Thermodynamics and the moment map

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Abstract

We give a thermodynamic interpretation of the moment map for toric varieties. The convexity properties of this map correspond to thermodynamical principles (concavity of the entropy functional) applied to a system with several Hamiltonians.

0 Introduction.

This elementary note is an exercise in generalizing the standard (Maxwell-Bolzmann-Gibbs) approach to thermodynamics, to the case when the energy function is vector valued. This case is similar to that of several commuting Hamiltonians, familiar in the theory of integrable systems.

It turns out that the mean energy function of such “higher-dimensional thermodynamics” is basically the same as the moment map in the theory of toric varieties. Low-temperature limit of the standard theory generalizes to the “tropical limits” near vertices of the convex polytope given by the image of the moment map. Convexity properties of the moment map correspond to fundamental thermodynamic principles such as concavity of the entropy functional.

Relation of thermodynamics with tropical geometry have recently begun to attract some interest from various directions [3, 5]. In particular, the observation that tropical geometry corresponds, thermodynamically, to the low-temperature limit (in contrast with the name “tropical” which suggests the opposite) has been made by I. Itenberg and G. Mikhalkin in [3]. Consideration of vector inverse temperature as in this note, makes this observation even more clear.

I am grateful to G. Mikhalkin for stimulating discussions.
1 Reminder on usual thermodynamics (one Hamiltonian).

We start by reviewing the standard material on statistical thermodynamics, see [4, 7], with some extra emphasis on logical structure.

A. The Gibbs distribution. Consider a thermodynamical system such as a gas, with the (large but finite) set of states $A$. According to the fundamental principle of Boltzmann, the statistical behavior of the system is completely determined by the knowledge of the energies of various states, i.e., by the choice of a function $E : A \rightarrow \mathbb{R}$. To find this behavior, one forms the Boltzmann partition function

$$Z(\beta) = \sum_{\omega \in A} e^{-\beta E(\omega)}, \quad \beta = \frac{1}{kT},$$

where $T$ is the absolute temperature and $k$ is the Boltzmann constant. This is a finite sum of exponents, so it is well-defined and positive for all real values of $\beta$. The Gibbs probability distribution is given by

$$p_\omega(\beta) = \frac{e^{-\beta E(\omega)}}{Z(\beta)}, \quad \sum_\omega p_\omega(\beta) = 1.$$

The interpretation of $p_\omega(\beta)$ is as follows. Let us heat the system to temperature $T = 1/k\beta$ and wait till it arrives at a “thermodynamical equilibrium”. Then $p_\omega(\beta)$ is the probability that the system is at the state $\omega$.

By an observable we mean simply a function $O : A \rightarrow \mathbb{R}$. The Gibbs distribution gives rise to the mean value of $O$, which is a function

$$\langle O \rangle = \langle O \rangle(\beta) = \sum_{\omega \in A} p_\omega(\beta) \cdot O(\omega).$$

In particular, we have the mean value of the energy

$$\langle E \rangle(\beta) = \frac{\sum_{\omega \in A} E(\omega) \cdot e^{-\beta E(\omega)}}{\sum_{\omega' \in A} e^{-\beta E(\omega')}} = -\frac{d}{d\beta} \log Z(\beta).$$

Let $E_{\min}, E_{\max}$ be the minimal and maximal values of $E$. For simplicity assume that each of these values is attained at one state: $\omega_{\min}, \omega_{\max}$. In the low temperature limit $\beta \to +\infty$ the value $\langle E \rangle(\beta)$ approaches $E_{\min}$, as $p_{\omega_{\min}}(\beta)$ approaches 1. The state $\omega_{\min}$ usually has a clear physical meaning.
and is called the ground state. Similarly, in the other limit $\beta \to -\infty$ we have that $\langle E \rangle(\beta) \to E_{\text{max}}$. In fact, we have

**Proposition 1.5.** The function $\langle E \rangle(\beta)$ defines a monotone decreasing diffeomorphism from $\mathbb{R}$ to the open interval $(E_{\text{min}}, E_{\text{max}})$.

