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STATISTICAL MECHANICS OF EQUILIBRIUM
AND NONEQUILIBRIUM PHASE TRANSITIONS:
THE YANG–LEE FORMALISM

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Showing that the location of the zeros of the partition function can be used to study phase transitions, Yang and Lee initiated an ambitious and very fruitful approach. We give an overview of the results obtained using this approach. After an elementary introduction to the Yang–Lee formalism, we summarize results concerning equilibrium phase transitions. We also describe recent attempts and breakthroughs in extending this theory to nonequilibrium phase transitions.

Keywords: Phase transitions; critical phenomena; Yang–Lee formalism; equilibrium phase transitions; nonequilibrium phase transitions.

1. Introduction

Boiling of water, denaturation of a protein, or formation of a percolation cluster in a random graph are examples of phase transitions. Description and understanding of these ubiquitous phenomena, that appear in physics, biology, or chemistry, remains one of the major challenges of thermodynamics and statistical mechanics.

The simplest and relatively well-understood phase transitions appear in systems in thermal equilibrium with their environment. A prototypical example of such an *equilibrium phase transition* is the liquid-gas transition. Crossing the coexistence curve, by varying e.g., the temperature, one can move between vapor and liquid phases. Such a transition is called first-order (or discontinuous) because in the framework of thermodynamics this phenomenon is understood in terms of thermodynamic potentials showing discontinuities in their first derivatives with respect

to the control parameters. The coexistence line terminates at a particular point, the critical point, where the two phases become undistinguishable. Close to this point, second derivatives of the thermodynamic potential exhibit power-law singularities and this indicates a second-order (or continuous) phase transition. In the late fifties, giving a microscopic description of first- and second-order phase transitions became a challenge that culminated in the development of scaling theories and then renormalization group methods. Although these techniques are computationally very effective and reliable, they do not explain all the aspects of phase transitions. In particular, it is not clear how free energy can develop singularities at the first-order phase transitions. To address this problem, Yang and Lee devised an approach where the partition function (that is used to calculate the thermodynamic potentials) is considered as a function of complex control parameters. Singularities of the thermodynamic potentials, given as zeros of the partition function, were then shown to accumulate exactly at the transition point. This approach, that was later on generalized and extended to various systems, provides a lot of information about equilibrium phase transitions.

However, an equilibrium system is rather often only an abstract idealization. Typically, a given system is not in equilibrium with its environment, but is exchanging matter and/or energy with it; fluxes are present in the system. The usual way to describe the physics of such a system is to write down a master equation for the time-dependent probability that a given mesoscopic state is realized at time t. The physics is then embedded in the transition rates between these mesoscopic states. In the long-time limit the system eventually settles into a steady-state and, depending on the values of some control parameters or the initial configuration, different nonequilibrium steady states (NESS) can be reached, and sometimes a breaking of ergodicity takes place. Upon varying some control parameters the system may change its steady state and this is called a *nonequilibrium phase transition.* In the particular situation in which the so-called detailed balance condition is fulfilled, one recovers the case of equilibrium phase transitions. Our understanding of NESS from a microscopic point of view is not as advanced as for equilibrium. Accordingly, it is legitimate to try to extend the Yang–Lee theory to NESS. It was argued recently, and illustrated on several examples, that Yang–Lee ideas should apply, at least to some extent, to nonequilibrium phase transitions.

This review provides an overview of the Yang–Lee theory for equilibrium phase transition and describes recent advances in applying it to nonequilibrium systems. In addition, we included an extensive bibliographical list that offers an interested reader the relevant references where one may find further details on a more specific subject. Although not exhaustive, the bibliography we are proposing covers all the relevant aspects and recent progress in the field. Our presentation is elementary and intuitive, and we omitted a number of technical details.

The structure of our paper is as follows. The first part of this review is devoted to the description of the Yang–Lee theory for equilibrium phase transitions.

A first paragraph is devoted to the question of the role played by the thermodynamic limit. Then the general Yang–Lee theory for the grand-canonical partition function is discussed. The celebrated Circle theorem is revisited, as well as its generalization to different models. Several aspects of the characterization of the critical behavior in terms of the Yang–Lee zeros are analyzed (density of zeros near criticality, Yang–Lee edge singularity, finite size effects). A brief discussion of the relation between the Pirogov–Sinai theory and the Yang–Lee zeros for first-order transitions is given. Then the problem of the Fisher zeros of the canonical partition function is revisited. Finally, the Potts model is discussed in order to compare several possible types of description of the phase transitions within the Yang–Lee formalism.

The second part of this review is devoted to the question of extending Yang–Lee formalism to NESS phase transitions. In a first paragraph, the description in terms of a master equation is given, and the question of detailed balance discussed. Then the problem of a possible candidate for nonequilibrium steady-state partition function is approached. Applications to driven-diffusive systems, reaction-diffusion systems, directed percolation models, and systems exhibiting self-organized criticality are reviewed. The connection with equilibrium system with long-range interactions is also considered. Finally, some conclusions and perspectives are given in the last paragraph.

PART I: EQUILIBRIUM PHASE TRANSITIONS

2. Phase Transitions and the Thermodynamic Limit

When one varies a control parameter (e.g., the temperature or an external field), a physical system can exhibit a qualitative change of its equilibrium state, i.e., it can undergo a *phase transition*. In the framework of thermodynamics such a phase transition shows up as a discontinuity or a singularity of physical observables (e.g., specific heat, susceptibility, etc.) as functions of the control parameter. A characteristic thermodynamic potential or some of its derivatives are discontinuous or singular, thus *nonanalytic* at the transition point.

How is it possible to understand this phenomenon from a microscopic perspective? From the point of view of the equilibrium statistical mechanics, the thermodynamic potentials can be expressed in terms of some properties of the microstates in the phase space of the system, that are determined by the microscopic interactions between the constituents of the system (particles, spins, etc.), as well as by the externally imposed constraints — like a fixed value of a control parameter. More explicitly, the characteristic potential is proportional to the *logarithm of the partition function* of the system. This partition function is a sum of the statistical weights over different configurations that are accessible to the system in the phase space under the given constraints, and these statistical weights are positively defined

analytic functions of the control parameter.[a] If the sum contains a finite number of such statistical weights, then the partition function is finite, and its logarithm, i.e., the corresponding characteristic potential, is an analytic function of the control parameter, and therefore no phase transition is possible. To obtain a nonanalyticity of the characteristic potential, the partition function should thus necessarily become zero for a certain value of the control parameter. However, as justified above, this cannot happen in a finite system. A nonanalytic behaviour could only be obtained for a system containing an infinite number N of constituents, and thus one has to work in the so-called *thermodynamic limit*, in which both $N \rightarrow \infty$ and the volume of the system $V \rightarrow \infty$, such that the density $n = N/V$ is constant.

One may object that all the systems in nature are finite. However, because of the huge number of its components (of the order of Avogadro's number), any macroscopic system behaves, from an experimental point of view, like an infinite system (except eventually in a very narrow domain in the vicinity of the transition point). The effects of the finite-size of the system on the appearance and properties of the phase transition will be subject of further discussion in Sec. 10.

To summarize, the presence of a phase transition, from a statistical mechanics point of view, should be related to the vanishing of the partition function for a certain value of the control parameter. Thus, one has to look for the zeros of the partition function, and such zeros should only show up in the thermodynamic limit.

Let us briefly comment now on the properties of the interaction potential between the constituents of the system that allow for the existence of a correct thermodynamic limit.[b] Roughly speaking (see Refs. 1–5 for further technical details), for systems with two-body central interactions, the interaction potential $u(r)$ (with r the distance between the particles) has to obey the following three conditions:

(i) The intermolecular forces have to approach zero rapidly enough for large inter-particle separations, i.e., in terms of the interaction potential, $|u(r)| \leqslant C_1/r^{d+\varepsilon}$

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[a]For example, consider a system in equilibrium with a heat bath at temperature T (that represents a control parameter in this case). The free energy (which is the characteristic potential) is proportional to the logarithm of the canonical partition function, that is defined as a sum over all the microstates α of the Boltzmann weight $\exp(-E_\alpha/k_B T)$, where E_α is the energy of the microstate α.

[b]For such a system, under some supplementary constraints on the regularity of its frontier, taking the thermodynamic limit $N \rightarrow \infty$, $V \rightarrow \infty$ at fixed $n = N/V$ implies that: (i) The various statistical ensembles are equivalent, and the relevant thermodynamic parameters are thus uniquely defined. For example, the pressure has the same thermodynamic limit, positively definite, in both the canonical and grand-canonical ensembles. (ii) The values of the thermodynamic potentials (energy, free energy, grand-canonical potential, enthalpy, etc.) *per particle* are finite. The system enjoys the additivity property, which means that its total Hamiltonian is the sum of the Hamiltonians of any combination of macroscopic parts taken separately (i.e., one can safely neglect the surface interaction energy between macroscopic component parts) – and so do all the thermodynamic potentials (free energy, enthalpy, etc.). (iii) The thermodynamic stability of the system is ensured, i.e., the thermodynamic potentials enjoy the required conditions of convexity/concavity. For example, the compressibility coefficient is positive, which means the pressure is a non-decreasing function of the particle-number density n. (iv) The effects of the boundaries (e.g., surface energy or tension) are extinguished, and we speak only of bulk effects.

as $r \to \infty$ (with $C_1 > 0$ and ε positive constants), where d is the dimension of the system. Such systems are currently called *short-range interaction* systems.

(ii) The potential $u(r)$ should have a repulsive part for small enough values of r (preventing the system from collapse at high particle number densities). Throughout this paper, we shall consider systems with a *hard-core* interparticle repulsion at small distances, $u(r) = \infty$ for $r < r_0 \sim b^{1/d}$ (where b is the single-particle excluded volume), which means that a system of volume V can accommodate a *finite* maximum number of particles $M = V/b$.[c]

(iii) Finally, the interaction potential has to be everywhere bounded from below, $u(r) \geqslant -u_0$ whatever r is (with u_0 a positive constant).

Note a rather general result concerning the *one-dimensional equilibrium systems with short range interactions*, namely van Hove's theorem,[1,5,7] according to which *no phase transition is possible* in such systems, in contrast to what happens generically in corresponding nonequilibrium systems (see Ref. 8 for a brief review). A recent critical discussion[9] of this result allowed us to highlight some exceptions to this theorem, but we shall not be concerned here with these rather pathological situations.

Many physical situations can be modeled by interaction potentials with the characteristics (i)–(iii) above. There are, however, a few exceptions. The most salient example is that of the systems with long-range interactions (or non-additive systems), which include, e.g., systems with gravitational or Coulombian forces [see Ref. 6 for a modern review of their (thermo)dynamical properties studies]. Such systems exhibit an unequivalence of the statistical ensembles, and it is not clear yet how to apply the concepts of the Yang–Lee theory (as described below) to their phase transitions. We will not address them further here. A limiting case of such systems is that of mean-field interactions, on which we will briefly comment in Secs. 7.2, 12 and 13.3.

3. Yang–Lee Zeros of the Grand-Canonical Partition Function: The General Framework

We shall address here two problems, namely:

(A) The location of the phase transition point: How, when knowing the partition function (in the thermodynamic limit), can one locate a phase transition point by investigating the zeros of this partition function with respect to the control parameter of the system.

(B) The characteristics of the transition: How can one extract information on the nature of the phase transition (e.g. if it is a discontinuous or continuous one) from the properties and distribution of these zeros.

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[c]As shown in Ref. 3, one can relax the hard-core condition to $u(r) \geqslant C_2/r^{d+\varepsilon}$ as $r \to 0$ (with C_2 and ε positive constants), but we will not consider this situation here.

The presentation in this section follows, with slight modifications, the same general lines of thought as in Ref. 10.

(A) The location of the phase transition point. Let us start with this first problem and concentrate on the case of a generic system with short-range interactions as described above, for which the thermodynamic limit is well-defined. For concreteness, and following the original papers of Yang and Lee,[11,12] we consider here the *grand-canonical* description of the system. The corresponding partition function, for a given volume V and a fixed temperature T, is expressed as:

$$\Xi_V(T, z) = \sum_{m=0}^{M} Z_m(T) z^m \,, \tag{1}$$

where $M = V/b$ (with b the single-particle excluded volume) is the maximum number of particles that can be accommodated in the system (as determined by the hard-core part of the binary interaction potential); $Z_m(T)$ is the canonical partition function of the system with fixed number of particles m; and finally z is the *fugacity* of the system,

$$z = \exp(\mu/k_B T) \,, \tag{2}$$

which is obviously a real, positive quantity expressed in terms of μ, the chemical potential of the system in contact with an external reservoir of particles; k_B is Boltzmann's constant.

One notices that $\Xi_V(T, z)$ is a polynomial of M-th order in the fugacity z. Let us consider its *roots*, i.e., the solutions of $\Xi_V(T, z) = 0$; according to the fundamental theorem of algebra, there are M such roots, $z_i = z_i(T)$, with $i = 1, \ldots, M$. Moreover, because the coefficients of all the powers of z in the expression of $\Xi_V(T, z)$ are real and positive, all these roots $z_i(T)$ appear in *complex-conjugated pairs in the complex-fugacity plane, away from the real, positive semi-axis*. One can express $\Xi_V(T, z)$ in terms of these roots,

$$\Xi_V(T, z) = \xi \prod_{i=1}^{M} \left[1 - \frac{z}{z_i(T)} \right] \tag{3}$$

(where ξ is a multiplicative constant, that we shall ignore in the foregoing), and the corresponding finite-size grand-canonical potential $\Omega_V = -k_B T \ln \Xi_V = -P_V V$ leads to the following expression of the finite-size pressure P_V:

$$P_V(z) = k_B T \frac{1}{V} \sum_{i=1}^{M} \ln \left[1 - \frac{z}{z_i(T)} \right] . \tag{4}$$

Note that throughout this section we shall consider the *temperature T as a fixed parameter*, and therefore all the quantities like $P_V(z)$, $\rho(z)$, $P(z)$, $\varphi(z)$, $\psi(z)$, $\lambda(s)$, as well as $\mathcal{C}$ (see below) are *temperature-dependent*.

Let us consider now the *complex extension of $P_V(z)$*, that is defined through Eq. (4) above for all *complex z with the exception of the points z_i*. From the standard

theory of the complex-variable functions, one can deduce that $P_V(z)$ is analytical (infinitely differentiable) over any region of the complex-z plane that is free of zeros of the partition function. Therefore, a nonanaliticity of $P_V(z)$ at a complex point z_0 appears if and only if in any arbitrarily small region around z_0 one finds at least one root of the partition function (or, in other terms, if and only if there is an accumulation of the roots of the partition function in the vicinity of z_0). If, moreover, z_0 lies on the physically accessible real positive semi-axis, this corresponds to a phase transition in the system.

Once more, one realizes that such conditions cannot be accomplished in a finite-size system. Let us then turn to the thermodynamic limit, where one might eventually expect a possible accumulation of the roots of the partition function toward the real positive semi-axis.

