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On the fine structure of minimizers in the Allen-Cahn theory of phase transitions

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Motivation

In the theory of phase transitions the Allen-Cahn functional

$$J_\Omega^\epsilon(v) = \int_\Omega \left(\epsilon \frac{|\nabla v|^2}{2} + \frac{1}{\epsilon} W(v)\right) dx, \quad v \in H^1, \quad 0 < \epsilon << 1,$$

$\Omega \subset \mathbb{R}^n$ a smooth domain, $W : \mathbb{R}^m \to \mathbb{R}$ a smooth nonnegative potential which vanishes on a finite set

$$\{W = 0\} = A = \{a_1, \ldots, a_N\},$$

is a model for the free energy of substance which can exist in N equally preferred phases: the zeros of W. The associated parabolic equation is a model for phase separation

$$u_t = \epsilon^2 \Delta u - W_u(u).$$

A basic step: the characterization of minimizers u^ϵ of J_Ω^ϵ:

$$J_\Omega^\epsilon(u^\epsilon) = \min_{v \in \mathscr{A}} J_\Omega^\epsilon(v).$$

Standard arguments of variational calculus yield existence of a minimizer u^ϵ for different choices of the admissible set $\mathscr{A}$ which may include a mass constraint

$$\frac{1}{|\Omega|}\int_\Omega v dx = m, \text{ for some } m \in \mathbb{R}^m,$$

or a Dirichlet condition

$$v|_{\partial\Omega} = v_0^\epsilon, \text{ for some } v_0^\epsilon : \partial\Omega \to \mathbb{R}^m.$$

Once existence is known, a challenging mathematical problem is the understanding of the fine structure of u^ϵ. In particular the effect of:

- the shape of Ω,
- the mass constraint and the boundary datum v_0^ϵ,
- the connections among the zeros of W and of the surface tensions $\sigma_{aa'}$, of these connections.

The diffuse interface $\mathscr{I}^\epsilon$

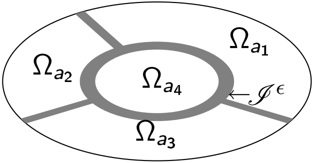
$$\mathscr{I}^\epsilon = \{x \in \bar{\Omega} : \min_{a \in A} |u^\epsilon(x) - a| > \delta\}, \quad \delta = \delta_\epsilon,$$

separates the phases

$$\Omega_a = \{x \in \Omega : |u^\epsilon(x) - a| \leq \delta\}, \quad a \in A.$$

and determines the structure of u^ϵ. Note that $J_\Omega^\epsilon(u^\epsilon) \leq C$ implies

$$|\mathscr{I}^\epsilon| \leq C \frac{\epsilon}{\delta^2} \text{ and } |\mathscr{I}^\epsilon| \xrightarrow{\epsilon} 0, \quad \delta = \epsilon^\alpha, \ \alpha \in (0, \frac{1}{2}).$$



- For the constrained problem Baldo (1990), using Γ-convergence, proved

$$u^\epsilon \xrightarrow{L^1} u^0 \quad \Rightarrow \quad u^0 = \sum_{a\in A} a\mathbb{I}_{S_a}$$

and $\{S_{a_1},\ldots,S_{a_N}\}$ minimizes $\sum_{a,a'\in A}\sigma_{aa'}H^{n-1}(\partial^* S_a\cap\partial^* S_{a'})$ in the set of partitions of Ω that satisfy $\sum_{a\in A} a|S_a| = m$.

$-$ We can ask if, as the jump set of u^0, also $\mathscr{I}^\epsilon$ enjoys some minimality property.

- A deep result on the structure of stable critical points for the constrained problem (for $m=1$, $N=2$ and $A=\{a_-,a_+\}$) is due to Sternberg and Zumbrun (1998). They showed that: Ω strictly convex, $0<\epsilon<<1$ and $\delta_\epsilon=\epsilon^k$ with $k>0$ sufficiently large, imply

$$\mathscr{I}^\epsilon \quad \text{is a connected set.}$$

Dirichlet conditions: a Theorem on the connectivity of $\mathscr{I}^{\epsilon}$

Set

$$\Gamma_a^{\epsilon} = \{x \in \partial\Omega : |v_0^{\epsilon}(x) - a| \leq \delta\}.$$

Assume:

1) $\Omega \subset \mathbb{R}^n$ is homeomorphic to a ball.