**Proof:** We need only to show that $\langle E \rangle(\beta)$ is monotone decreasing. But

$$\langle E \rangle'(\beta) = \frac{1}{Z(\beta)^2} \sum_{\omega, \omega' \in A} (-E(\omega)^2 + E(\omega)E(\omega')) e^{-\beta(E(\omega) + E(\omega'))}.$$  

For an unordered pair $\{\omega \neq \omega'\}$ the two coefficients at $e^{-\beta(E(\omega) + E(\omega'))}$ sum to $-(E(\omega) - E(\omega'))^2 \leq 0$, while for $\omega = \omega'$ the coefficient vanishes. So unless all the $E(\omega)$ are equal to each other, the derivative is strictly negative. \(\square\)

**B. Derivation of the Gibbs distribution.** For future convenience, we sketch here the classical derivation of (1.2). As many thermodynamical arguments, it assumes two levels of microscopicity. That is, although the set $A$ is already supposed to be very large, $|A| \gg 0$, and involve microscopic degrees of freedom, we now assume that we have a much larger number $N \gg |A|$ of “truly microscopic” particles which can be distributed among the states $\omega \in A$, possibly many at a time. Each such way of distributing particles is called a microstate.\(^2\) We further assume (this corresponds to the classical and not quantum approach to the problem) that the particles distributed are distinguishable from each other. This means that we can think of microstates as being sequences $\xi = (\xi_1, ..., \xi_N)$ of elements of $A$, forming the Cartesian power $A^N$.

Since we want to determine a probability distribution (measure) on $A$, consider first the space $\Delta^A$ of all such measures. This is a simplex of dimension $|A| - 1$. Fix an arbitrary $p = (p_\omega)_{\omega \in A} \in \Delta^A$ and equip $A^N$ with the product measure. For a microstate $\xi \in A^N$ as above let $N_\omega(\xi) = |\{i : \xi_i = \omega\}|$ be the number of particles in the state $\omega$, so the observed probability of being in the state $\omega$ (observed at $\xi$) is $q_\omega(\xi) = N_\omega(\xi)/N$. Fix a partition $N = \sum_{\omega \in A} n_\omega$, $n_\omega \in \mathbb{Z}_+$. Then the set of $\xi \in A^N$ such that $N_\omega(\xi) = n_\omega$ has

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\(^1\)This is not the high temperature limit but rather the non-physical limit of $T$ approaching 0 from the negative direction. The limit $T \to +\infty$ corresponds to $\beta \to 0$, when all the states become equally probable.

\(^2\) The “thermostat” in standard discussions of equilibrium thermodynamics is a device for producing these microstates.
the measure (probability)

\[ N! \prod_{\omega \in A} \frac{p_{\omega}^{n_{\omega}}}{n_{\omega}!}, \]

as the measure of any single such \( \xi \) is \( \prod p_{\omega}^{n_{\omega}} \), while the number of these \( \xi \) is the multinomial coefficient. Using the Stirling approximation

\[ \log(n!) \sim n(\log(n) - 1), \quad n \gg 0, \]

we approximate the logarithm of (1.6) by

\[ N \sum_{\omega \in A} q_{\omega}(\log(p_{\omega}) - \log(q_{\omega})), \quad q_{\omega} = n_{\omega}/N. \]

Notice the following fact.

**Lemma 1.8.** Let \( p \in \Delta^A \) be given. Then

\[ \max_{q \in \Delta^A} \sum_{\omega \in A} q_{\omega}(\log(p_{\omega}) - \log(q_{\omega})) = 0, \]

and the maximum is achieved for \( q = p \).

**Proof:** The function of \( q \in \Delta^A \) which we seek to maximize, is concave, approaches \(-\infty\) at the boundary and has a critical point at \( q = p \), which must then be the absolute maximum. \( \square \)

Therefore, the most probable microstates will be those \( \xi \) for which each \( q_{\omega}(\xi) = p_{\omega} \). Such \( \xi \) are called *equilibrium microstates*. In the case when the \( p_{\omega} = n_{\omega}/N \) are rational, their number is the multinomial coefficient, which we interpolate for arbitrary \( p \in \Delta^A \), using the Gamma function, by

\[ N(\log(N) - 1) - \sum_{\omega} Np_{\omega}(\log(Np_{\omega}) - 1)) = -N \sum_{\omega} p_{\omega} \log(p_{\omega}). \]

\[ ^3\]This is, essentially, the law of large numbers of probability theory. Up to now, consideration of microstates was formally identical with that of \( N \) independent trials of a random event such as a roll of dice.
Recall that for a probability distribution $p \in \Delta^A$ its *entropy* is defined as
\begin{equation}
S(p) = -\sum_{\omega \in A} p_\omega \log(p_\omega).
\end{equation}

