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Tropical limit in statistical physics

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ABSTRACT

Tropical limit for macroscopic systems in equilibrium defined as the formal limit of Boltzmann constant $k \to 0$ is discussed. It is shown that such tropical limit is well-adapted to analyze properties of systems with highly degenerated energy levels, particularly of frustrated systems like spin ice and spin glasses. Tropical free energy $F_{tr}(T)$ is a piecewise linear function of temperature T, tropical entropy is a piecewise constant function and the system has energy for which tropical Gibbs' probability has maximum. Properties of systems in the points of jump of entropy are studied. Systems with finite and infinitely many energy levels and phenomenon of limiting temperatures are discussed.

1. Introduction

Singular (nonanalytic) limits of various types have shown up many times in physics and mathematics. Maslov's dequantization [1–3], ultra-discrete integrable systems [4–8] and tropical geometry [9–13] are three apparently disconnected fields where such a limit was most actively studied during the last twenty years. Nowadays all of them are viewed as the different faces of the so-called tropical mathematics (see e.g. [14–16]). Tropical limit is characterized by a highly singular limiting behavior of the type $x = \exp\left(\frac{x_{tr}}{\varepsilon}\right)$ as the parameter $\varepsilon \to 0$. Elements x_{tr} form an idempotent semiring with the tropical addition $\oplus$ and multiplication $\odot$ defined by $x_{1tr} \oplus x_{2tr} = \lim_{\varepsilon\to 0}\left(\varepsilon \ln\left(\exp\frac{x_{1tr}}{\varepsilon} + \exp\frac{x_{2tr}}{\varepsilon}\right)\right) = \max\{x_{1tr}, x_{2tr}\}$ and $x_{1tr} \odot x_{2tr} = \lim_{\varepsilon\to 0}\left(\varepsilon \ln\left(\exp\frac{x_{1tr}}{\varepsilon}\cdot \exp\frac{x_{2tr}}{\varepsilon}\right)\right) = x_{1tr} + x_{2tr}$ [9–16].

It was already noted in [13,17–21] that statistical physics seems to be the part of physics most naturally adapted to consider the tropical limit. Indeed, free energy F of the macroscopic system in equilibrium is given by the formula [22]

$$F = -kT \ln \sum_n g_n \exp\left(-\frac{E_n}{kT}\right) \tag{1.1}$$

where k is the Boltzmann constant, T is the absolute temperature, $\{E_n\}$ is the energy spectrum of the system, g_n are statistical weights (degeneracies) of the corresponding levels E_n and the sum is performed over different energy levels. Thus, in the limit $kT \to 0$ one has the tropical sum in the r.h.s. of the formula (1.1) and E_n and $F(kT \to 0)$ become elements of idempotent semiring referred to in [21] as the thermodynamic semiring. In the papers [13,19–21] the tropical limit was identified with the limit $T \to 0$. With such a choice tropical free energy is equal to E_{min} and entropy $S_{tr} = 0$ for the systems with finite g_n.

In this paper we argue that the formal limit $k \to 0$ is a more appropriate avatar of tropical limit in statistical physics. At first glance the separation of k and T seems to be artificial and irrelevant since the r.h.s. of (1.1) and Gibbs' distribution

$$w_n = \frac{\exp\left(-\frac{E_n}{kT}\right)}{\sum_m g_m \exp\left(-\frac{E_m}{kT}\right)} \tag{1.2}$$

contain only the product kT. It is indeed so for systems with finite g_n.

An observation is that there exists a wide class of systems with exponentially large degeneracies g_n for which the situation is quite different. In 1935 L. Pauling [23] showed that the degeneracy of the ground state of the ice is given by $g_0 = \exp(N \ln \frac{3}{2})$, where N is the number of molecules. So the ice has (residual) entropy $S_0 \sim kN \ln \frac{3}{2}$ at $T = 0$ that is in good agreement (with 2–3% accuracy) with experimental data [24]. Several other systems like spin ices and spin glasses have exponentially large degeneracies of ground and excited states of the type $g_n = \exp(a_n N)$ with certain constants a_n (see e.g. [22,25–33]). In the thermodynamic limit $N \to \infty$ such g_n have a typical tropical behavior. A natural way to formalize this limit is to represent exponentially large degeneracies as $g_n = \exp\frac{S_n}{k}$ with finite S_n and $k \to 0$. Physically it corresponds to the limit $N \to \infty$, $k \to 0$ with $k \cdot N =$constant (gas constant R) and $S_n = a_n R$.

