Uniqueness of local minimizers for crystalline variational problems

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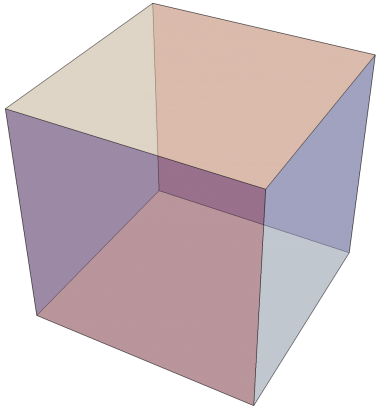
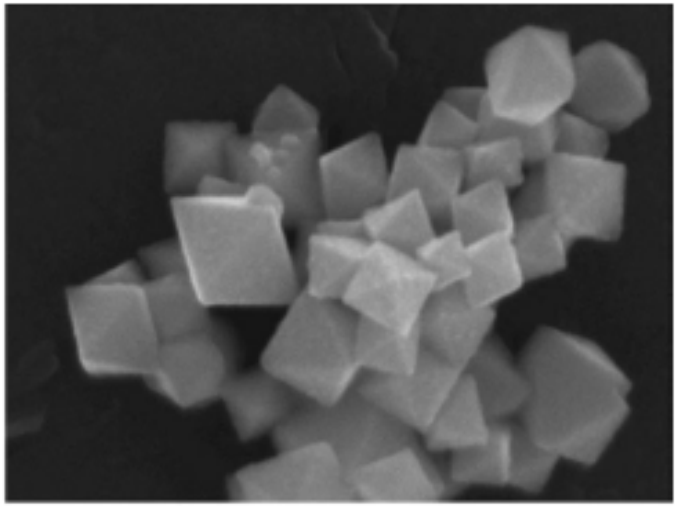
Introduction

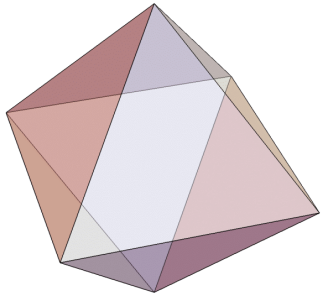
- **Crystalline variational problem**: Study on equilibrium surfaces for anisotropic (surface) energy of which the minimizer among surfaces enclosing the same volume is a polyhedron.
- **The origin of the above name**: Single crystals are usually polyhedra, and each of them is a local minimizer of such a variational problem.
- **Our main result** is the uniqueness of local minimizer!
  Consider any crystalline variational problem whose minimizer with volume constraint is a regular polyhedron. Then, roughly speaking, we proved any local minimizer is the global minimizer!



salt crystal (cube)



nanocrystals of CeO_2
(Asahina, Takami, et al., 2011)