As V and therefore $M = V/b$ increase, the location of the roots z_i changes, and in the *thermodynamic limit* they accumulate in a certain region $\mathcal{C}$ of the complex-z plane, with a local density $\rho(z)$. Of course, in view of its significance, $\rho(z)$ is a *real-valued, non-negatively defined function* on $\mathcal{C}$, identically zero for any z outside $\mathcal{C}$, which is normalized as

$$\int_{\mathbf{R}^2} \rho(z)\, dz = \int_{\mathcal{C}} \rho(z) dz = \frac{M}{V} = \frac{1}{b}, \tag{5}$$

and thus it is integrable over any bounded region of the complex-z plane.[d] Moreover, the symmetry property of the roots with respect to the real axis is preserved in the thermodynamic limit, and leads to the following property of the density of zeros:

$$\rho(z) = \rho(z^*) \tag{6}$$

[where $(\cdots)^*$ denotes complex-conjugation], i.e., $\mathcal{C}$ is symmetric with respect to the real axis. Note also that the region $\mathcal{C}$ depends on the temperature T, and, of course, its characteristics are specific to each system. For all the points z outside the region $\mathcal{C}$, one can define the thermodynamic limit of the complex extension of the pressure, $P(z) = \lim_{V \to \infty} P_V(z)$, a *complex-valued* quantity expressed as

$$P(z) = k_B T \int dz' \rho(z') \ln\left(1 - \frac{z}{z'}\right), \tag{7}$$

which is, of course, a multi-valued function. Let us consider its real part (up to a factor $k_B T$)

$$\varphi(z) \equiv \frac{1}{k_B T} \mathcal{R}e\, P(z) = \int dz' \rho(z') \ln\left|1 - \frac{z}{z'}\right|. \tag{8}$$

Since $\ln|z|$ (with $z = x + iy$; $x, y \in \mathbf{R}$) is the Green's function of the two-dimensional Laplacian $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$, by applying the Laplacian to the above equation,

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[d]As already mentioned in Sec. 2, we shall consider here only systems with a hard-core interparticle repulsion at small distances, i.e., with a non-zero single-particle excluded volume b. Most of the litterature on the subject is limited to this situation; see Ref. 22 for an exception.

one finds that:

$$\rho(z) = \frac{1}{2\pi}\,\Delta\varphi(z)\,. \tag{9}$$

This means that $\varphi(z)$ is the electrostatic potential associated to a distribution of charges of density $\rho(z)$. This analogy is very useful since it allows the direct transcription of well-known results from electrostatics. In particular, since $\rho(z)$ is integrable even on regions containing parts of $\mathcal{C}$, the function $\varphi(z)$ can be extended through *continuity* over the entire complex-z plane. The equipotential surfaces are thus given by $\varphi(z) = $ constant. Still in this analogy with electrostatics, the imaginary part of $P(z)/k_B T$,

$$\psi(z) \equiv \frac{1}{k_B T}\mathcal{I}m\,P(z) \tag{10}$$

(defined modulo 2π) determines, through the condition $\psi(z)=$constant, the lines of force of the electrostatic field generated by the distribution of charges $\rho(z)$, and the intensity of the field is given as $\nabla\varphi(z)$ and is, of course, discontinuous on $\mathcal{C}$, see point (ii) below for further details. Note also that

$$\varphi(z) = \varphi(z^*) \quad \text{and} \quad \psi(z) = -\psi(z^*)\,, \tag{11}$$

which result directly from the symmetry property (6) of the distribution of zeros.

Suppose now that the known partition function of the system indicates that $\varphi(z)$ has, for example, two distinct analytical expressions $\varphi_1(z)$ and $\varphi_2(z)$ in two different regions of the complex-z plane. But since $\varphi(z)$ has to be continuous over the entire plane, there should be a matching region between these expressions, and, of course, this region can be nothing else than $\mathcal{C}$. Indeed, since $\varphi_{1,2}$ are different functions, there appears the possibility of a nonanaliticity of φ (and thus of $P(z)$) at the matching points. Then the location of $\mathcal{C}$ is given by the condition:

$$\varphi_1(z)\Big|_{\mathcal{C}} = \varphi_2(z)\Big|_{\mathcal{C}}\,, \quad \text{i.e.,} \quad \mathcal{R}e\,P_1(z)\Big|_{\mathcal{C}} = \mathcal{R}e\,P_2(z)\Big|_{\mathcal{C}}\,. \tag{12}$$

If the region $\mathcal{C}$ intersects the real positive semi-axis at some point z_0, and/or there is an accumulation of zeros in the vicinity of z_0, then we have a phase transition in the system, and

$$\mathcal{R}e\,P_1(z_0) = \mathcal{R}e\,P_2(z_0)\,, \tag{13}$$

the real part of the complex-valued pressure is *continuous* at the transition point.

Of course, depending on the shape of $\mathcal{C}$, several transition points may appear, for different values of the fugacity; one can also encounter the phenomenon of multiple phase coexistence — like, for example, the appearance of triple points through the coalscence, at some temperature, of two simple (two-phase) transition points. Moreover, recall that $\mathcal{C}$ depends on the temperature, and from here there appears the possibility of the existence of a critical temperature T_c, such that for any $T < T_c$ the zeros of the partition function accumulate in the vicinity of the real positive semi-axis (i.e., there is a phase transition in the system), while for any $T > T_c$ the

zeros of the partition function are no longer accumulating in the vicinity of the real positive semi-axis, i.e., a phase transition is no longer possible.

We thus answered the point (A) concerning the formal frame for the description of the appearance of the phase transitions — at least, for the time being, in the grand-canonical ensemble.

(B) The characteristics of the transition. In order to answer the second question, namely the quantitative connection between the nature of the phase transition and the distribution of zeros of the partition function, let us suppose for the moment that $\mathcal{C}$ is a *smooth curve* in the vicinity of the transition point z_0. As it can be seen below, on some concrete prototypical examples of physical systems, this is rather often the case for the zeros of the grand-canonical partition function in the complex-fugacity plane — the so-called *Yang–Lee zeros*.

Following the arguments in Refs. 10, 13–15 and 17–19, let us consider a parametrization of the curve $\mathcal{C}$ in the vicinity of z_0, with the parameter s measuring the anti-clockwise oriented distance from z_0 along the curve ($s = 0$ at $z = z_0$), (see Fig. 1).

Let $\lambda(s)$ denote the line density of zeros along $\mathcal{C}$. Then, according to Gauss' theorem, one has for a point z on the curve

$$\frac{1}{2\pi}[\boldsymbol{\nabla}\varphi_2(z) - \boldsymbol{\nabla}\varphi_1(z)] \cdot \hat{\mathbf{n}}\Big|_{\mathcal{C}} = \lambda(s)\,, \tag{14}$$

where $\hat{\mathbf{n}} = \hat{\mathbf{n}}(s)$ is the unit vector normal to $\mathcal{C}$ (oriented from region "1" to region "2") at that point z. In view of the Cauchy–Riemann properties of the analytical
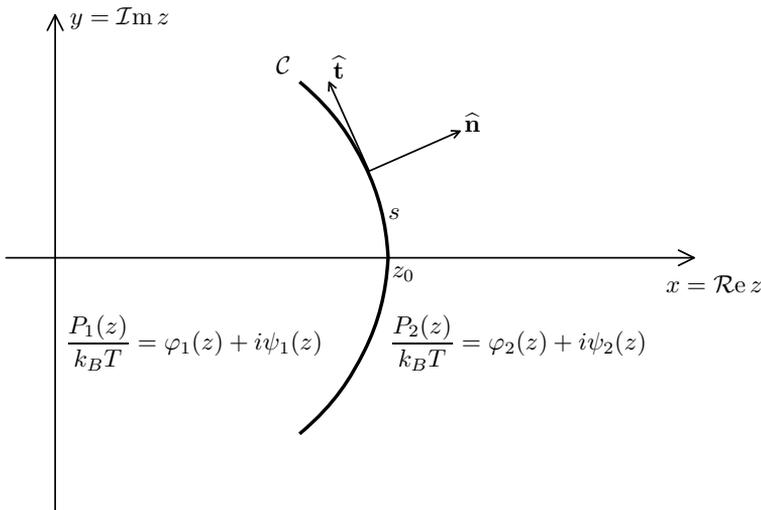

Fig. 1.   Schematic representation of the location $\mathcal{C}$ of the Yang–Lee zeros in the vicinity of a transition point z_0, meant to illustrate the notations in the main text.

functions $P_{1,2}(z)$, one has

$$\boldsymbol{\nabla}\varphi_{1,2}(z)\cdot\hat{\mathbf{n}}\Big|_{\mathcal{C}} = \boldsymbol{\nabla}\psi_{1,2}(z)\cdot\hat{\mathbf{t}}\Big|_{\mathcal{C}} \tag{15}$$

where

$$\psi_{1,2}(z) = \frac{1}{k_B T}\mathcal{I}m\,P_{1,2}(z) \tag{16}$$

are the imaginary parts of $P_{1,2}(z)/k_B T$ (defined modulo 2π), and $\hat{\mathbf{t}} = \hat{\mathbf{t}}(s)$ is the unit vector tangent to $\mathcal{C}$. This leads finally to

$$\lambda(s) = \frac{1}{2\pi}\frac{d}{ds}[\psi_2(z) - \psi_1(z)]\Big|_{\mathcal{C}}\,, \quad i.e., \quad \lambda(s) = \frac{1}{2\pi k_B T}\frac{d}{ds}[\mathcal{I}m\,P_2(z) - \mathcal{I}m\,P_1(z)]\Big|_{\mathcal{C}} \tag{17}$$

where d/ds denotes the directional derivative along the curve. In particular, at the transition point z_0, the discontinuity in the directional derivative of the imaginary part of the complex-valued pressure is determined by the local linear density of zeros,

$$\frac{1}{2\pi k_B T}\frac{d}{ds}[\mathcal{I}m\,P_2(z) - \mathcal{I}m\,P_1(z)]\Big|_{z=z_0} = \lambda(0)\,. \tag{18}$$

The relationships (12), (13), (17) and (18) will allow us to establish the nature of the phase transition, i.e., whether it is discontinuous (or first-order) or continuous — i.e., second- or higher-order in the classical *Ehrenfest classification scheme*.

Let us consider the Taylor expansion around z_0 of the complex-valued pressure on both sides of the curve $\mathcal{C}$, i.e.,

$$\frac{1}{k_B T}P_{1,2}(z) = \frac{1}{k_B T}P(z_0) + a_{1,2}(z - z_0) + b_{1,2}(z - z_0)^2 + \mathcal{O}((z - z_0)^3)\,. \tag{19}$$

In order for the pressure to be real on the real z axis, all the coefficients of the development have to be real. From the condition (12), one finds that the equation for the curve $\mathcal{C}$ is given by

$$(a_2 - a_1)(x - z_0) + (b_2 - b_1)[(x - z_0)^2 - y^2] + \mathcal{R}e[\mathcal{O}(z - z_0)^3] = 0\,, \tag{20}$$

where x and y are the real, respectively the imaginary part of z. Several situations may appear.

(i) *First-order phase transition*. If $a_2 \neq a_1$ then the complex-valued pressure has a discontinuity in its first derivative and the transition is of first-order. If, moreover, $b_2 \neq b_1$, then in the vicinity of the transition point z_0 the curve $\mathcal{C}$ is a hyperbola,

$$y^2 = (x - z_0)^2 + \frac{a_2 - a_1}{b_2 - b_1}(x - z_0) \tag{21}$$

whose tangent in z_0 is parallel to the imaginary axis, i.e., $\mathcal{C}$ crosses the real axis smoothly at an angle $\pi/2$. Using Eq. (18) we find the density of zeros at z_0,

$$\lambda(0) = \frac{a_2 - a_1}{2\pi}\,, \tag{22}$$

i.e., the density of zeros at the transition point of a first-order phase transition is nonzero.

(ii) *Second-order phase transition.* If $a_2 = a_1$, but $b_2 \neq b_1$, then the curve $\mathcal{C}$ obeys the equation

$$y = \pm(x - z_0)\,, \tag{23}$$

i.e., in the vicinity of z_0 it consists of two straight lines that make an angle of $\pm\pi/4$ with the real axis (and $\pi/2$ between them) and meet at z_0. From Eq. (17) we find that

$$\lambda(s) = \frac{b_2 - b_1}{\pi}\,|s| + \mathcal{O}(s^2)\,, \tag{24}$$

i.e., the desity of zeros is decreasing linearly to zero when approaching the transition point z_0 ($s = 0$).

(iii) *Higher-order phase transitions.* If the discontinuities appear at higher orders in the derivatives of the complex-valued pressure, then one can repeat the above type of reasoning to find the equation of $\mathcal{C}$ and the density of zeros in the vicinity of the transition point z_0. In general, if the transition is of n-th order ($n \geqslant 3$), then the density of zeros is zero at the transition point, $\lambda(s) \sim |s|^{n-1}$, and the curve $\mathcal{C}$ does not cross smoothly the real axis, but approaches it at an angle $\pm\pi/2n$ from above and below.

Resuming, we managed therefore to respond the two main questions:

(A) The accumulation of zeros of the partition function along the (physically acessible) real, positive semi-axis of the complexified fugacity z indicates the location of the phase transition point(s);

(B) The density of zeros near such an accumulation point determines the order of the transition (according to Ehrenfest's classification scheme) at that point.

In this section we discussed the zeros Yang–Lee zeros of the grand-canonical partition function in the complex-fugacity plane. One can, of course, address the following legitimate question: how can one extend this type of formalism in order to study phase transitions in other statistical ensembles (e.g., the canonical one). Indeed, in view of the equivalence of these ensembles in the thermodynamic limit, one is entitled to expect similar results on the location and characteristics of the phase transitions whatever the ensemble used in the description of the system. Before addressing this important problem in Sec. 12 below, let us add a few more relevant comments on the Yang–Lee zeros.

4. Grand-Canonical Partition Function Zeros and the Equation of State

We saw from above that knowing the distribution $\rho(z)$ of the zeros of the grand-canonical partition function in the thermodynamic limit, one can compute the

complex-valued pressure $P(z)$ through Eq. (7),

$$P(z) = k_B T \chi(z) \,, \tag{25}$$

with

$$\chi(z) \equiv \int dz' \rho(z') \ln\left(1 - \frac{z}{z'}\right) \,, \tag{26}$$

that is analytical everywhere outside $\mathcal{C}$. Also, the complex-valued particle-number density $n(z)$ follows from the complex extension of

$$n(z) = \lim_{V \to \infty} \frac{\partial}{\partial \ln(z)} \frac{1}{V} \ln \Xi_V \tag{27}$$

as:

$$n(z) = z \frac{d\chi(z)}{dz} = z \int dz' \frac{\rho(z')}{z - z'} \,, \tag{28}$$

for all complex z outside $\mathcal{C}$. When z is *real and positive* (and outside the possible intersections of $\mathcal{C}$ with the real positive semi-axis that corresponds to phase-transition points), Eqs. (25) and (28) [with $\chi(z)$ given by Eq. (26) as a functional of $\rho(z)$] are parametric expressions of the *equation of state* of the system. Recall also that $\rho(z)$ and $\mathcal{C}$, and therefore $\chi(z)$ are *temperature-dependent*, see Sec. 3, and thus the structure of these parametric equations is actually quite intricate. Of course, one can, in principle, eliminate z between the two equations and find the explicit form of $P = P(n, T)$ (for the different regions of the real-positive semi-axis of z outside $\mathcal{C}$, i.e., free of transition points).

