Phase Transitions with a Minimal Number of Jumps in the Singular Limits of Higher Order Theories

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A Minimization Problem

$$\inf_{\varphi \in L^\infty_{\text{per}}} \int_0^L W(\varphi(s), \vartheta(s))\, ds$$

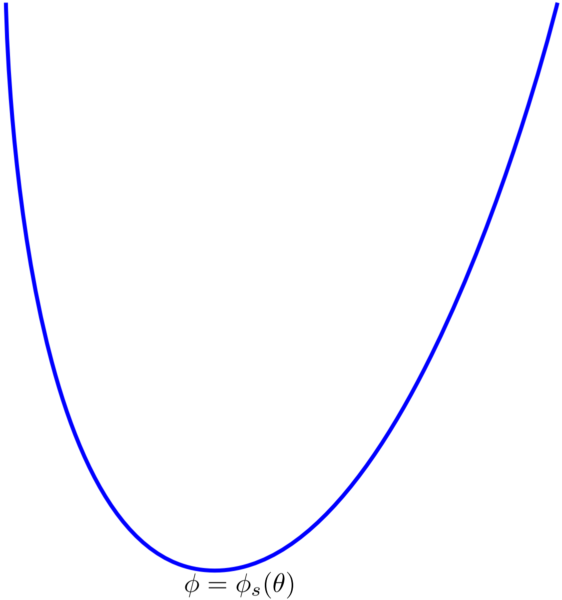
Class of Functions W Parametrized by $\theta \in \mathbb{R}^n$

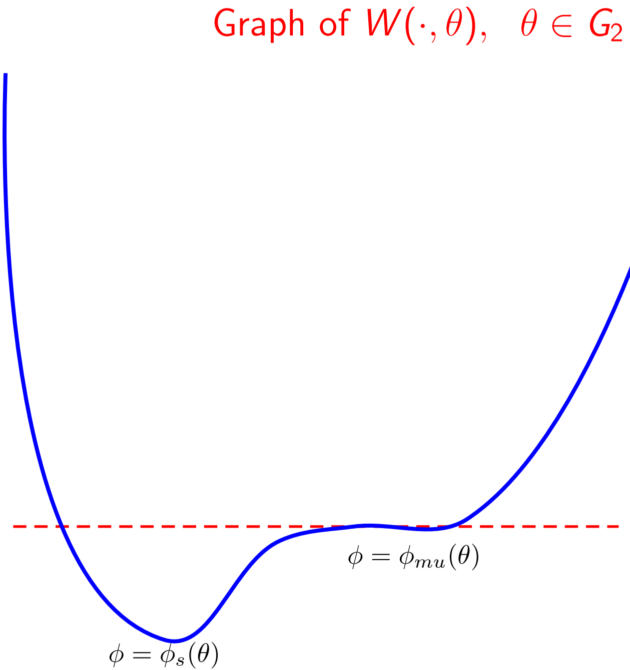
- For all $\theta \in \mathbb{R}^d$,

$$W(\phi, \theta) \to \infty \text{ as } \phi \searrow 0 \text{ or as } \phi \nearrow \infty$$

