Visualization of Wulff's crystals

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Abstract. In this extended abstract, we deal with Wulff's construction and the graphical representation of Wulff's crystals and their surface energy functions as *potential surfaces*.

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INTRODUCTION

According to *Wulff's principle* [1], the shape of a crystal is uniquely determined by its surface energy function. A surface energy function is a real valued function depending on a direction in space.

Let ∂B^n denote the unit sphere in euclidean $\mathbb{R}^{n+1}$, that is,

$$\partial B^n = \left\{ \vec{x} = (x_1, x_2, \ldots, x_{n+1}) \in \mathbb{R}^{n+1} : \|\vec{x}\|_2 = \left(\sum_{k=1}^{n+1} x_k^2 \right)^{1/2} = 1 \right\},$$

and let $F : \partial B^n \to \mathbb{R}$ be a surface energy function. Then, we may consider the set $PM = \{\vec{x} = F(\vec{e})\vec{e} \in \mathbb{R}^{n+1} : \vec{e} \in \partial B^n\}$ as a natural representation of F.

If $n = 1$, then $\vec{e} = \vec{e}(u) = (\cos u, \sin u)$ for $u \in (0, 2\pi)$ and we obtain a *potential curve* with a parametric representation

$$PC = \{\vec{x} = f(u)(\cos u, \sin u) : u \in (0, 2\pi)\}, \text{ where } f(u) = F(\vec{e}(u)).$$

If $n = 2$, then

$$\vec{e} = \vec{e}(u^1, u^2) = (\cos u^1 \cos u^2, \cos u^1 \sin u^2, \sin u^1), \text{ for } (u^1, u^2) \in R = (-\pi/2, \pi/2) \times (0, 2\pi),$$

and we obtain a *potential surface* with a parametric representation

$$PS = \{\vec{x} = f(u^1, u^2)(\cos u^1 \cos u^2, \cos u^1 \sin u^2, \sin u^1) : (u^1, u^2) \in R\},$$

where $f(u^1, u^2) = F(\vec{e}(u^1, u^2))$.

WULFF'S PRINCIPLE AND PARAMETRIC REPRESENTATIONS FOR WULFF'S CRYSTALS

Wulff gave a geometric principle of construction for crystals [1].

Theorem 1 (Wulff's principle) *For every $\vec{e} \in \partial B^n$, let $E_{\vec{e}}$ denote the hyperplane orthogonal to $\vec{e}$ and through the point P with position vector $\vec{p} = F(\vec{e})\vec{e}$, and $H_{\vec{e}}$ be the half space which contains the origin 0 and has the boundary $E_{\vec{e}} = \partial H_{\vec{e}}$. Then, the crystal C_F which has F as its surface energy function is uniquely determined and given by $C_F = \bigcap_{\vec{e} \in \partial B^n} H_{\vec{e}} = \bigcap_{\vec{e} \in \partial B^n} \{\vec{x} : \vec{x} \bullet \vec{e} \leq F(\vec{e})\}$.*

Since Wulff's construction in Theorem 1 is far from applicable for the graphical representation of crystals, we give two results which are more useful.

Theorem 2 ([2, Theorem 5.3]) *Let $F : \partial B^n \to \mathbb{R}^+$ be a continuous function. Then, a point X is on the boundary ∂C_F of Wulff's crystal C_F corresponding to F if and only if $F(\vec{e}) \geq \vec{x} \bullet \vec{e}$ for all $\vec{e} \in \partial B^n$ and $F(\vec{e}_0) = \vec{x} \bullet \vec{e}_0$ for some $\vec{e}_0 \in \partial B^n$.*