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Thus, representing the degeneracies g_n as $g_n = \exp\frac{S_n}{k}$ and defining $F_{tr} = \lim_{k\to 0} F$, one has at $T > 0$

$$F_{tr}(T) = -T\sum_n \oplus\left(-\frac{F_n}{T}\right) = \min\{F_1, F_2, \dots, F_n, \dots\} \qquad (1.3)$$

where $F_n = E_n - TS_n$ is a "microscopic" free energy associated with the energy level E_n. So $F_{tr}(T)$ is a piecewise linear function of temperature T. This leads to various consequences. For instance, the tropical entropy $S_{tr} = -\frac{\partial F_{tr}}{\partial T} = S_{n_{min}}$ where n_{min} is the index of minimal free energy $F_{n_{min}}$ at temperature T in the case when the minimum is attained only once. So S_{tr} is a piecewise constant function of T. The value $S_{tr}(T=0)$ is the residual entropy of the macroscopic system at $T=0$. At certain singular values of T S_{tr} exhibits jumps (entropy drop). Depending on the system it happens either at positive or negative temperatures.

These properties of the tropical limit $k\to 0$ trace quite well certain characteristic features of various frustrated systems similar to spin ices and spin glasses. In contrast in the tropical limit defined as $T\to 0$ [13,19–21] one has $F(T\to 0) = E_1$ and the above-mentioned properties are not visible.

This is the main evidence in favor of the definition of the tropical limit as $k\to 0$. The second reason is that in such a limit the basic thermodynamic equations, like the first law $dE = TdS - pdV$ and relations between thermodynamic potentials, remain unaltered leaving temperature T to be a free positive or negative parameter. In addition the limit $k\to 0$ resembles very much that of $\hbar\to 0$ in Maslov's dequantization.

Tropical limit of Gibbs' distribution (1.2) has rather interesting properties too. Tropical probability $w_{n,tr} = \lim_{k\to 0}(k\cdot\ln w_n)$ takes values in the interval $(-\infty, 0]$ and is equal to

$$w_{n,tr} = -S_n + \frac{F_{tr} - F_n}{T}. \qquad (1.4)$$

The tropical probability $W_{n,tr}$ for the system to have energy E_n is

$$W_{n,tr} = w_{n,tr} + S_n = \frac{F_{tr} - F_n}{T} \qquad (1.5)$$

and it is normalized by the condition $\sum_n \oplus W_{n,tr} = 0$.

These tropical Gibbs' distributions describe fine structure of the states with exponentially small usual probabilities $w_n \sim \exp\left(-\frac{S_n}{k}\right)$. It is shown that tropical probabilities and entropy have a peculiar behavior at the singular values T^* of temperature at which jump of S_{tr} is observed.

Systems with finitely many energy levels are considered as illustrative examples. Tropical limit of the systems with infinite number of energy levels, the phenomenon of limiting temperatures and existence of intervals of forbidden temperatures are discussed too.

It is noted that the limit $k\to 0$ viewed as the limit of vanishing white noise for systems with finite degeneracies has been discussed in a different context in [34].

The paper is organized as follows. In Section 2 general definitions and formulas are presented. Singularities appearing in tropical limit are analyzed in next Section 3. Systems with finite number of energy levels are considered in Section 4. In Section 5 the systems with infinitely many energy levels bounded and unbounded from below and the existence of limiting temperatures are discussed.

2. Tropical Gibbs' distribution and free energy

So we will consider macroscopic systems in equilibrium and will study their limiting behavior as (formally) $k\to 0$. Introducing the energy level "entropy" $S_n = k\ln g_n$ and assuming that S_n are finite, one has the following form of partition function

$$Z = \sum_{n\geq 1}\exp\left[\frac{1}{k}\left(S_n - \frac{E_n}{T}\right)\right] = \sum_{n\geq 1}\exp\left(-\frac{F_n}{kT}\right) \qquad (2.1)$$

where $F_n \equiv E_n - TS_n$ is the "energy-level" free energy and energies E_n are ordered as $0 < E_1 < E_2 < \dots$. One observes that the degeneracies $g_n = \exp\frac{S_n}{k}$ with finite $S_n > 0$ and Boltzmann weights $\exp\left(-\frac{E_n}{kT}\right)$ behave quite differently as $k\to 0$. So in the tropical limit we will have sort of Bergmann's logarithmic limit set [35].