However, one has to realize that the problem of determining the distribution of complex zeros $\rho(z)$ is an extremely difficult task, even in the simplest known-cases like, e.g., a one-dimensional lattice gas with nearest-neighbor attractive interactions,[12] a gas of hard rods,[22] a mean-field lattice gas.[40,41] It is of interest, therefore, to address the following problem. Suppose that we are given an certain equation of state $P = P(n, T)$; using the parametrization of Eqs. (25) and (28), one can find a closed nonlinear first-order differential equation for the function $\chi(z)$, which, by integration, leads generically to a functional equation of the form

$$\mathcal{F}(\chi, z) = 0 \,, \tag{29}$$

(for real positive z). Let us extend it, by definition, to the whole complex-z plane. Would it then be possible to solve it and, once $\chi(z)$ is found, to determine the region $\mathcal{C}$ of accumulation of zeros of the grand-canonical partition function? Supposing that $\mathcal{C}$ is a smooth curve, would it be then possible to find, through Eqs. (26) or (17), the corresponding density of zeros $\rho(z)$ of the grand-canonical partition function of the system?

This is currently called *the inverse problem* (in analogy with the inverse problem in electrostatics), and it has been addressed in several papers on various specific systems, see Refs. 20 and 21 (two models of Ising ferromagnets),[22] (a Tonks gas of hard rods and a gas with a weak long-range repulsion),[31] (Tonks gas),[23,24,27−30]

(the van der Waals gas),[25] (a lattice gas with a hard-core repulsion extended over several lattice sites),[32,33] (Takahashi lattice gas),[34] (point particles with logarithmic interactions), and even in an experimental setup, see Ref. 35 (for a two-dimensional Ising ferromagnet).

The answer to this issue is related to the considerations in the previous section and, being rather technical, will not be given here in detail; we refer the reader to the set of four papers by Ikeda, Refs. 36–39, for a rigorous approach of the problem (and also some illuminating examples, like various systems with circular distributions of zeros, see Sec. 7 below; the ideal Fermi–Dirac gas; and the ideal Bose-Einstein gas). Roughly, an equation of type (29) has as solutions one or several complex-valued functions, which may have one or several Riemann surfaces (i.e., are in general multi-valued functions), with branching points corresponding to $dz/d\chi = 0$. One has to try to match these different Riemann sheets, along the curve $\mathcal{C}$, so that several mathematically and physically necessary conditions are fulfilled by the resulting patch-function $\chi(z)$:

 (i) The branching points belong to $\mathcal{C}$;
 (ii) The real part of $\chi(z)$ ($\varphi(z)$ in the notations of the previous section) has to be continuous in the whole z plane;
(iii) $\chi(z)$ is real and continuous on the real positive semi-axis and has the value given by Eq. (25);
(iv) The integration constant result from the infinite-dilution (ideal gas) limit, $\chi(z) \sim z$ for $z \to 0$;
 (v) The quantity $\rho(z)$, as defined by Eq. (17), has to be real-valued and non-negative for all z on $\mathcal{C}$.

The discontinuities in the imaginary part of $\chi(z)$ ($\psi(z)$ in the notations of the previous section) appear thus across the charged contour $\mathcal{C}$ originating from matching the different Riemann sheets of the multi-valued solutions of (29). In the particular case when the solution of Eq. (17) is a single multi-valued function, the domain $\mathcal{C}$ of the zeros of the partition function reduces to the branching points. One has to note, however, that for a general functional relation (29) there is no guarantee of the uniqueness of the domain $\mathcal{C}$, and also that rather often the explicit construction of $\mathcal{C}$, and thus the calculation of $\rho(z)$ are not possible, except for limiting cases, e.g., in the vicinity of the branching points.

5. The Lattice Gas and the Ising Model in a Magnetic Field

Before proceeding to the next sections with a discussion of the domain $\mathcal{C}$ of accumulation of zeros of the grand-canonical partition function, let us recall a well-known classical result of equilibrium statistical mechanics, namely that the problem of a discrete lattice gas (with nearest-neighbor interactions) is mathematically equivalent to the problem of an Ising model (with nearest-neighbor interactions) in an uniform magnetic field (see e.g. Refs. 4 and 12 for a detailed description). In

particular, the expression of the *grand-canonical* partition function of the lattice gas
is identical to the expression of the *canonical* partition function of the Ising model
in magnetic field (at the same fixed temperature T). The search of the complex
roots of the grand-canonical partition function of the gas in the complex-fugacity
plane amounts to the search of the complex roots of the canonical partition function
of the Ising model in the plane of the complex variable $z = \exp(-2H/k_B T)$ (in the
appropriate units for the field and the temperature), that is related to a *complex
magnetic field intensity H*.

Therefore, based on this one-to-one correspondence, in the foregoing we will
speak either of a discrete lattice gas, or of an Ising model in a magnetic field.

6. Yang–Lee Zeros and the Transfer Matrix Formalism

For one-dimensional Ising lattice systems with finite-range interactions, in a mag-
netic field H, it is customary to compute the partition function using the *transfer-
matrix* technique. The canonical partition function for N spins can be written as:

$$Z_N = \lambda_1^N + \lambda_2^N + \cdots + \lambda_k^N \,, \tag{30}$$

where λ_i, with $i = 1, \ldots, k$, are the k eigenvalues of the $k \times k$ transfer ma-
trix of the system. Besides being dependent on the reduced coupling constants
(i.e., the coupling constants divided by $k_B T$) between the spins, these eigenval-
ues depend on the value of the magnetic field H, or, equivalently, on the fugacity
$z = \exp(-2H/k_B T)$, $\lambda_i = \lambda_i(z)$, $i = 1, \ldots, k$. Let us consider the free energy per
spin, $F = -k_B T \ln Z_N/N$, and its extension to the plane of the complex fugacity.
In the thermodynamic limit, only the eigenvalue of highest modulus contribute to
the free energy. Suppose now that in two different regions of the complex-z plane
two different eigenvalues, $\lambda_1(z)$, respectively $\lambda_2(z)$ assume the largest modulus.
Since the real part of the free energy (per spin) has to be continuous throughout
the whole z plane — see the discussion in Sec. 3 in the light of the correspondence
between Ising systems and lattice gases, Sec. 5 — it follows that the location $\mathcal{C}$ of
the zeros of the partition function in the complex-z plane is given by the condition
of matching of the modulus of these two eigenvalues of the transfer matrix:

$$\left.|\lambda_1(z)|\right|_{\mathcal{C}} = \left.|\lambda_2(z)|\right|_{\mathcal{C}} \,, \tag{31}$$

which is the equivalent of Eq. (12) in the present frame. Of course, in view of the
van Hove theorem (Sec. 2) for the systems with short-range interactions that we are
considering here, no phase transition is possible, i.e., $\mathcal{C}$ does not have any accumula-
tion point on the real positive semi-axis for such systems. This matching condition
between eigenvalues might be useful for the construction of $\mathcal{C}$, (see e.g. Ref. 45 and
110 for a few examples). A more rigorous discussion of this type of approach for a
wide class of lattice gases can be found in Ref. 48.

7. The Circle Theorem for the Yang–Lee Zeros

The general frame discussed in Sec. 3 above is applicable to all the systems — within, of course, the mentioned restrictions that refer, essentially, to the existence of the thermodynamic limit (see Sec. 2). However, as already mentioned, the shape of the domain $\mathcal{C}$ of the accumulation of zeros of the grand-canonical partition function in the complex-fugacity plane, besides being *temperature-dependent*, is *specific to each system*, and *a priori* one might expect it to have a rather intricate structure. It is therefore a rather amazing result that, for a quite general class of systems, this region $\mathcal{C}$ can be proven rigorously to *lie on the unit circle* $|z| = 1$ in the complex-fugacity plane. This is the celebrated Circle theorem that was first demonstated by Yang and Lee (see Ref. 12, for a rather restricted class of Ising systems). The beauty and simplicity of this result attracted a lot of research afterwards, and led to its generalization to many other situations and models, see below. Note, however, that no general statement can be made about the density of zeros on the unit circle, which is characteristic to each system and, of course, temperature-dependent.

7.1. *The original Yang–Lee Circle theorem*

The system originally considered by Yang and Lee (see Refs. 12, 72 and 26) consists of an ensemble of N Ising 1/2-spins σ_i $(i = 1, \ldots, N)$:

(i) that are placed on a d-dimensional lattice;
(ii) with pair ferromagnetic interactions between them, of coupling constants $J_{ij} \geqslant 0$ $(i \neq j = 1, \ldots, N)$;
(iii) that are subject to a (eventually inhomogeneous) magnetic field.

The corresponding Hamiltonian[e]

$$\mathcal{H} = -\sum_{i<j} J_{ij}\sigma_i\sigma_j - \sum_i H_i\sigma_i \tag{32}$$

leads to a canonical partition function $Z_N = Z_N(z_1, z_2, \ldots, z_N)$ that is a multinomial in the fugacities

$$z_i = \exp(-2H_i/k_B T) \tag{33}$$

(H_i being the value of the magnetic field acting on the spin σ_i). In the particular case of a homogeneous magnetic field $H_i = H$ for all i, the partition function is simply a polynomial of degree N in the fugacity $z = \exp(-2H/k_B T)$. Under the supplementary hypothesis

(iv) $|z_i| \leqslant 1$ for all $i = 1, \ldots, N$

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[e]Of course, alternatively, one can consider the equivalent lattice gas model, which corresponds to an uniform magnetic field.

one can prove the *Circle theorem*: the zeros of the partition function in the $2N$-dimensional space of complex z_i lie all on the unit circle,

$$Z_N = 0 \rightarrow |z_1| = |z_2| = \cdots = |z_N| = 1 \,, \tag{34}$$

which amounts to saying that these roots correspond to strictly imaginary (or zero) values of the magnetic field intensity H_i, $i = 1, \ldots, N$. In the particular case of a homogeneous magnetic field, all the N roots of $Z_N = 0$ lie on the unit circle $|z| = 1$ in the complex-z plane, i.e., appear for N strictly imaginary (or zero) values of H. The theorem remains valid in the thermodynamic limit, when the zeros form a dense set $\mathcal{C}$ on the unit circle, characterized by the linear density λ. Of course, an immediate consequence of this theorem is the well-known classical result that a phase transition might appear in such a system, at a fixed finite temperature T, only in zero magnetic field.

Note that:

(i) The dimensionality of the lattice does not play any role in the demonstration of the theorem, which is thus valid in any dimension. Moreover, the size and the structure of the lattice, its regularity, periodicity, translational symmetry do not play any role either in the obtention of the result.

(ii) The ferromagnetic interactions are not restricted to first neighbors. However, they should decrease sufficiently rapidly with the distance in order to ensure the existence of the appropriate thermodynamic limit (see the discussion in Sec. 2).

Indeed, the demonstration of this theorem,[12] that will not be reproduced here, rely on some properties of the Hamiltonian that are independent of the dimension and of the range of the interactions; besides the ferromagnetic character of the interspin interaction, an essential necessary ingredient is the *spin-reversal symmetry* of the system, i.e., the invariance of its Hamiltonian with respect to global inversion of the spins and of the (inhomogeneous) magnetic field, which leads to the following symmetry property of the canonic partition function:

$$Z_N(z_1, z_2, \ldots, z_N) = z_1 z_2 \cdots z_N Z_N(z_1^{-1}, z_2^{-1}, \ldots, z_N^{-1}) \,. \tag{35}$$

Later on, Asano, in Refs. 53 and 54, introduced a new, more general technique for the study of the location of the zeros of the grand-canonical partition function. This method was often used to prove the Circle theorem for various systems (see below), but it was also extended by Ruelle, (see Refs. 73 and 74), so as to permit statements about regions other than the unit circle.

7.2. *Generalizations of the Circle theorem to other systems and models*

We shall briefly present below some of the systems for which it was shown, using various methods, that the Circle theorem is valid.

(A) Modified Ising ferromagnets, which include:

(i) *Ising ferromagnets of arbitrary spin*, see Refs. 49, 50 and 52. The basic idea for the extension is that the higher-spin "atom" is a cluster of 1/2-spin "atoms", that are coupled together through a suitable ferromagnetic interaction. This representation leads to an effective, temperature-dependent, 1/2-spin Ising Hamiltonian and from here to the Circle theorem. Once demonstrated this result for any finite value of the spins, one can extend it to the classical limit or infinite-spin limit (see Ref. 59).

(ii) *Diluted Ising ferromagnets.* Consider a lattice whose sites are either occupied by a spin 1/2 (with a probability p), or by a non-magnetic atom (with probability $1 - p$); p is thus equal to the concentration of spins on the (infinite) lattice. As shown in Refs. 60 and 61, for a ferromagnetic coupling between the spins, and in a homogenous magnetic field H, the zeros of the partition function correspond to purely imaginary (or zero) values of H. This result can be extended to higher-spin cases.

(iii) *Ising models with many-spin interactions.* Ising lattice systems with interactions involving three or more sites — i.e., whose Hamiltonian comprises interaction terms of the form $-J_{ij\ldots k}\sigma_i\sigma_j\cdots\sigma_k$, where $i \neq j \neq \cdots \neq k$ correspond to different lattice sites, and $J_{ij\ldots k}$ is the coupling constant between these sites — have been used to model a variety of physical situations, like, for example, some binary alloys,[84] lipid bilayers,[85] and gauge-field theory models.[86] These systems have rich phase diagrams, and Monte–Carlo results indicate the presence of phase transitions at nonzero values of the magnetic field for a number of these systems (see e.g. Refs. 87 and 88). However, in view of their complexity, very few analytically rigorous results are known. In Ref. 55 it is shown that for a set of many-spin interactions of finite range, under some conditions on the coupling constants, and also some spin-inversion symmetry conditions, the Circle theorem holds (at least) up to a certain temperature (that is determined by the coupling constant and does not depend on the number of spins in the system). The example of four-spin interactions shows explicitly that the zeros leave the unit circle at large-enough temperatures. Qualitative arguments suggest that this is the case for other systems with multi-spin interactions, (see also Ref. 83).

(iv) *Ising models on hierarchical lattices.* In Ref. 89 a rescaling formalism is used in order to study the location of the Yang–Lee zeros for 1/2-spin and 1-spin Ising chains on two- and three-dimensional Sierpinski gaskets, as well as on 3-simplex and 4-simplex lattices. The Circle theorem is shown to hold for nearest-neighbor ferromagnetic interactions, but is no longer valid at high temperatures when four-spin interactions are included, see also point (iii) above. References 90 and 91 address the problem of the Yang–Lee zeros of the Ising nearest-neighbor ferromagnetic model on a Cayley tree. The Julia set of the renormalization transformation of the model gives the thermodynamic limit of the partition function zeros distribution. This one lies on the unit circle, and is multi-fractal in nature, with a temperature-dependent generalized dimension;

below T_c the Julia set is the unit circle (i.e., it has dimension $D = 1$), and above T_c the Julia set is a Cantor set (with a dimension $D(T) < 1$ decreasing with the temperature) on the unit circle. When multi-site interactions are included, these zeros leave the unit circle, (see Ref. 92).

(v) *Aperiodic Ising models.* References 93–95 discuss various one- and two-dimensional examples of Ising spins with nearest-neighbor interactions on aperiodic lattices. The interaction constant can take only two values, $J_{a,b}$, distributed on the lattice according to some generating rule. In $1D$ case, for example, the actual distributions of the two coupling constants $J_{a,b}$ along the chain is determined by an infinite "word" in the letters "a" and "b" which is obtained as the unique limit of certain two-letter substitution rules (like, e.g., the Fibonacci or the Thue–Morse rules). If both $J_{a,b}$ are positive (ferromagnetic coupling), then although the zeros still lie on the unit circle, their distribution has a fractal structure (that, of course, disappears when $J_a = J_b$), as shown by the integrated density of the zeros along the circle. Thus such systems may be regarded as intermediate between regular and hierachical models.