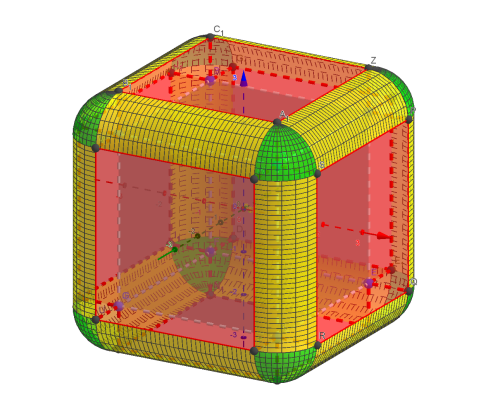


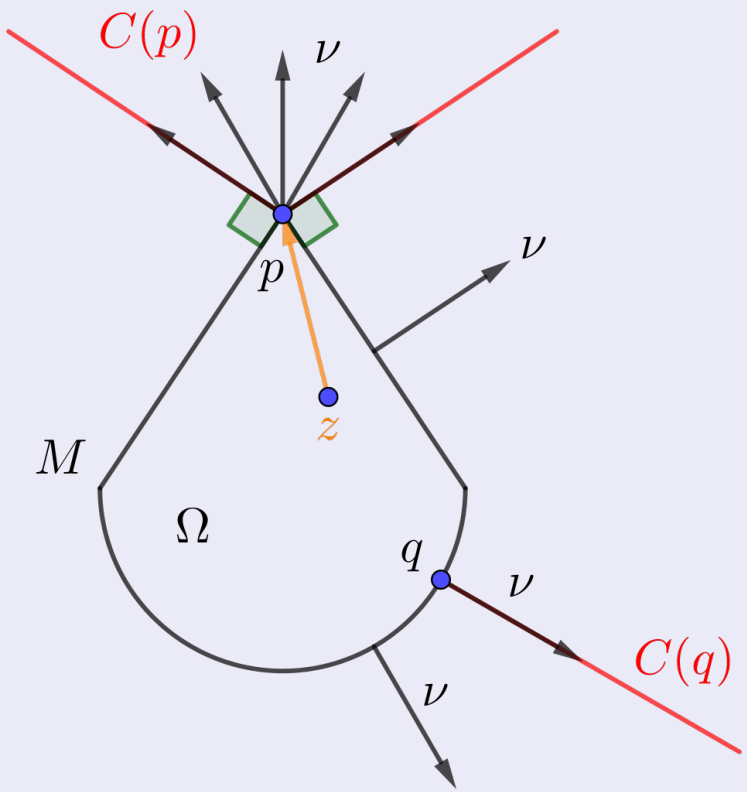
regular octahedron

- **Difficulty**: Equilibrium surfaces are **not** smooth. They have edges and vertices. Moreover, if the global minimizer has a flat face or a straight edge, then the anisotropic energy is **not** differentiable!
- **Our idea**: We adopt "multi-valued unit normal vector" at edges and vertices of considered surfaces.

Definition 1 (Multi-valued unit normal vector)

Let M be a piecewise-C^1 convex surface in $\mathbb{R}^3$. Denote by Ω the closed domain bounded by M. For a point p in M, a vector n is called an outer normal at p if n satisfies $\langle p - z, n \rangle \geq 0$ for any point z on Ω. $\nu(p) = n(p) / \|n(p)\|$ is called an outer unit normal at p. If $q \in M$ is a regular point of M, $\nu(q)$ is the usual outward-pointing unit normal at q.





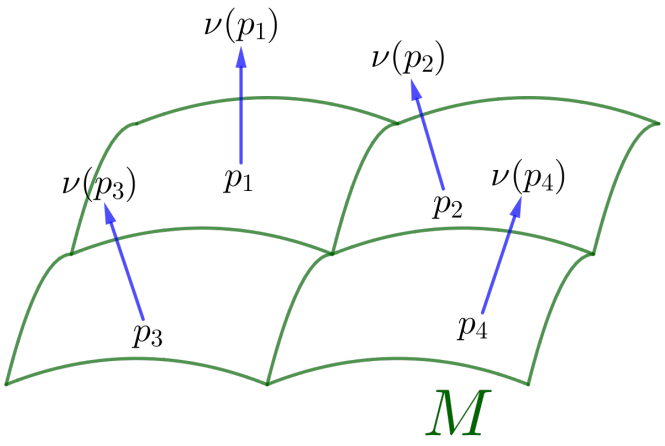
Anisotropic surface energy and the Wulff shape

- $\gamma : S^2 \to \mathbb{R}_{>0} := \{x \in \mathbb{R}; x > 0\}$: a positive continuous function
  ($S^2 = \left\{\nu \in \mathbb{R}^3; \|\nu\| = 1\right\}$: a unit sphere in $\mathbb{R}^3$)
  $\rightsquigarrow$ This γ is a mathematical model of anisotropic surface energy density.
- M: a piecewise smooth surface in $\mathbb{R}^3$
- $\nu : M \to$ " S^2 ": a (multi-valued) unit normal on M
- $\mathcal{F}_\gamma(M) := \int_M \gamma(\nu)\, dA$: the anisotropic energy of M
  (dA: the area element of M)
  Special case: $\gamma \equiv 1 \Rightarrow \mathcal{F}_\gamma(M)$: the area of the surface M