2) There is a subset $\tilde{A} \subset A$ such that

$v_0^{\epsilon}(\partial\Omega) \cap B_{\delta_0}(a) = \emptyset$ for $a \in A \setminus \tilde{A}$.

Γ_a^{ϵ}, $a \in \tilde{A} \subset A$ is homeomorphic to a n-1 ball,

3) $\delta = \delta_{\epsilon}$ is a regular value in the sense of Sard Lemma.

Then

$$\mathscr{I}^{\epsilon} \quad \text{is a connected set.}$$

Main points of the proof

- A maximum principle for minimizers (Alikakos et altri 2012).
  Assume that $E \subset \mathbb{R}^n$ is open bounded with Lipshitz boundary and let u^ϵ be a minimizer. Then, for small $\delta > 0$

$$|u^\epsilon(x) - a| \leq \delta, \;\; x \in \partial E \quad \Rightarrow \quad |u^\epsilon(x) - a| < \delta, \;\; x \in E.$$

- A topological Lemma (Czarnecki et altri 2001)
  If $E \subset \mathbb{R}^n$ is a domain (open bounded and connected) then ∂E is connected if and only if the complement $E' = \mathbb{R}^n \setminus E$ is connected.

Let ω^ϵ a connected component of $\Omega \setminus \mathscr{I}^\epsilon$. The definition of $\mathscr{I}^\epsilon$ implies

$$|u^\epsilon(x) - a| \leq \delta, \quad x \in \partial\omega^\epsilon, \quad \text{for some} \;\; a \in A.$$

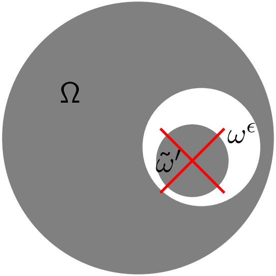
Assume that $(\omega^\epsilon)'$ contains a bounded component $\tilde{\omega}'$. Then

$$\partial\tilde{\omega}' \subset \partial(\omega^\epsilon)' = \partial\omega^\epsilon.$$

and, in contradiction with $\tilde{\omega}' \subset (\omega^\epsilon)'$, the Maximum Principle implies

$$|u^\epsilon(x) - a| < \delta, \quad x \in \tilde{\omega}'.$$

$\Rightarrow$ $(\omega^\epsilon)'$ coincides with its unbounded connected component.



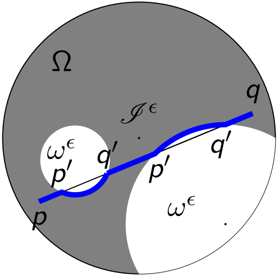
Then the topological Lemma

$\Rightarrow \quad \partial\omega^\epsilon$ is connected

Let Φ a family of connected components ω^ϵ of $\Omega \setminus \mathscr{I}^\epsilon$. Then

$$\mathscr{I}^\epsilon_\Phi = \Omega \setminus \cup_{\omega^\epsilon \in \Phi} \omega^\epsilon \quad \text{is a connected set.}$$

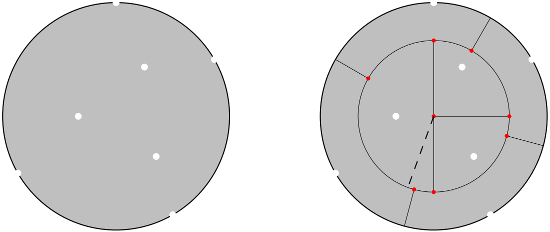
Ω connected $\Rightarrow$: given $p, q \in \mathscr{I}^\epsilon_\Phi$ there is an arc in Ω that connects p to q. The connectivity of $\partial\omega^\epsilon$ implies: if p' and q' are the extremes of a subarc contained in ω^ϵ, the subarc can be replaced by an arc in $\partial\omega^\epsilon$. In particular $\mathscr{I}^\epsilon$ is connected



