Geometric variational problems of statistical mechanics and of combinatorics

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Abstract

We present the geometric solutions of the various extremal problems of statistical mechanics and combinatorics. Together with the Wulff construction, which predicts the shape of the crystals, we discuss the construction which exhibit the shape of a typical Young diagram and of a typical skyscraper.

1 Introduction

1.1 Statistical mechanics

The variational problems of statistical mechanics we are going to discuss here are those related to the formation of a droplet or a crystal of one substance inside another. The question here is: what shape such a formation would take? The statement that such shape should be defined by the minimum of the overall surface energy subject to the volume constraint was known from the times immemorial. In the isotropic case, when the surface tension does not depend on the orientation of the surface, and so is just a positive number, the shape in question should be of course spherical (provided we

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neglect the gravitational effects). In a more general situation the shape in question is less symmetric. The corresponding variational problem is called the Wulff problem. Wulff formulated it in his paper [W] of 1901, where he also presented a geometric solution to it, called the Wulff construction (see section 2.2 below).

This Wulff construction was considered by the rigorous statistical mechanics as just a phenomenological statement, though the notion of the surface tension was among its central notions. The situation changed after the appearance of the book [DKS]. There it was shown that in the setting of the canonical ensemble formalism, in the regime of the first order phase transition, the (random) shape occupied by one of the phases has asymptotically (in the thermodynamic limit) a non-random shape, given precisely by the Wulff construction! In other words, a typical macroscopic random droplet looks very close to the Wulff shape. The results of the book [DKS] are restricted to the 2D Ising ferromagnet at low temperature, though the methods of the book are suitable for the rigorous treatment of much more general two-dimensional low-temperature models. Physical intuition is that as soon as there is phase coexistence, these results should be valid. It was proven in [I1, I2, IS] to be the case for the 2D Ising model at all subcritical temperatures. Some results for the higher dimensional case were obtained in [Be, CeH]. For the independent percolation the corresponding results were obtained in [ACC] for the 2D case, and in [Ce] in the 3D case.

1.2 Combinatorics.

The main content of the present paper concerns the problems arising in combinatorics, so in this section we describe some of them in more details.

A partition $p$ of an integer $N$ is a collection of non-negative integers $n_1 \geq n_2 \geq ... \geq n_k \geq ...$, such that $\sum_{i=1}^{\infty} n_i = N$. It can be specified by the sequence $\{r_k\}$ of integers, with $r_k = l$ iff exactly $l$ elements of $p$ equal $k$. It can also be described by the monotone function

$$\phi_p(y) = \sum_{k=\lceil y \rceil}^{\infty} r_k.$$ 

Its graph $G[\phi_p]$ provides a graphical description of $p$ and is called a (2D) Young diagram.
Similarly, a plane partition $P$ of an integer $N$ is a two-dimensional array of non-negative integers $n_{ij}$, such that for any $i$ we have $n_{i1} \geq n_{i2} \geq \ldots \geq n_{ik} \geq \ldots$, for any $j$ we have $n_{1j} \geq n_{2j} \geq \ldots \geq n_{kj} \geq \ldots$, while again $\sum_{i,j=1}^{\infty} n_{ij} = N$. One defines the corresponding function $\phi_P(y_1, y_2)$ in the obvious way. The function $\phi_P(y_1, y_2)$ is monotone in each variable. Its graph $G[\phi_P]$ is called a 3D Young diagram or a skyscraper.

Many more objects of a similar type can be defined. For example, one can put restrictions on how the steps of the stair $G[\phi_P]$ can look: they can not be longer than 3 units, and their heights can be only 1,2 or 5, say. The same freedom is allowed in 3D, and above.

Let us fix the number $N$, choose the kind of diagrams we are interested in, and consider the corresponding set $\mathcal{D}_N$ of all these diagrams. There are finitely many of them, so we can put a uniform probability distribution on $\mathcal{D}_N$. (Here, again, variations are possible.) The question now is the following: how the typical diagram from the family $\mathcal{D}_N$ looks like, when $N \to \infty$?