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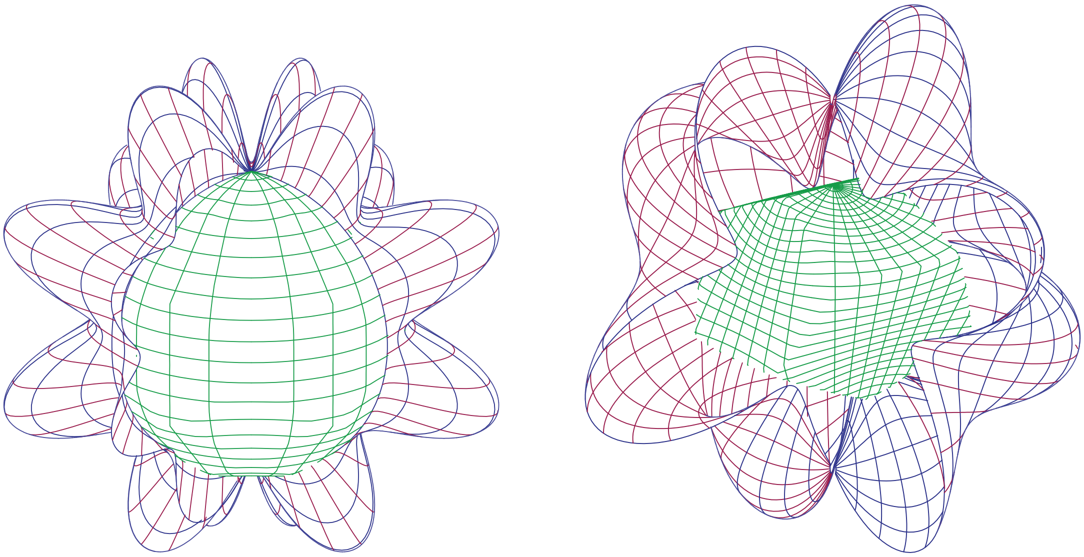

FIGURE 1. Wulff's crystals constructed by Theorems 2 and 3

Theorem 3 ([2, Theorem 5.4]) *Let $F : \partial B^n \to \mathbb{R}^+$ be a continuous function and $CF : \partial B^n \to \mathbb{R}^+$ be defined by*

$$CF(\vec{e}) = \inf\left\{F(\vec{u})(\vec{e} \bullet \vec{u})^{-1} : \vec{u} \in \partial B^n \text{ and } \vec{e} \bullet \vec{u} > 0\right\}.$$

Then, the boundary ∂C_F of Wulff's crystal corresponding to F is given by

$$\partial C_F = \{\vec{x} = CF(\vec{e})\vec{e} \in \mathbb{R}^{n+1} : \vec{e} \in \partial B^n\}; \tag{1}$$

in particular, if $n = 2$, then a parametric representation for the boundary ∂C_F of Wulff's crystal corresponding to F is

$$\vec{x}(u^1, u^2) = CF(\vec{e}(u^1, u^2))\vec{e}(u^1, u^2), \tag{2}$$

for $(u^1, u^2) \in R = (-\pi/2, \pi/2) \times (0, 2\pi)$.

Although we have used both Theorems 2 and 3 to develop algorithms and programmes for the graphic representation of Wulff's crystals, in some cases a parametric representation can explicitly be given for the boundary of a Wulff's crystal, that is, for the function CF. One such case is when the function F is equal to a norm in three–dimensional space. If $F = \|\cdot\|$, then the boundary of Wulff's crystal corresonding to F is given by the dual norm of $\|\cdot\|$.

Corollary 4 ([2, Corollary 5.5]) *Let $\|\cdot\|$ be a norm on $\mathbb{R}^{n+1}$ and, for each $\vec{w} \in \partial B^n$, let $\phi_{\vec{w}} : \mathbb{R}^{n+1} \to \mathbb{R}$ be defined by $\phi_{\vec{w}}(x) = \vec{w} \bullet \vec{x} = \sum_{k=1}^{n+1} w_k x_k$ ($\vec{x} \in \mathbb{R}^{n+1}$). Then, the boundary $\partial C_{\|\cdot\|}$ of Wulff's crystal corresponding to $\|\cdot\|$ is given by*

$$\partial C_{\|\cdot\|} = \left\{\vec{x} = \frac{1}{\|\phi_e\|^*} \cdot \vec{e} \in \mathbb{R}^{n+1} : \vec{e} \in \partial B^n\right\}, \tag{3}$$

where $\|\phi_{\vec{e}}\|^*$ is the norm of the functional $\phi_{\vec{e}}$, that is, the dual norm of $\|\cdot\|$.