The following is known:

Fact 1 (J. E. Taylor, 1978)

There is a unique minimizer of $\mathcal{F}_\gamma$ among closed surfaces enclosing the same volume in $\mathbb{R}^3$ (up to translation). It is a convex surface which is called the Wulff shape or its homothety.



piecewise smooth surface M

Wulff shape W_γ

- $W_\gamma = \partial\left(\bigcap_{\nu\in S^2}\left\{X\in\mathbb{R}^3;\langle X,\nu\rangle\le\gamma(\nu)\right\}\right)$

Convex energy density function γ

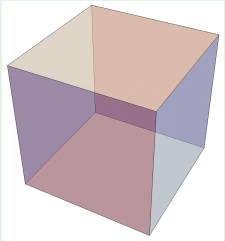
- $\forall W$: a convex closed surface in $\mathbb{R}^3$ with the origin inside,
  $\exists\gamma$: an energy density function s.t. W is the Wulff shape.
- γ is **not** necessarily unique.
- The smallest γ is called the support function of W.
- And its homogeneous extension to $\mathbb{R}^3$ is a convex function.

Remark 1

Assume W has a flat face f (resp. straight edge e). Then, γ is **not** differentiable at any $\nu\in S^2$ that is orthogonal to f (resp. to e).

Example 1

$\gamma(\nu) = |\nu_1| + |\nu_2| + |\nu_3| \quad\Rightarrow\quad W_\gamma$ is the cube.



Main theorem

Theorem 1 (Uniqueness of local minimizers for crystalline variational problems)

Let W be a regular polyhedron with the origin at the center. And let γ be the support function of W and let M be a piecewise-C^1 convex closed surface. Then, M is a local minimizer of $\mathcal{F}_\gamma(M) = \int_M \gamma(\nu)\, dA$ for all volume-preserving variations if and only if $M = W$ (up to homothety and translation).

Outline of the proof of the Main theorem

Assume

- W: a regular polyhedron
- $\gamma : S^2 \to \mathbb{R}_{>0}$: the support function of W
- η: the outer unit normals of W
- η is multi-valued on vertices and edges.

Assume

- M: a piecewise-C^1 surface
- ν: the outer (multi-valued) unit normals of M

A mapping

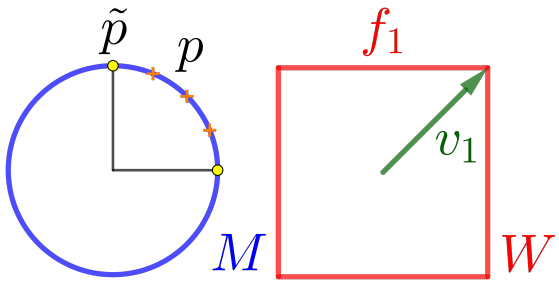
$\xi : M \to W$ (multi-valued) anisotropic Gauss map of M

is defined as follows:

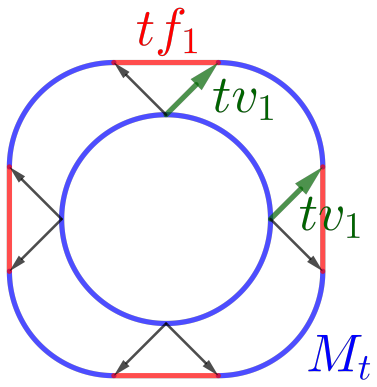
$$\xi(p) := \eta^{-1}(\nu(p)), \quad \forall p \in M.$$