(vi) *Mean-field Ising model.* In Refs. 40–43, the problem of the Yang–Lee zeros for the Temperley-Husimi model of a lattice gas is addressed, or for the equivalent mean-field Ising model in a magnetic field, which, of course, is known to exhibit a first-order phase transition, with a critical temperature T_c. The partition function zeros lie on the unit circle in the complex-fugacity plane, and one can compute analytically the corresponding density. A direct comparison with Mayer's cluster expansion theory[97−99] shows that the non-analiticity point in Mayer's series does not coincide with the true transition point as obtained from the Yang–Lee theory, (see related comments in, e.g. Refs. 11, 20 and 100). See also Ref. 101 for an approach using the Yang–Lee zeros of a restricted partition function for the study of the metastable states of long-range (and their mean-field limit) Ising models.

(B) Heisenberg spin models. The technique of studying the Yang–Lee zeros that was introduced by Asano in Refs. 53 and 54 was also used by Suzuki and Fisher in Ref. 55, their studies being devoted to the extension of the Circle theorem to quantum 1/2-spin systems in a magnetic field. More precisely, they considered the following *fully anisotropic* Heisenberg Hamilonian for a system of N spins of components $\sigma_i^{x,y,z}$, $i = 1, \ldots, N$, in a magnetic field:

$$\mathcal{H} = -\sum_{i<j}(J_{ij}^x\sigma_i^x\sigma_j^x + J_{ij}^y\sigma_i^y\sigma_j^y + J_{ij}^z\sigma_i^z\sigma_j^z) - \sum_i(H_i^x\sigma_i^x + H_i^y\sigma_i^y + H_i^z\sigma_i^z)\,, \quad (36)$$

where $J_{ij}^{x,y,z}$ are the (anisotropic) coupling constants and $H_i^{x,y,z}$ are the (non-uniform) components of the magnetic field in the x, y and z directions. Consider that $H_i^z \equiv H\mu_i$, with μ_i non-negative constants (for all $i = 1, \ldots, N$), and that the coupling constants obey the following set of inequalities

$$J_{ij}^z \geqslant |J_{ij}^x| \quad \text{and} \quad J_{ij}^z \geqslant |J_{ij}^y| \quad \text{for all} \ \neq j = 1, \ldots, N\,, \quad (37)$$

which correspond to the so-called[55] *ferromagnetic Heisenberg model with dominant $z - z$ coupling.* Then one can prove that the zeros of the partition function $Z_N = \text{Tr}[\exp(-\mathcal{H}/K_B T)]$ as a function of H lie all on the imaginary-H axis for all N, and do so also in the thermodynamic limit. This result was generalized further in Ref. 55 for quantum models with spin greater than $1/2$ (note that some preliminary results have already been obtained in Ref. 56), and also to the classical Heisenberg system of infinite spins (see Ref. 59); see also Ref. 61 for a temptative relaxation of the corresponding conditions (36) on the coupling constants in the classical limit. In Ref. 59 it was also shown that the Circle theorem holds for a *two-sublattice antiferromagnet of arbitrary spin, in terms of the staggered magnetic field intensity.*

(C) Monomer-dimer models. Consider a lattice of N sites or vertices, connected through $N(N-1)/2$ edges; one associates to the edge connecting the vertices i and j a weight w_{ij}, and to a vertex i a weight x_i (of course, w_{ij} and x_i are non-negative numbers for all $i \neq j = 1, \ldots, N$). A dimer-monomer covering of this lattice corresponds to (i) placing dimers on the edges such that no two dimers share a common vertex (i.e., no vertex has more than one dimer); (ii) placing monomers on all the remaining vertices, i.e., the vertices that are not adjacent to a dimer. The statistical weight of such a covering is then the product of all the weights w_{ij} of the edges covered by the dimers times the weights x_i of all the vertices covered by a monomer. The partition function $Z_N = Z_N(\{w_{ij}\}, \{x_i\})$ of the system is then the sum of the weights of all the possible coverings. These models correspond to a huge variety of physical situations, (see e.g. Ref. 64 for an overview).

References 61–65 address the problem of the zeros of the partition function of the monomer-dimer system. It is shown that, for given non-negative w_{ij}, Z_N cannot be zero if $\mathcal{R}e(x_i) > 0$ for all $i = 1, \ldots, N$ or if $\mathcal{R}e(x_i) < 0$ for all $i = 1, \ldots, N$. In particular, if $x_i \equiv x$ for all $i = 1, \ldots, N$, this leads to the conclusion that the zeros of Z_N appear on the imaginary-x axis (or at $x = 0$), a result that holds also in the appropriate thermodynamic limit. This corresponds to the absence of a phase transition in the monomer-dimer system, except, eventually, at $x = 0$, which corresponds to a maximum density of dimers. Connections with Ising and Heisenberg spin models are also discussed.

(D) Ferroelectric models. In Refs. 55, 57 and 58 it was shown that the Slater-type models for ferroelectricity[102] can be mapped onto Ising models with at most four-spin interactions. Therefore, the Yang–Lee zeros lie on the unit circle at low temperatures, but leave it at the critical temperature T_c. A modified Slater model, and an antiferromagnetic model are also discussed from the perspective of the Yang–Lee theory, and their distributions of zeros on the unit circle, for finite-size lattices, are investigated numerically.

(E) Quantum fields. References 66–71 show that some Euclidian quantum fields can be approximated by generalized Ising models on a lattice, with a given probability distribution of the spins (that may be discrete or continuous, but has to obey

certain symmetry properties), and with a self-interaction of the spins. In particular, the Yang–Lee Circle theorem is shown to hold for the considered systems, see the above-cited references for further details.

For all these systems for which the Circle theorem holds, using the notations in Sec. 3 one can say that the curve $\mathcal{C}$ lies on the unit circle $|z| = 1$, and can be parametrized by the trigonometric angle θ. Correspondingly, the density of zeros $\lambda = \lambda(\theta) = \lambda(-\theta)$ [in virtue of the symmetry property (6)], and it is nonzero on two arches of the unit circle defined by $\theta_0 \leqslant |\theta| \leqslant \pi$, where $\theta_0 > 0$ is a function of temperature (see also Sec. 9.2). The normalization condition (5) for the density of zeros reads simply

$$2 \int_{\theta_0}^{\pi} \lambda(\theta) d\theta = b \,. \tag{38}$$

The complex pressure (7) becomes

$$P = k_B T \int_{\theta_0}^{\pi} \lambda(\theta) \, \ln(z^2 - 2z \cos \theta + 1) d\theta \,, \tag{39}$$

and the complex particle-number density (28) is

$$n = 2z \int_{\theta_0}^{\pi} \lambda(\theta) \frac{z - \cos \theta}{z^2 - 2z \cos \theta + 1} \, d\theta \,. \tag{40}$$

Note, however, that the density of zeros $\lambda(\theta)$ is known analytically in very few cases (e.g., the one-dimensional Ising model with nearest-neighbor interactions, see Ref. 12; the mean-field Ising model, Refs. 40 and 41), and was computed numerically in few other cases (see Ref. 21 for such a calculation for the Ising ferromagnets on a two-dimensional square lattice, and on a three-dimensional diamond lattice, respectively), and thus the practical use of these relationships is rather restricted.

7.3. *Griffiths inequalities*

Note also a very important by-product of the Circle theorem, namely the demonstration of various *Griffiths-type inequalities*, i.e. inequalities between spin-correlation functions, (see Refs. 50, 51, 53, 54, 66, 67, 69, 70, 75 and 76). The simplest to demonstrate are the Griffiths–Kelly-Sherman[77−80] (GKS) inequalities. They were first obtained using the Circle theorem in Refs. 50 and 51 for an Ising $1/2$-spin ferromagnet in a magnetic field $H \geqslant 0$, as:

$$\langle \sigma_A \sigma_B \rangle \geqslant 0 \quad \text{(the first-type GKS inequality)} \tag{41}$$

$$\langle \sigma_A \sigma_B \sigma_C \sigma_D \rangle \geqslant \langle \sigma_A \sigma_B \rangle \langle \sigma_C \sigma_D \rangle \quad \text{(the second-type GKS inequality)}, \tag{42}$$

where $\sigma_{A,B,C,D}$ are the products of the spins inside the (multi-site) regions A, B, C, D of the lattice, respectively; $\langle \cdots \rangle$ denotes the mean over the statistical ensemble. These inequalities were generalized, on the basis of Yang–Lee Circle theorem, to higher-spin systems,[50] Heisenberg ferromagnets,[53,54] and systems with arbitrary even spin distributions.[67]

The Griffiths–Hurt-Sherman[81] (GHS) inequality

$$\langle \sigma_A \sigma_B \sigma_C \rangle \leqslant \langle \sigma_A \rangle \langle \sigma_B \sigma_C \rangle + \langle \sigma_C \rangle \langle \sigma_A \sigma_B \rangle + \langle \sigma_B \rangle \langle \sigma_C \sigma_A \rangle - 2 \langle \sigma_A \rangle \langle \sigma_B \rangle \langle \sigma_C \rangle \quad (43)$$

was demonstrated for various systems, using the Circle theorem, in Refs. 66, 69 and 70. It has several interesting implications, the concavity of the average magnetization as a function of H; the monotonicity of the correlation length as a function of the magnetic field; the well-known result on the absence of phase-transition for $H > 0$; some inequalities for the critical exponents; (see e.g., Refs. 76 and 82). More complicated inequalities on the correlation functions, involving the Circle theorem, are treated in Refs. 69 and 75.

8. Further Results on the Yang–Lee Zeros Location

As already mentioned, the papers by Asano, Refs. 53 and 54, and later on their elegant generalization by Ruelle, Refs. 73 and 74, lead to a criterion for the location of the Yang–Lee zeros in the complex-fugacity plane for a fairly large number of systems. This criterion, as well as ad-hoc methods adapted for the system under study (e.g., the transfer-matrix formalism for the one-dimensional lattice systems, see Sec. 6), and sometimes numerical results allowed us to approach several systems and to draw some general conclusions. A first remark would be that usually the distribution of Yang–Lee zeros in the complex-fugacity plane is well behaved, i.e., in the thermodynamic limit the zeros are distributed densely on an ensemble of smooth curves.

(A) Ising systems with multi-spin interactions. A rather general result refers to the fact that the Circle theorem does not hold at high temperatures, (see points (iii) and (iv) for modified Ising models in the previous section). A rigorous study of the regions in the complex-magnetic plane that are *free* of zeros of the partition function is carried in Ref. 83 for two very general classes of multisite interaction systems, namely (i) systems having ferromagnetic interactions involving even numbers of sites, and (ii) systems with, again, ferromagnetic interactions involving even numbers of sites and, in addition, either ferromagnetic or antiferromagnetic interactions involving odd numbers of sites. Each site may interact with a finite number of other sites. As for the case of the Circle theorem, the dimension and the specific type of lattice do not come into play. It is shown that: (i) For systems of the first type, there is an interval of the real H axis, $(-C(T), C(T))$ (with $C(T) > 0$ that depends on the strength of the ferromagnetic couplings) outside which there is no phase transition. $C(T)$ goes to zero as $T \to 0$, and hence the interval shrinks to $H = 0$. (ii) For systems of the second type, when the interaction involving odd numbers of sites is antiferromagnetic, there is an interval on the real H axis $(-\infty, -C(T))$ in which no phase transition occurs; when the interaction involving odd numbers of sites is ferromagnetic, there is no phase transition for real $H \in (C(T), \infty)$. Here again $C(T)$ is a positive parameter, depending on temperature and on the interaction constants, that goes to zero in the zero-temperature limit. These general

results put clear constraints on the region of the plane temperature-magnetic field where one is entitled to look for a possible phase transition for such systems with multi-spin interactions.

(B) Ising systems with antiferromagnetic interactions or, equivalently, lattice gases with repulsive interactions. Various Ising lattice systems with antiferromagnetic interactions have been considered in Refs. 22 (a Tonks gas of hard rods and a gas with a weak long-range repulsion),[31] (Tonks gas),[25] (a lattice gas with a hard-core repulsion extended over several lattice sites),[103] (a hard-core lattice gas on an $M \times \infty$ square lattice),[26,170] (Ising antiferromagnet),[59] (a two-sublattice antiferromagnet),[105] (Ising ferromagnet on a bipartite lattice),[44,45] (Ising lattices with various combinations of ferromagnetic and antiferromagnetic couplings),[46] (Fisher and Temperley lattice gases),[47] (one-dimensional XY model),[106] (antiferromagnetic Husimi-Temperley model),[63] (lattice gases with all the zeros of the partition function on the real negative semi-axis of the fugacity),[104] (various lattice systems of rigid molecules),[107] (various Ising antiferromagnets),[109] (numerical results on finite square-lattice Ising antiferromagnets). Different approaches are used; those that lie from the very abstract rigorous mathematical ones to approximate analytical ones in solving the inverse problem (Sec. 4), and to numerical methods. The generic emerging result is that, due to the presence of the antiferromagnetic coupling (or, equivalently, of the repulsive part of the lattice gas interparticle interaction), a part of the Yang–Lee zeros lie on the real negative semi-axis of the fugacity z (for finite systems, as well as in the thermodynamic limit, when eventually these zeros occupy densely a whole portion of the negative semi-axis). The other details of the distribution of the zeros are, of course, specific to the details of the considered model (i.e., range of interactions, whether the coupling is mixing ferromagnetic and antiferromagnetic features, etc.). The locus of zeros and even the density of zeros were sometimes computed analytically.

(C) Degenerated Ising spins. In Ref. 110 the case of a a one-dimensional, nearest-neighbor interactions, spin-1 Ising system that has a *spin degeneracy*, i.e., for which each spin variable S can take either of the values values $S = 1, 0, -1$ with a certain weight (degeneracy) $g(1)$, $g(0)$, $g(-1)$ is discussed. It is shown that the corresponding Yang–Lee zeros do not lie, in general, on the unit circle in the complex-fugacity plane. The conditions under which one recovers the Circle theorem are discussed, (see also Refs. 50, 111 and 112).

(D) Van der Waals gas. Several papers were devoted to this prototypical model of non-ideal gas that can be seen as the continuum limit of a lattice gas with weak, long-ranged attractive forces, (see Ref. 25). References 23, 24, 27–30 addressed the problem of the distribution of Yang–Lee zeros, showing that:

(i) For infinite temperature the zero distribution is located on part of the real negative semi-axis of the fugacity;

(ii) With decreasing temperature the distribution branches off the real axis, circumventing the origin symmetrically, on both sides;

(iii) Below the critical temperature T_c the distribution forms a closed curve around the origin, with a diameter decreasing exponentially to zero as $T \to 0$;

(iv) An additional tail of the distribution remains on the negative real axis, but with a density of zeros going linearly to zero as $T \to 0$.

This tail is connected to the repulsive-core singularity of the van der Waals interaction potential, (see Ref. 113 for a discussion). The density of zeros was computed analytically in some limiting cases, e.g., in the vicinity of the branching points.

