partial^* E; \mathbb{R}_+)$, we define the *total mass*

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For $m > 0$, we define the *admissible class of competitors*

$$\mathrm{Cl}(m) := \left\{ (E,u) \,:\, E \text{ is a set of finite perimeter}, \; u \in L^1(\partial^* E; \mathbb{R}_+) \,, \; \mathcal{M}(E,u) = m \right\} .$$

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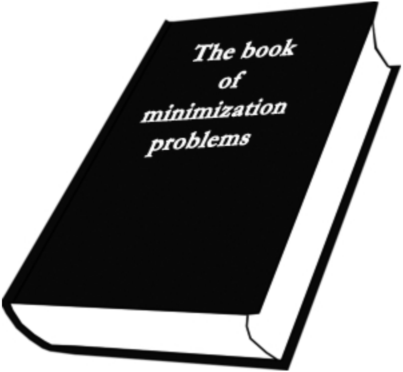
We are interested in the following *constrained* minimization problem

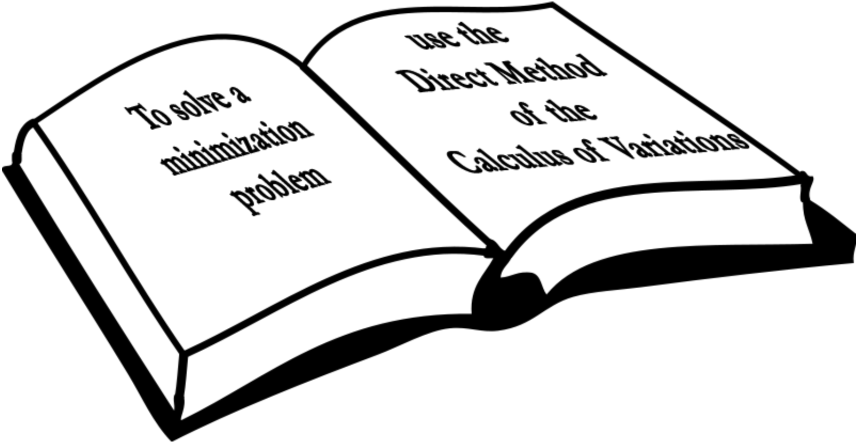
$$\gamma_m := \inf \left\{ \mathcal{F}(E, u) = \int_{\partial^* E} \psi(u) \, \mathrm{d}\mathcal{H}^{N-1} \, : \, (E, u) \in \mathrm{Cl}(m) \right\} ,$$

Equilibria configurations

Equilibria configurations



Equilibria configurations



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by applying Jensen's inequality

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where

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Achtung! Volume constraint

$$\mathcal{M}(E,u) = \rho|E| + \overline{u}\mathcal{H}^{N-1}(\partial^* E) = m\,.$$

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Remark

Non-uniqueness of the solution: different size of balls (other than translation invariance).

Is the energy l.s.c.?

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The pacman example

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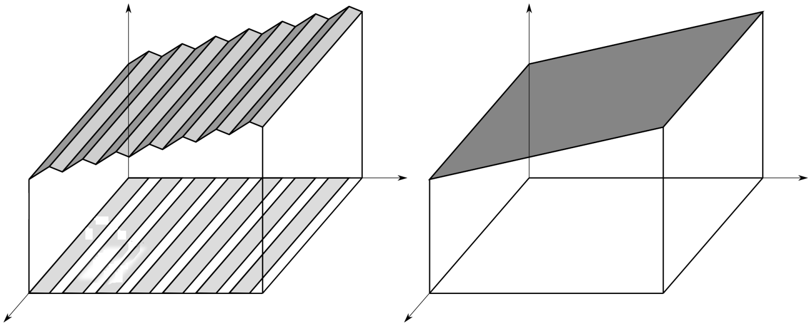

The wriggling example

The extended energy

$$(E, u)$$

E set of finite perimeter

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$$\mathcal{F}(E,\mu) := \begin{cases} \displaystyle\int_{\partial^* E} \psi(u)\ \mathrm{d}\mathcal{H}^{N-1} & \text{if } \mu = u|D\mathbb{1}_E| \text{ with } u \in L^1(\partial^* E;\mathbb{R}_+)\,, \\ +\infty & \text{otherwise}\,, \end{cases}$$

where E is a set with finite perimeter
μ is a non-negative finite Radon measure on $\mathbb{R}^N$
in brief $(E,\mu) \in \mathfrak{S}$.

