The infinite limit as an eliminable approximation for phase transitions

Vincent Ardourel

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Abstract 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, we argue for the plausibility for eliminating the infinite limit for studying phase transitions. We offer a new account for phase transitions in finite systems, and we argue for the use of the infinite limit as an approximation for studying phase transitions in large systems.

Keywords infinite idealizations · phase transitions · finite systems · ineliminability · approximation · zeros of partition function

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. Our emphasis). This assertion underlies many discussions concerning emergence and reduction in statistical mechanics (Battermann 2005, 2011; Liu 1999, 2001, Jones 2006, Mainwood 2006 among others), such as Batterman's (2011):

> Consider phase transitions and critical phenomena. Such qualitative changes of state, as we will argue below, *cannot be reductively explained*

V. Ardourel
Université catholique de Louvain, ISP – CEFISES
E-mail: vincent.ardourel@gmail.com

> 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. Our 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, we deal with Menon and Callender's proposal in depth. For that purpose, we focus on one of these theories, which studies phase transitions from the distribution of zeros of the complex partition function in finite systems (Borrmann et al. 2000). Based on this theory, we claim that the elimination of the infinite limit for studying phase transitions in statistical mechanics is highly plausible. In addition, we examine the consequences of this theory for the concept of phase transition, and we 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, we explain why the infinite limit is widely claimed to be ineliminable for studying phase transitions (PTs) in statistical mechanics (Section 2). Then, we give an overview our main claim about the eliminability of the infinite limit in PTs, and we contextualize it within the literature (Section 3). Next, we stress the need for a theory of PTs without the infinite limit by tackling the question of PTs in small systems (Section 4). We 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, we 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, we 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 our argument, we 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 coworkers (1967, 1968, 1969a, 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 $E = n\epsilon$ with $n = 0, 1, 2, ..., M$. 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 $z = e^{-\beta\epsilon}$. 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:

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

[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).

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:

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

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 and Evans 2003, p. 465. Our 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:

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

[2] Similarly, according to Le Bellac (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) where $\rho(z)$ is the local density of zeros in the complex plane. Consequently, the study of the expression of $h(z)$ allows a characterization of PTs. For that purpose, a potential $\phi(z)$ is defined as the real part of the complex free energy. It can be shown that it satisfies the equation:

$$\rho(z) = \frac{1}{2\pi}\nabla^2\phi(z) \tag{5}$$

which is analogous to an equation from electrostatics between the density of electric charges and the electrostatic potential. Blythe and Evans (2003) show that the characterization of phase transitions is derived from this analogy. The potential function $\phi(z)$ of two complex regions ϕ_1 and ϕ_2 satisfies some continuity conditions at the boundary. A linear density $\mu(s)$ of zeros along the curve – parametrized by the arc length s along the curve – is then defined from which PTs are characterized (see Fig. 1). PTs occur at $s = 0$. More precisely,

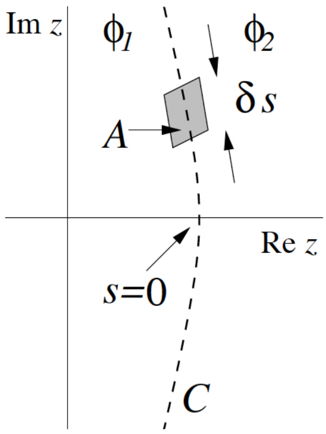

Fig. 1 Two complex potential functions separated by a dense line of zeros of the partition function. The phase transition occurs when the arc length s equals zero. Figure extracted from (Blythe and Evans 2003, p. 466).

it is shown that *first order* PTs occur when the curve of zeros is parallel to the imaginary axis close to $s = 0$, and are characterized by a certain value of $\mu(0)$. For *second order* PTs, the curve also becomes a straight line close to $s = 0$ but with an angle, and the density $\mu(s)$ decreases linearly to zero when approaching the transition $s = 0$. For n^{th} *order* PTs ($n > 2$), the curve approaches the real axis at angle $\pi/(2n)$, and the density $\mu(s)$ varies with s^{n-1}.

Thus, Yang-Lee formalism allows us to recover the singularities of the free energy, and thereby the PTs of thermodynamics by studying the zeros of the partition function. It also allows us to understand why the thermodynamic limit is required to obtain such singularities: PTs are characterized by *real-valued singularities* of the partition function, which can only appear in the infinite limit.[3]

Rather surprisingly, as we will argue below in Section 5, it is nevertheless possible to develop an approach for studying PTs *without* the infinite limit from Yang-Lee formalism. But before discussing this approach, let us clearly explain the motivation of our project in this paper.

3 Idealization, approximation, and eliminability

This section provides an overview of our main claim on PTs and contextualizes it within the literature. To put it succinctly, we claim that *it is highly plausible to eliminate the infinite limit to study PTs in SM.* The rest of the paper will be essentially dedicated to argue for this claim.

To begin with, let us recall a recent debate on the role of the infinite limit in PTs. As we have seen in the Introduction, Batterman (2005, 2011), among others, argues that infinite *idealizations* are required to describe PTs within SM, which allows him, in turn, to claim that PTs are emergent phenomena. This position contrasts with the ones promoted by Butterfield (2011) and Norton (2012). They claim that PTs do not actually require infinite idealizations. In particular, they distinguish between the use of *limit systems*, which are systems with infinite components and accordingly that involve infinite idealizations, and the use of *limit properties* or *limit quantities*, which are the limits of some properties or quantities of the system.[4] In that case, some functions are evaluated in the limit but without assuming that the system is infinite. This corresponds to the infinite *approximations* of Norton's terminology.

According to Butterfield and Norton, SM only requires limit quantities and limit properties for studying PTs, and not limit systems. Accordingly, there are no infinite idealizations. However, since they agree with the mandatory use of the infinite limit for studying PTs, they maintain a kind of ineliminability claim for defining PTs in SM. With Norton's terminology, one would claim that infinite *approximations* cannot be eliminated. Our claim is more radical: we will argue that not only infinite idealizations but even infinite approximations are eliminable, or at least, that this elimination is highly plausible.

[3] Mainwood (2006), who argues for the ineliminability of the infinite limit for studying PTs, emphasizes the importance of this Yang-Lee formalism:

> This sort of analysis of the density of zeroes in the complex plane, and thereby the nature of the singularities in the free energy, tells us a great deal about how the derivatives of the free energy behave in the TD limit. Since in statistical mechanics, macroscopic quantities are obtained from derivatives of the free energy, this in turn yields information about the properties of a substance as it approaches a phase transition [...] Yet the Lee-Yang analysis also shows clearly that a phase transition – defined as a discontinuity in the free energy – cannot appear in a finite N system of the type considered. (Mainwood 2006, p. 218)

[4] Butterfield (2011) uses the term 'quantity' and Norton uses the term 'property' but the distinction is similar. See (Shech 2015, p. 1066).

Our analysis thus will contrast with both Butterfield and Norton as follows. Their indispensabilist claim comes from the analysis of the *traditional* theory of PTs, with which we perfectly agree. In Section 7, we will label the concept of PTs at stake as *thermodynamic* PTs. Instead, our elimininativist claim will be based on an *unconventional* theory of PTs that does not appeal at all to the infinite limit, namely the finite DOZ approach of PTs (see Section 5). It will involve a concept of *finite* PTs that will be clarified and contrasted with thermodynamic PTs in Section 7.[5] Finally, it has to be noted that even if one does not endorse the claim that infinite limits in PTs are approximations, and still maintains that they are idealizations, our analysis remains useful. It supports an account of infinite idealizations in PTs as "Galilean idealizations", i.e. idealizations that can be de-idealized, such as a frictionless plane in the models of classical mechanics (McMullin 1985).