(E) $\pm J$ Ising model for spin glasses. Reference 114 discusses a numerical technique for obtaining the distribution of Yang–Lee zeros of the disordered symmetric $\pm J$ Ising model (i.e., an Ising lattice for which the coupling constant between two neigbour sites is chosen at random as J or $-J$), in two and three dimensions. This distribution of zeros, which determines the analytical properties of the configuration-averaged free energy, is the superposition of the zeros of the partition function corresponding to each configuration of the coupling constants. The zeros are not distributed on smooth curves, and it seems that in the thermodynamic limit they occupy (densely or not, the question is not clarified yet) a whole region of the complex-z plane. The computation of the corresponding configuration-averaged free energy allows to approach some problems of this short-range spin glass model — like the existence of the Griffiths singularity (a non-analytic behaviour in the paramagnetic phase of a random or diluted Ising ferromagnet, see Ref. 115) and of the Almeida-Thouless transition line, Ref. 116.

9. Yang–Lee Zeros and the Critical Behaviour

For simplicity, the considerations in this section address the particular case of a system for which the Circle theorem is valid. However, they can be adapted, with some modifications, to more general locations of Yang–Lee zeros. For example, instead of the Yang–Lee edge angle θ_0 in Sec. 9.2, one should consider, in general, the smallest distance between the ensemble $\mathcal{C}$ of zeros and the critical point.

9.1. *Density of zeros near criticality*

In the vicinity of a critical point, the thermodynamic quantities, as well as the correlation functions, exhibit power-law behaviours associated with a set of critical exponents. For example, for an Ising model one has:

• For the (zero field) specific heat

$$c(t) \sim t^{-\alpha}, \quad \text{for } t > 0 \tag{44}$$

and

$$c(t) \sim |t|^{-\alpha'}, \quad \text{for } t < 0 ; \tag{45}$$

- For the spontaneous magnetization

$$m(t) \sim |t|^{\beta}, \quad \text{for } t < 0 ; \tag{46}$$

- For the isothermal susceptibility in zero field

$$\chi(t) \sim t^{-\gamma}, \quad \text{for } t > 0 \tag{47}$$

and

$$\chi(t) \sim |t|^{-\gamma'}, \quad \text{for } t < 0 ; \tag{48}$$

- For the field dependence of the magnetization at criticality

$$m(h, t = 0) \sim h^{\delta} ; \tag{49}$$

- For the correlation length

$$\xi(t) \sim t^{-\nu}, \quad \text{for } t > 0 \tag{50}$$

and

$$\xi(t) \sim |t|^{-\nu'}, \quad \text{for } t < 0 ; \tag{51}$$

- Finally, for the long-distance spin-spin correlation function at criticality:

$$G_2(r, t) \sim \frac{1}{r^{(d+2-\eta)}} , \tag{52}$$

where $t = (T/T_c - 1)$ is the reduced temperature (T_c being the critical temperature). The nine critical exponents α, α', β, γ, γ', δ, ν, ν' and η are not independent, and the scaling laws reduce the number of independent exponents to two.[117]

In the framework of the Yang–Lee theory, all the above quantities can be expressed in terms of the density of zeros, e.g., $\lambda(\theta, t)$ for an Ising-like system for which the Circle theorem is valid. In the critical region, $\lambda(\theta, t)$ should take a particular scaling form in order to reproduce the above behaviours. A large body of work has been devoted to the study of this scaling form (see Refs. 52, 118–123, and the main result is that:

$$\lambda(\theta, t) = |t|^{\beta} \psi(\theta t^{-(\beta+\gamma)}) , \tag{53}$$

in the region of the unit circle $\theta_0(t) \leqslant |\theta| \leqslant \pi$ where the density of zeros is different from zero [see Eq. (38) and above it]; $\psi(x)$ is a positively-defined function, that is finite and nonzero at $x = 0^{\pm}$. Thus, the critical exponent β can be extracted from the scaling behavior of $\lambda(\theta, t)$ in the vicinity of the critical point.

9.2. *Yang–Lee edge singularity*

Let us consider again a model for which the Circle theorem is valid, as for example an Ising-like model. For a temperature $t > 0$, a gap will show up in the density of zeros $\lambda(\theta, t)$. No zeros are present in an interval $[-\theta_0(t), \theta_0(t)]$ or, correspondingly, in a purely imaginary external field interval $[-iH_0, +iH_0]$ (with $H_0 = k_B T \theta_0 / 2$ in

the appropriate units, see Sec. 5). This gap reduces to zero when the temperature descends to the critical value and below. Kortman and Griffiths[21] were the first to point out the interest to investigate the behavior of $\lambda(\theta, t > 0)$ for θ close to the points $\pm\theta_0(t)$, called the *Yang–Lee edges*. A large literature addressed this question, (see Refs. 113, 124, 125, 127–130), leading to the following picture. The edge singularity should be regarded merely as an usual critical point occuring with a purely imaginary field iH. It turns out that

$$\lambda(\theta, t > 0) \sim |\theta - \theta_0(t)|^\sigma, \quad \text{for } \theta \to \theta_0(t)^+. \tag{54}$$

Renormalization group arguments demonstrate that the appropriate model describing the edge singularity is the so-called ϕ^3 field theory.[131] The exponent σ is simply related to the thermodynamic exponent δ:

$$\sigma = \delta^{-1}. \tag{55}$$

The upper critical dimension (above which mean-field predictions are correct) is $d_u = 6$. Moreover, the above power law behavior is valid for all temperatures $T > T_c$, and also for all $\mathcal{O}(n)$ models. Indeed, the presence of the magnetic field breaks the original $\mathcal{O}(n)$ symmetry and thus the behavior becomes Ising-like. Note moreover that the critical theory of the Yang–Lee edge in two dimensions corresponds to a rather simple realization of conformal symmetry.[126]

Therefore, the behaviour of the density of zeros near the critical edge provides a second independent critical exponent δ. The knowledge of β and δ, and of the scaling laws characterizes completely the critical behaviour of the system.

10. Finite-Size Scaling and Yang–Lee Zeros

As we have seen from above, the density of zeros near the critical edge and at criticality contains all the information concerning the critical behavior of a given system. However, an analytical expression for the density of zeros can be obtained only for some particular simple systems. For more complicated cases, the density of zeros has to be computed numerically on finite systems. It is thus important to understand the role played by the finiteness of the systems.

The finite-size scaling theory provides a powerful tool in interpreting finite-size systems data. The theory was first developped for continuous phase transitions based on phenomenological arguments.[132] A more modern presentation is based on a renormalisation group approach.[133] The key hypothesis is based on the premise that only two different scales matter, namely: ξ, the correlation lenght in an infinite system, and L, the characteristic linear extent of the finite-size system. The case of finite-size effects in first-order phase transition is somehow more subtle as discussed by Fisher and Berker.[134] However, scaling at a first-order transition can be treated in a similar manner as the one for a second-order transition with the temperature and magnetic anomalous dimensions, y_t and y_h, assuming the maximal values $y_t = y_h = d$, where d is the dimension of the system.

For a finite-size system of size L the singular part of the magnetization has the form

$$m(t, h, L) = L^{-d+y_h} m(tL^{y_t}, hL^{y_h}) \tag{56}$$

where $h \equiv 2H/k_B T$. Then the density of zeros scales as

$$\lambda(\theta, t, L) = L^{-d+y_h}\lambda(\theta L^{y_h}, tL^{y_t})\,. \tag{57}$$

At the critical temperature $t = 0$ one has

$$\lambda_c(\theta, L) = L^{-d+y_h}\lambda_c(\theta L^{y_h})\,, \tag{58}$$

which implies for the infinite system

$$\lambda_c(\theta) \sim |\theta|^{1/\delta}\,. \tag{59}$$

For $t > 0$, the angle of the Yang–Lee edge (see Sec. 9.2) for finite systems, $\theta_0(t, L)$, scales as

$$\theta_0(t, L) = L^{-y_h}\theta_0(tL^{y_t})\,, \tag{60}$$

leading, for $L \to \infty$, to

$$\theta_0 \sim t^{\beta+\gamma}\,. \tag{61}$$

Finite-size scaling for the density of Yang–Lee zeros $\lambda(\theta, t, L)$ has been discussed by Alves *et al.*[172] for the three-dimensional Ising model, by Kenna *et al.*[194,196,201] for the four-dimensional Ising model and for the $\mathcal{O}(N)\,\phi^4$ theory at the upper critical dimension.[205] Creswick and Kim[135,197] have analyzed the critical properties of the two-dimensional Ising model by computing exactly the partition function of systems of sizes $4 \leqslant L \leqslant 10$ and by extrapolating the data using a Bulirsch–Stoer (BST) algorithm.[136] Janke and Kenna[198,204] have recently developed a novel numerical technique which allows us to determine both the latent heat in the case of a first-order transition and the specific heat exponent α in the case of a second-order transition. The main point is the study the so-called *cumulative distribution of zeros*, that is defined as:

$$\Lambda_L(r, t) = \int_0^r \lambda(s, t, L)ds\,. \tag{62}$$

This approach has been successfully applied to the study of $2d$ and $3d$ Ising models, $d = 2$, $q = 10$ Potts model (see Sec. 13), and lattice gauge theories.

11. Pirogov–Sinai Theory and Yang–Lee Zeros for First-Order Phase Transitions

A recent series of papers (see Refs. 137–141) addresses the problem of a more direct connection of the Yang–Lee zeros with the (complex extension of the) free

energy and the discontinuities of its derivatives, for *general*[f] lattice spin models in a magnetic field, that present first-order phase transitions. The departure point is the Pirogov–Sinai formalism for the phase diagram of the system (see Refs. 142 and 143). Its basic hypothesis are the existence of a finite number of ground states (which are the thermodynamic phases) of the system, and of the availabilty of an appropriate contour representation, i.e., the fact that the partition function can be written as the sum over the partial partition functions of each phase. Roughly speaking, this corresponds to the fact that, for a system with $\mathcal{P}$ possible phases ($\mathcal{P} = 1, 2, 3, \ldots$), the probability distribution for the *order parameter* (the magnetization) conjugated to the external field H has $\mathcal{P}$ peaks; the partition functions corresponding to the different phases can be evaluated from the position and width of these peaks (which depend on the control parameters temperature and magnetic field H). The total partition function is then expressed as

$$Z_N(z) = \sum_{l=1}^{\mathcal{P}} g_l \exp[-V f_l(z)/k_B T] + \mathcal{O}(\exp(-L/L_0)), \qquad (63)$$

where N is the number of spins; $f_l(z)$ is the complex extension of the thermodynamic free energy per unit volume of phase l, as a function of the complex fugacity $z = \exp(-2H/k_B T)$; g_l is the degeneracy of phase l; $V = L^d$ is the volume of the lattice of linear extension L and dimension d; and L_0 is of the order of the correlation length. Let us suppose here, for simplicity, the absence of triple or higher-order coexistence points (the theory can be extended to include these cases, too), i.e., for any values of the control parameters (T, H) the probability distribution function of the order parameter do not have more than two peaks. Then by inspection of Eq. (63) one realizes that the zeros of the partition function in the complex-z plane arise, up to order $\mathcal{O}(\exp(-L/L_0))$, from a destructive interference of pair of terms of the sum, $q_l \exp(-V f_l/k_B T)$ and $q_p \exp(-V f_p/k_B T)$, $l \neq p = 1, \ldots, \mathcal{P}$. So, each zero of $Z_N(z)$ in the complex-fugacity plane lies in a vicinity of the order $\mathcal{O}(\exp(-L/L_0))$ of a solution of the equations corresponding to this condition of destructive interference:

$$\mathcal{R}e\, f_l(z) - (k_B T/V) \ln g_l = \mathcal{R}e\, f_p(z) - (k_B T/V) \ln g_p\,,$$
$$V/k_B T[\mathcal{I}m\, f_l(z) - \mathcal{I}m\, f_p(z)] = \pi \bmod 2\pi\,, \quad l \neq p = 1, \ldots, \mathcal{P}\,. \qquad (64)$$

In the thermodynamic limit, the zeros concentrate asymptotically on the *phase coexistence curves* $\mathcal{R}e\, f_l(z) = \mathcal{R}e\, f_p(z)$, and the corresponding local density of zeros is given by $\rho(z) = (2\pi k_B T)^{-1} d[f_l(z) - f_k(z)]/dz$. Practically, this means that the zeros of the partition function can indeed be expressed in terms of the complex free energy and of the discontinuities in its derivatives. References 137 and 139 illustrate the application of this rather abstract-looking method to three examples, the low

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[f] "General" means here systems with no particular symmetry properties like, e.g., the spin-inversion symmetry invoked in deriving the Circle theorem.

temperature Ising and Blume–Capel, and the q-state Potts model in the limit of large q.

12. Fisher Zeros of the Canonical Partition Function

In a review article written in 1965 (Ref. 4), Fisher suggested the analysis of the phase trasitions in the frame of the *canonical* ensemble, through the study of the distribution of the zeros of the canonical partition function in the plane of the complex temperature — i.e., what we call today *Fisher's zeros*. Indeed, in view of the equivalence of the various statistical ensembles in the thermodynamic limit, one should be able to equally characterize a phase transition in any of these ensembles. As in the grand-canonical case, the Fisher zeros will lie off the real positive temperature semi-axis for a finite system, but may close up on this semi-axis in the thermodynamic limit; the point T_c where a limiting line of zeros cuts the semi-axis will locate a *critical point*. Fisher illustrated this idea in Ref. 4 on the two-dimensional square-lattice Ising model, with isotropic nearest-neighbor interactions, in the absence of the external magnetic field, whose partition function is known analytically since Onsager (see Ref. 144). Fisher found that the zeros of the canonical partition function lie on an unit circles in the plane of the complex variable $v = \sinh(2J/k_B T)$, where $J > 0$ is the ferromagnetic coupling constant, and T is the *complex* temperature. These circles cut the real-v axis in $v = \pm 1$; the point $v = +1$ corresponds to the ferromagnetic transition, and $v = -1$ corresponds to the antiferromagnetic phase transition point (in agreement with the $\pm J$ symmetry property of the square lattice in zero magnetic field).

The concept of Fisher zeros (both in the absence and in the presence of a magnetic field), which seems to follow closely that of the Yang–Lee zeros studies, was rapidly set-up in its general frame, including the relevance of the thermodynamic limit, the location of the critical point, Refs. 4, 145 and 146, and the characterization of the transition, see Refs. 13–19. The (often tacit) underlying assumption of these abstract studies on the characteristics of the transition is that in the thermodynamic limit the Fisher zeros fall on smooth, complex-conjugate curves, at least in some vicinity of the critical point. In particular, provided that this is indeed the case, Itzykson *et al.* (see Ref. 147), proved two very strong general statements for Ising systems, namely: (i) These complex-conjugate curves in the absence of a magnetic field, in the vicinity of the critical point, form an angle with the real temperature axis that is a universal known function of the critical exponent α (of the specific heat) and of the ratio of the specific heat amplitudes below and above the critical point. (ii) The angle (with respect to the real temperature axis) at which these zeros curves (in the vicinity of the critical point) depart when a real, weak magnetic field is switched on is an universal function of the critical exponents β (of the spontaneous magnetization) and δ (of the relation between field and magnetization at the critical temperature).