The first problem of that type was solved in the paper [VK], see also [V1, V2, DVZ]. It was found there, that the typical 2D Young diagram under statistics described above, if scaled by the factor $(1/\sqrt{N})$, tends to the curve

$$\exp\left\{-\frac{\pi}{\sqrt{6}} x \right\} + \exp\left\{-\frac{\pi}{\sqrt{6}} y \right\} = 1. \quad (1)$$

More precisely, for every $\epsilon > 0$ the probability that the scaled Young diagram would be within distance $\epsilon$ from the curve (1), goes to 1 as $N \to \infty$.

The heuristic way to obtain (1) (and similar results) is the following:

i) Let $A = (a_1, a_2), B = (b_1, b_2)$ be two points in $\mathbb{Z}^2$, with $a_1 < b_1, a_2 > b_2$. We can easily see that the number $\#(A, B)$ of lattice staircases, starting from $A$, terminating at $B$, and allowed to go only to the right or down, is given by

$$\binom{b_1-a_1+(a_2-b_2)}{(b_1-a_1)}.$$ 

Therefore one concludes by using the Stirling formula that

$$\lim_{|B-A| \to \infty} \frac{1}{|B-A|} \ln \#(A, B) = h(n_{AB}). \quad (2)$$

Here $n_{AB}$ is the unit vector, normal to the segment $[A, B]$, and for $n = (n_1, n_2), \alpha = \frac{n_1}{n_1+n_2}$, the entropy function $h(n) = - (\alpha \ln \alpha + (1-\alpha) \ln (1-\alpha))$.

ii) One argues that the number of Young diagrams of the area $N$ scaled by $\sqrt{N}$, “going along” the monotone curve $y = c(x) \geq 0$ with integral one,
is approximately given by

\[
\exp \left\{ \sqrt{N} \int h \left( \frac{-c'(x)}{\sqrt{1 + (c'(x))^2}}, \frac{1}{\sqrt{1 + (c'(x))^2}} \right) \sqrt{1 + (c'(x))^2} dx \right\}.
\]

(3)

\[\text{iii)}\) Assuming that indeed the model under consideration exhibits under a proper scaling some typical behavior, described by a nice smooth non-random curve (or surface) \(C\), one comes to the conclusion that the curve \(C\) should be such that the integral in (3), computed along \(C\), is maximal compared with all other allowed curves.

In general case one is not able to write down the corresponding entropy function precisely. The only information available generally is the existence of the limit of the type of (2), by a subadditivity argument. It should be stressed that even when the variational problem for the model is known, the main difficulty of the rigorous treatment of the model is the proof that indeed it does exhibit a nontrivial behavior after a proper scaling.

The above program was realized in [V1, V2], see also [DVZ], for the 2D case described above and for some other cases. In [B] a class of more general 2D problems was studied. The first 3D problem was successfully studied in [CKP]. The method of the last paper can also solve the skyscraper problem, as is claimed in [Ke].

When compared with the situation in statistical mechanics, the combinatorial program and its development look very similar. The only difference is that the counterpart of the Wulff construction was not designed in combinatorics, probably because there was no heuristic period there. In this note we fill this lack of parallelism by presenting such a construction. It provides, like the Wulff one, the geometric solution to the corresponding variational problem under minimal restrictions on the initial data, and also proves the uniqueness of the solution.

In the next section we first remind the reader about the Wulff minimizing problem (sect. 2.1) and the Wulff construction (sect. 2.2), which solves this problem, and then present the corresponding maximizing problem of combinatorics (sect. 2.3) and the geometric construction for its solution (sect 2.4), which is our main result. We give the proof in the section 3.