Let us make clear a related point with regard to the debate on PTs and the infinite limit. Butterfield (2011), based on Mainwood's (2006) work, defends a twofold claim. One the one hand, some behaviours in PTs are *deducible* from the SM *in the infinite limit*. Singularities and non-analyticities of some thermodynamic quantities can only be deduced with the infinite limit, as we have seen with the Yang-Lee theory. In that sense, the infinite limit is indispensable – even if it is not an idealization. On the other hand, these behaviours can be understood "more weakly" and occur before the infinite limit (Butterfield 2011, p. 1129). For instance, as the number N of spins increases, the change in the magnetization in an Ising model occurs more and more abruptly. In that sense, emergent behaviours can occur before the limit.

Butterfield therefore endorses a definition on PTs in N-finite systems provided by Mainwood (2006, p. 238). Although the free energy F_N of a N-finite system S has no singularities, "Phase transitions occur for a finite system in state S if and only if $F_\infty(S)$ has a singularity." PTs are thus defined as behaviours of *finite* systems that require quantities, however, to be taken in the infinite limit. According to Mainwood, this definition allows him to avoid Callender's (2001) paradox of phase transitions.[6] Nevertheless, he mentions a possible difficulty (Mainwood 2006, p. 242). This definition would allow PTs to occur in very small systems, such as a lattice of four Ising spins (since F_∞ of such a small system would have a singularity). However, extra requirements might be added in order to avoid this problem, such as 'N having to be large enough'. Even though 'large enough' is a vague concept, it is clear that four molecules of H_2O would not be enough to boil, but 10^{23} can.

Although we are very sympathetic to this account of PTs in finite systems, our paper offers an alternative account of PTs in finite systems. First of all, even if four molecules of H_2O would not boil, this does not mean that PTs, or behaviour thats look like PTs, cannot happen in small systems. As we will argue below, small systems can display PTs, or behaviour thats look

[5] See Fraser (2016) for a distinct discussion about the eliminability of the thermodynamic limit in spontaneous symmetry breaking phenomena.

[6] See also Bangu (2009) and Shech (2013) on this paradox.

like PTs, depending on the system at stake (Section 4). This point might thus reinforce Mainwood and Butterfield's account (since the difficulty lies on PTs in small systems). However, when N-finite systems are small, quantities defined in the infinite limit (with $F_\infty(S)$) could ostensibly differ from observed and theoretical quantities in small N system. In other words, using F_∞ to define PTs in small systems could lead to wrong empirical predictions. Our approach thus provides the opportunity to account for PTs in finite systems that do not appeal to quantities defined in the infinite limit. Only finite quantities are required to define PTs in finite systems. However, when N-finite systems becomes large, our approach should be compatible with Mainwood and Butterfield account. But we will maintain our different perspective, which provides a *general framework* for PTs in all finite systems, from very small to large thermodynamic systems. For large finite systems, we will maintain that the infinite limit is not required to define PTs. We will rather argue that, in that case, the infinite limit is a reliable *approximation* to define and study PTs (Section 7).

4 Phase transitions in small systems

This section highlights a point that has not been sufficiently mentioned in the philosophical literature about PTs: small systems can display PTs or, *strictly speaking* at this stage of the paper, something that *looks like* PTs. Like in large systems, thermodynamic properties exhibit abrupt changes in small systems. These changes are nevertheless smoother, and the corresponding peaks less sharp than in large systems. More to the point, scientists are able to show that, in some cases, the use of an infinite limit leads to *wrong* predictions about the changes of properties in small systems. This point challenges the presumed mandatory use of the infinite limit to study these small systems. A philosophical moral of this section would be that a theory of PTs that could accommodate the behaviour of these small finite systems would be a more general theory of PTs. Sections 5-7 will be devoted to offer such an account.

First of all, the case of Ising models to describe ferromagnetic behaviours is very informative. Since the 1960's, finite-size corrections for spin lattices have attracted widespread attention. For example, in the case of two-dimensional lattices, exact results can be achieved for finite systems. In particular, Ferdinand and Fisher (1969) have shown that the temperatures for which the specific heat per spin is maximum are different in finite systems, viz. T_{max}, and with the infinite limit, viz. T_c. The relative difference between these temperatures varies with $1/N$. Yet Ising models are not relegated to describe only large systems, such as magnets with 10^{23} spins. Current scientific research is driven by the study of small systems, and the use of Ising models without the infinite limit might be crucial. For example, it is plausible that systems with only a hundred spins can be used to study some phenomena. In that case, T_c might not be a sufficiently accurate temperature for studying such systems. As we can see in Figure (2), a system with *only* $16 \times 16 = 256$ spins,

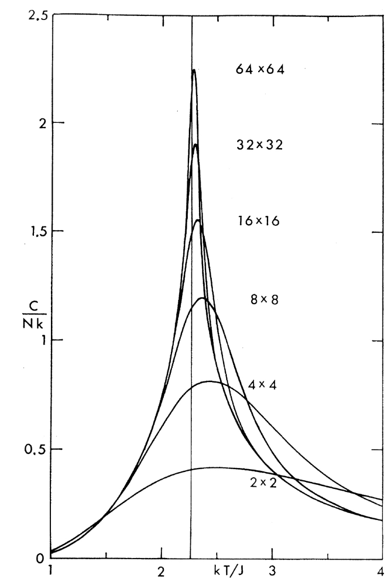

Fig. 2 The specific heat per spin for small Ising lattices; exact results for the $N \times N$ square lattice with periodic boundary conditions are displayed for $N = 2$, 4, 8, 16, 32, and 64. The limiting critical point is marked by a vertical line. Figure extracted from (Ferdinand and Fisher 1969, p. 834).

for instance, exhibits a peak for the specific heat. This is very far from 10^{23} spins. This exemplifies how small systems can display physical behaviours, viz. abrupt changes in variables, which are very similar to those displayed in large systems. This similarity should lead us to classify both physical phenomena as belonging to the same kind, differing only by degree, not by kind.

It has to be noticed that such finite approaches to describe changes of behaviours in small systems are demanded by a whole category of systems, e.g. where surface effects are relevant. Many areas of physics, such as soft matter and condensed matter require such a treatment, e.g., to study clusters or biomolecules. An example can be found in transitions in folding proteins, i.e. transitions from one configuration to another protein configuration. There are studies based on lattice model proteins. In this context, the use of an infinite limit is not considered relevant by some authors: "for proteins, the thermodynamic limit is meaningless *due to their moderate sizes.* The generally interesting single-domain proteins have a *size near several hundred residues*, which obviously is far from the thermodynamic limit. The thermodynamic limit for proteins cannot be realized or approached in nature" (Wang and Wang 2003, p. 2956. Our emphasis).

To conclude our discussion about abrupt changes of properties in small systems, let us turn to a more quantitative analysis based on the case of

Bose-Einstein (BE) condensation.[7] BE condensation is generally viewed as a genuine example of PTs, i.e. that require the thermodynamic limit to be obtained. For example, according to Kadanoff "qualitative changes in physical behaviour, called 'phase transitions', are always accompanied by infinities in thermodynamic derivatives. *This phase transition of non-interacting bose gas is no exception.*"(2000, p. 203. Our emphases).[8]

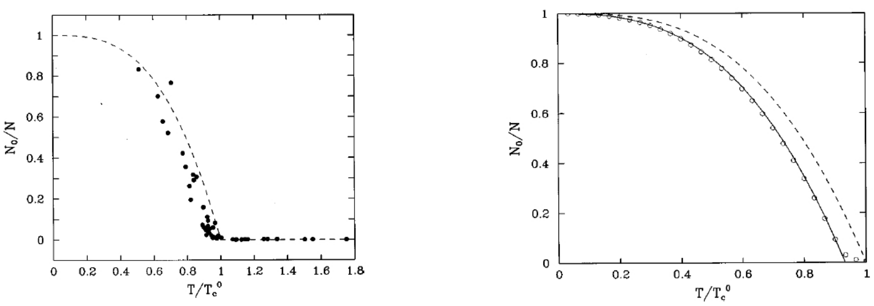

Fig. 3 Formation of Bose-Einstein condensates in small systems. The occupation number of the ground state is studied with respect to the temperature. On the left, circles are the experimental results of Ensher et al. (1996) with $N = 40\,000$ atoms. On the right, the solid line corresponds to the calculations for finite systems ($N = 1000$ atoms), and the dashed line refers to the thermodynamic limit. Figures extracted from (Dalfavo et al. 1999, p. 470).