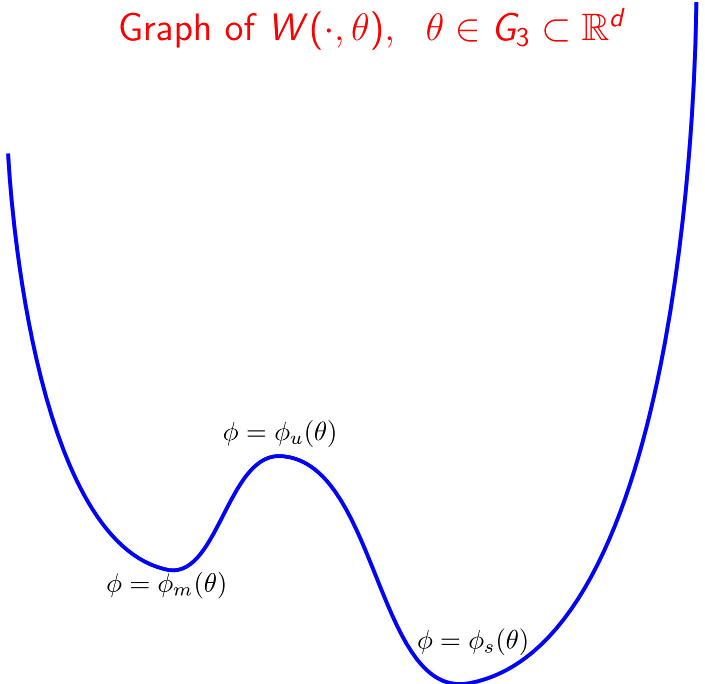
- $W(\cdot, \theta)$ has never more than three critical points, depending on the value of $\theta \in \mathbb{R}^d$
- $\mathbb{R}^d = G_1 \cup G_2 \cup G_3$ and $G_3^0 \subset G_3$, defined as follows:

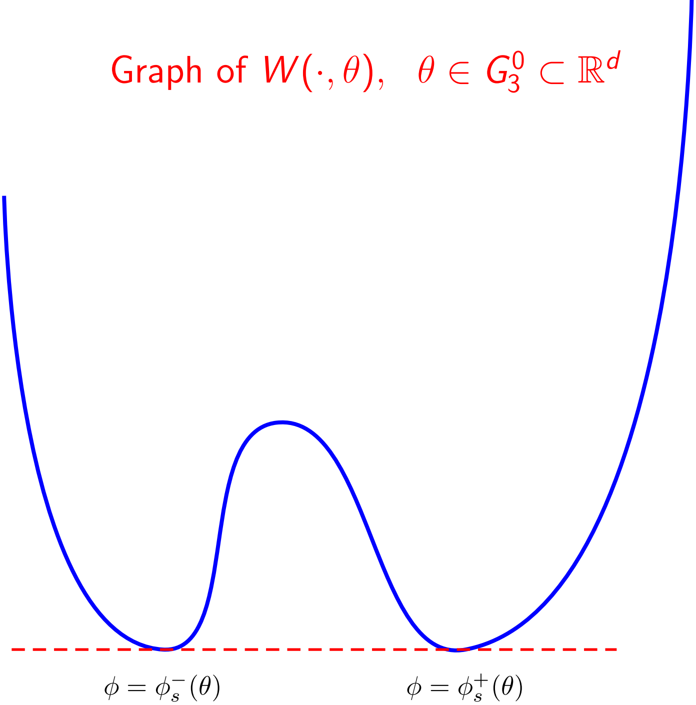
Graph of $W(\cdot, \theta)$, $\theta \in G_1 \subset \mathbb{R}^d$




Graph of $W(\cdot, \theta)$, $\theta \in G_2$
$\phi = \phi_{mu}(\theta)$
$\phi = \phi_s(\theta)$

Graph of $W(\cdot, \theta)$, $\theta \in G_3 \subset \mathbb{R}^d$




Graph of $W(\cdot,\theta)$, $\theta \in G_3^0 \subset \mathbb{R}^d$
$\phi = \phi_s^-(\theta)$
$\phi = \phi_s^+(\theta)$

Minimizers

When $\vartheta : \mathbb{R} \to \mathbb{R}^d$ is a given continuous L-periodic function

$$\inf_{\varphi \in L^\infty_{\text{per}}} \int_0^L W(\varphi(s), \vartheta(s))\, ds$$

is attained at a minimizers φ; indeed

- If $\vartheta(s)$ is never in G_3^0, then the minimizer is unique, continuous and $\varphi(s)$ is the global minimizer of $W(\cdot, \vartheta(s))$.
- If $\vartheta(s)$ crosses G_3^0 transversally at s_0, then φ must jump through $|\phi^-(\vartheta(s_0)) - \phi^+(\vartheta(s_0))|$ at s_0 .
- If $\vartheta(s) \in G_3^0$ for $s \in [a, b]$, then $\varphi(s)$ can take any value between $\phi^-(\vartheta(s))$ and $\phi^+(\vartheta(s))$ on $[a, b]$
- For a general function ϑ, minimizers need not be continuous and may have infinitely many jumps.

