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The infinite limit as an eliminable approximation for phase transitions

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A B S T R A C T

It is generally claimed that infinite idealizations are required for explaining phase transitions within statistical mechanics (e.g. Batterman 2011). Nevertheless, Menon and Callender (2013) have outlined theoretical approaches that describe phase transitions without using the infinite limit. This paper closely investigates one of these approaches, which consists of studying the complex zeros of the partition function (Borrmann et al., 2000). Based on this theory, I argue for the plausibility for eliminating the infinite limit for studying phase transitions. I offer a new account for phase transitions in finite systems, and I argue for the use of the infinite limit as an approximation for studying phase transitions in large systems.

1. Introduction

It is generally claimed that infinite idealizations are necessarily required for explaining phase transitions within statistical mechanics. For example, Kadanoff demands: "The existence of a phase transition *requires an infinite system*. No phase transitions occur in systems with a finite number of degrees of freedom" (2000, p. 238. My emphasis). This assertion underlies many discussions concerning emergence and reduction in statistical mechanics (Batterman, 2005, 2011; Liu, 1999, 2001; Jones, 2006; Mainwood, 2006; Morrison, 2012 among others), such as Batterman's (2011):

> Consider phase transitions and critical phenomena [...]. Such qualitative changes of state, as I will argue below, *cannot be reductively explained* by the more fundamental theories of statistical mechanics. They are indeed *emergent phenomena*. The reason for this (rather dramatic) negative claim has to do with the fact that such changes *require certain infinite idealizations*. (p. 1033. My emphases)

The core of the argument is that statistical mechanics is not capable of describing phase transitions without using infinite idealizations. Phase transitions cannot be explained by statistical mechanics with finite systems only and, accordingly, they are claimed to be emergent phenomena.

Nevertheless, Menon and Callender (2013) have recently pointed out theoretical approaches that attempt to describe phase transitions without using the infinite limit. Such approaches might lead to a revision of the antireductionist views about thermodynamics:

> [A]re phase transitions actually explanatorily irreducible? The answer hangs on whether de-idealization can be achieved within finite-*N* statistical mechanics. We believe that it can be. We have already hinted at one possibility. (2013, p. 211)

Menon and Callender propose that phase transitions might not be emergent phenomena or, at least, that they are compatible within a broadly construed reductionist project. To show this compatibility, they present several theoretical approaches capable of accounting for phase transitions in finite systems without the infinite limit. However, Menon and Callender do not aim at investigating these approaches in detail, but rather at giving only an overview. In this paper, I deal with Menon and Callender's proposal in depth. For that purpose, I focus on one of these theories, which studies phase transitions from the distribution of zeros of the complex partition function in finite systems (Borrmann, Mülken & Harting, 2000). Based on this theory, I claim that the elimination of the infinite limit for studying phase transitions in statistical mechanics is highly plausible. In addition, I examine the consequences

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of this theory for the concept of phase transition, and I clarify how the infinite limit is an approximation. More generally, this paper offers a new account for phase transitions in finite systems without using the infinite limit.

The paper is organized as follows. First, I explain why the infinite limit is widely claimed to be ineliminable for studying phase transitions (PTs) in statistical mechanics (Section 2). Then, I give an overview my main claim about the eliminability of the infinite limit in PTs, and I contextualize it within the literature (Section 3). Next, I stress the need for a theory of PTs without the infinite limit by tackling the question of PTs in small systems (Section 4). I then investigate such a possible finitisitic theory, viz. the theory of finite distribution of zeros (Section 5). The next section is then devoted to discuss several applications of this theory to provide evidence for its viability and interest to describe PTs (Section 6). Finally, I investigate the consequences of this theory with regard to the concept of PT. Based on the relationship between this theory and Yang-Lee's approach, I argue for the use of the infinite limit as an approximation for PTs when finite systems are large (Section 7).

2. Ineliminability of the infinite limit and Yang-Lee's theory

To properly situate my argument, I must first clarify why the infinite limit is usually claimed to be ineliminable for studying PTs within statistical mechanics (SM). In thermodynamics, the mathematical signatures of PTs are singularities for thermodynamic potentials. For example, within the Ehrenfest classification, first order PTs correspond to a discontinuity in the first derivative of a thermodynamic potential; second order PTs occur when there is a discontinuity in a second derivative; and, so on. In SM, PTs are described with the partition function Z used to define thermodynamic potentials like the free energy $F = -k_B \ln(Z)$. The main point is that this free energy F exhibits singularities only within the thermodynamic limit.