However, very few atoms lead to an abrupt change of the properties of a quantum gas (Fig. 3, on the left). According to physicists:

> [The] experiments have been carried out with a maximum of about 10^7 atoms. As a consequence, the thermodynamic limit is never reached exactly. A first effect is the lack of discontinuities in the thermodynamic functions. Hence Bose-Einstein condensation in these trapped gases is *not, strictly speaking*, a phase transition.
> In practice, however, the macroscopic occupation of the lowest state occurs rather abruptly as temperature is lowered and can be observed, as clearly shown in (Fig. 3 on the left). The transition is actually rounded with respect to the predictions of the $N \to \infty$, but this effect, though interesting, is small enough to make the words *transition* and *critical temperature meaningful even for finite-sized systems.*(Dalfavo et al. 1999, p. 470. Our emphases)

Dalfavo et al. claim that these experimental results are not, strictly speaking, PTs. This agrees with the distinction made by Le Bellac between "BE conden-

[7] BE condensates are states of non-interacting (ideal) quantum gases of bosons cooled to temperatures very close to absolute zero. Under such conditions, a large fraction of bosons occupy the lowest quantum state, at which point that macroscopic quantum phenomena become apparent.

[8] See also (Le Bellac et al. 2004, p. 300-303).

sation" and "formation of BE condensate"(Le Bellac 2007, p. 572). The first one is a genuine PT, defined within the thermodynamic limit, whereas the second one corresponds to a finite fraction of particles in the lowest quantum state. However they stress that a critical temperature T_c for finite N-systems, according to which a large portion of atoms goes to the lowest quantum state, can be rigorously defined in agreement with these experiments (Grossmann et al. 1995, Ketterle and Druten 1996).

More to the point, the shift between the critical temperature T_c for finite N-systems and the critical temperature T_c^0 when N tends to infinity can be rigorously calculated and varies with $\delta T_c^0/T_c^0 \approx N^{-1/3}$ (see Fig. 3, on the right). This equation shows that the quantitative predictions for the critical temperature of finite systems with the infinite limit are misleading. The gap between the predictions in the thermodynamic limit (the dashed line in the Fig. 3, on the left) and the theoretical predictions for finite systems (the solid line in the Fig. 3, on the left) is well-confirmed by experiments. For instance, this is empirically well-confirmed for 40 000 atoms at 280 nK, $T_c = 0.94(5)T_c^0$. This difference is not negligible at all.

But, how should one deal with these changes of behaviours in small systems? A first possibility would be merely to deny that such small systems display genuine PTs. For example, applied to the case of BE models, large systems would exhibit 'BE condensation' and small systems only 'formation of BE condensates'. Following Mainwood's definition of PTs in finite systems, extra requirements should be added in order to put aside such small systems. But this strategy might be ad hoc and unsatisfactory because the separation between small systems and large systems is not clear. Physics models, such as Ising models, can be used to study finite systems from the very small to the very large. The only behavioural difference of all these systems is by degree: as N increases, abrupt changes and peaks become increasingly sharp. Another strategy would be to provide a general account of PTs in N-finite systems that would apply to small as well as very large systems. Since the problem of erroneous predictions in small systems comes from the reference of limit properties, such an account would have to avoid this reference. The remainder of the paper argues for such an account.

5 The theory of finite Distribution of Zeros

Menon and Callender (2013) offer theoretical approaches for studying phase transitions in SM without using the infinite limit:

> There are already several proposals for finite-particle accounts of phase transitions. These are sometimes called *smooth phase transitions.* The research is ongoing, but what exists already provides evidence of the existence of thermodynamic phase transitions in finite systems. (2013, p. 206)

Menon and Callender discuss two approaches, viz. the *back bending* approach (Wales and Berry 1994, Gross and Votyakov 2000, Chomaz et al. 2001) and the *finite Distribution of Zeros* (DOZ) approach (Borrmann et al. 2000, Mülken et al. 2001, Stamerjohanns et al. 2002). The first one deals with PTs in microcanonical ensemble. In that case, PTs in finite systems are identified by studying the curvature of the microcanonical entropy. PTs occur when the entropy curve is convex or when the heat capacity is negative for certain values. The second approach deals with PTs in canonical and grand-canonical ensembles. We focus on this approach. First, as far as we know, the back bending theory allows us to define only first order PTs, which is a severe limitation. Instead, the finite DOZ approach holds for any PTs. Second, we will show that the finite DOZ approach is a straightforward extension of Grossmann's and Yang-Lee's approach. This allows us to understand why and how the no-go Yang-Lee's results can thus be avoided.

5.1 Determining phase transitions in finite systems

Borrmann and coworkers introduce their theory of PTs in finite systems as follows:

> Our ansatz presented in this letter is based on earlier works of Lee and Yang and Grossmann et al. who gave a description of phase transitions by analyzing the distributions of zeros (DOZ's) of the grand canonical and the canonical partition function in the complex temperature plane. For macroscopic systems this analysis merely contributes a sophisticated view of the thermodynamic behavior of the investigated system. We will show that for small systems the DOZ's are able to reveal the thermodynamic secrets of small systems in a distinct manner. (Borrmann et al. 2000, p. 3511)

Borrmann et al.'s approach to PTs relies on Yang-Lee and Grossmann formalism introduced in Section 2. Borrmann and coworkers offer a finite version of it. They study the DOZ of the partition function and the characterization of PTs, but for *finite* systems. Let us make clear how they proceed in the case of the canonical approach of SM.

First of all, a complex partition function $Z(\mathcal{B})$ is introduced as follows, for which $\mathcal{B}$ is the complex inverse temperature defined as $\mathcal{B} = \beta + i\tau$ with $\beta = 1/k_B T$:

$$Z(\mathcal{B}) = \int dE\,\Omega(E)e^{-\mathcal{B}E} \tag{6}$$

Under some assumptions and mathematical manipulations, the partition function is written as:[9]

$$Z(\mathcal{B}) = \alpha(\mathcal{B}) \prod_{k\in\mathbb{Z}} \left(1 - \frac{\mathcal{B}}{\mathcal{B}_k}\right) e^{\left(\frac{\mathcal{B}}{\mathcal{B}_k}\right)} \tag{7}$$

[9] In particular, the product theorem of Weierstrass and the theorem of Mittag-Leffler is used, which relate integral functions of $Z(\mathcal{B})$ to their zeros (Titchmarsh 1964).

where $\mathcal{B}_k$ are the complex zeros of the partition function, and k an integer that ranges between a finite set. This expression for the partition function corresponds to the Eq. (2) of the Yang-Lee formalism, but in the canonical case.[10] In Yang-Lee and Grossmann formalism, the study of the DOZ allows to define a thermodynamic PT from a number of zeros that extends to infinity along a line corresponding to separation between two domains of complex functions (See Fig. 4, on the right). With the finite DOZ approach, PTs are identified from the *finite* DOZ:

> In the *thermodynamic limit* different regions of holomorphy separate different phases by *dense lines of zeros*. In *finite systems* the zeros do *not become dense* on lines which leads to a less sharp separation of different phases. We interpret the zeros as boundary posts between two phases. (Mülken and Borrmann 2001, p. 024306. Our emphases.)