The function $S$ is a concave function on the simplex $\Delta^A$, equal to 0 at the boundary, and achieving the maximim at the barycenter. Thus, thermodynamically,
\begin{equation}
S \approx \frac{\log(\text{Number of equilibrium microstates})}{N}, \quad N \gg |A|.
\end{equation}

Now, the main thermodynamic principle used to deduce the Gibbs distribution is that the number of equilibrium microstates should be as large as possible, while maintaining the desired mean value of energy. That is, take a point $E \in (E_{\text{min}}, E_{\text{max}})$ and look at all probability distributions $p \in \Delta^A$ satisfying
\begin{equation}
\langle E \rangle_p := \sum_{\omega} p_\omega E(\omega) = E.
\end{equation}

The above principle implies (1.2) in virtue of the following fact.

**Proposition 1.13.** Among the distributions $p$ satisfying (1.12), the maximal entropy is achieved by the Gibbs distribution $p(\beta)$, where $\beta \in \mathbb{R}$ is the unique number such that $\langle E \rangle(\beta)$ as defined by (1.4), is equal to $E$.

**Proof:** The constraint (1.12) defines a hyperplane section of the simplex $\Delta^A$, a convex polytope, denote it $P$. The restriction $S|_P$ is a strictly concave function, equal to 0 at the boundary. So it has a unique critical point inside $P$, and this point is the global maximum. By the Lagrange multiplier method, this critical point is characterized as a point $p \in \Delta^A$ which satisfies the constraint (lies in $P$) and at which the differential of $S$ is proportional to the differential of the constraint. On $\Delta^A$ we have $\sum_{\omega} dp_\omega = 0$, therefore $dS = -\sum_{\omega} \log(p_\omega)dp_\omega$, and the condition of proportionality reads:
\begin{equation}
-\sum_{\omega} \log(p_\omega)dp_\omega = \lambda \sum_{\omega} E(\omega)dp_\omega.
\end{equation}

But this condition is satisfied by $p_\omega = p_\omega(\beta)$ as defined in the statement of the proposition, with $\lambda = \beta$. Indeed, $\log p_\omega(\beta) = -\beta E(\omega) - \log Z(\beta)$, so in virtue of $\sum_{\omega} dp_\omega = 0$, the LHS of (1.14) is equal to $\beta \sum_{\omega} E(\omega)dp_\omega$. \qed
C. Entropy, energy and temperature. One can object that the above derivation of the Gibbs distribution (1.2) is somewhat circular. It does explain, from clear principles, the behavior of \( p = (p_\omega)_{\omega \in A} \) as a function of the mean energy \( E \), but not of \( \beta \) or of temperature. In fact, \( E \) and \( \beta \) are supposed to be related by the formula (1.4) which depends on (1.2). This is not surprising since we have not used any meaningful features of the concept of “temperature”.

A mathematically satisfying way of dealing with this issue is to consider the temperature as a secondary quantity, and to define it in terms of more fundamental quantities such as energy. A standard definition like this (see, e.g., [4]) says that the inverse temperature (i.e., \( \beta \)) is “the derivative of the entropy with respect to the energy”. Mathematically, this definition (or, rather, its consistency) amounts to the following general fact about exponential sums.

**Proposition 1.15.** Consider \( \beta \) as a function of \( E \in (E_{\min}, E_{\max}) \) by inverting the diffeomorphism of Proposition 1.5. Let \( S(E) \) be the entropy of the Gibbs distribution \( p(\beta(E)) \). Then \( dS/dE = \beta(E) \).

In particular, \( S(E) \) is a concave function on \([E_{\min}, E_{\max}]\), equal to 0 at both ends, with the derivative at these points being \( \pm \infty \).