Anisotropic parallel surfaces M_t of M are defined as

$$M_t(p) := p + t\xi(p), \quad p \in M.$$



$$\xi(p) = v_1,$$
$$\xi(\tilde{p}) = f_1.$$



Let M be a local minimizer of $\mathcal{F}_\gamma$ for all volume-preserving variations. We may assume $V(M) = V(W)$. Take $r(t) > 0$ so that $\tilde{M}_t := r(t) M_t$ satisfies $V\left(\tilde{M}_t\right) = V(M)$. Then, $\tilde{M}_0 = M$, and we can prove

$$\left.\frac{d\mathcal{F}_\gamma\left(\tilde{M}_t\right)}{dt}\right|_{t=0} \leq 0,$$

here "=" $\Leftrightarrow M = W$ (up to translation). Therefore, if M is a local minimizer of $\mathcal{F}_\gamma$, then M must coincide with W (up to translation), which proves the following.

Theorem 1 (Uniqueness of local minimizers for crystalline variational problems)

Let W be a regular polyhedron with the origin at the center. And let γ be the support function of W and let M be a piecewise-C^1 convex closed surface. Then, M is a local minimizer of $\mathcal{F}_\gamma(M) = \int_M \gamma(\nu)\, dA$ for all volume-preserving variations if and only if $M = W$ (up to homothety and translation).

Preceding research

The uniqueness of local minimizers was proved,

- for $W = S^n$, by Barbosa-do Carmo (1984).
- for W is smooth and strictly convex, by B. Palmer (1998).

Concluding remarks: We defined

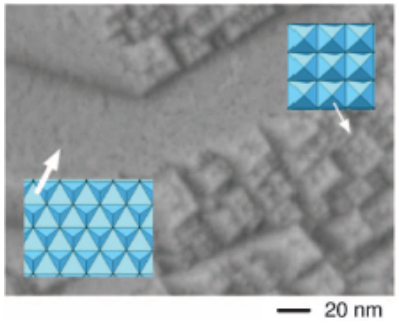
- anisotropic surface energy,
- multi-valued unit normals for piecewise-C^1 surfaces,
- multi-valued anisotropic Gauss map for piecewise-C^1 surfaces.

We proved:

- If the Wulff shape W_γ (the absolute minimizer) is a regular polyhedron, then any convex local minimizer is a homothety of W_γ.

Application to material science

- A single crystal of $\mathrm{CeO_2}$ usually forms a regular octahedron.
- Inner structure of nanocrystals of $\mathrm{CeO_2}$ in the water consists of regular octahedra and regular tetrahedra (Asahina, Takami, et al., 2011).
- If the energy density of $\mathrm{CeO_2}$ is convex, from the Main theorem, these regular tetrahedra are **not** single crystals of $\mathrm{CeO_2}$. $\Rightarrow$ They are expected to be air or water.



nanocrystals of $\mathrm{CeO_2}$
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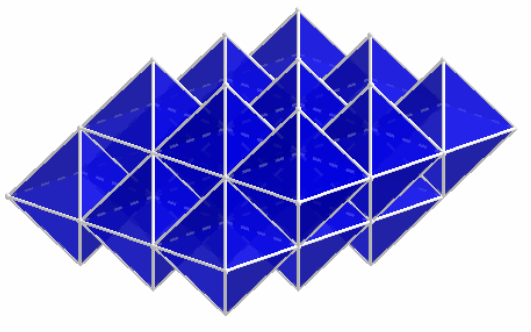
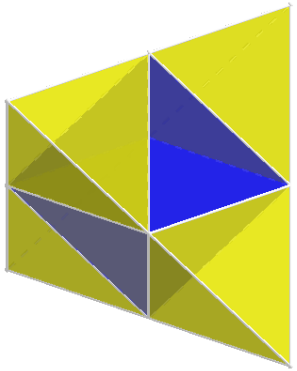


regular octahedra:
single crystals of $\mathrm{CeO_2}$



regular tetrahedra:
air or water

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