Within the finite DOZ approach, PTs in finite systems correspond to an increasing finite number of zeros with N that align along a curve (see Fig. 4, on the left). This curve approaches the real axis with an angle ν with respect to

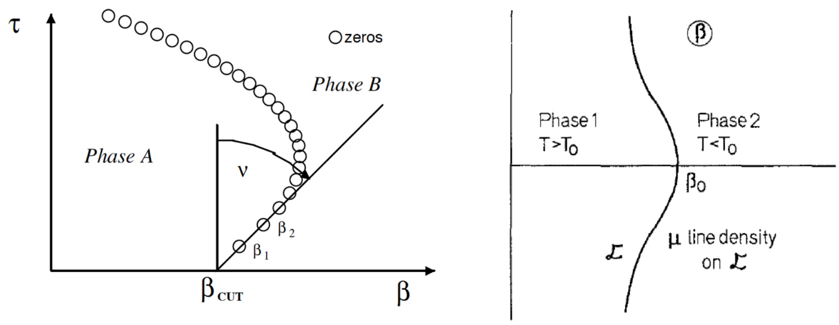

Fig. 4 Zeros of the partition function for finite systems (on the left) and infinite systems (on the right). In both cases, finite and dense series of zeros are interpreted as the boundary between two phases. On the left, the figure is extracted from (Stamerjohanns et al. 2002, p. 053401-2). On the right, the figure is extracted from (Grossmann and Rosenhauer 1969a, p. 440).

the imaginary axis.

This geometrical characterization of PTs from the finite DOZ is completed by a quantitive analysis. The free energy $F(\mathcal{B}) = -\mathcal{B}^{-1}\ln(Z(\mathcal{B}))$ and other quantities, such as heat capacity, can indeed be derived from the finite DOZ. For example, the heat capacity is derived from the free energy and corresponds to:

$$C_V(\mathcal{B}) = C_1(\mathcal{B}) - \sum_{k\in\mathbb{Z}} \left(\frac{k_B \mathcal{B}^2}{(\mathcal{B}_k - \mathcal{B})^2} \right) \tag{8}$$

[10] For that reason, the approach provided by Borrmann et al. is actually a straightforward extension of Grossmann and coworkers' approach (1967, 1968, 1969a, 1969b).

The zeros of partition function are the poles of free energy and heat capacity. Since the major contributions to the specific heat come from the zeros close to the real axis, an increasing number of zeros approaching the real axis leads to a rising peak in the specific heat (Borrmann et al. 2000, p. 3512). The study of specific heats, or other quantities derived from the finite DOZ, can thus provide empirical signatures for PTs in finite systems (See Fig. 5, on the right).

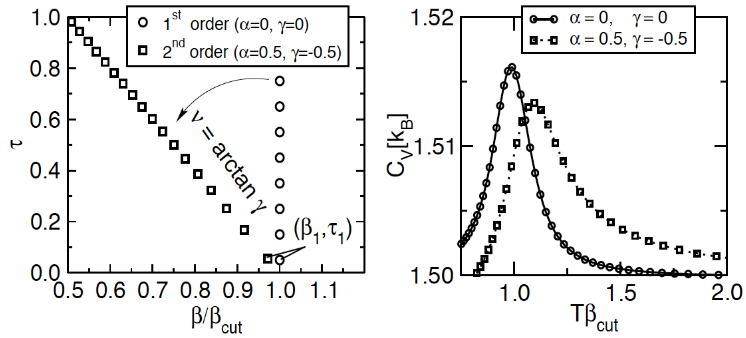

Fig. 5 Examples of finite distributions of zeros for first and second order phase transitions (on the left) with the corresponding calculated specific heats (on the right). (Stamerjohanns et al. 2002, p. 053401-2).

5.2 Classification of phase transitions

Following Grossman et al.'s scheme, a classification for finite PTs by studying the properties of the finite DOZ is obtained. This classification is a straightforward finite version of Grossmann et al's classification. For that purpose, a local density of zeros $\phi(\tau_k)$ at the zero $\mathcal{B}_k$ is defined as the average of the inverse distances between $\mathcal{B}_k$ and its neighboring zeros:

$$\phi(\tau_k) = \frac{1}{2}\left(\frac{1}{|\mathcal{B}_k - \mathcal{B}_{k-1}|} + \frac{1}{|\mathcal{B}_{k+1} - \mathcal{B}_k|}\right) \tag{9}$$

with $k = 2, 3, ..., M$ labelling the zeros. Following Yang and Lee and Grossmann et al. on the expression of the local DOZ as a power law of a parameter α, Borrmann et al. assume that the local finite DOZ satisfies $\phi(\tau_k) \sim \tau_k^\alpha$.[11]

[11] In Grossmann's approach, this assumption is made clear as follows:

> We shall show that the whole variety of phenomenologically known types of phase transitions with respect to T may be described by an appropriate choice of the density function $\mu(y, \gamma, v)$. [...] First we derive some general results for the density function $\mu(y)$ and show, that already a simple power law $\mu(y) \approx y^\alpha$ describes for various exponents α phase transitions of various (conventional) order. One thus

An estimation of this parameter α close to the real axis is thus provided by:

$$\alpha = \frac{\ln \phi(\tau_3) - \ln \phi(\tau_2)}{\ln \tau_3 - \ln \tau_2} \tag{10}$$

In addition, an estimation of the crossing angle between the finite DOZ and the imaginary axis $\nu = \arctan \gamma$ is given by $\gamma = (\beta_2 - \beta_1)/(\tau_2 - \tau_1)$.

Since τ_1, which is the imaginary part of the first zero, is non-zero, Borrmann et al. provide a classification for finite PTs from the two parameters α, γ (See Fig. 5, on the left). If $\alpha = 0$ and $\gamma = 0$, the PT is a *first order* PT. This means that the zeros align along a perpendicular line to the real axis. A *second order* PT is characterized by $0 < \alpha < 1$, γ arbitrary, and for a *highter order* PT, $\alpha > 1$, γ arbitrary.[12] As Borrmann et al. emphasize, this classification is an extension of the one provided by Grossmann and coworkers that fits with the Ehrenfest classification: "the classification of phase transitions in finite systems by γ, α, and τ_1,which reflects the finite size effects, is a straightforward extension of the Ehrenfest scheme" (Borrmann et al. 2000, p. 3512).[13] Indeed, the difference between Borrmann et al.'s and Grossmann et al's classifications lies in the value of τ_1. For finite systems, τ_1 is non-zero, and when the number of components N tends to infinity, τ_1 tends toward zero. Therefore, the Ehrenfest classification is a particular case within Borrmann et al.'s framework for which τ_1 tends towards zero.

6 Applications of finite DOZ theory

Having introduced the theoretical and conceptual principles on the finite DOZ theory of PTs, we now provide evidence for the usefulness and viability of this theory. For that purpose, we discuss several applications. We begin with the case of the Ising model of ferromagnetism before discussing the case of BE condensation, and afterwards refer to studies in biophysics small systems. We thus exemplify cases of what we call *finite* PTs, instead of *thermodynamic* PTs, a distinction that will be further discussed in Section 7.

6.1 Ising model of ferromagnetism

Some of the most popular thermal PTs are the one which occur in ferromagnets. These PTs are usually described with the Ising model. It corresponds to

> could *classify* the phase transitions with respect to the temperature T at fixed v by the order α (Grossmann and Rosenhauer 1967, p. 146)

The notations are here different. Our ϕ corresponds to μ, and our τ corresponds to their y.