Piecewise Regular Minimizers

For a piecewise regular minimizer there is a sequence $\{S_n\}$:

- invariant with respect to $s \to s + L$
- $0 < k \leq S_{n+1} - S_n \leq K < \infty \ \forall \ n$.
- $\vartheta(S_n) \in G_3^0$, $n \in \mathbb{Z}$,
- $\varphi \in H^1(S_n, S_{n+1})$ for all n
- $\lim\limits_{s \to S_n \pm 0} \varphi(s) \in \{\phi_s^-(\vartheta(S_n)), \quad \phi_s^+(\vartheta(S_n))\}$
- The function φ has a jump at S_n with magnitude

$$\phi_s^+(\vartheta(S_n)) - \phi_s^-(\vartheta(S_n))$$

More about the Set $G_3^0 \subset \mathbb{R}^d$

If W is real-analytic, G_3^0 is a real-analytic variety.
More generally, G_3^0 is typically the closure of a union of manifolds with dimensions $d-1$, or less (except in non-generic situations possibly due to symmetries)
When $d=1$, G_3^0 is often a discrete set of points.
Let B be smooth and strictly increasing

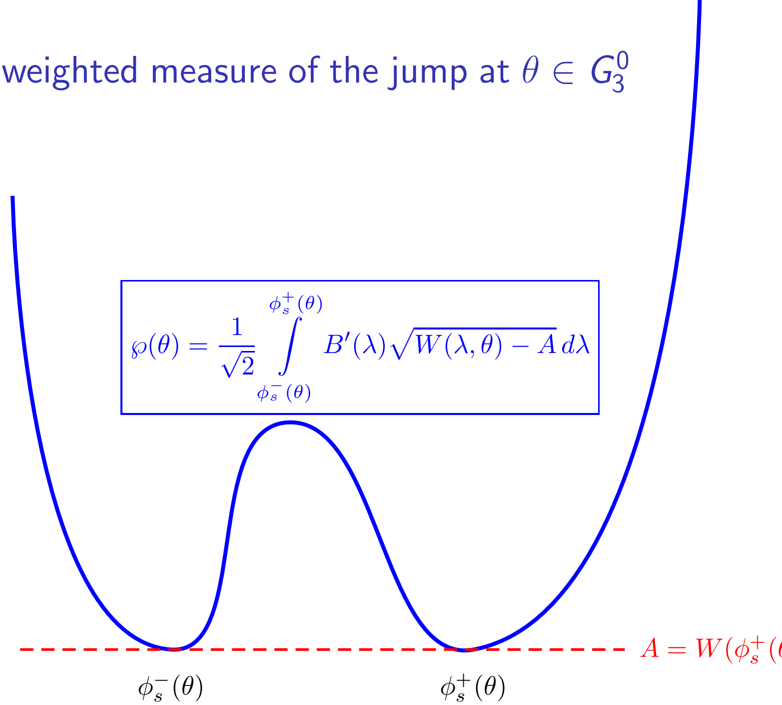
A weighted measure of the jump at $\theta \in G_3^0$

$$\wp(\theta) = \frac{1}{\sqrt{2}} \int_{\phi_s^-(\theta)}^{\phi_s^+(\theta)} B'(\lambda)\sqrt{W(\lambda,\theta)-A}\,d\lambda$$

where $A = W(\phi_s^{\pm}(\theta),\theta)$ Our hypotheses on B and W guarantee that $\wp(\theta)$ is bounded below by a positive constant, $\theta \in G_3^0$.
If $d=1$ and G_3^0 is a discrete set of points, then $\wp$ takes a finite set of positive values