Restricting to $2D$: $\Omega \subset \mathbb{R}^2$

δ a regular value, the IFT and $\omega^\epsilon \subset \Omega \subset \mathbb{R}^2 \Rightarrow \partial\omega^\epsilon$ is a C^1 curve. Actually a Jordan curve since $\partial\omega^\epsilon$ is connected. It follows that ω^ϵ is homeomorphic to a ball. $u^\epsilon|_{\partial\Omega} = v_0^\epsilon$ implies that $\tilde{N} = \sharp\tilde{A}$ of the $\partial\omega^\epsilon$ have an arc in common with $\partial\Omega$.

$\Rightarrow \mathscr{I}^\epsilon$ is homotopically equivalent to a closed ball deprived of $N = \sharp A$ points, $\tilde{N} = \sharp\tilde{A}$ of which on the boundary.



$N = 7$

$\tilde{N} = 4$

$n_b = 8$

$n_s = 14$

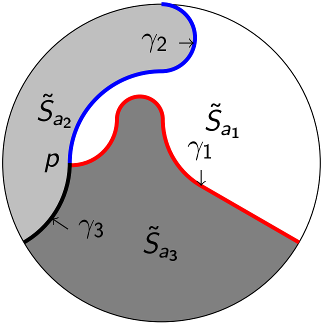
$\exists$ a network $\tilde{\mathscr{G}}^\epsilon \subset \mathscr{I}^\epsilon$ with $n_b = 2(N-1) - \tilde{N}$ branching points of triple junction type and $n_s = 3(N-1) - \tilde{N}$ arcs that separate the phases: $\Omega \setminus \tilde{\mathscr{G}}^\epsilon = \cup_a \tilde{S}_a$ and $\Omega_a^\epsilon \subset \tilde{S}_a$.

Exponential decay

- Let u^1 be a minimizer of J^1_E, $O \subset E$ and $a \in A$. Assume $x \in O,\ a' \in A \setminus \{a\} \ \Rightarrow\ |u^1(x) - a'| > \delta$. Then given $\eta > 0$, $r \geq r_\eta$ and $B_r(y) \subset O \ \Rightarrow |u^1(y) - a| \leq \eta$.

This applies to $\tilde{S}_a$ yielding (for some $k_\delta, K_\delta > 0$)

$$|u^\epsilon(x) - a| \leq K_\delta e^{\frac{k_\delta}{\epsilon} d(x,\partial\tilde{S}_a)} \quad x \in \tilde{S}_a.$$



$$N = \tilde{N} = 3$$

$$n_b = 2(N-1) - \tilde{N} = 1$$

$$n_s = 3(N-1) - \tilde{N} = 3$$

The optimal network $\mathscr{G}^\epsilon$

- There exist infinitely many networks $\tilde{\mathscr{G}}^\epsilon$ with the properties described above.
Is there an optimal choice?
The networks $\tilde{\mathscr{G}}^\epsilon$ can be classified in a finite number of types. If γ_i, $i = 1, \ldots, n_s$ are the arcs of $\tilde{\mathscr{G}}^\epsilon$, then there are a_i and a_i'

$$\gamma_i \subset \partial\tilde{S}_{a_i} \cap \partial\tilde{S}_{a_i'}.$$

A natural choice is to associate to each network $\mathscr{G}$ the number

$$\mathscr{F}(\mathscr{G}) = \sum_{i=1}^{n_s} \sigma_{a_i a_i'} |\gamma_i|.$$

It can be shown that there exists a network $\mathscr{G}^\epsilon$ which minimizes $\mathscr{F}$. The minimum $\mathscr{F}(\mathscr{G}^\epsilon)$ can be regarded as a weighted length of $\mathscr{I}^\epsilon$.