[12] Unlike Grossmann et al.'s works, α actually satisfies more generally $\alpha \leq 0$ for first order PTs. (Stamerjohanns et al. 2002, p. 053401-2).

[13] For details, see Grossmann and Rosenhauer (1967, p. 146 and p. 151).

N spins S_i located on a lattice. With the presence of an external magnetic field h, the system is described with the following Hamiltonian:

$$H = -J \sum_{\langle i,i \rangle} S_i S_j - h \sum_{i=1}^{N} S_i \tag{11}$$

J is the effective coupling constant between spins, which describes local interaction between spins with $\langle i, i \rangle$ indicating a sum over the nearest neighbors.

Let us briefly recall how ferromagnetic PTs are usually studied in SM thermodynamic limit. Depending on the values of the external magnetic field and the temperature, the magnetization M of the system changes. The system can go from a positive magnetization to a negative magnetization, or a zero magnetization. These PTs have led to intense discussions in the philosophical literature because they are paradigmatic cases of PTs with symmetry breaking (e.g., Batterman 2005, Butterfield and Bouatta 2012). More precisely, there are *first order* and *second order* PTs.[14] For example, let us focus on PTs with respect to change of the external field h, the temperature T being kept fixed. In that case, if $T < T_c$, with T_c the critical temperature (also called the Curie temperature), there is a PT between a ferromagnetic state with positive magnetization and a ferromagnetic state with negative magnetization. The value of the magnetization M changes abruptly, with a *discontinuity* at $h = 0$. This is a *first order* PT. If $T = T_c$, the positive magnetization decreases *smoothly* when h decreases. The ferromagnetic magnet becomes paramagnetic. This smooth change of value of M, also called a *continuous* PT, is a *second order* PT.

Let us turn now to the study of these PTs with the finite DOZ theory, which we call *finite* PTs. This theory is used by Kim (2006) to investigate ferromagnetic PTs with an external field h vanishing in small systems. Ising models on $L \times L$ square lattices are used, where L ranges from 8 to 16. The author shows that the finitistic theory allows us to identify clearly both kinds of PTs for these small systems from Borrmann et al.'s classification. More precisely, for each lattice size, the finite DOZ of the partition function is calculated. The value of the parameter α is then extracted from which the order of PTs can be determined. The author concludes as follows:[15]

> Figure 6 shows the results of α_ϕ [...] at $T = 1$ first-order phase transition, $T = 2.2$ weak first-order phase transition, and $T_c = 2.269$ second-order phase transition for the Yang-Lee zeros of the square-lattice Ising ferromagnet. [...] [T]he approach clearly identif[ies] the first-order and

[14] See for example Yeomans (1992, p. 21), Kadanoff (2000, p. 212), or Selinger (2016, p. 14). For a clear 3-d representation of the phase diagram of the Ising model of ferromagnetism, with M, h and T, see Selinger (2016, p. 20).

[15] In his paper, Kim compares different finite approaches. For the sake of this paper, we only focus on Borrmann et al.'s approach. That is why there are omissions and minor modifications in the quotation. We also must note that the parameter α in Borrmann et al.'s theory is named α_ϕ in Kim's paper.

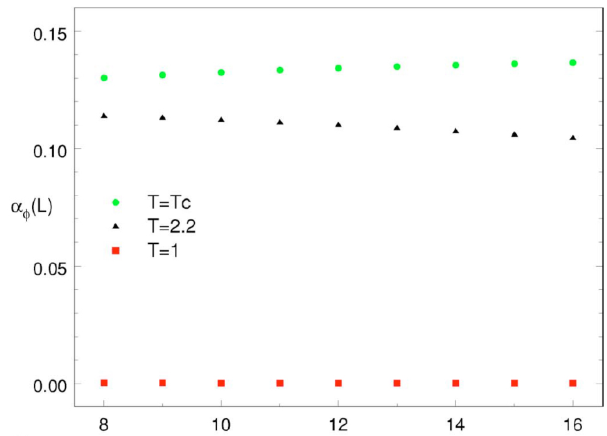

Fig. 6 Values of α (here named α_ϕ) obtained for Ising ferromagnets on the $L \times L$ square lattices with $L = 8$ to 16 and $T = 1$, $T = 2.2$ and $T_c = 2.269$. Figure extracted from (Kim 2006, p. 6).

> second-order phase transitions. In particular, the finite-size results at $T = 1$ are perfect. (Kim 2006, p. 6. Our emphasis)

Let us begin to comment on the two extreme cases, viz. $T = 1$ and $T = T_c$. The first case $T = 1$ corresponds to the domain where $T < T_c$. In that case, it is shown that α equals 0 for all the lattice sizes (red dots in Figure 6). Following Borrmann et al.'s classification, this corresponds to a *first order* PT. This is a perfect extension of the usual classification based on the infinite limit to small finite systems. In the case where $T = T_c$, it is shown that $0 < \alpha < 1$ for all the lattice sizes (green dots in Figure 6). This corresponds to a *second order* PT with Borrmann et al.'s classification. Again, the usual classification based on the infinite limit is successfully extended to these small systems.

Let us turn now to the apparent problematic but very interesting case for which $T = 2.2$. This corresponds to the domain where $T < T_c$ when T is very close to T_c, with a relative difference of 3%. It is shown that $0 < \alpha < 1$ (black dots in Figure 6). Following Borrmann et al.'s classification, this corresponds to a *second order* PT. In that case, as Kim notes, this is not an extension of the usual classification based on the infinite limit, for which the PT at $T = 2.2$ is a *first order*. How should we interpret this case? According to us, this result does not refute Borrmann et al.'s theory at all. It rather reveals again that, in a finite theory of PTs, changes in properties are gradual rather than abrupt.[16] What has to be clearly emphasized is this result occurs when T *approaches* the critical temperature. According to Kim, it happens for "weak first-order" thermodynamic PTs, which are first-order PTs with very large

[16] This result might be also related to an effect that occurs in very small systems, discussed in Section 7.1, according to which the definition of the temperature at which the PTs occur might be ambiguous.

but finite correlation length, because of approaching the critical temperature. It is thus not surprising at all that very small systems are not in a clear first order or second order PT when they are *close to the critical regime*. Large (but finite) correlations can be correlations with *all* the components for very small systems. Moreover, we emphasize that when the number of spins increases, α decreases (see black dots Figure 6). It is thus expected that, as systems become larger, the distinction between first and second order PTs for finite systems become clearer the closer they get to their critical regime.

6.2 The case of Bose-Einstein condensation

The finite DOZ theory is also able to deal with another kind of PTs, viz. Bose-Einstein condensation.[17] This section is devoted to show how the finite DOZ theory deals with small ideal bose gas systems. First of all, as we will see, numerical simulations provide evidence that the finite DOZ can be used in practice to study PTs in small systems. Second, they support the idea that a gas of bosons can exhibit not only 'formation of BE condensates' but also 'BE condensation', if we endorse our new definition for PTs from the finite DOZ approach, viz. *finite* PTs.

First, in agreement with experiments on small systems, the numerical simulations from the finite DOZ theory predict that there are two phases for such quantum gases even for very small gases. Figure 7 corresponds to the DOZ for $N = 100$ and 200 components. We can see how the zeros align along a curve that separates two domains of holomophy, each of them interpreted as the two phases of the system. The white part corresponds to the normal phase and the grey part to the condensed phase. As expected, the number of zeros increases with the number of components.