A weighted measure of the jump at $\theta \in G_3^0$

$$\wp(\theta) = \frac{1}{\sqrt{2}} \int_{\phi_s^-(\theta)}^{\phi_s^+(\theta)} B'(\lambda)\sqrt{W(\lambda,\theta) - A}\, d\lambda$$



Counting Jumps

The *actual number of jumps of φ per period* is

$$\mathcal{N}(\varphi) = \sum_{[0,L)\cap\{S_n\}} 1 = \mathrm{card}\ \mathcal{Q}(\varphi)$$

The *weighted number of jumps of φ per period* is

$$\mathcal{W}(\varphi) = \sum_{s\in\mathcal{Q}(\varphi)} \wp(\vartheta(s)),$$

where

$$\boxed{\mathcal{Q}(\varphi) = [0, L) \cap \{S_n : n \in \mathbb{N}\}}$$

Let

$$\mathcal{W}_{\min} = \inf\{\mathcal{W}(\varphi) : \varphi \text{ is piecewise regular}\}$$

Minimal Number of Jumps

Lemma

If there exists a piecewise regular minimizer,
then there exists a piecewise regular minimizer with a minimal weighted number of jumps.
Let

$$\mathcal{N}^* = \max_{\varphi_{\mathsf{min}}} \mathcal{N}(\varphi_{\mathsf{min}}),$$

where the maximum of the actual number of jumps is taken over all piecewise regular minimizers with minimal weighted number of jumps.
Then there exists $\delta > 0$ such that $\mathcal{N}(\varphi) \leq \mathcal{N}^*$ if $\mathcal{W}(\varphi) \leq \mathcal{W}_{\min} + \delta$.

Regularized Variational Problems

Suppose throughout that $E \subset (0, \infty)$ has a limit point at 0

We are interested in how often piecewise regular minimizers arise as limits of regularized problems

Let H^1_{per} denote the Sobolev space of L-periodic functions which, with their weak derivatives, are in $L^2_{\text{loc}}(\mathbb{R})$

Let $\vartheta_\varepsilon \rightharpoonup \vartheta$ in $(H^1_{\text{per}})^d$ as $E \ni \varepsilon \searrow 0$, $d \geq 1$

For $\varepsilon \geq 0$ consider the non-autonomous variational problem for an L- periodic function $\varphi : \mathbb{R} \to \mathbb{R}$

$$\mathfrak{E}(\varepsilon) = \inf_{\varphi \in H^1_{\text{per}}} \int_0^L \Big(\frac{\varepsilon}{2} (B(\varphi)')^2 + W(\varphi, \vartheta_\varepsilon) \Big) \, ds$$

where B is a strictly increasing smooth function

The Euler-Lagrange Equation

Suppose that $\varepsilon > 0$ and that $\mathfrak{E}(\varepsilon)$ is attained at φ_ε:

$$\mathfrak{E}(\varepsilon) = \int_0^L \Big(\frac{\varepsilon}{2}(B(\varphi_\varepsilon)')^2 + W(\varphi_\varepsilon, \vartheta_\varepsilon)\Big)\, ds$$

Then φ_ε satisfies the Euler-Lagrange equation

$$\varepsilon B'(\varphi_\varepsilon(s))(B'(\varphi_\varepsilon)\varphi_\varepsilon')'(s) - \partial_\phi W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s)) = 0 \text{ on } \mathbb{R}$$