Tropical limit of probability w_n, in general, is naturally associated with its singular behavior of the form $w_n = \tilde{w}_n\cdot\exp\frac{w_{n,tr}}{\varepsilon}$ with small positive parameter ε, $0 < \tilde{w}_n \leq 1$ and $w_{n,tr} = \lim_{\varepsilon\to 0}(\varepsilon\ln w_n)$. Tropical probability $w_{n,tr}$ varies in the interval $(-\infty, 0]$. The interval $0 < w_n \leq 1$ collapses into $\{0\}$ while exponentially small usual probabilities w_n are represented by the whole semi-line $(-\infty, 0)$ for $w_{n,tr}$ and numbers $\tilde{w}_n$. The meaning of the quantities $w_{n,tr}$ and $\tilde{w}_n$ is clarified by the formula $\ln w_n = \frac{w_{n,tr}}{\varepsilon} + \ln\tilde{w}_n + \dots$. So singular behavior under consideration is characterized by a simple pole behavior of $\ln w_n$ as a function of the small parameter ε: $w_{n,tr}$ is the residue at this pole while $\ln\tilde{w}_n$ is the first regular nondominant term. In generic regular case it is sufficient to consider the dominant pole term and, hence, the tropical probability $w_{n,tr}$. Contribution of nondominant term $\ln\tilde{w}_n$ becomes crucial, as we shall see, in the singular situations when limit $\varepsilon\to 0$ ceases to be uniquely defined.

Under the assumption that all F_n are distinct the tropical limit of Gibbs' probabilities (1.2) is given by ($\varepsilon = k$)

$$\begin{aligned} w_{n,tr} &= -\frac{E_n}{T} - \max\left\{-\frac{F_1}{T}, -\frac{F_2}{T}, \dots\right\} \\ &= -S_n - \frac{F_n}{T} + \min\left\{\frac{F_1}{T}, \frac{F_2}{T}, \dots\right\} \end{aligned} \qquad (2.2)$$

Denoting $\left(\frac{F}{T}\right)_{min} := \min\left\{\frac{F_1}{T}, \frac{F_2}{T}, \dots\right\}$, one gets

$$w_{n,tr} = -S_n - \frac{F_n}{T} + \left(\frac{F}{T}\right)_{min}. \qquad (2.3)$$

Normalization condition for these tropical probabilities is the limit $k\to 0$ of the condition $\sum_n g_n\cdot w_n = 1$ and it is given by

$$\sum_n \oplus\left(S_n + w_{n,tr}\right) = 0. \qquad (2.4)$$

In particular, for $n = n_0$ such that $\frac{F_{n_0}}{T} = \left(\frac{F}{T}\right)_{min}$, one has

$$w_{n_0,tr} = -S_{n_0}. \qquad (2.5)$$

So, the entropies S_{n_0} are, in fact, the tropical Gibbs' probabilities to find the system in certain state with energy E_{n_0}. Probability W_n for the system to have energy E_n at small k and $T > 0$ is equal to $W_n = g_n\exp\frac{w_{n,tr}}{k} = \exp\frac{W_{n,tr}}{k}$ and, hence, tropical probability $W_{n,tr}$ for the system to have energy E_n is equal to

$$W_{n,tr} = \frac{F_{tr} - F_n}{T}. \qquad (2.6)$$

These tropical probabilities obey the normalization condition $\sum_n \oplus W_{n,tr} = \max\{W_{n,tr}\} = 0$. Also in the limit $k\to 0$ for usual probabilities one gets $W_{n_0} = 1$ and $W_{n\neq n_0} = 0$ and the tropical energy E_{tr} of the system is

$$E_{tr} = \lim_{k\to 0}\left(\sum_{n\geq 1} W_n E_n\right) = E_{n_0}. \qquad (2.7)$$

The tropical Gibbs' distribution provides us with the fine description of the energy levels.

Tropical limit of the free energy (1.1) is given by