However, despite some exceptions (like, e.g., the above-cited Onsager–Ising model), the above assumption on the location of Fisher zeros is rarely fulfilled (see e.g. Ref. 148 for a discussion of this point). The rule seems to be that the Fisher zeros in the thermodynamic limit occupy densely some whole areas in the complex-temperature plane, delimited by curves on which the density of zeros may diverge. Nothing like a Circle theorem or an Asano–Ruelle type of argument exists for Fisher zeros, because the canonical partition function with respect to a variable of the type $v = \sinh(2J/k_B T)$ (where J is a typical interaction constant of the model, and T is the complex temperature) does not have the polynomial structure the grand-canonical partition function has with respect to the fugacity z. In fact, there are three elements that render the study of Fisher zeros more complicated than that of Yang–Lee zeros:

(i) The first element is that the location of the Fisher zeros is strongly dependent on the details of the system (dimension, interaction between the components of the system, etc.). For example, Fisher zeros for the Onsager–Ising model have completely different location than the Fisher zeros of the corresponding anisotropic ferromagnet. This general feature is, of course, in relation with the fact that the critical temperature T_c is a quantity that varies from one system to another.

(ii) In general, the zeros for a *finite* system are not necessarily located in the region of the complex plane occupied densely by the Fisher zeros in the thermodynamic limit. See, for example, the case of a mean-field Ising ferromagnet, in Refs. 101, 149–153, where the location of the Fisher zeros in the thermodynamic limit is interpolated from that corresponding to larger and larger finite systems.

(iii) The third point is that very often, the location of the Fisher zeros, even in the thermodynamic limit, is not well behaved, i.e., it does not correspond to smooth curves in the complex-v plane, but rather to a combination of curves and densely-covered regions of the plane (like, for example, for the very simple example of an anisotropic ferromagnet on a square lattice, see e.g. Ref. 148).

These elements explain the scarcity of exact analytical results on the Fisher zeros (as compared to the Yang–Lee zeros), the predominance of numerical results, and thus the importance of finite-size scaling arguments in the study of the characteristics of the transition by means of Fisher zeros. Without entering into details, let us give a few examples of the systems that were studied in the literature:

(A) Ising models with nearest-neighbor ferromagnetic interactions, including:

(i) Two-dimensional finite $m \times n$ isotropic square lattices, in zero magnetic field,[154,155] (see also Ref. 156 for a discussion of the role of boundary conditions). Reference 157 generalizes the result of Fisher[4] on the circular location of the zeros to $m \times \infty$ rectangular lattices with (asymmetric) self-dual bound-

ary conditions, and closed form expression of the density of zeros are obtained
for $m = 1, 2$.

(ii) The Onsager–Ising model in an external, symmetry-breaking magnetic field of
complex value $H/k_BT = \pm i\pi/2$, whose exact partition function in the thermo-
dynamic limit was first presented by Lee and Yang in Ref. 12, was approached
from the point of view of the complex-temperature zeros in Refs. 158 and
159. The density of Fisher zeros is discussed in Ref. 160 (also for the cases of
triangular, honeycomb, and Kagomé lattices).

(iii) The corresponding problem in a *real* nonzero magnetic field was approached
numerically and analytically (with low-temperature series expansions) in
Refs. 159 and 170. It was found that the density of Fisher zeros diverges at
a non-physical critical point, the *Fisher edge singularity* that can be consid-
ered as the equivalent of the Yang–Lee edge singularity (see Sec. 9), as also
discussed in Ref. 161.

(iv) The loci of the Fisher zeros in the thermodynamic limit of two-dimensional
systems on honeycomb, triangular, diced, and Kagomé lattices, in the absence
of the magnetic field, were described in Ref. 162. Reference 160 discusses the
corresponding density of the Fisher zeros.

(v) Two-dimensional Ising systems on square, triangular, and honeycomb lattices
are investigated both in the isotropic and *anisotropic* cases, for finite systems,
and in the thermodynamic limit, in zero magnetic field, in Refs. 148, 163–168.
It is concluded that, in general, the Fisher zeros occupy densely the complex-
v plane in the thermodynamic limit, and the corresponding density is also
discussed.

(vi) Fisher zeros for finite three-dimensional isotropic, cubic-lattice Ising ferromag-
nets, in zero magnetic field, as well as estimates (based on finite-size scaling
arguments) of their densities were discussed at various levels, in Refs. 169–172.

(B) Higher-spin Ising model. Ising models of spin $S = 1, 3/2, 2, 5/2$ and 3 have
been calculated in Ref. 173 for a two-dimensional Ising model on a square lattice,
for various lattice sizes, in zero magnetic field. The temperature-dependence, as
well as the asymmetry in the specific heat amplitude above and below the critical
point are estimated from the Fisher zeros distribution.

(C) Mean-field spin models. The problem of the Fisher zeros for mean-field
1/2-spin Ising models — including the relation with critical exponents, finite-size
scaling aspects, the use of a partial distribution function in order to characterize
the metastable behavior, the relationship with long-range interaction systems —
was approached in Refs. 43, 101, 149–153. The exact locus of the Fisher zeros for
the mean-field spherical model was obtained in Ref. 174. See also Ref. 175 for an
Ising-type mean-field model for a polypeptide with helix-coil transition.

(D) Antiferromagnetic Ising models. References 170 and 176 obtain numeri-
cally the location of the Fisher zeros for a finite Ising antiferromagnet on a square
lattice, for different values of the external magnetic field and different extensions

of the lattice. It is inferred that in the thermodynamic limit these zeros have an accumulation point on the real axis, corresponding to the antiferromagnetic critical point.

(E) Heisenberg ferromagnets. References 177–179 discuss the thermodynamic functions (such as energy, specific heat, magnetization, and susceptibility) that have been computed numerically, using Fisher zeros distributions, for finite three-dimensional Heisenberg models with different anisotropy constant parameters, including both ferromagnetic and antiferromagnetic couplings.

(F) Ising models on hierarchical lattices. The location, fractal nature, and density of Fisher zeros for Ising models on various such lattices are studied in Refs. 180, 181 (diamond hierarchical lattice),[182,92] (Cayley trees),[89,183,184] (Sierpinski gaskets and 3- and 4-simplex lattices). We also refer the reader to a short, comprehensive review of Itzykson *et al.* on this subject.[185]

(G) Ising models on aperiodic lattices. References 93–96 discuss the Fisher zeros for several such one- and two-dimensional Ising aperiodic lattices, with coupling constants generated according some predefined algorithms (see also Sec. 8).

(H) $\pm J$ Ising spin model. In Refs. 186 and 187 there are presented numerical results on the corresponding Fisher zeros for two- and three-dimensional lattices of different sizes. More extended simulations in Ref. 188 seem to indicate a fractal nature of the distribution of zeros.

(I) Random energy model. The random energy model is one of the simplest, exactly-solvable, *disordered* model that contains some physics of the spin glasses (see Ref. 189). It is equivalent to a spin model with multispin interactions exhibiting a low-temperature spin glass phase. Its Fisher zeros were studied numerically and analytically in Refs. 190 and 191, and they were found to occupy densely lines and extended areas of the complex-temperature plane.

Most of the above-cited references invoke finite-size scaling arguments in order to infer the properties of the Fisher zeros (location zone, position of the critical point of the transition, density, etc.) in the thermodynamic limit from those obtained numerically for finite-size systems. A long list of references concentrate precisely on the *finite-size scaling* theory for Fisher zeros (and, sometimes, they also address the same problem for the Yang–Lee zeros) (see Refs. 192–194, 196–206).

13. Potts Model: What to Complexify?

The Potts model (so named after R. B. Potts who first studied it in his 1951 Ph.D. thesis at Oxford) is a generalization of the Ising model to more-than-two-component spins, and, due to its complex behavior, as well as the various experimental realizations, has been a subject of intense research during the last 30 years (see Ref. 207 for a review). The q-state Potts model consists of q-components spins, i.e., spins

that can point in the q symmetric directions of a hyperthetraedron in $(q-1)$ dimensions, described by the unit vectors $\mathbf{s}^\alpha$, $\alpha = 0, \ldots, q-1$; these spins are placed on a lattice, and the corresponding Hamiltonian $\mathcal{H}$ of the system in the presence of a magnetic field H is expressed as:

$$\mathcal{H} = -\varepsilon \sum_{\langle ij \rangle} \delta(\mathbf{s}_i, \mathbf{s}_j) - H \sum_i \delta(\mathbf{s}_i, \mathbf{s}^Q). \tag{65}$$

Here $\mathbf{s_i}$ is the direction of the i-th spin as discussed above; ε is the coupling constant (which is *ferromagnetic* if $\varepsilon > 0$, and *antiferromagnetic* if $\varepsilon < 0$); $\langle ij \rangle$ indicates nearest-neighbor pairs; δ is the Kronecker delta; and $\mathbf{s^Q}$ is a fixed direction amongst the q possible ones (one says that the field H is coupled to the spin-state Q). The model can be modified to include multi-site interactions.

Using its representation in terms of a graph with colored edges, Potts model can be generalized to *arbitrary, non-integer values of q*. It is connected with other interesting models of statistical mechanics. Potts model with $q = 4$ is known as Ashkin–Teller model;[208] the case $q = 2$ corresponds to the usual Ising model; $q = 1$ model is in correspondence with the percolation process; $q = 1/2$ can be related to a dilute spin glass model; finally, the $q = 0$ limit relates to the Kirchhoff resistor network problem.

The nature of the order-disorder phase transition in Potts model depends — besides on the ferromanetic or antiferromagnetic nature of the model — both on the dimension d and on the value of q. For example, for the ferromagnetic model in the absence of a magnetic field, for $d = 2$ there is a second-order phase transition when $q = 2, 3, 4$, while for $q > 4$ the transition is first-order. There exists a dimension-dependent critical value of q, $q_c(d)$, above which the transition is mean-field like — either of the first order if $q > \max(2, q_c)$ or continuous if $q_c \leqslant q \leqslant 2$. The few exactly-known points are $q_c(2) = 4$ (Ashkin–Teller), $q_c(4) = 2$ (Ising), $q_c(6) = 1$ (percolation). Besides the $q = 2$ (Ising) case, the $q = 3$ and $q = 4$ models have a rather well-studied phase diagram, which proved to be dimension-dependent.

The location and characteristics of the phase transition(s) — that are known analytically only in few cases — can be studied, essentially numerically, in the Yang–Lee formalism. The canonical partition function, in the general case, is a function of three control parameters: the magnetic field intensity H, the temperature T, and the parameter q of the model. One can therefore consider the complex extension of the partition function and the corresponding zeros either with respect to the complex magnetic field (Yang–Lee zeros), or the complex temperature (Fisher zeros), or, moreover, with respect to the complex q — the so-called *Potts zeros*.

13.1. *Yang–Lee zeros*

A first category of studies was done on the zeros of the partition function in the plane of the complex magnetic field, at fixed temperature and real value of the parameter q of the Potts model, for various dimensions d and types of lattices.

The one-dimensional lattice was studied in the references cited below using a transfer-matrix technique. It was shown[211] that for $1 < q < 2$ the zeros lie inside the unit circle in the complex fugacity plane, while for $q > 2$ they lie outside the unit circle for finite temperature; $q = 2$ corresponds to the Circle theorem for the Ising system. The situation $q < 1$ is somehow pathological,[210,213] since for all the temperatures the zeros lie (in part or completely, depending on T) on the real axis, and accumulate around a certain point of the real axis. This would mean that one obtains a second-order phase transition at finite temperature, and in the presence of a real magnetic field; however, the eigenvalues of the transfer matrix — which give the correlation length — are not real. $q = 1$ is a particular limiting case. The discussion of a tricritical point and its connection with a special type of Yang–Lee edge singularity is given in Ref. 209 for $q = 3$ Potts model. Reference 212 demonstrates a connection between the locus of the Yang–Lee zeros and the Julia set of the logistic map associated with the renormalization transformation of the lattice (and idea already present in the study of Ising models on hierachical lattices, see above). Finally, Ref. 214 presents a recursive method (adapted from the theory of dynamical systems) for the computation of the partition function zeros.

The two- and three-dimensional models on regular lattices are discussed in Refs. 216, 217 and 211, and they are shown[211] to have the same type of behavior with respect to q as the one-dimensional lattices. Yang–Lee zeros on recursive Bethe lattices are studied in Ref. 218 for noninteger values of q.

13.2. *Fisher zeros*

As already mentioned in Sec. 12, the Fisher zeros are much more sensitive than the Yang–Lee zeros to the details of the interactions (type of lattice, dimensionnality), and also to finite-size effects (like boundary conditions), and this explains the large number of (essentially numerical) papers devoted to the study of various specific models.

For the one-dimensional lattices with arbitrary q it was shown in Ref. 210 that the zeros in the complex field plane can be related, through a kind of duality transformation, to the zeros in the complex temperature plane. Potts models on square lattices are discussed, e.g., in Refs. 108, 219 and 220, in the absence of a magnetic field and for various values of q. In the region where $\mathcal{R}e[\exp(\varepsilon/k_B T)] < 1$, Fisher zeros lie on the circle $|\exp(\varepsilon/k_B T) - 1| = \sqrt{q}$, while outside this region the zeros are no longer ocuppying this circle and lead to the existence of (nonphysical) points at which the magnetization and susceptibilities diverge — the *Fisher edges*. The problem of the Fisher edges is also discussed in Refs. 161, 214, 221–223, both in the absence and presence of an external magnetic field.

Finally, a large body of literature addresses these problems on various other lattices — strips of square lattices,[224,225] honeycomb, triangular, and Kagomé lattices,[226]–228 and recursive Bethe lattices.[215,218]

13.3. *Potts zeros*

As already mentioned, Potts model can be extended to arbitrary, continuous values of q (through the so-called Kasteleyn–Fortuin[229] representation). Thus the canonical partition function becomes a function of the parameter q, and this gives the motivation for the analysis of its zeros in the plane of complex q — the *Potts zeros*. The physical relevance of such an approach may be somewhat unclear at first sight. However, in Ref. 222 it is shown that one can find a similarity between the scaling property of complex-q zeros and the den Nijs[230] expression for the thermal critical exponent; in Ref. 223 it is shown that a Circle theorem holds for a certain range of intensity of the applied magnetic field, while for other ranges the Potts zeros lie on the positive real axis (without necessarily being accumulation, i.e., phase-transition points). A *Potts edge* exists, analogous to the Yang–Lee and Fisher edges. Several types of lattices are considered in Refs. 214, 224, 225 and 228. Finally, $1D$ long-range interaction and the mean-field cases are approached in Ref. 231, with a discussion of the phase transition point and of finite-size effects.

While most of the above-cited references address the case of the ferromagnetic Potts model, there is a non-negligible amount of work dedicated to the *antiferromagnetic* case (see Refs. 108, 213, 222–224 and 228). In particular, the canonical partition function in the $T \to 0$ limit reduces to chromatic polynomials in q, that have a relevance in the theory of graphs.[232]

PART II: NONEQUILIBRIUM STEADY-STATE PHASE TRANSITIONS

14. Generalities

The study of nonequilibrium systems reveals its importance once one realizes that equilibrium in nature is merely an exception rather than the rule, and that most of the qualitative, structural changes (like, for example, pattern formation) that one encounters in various systems take place under nonequilibrium conditions.

From a macroscopic point of view, roughly speaking, a nonequilibrium system is the set of fluxes of various characteristic quantities (e.g. number of particles, energy, etc.) inside the system and between the system and its surroundings. Let us try to give a more precise, quantitative meaning of the notion of nonequilibrium system from a microscopic point of view, in the frame of a stochastic description of the system in the corresponding configuration space. Of course, as for equilibrium systems, this probabilistic description is imposed by the huge number of microscopic degrees of freedom, and by the practical necessity of describing the system in terms of a few relevant measurable quantities.