The limiting equation, with $\varepsilon = 0$ is

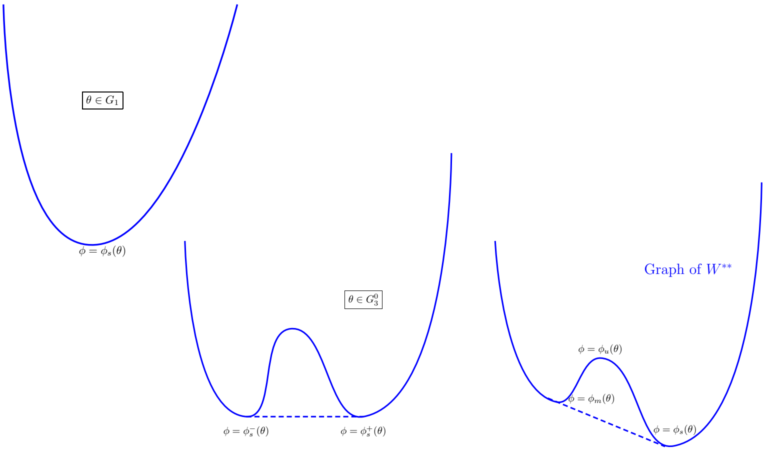
$$\partial_\phi W(\varphi(s), \vartheta(s)) = 0 \text{ on } \mathbb{R}$$

Our purpose is to study the limit as $\varepsilon \searrow 0$ of φ_ε

A peculiarity of the problem is that a weak* limit of φ_ε need not satisfy the limiting equation with $\varepsilon = 0$

It satisfies a relaxed form of the limiting equation instead.

W^{**} - the relaxation of W



Example: Cahn-Hilliard Theory

from phase separation theory

$$W(\varphi, \vartheta) = \frac{1}{4}(\varphi^2 - 1)^2 - \vartheta\varphi,$$

where ϑ is the chemical potential.
If φ and ϑ are L-periodic, the total mesoscopic energy per period is

$$\mathcal{J}_\varepsilon(\varphi) := \int_0^L \left(\frac{\varepsilon}{2}\varphi'^2 + \frac{1}{4}(\varphi^2 - 1)^2 - \vartheta\varphi \right) dx, \quad \varepsilon > 0,$$

$\varepsilon\varphi'^2/2$ corresponds to the energy of phase interactions
small $\sqrt{\varepsilon}$ characterizes the width of interfaces between phases
Critical points of $\mathcal{J}_\varepsilon$ satisfy

$$-\varepsilon\varphi''(x) + \varphi(x)^3 - \varphi(x) = \vartheta(x), \quad x \in \mathbb{R}.$$

Questions in Cahn Hilliard Theory

Two questions about weak* limits in L^∞_{per} of minimizers as $\varepsilon \to 0$

(1) How to characterise weak* limits of minimizers ?

(2) Is there is a so-called macroscopic variational problem with minimizers that coincide with these weak* limits?

A common belief is that both issues can be resolved using Γ-convergence theory,

We think that this is not always the case

Gamma Convergence

on a Metric Space X

A sequence of functionals $F_\varepsilon : X \to [\alpha, \infty]$, $\alpha > -\infty$ has Γ-limit $F : X \to [\alpha, \infty]$ if,
for every φ_0 and $\varphi_\varepsilon \to \varphi_0$,

$$F(\varphi_0) \leq \liminf_{\varepsilon \to 0} F_\varepsilon(\varphi_\varepsilon)$$

and there exists a sequence $\bar{\varphi}_\varepsilon \to \varphi_0$ so that

$$F(\varphi_0) = \lim_{\varepsilon \to 0} F_\varepsilon(\bar{\varphi}_\varepsilon).$$

Let $\mathcal{M}F_\varepsilon$ and $\mathcal{M}F$ be the set of minimizers of F_ε and F respectively
$\mathcal{L}F$ be the limit points of sequences $x_\varepsilon \in \mathcal{M}F_\varepsilon$ as $\varepsilon \to 0$
It is clear that $\mathcal{L}F \subset \mathcal{M}F$, but they are not equal in general.