Second, Figure 8 shows that quantitative predictions on BE systems can be calculated from the zeros of the partition function. On the one hand, Figure 8a corresponds to the occupation number of the lowest state for a system of 120 atoms with respect to the temperature. This is in agreement with the experimental results discussed in Section 4 (see Fig. 3). On the other hand, Figure 8b shows the specific heat with respect to temperature of different systems. We see humps in the specific heats, which can be used as empirical signature for finite PTs. As we have seen, these peaks come from zeros that approach the real axis. Besides, maxima of specific heats depend on the number of components, in agreement with the experimental results that show that critical temperatures depend on the number of components. More to the point, according to Borrmann and coworkers, their "calculations [about PTs in BE

[17] One might not regard BEC as an archetype for thermal phase transition. Unlike the previous PTs in ferromagnets, the BEC results from the details of quantum statistics, rather than the strong interactions of the parts of a system. We thank one of the anonymous reviewers for calling our attention to this point. Since the BEC is nevertheless usually claimed to be a genuine PT, in the sense that it requires the infinite limit to be obtained (see Kadanoff 2000, p. 203 or Le Bellac et al. 2004, p. 300-303), we have to see how the finite DOZ deals with this transition.

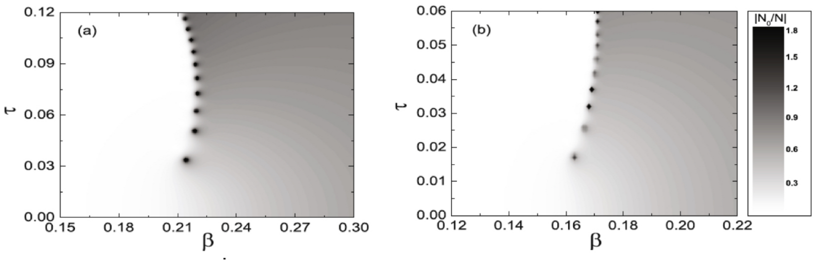

Fig. 7 Contour plots of the ground-state occupation number in the complex temperature plane for an ideal Bose condensate with (a) $N = 100$ and (b) $N = 200$ particles confined in a 3D quartic potential. Figures extracted from (Wang and He 2011, p. 75)

gases] are in very good agreement with recent theoretical works, not only qualitatively but also quantitatively" (Mülken et al. 2001, p. 013611-6). These theoretical results (Grossmann and Holthaus 1995a) are closely related with those discussed in Section 4 from which rigorous critical temperatures in finite systems are calculated (Ketterle and Druten 1996).[18]

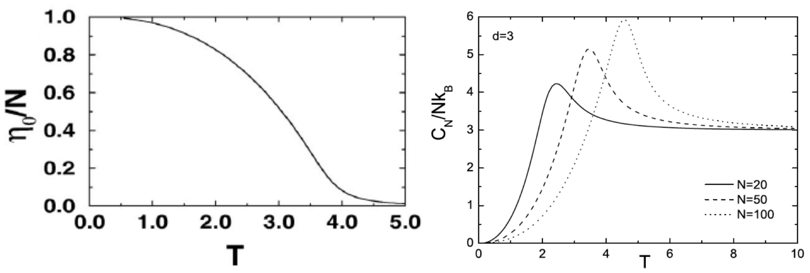

Fig. 8 On the left, the occupation number of the ground state with respect to the temperatures for a 120-particle harmonically trapped ideal Bose gas (Mülken et al. 2001, p. 013611-3). On the right, the specific heat per particle with respect to temperature for a $3-d$ quartic potential for $N = 20$, 50, and 100 components (Wang et al. 2012, p. 84).

Finally, from numerical computations of the parameters τ_1, α, γ, the finite PT of ideal BE gases is identified as a third order PT. This order is extracted from the values α and γ (Fig. 9a), in particular since α is superior to 1. Figure 9b is characteristic of a *finite* PT since τ_1 is a strictly positive quantity. This quantity decreases as the number N of components increases, τ_1 varying approximately with N^{-1}. As we will argue below in Section 7.2, this exemplifies

[18] Actually, the theoretical works of Grossmann and Holthaus (1995a) and Ketterle and Druten (1996) are so close that Ketterle and Druten (1996) add the following note at the end of their paper: "After submission of this work we learned that Equations 6 and 11 were derived independently by Grossmann and Holthaus (1995a)"(Ketterle and Druten 1996, p. 559).

that the finite DOZ approach allows us to recover Yang-Lee's and Grossmann's approach by using the infinite limit. In addition, we mention that the finite

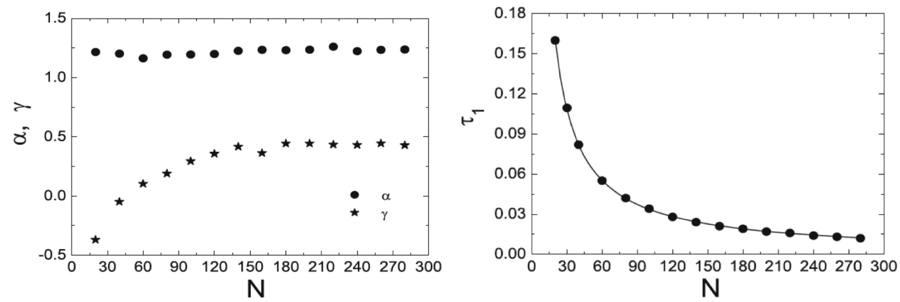

Fig. 9 (a) On the left, parameters α (circles) and γ (starts) vs. particle number N for an ideal Bose gas in a $3-d$ quartic potential. (b) On the right, parameter τ_1 vs. particle number N (Wang and He 2011, p. 75 and p. 76).

DOZ theory can be used to study not only ideal Bose gases but also weakly interacting Bose systems. In that case, it is shown, for example, that such small systems exhibit PTs from a normal phase to a one-vortex phase, which is identified as a first order PT (Dean and Papenbrock 2002).[19]

6.3 Phase transitions with biomolecules

To finish this section devoted to applications of the finite DOZ theory, we briefly emphasize this theory's ability to describe PTs in other small systems. Our goal here is to indicate the potential plurality of scientific domains in which the finite DOZ can be used. As we have mentioned in Section 4, transitions in folding proteins are discussed in the scientific literature. Yet since proteins are only made of a few components, the thermodynamic limit might be misleading to describe them. This is why some researchers turn to the finite DOZ theory to study them:

> For protein-like model systems, it [the finite DOZ theory] is a powerful way to extract information of the transition via the study on the partition function zeros. In this work, we report a study on the features of folding transitions of lattice model proteins based on the partition function zeros. [...] The order of the transition is discussed on the basis of the partition function zeros. [...] The transition temperature and the strength of the transition directly relate to the intercept and the slope of the local distribution of the zeros near the real axis. The conventional

[19] There are also studies of the finite DOZ theory on the PTs between different isomers of Argon clusters (Borrmann et al. 2000) or in PTs in small magnetic clusters (Stamerjohanns et al. 2002).

characterization of proteins is assessed from their correlations with the related parameters to the zeros. (Wang and Wang 2003, p. 2952)

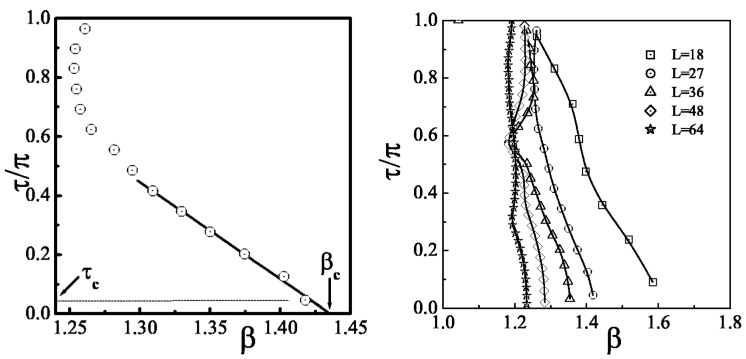

Fig. 10 On the left, the DOZ of a folding protein lattice model. The zeros near the real axis lie on a straight line, from which the inverse temperature β_c of the transition of configuration is extracted. This corresponds to a second order PT. On the right, the DOZ for another theoretical model, and with chains with different lengths of $L = 18, 27, 36, 48$, and 64. Figures extracted from (Wang and Wang 2003, p. 2952).