The topology

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We say that $((E_k, \mu_k))_{k\in\mathbb{N}} \subset \mathfrak{S}$ *convergence* to $(E, \mu) \in \mathfrak{S}$ if

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Lemma

The above topology is metrizable.

Necessary conditions for l.s.c.

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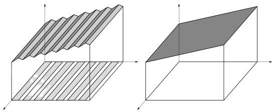

oscillating phenomena

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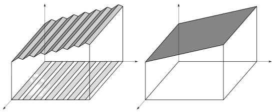

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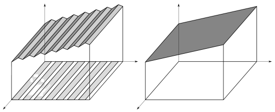

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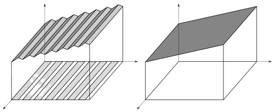

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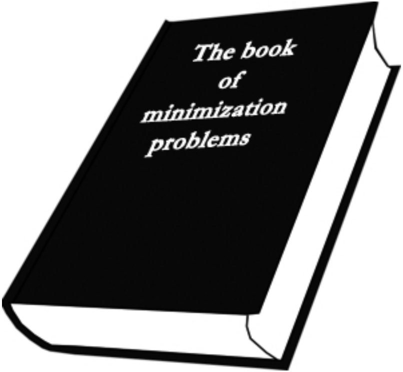

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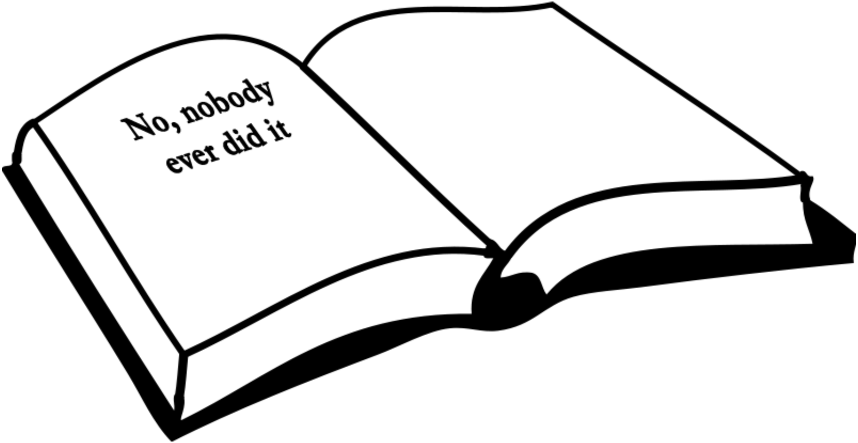

Convex subadditive envelope

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Let $\psi : \mathbb{R} \to \mathbb{R}$. We say that ψ is *subadditive* if for every $r, s \in \mathbb{R}$,

$$\psi(r + s) \leq \psi(r) + \psi(s)\,.$$

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Definition

Let $\psi : [0,\infty) \to \mathbb{R}$ be a function. We define its *convex subadditive envelope* $\overline{\psi} : [0,\infty) \to \mathbb{R}$ as

$$\overline{\psi}(s) := \sup\{\, f(s) \;:\; f : [0,\infty) \to \mathbb{R} \text{ is convex, subadditive and } f \leq \psi \,\}\,.$$

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$$\overline{\psi}(s) = \sup\{\, a_j s + b_j \;:\; j \in \mathbb{N}\,,\; b_j \geq 0 \,\}\,.$$

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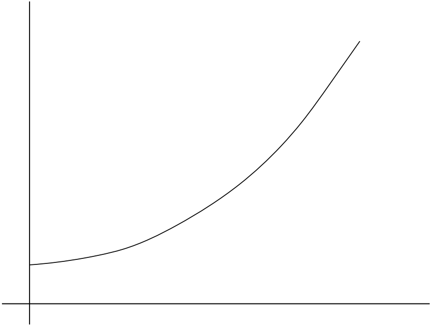