**Proof:** This is an immediate consequence of the identification of \( \beta \) with the Lagrange multiplier in (1.14). Indeed, for any constrained maximum problem \( \max_{g(x) = c} f(x) \) the value of the Lagrange multiplier \( \lambda = \lambda(c) \) has the interpretation as the derivative, with respect to \( c \), of the constrained maximum value (this derivative is called, in the language of applied math, the “effective price of the resource represented by the constraint”, see, e.g., [6]).

2 Thermodynamics with several Hamiltonians.

A. The Gibbs distribution for several Hamiltonians. We now assume that the set of states \( A \) is equipped with not one, but several “energy functionals” \( E_1, \ldots, E_n : A \to \mathbb{R} \), which we combine into one vector valued function \( E : A \to \mathbb{R}^n \). To these energy functionals there correspond \( n \) “inverse temperatures” \( \beta_1, \ldots, \beta_n \), which we combine into one vector quantity \( \beta \) lying in the dual space \( \mathbb{R}^{n*} \).

For simplicity we assume that \( E \) defines an embedding of \( A \) into \( \mathbb{R}^n \). We can then think of \( A \) as being a subset of \( \mathbb{R}^n \) to begin with, and sometimes
drop $E$ from the notation, thinking of it as just the inclusion map. With these conventions, we write the partition function and the Gibbs distribution

$$Z(\beta) = \sum_{\omega \in A} e^{-(\beta, \omega)}, \quad p_\omega(\beta) = \frac{e^{- (\beta, \omega)}}{Z(\beta)}, \quad \beta \in \mathbb{R}^{n^*}.$$  

As in (1.3), the Gibbs distribution can be used to define the mean value of any observable $O$ on $A$. In particular, taking for $O$ the vector valued function (embedding) $E : A \to \mathbb{R}^n$, we have the mean energy map

$$\langle E \rangle : \beta \mapsto -\langle E \rangle(\beta) = \frac{\sum_{\omega \in A} \omega \cdot e^{-(\beta, \omega)}}{\sum_{\omega' \in A} e^{- (\beta, \omega')}} = -\nabla_{\beta} \log Z(\beta).$$

Here $\nabla_{\beta}$ means the vector of gradient with respect to $\beta$, i.e., the differential of a function considered as a vector in the dual space. Thus $\langle E \rangle : \mathbb{R}^{n^*} \to \mathbb{R}^n$. Let $Q \subset \mathbb{R}^n$ be the convex hull of $A$, and $Q^0$ be the interior of $Q$. Since $(p_\omega(\beta))_{\omega \in A}$ is a probability distribution on $A$ with all components nonzero, we see that $\langle E \rangle$ maps $\mathbb{R}^{n^*}$ into $Q^0$. We can now generalize the thermodynamic formalism of the previous section as follows.

**Proposition 2.3.** (a) The map $\langle E \rangle : \mathbb{R}^{n^*} \to Q^0$ is a diffeomorphism.

(b) For any $E \in Q^0$ let $P_E$ be the set of probability distributions $p \in \Delta^A$ satisfying the constraints

$$\langle E \rangle_p := \sum_{\omega \in A} p_\omega \cdot \omega = E.$$  

Let $\beta(E) \in \mathbb{R}^{n^*}$ be unique such that $\langle E \rangle(\beta) = E$. Then the Gibbs distribution $p(\beta) = (p_\omega(\beta))$ defined above, has maximal entropy among all the distributions from $P_E$.

(c) Let $S(E)$ be the entropy of the distribution $p(\beta(E))$. Then $\nabla_{E} S(E) = \beta(E)$.

(d) The functions $-\log Z(\beta)$ on $\mathbb{R}^{n^*}$ and $S(E)$ on $Q^0 \subset \mathbb{R}^n$ are concave and are the Legendre transforms of each other.

Note that part (b) shows that the “vector” Gibbs distribution (2.1) has the same thermodynamic significance as the more standard one (1.2).

The proof of the proposition will be given later in this section.
B. Example: toric varieties and the moment map. Assume that \( A \) lies in \( \mathbb{Z}^n \subset \mathbb{R}^n \). The exponential \( e^{-(\beta, \omega)}, \omega \in A \), then becomes a Laurent monomial \( z^\omega = \prod z_i^{\omega_i} \) in the variables \( z_i = e^{-\beta_i} \). Real values of \( \beta \) correspond to \( z \in \mathbb{R}^*_+ \), where \( \mathbb{R}^*_+ \) is the set of positive real numbers.