Remark 5 *For $n = 2$, we obtain from (2) and (3) the following parametric representation for Wulff's crystal corresponding to a norm $\|\cdot\|$ in $\mathbb{R}^3$*

$$\vec{x}(u^1, u^2) = C_{\|\cdot\|}\left(\vec{e}(u^1, u^2)\right) \cdot \vec{e}(u^1, u^2) = \frac{1}{\|\phi_{\vec{e}}\|^*} \cdot \vec{e}(u^1, u^2), \text{ for } (u^1, u^2) \in R;$$

the potential surface has a parametric representation

$$\vec{y} = F(\vec{e}(u^1, u^2)) \cdot \vec{e}(u^1, u^2) = \|\vec{e}(u^1, u^2)\| \cdot \vec{e}(u^1, u^2), \text{ for } (u^1, u^2) \in R.$$

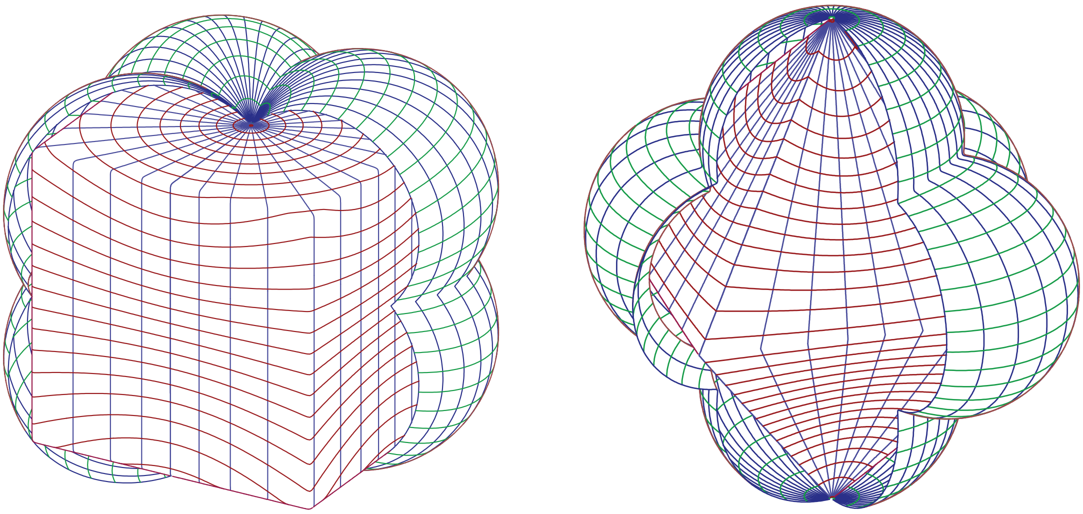

FIGURE 2. Wulff's crystals corresponding to the ℓ_1 and ℓ_∞ norms

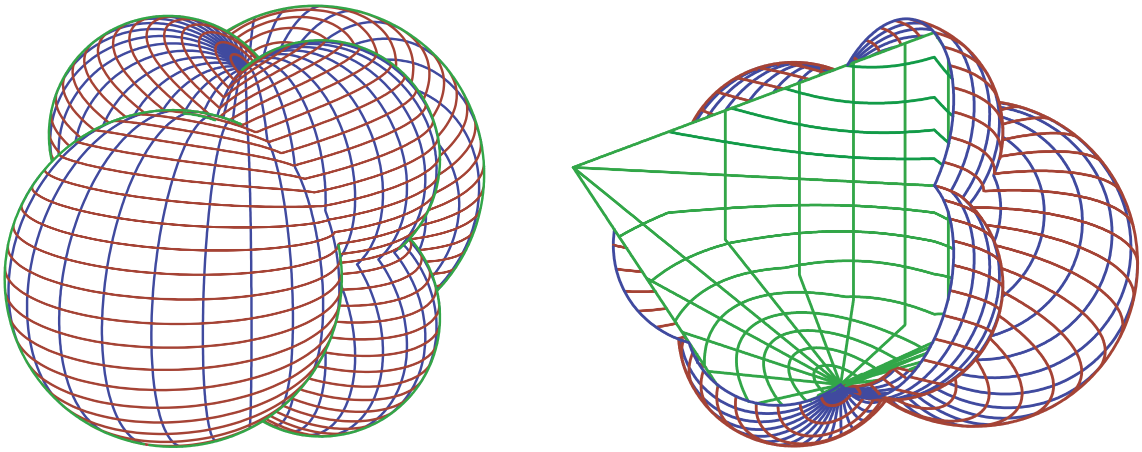

FIGURE 3. Potential surface of the $w_\infty(\Lambda)$ norm and potential surface with corresponding Wulff's crystal

Example 6 *As a first example, we represent the potential surfaces and corresponding Wulff's crystals for the ℓ_1 and ℓ_∞ norms $\|\cdot\|_1$ and $\|\cdot\|_\infty$ given