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

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A Minimization Problem

\[
\inf_{\varphi \in L_{\text{per}}^\infty} \int_0^L W(\varphi(s), \vartheta(s)) \, ds
\]

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

- For all \( \theta \in \mathbb{R}^d \),
  \[
  W(\phi, \theta) \to \infty \quad \text{as} \quad \phi \downarrow 0 \quad \text{or as} \quad \phi \uparrow \infty
  \]

- \( W(\cdot, \theta) \) 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 $W(\cdot, \theta), \quad \theta \in G_2$

$\phi = \phi_{mu}(\theta)$

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

\[
\phi = \phi_u(\theta) \\
\phi = \phi_m(\theta) \\
\phi = \phi_s(\theta)
\]
Graph of $W(\cdot, \theta)$, $\theta \in G^0_3 \subset \mathbb{R}^d$
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 $\varphi$; indeed

- If $\vartheta(s)$ is never in $G^0_3$, then the minimizer is unique, continuous and $\varphi(s)$ is the global minimizer of $W(\cdot, \vartheta(s))$.
- If $\vartheta(s)$ crosses $G^0_3$ transversally at $s_0$, then $\varphi$ must jump through $|\phi^-(\vartheta(s_0)) - \phi^+(\vartheta(s_0))|$ at $s_0$.
- If $\vartheta(s) \in G^0_3$ 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 $\vartheta$, minimizers need not be continuous and may have infinitely many jumps.
For a piecewise regular minimizer there is a sequence \( \{ S_n \} \):

- invariant with respect to \( s \to s + L \)
- \( 0 < k \leq S_{n+1} - S_n \leq K < \infty \) \( \forall \ n \).
- \( \vartheta(S_n) \in G^0_3, \ n \in \mathbb{Z}, \)
- \( \varphi \in H^1(S_n, S_{n+1}) \) for all \( n \)
- \( \lim_{s \to S_n \pm 0} \varphi(s) \in \{ \phi_s^-(\vartheta(S_n)), \ \phi_s^+(\vartheta(S_n)) \} \)
- The function \( \varphi \) 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 $\theta \in G_3^0$

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

where $A = W(\phi_s^{\pm}(\theta), \theta)$ Our hypotheses on $B$ and $W$ guarantee that $\phi(\theta)$ 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 $\phi$ takes a finite set of positive values
A weighted measure of the jump at $\theta \in G_3^0$:

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

$$
A = W(\phi_s^+ (\theta))
$$
Counting Jumps

The **actual number of jumps of** \( \varphi \) **per period** is

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

The **weighted number of jumps of** \( \varphi \) **per period** is

\[
\mathcal{W}(\varphi) = \sum_{s \in Q(\varphi)} \varphi(\vartheta(s)),
\]

where

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

Let

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

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

Let

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

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 \( N(\varphi) \leq N^* \) if \( W(\varphi) \leq W_{\text{min}} + \delta \).
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 $H^1_{\text{per}}$ 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 $\varphi : \mathbb{R} \to \mathbb{R}$:

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

where $B$ is a strictly increasing smooth function.
The Euler-Lagrange Equation

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

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

Then $\varphi_\varepsilon$ satisfies the Euler-Lagrange equation

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

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

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

Our purpose is to study the limit as $\varepsilon \downarrow 0$ of $\varphi_\varepsilon$

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

It satisfies a relaxed form of the limiting equation instead.
$W^{**} -$ the relaxation of $W$

$\theta \in G_1$

$\phi = \phi_s(\theta)$

$\theta \in G_3^0$

$\phi = \phi^+_s(\theta)$

Graph of $W^{**}$

$\phi = \phi^+_m(\theta)$

$\phi = \phi_s(\theta)$
Example: Cahn-Hilliard Theory
from phase separation theory

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

where \( \vartheta \) is the chemical potential.
If \( \varphi \) and \( \vartheta \) are \( L \)-periodic, the total mesoscopic energy per period is

\[ J_\varepsilon(\varphi) : = \int_0^L \left( \frac{\varepsilon}{2} \varphi'^2 + \frac{1}{4}(\varphi^2 - 1)^2 - \vartheta \varphi \right) \, dx, \quad \varepsilon > 0, \]

\( \varepsilon \varphi'^2 / 2 \) corresponds to the energy of phase interactions
small \( \sqrt{\varepsilon} \) characterizes the width of interfaces between phases
Critical points of \( J_\varepsilon \) 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 $L^\infty_{\text{per}}$ of minimizers as $\varepsilon \to 0$

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

(2) Is there 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 $\Gamma$-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 $\Gamma$-limit $F : X \to [\alpha, \infty]$ if, for every $\varphi_0$ 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 $F_\varepsilon$ 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 $F_\varepsilon$ 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 $\Gamma$-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 $\mathcal{MF}$ and $\mathcal{LF}$

$\vartheta$ is a given, continuous $L$-periodic function

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

Problem I: to minimize

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

Problem II: to minimize

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

If $\vartheta$ in $J_\epsilon$ is replaced by $\sqrt{\epsilon} \vartheta$, problem I is transformed into problem II but there is an essential difference between the two as they stand
and its Minimizers

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

The \( \Gamma \)-limit \( J \) of \( J_\varepsilon \) is

\[
J(\varphi) =: \Gamma- \lim J_\varepsilon(\varphi) = \int_0^L W^{**}(\varphi, \vartheta) \, ds,
\]

where \( W^{**}(\cdot, \theta) \) denotes the convex envelope of \( W(\cdot, \theta) \).

Since \( W \) is bounded below, the set of minimizers of \( J \) is non-empty and there are various possibilities.