2 Statement of results
2.1 Wulff minimizing problem.

Let $S^d \subset \mathbb{R}^{d+1}$ denote the unit sphere, and let the real function $\tau$ on $S^d$ be given. We suppose that the function is continuous, positive: $\tau (\cdot) \geq \text{const} > 0$, and even: $\tau (n) = \tau (-n)$. Then for every hypersurface $M^d \subset \mathbb{R}^{d+1}$ we can define the Wulff functional

$$W_\tau (M^d) = \int_{M^d} \tau (n_x) \, ds_x,$$

(4)

Here $x \in M^d$ is a point on the manifold $M^d$, the vector $n_x$ is the unit vector parallel to the normal to $M^d$ at $x$, and $ds$ is the usual volume $d$-form on $M^d$, induced from the Riemannian metric on $\mathbb{R}^{d+1}$ by the embedding $M^d \subset \mathbb{R}^{d+1}$. Of course, we need to assume that the normal to $M^d$ is defined almost everywhere, i.e. that $M^d$ is smooth enough. Let now $D_q$ be the collection of all closed hypersurfaces $M^d$, embedded in $\mathbb{R}^{d+1}$, and such that the volume $\text{vol} (M^d)$ inside $M^d$ equals $q$. The Wulff problem consists in finding the lower bound of $W_\tau$ over $D_1$:

$$w_\tau = \inf_{M \in D_1} W_\tau (M),$$

(5)

as well as the minimizing surface(s) $W_\tau$, such that $W_\tau (W_\tau) = w_\tau$, if it exists. It turns out that the above variational problem indeed can be solved. It has a unique solution, which is given by the following

2.2 Wulff construction ([W]).

The minimizer $W_\tau$ can be obtained as follows. For every $n \in S^d$, $\lambda > 0$ define the half-space

$$L^<_\tau (n; \lambda) = \{ x \in \mathbb{R}^{d+1} : (x, n) \leq \lambda \tau (n) \},$$

(6)

and let

$$K^<_\tau (\lambda) = \bigcap_{n \in S^d} L^<_\tau (n; \lambda),$$

(7)

$$M_\tau (\lambda) = \partial (K^<_\tau (\lambda)).$$

(8)

The bodies $K^<_\tau (\lambda)$ are called Wulff bodies. We define $\lambda_1$ as the value of $\lambda$, for which $\text{vol} (M_\tau (\lambda)) = 1$. Then we define $W_\tau = M_\tau (\lambda_1)$. The surface $W_\tau$ is called the Wulff shape. This is the minimizer we are looking for.
The paper [12] contains a simple proof that \( W_\tau (W_\tau) \leq W_\tau (M) \) for every \( M \in D_1 \). The uniqueness of the minimizing surface is proven in [11]. It is known that in dimension 2 the minimizing surface \( W_\tau \) of the functional \( W_\tau \) is not only unique, but also is stable in the Hausdorff metric; for the proof, see [DKS], Sect. 2.4.

### 2.3 Maximizing problem.

In a dual problem we again have a function \( \eta \) of a unit vector, but this time it is defined only over the subset \( \Delta^d = S^d \cap \mathbb{R}^{d+1}_+ \) of them, lying in the positive octant. We suppose again that the function is continuous and nonnegative: \( \eta (\cdot) \geq 0 \). We assume additionally that

\[
\eta (n) \to 0 \text{ uniformly as } n \to \partial \Delta^d.
\]  

(9)

Let now \( G \subset \mathbb{R}^{d+1}_+ \) be an embedded hypersurface. We assume that for almost every \( x \in G \) the normal vector \( n_x \) is defined, and moreover

\[
n_x \in \Delta^d \text{ for a.e. } x \in G.
\]  

(10)

Then we can define the functional

\[
\mathcal{V}_\eta (G) = \int_G \eta (n_x) \, ds_x.
\]  

(11)

In analogy with the section 2.1 we introduce the families \( \bar{D}_q, q > 0 \), of such surfaces \( G \) as follows:

- \( G \in D_q \) iff
  - \( i) \) \( G \) splits the octant \( \mathbb{R}^{d+1}_+ \) into two parts, with the boundary \( \partial \mathbb{R}^{d+1}_+ \) belonging to one of them,
  - \( ii) \) the \(((d + 1))-dimensional\) volume of the body \( Q (G) \), enclosed between \( \partial \mathbb{R}^{d+1}_+ \) and \( G \), equals \( q \). In what follows we denote the volume of \( Q (G) \) by \( \text{vol} (G) \).