A configuration ω of the system represents a set of relevant mesoscopic variables, corresponding to the degree of coarse-graining of the adopted description. The ensemble of the accessible configurations, according to the constraints imposed on the system, form the corresponding configuration space. The system is jumping

between the configurations according to some prescribed stochastic transition rules. The state of the system at a time t is given by the probability distribution $P(\omega, t)$ associated to the set of possible configurations $\{\omega\}$. Suppose now that the level of coarse-graining is such that the evolution of the system is Markovian (this is the only type of systems that we shall be dealing with in the foregoing). The evolution of the probability distribution function can be described by a master equation with a set of transition rates between the configurations, $\{\mathcal{W}(\omega \to \omega')\}$:[g]

$$\frac{dP(\omega, t)}{dt} = \sum_{\omega' \neq \omega} [\mathcal{W}(\omega' \to \omega)P(\omega', t) - \mathcal{W}(\omega \to \omega')P(\omega, t)]. \tag{66}$$

Let us consider the long-time behavior of the system. The dynamics can be such that no stationary state is reached (e.g., the system may exhibit a limit-cycle or a chaotic-like behaviour). On the contrary, suppose that the system reaches a *stationary state*, i.e., the probability distribution of the possible configurations becomes time-independent, $P_s(\omega)$. The stationarity condition in the configuration space is that the total flow of probability into configuration ω is balanced by the corresponding outgoing flow,

$$\sum_{\omega' \neq \omega} [\mathcal{W}(\omega' \to \omega)P_s(\omega') - \mathcal{W}(\omega \to \omega')P_s(\omega)] = 0 \quad \text{for all } \omega. \tag{67}$$

One realizes that an equilibrium state is a very particular case of stationary state. Besides the independence on time of the characteristic quantities of the system, there is no macroscopic exchange between the system and its surroundings, i.e., no flow runs through the system and its borders. From a stochastic point of view, this corresponds to the *detailed-balance* condition in the configuration space,

$$\mathcal{W}(\omega' \to \omega)P_s(\omega') = \mathcal{W}(\omega \to \omega')P_s(\omega) \quad \text{for all } \omega, \omega', \omega \neq \omega', \tag{68}$$

i.e., the balance of probability flow between *any pair of configurations*.

On the contrary, a *nonequilibrium stationary state* corresponds to *probability flow loops* in the configuration space, i.e., to the *breaking of detailed balance* for certain configurations ω, ω',

$$\mathcal{W}(\omega' \to \omega)P_s(\omega') \neq \mathcal{W}(\omega \to \omega')P_s(\omega). \tag{69}$$

These probability flow loops lead to the observed flows of macroscopic quantities through the system and its borders. In particular, note that in order to maintain a system in a nonequilibrium state continuous exchanges with its surroundings are necessary, i.e., the system is necessarily *opened*.

One should realize that for such stochastic models the physics is embedded in the transition rates that are chosen on "reasonable" backgrounds according to the nonequilibrium phenomena one wishes to describe. It seems thus that one has a

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[g]One can consider the more general case when these transition rates are time-dependent but, for simplicity, here we shall limit ourselves to the case of constant transition rates.

high degree of freedom in the choice of the transition rates that lead to a nonequi-
librium stationary states although it has been argued recently[233−235] (on the basis
of Jaynes' MaxEnt principle extended to nonequilibrium situations) that there are
rather severe restrictions on this choice.

To sum up, *breaking of detailed balance is the general characteristic of stochastic
systems in a nonequilibrium steady-state.*

15. A Partition Function for Nonequilibrium Stationary States

Phase transitions in nonequilibrium steady states are sometimes accompanied, as
in the equilibrium case, by a *breaking of ergodicity* of the system, i.e., by the fact
that the asymptotic stationary state of the system is not uniquely-defined, but
depends on its initial configuration. This means that Eq. (67), for certain values of
the transition rates (depending on the control parameters of the system), admits
more than one solutions for the stationary probability distribution $P_s(\omega)$, and,
correspondingly, the stationary properties of the system (e.g., the mean values of
the characteristic parameters and of their stationary flows throughout the system)
differ from one phase to another.

The problem we address now is whether there exists any possibility to define
a partition function for the nonequilibrium systems, that allows for the character-
ization of a nonequilibrium phase transition between stationary states in a way
that is analogous to that described in Part I for the equilibrium cases. The answer,
in a rather general frame, was given in Ref. 10, and we present here the relevant
arguments, (see also Refs. 8, 236, 237 and 239).

For simplicity, define the *transition matrix*[238] $[W(\omega, \omega')]$, whose off-diagonal
terms are equal to the transition rates $W(\omega, \omega') = \mathcal{W}(\omega' \to \omega)$ and the diagonal
terms are $W(\omega, \omega) = -\sum_{\omega'} \mathcal{W}(\omega \to \omega')$, so that the evolution equation (66) for
the probability density reads

$$\frac{dP(\omega, t)}{dt} = \sum_{\omega'} W(\omega, \omega') P(\omega', t) \,, \tag{70}$$

and it preserves the normalization condition $\sum_{\omega} P(\omega, t) = 1$. The stationarity con-
dition (67) reads

$$\sum_{\omega'} W(\omega, \omega') P_s(\omega') = 0 \,, \quad \text{for all } \omega \,. \tag{71}$$

Suppose now that the control parameters of the system are such that there is
a unique steady state. Then, according to the Perron–Frobenius theorem, there
exists a single eigenvalue of the transition matrix that is equal to zero, and the
corresponding eigenvector gives the stationary-state probabilities of the various
configurations $P_s(\omega)$. All the other eigenvalues $\{\lambda_i\}$ of the transition matrix have
negative real parts, $\mathcal{R}e\,\lambda_i > 0$, and each of them corresponds to an eigenvector of
the transition matrix that relaxes exponentially to zero within a time-scale of the
order $1/|\mathcal{R}e\,\lambda_i|$.

Because of the zero eigenvalue of the transition matrix, the linear set of equations (71) is underdetermined, and therefore one can obtain from it only the *relative statistical weights* $f_s(\omega)$ of the various configurations. However, one can define the *normalization factor*

$$Z = \sum_{\omega} f_s(\omega)\,, \tag{72}$$

such that

$$P_s(\omega) = \frac{1}{Z} f_s(\omega)\,. \tag{73}$$

This normalization factor is related to the nonzero eigenvalues of the transition matrix, more precisely (up to a multiplicative factor),[h]

$$Z = \prod_{\lambda_i \neq 0} (-\lambda_i)\,. \tag{74}$$

This is the key relationship that allows to propose Z *as a candidate for a nonequilibrium steady-state partition function* that can give informations on the appearance of a phase transition in the system.

Indeed, suppose that one varies the control parameters (and thus the transition rates, as well as the corresponding eigenvalues of the transition matrix) so that the system is driven toward a nonequilibrium phase transition. A new stationary state appears in the system, and, correspondingly, at a phase transition one is expecting the appearance of a diverging time scale related to this new slow-mode that sets in. This means that one of the eigenvalues λ_i that is associated to this mode goes to zero as one approaches the phase transition point and thus, by virtue of Eq. (74), so does the normalization factor Z.

It seems therefore meaningful to try to locate the nonequilibrium phase transition points through the analysis of the zeros of the normalization factor Z. However, the legitimacy of this approach has to be checked on several known exactly-solvable models before trying to use it for further predictions. Several classes of nonequilibrium systems were discussed in the litterature using this approach, and we briefly review them here, following for the most the original work of Blythe and Evans.[10]

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[h]In order to obtain this result, note that the characteristic polynomial of the transition matrix reads (up to a multiplicative factor)

$$\det(\lambda I - W) = \left[\det(W) + \lambda \sum_{\omega} f_s(\omega) + \mathcal{O}(\lambda^2)\right]\,.$$

Given that $\det(W) = 0$, and $Z = \sum_{\omega} f_s(\omega)$, one has:

$$Z = \lim_{\lambda \to 0} \frac{\det(\lambda I - W)}{\lambda} = \lim_{\lambda \to 0} \frac{1}{\lambda} \prod_{\text{all } \lambda_i} (\lambda - \lambda_i) = \prod_{\lambda_i \neq 0} (-\lambda_i)\,.$$

Recall at this point that Z is defined up to a multiplicative factor,[i] that depends on the method adopted to solve Eqs. (71); this factor (which is common to all the stationary states weights f_s) is generally a polynomial in the transition rates $\mathcal{W}(\omega \to \omega')$, and therefore may introduce additional zeros to Z. However, one expects that these zeros are not physically relevant, and this can be checked on the models that are discussed below.

16. Driven Diffusive Systems

Most of the studies on the applicability of Yang–Lee theory to nonequilibrium phase transitions refer to simple models of systems with diffusion and drift, mostly because they were intensively studied in the last years and many results are known for their stationary states and phase diagrams.

16.1. *Stochastic single-species models*

Such models belong to the class of the so-called *Asymmetric Simple Exclusion Process* (ASEP). These are interacting-particle systems, with a single species of particles without internal degrees of freedom, and with hard-core two-body interactions between nearest-neighbor sites on a one-dimensional lattice. This hard-core interaction with excluded volume is expressed by the condition that each lattice site may be occupied by at most one particle. Therefore, this class of models may be described by a set of occupation numbers $\{n_1, n_2, \ldots, n_L\}$, where $n_k = 0, 1$ is the number of particles on site k of a lattice of L sites. The particles may jump at random, according to some prescribed stochastic rules, by one lattice site, with a bias in the right/left transition probabilities. The system is maintained in a nonequilibrium stationary state, with a constant particle flow along it, by continuous injection and extraction of particles at its two borders. The specificity of each model is embedded in the prescribed stochastic dynamics, i.e., in the probabilities for the changes of the configuration of a pair of neighboring sites k and $k + 1$, and also in the continuous or discrete (parallel or sequential) character of the dynamics (see e.g. Refs. 240 and 241 for an overview).

The *totally asymmetric exclusion process* (TASEP) with open boundaries is perhaps the simplest exactly solvable model with a nontrivial stationary behavior that includes both a first-order and continuous phase transitions, and, in view of its prototypical character, we will describe it here in some detail (see also Refs. 10 and 242).

In its *continuos-time* variant, in an infinitesimal time interval dt, one can have one of the following transitions: a particle may hop to the right with probability dt (i.e., with transition rate equal to unity), provided the receiving site is

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[i]Note that such a spurious multiplicative factor may appear also in equilibrium systems, e.g., through a uniform shift of the energy scale.

empty; or a particle is injected at the left border (leftmost lattice site) with probability αdt (provided the left border is empty); or a particle at the right border is removed from the system with probability βdt (provided the right border contains a particle). Obviously, the injection and extraction rates, α and β, are the control parameters that determine the stationary state of the system, which can be characterized through the density profile, i.e., the set of mean occupation numbers of the lattice site, $\langle n_k \rangle$, $k = 1, \ldots, L$. The stationary flow of particles $J = J(\alpha, \beta)$ exhibits non-analiticities *in the thermodynamic limit* of an infinite lattice $L \to \infty$, as one varies α and β, and these non-analiticities correspond to phase transitions in the system. The phase diagram consists of three regions: (i) A high-density phase with a density profile that decays exponentially toward the right boundary. In this phase the current $J = \beta(1 - \beta)$ is controlled by the rate at which the particles are removed from the system, $\beta < \min(\alpha, 1/2)$. (ii) A low density phase, with a density profile that has an exponential decay towards the left boundary. The current $J = \alpha(1 - \alpha)$ is again controlled by the smallest of the two rates, $\alpha < \min(\beta, 1/2)$. At the first-order transition line $\alpha = \beta < 1/2$, the current exhibits a discontinuity in its first derivative. The system presents a *shock* separating regions of high and low densities, and this is an example of *phase coexistence* at a nonequilibrium first-order phase transition. (iii) The third phase, for $\alpha, \beta > 1/2$, is called the maximum current phase, since the current assumes throughout the constant value $J = 1/4$, which is the largest possible current for any combination of α and β. The density profile decays *as a power-law* from both boundaries, and therefore the transitions from either phase (i) or phase (ii) are accompanied by diverging lengthscales. Moreover, J has a discontinuity in its second derivative, and this corresponds to a second-order phase transition.

The normalization factor for the TASEP is

$$Z_L(\alpha, \beta) = \sum_{\ell=1}^{L} \frac{\ell(2L - 1 - \ell)!}{L!(L - \ell)!} \frac{(1/\beta)^{\ell+1} - (1/\alpha)^{\ell+1}}{1/\beta - 1/\alpha} , \tag{75}$$

and the current $J = Z_{L-1}/Z_L$. In the thermodynamic limit $\ln Z_L \approx -L \ln J$, i.e., $\ln J$ plays the role of a free energy density for the nonequilibrium partition function Z_L. From here it is routine to apply the Yang–Lee procedure to Z_L. For example, keeping β as a parameter, one finds that the zeros of Z_L in the plane of the complex variable α lie on a smooth curve, and accumulate at the phase transition point α_c on the real positive semiaxis when L is increased towards the thermodynamic limit. Depending on the value of β, one has: (i) If $\beta < 1/2$, the curve of zeros passes smoothly, with a nonzero density of zeros, through the transition point $\alpha_c = \beta$, corresponding to a first-order phase transition (see Sec. 3); (ii) If $\beta > 1/2$, the density of zeros decays to zero as one approaches the transition point

$\alpha_c = 1/2$, and the zero-lines approach the transition point at angles $\pi/4$ with the real axis (thus meeting at a right angle), indicating therefore a second-order phase transition.

Therefore, the example of TASEP seems to indicate that it is legitimate to study the zeros of the normalization factor Z, in the plane of one complexified control parameter and in the thermodynamic limit, in order to get the location of a nonequilibrium phase transition point. Moreover, the distribution of these zeros offers informations on the characteristics of the transition — exactly as in the equilibrium case.

The same conclusions hold for the time-continuous *partially asymmetric exclusion process* (PASEP), for which the particles have a nonzero probability to jump to the left, corresponding to a transition rate q. The PASEP thus has a supplementary control parameter q, and one can follow the change in the locus of the partition function zeros in the complex-α plane (at fixed value of β) with changing q. Also, one could look for the zeros of Z in terms of complex q (at fixed values of α and β). In particular, at $q = 1$ (when there is no bias between right and left transitions), one transits to a regime of zero-current in the thermodynamic limit, and this phase transition should manifest as an accumulation of the complex-q zeros in the vicinity of $q = 1$, a scenario that has still to be verified (see Ref. 268 for some more comments on this phase transition).

Two types of *discrete-time* variants of TASEP were discussed recently in the frame of Yang–Lee formalism for phase transitions, namely:

(i) The *parallel-update* TASEP[j] (see Ref. 247). At each time step particles are introduced with a probability α at the left border (if this first site is empty) and are extracted with probability β at the right border (if this last site is occupied); moreover, the particles in the bulk can jump to the right with probability p (if the right space is empty), or remain still with probability $1 - p$. This update is applied to all particles *simultaneously*. Here again one can compute exactly the normalization factor $Z = Z(\alpha, \beta, p)$, and look for its zeros in the complex-α plane at fixed β and p. The phase diagram is similar to that of the continuous-time TASEP; there are three phases, separated, respectively, by two continuous-transition lines at α or $\beta = 1 - \sqrt{1 - p}$, and a first-order transition line at $\alpha = \beta < 1 - \sqrt{1 - p}$. Thus, the zeros of Z in the complex-β plane also behave similarly. One can also look at zeros of Z in the complex-p plane (at fixed values of α and β); their locus is a cardioid, with the transition point appearing as a cusp on the real positive semiaxis.