The monomial \( z^\omega \) makes sense for any \( z \in (\mathbb{C}^*)^n \). Consider the complex vector space \( \mathbb{C}^A \) with basis \( e^\omega, \omega \in A \) and let \( \mathbb{P}^A \) be its projectivization. A vector of \( \mathbb{C}^A \) is thus a tuple \((a_\omega)_{\omega \in A}\). The torus \((\mathbb{C}^*)^n\) acts on \( \mathbb{C}^A \) and \( \mathbb{P}^A \) by

\[
z \cdot e_\omega = z^\omega e_\omega.
\]

In particular, we consider the orbit \( X_\Lambda^+ \subset \mathbb{P}^A \) of the point represented by \( 1 = (1)_{\omega \in A} \in \mathbb{C}^A \) and let \( X_\Lambda \subset \mathbb{P}^A \) be the projective toric variety defined as the closure of \( X_\Lambda^+ \).

Assume for simplicity that \( A \) generates \( \mathbb{Z}^n \) as an affine lattice, i.e., there is no smaller integer affine sublattice in \( \mathbb{Z}^n \) containing \( A \). Then the action of \( \mathbb{C}^n \) on \( \mathbb{P}^A \) is faithful, in particular, the action map

\[
z \mapsto z \cdot 1 = (z^\omega)_{\omega \in A}
\]

identifies \((\mathbb{C}^*)^n\) with \( X_\Lambda^+ \). This image is known as the positive part of the toric variety \( X_\Lambda \). Clearly, \( X_\Lambda^+ \) consists of the points of the form \( x(\beta) = (e^{-(\beta, \omega)})_{\omega \in A} \) for all \( \beta \in \mathbb{R}^{n*} \).

The action of the compact part \((S^1)^n\) of the torus \((\mathbb{C}^*)^n\) on the projective space \( \mathbb{P}^A \) preserves the standard Fubini-Study Kähler metric and gives rise to the moment map

\[
\mu_P : \mathbb{P}^A \to \mathbb{R}^n, \quad (a_\omega)_{\omega \in A} \mapsto \frac{\sum_{\omega \in A} \omega \cdot \|a_\omega\|^2}{\sum_{\omega \in A} \|a_\omega\|^2},
\]

see, e.g., [2]. The image of this map is the polytope \( Q = \text{Conv}(A) \). Let \( \mu_X^+ \) be the restriction of \( \mu_P \) to \( X_\Lambda^+ \). Using the above parametrization of \( X_\Lambda^+ \) by the \( x(\beta) \), we write \( \mu_X^+ \) as a map from \( \mathbb{R}^{n*} \) to \( Q \), and find that

\[
\mu_X^+(\beta) = \frac{\sum_{\omega \in A} \omega \cdot e^{-(2\beta, \omega)}}{\sum_{\omega \in A} e^{-(2\beta, \omega)}} = \langle E(2\beta) \rangle
\]

is nothing but the mean energy of the twice scaled \( \beta \), with respect to the Gibbs distribution (2.1). Proposition 2.3(a) reduces then to the well known fact about toric varieties: that the moment map defines a diffeomorphism from the positive part to the interior of the defining polytope, see [1], [2].
C. Direct and inverse images of concave functions. To give a natural proof of Proposition 2.3, we start with some general remarks. By a convex body we will mean a convex subset $P$ of some finite-dimensional affine space $V$ over $\mathbb{R}$. For such $P$ we denote by $\text{Conc}(P)$ the space (semigroup) of concave functions $f : P \to \mathbb{R}$ which are proper, i.e., such that each level set $f^{-1}(c)$ is compact. Any such function achieves a maximum on $P$.

By an admissible embedding of convex bodies $i : P' \to P$ we mean an injective map induced by an affine embedding of ambient affine spaces $V' \hookrightarrow V$, so that $P' = V' \cap P$. In this case for any $f \in \text{Conc}(P)$ we have the inverse image (restriction) $i^* f = f|_{P'}$ which again lies in $\text{Conc}(P')$.