For example, let \( f (y) \geq 0 \) be a function on \( \mathbb{R}^{d}_+ \), non-increasing in each of \( d \) variables, and \( G [f] \subset \mathbb{R}^{d+1}_+ \) be its graph. Then

\[
\text{vol} (G [f]) = \int_{\mathbb{R}^{d}_+} f (y) \, dy,
\]  

(12)

so if \( \int_{\mathbb{R}^{d}_+} f (y) \, dy = q \), then \( G [f] \) is an element of \( \bar{D}_q \), provided the function \( f \) is sufficiently smooth.
Our problem now is to find the *upper bound* of $\mathcal{V}_\eta$ over $\bar{D}_1$:

$$v_\eta = \sup_{G \in \bar{D}_1} \mathcal{V}_\eta(G),$$  \hspace{1cm} (13)

as well as the maximizing surface(s) $V_\eta \in \bar{D}_1$, such that $\mathcal{V}_\eta(V_\eta) = v_\eta$, if possible. Note that the last problem differs crucially from (5), since here we are looking for the *supremum*. In particular, this upper bound evidently diverges if taken over all surfaces, and not only over "monotone" one, in the sense of (10), unlike in the problem (5).

It turns out that there exists a geometric construction, which provides a solution to the variational problem (13), in the same way as the Wulff construction solves the problem (5).

### 2.4 The main result.

For every $n \in \Delta^d, \lambda > 0$ define the half-space

$$L^\eta_\eta(n; \lambda) = \{ x \in \mathbb{R}^{d+1} : (x, n) \geq \lambda \eta(n) \},$$  \hspace{1cm} (14)

and let

$$K^\eta_\eta(\lambda) = \bigcap_{n \in \Delta^d} L^\eta_\eta(n; \lambda)$$  \hspace{1cm} (15)

$$G_\eta(\lambda) = \partial \left( K^\eta_\eta(\lambda) \right).$$  \hspace{1cm} (16)

Because of (8), the surfaces $G_\eta(\lambda)$ are graphs of functions, $f_\eta^\lambda(y), y \in \mathbb{R}^d$, i.e. $G_\eta(\lambda) = G[f_\eta^\lambda]$.

**Theorem 1** Suppose the integrals $\text{vol}(G_\eta(\lambda))$ (see (12)) are converging. Then the functional $\mathcal{V}_\eta$ has a unique maximizer, $V_\eta$, over the set $\bar{D}_1$. It is given by the above construction (16):

$$V_\eta = (G_\eta(\lambda_1)) \equiv G[f_\eta^\lambda_1],$$

where $\lambda_1$ satisfies $\text{vol}(G_\eta(\lambda_1)) = 1$, and the maximum of the functional $v_\eta = \mathcal{V}_\eta(V_\eta)$, (see (13)). If the integrals $\text{vol}(G_\eta(\lambda))$ diverge, then $v_\eta = \infty$.

As we already said in the introduction, in all known cases the heuristic arguments of the Section 1.2 turn out to be correct, and are validated by corresponding (sometime quite hard) theorems proven. For example, they are valid for the problem of finding the asymptotic shape of the Young diagram, described in the Section 1.2, as was proven in [VK, V1, V2]. Therefore, the following statement holds:
Corollary 2 In the notations of the theorem above, the curve \( \exp \left\{ -\frac{\pi}{\sqrt{6}} x \right\} + \exp \left\{ -\frac{\pi}{\sqrt{6}} y \right\} = 1 \) from the formula (4) coincides with the curve \( G_h(\lambda_1) \), given by our construction applied to the function \( \eta(n) = h(n) \) from the formula (3).

Of course, this statement can also be easily checked directly.

3 The proof of the Theorem.

We start with the case of finite volumes: \( \text{vol}(G_\eta(\lambda)) < \infty \) for all \( \lambda \).