A possible approach to the fine structure of u^ϵ

1. Determine a free optimal network $\hat{\mathscr{G}}$ and a sharp upper bound of the form
   $J^\epsilon_\Omega(u^\epsilon) \le \mathscr{F}(\hat{\mathscr{G}}) + C\epsilon^\mu,\ \mu \in (0,1).$
2. Show that, if $\mathscr{G}$ is a network which coincides with $\hat{\mathscr{G}}$ on $\partial\Omega$ and is not contained in a h-neighborhood of $\hat{\mathscr{G}}$, then
   $\mathscr{F}(\mathscr{G}) - \mathscr{F}(\hat{\mathscr{G}}) \ge ch^2.$
3. Construct a sharp lower bound of the form
   $J^\epsilon_\Omega(u^\epsilon) \ge \mathscr{F}(\mathscr{G}^\epsilon) - C\epsilon^\mu,\ \mu \in (0,1).$
4. Deduce from 1 and 3 and the geometric inequality 2

   $$\mathscr{F}(\mathscr{G}^\epsilon) - C\epsilon^\mu \le J^\epsilon_\Omega(u^\epsilon) \le \mathscr{F}(\hat{\mathscr{G}}) + C\epsilon^\mu$$

   $$ch^2 \le \mathscr{F}(\mathscr{G}^\epsilon) - \mathscr{F}(\hat{\mathscr{G}}) \le 2C\epsilon^\mu \quad \Rightarrow h \le C\epsilon^{\frac{\mu}{2}}.$$

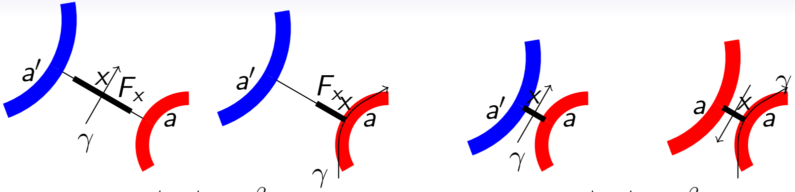
Associate to $\hat{\mathscr{G}}$ a map $\hat{v}^\epsilon$ that satisfies

$$\hat{v}^\epsilon \sim a, \;\; x \in \hat{S}_a, \;\; d(x, \partial \hat{S}_a) \geq \epsilon |\ln \epsilon|,$$
$$\hat{v}^\epsilon(x + s\nu_x) = \bar{u}_{aa'}(\frac{s}{\epsilon}), \;\; |s| < \epsilon |\ln \epsilon|, \;\; x \in \partial \hat{S}_a \cap \partial \hat{S}_{a'}.$$

where ν_x is the normal vector to $\hat{\mathscr{G}}$ at x and $\bar{u}_{aa'}$ the connection a to a' and $\Omega \setminus \hat{\mathscr{G}} = \cup_a \hat{S}_a$. It follows

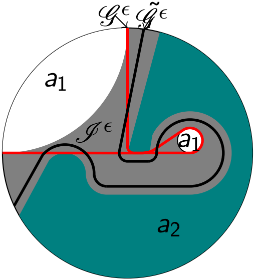
$$J^\epsilon_\Omega(u^\epsilon) \leq J^\epsilon_\Omega(\hat{v}^\epsilon) \leq \mathscr{F}(\hat{\mathscr{G}}) + \epsilon |\ln \epsilon|.$$

The lower bound. For $x \in \mathscr{G}^\epsilon$, ν_x a unit vector orthogonal to $\mathscr{G}^\epsilon$ at x denote F_x the connected component of $\{x + t\nu_x : |t| < \epsilon^\beta\} \cap \bar{\mathscr{I}}^\epsilon$ that contains x. Since $|\mathscr{I}^\epsilon| \leq \frac{\epsilon}{\delta_\epsilon^2} = \epsilon^{1-2\alpha}$, we expect that for most $x \in \gamma_i$ the extremes of F_x lie on $\Omega^\epsilon_{a_i}$ and $\Omega^\epsilon_{a'_i}$ with a_i, a'_i determined by $\gamma_i \subset \partial S^\epsilon_{a_i} \cap \partial S^\epsilon_{a'}$.