In the mesoscopic theory of phase transitions F_ε would represent the total free energy and $\varphi_\varepsilon \in \mathcal{M}F_\varepsilon$ the corresponding stable equilibrium states.
If a macroscopic theory is to be regarded as a limit of mesoscopic theory, then macroscopic stable equilibria should belong to $\mathcal{L}F$ with the Γ-limit F interpreted as macroscopic free energy.
The validity of such an approach depends on the size of $\mathcal{M}F \setminus \mathcal{L}F$.
If it is not empty, an additional selection principle is needed to identify the solutions of the macroscopic problem that are relevant to the mesoscopic theory
particularly if $\mathcal{L}F$ is small in $\mathcal{M}F$

Examples of different relations between $\mathcal{M}F$ and $\mathcal{L}F$

ϑ is a given, continuous L-periodic function

$L^p_{\rm per}$ or $L^\infty_{\rm per}$ is the space of L-periodic functions with restrictions that are $p^{\rm th}$-power integrable or essentially bounded on $(0, L)$
Problem I: to minimize

$$\mathcal{J}_\varepsilon(\varphi^*) = \min_{\varphi \in L^4_{\rm per}} \mathcal{J}_\varepsilon(\varphi) := \int_0^L \left\{ \varepsilon {\varphi'}^2 + \frac{1}{4}(\varphi^2 - 1)^2 - \varphi\vartheta \right) ds.$$

Problem II: to minimize

$$\mathfrak{J}_\varepsilon(\psi^*) = \min_{\psi \in L^4_{\rm per}} \mathfrak{J}_\varepsilon(\psi) := \int_0^L \left(\sqrt{\varepsilon} {\psi'}^2 + \frac{1}{4\sqrt{\varepsilon}}(\psi^2 - 1)^2 - \psi\vartheta \right) ds.$$

If ϑ in $\mathcal{J}_\varepsilon$ is replaced by $\sqrt{\varepsilon}\vartheta$, problem I is transformed into problem II
but there is an essential difference between the two as they stand

$\mathcal{J}$ and its Minimizers

$X = L^4_{\text{per}}$ with the weak topology - bounded sets are metrizable

The Γ-limit $\mathcal{J}$ of $\mathcal{J}_\varepsilon$ is

$$\mathcal{J}(\varphi) =: \Gamma\text{-}\lim \mathcal{J}_\varepsilon(\varphi) = \int_0^L W^{**}(\varphi, \vartheta)\, ds,$$

where $W^{**}(\cdot, \theta)$ denotes the convex envelope of $W(\cdot, \theta)$.
Since W is bounded below, the set of minimizers of $\mathcal{J}$ is non-empty and there are various possibilities.

- The minimizer may be unique as when the set of zeros of ϑ is discrete
- Alternatively, there may be an infinite set of minimizers, as when ϑ vanishes on some interval.
- A minimizer may be discontinuous at every point of such an interval.

$\mathfrak{J}$ and its Minimizers

$X = L^4_{\text{per}}$ with the weak topology - bounded sets are metrizable

$$\Gamma\text{-}\lim \mathfrak{J}_\varepsilon(\psi) = \mathfrak{J}(\psi) := \begin{cases} \wp_0 \mathcal{N}(\psi) - \int_0^L \psi\vartheta \, ds \text{ if } |\psi| = 1 \\ \text{almost everywhere on } [0, L) \\ \text{and } \psi \text{ is piecewise constant,} \\ \\ +\infty \qquad \text{otherwise,} \end{cases}$$

where $\mathcal{N}(\psi)$ is the number of discontinuities of ψ in $[0, L)$ and

$$\wp_0 = 2\int_{-1}^{1} \sqrt{\frac{1}{4}(\phi^2 - 1)^2} d\phi = \frac{4}{3}.$$

Elements of $\mathcal{M}\mathfrak{J}$ are piecewise constant functions ψ with a finite number of jumps and $\mathcal{N}(\psi)\wp_0$ is a weighted count of jumps per period.

Roughly speaking the first term strives to minimize the number of jumps, but this process is controlled by ϑ.

A difference between $\mathcal{M}\mathfrak{J}_\varepsilon$ and $\mathcal{M}\mathcal{J}_\varepsilon$

Elements of $\mathcal{M}\mathfrak{J}_\varepsilon$ have a regularity property independent of ε because the set

$$\{\Phi(\psi_\varepsilon)\,\psi_\varepsilon \in \mathcal{M}\mathfrak{J}_\varepsilon,\ \varepsilon \in (0,1)\}\,, \quad \text{where} \quad \Phi(\phi) = \int_0^\phi |s^2 - 1|\,ds,$$

is bounded in the Sobolev space $W^{1,1}_{\mathrm{per}}$.
In contrast, *minimizers of $\mathcal{J}_\varepsilon$ have no regularity independent of ε*.