Justifying the mandatory use of the thermodynamic limit usually involves referring to the works of Yang and Lee (1952), Fisher (1965), and Grossmann and Rosenhauer, 1967, Grossmann, 1968, Grossmann and Rosenhauer, 1969a, Grossmann and Lehmann, 1969b on the zeros of the partition function. For example, according to Jones (2006), “The idealizations that occur in the [Yang-Lee] accounts of phase transitions […] are ineliminable”(p. ii). Or similarly, according to Mainwood (2006), “Perhaps the clearest example of the ineliminability of the infinite nature of the models is to be found in Lee-Yang theory”(p. 7). This section is dedicated to introduce this theory since its importance in the literature. In addition, as it will become clear below, this introduction foreshadows how a theory of PTs without the infinite limit can be built (see Section 5).

2.1. Infinite limit and non-analyticities

For the sake of simplicity, let us illustrate Yang and Lee formalism on the case of a model of N spins in the canonical ensemble.[1] The energy of the system can take the values $E = n\varepsilon$ with $n = 0, 1, 2, \ldots, M$. The partition function is:

$$Z_N(z) = \sum_{n=0}^{M} g(n) z^n \tag{1}$$

where $g(n)$ is the number of microstates corresponding to the n^{th} energy level and $z = e^{-\beta\varepsilon}$. Since the $g(n)$ are positive, there are not any zeros of $Z_N(z)$ that can be real and positive. However, the partition function has complex zeros z_n as it appears when it is factorized as:

$$Z_N(z) = \kappa \prod_{n=1}^{M} \left(1 - \frac{z}{z_n}\right) \tag{2}$$

with κ a constant that will be taken equals to 1. These zeros generally lie in the complex plane away from the positive real axis. Let us then define the complex free energy per spin for all complex z except the points $z = z_n$ as:

$$h_N(z) =_{def} \frac{\ln(Z_N)}{N} = \frac{1}{N} \sum_{n=1}^{M} \ln\left(1 - \frac{z}{z_n}\right) \tag{3}$$

These free energies $h_N(z)$ are regular complex functions around all points $z \neq z_n$ since they can be expanded in Taylor series. They can be differentiated infinitely many times. Under these conditions, it becomes clear that the infinite limit is required to possibly obtain singularities for $h_N(z)$. Blythe and Evans (2003) make this point clear:

> Since we identify a phase transition through a *discontinuity* in a derivative of the free energy, we see that such a transition can only occur at a point z_0 in the complex plane *if there is at least one zero of the partition function* $Z_N(z)$ within any arbitrarily small region around the point z_0. Clearly this scenario is *impossible if the number of zeros M is finite*, except at the isolated points z_n where the free energy exhibits a logarithmic singularity. Since such a point cannot lie on the positive real z axis, there is *no scope for a phase transition in a finite spin system*, such as the simple example (Eq. (1)). On the other hand, if the partition function zeros accumulate towards a point z_0 on the real axis as *we increase the number of spins N to infinity* there is the possibility of a phase transition. (Blythe & Evans, 2003, p. 465. My emphases)

It is impossible for the partition function Z_N to vanish since it is a sum of non-vanishing functions. Therefore it becomes impossible for $\ln(Z_N)$, and thus F_N to exhibit non-analyticities. The only possibility – but still not guaranteed – for the free energy F_N to diverge is that N tends to infinity.[2]

2.2. Defining phase transitions with the density of zeros

Yang-Lee formalism not only requires the use of the thermodynamic limit to recover PTs within SM it also, as will be seen now, provides an account for PTs by studying these zeros of the complex partition function.

In order to recover PTs, the free energy is taken within the thermodynamic limit. Accordingly, it is defined by rewriting the finite sum as an integral as follows:

$$h(z) = \lim_{N\to\infty} h_N(z) = \int dz' \rho(z') \ln\left(1 - \frac{z}{z'}\right) \tag{4}$$

[1] This section is based on Blythe and Evans (2003, p. 464). Mainwood (2006, p. 214) also introduces Yang-Lee's approach in this way. See also Butterfield and Bouatta (2012, pp. 8–10).

[2] Similarly, according to Le Bellac, Mortessagne, & George Batrouni, 2004: “For finite N, Z_N is an analytic function of z which does not vanish, so that $\ln(Z)$ and all thermodynamic functions are analytic functions of z. Since a phase transition is characterized by non-analytic behaviour of the thermodynamic functions, it can only occur in the thermodynamic limit N to infinity.” (Le Bellac et al. 2004, p. 182).

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