These studies are based on three-dimensional cubic lattice models with local interactions. With several assumptions, an energy E of the conformation for the model chain is defined. Without going into technical details, we point out that features on the model are extracted from the finite DOZ theory. As an example, the orders of PTs following the classification of Borrmann et al.'s are studied depending on different assumptions on interactions, and the lengths of the model chains (see Fig. 10).

After having provided evidence in favor of the finite DOZ approach in Section 6, we stipulate the philosophical consequences of this theory on the concept of PT, and the role of the infinite limit for studying PTs.

7 Finite and thermodynamic phase transitions

The development of the finite DOZ approach allows us to argue for eliminating the infinite limit to define PTs within SM. Nevertheless, such an eliminativist claim raises issues about the concept of PT at stake, and the role of the infinite limit in SM. In the finite DOZ theory, PTs are described *without* limit properties, i.e., without using infinite limits applied to functions of the partition function Z_N, such as free energy or specific heat. By contrast, in Yang-Lee's theory, PTs are described *with* limit properties, which are mandatory. This difference compels us to argue for two different concepts of PTs. Yang-Lee and Grossmann et al. deal with *thermodynamic* PTs, which are PTs defined within thermodynamics or within SM in the infinite limit. Instead, the finite

DOZ theory deals with *finite* PTs or *smooth* PTs, defined within SM without infinite limits. This section is dedicated to characterize and discuss this concept of *finite* PTs before clarifying in what sense the infinite limit becomes an *approximation* for large finite-N systems.

7.1 Characterization of finite phase transitions

Menon and Callender (2013) suggest a definition for PTs from the finite DOZ theory:

> A phase transition occurs when the zeros of the canonical partition function align perpendicularly to the real temperature axis and the density scales with the number of particles. (2013, p. 208)

Starting from this definition, we suggest a few modifications to better characterize finite PTs. First of all, Menon and Callender do not seem to endorse a distinction between *finite* PTs and *thermodynamic* PTs. Conversely, we do stress this distinction. Furthermore, Menon and Callender's definition holds only to first order PTs. As we have seen, the signature of first order PTs involves zeros aligning *perpendicularly* to the real temperature axis (see Section 5.2). For higher orders, the zeros line up at an angle with the real axis. Accordingly, we suggest to characterize finite PTs as follows:

> *A finite phase transition occurs when the zeros of the canonical partition function align close to the real temperature axis and the density scales with the number of particles.*

This modification allows us to deal with PTs of any order (see Figure 11a). Additionally, we stress that both Menon and Callender and our revised characterizations of finite PTs lead to empirical signatures for finite PTs. The specific heats indeed exhibit humps when the zeros align close to the real temperature axis (see Figure 11b). As we have seen, this is due to the fact that the major contributions to the specific heat come from zeros close to the real axis.

This characterization is not however without any problems. First of all, the statement that the zeros of the partition function are 'close' to the real axis, or 'approach' the real axis is vague. It raises the question of how close the zeros have to be, and consequently how large a finite system has to be, before a finite PT can be said to occur.[20] This question does not receive a clear cut answer. We nevertheless stress that there is a minimal number of zeros required to characterize a finite PT. The four first complex zeros are indeed needed to evaluate the parameter α, which is defined with the equations (9) and (10). A small system with less than four zeros, therefore, could not be treated by the finite DOZ theory. But, four zeros might not even be enough in practice. We stress that finite PTs are more accurately identified and characterized as the number of components increases, making the minimal number of components to have a clear finite PT difficult to discern. This depends on systems. For

[20] We thank one of the anonymous reviewer for pointing out this issue.

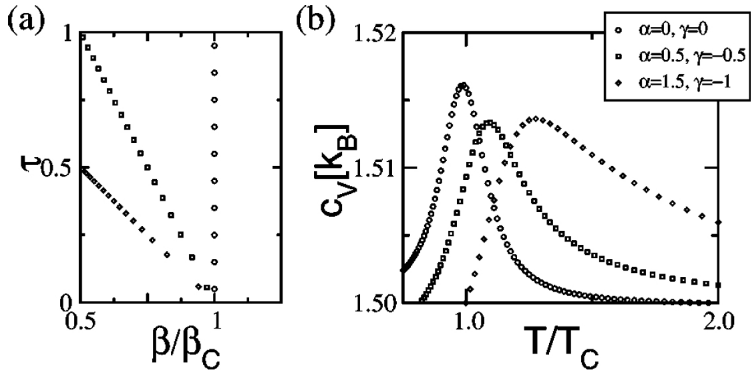

Fig. 11 Plot of (a) generated zeros lying on straight lines to simulate first- ($\alpha = 0$ and $\gamma = 0$), second- ($\alpha = 0.5$ and $\gamma = -0.5$),and third- ($\alpha = 1.5$ and $\gamma = -1$) order phase transitions and (b) the appropriate specific heats per particle. Figure extracted from (Mülken et al. 2001, p. 013611-3).

example, as we have seen in the case of Ising models, one can clearly identify a first order PT with *only* $8 \times 8 = 64$ spins if the systems are far from the critical regime (Section 6.1). But for small systems approaching the critical temperature, larger systems are needed to clearly identify the first order PT.

Second, characterizing finite PTs raises an issue that we could call *the problem of transition temperatures.* According to the authors of the finite DOZ theory:

> The definition of a critical temperature β_c in small systems is crucial and *ambiguous* since no thermodynamic properties diverge. Thus, different definitions are possible. We define the critical temperature as β_{cut} (Mülken et al 2001, p. 2. Our emphasis.)

The definition of the temperature at which the PT occurs is indeed ambiguous.[21] There are at least three possibilities to define the inverse transition temperature β_c. First, following Borrmann and collaborators, one can define this temperature as β_{cut} , which is the point where the continuation of this zeros crosses the real axis of temperature. But one could also define it as β_1, i.e. the real part of the first zero. And one could also use $\beta(C_{v,max})$, which is the inverse temperature at which the specific heat is maximum. These three definitions are possible since they are similar within small systems (see Figure 12) as they are expected to converge in the thermodynamic limit (Mülken et al 2001, p. 013611-2).[22] However, this ambiguity still raises the question of which definition has to be chosen. This choice is problematic since it seems to imply

[21] Unlike Borrmann et al. we make the difference between a transition temperature (when a PT occurs) and a critical temperature (when the system is at the critical point) in order to make this discussion compatible with Ising models (see Section 6.1).

[22] It is shown at least that β_{cut} and β_1 converge in the thermodynamic limit: "In the thermodynamic limit, both definitions coincide"(Mülken et al 2001, p. 013611-2).