$|F_x| \geq \epsilon^\beta$ $|F_x| < \epsilon^\beta$

Let J_x be the energy of the restriction of u^ϵ to F_x.



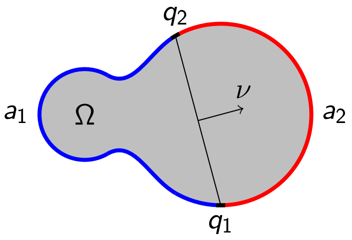
$N = \tilde{N} = 2,\ n_b = 0,\ n_s = 1$

The partition associated to $\mathscr{G}^\epsilon$

can be singular.

What can be said if Ω_a^ϵ is connected?

The simplest nontrivial case



Assumptions:

1. $A = \{W = 0\} = \{a_1, a_2, a_3\}$, and $\sigma_{a_1 a_2} < \sigma_{a_1 a_3} + \sigma_{a_1 a_3}$,

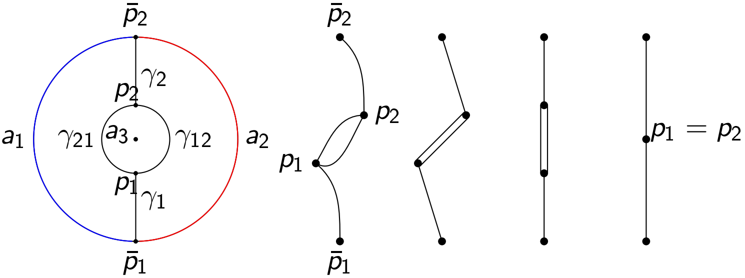
   where $\sigma_{a_i a_j} = \int_{\mathbb{R}} |\bar{u}'_{a_i a_j}|^2$, $\bar{u}_{a_i a_j}$ heteroclinic $a_i \to a_j$

2. $v_0^\epsilon \sim \bar{u}_{a_i a_j}((x - q_1) \cdot \nu)$, $x \in \partial\Omega$,

3. $\Omega^\epsilon_{a_i} = \{|u^\epsilon(x) - a_i| \leq \delta = \epsilon^\alpha\}$ is connect

The networks $\mathscr{G}^\epsilon$ and $\hat{\mathscr{G}}$.

$$N = 3, \tilde{N} = 2 \qquad \Rightarrow \qquad n_b = 2, n_s = 4$$



$$\mathscr{F}(\mathscr{G}^\epsilon) = \sigma_{a_1 a_2}(|\gamma_1| + |\gamma_2|) + \sigma_{a_1 a_3}|\gamma_{21}| + \sigma_{a_2 a_3}|\gamma_{12}|.$$

$$\mathscr{F}(\hat{\mathscr{G}}) = \sigma_{a_1 a_2}|\bar{p}_1 - \bar{p}_2|.$$

The upper bound for $J^\epsilon_\Omega(u^\epsilon)$

The characterization of $\mathscr{F}(\hat{\mathscr{G}})$ suggests $\hat{v}^\epsilon = \bar{u}_{a_1 a_2}((x - q_1)\cdot\nu)|_\Omega$ as a good test function

$$J^\epsilon_\Omega(u^\epsilon) \leq J^\epsilon_\Omega(\hat{v}^\epsilon) \leq \sigma_{a_1 a_2}|q_1 - q_2| + \epsilon|\ln\epsilon| \ \leq \mathscr{F}(\hat{\mathscr{G}}) + \epsilon|\ln\epsilon|$$

A geometric inequality: if $\mathscr{G} \not\subset h-$ neighborhood of $\hat{\mathscr{G}}$, then

$$\mathscr{F}(\mathscr{G}) - \mathscr{F}(\hat{\mathscr{G}}) \geq ch^2,$$

If we derive a lower bound of the form

$$J^\epsilon_\Omega(u^\epsilon) \geq \mathscr{F}(\mathscr{G}^\epsilon) - \epsilon^\mu, \ \mu \in (0,1),$$

then the upper bound and the geometric inequality imply

$$\epsilon^\eta \geq \mathscr{F}(\mathscr{G}^\epsilon) - \mathscr{F}(\hat{\mathscr{G}}) \geq ch^2, \ \Rightarrow \ h = \epsilon^{\frac{\mu}{2}}.$$

The lower bound for $J^{\epsilon}_{\Omega}(u^{\epsilon})$

The minimality of $\mathscr{G}^{\epsilon}$ $\Rightarrow$ that locally $\mathscr{G}^{\epsilon}$ is either rectilinear or F_x and the center of curvature lie on opposite sides.