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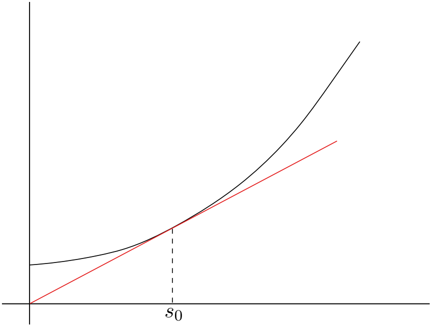

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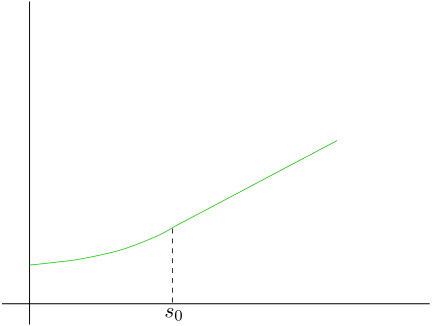

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$$\overline{\mathcal{F}}(E, \mu) := \int_{\partial^* E} \overline{\psi}\,(u)\ \mathrm{d}\mathcal{H}^{N-1} + \Theta \mu^s(\mathbb{R}^N)\,,$$

where we write $\mu = u\mathcal{H}^{N-1} \llcorner \partial^* E + \mu^s$ using the Radon-Nikodym decomposition.

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Theorem

$\overline{\mathcal{F}}$ is the relaxed functional of $\mathcal{F}$ w.r.t. the topology in $\mathfrak{S}$.

Relaxation - liminf inequality

Liminf inequality:

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The functional $\overline{\mathcal{F}}$ is lower semi-continuous w.r.t. the topology in $\mathfrak{S}$.

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where $\mu_k := u_k \mathcal{H}^{N-1} \llcorner \partial^* E$.

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By the l.s.c. of $\bar{\mathcal{F}}$ we obtain that

$$\liminf_{k\to\infty} \mathcal{F}(E_k, \mu_k) \geq \overline{\mathcal{F}}(E, \mu)\,.$$

Relaxation - idea for the recovery sequence

Recovery sequence: let $(E, \mu) \in \mathfrak{S}$. Write

$$\mu = u\mathcal{H}^{N-1} \llcorner \partial^* E + \mu^s = u|D\mathbb{1}_E| + \mu^s \,,$$

using the Radon-Nikodym decomposition. Then

$$\overline{\mathcal{F}}(E, \mu) = \int_{\partial^* E} \overline{\psi}\,(u) \;\mathrm{d}\mathcal{H}^{N-1} + \Theta \mu^s(\mathbb{R}^N)\,.$$

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We will construct:

(i) (F_k, v_k) with $(F_k, v_k) \to (E, u|D\mathbb{1}_E|)$ such that

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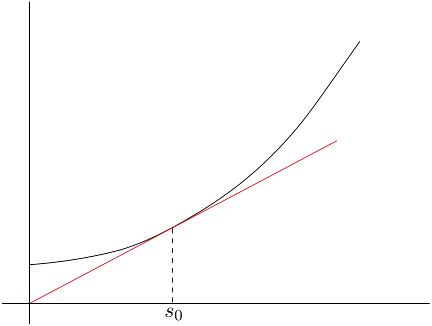

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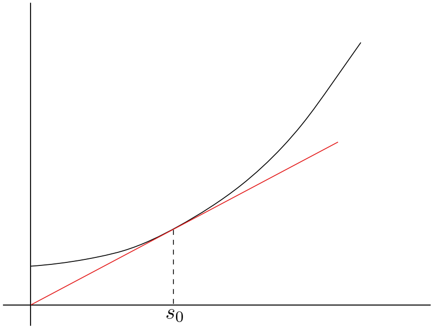

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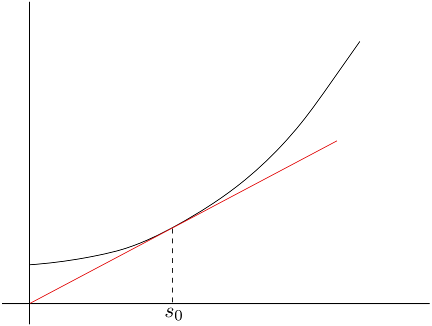

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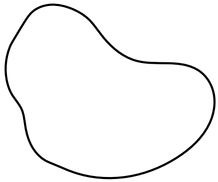