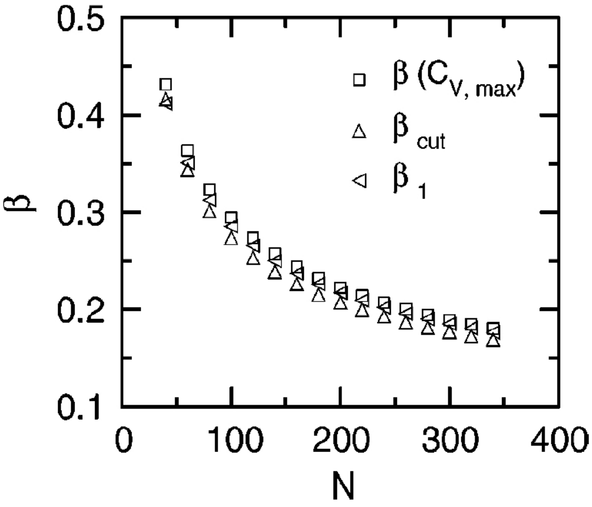

Fig. 12 Comparison between three different approaches to define a transition temperature for phase transitions in finite systems. Figure extracted from (Mülken et al. 2001, p. 013611-6).

that that the definition of the transition temperature is conventional. We do not offer a final answer to this problem. Perhaps, it will receive an empirical answer after further investigation. Nevertheless, we suggest a possible way to deal with this problem. After all, it is not mandatory for *finite* PTs to be characterized by a single value for the transition temperature. Finite PTs might be characterized by a *range* of temperatures, an interval of temperatures for which PTs appear smooth. The size of the temperature interval would decrease when the number of components increases, and would tend to a single value in the infinite limit. Small systems exhibit such important fluctuations, but they do not exhibit divergence or very sharp changes of properties. Therefore, since we endorse a concept of finite PTs that differs from the concept of thermodynamic PTs, we do not see why a single transition temperature should be required to characterize the changes of behaviours in finite systems.

Before examining the relationship between finite and thermodynamic PTs in the next section, we stress that we have put aside an aspect of the infinite limit in PTs. We have focused on the identification, classification and characterization of PTs in finite systems without using the infinite limit. But one might need the infinite limit to extract information on critical exponents. This might require the use of the infinite limit and the framework of renormalization group, which is important to address the question of universality and emergence of critical phenomena (e.g. Batterman 2000, 2011). We leave this topic open for further study. Nevetherless, at this stage of our analysis of the finite DOZ theory, we would like to make two comments. First of all, as far we know, there is not much scientific work on this aspect, leaving the question of how to deal with critical exponents within the finite DOZ theory a scientific and open question. However, the relationship between the parameter α and the critical exponents in thermodynamic PTs suggests the direction of future research because:[23]

$$C_v \approx (\beta - \beta_c)^{\alpha-1} \tag{12}$$

Since the parameter α in Borrmann et al.'s approach is extracted from the finite DOZ, this finite DOZ might contain information on critical exponents. Our second comment is more philosophical. In the case of small systems, one might wonder whether divergences involved in critical exponents might be relevant. As Mülken et al. point out "since critical indices are used to describe the shape of a divergency at the critical point, an extension to small systems seems to be more or less academic"(2001, p. 3). As we have seen, peaks are smooth in small systems. This might lead to the consequence that universality might be not concerned with small systems, at least understood via critical exponents. For very large systems, however, peaks are sharper. In those cases divergences provided in the infinite limit are good approximations. The infinite limit might thus be used to evaluate the critical exponents of these finite large systems. But this procedure might be compatible if viewing the infinite limit as a convenient mathematic tool, used for practical purposes as we point out it in the next section.

7.2 The thermodynamic limit as an approximation

In this final section we stress the relationship between the two concepts of *finite* PTs and *thermodynamic* PTs. We claim they are linked by an *approximation* relation, which is reliable for sufficiently large systems.

For that purpose, we emphasize that the finite DOZ theory and Yang-Lee's and Grossmann's theories are interlinked by the *thermodynamic limit*:

> The imaginary part τ_1 reflects the "discreteness" of the system. Thus, in the thermodynamic limit we have $\tau_1 \to 0$ and our scheme coincides with the scheme given by Grossmann and coworkers.(Stamerjohanns et al. 2002, p. 1)

We have seen that the theoretical predictions from the finite DOZ approach for small systems, such as Ising models or gases of bosons for example, differ quantitatively from predictions using the thermodynamic limit. From this perspective, finite PTs clearly differ from thermodynamic PTs. This difference reveals the distinction between the two concepts of PTs. However, when the number N of components is sufficiently large, the Grossmann et al's approach can be used for mathematical convenience to deal with systems described by the finite DOZ theory. Even if such large but finite systems are *described within* the finite DOZ approach, one can use an *approximate theory*, which

[23] See Equation (2.6) in Mülken et al. (2001, p. 3), which is related to Equation (17) in Grossmann and Rosenhauer (1969a, p. 443).

is Grossmann et al's theory. In such sufficiently large systems, the concept of thermodynamic PTs – provided by Grossmann et al's approach – is thus a good approximation for the concept of finite PTs – provided by the finite DOZ approach.

This view is unconventional in the sense that thermodynamic PTs are generally viewed as the genuine PTs. Finite systems-based methods using techniques like the Finite-Size-Scaling (FSS) are viewed as approximating methods (e.g. Barber 1983).[24] For example, according to Janke and Kenna (2001):

> Finite volume systems do [...] anticipate the presence of the phase transition as the thermodynamic limit is approached [...]. Numerical methods of identifying the order of a phase transition exploit this anticipation by including finite size scaling (FSS) of extrema of thermodynamic quantities which are singular in the thermodynamic limit at the transition point. The counterparts of these singularities in finite systems are smooth peaks, the shapes of which depend on the order and the strength of the phase transition. (Janke and Kenna 2001, p. 1212)

In that case, finite systems are viewed as *anticipating* genuine PTs, which have to be understood as *thermodynamic* PTs. There are indeed signatures in finite systems that indicate that such finite systems would exhibit a PT in the infinite limit. Finite-systems based numerical techniques exploit this property to study *thermodynamic* PT from numerical simulations of finite systems. Instead, in our view, we put forth the idea that *finite* PTs is a genuine concept of PTs for finite systems, and that thermodynamic PTs would be approximations of these *finite* PTs. Such approximations are accurate when N is sufficiently large and useful for practical purposes since theoretical calculations are often easier within the thermodynamic limit.

The development of the finite DOZ theory thus exemplifies the idea that SM is not doomed to define PTs with singularities or non-analyticities. Such an idea was already suggested by Callender (2001):

> After all, the fact that thermodynamics treats phase transitions as singularities does not imply that statistical mechanics must too. To assume that would be to take thermodynamics too seriously. It will now come as no surprise that we believe the source of this 'emergence' is again the result of a too-literal translation from thermodynamics to statistical mechanics. Thermodynamics represents (for pretty good reasons) phase transitions as singularities, and statistical mechanics (for pretty good pragmatic reasons) takes this to mean a non-analyticity in the partition function. But from a foundational perspective we cannot endorse this knee-jerk identification of mathematical definitions across levels. (p. 550)

The value of the finite DOZ theory can be found in how SM can indeed treat *in practice* PTs without singularities. Nevertheless we are not forced to endorse that the finite DOZ theory is the fundamental theory of PTs. The main reason

[24] See also Hüttemann et al. (2015, p. 187) for a discussion in a philosophical perspective.

is that there are several different approaches for finite PTs, like the back bending theory, but also topology of configuration space-based approaches (Kastner 2008), and possibly even other theories. It is not clear yet if there is one fundamental finite theory of PTs among these theories. Therefore, we are rather tempted to argue for a pluralistic account of finite PTs, where the different concepts of finite PTs should be linked to the concept of thermodynamic PTs within the infinite limit.

8 Conclusion

We argued against the received view that holds infinite idealizations as ineliminable when accounting for phase transitions in statistical mechanics. Conversely, we argued for the plausibility of eliminating the infinite limit for explaining phase transitions within statistical mechanics. In this framework, we offered a new account for phase transitions in finite systems that does not require the infinite limit. To do so, we focused on the finite distribution of zeros theory, which is of particular relevance because, first, it allows us to tackle the ineliminability results from Yang-Lee's and Grossman's theories, and second, to highlight on an approximation relation with Yang-Lee's and Grossman et al.'s theories when finite systems are large.

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