Set $\Phi^{\epsilon} = \cup_{x \in \mathscr{G}^{\epsilon}} F_x$ then, if the connectivity of $\Omega^{\epsilon}_{a_i}$ $\Rightarrow$ no b), we have $|\Phi^{\epsilon}| \geq \int_{\mathscr{G}^{\epsilon}} |F_x| dx$ and

$$J^{\epsilon}_{\Phi^{\epsilon}}(u^{\epsilon}) \geq \int_{\mathscr{G}^{\epsilon}} J_x dx \geq \int_{\mathscr{G}^{\epsilon -}} J_x dx, \; (J_x = J_{F_x}(u^{\epsilon}|_{F_x})$$

$$\mathscr{G}^{\epsilon -} = \{x \in \mathscr{G}^{\epsilon} : |F_x| < \epsilon^{\beta}\}, \qquad \mathscr{G}^{\epsilon +} = \{x \in \mathscr{G}^{\epsilon} : |F_x| \geq \epsilon^{\beta}\}.$$

- $\epsilon^{\beta}|\mathscr{G}^{\epsilon+}| \leq |\cup_{x\in\mathscr{G}^{\epsilon+}} F_x| \leq |\mathscr{I}^{\epsilon}| \leq \epsilon^{1-2\alpha}, \ (\delta_\epsilon = \epsilon^{\alpha}),$
  $\Rightarrow \quad |\mathscr{G}^{\epsilon+}| \leq \epsilon^{1-(2\alpha+\beta)}$

- $x \in \mathscr{G}^{\epsilon-} \quad \Rightarrow \quad J_x \geq \sigma_{a_i a_j} - \epsilon^{2\alpha}$

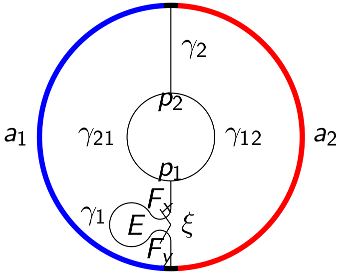
- $J^{\epsilon}_{\Omega}(u^{\epsilon}) \geq J^{\epsilon}_{\Phi^{\epsilon}}(u^{\epsilon}) \geq \int_{\mathscr{G}^{\epsilon-}} J_x dx$
  $\geq \sigma_{a_1 a_2}(|\gamma_1| + |\gamma_2|) + \sigma_{a_1 a_3}|\gamma_{21}| + \sigma_{a_2 a_3}|\gamma_{12}| - \epsilon^{\mu}$
  $= \mathscr{F}(\mathscr{G}^{\epsilon}) - \epsilon^{\mu}.$

From this and the geometric inequality it follows that $\mathscr{G}^{\epsilon}$ is contained in a $\epsilon^{\frac{\mu}{2}}$-neighborhood of $\mathrm{sg}[q_1, q_2]$. Moreover

$$||\gamma_1| + |\gamma_2| - |q_1 - q_2|| \leq \epsilon^{\mu},$$

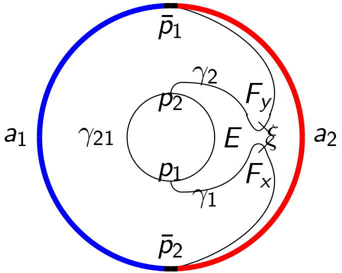
$$\max\{|\gamma_{12}|, |\gamma_{21}|\} \leq \epsilon^{\mu}.$$