- The minimizer may be unique as when the set of zeros of \( \vartheta \) is discrete
- Alternatively, there may be an infinite set of minimizers, as when \( \vartheta \) vanishes on some interval.
- A minimizer may be discontinuous at every point of such an interval.
$\mathcal{J}$ and its Minimizers

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

$$\Gamma\text{-}\lim J_\epsilon(\psi) = \mathcal{J}(\psi) := \begin{cases} 
\varphi_0 N(\psi) - \int_0^L \psi \vartheta \, ds & \text{if } |\psi| = 1 \\
\text{almost everywhere on } [0, L) \\
\text{and } \psi \text{ is piecewise constant,} \\
+\infty & \text{otherwise,}
\end{cases}$$

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

$$\varphi_0 = 2 \int_{-1}^1 \sqrt{\frac{1}{4}(\phi^2 - 1)^2} \, d\phi = \frac{4}{3}.$$

Elements of $\mathcal{M}\mathcal{J}$ are piecewise constant functions $\psi$ with a finite number of jumps and $N(\psi)\varphi_0$ 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 $\vartheta$. 
A difference between $\mathcal{M}\tilde{\mathcal{J}}_\varepsilon$ and $\mathcal{M}\mathcal{J}_\varepsilon$

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

$$\{\Phi(\psi_\varepsilon) \psi_\varepsilon \in \mathcal{M}\tilde{\mathcal{J}}_\varepsilon, \varepsilon \in (0, 1)\},$$

where $\Phi(\phi) = \int_0^\phi |s^2 - 1| \, ds$,

is bounded in the Sobolev space $W^{1,1}_{\text{per}}$.

In contrast, minimizers of $J_\varepsilon$ have no regularity independent of $\varepsilon$.

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
\[ A'_\varepsilon(s) = \partial_\vartheta W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s))\vartheta'_\varepsilon(s) \]
where the adiabatic variable
\[ A_\varepsilon(s) := W(\varphi_\varepsilon(s), \vartheta_\varepsilon(s)) - \frac{\varepsilon}{2} (B(\varphi_\varepsilon)'(s))^2. \]

and we have the estimates
\[ M^{-1} \leq \varphi_\varepsilon(s), \varphi(s) \leq M \text{ for } s \in \mathbb{R}, \quad \|A_\varepsilon\|_{H^1_{\text{per}}} \leq M, \]

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

The idea is to obtain a representation for weak* limits of solutions in terms of \( A \) and \( \vartheta \).
Of course \( \vartheta \) and \( A \) are both unknown.
The Result - in a Nut Shell

$LJ$ 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

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

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

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

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

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

Thus

\[
\{\vartheta_\varepsilon : \varepsilon \in E\} \text{ is weakly relatively compact in } (H^1_{\text{per}})^d,
\]

\[
\{\varphi_\varepsilon : \varepsilon \in E\} \text{ is weak* relatively compact in } L^\infty_{\text{per}}.
\]

Therefore, for a sequence of \( E \ni \varepsilon \downarrow 0 \),

\[
\vartheta_\varepsilon \rightharpoonup \vartheta \text{ in } (H^1_{\text{per}})^d \text{ and hence uniformly on } \mathbb{R},
\]

and \( \varphi_\varepsilon \rightharpoonup^* \varphi \text{ in } L^\infty_{\text{per}} \),

where \( \vartheta \) and \( \varphi \) depend on the sequence.
Bounding the Weighted Number of Jumps

Without variational characterization of $\varphi_\varepsilon$

Theorem

$$\liminf_{E \ni \varepsilon \downarrow 0} \frac{\sqrt{\varepsilon}}{2} \int_{[0,L]} (B(\varphi_\varepsilon(s))')^2 \, ds \geq \sum_{s \in \mathcal{O}} \varphi(\vartheta(s)),$$

where

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

If $\mathcal{O}$ is infinite, then both sides are infinite.
Recall that $\varphi(\vartheta(s))$ 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 $\varphi$. 
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 $\varphi$ of minimizers $\varphi_{\varepsilon}$ have a finite number of jumps?

We need a hypothesis on the dependence of $\vartheta_{\varepsilon}$ on $\varepsilon$.

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

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

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

This is automatic of $\vartheta_{\varepsilon}$ is a $C^1$-function of $\varepsilon$; in particular when $\vartheta_{\varepsilon} = \vartheta$, independent of $\varepsilon$. 
Asymptotic Behavior of the Energy

Recall that

\[ \mathcal{E}(\varepsilon) = \inf_{\varphi \in H^1_{\text{per}}} \int_0^L \left( \frac{\varepsilon}{2} (B(\varphi))'\right)^2 + W(\varphi, \vartheta_{\varepsilon}) \right) \, ds, \quad \varepsilon > 0, \]

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

Theorem

*If a piecewise regular minimizer \( \varphi \) exists then

\[
\limsup_{\varepsilon \searrow 0} \frac{\mathcal{E}(\varepsilon) - \mathcal{E}(0)}{\sqrt{\varepsilon}} \leq 2 \sum_{s \in Q(\varphi)} \varphi(\vartheta(S_n)) =: 2\mathcal{W}(\varphi)
\]

\( \mathcal{W}(\varphi) \) is the weighted number of jumps of \( \varphi \).
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 $L^\infty_{\text{per}}$ *to some function* $\varphi$, *then* $\varphi$ *is an actual minimizer with weighted number of jumps* $\mathcal{W}(\varphi) \leq \mathcal{W}_{\text{min}} + \delta$. 
Theorem
There exists a piecewise regular minimizer with a minimal weighted number of jumps.

Let

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

where the maximum number of actual jumps is taken over all piecewise regular minimizers with minimal weighted number of jumps.

Then, $N^* < \infty$ and for any $\delta > 0$, $E_\delta$ can be chosen such that

$$N(\varphi) \leq N^*$$

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