We will prove our theorem by showing that for any surface \( G \in \bar{D}_1, G \neq V_\eta \), which coincides with \( G[V_\eta] \) outside some big ball around the origin of \( \mathbb{R}^{d+1} \), we have
\[
\mathcal{V}_\eta(G) > \mathcal{V}_\eta(V_\eta).
\]

First, we need more detailed notation than in the previous section. For every \( x \in \mathbb{R}^{d+1}, n \in S^d, \kappa > 0 \) we define the half-spaces
\[
L^>(x, n; \kappa) = \{ y \in \mathbb{R}^{d+1} : (y - x, n) \geq \kappa \}
\]
and the planes
\[
L^\equiv(x, n; \kappa) = \{ y \in \mathbb{R}^{d+1} : (y - x, n) = \kappa \}.
\]
Let \( C \subset \mathbb{R}^{d+1} \) be a convex set, and \( x \in C \). The support function \( \tau_{x,C}(\cdot) \) is defined by
\[
\tau_{x,C}(n) = \inf \{ \kappa : L^>(x, n; \kappa) \cap C = \emptyset \};
\]
we put \( \tau_{x,C}(n) = \infty \) if \( L^>(x, n; \kappa) \cap C \neq \emptyset \) for all \( \kappa \). We denote by \( K \) the convex set \( K^>\eta(\lambda = \lambda_1) \), introduced in (13), and we use the notation \( G \) for the surface \( \partial(K) \).

Let \( \varepsilon > 0 \). Introduce the set \( \mathbb{R}_{\varepsilon}^{d+1} = \{ y = (y_1, \ldots, y_{d+1}) \in \mathbb{R}_{\varepsilon}^{d+1} : y_i \geq \varepsilon \} \), and define \( K(\varepsilon) = K \cap \mathbb{R}_{\varepsilon}^{d+1}, G(\varepsilon) = \partial(K(\varepsilon)) \). The family of the subsets \( \tilde{G}(\varepsilon) \equiv (G(\varepsilon) \cap G) \subset G \) is increasing, with \( \bigcup_{\varepsilon > 0} \tilde{G}(\varepsilon) = G \).

Let \( N = N(\varepsilon) \) be so big, that the cube \( B_N = \{ y = (y_1, \ldots, y_{d+1}) \in \mathbb{R}_{\varepsilon}^{d+1} : 0 \leq y_i \leq N \} \) contains the set \( \tilde{G}(\varepsilon) \). We denote by \( x_N \) the vertex \( (N, \ldots, N) \) of this cube. Consider the convex set \( \bar{U} = B_N \cap K(\varepsilon) \). We are going to define with its help a function \( T_N(n) = T_{N,\varepsilon}(n) \) on \( S^d \). First, let \( n \in -\left( \Delta^d \right) \); in other words, \( n \)
has all coordinates non-positive. Note that by definition the support plane
\(L = (x_N, n; \tau_{x_N, \tilde{U}} (n))\) intersects the set \(\bar{G} (\varepsilon)\). In case when this intersection
contains “inner” points of \(\bar{G} (\varepsilon)\), i.e. points not in \(\partial \bar{G} (\varepsilon) \equiv G \cap \partial (\mathbb{R}_+^{d+1})\), we put

\[
T_N (n) = - (x_N, n) - \eta (-n) > 0, \tag{17}
\]

where \(\eta\) is our initial function (17). We use the same definition (17) for
remaining \(n\)-s in \(\Delta^d\), for which the intersection
\(L = (0, -n; \eta (-n)) \cap \bar{G} (\varepsilon) \neq \emptyset\).

For future use we denote the set of \(n\)-s, where the function \(T_N\) is already
defined, by \((-\Delta^d)\); note that \(\Delta^d \rightarrow \Delta^d\) as \(\varepsilon \rightarrow 0\). For the remaining \(n \in - (\Delta^d \setminus \Delta^d)\) we define \(T_N (n) = \tau_{x_N, \tilde{U}} (n)\). For \(n\)-s in \(\Delta^d \setminus \Delta^d\) the function
\(T_N (n)\) is defined by applying multiple reflections in the coordinate planes.
In other words, the values \(T_N (\pm n_1, \pm n_2, ..., \pm n_{d+1})\) do not depend on the
choice of signs. Analogously, we define the convex set \(U\) as the union of \(\tilde{U}\)
and all its multiple reflections in coordinate planes shifted by \(x_N\).