$F_x \cap F_y = \emptyset$, for $x \neq y \in \mathscr{G}^\epsilon \setminus (B_{\epsilon^\eta}(p_1) \cup B_{\epsilon^\eta}(p_1))$

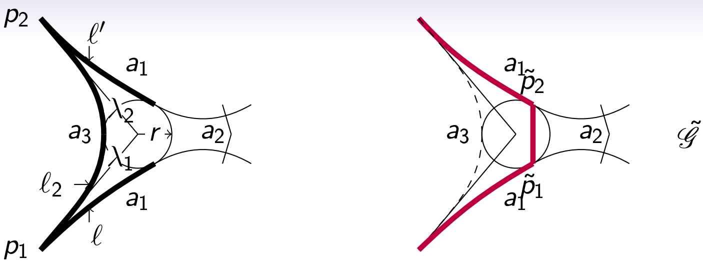


$\xi \in F_x \cap F_y$ for $x \neq y \in \gamma_1$

$E \subset \mathscr{I}^\epsilon$ and $E \cap \Omega_{a_2} = \emptyset$



$\xi \in F_x \cap F_y$ for $x \in \gamma_1$ and $y \in \gamma_2$



$$B_r \subset E \subset \mathscr{I}^\epsilon \quad \Rightarrow \quad r \leq \epsilon^{\frac{1}{2}-\alpha},$$

$$\Rightarrow |\ell - \lambda_1| \leq \epsilon^\mu, \quad |\ell' - \lambda_2| \leq \epsilon^\mu,$$

$$|\ell_2 - (\lambda_1 + \lambda_2)| \leq \epsilon^\mu.$$

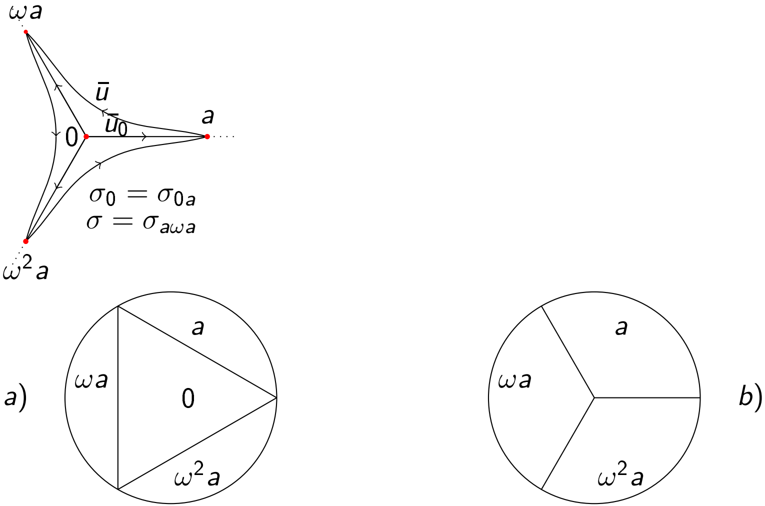
$$\Rightarrow \quad \mathscr{F}(\mathscr{G}^\epsilon) - \mathscr{F}(\tilde{\mathscr{G}})$$

$$= \sigma_{a_2 a_3} \ell_2 + \sigma_{a_2 a_1}(\ell + \ell') - \sigma_{a_1 a_3}(\ell + \ell') - \sigma_{a_2 a_3}|\tilde{p}_1 - \tilde{p}_2|$$

$$\geq (\sigma_{a_2 a_3} + \sigma_{a_2 a_1} - \sigma_{a_1 a_3})(\lambda_1 + \lambda_2) - \epsilon^\mu.$$

That contradicts the minimality of $\mathscr{G}^\epsilon$ unless $\lambda_1 + \lambda_2 \leq \epsilon^\eta$.

A potential with four zeros



$$1 < \frac{2\sigma_0}{\sigma} < \frac{1}{\sin\frac{\pi}{3}}$$

$$\frac{2\sigma_0}{\sigma} > \frac{1}{\sin\frac{\pi}{3}}$$