by $\|\vec{x}\|_1 = |x_1| + |x_2| + |x_3|$ and $\|\vec{x}\|_\infty = \max_{1\le k\le 3}|x_k|$ for $\vec{x} = \{x_1, x_2, x_3\}$. The two pictures in Figure 2 are* dual *to one another.*

Example 7 *Finally, we represent some potential surfaces and the corresponding Wulff's crystals for the norm $\|\cdot\|_{w_\infty(\Lambda)}$ and for the dual norm $\|\cdot\|_{\mathscr{W}(\Lambda)}$* ([3, Proposition 5.3, Theorem 5.5])*. We identify the sequences $x = (x_k)_{k=1}^\infty$ with the three–dimensional vectors $\vec{x}$ given by their three–sections $x^{[3]}$, that is $\vec{x} = (x_1, x_2, x_3)$. We also choose $\Lambda = (1,2,3,4)$ in each picture (Figures 3 and 4).*

Further studies on Wulff's crystals and their graphical representations can be found in [4].

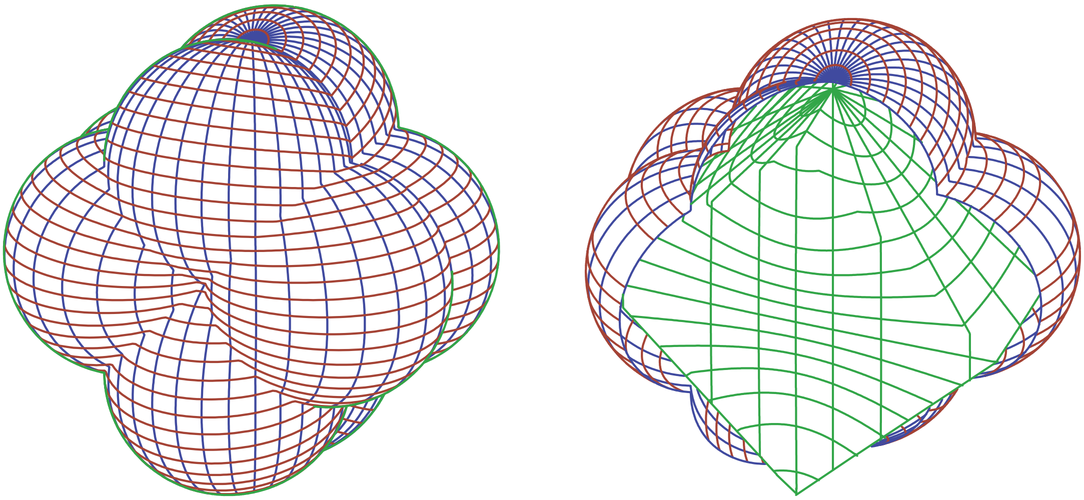

FIGURE 4. Potential surface of the $\mathscr{W}(\Lambda)$ norm and potential surface with corresponding Wulff's crystal

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