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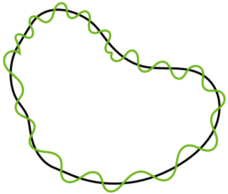

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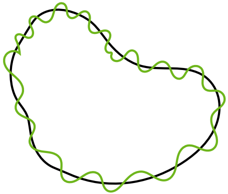

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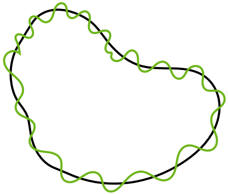

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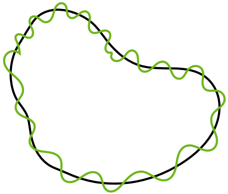

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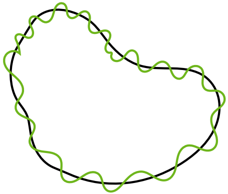

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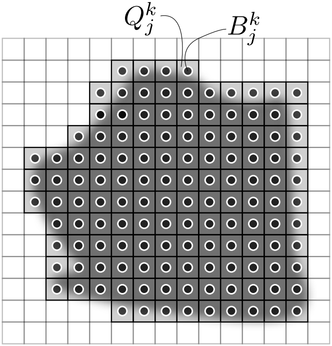

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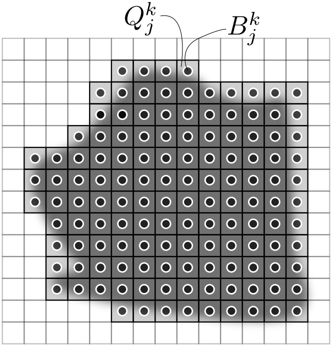

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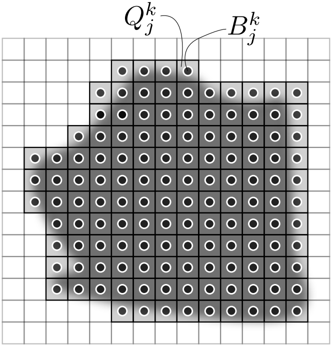
Consider $H^k := \cup_{j\in\mathbb{N}} B_j^k$. We apply the wriggling process to H^k –> done!



Minimization of the relaxed functional

Definition

Give $(E, \mu) \in \mathfrak{S}$, we define the *total mass*

$$\overline{\mathcal{M}}(E, \mu) := \rho|E| + \mu(\mathbb{R}^n)\,.$$

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We are interested in the following constrained minimization problem

$$\overline{\gamma}_m := \inf\{\,\overline{\mathcal{F}}(E,\mu) \,:\, (E,\mu) \in \overline{\mathrm{Cl}}(m)\,\}\,.$$

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$$\overline{\mathcal{F}}(B_R, c) = \overline{\gamma}_m = \gamma_m \, .$$

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Remark

Due to the presence of the singular part of the measure, minimizers of $\overline{\mathcal{F}}$ have less structure than minimizers of $\mathcal{F}$.

A diffuse phase approximation of the energy

For $\varepsilon > 0$ define the *diffuse energy* $\mathcal{F}_\varepsilon : W^{1,2}(\mathbb{R}^N) \times C(\mathbb{R}^N) \to [0, +\infty]$ as

$$\mathcal{F}_\varepsilon(\phi, u) := \int_{\mathbb{R}^N} \left(\frac{1}{\varepsilon} W(\phi) + \varepsilon |\nabla \phi|^2 \right) \psi(u) \mathrm{d}x \,.$$

where $W : \mathbb{R} \to \mathbb{R}$ is a double well potential.

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A discrete non-local approximation of the energy

Fix $R > 0$. For $n \in \mathbb{N}$ let $X_n := \{x_1, \dots, x_n\} \subset \mathbb{R}^N$ be such that x_i are chosen randomly in $B_R(0)$ uniformly.

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Theorem (True at 93% (2% more w.r.t. last week!))

If $\epsilon_n \to 0$ with a certain rate, then $\mathcal{F}_n^{(p)} \xrightarrow{\Gamma} c_{\eta,p,W} \overline{\mathcal{F}}$.

Ongoing project/Future plans

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- include more effects in the energy (more general materials)

Thank you for your attention!