An analysis of the relation between $\mathcal{M}\mathcal{J}$ and $\mathcal{L}\mathcal{J}$ is consequently more difficult and is our concern here

To Get Around This

note that the Euler-Lagrange equation implies that $\mathcal{A}_\varepsilon'(s) = \partial_\vartheta W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s))\vartheta_\varepsilon'(s)$ where the adiabatic variable

$$\mathcal{A}_\varepsilon(s) := W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s)) - \frac{\varepsilon}{2}\big(B(\varphi_\varepsilon)'(s)\big)^2.$$

and we have the estimates

$$M^{-1} \le \varphi_\varepsilon(s),\ \varphi(s) \le M \text{ for } s \in \mathbb{R}, \quad \|\mathcal{A}_\varepsilon\|_{H^1_{\text{per}}} \le M,$$

Therefore, if periodic solutions φ_ε converge weak* in L^∞_{per} to φ, then, after passing to a subsequence, $(\mathcal{A}_\varepsilon, \vartheta_\varepsilon)$ converges weakly in $(H^1_{\text{per}})^{d+1}$ to some $(\mathcal{A}, \vartheta)$.

The idea is to obtain a representation for weak* limits of solutions in terms of $\mathcal{A}$ and ϑ

Of course ϑ and $\mathcal{A}$ are both unknown

The Result - in a Nut Shell

$\mathcal{LJ}$ under the assumption that the limiting problem, with $\varepsilon = 0$, has at least one piecewise continuous minimizer

There exists a set $E \subset (0,1)$ which is Lebesgue dense at 0

$$\lim_{t \searrow 0} \frac{\operatorname{meas} E \cap [0,t]}{t} = 1$$

with the following property:
Elements of $\mathcal{LJ}$ which arise from sequences in E are true minimizers of

$$\boxed{\inf_{\varphi \in L^\infty_{\text{per}}} \int_0^L W(\varphi(s), \vartheta(s))\, ds}$$

not only of the relaxed problem
and are piecewise continuous functions with the minimal weighted number of jumps

Ignoring Variational Structure

Suppose that $\vartheta_\varepsilon,\ \varepsilon \in E$ is bounded in $(H^1_{\text{per}})^d$, and that

$$\varepsilon B'(\varphi_\varepsilon(s))(B'(\varphi_\varepsilon)\varphi_\varepsilon')'(s) - \partial_\phi W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s)) = 0 \text{ on } \mathbb{R},$$

It is easily shown that

$$\|\vartheta_\varepsilon\|_{(H^1_{\text{per}})^d} \le M \quad \Rightarrow \quad C(M)^{-1} \le \varphi_\varepsilon(s) \le C(M) \text{ for } s \in \mathbb{R},$$

Thus
$\{\vartheta_\varepsilon : \varepsilon \in E\}$ is weakly relatively compact in $\left(H^1_{\text{per}}\right)^d$,
$\{\varphi_\varepsilon : \varepsilon \in E\}$ is weak* relatively compact in L^∞_{per}.
Therefore, for a sequence of $E \ni \varepsilon \searrow 0$,

$$\vartheta_\varepsilon \rightharpoonup \vartheta \text{ in } (H^1_{\text{per}})^d \text{ and hence uniformly on } \mathbb{R},$$
$$\text{and } \varphi_\varepsilon \rightharpoonup^* \varphi \text{ in } L^\infty_{\text{per}},$$

where ϑ and φ depend on the sequence.