It follows from the definitions above that the set \(U\) is nothing else but
the shift of the Wulff body \(K^\varepsilon_{TN} (1)\) by the vector \(x_N\). According to what was
said in the section 2.2, for every \(M \in D_{\text{vol}(\partial U)\setminus \partial U}^\varepsilon, M \neq \partial U,\)

\[
\mathcal{W}_{TN} (\partial U) < \mathcal{W}_{TN} (M), \tag{18}
\]

Consider now an arbitrary hypersurface \(H\), such that \(\partial H = \partial \bar{G} (\varepsilon)\), while the
set \(\nu (H)\) of its unit normal vectors belongs to the subset \(\Delta^d \subset \Delta^d\) (which is
the case for the surface \(\bar{G} (\varepsilon)\) itself). Then for any such \(H\)

\[
\mathcal{V}_H (H) + \mathcal{W}_{TN} (H) = N \sqrt{d} \text{vol} \left( \pi \left( \partial \bar{G} (\varepsilon) \right) \right), \tag{19}
\]

where \(\pi \left( \partial \bar{G} (\varepsilon) \right)\) is the projection of the “curve” \(\partial \bar{G} (\varepsilon)\) (of codimension 2) on
the hyperplane \(\{y : y_1 + ... + y_{d+1} = 0\} \subset \mathbb{R}_+^{d+1}\), and where \(\text{vol} \left( \pi \left( \partial \bar{G} (\varepsilon) \right) \right)\)
is the ((\(d-1\))-dimensional) volume inside it. The relation (19) follows from
(17). Therefore the minimality property (18) of the functional \(\mathcal{W}_{TN}\) on the
surface \(\bar{G} (\varepsilon)\) implies the maximality property of the functional \(\mathcal{V}_H\) on the
same surface!

The uniqueness statement for \(\mathcal{V}_H\) is therefore a corollary of the uniqueness
for \(\mathcal{W}\).

It remains now to consider the question when the volumes \(\text{vol} (G_H (\lambda))\)
are infinite for all \(\lambda\). We are going to show that in that case \(v_H = \infty\). To make
things look simpler, we restrict ourselves to the 2D case. Let \( G \subset G_\eta(1) \) be an arc, and consider the “triangle” \( \Delta(G) \subset \mathbb{R}^2 \), made from all the points of all the segments joining the origin to the curve \( G : \)

\[
\Delta(G) = \bigcup_{x \in G} [0, x].
\]

It is straightforward to see that

\[
\text{vol}(\Delta(G)) = \frac{1}{2} \nu_\eta(G).
\]

We now will present the family \( G_\gamma \in \bar{D}_1 \), such that \( \nu_\eta(G_\gamma) \to \infty \) as \( \gamma \to 0 \). Namely, for every \( \lambda \) we define the number \( N(\lambda) \) to be the size of the square \( B(\lambda) = \{ y \in \mathbb{R}^2 : 0 \leq y_i \leq N(\lambda) \} \) for which \( \text{vol}(Q(G_\eta(\lambda)) \cap B(\lambda)) = 1 \), and we put \( G_\gamma \) to be the part of the boundary of the intersection \( Q(G_\eta(\gamma)) \cap B(\gamma) \), which is visible from the point \((2N(\gamma), 2N(\gamma))\), say. The curve \( G_\gamma \) consists of a certain arc \( \bar{G}_\gamma \) of the curve \( G_\eta(\gamma) \) and two small segments, joining its endpoints to the coordinate axes. By construction, \( \text{vol}(\Delta(\bar{G}_\gamma)) > \frac{1}{3} \). On the other hand, \( \text{vol}(\Delta(\bar{G}_\gamma)) = \frac{2}{3} \nu_\eta(\bar{G}_\gamma) \), which implies that

\[
\nu_\eta(\bar{G}_\gamma) > \frac{2}{3\gamma}.
\]

\[\blacksquare\]

4 Conclusion

In this paper we have described the explicit geometric construction, which predicts the asymptotic shape of some combinatorial objects. It is worth mentioning that the method presented should work whenever the underlying probability measure has certain locality property, namely that the distant portions of the combinatorial object under consideration are weakly dependent. This locality property is in fact the key feature behind the results obtained in the papers cited above. It also holds for the corresponding problems of statistical mechanics, like the validity of the Wulff construction, and is crucial there as well.

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