Similarly, by an admissible surjection of convex bodies $j : P \to P''$ we mean a surjective map induced by an affine surjection $J : A' \to A''$ of ambient affine spaces. In this case for any $f \in \text{Conc}(P)$ we have the direct image which is the function $j_* f$ on $P''$ defined by

$$ (j_* f)(p'') = \max_{j(p) = p''} f(p). $$

**Example 2.7.** One can take $P = V$ to be a finite-dimensional vector space over $\mathbb{R}$ and $f$ to be a negative definite quadratic form on $V$. Then, for any linear surjection $j : V \to V''$, the direct image $j_* f$ is a negative definite quadratic form on $V''$. The integration, along the fibers of $j$, of the Gaussian function $e^{f(p)}$ on $V$ gives, up to a constant, the Gaussian function $e^{(j_* f)(p'')}$. On $V''$.

For a general $f \in \text{Conc}(P)$ and an admissible surjection $j : P \to P''$ the function $e^{j_* f}$ is the leading term, as $h \to 0$, of the function on $P''$ obtained by integrating $e^{f(p)/h}$ along the fibers of $j$.

The following is then elementary.

**Proposition 2.8.** (a) The function $j_* f$ belongs to $\text{Conc}(P'')$.

(b) (Base change) Let

$$
\begin{array}{ccc}
P_2 & \xrightarrow{i} & P_1 \\
\downarrow j_2 & & \downarrow j_1 \\
P'_2 & \xrightarrow{i'} & P'_1
\end{array}
$$

be a Cartesian square of convex bodies, such that $i, i'$ are admissible embeddings and $j_1, j_2$ are admissible surjections. Then for any $f \in \text{Conc}(P_1)$ we have the equality $(j_1)_* i^* f = (i')^* (j_2)_* f$ of concave functions on $P'_2$. \qed
D. Proof of Proposition 2.3. Consider the admissible surjection of convex bodies

\[ \pi : \Delta^A \rightarrow Q, \quad p \mapsto \langle E \rangle_p = \sum_{\omega \in A} p_\omega \cdot \omega. \]

Fix \( E \in Q^0 \). The fiber \( \pi^{-1}(E) \) is the set \( P_E \) of part (b) of the proposition. Consider the entropy function \( S \in \text{Conc}(\Delta^A) \) defined by (1.10). It is strictly concave, so the restriction of \( S \) to \( \pi^{-1}(E) \) achieves maximum at a unique interior point; denote this point \( \tilde{p}(E) \). This point is, furthermore, the unique critical point of \( S \) on \( \pi^{-1}(E) \). Consider also the direct image function \( \pi_* S \in \text{Conc}(Q) \).

The location of the critical point can be found by the Lagrange multiplier method for \( n \) constraints: the differential of \( S \) at \( \tilde{p}(E) \) should be a linear combination of the differentials of the individual scalar constraints, i.e., to have the form \( (\lambda, d\pi) \) for some \( \lambda \in \mathbb{R}^n \). Further, we have the \( n \)-constraint interpretation of the Lagrange multipliers as minus the partial derivatives of the maximal value with respect to the constraints, see again [6]. This means that \( \lambda = \lambda(E) \) is equal to the gradient (differential) of the strictly convex function of \( \pi_* S \) at the point \( E \).

Next, look at the Gibbs distribution \( p(\lambda(E)) \). We see that \( p(\lambda(E)) \) is a critical point of \( S \) on \( \pi^{-1}(E) \), so it is equal to \( \tilde{p}(E) \). This implies that \( \lambda(E) = \beta(E) \) is the inverse to the map \( \beta \mapsto \langle E \rangle(\beta) \) which is therefore a diffeomorphism, thus proving part (a) of the proposition. In particular, the function \( S(E) \) of part (c) is the same as \( \pi_* S \). Since \( p(\lambda(E)) = \tilde{p}(E) \), this implies part (b). Part (c) follows since \( \lambda(E) = \nabla_E(\pi_* S) \) by definition. Finally, the Legendre transform relation between the functions \( -\log Z(\beta) \) and \( S(E) = \pi_* S \) in part (d) is equivalent to the fact that their gradients define mutually inverse diffeomorphisms, as we have shown that \( \langle E \rangle = \nabla_\beta(-\log Z) \) is inverse to \( \nabla_E(\pi_* S) \).

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