Bounding the Weighted Number of Jumps

Without variational characterization of φ_ε

Theorem

$$\boxed{\liminf_{E \ni \varepsilon \searrow 0} \frac{\sqrt{\varepsilon}}{2} \int\limits_{[0,L]} \left(B(\varphi_\varepsilon(s))'\right)^2 ds \geq \sum_{s \in \mathcal{O}} \wp(\vartheta(s)),}$$

where

$$\mathcal{O} = \{s \in [0, L) : \varphi \textit{ is discontinuous}\}.$$

If $\mathcal{O}$ is infinite, then both sides are infinite.
Recall that $\wp(\vartheta(s))$ is bounded below by a positive constant.
Therefore if left side tends to zero as $\varepsilon \to 0$, the limit is continuous.
In general: he left hand limit bounds the number of jumps of the weak* limit function φ.

Limiting Behaviour of Minimizers

- Suppose the $\varepsilon = 0$ variational problem has at least one piecewise regular minimizer with a finite number of jumps

Does the weak* limit φ of minimizers φ_ε have a finite number of jumps?
We need a hypothesis on the dependence of ϑ_ε on ε

$$\|\vartheta_\varepsilon - \vartheta\|_{(L^1_{\mathrm{per}})^d} = o\big(\sqrt{\varepsilon}\big) \text{ as } \varepsilon \searrow 0$$

and, for almost all $\varepsilon \in (0,1)$,

$$\liminf_{\lambda \searrow 0} \frac{\|\vartheta_{\varepsilon-\lambda} - \vartheta_\varepsilon\|_{(L^1_{\mathrm{per}})^d}}{\lambda} = \Lambda(\varepsilon) \text{ where } \sqrt{\varepsilon}\Lambda(\varepsilon) \to 0.$$

This is automatic of ϑ_ε is a C^1-function of ε; in particular when $\vartheta_\varepsilon = \vartheta$, independent of ε

Asymptotic Behavior of the Energy

Recall that

$$\mathfrak{E}(\varepsilon) = \inf_{\varphi \in H^1_{\text{per}}} \int_0^L \Big(\frac{\varepsilon}{2} (B(\varphi)')^2 + W(\varphi, \vartheta_\varepsilon) \Big)\, ds, \quad \varepsilon > 0,$$

$$\mathfrak{E}(0) = \int_0^L \mathcal{A}(s)\, ds \text{ where } \mathcal{A}(s) = \inf_\phi W(\phi, \vartheta(s)).$$

Theorem

If a piecewise regular minimizer φ exists then

$$\boxed{\limsup_{E \ni \varepsilon \searrow 0} \frac{\mathfrak{E}(\varepsilon) - \mathfrak{E}(0)}{\sqrt{\varepsilon}} \le 2 \sum_{s \in \mathcal{Q}(\varphi)} \wp(\vartheta(S_n)) =: 2\mathcal{W}(\varphi)}$$

$\mathcal{W}(\varphi)$ is the weighted number of jumps of φ

Minimal Principle

Our main corollary of these observations is that, *almost always,* solutions to the variational problem converge weak* to piecewise regular minimizers with a minimal number of jumps, in the following sense:

Theorem

For any $\delta > 0$ there is a set $E_\delta \subset (0,1]$ which is dense at 0 with the following property.
If a sequence $\{\varphi_{\varepsilon_n}\}$, $E_\delta \ni \varepsilon_n \to 0$, of minimizers converges weak in L^∞_{per} to some function φ, then φ is an actual minimizer with weighted number of jumps $\mathcal{W}(\varphi) \leq \mathcal{W}_{\min} + \delta$.*

Theorem

There exists a piecewise regular minimizer with a minimal weighted number of jumps.
Let

$$\mathcal{N}^* = \max_{\varphi_{\min}} \mathcal{N}(\varphi_{\min}),$$

where the maximum number of actual jumps is taken over all piecewise regular minimizers with minimal weighted number of jumps.
Then, $\mathcal{N}^* < \infty$ and for any $\delta > 0$, E_δ can be chosen such that

$$\mathcal{N}(\varphi) \leq \mathcal{N}^*$$

where $\mathcal{N}(\varphi)$ is the actual number of jumps of φ in the preceding theorem.