(ii) The *sublattice-parallel update* TASEP with the supplementary constraint of fixed average density of particles in the system, $\rho = M/L$ (where M is the

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[j]This is a special case of the famous Nagel–Schreckenberg model for traffic flow [K. Nagel and M. Schreckenberg, *J. Phys. I. France* **2**, 2221 (1992)], in which the TASEP phase transitions can be considered as jamming transitions.

total number of particles on the lattice of length L) was studied in Ref. 246. In this model, at the first-time step, besides the injection and extraction of the particles at the borders with probabilities α and β, respectively, all the particles on odd sites jump to the right with probability one (if the site to the right is empty); at the next step, all the particles on even sites jump to the right with probability one (again, if the receiving site is empty). Then one repeats this two-stage process. The phase diagram of this model in the thermodynamic limit contains three phases, namely a high-density phase and a low-density phase (as for the continuous-time TASEP), and a *shock phase*, characterized by existence of shocks in the particle-density profile. This shock phase has second-order transition borders with the high and low density phases, and this is confirmed by the behavior of the zeros of Z in the complex-α plane, for various fixed values of β and ρ.

The problem of finite-size scaling and universality for several variants of *discrete-time* TASEP was addressed recently in Ref. 248. In the thermodynamic limit, in general (i.e., whatever the adopted update rule), both first and second order boundary-induced transitions between the steady-states are encountered, and one derives finite-size scaling expressions for the current J, for the mean local particle density, as well as for the zeros of the normalization factor Z in the complex plane of the injection α extraction β rate of particles at the borders. In particular, simulations suggest that the smallest distance between the locus of these zeros and the critical point α_c/β_c has a power-law behavior $\sim L^{-1/\nu}$, where ν (as in the equilibrium systems) is the critical exponent of the bulk correlation length for the nonequilibrium phase transition.

16.2. *Two-species models*

Actually, there are two slightly different variants of the same model that were studied, from the point of view of the Yang–Lee approach, in Refs. 249 and 250. As described in Ref. 249, the model consists of two types of particles, A and B, of fixed numbers N_A and N_B, that diffuse in opposite directions on a one-dimensional L-site lattice with periodic boundary conditions. Specifically, particles of type A jump to the right and particles of type B jump to the left, both with unit transition rates, provided that the destination site is empty. Also, if on neighbor sites, the A and B particles exchange places, $A+B \to B+A$ with transition rate q, and $B+A \to A+B$ with unit transition rate. The bias parameter q is thus the control parameter of the system (at fixed particle densities $\rho_{A,B} = N_{A,B}/L$), and as long as $q \neq 1$ the system can reach a nonequilibrium stationary state with a stationary nonzero flow of particles throughout the system. Arndt[249] studied the phase diagram in the particular case of equal particle densities $\rho_A = \rho_B \equiv \rho = M/L$ in terms of the Yang–Lee formalism. Since the normalization factor $Z_L(q, \rho)$ was not known analytically at that moment, Arndt went to the numerical study of a grand-canonical partition

function

$$\Xi_L(z,q) = \sum_{M=0}^{M_{\max}=L/2} z^M Z_L(q, M/L) \tag{76}$$

in the plane of the complex fugacity z. From these studies of the zeros on finite-size systems (with L up to 100), he inferred the existence, in the thermodynamic limit, of a first-order phase transition at some point $q_c(\rho) > 1$, between a mixed phase (corresponding to a condensate made of both A and B particles; a block of empty sites, with a few residual A or B particles, occupies the rest of the system) and a disordered phase (with uniform density profiles of both species and no spatial condensation).

However, it was shown later (see Refs. 10, 251 and 252), through an exact calculation of the grand-canonical partition function in the thermodynamic limit, that no phase transition, rigorously speaking, appears in the system. When one varies the control parameters, there appears, instead, a very abrupt increase in the correlation length to an anomalously large value — of the order $\mathcal{O}(10^{70})$ sites, which, however, if finite. Although very spectacular, this phenomenon does not seem to be extremely rare, since it can be argued (see e.g. Ref. 252) that it is generated when the dynamics of the model is such that small domains tend to be suppressed in the steady-state distribution.

Thus, the extrapolation done by Arndt from numerical results on finite-size systems toward the thermodynamic limit is unreliable. One should therefore be aware of the possible appearance of such extremely large correlation lengths in the nonequilibrium systems, correlations that may lead to a false impression of the existence of a phase transition when investigating (numerically) systems with sizes less or comparable to the correlation length.

Note also[10] that studying the zeros of this grand-canonical partition function in the complex fugacity plane amounts, from a physical point of view, at placing the lattice in equilibrium with a reservoir of particles, and thus (despite the claim in the title of Ref. 249) at studying an equilibrium system.

Reference 250 reconsidered the same model in the exactly-solvable case $N_B = 1$, i.e., of a single impurity present in the system. Using a matrix-product formalism, one can compute the corresponding normalization factor $Z_L(q, \rho)$ at fixed density ρ of the A particles. Studying the behaviour of $Z_L(q, \rho)$ in the thermodynamic limit, one deduces the existence of two stationary phases of the system, namely, (i) a *jammed phase* for $q < 2\rho$, when the impurity provokes a macroscopic shock (error-function like) in the density profile of A particles; (ii) and a *power-law phase* for $q > 2\rho$, when the impurity has a short-range effect on the system, such that the density profile of A-s has an exponential behaviour, with a correlation length $\sim |\ln(q_c/q)|^{-1}$ that diverges when q approaches the critical value $q_c = 2\rho$. This result is confirmed by the study of the location and distribution of zeros of $Z_L(q, \rho)$ in the complex-q plane (at fixed value of ρ), that predicts correctly the second-order phase transition point between the two phases, as well as its characteristics.

17. Simple Reaction-Diffusion Models

These stochastic models are characterized by the fact that, contrary to the driven-diffusive systems discussed above, the number of particles is not conserved by the dynamics, i.e., there are some reactions inside the system. One such model, which results through a simple modification of the continuous-time ASEP, is the *coagulation-decoagulation model* with open boundaries (see Ref. 243). It consists of particles that diffuse, coagulate (two neighbor particles merge into a single one), and decoagulate (one particle splits into two neighbor particles) preferentially, e.g., in the leftward direction. More precisely, in the simplified model in Ref. 244, they (i) diffuse to the left and right with rates q and q^{-1} respectively; (ii) coagulate at the left $A + A \to A + 0$ with rate q and at the right $A + A \to 0 + A$ with rate q^{-1}; (iii) decoagulate to the left $0 + A \to A + A$ with rate γq and at the right $A + 0 \to A + A$ with rate γq^{-1}. Here, $q > 1$ in order to assure the leftward preference of the processes. Besides this, there is an injection and an extraction of particles solely at the left border, with rates α and β. This model, for which the normalization factor Z can be computed exactly when $\alpha = (q^{-1} - q + \beta)\gamma$, exhibits a first-order phase transition between a low-density and a high-density phase. The roots of Z in the complex-q plane are studied (for fixed β and γ), and Yang–Lee theory is shown to hold, describing correctly both the location and the nature of the phase transition.

A variant of this model with reflecting boundary conditions, instead of the open boundaries, was studied in Ref. 244. The model in this case has two control parameters, q and γ, at a fixed particle-density ρ. The system has two second-order phase transition points, at $q_c = 1/\sqrt{1 - \rho}$ and $q'_c = 1/q_c = \sqrt{1 - \rho}$. The reason of the existence of these two transition points is simply the invariance of Z under the transformation $q \to q^{-1}$. Note that γ plays no role in the location of the phase transition points. Again the Yang–Lee formalism predicts correctly these results.

Reference 245 offered recently a unified frame, based on the matrix-product formalism, for the study of the nonequilibrium steady-state phase transitions of three families of one-dimensional nonequilibrium models with opened boundaries. Besides the TASEP and a generalization of the above-described coagulation-decoagulation model, it also discusses the *asymmetric Kawasaki–Glauber process* (AKGP). The latter corresponds to a (totally) asymmetric diffusion of the particles (Kawasaki spin-exchange dynamics), combined to death to the left and right $A + 0 \to 0 + 0$, $0 + A \to 0 + 0$, and to branching to the left and right $A + 0 \to A + A$, $0 + A \to A + A$. These two last processes represent a variant of the spin-flip Glauber dynamics. Moreover, a steady-state current is maintained through the injection and extraction of particles at the borders. For special values of the corresponding transition rates, one can estimate the normalization factor Z, and study its Yang–Lee zeros (however, the paper does not concentrate further on this neither for the AKGP, nor for TASEP, but only for the extended coagulation-decoagulation model).

18. Directed Percolation

An important type of nonequilibrium phase transitions is represented by the *absorbing-state phase transitions*, which take place when a system, during its evolution, reaches a configuration (a so-called absorbing state) in which it remains trapped forever. Phenomena of this type are present in a wide variety of physical, chemical, biological systems (see Refs. 253–255 for recent reviews). It has been conjectured recently that a large group of such models fall into the *directed-percolation (DP) universality class* (see Refs. 256 and 257). A simple example of such a model is a reaction-diffusion system on a one-dimensional lattice, with a competition between the reproduction of particles, i.e., a (symmetric) decoagulation, $A+0 \rightarrow A+A$ or $0+A \rightarrow A+A$, and the death of particles, i.e., a spontaneous decay $A \rightarrow 0$. This competition is controlled by some external parameter p; if its value is below a certain threshold $p < p_c$, the system reaches an absorbing state (empty lattice) with certainty; otherwise the system remains active forever in the thermodynamic limit of an infinite-lattice. The corresponding phase transition is a continuous one.

In order to study the applicability of the Yang–Lee theory to this class of nonequilibrium phase transition, it is natural to turn to the original *directed percolation model* (see Refs. 10, 259–261). In order to fix the ideas, let us consider the two-dimensional case — although the process can be defined on general d-dimensional lattices. The system consists of a finite square lattice with L rows that has one site, the apex O, on the first row, two sites on the second row, etc., up to a total of $L(L+1)/2$ sites. Bonds between the sites are opened with probability p, and closed with probability $1-p$. At the initial moment, a particle is placed on the apex; at each time step this particle jumps on a site of the next lower level, provided the corresponding bond is opened. The sites connected by a continuous percolation path (i.e., by a succession of opened bonds) are said to belong to the same percolation cluster. One is interested by the *percolation (or survival) probability* $P_L(p)$ that at least one site on the level L is connected to the apex through a percolation path; $P_L(p)$ is obtained by considering all the possible bond configurations. The order parameter, defined for an infinite lattice $L \rightarrow \infty$, is $P_\infty(p)$, which is the probability of having an infinite cluster (i.e., a cluster that goes from the apex all the way down the lattice) for a given bond probability p. If $p < p_c$, then $P_\infty(p)$ is zero, i.e., there are no infinite percolation clusters in the system (that means that one can always, i.e., with probability one, find a row, sufficiently far from the origin, that is not connected to the apex through any percolation path). For $p > p_c$, however, $P_\infty(p)$ becomes nonzero, and in the vicinity of the critical point it has a power-like behavior,

$$P_\infty(p) \sim (p - p_c)^\beta \,, \tag{77}$$

with an universal exponent β. In addition, the DP process is characterized by a transversal correlation length $\xi_\perp$ perpendicular to the percolation flow, and a

longitudinal correlation lenght $\xi_\|$ along the percolation flow, that diverge both when p approaches its critical value p_c,

$$\xi_\perp \sim |p - p_c|^{-\nu_\perp} , \quad \xi_\| \sim |p - p_c|^{-\nu_\|} . \tag{78}$$

A continuous transition takes place at p_c. Although DP can be defined and simulated easily, no analytical solution exists for it (neither for any of the models pertaining to the DP universality class) in dimension d lower than the critical dimension $d_c = 6$. Therefore, one has to use numerical estimates of the critical exponents. Currently, the best estimates[258] in $d = 2$ are $\beta = 0.27649$, $\nu_\perp = 1.096854$, and $\nu_\| = 1.733847$; the percolation threshold depends both on the spatial dimension and the type of array, and for $d = 2$ on a square lattice the best estimation of it is $p_c = 0.6447001$.

Attempts to describe this phase transition in the Yang–Lee formalism were done in Refs. 259–261, by considering the zeros of $P_L(p)$ in the plane of complex p, for dimensions $L \leqslant 15$, and looking for their accumulation points when one increases L, i.e., when one goes towards the thermodynamic limit. These zeros do not lie on a single smooth curve (as it was the case for the other nonequilibrium systems discussed above), but on a sequence of curves that tend to intersect at the critical point. Also, the results in Refs. 259–261 suggest a fractal structure of the distribution of these zeros (but this aspect deserves further investigation). From these numerical results, the authors infer the values of p_c, and (using finite-size scaling arguments) also the longitudinal exponent $\nu_\|$.

It should be noted, however, that the partition function $P_L(p)$ has some properties that render it qualitatively different from the other nonequilibrium partition functions considered above. A first remark[259,262] is that the survival probability $P_L(p)$ can be represented formally as the partition function of a system of Ising spins, with two- and three-spin plaquette interactions, on a pyramid-shaped lattice. However, some of these three-spin interactions have an infinite energy, and thus the usefulness of such a mapping is questionable. Also, one encounters some problems with the definition of a thermodynamic limit and of an extensive free energy of the system, since, on one hand, $P_L(p)$ does not grow exponentially with the size of the system, and on the other hand $\lim_{L\to\infty} P_L(p) = 0$ for $0 \leqslant p < p_c$, and it is not clear how to define a free energy density in this case. This illustrates some of the difficulties related to the extension of equilibrium concepts to nonequilibrium situations.

19. Self-Organized Criticality

Two recent studies,[263,264] addressed the problem of the applicability of the Yang–Lee formalism to self-organized criticality (SOC). Roughly speaking, a system that exhibits SOC is a nonequilibrium system (subject to external stationary nonequilibrium constraints) characterized by the fact that, in the thermodynamic limit, it reaches a stationary state with *scale invariance and power-law statistics*. One

should underline that this nonequilibrium state is reminiscent of equilibrium critical states. However, contrary to these ones, this stationary critical state is reached solely through the internal dynamics of the system in response to the external constraints, without the fine-tuning of the control parameters that is required for the equilibrium criticality. There is a huge body of literature devoted to this topic (see Ref. 265 for a pedagogical overview of the field).

The papers of Cessac *et al.* then raise the legitimate question whether this spontaneous criticality manifests itself in the properties of the distributions of complex zeros of a properly defined partition function for the stationary state, i.e., if these zeros have an accumulation point when the size of the system is increased to infinity, without any manipulation of the parameters of the system.

The dynamics of SOC systems occurs in avalanche-like events; one can define a set of observables (size, duration, etc.) characterizing these avalanches. In a finite system of size L such an observable $\mathcal{V}$ can take a finite set of values, up to a maximum finite value N_L, $\mathcal{V} = 0, 1, \ldots, N_L$, according to a stationary probability distribution $P_L(\mathcal{V} = n)$. Let us consider the generating function of this distribution (the grand-canonical partition function),

$$\Xi_L(z) = \sum_{i=1}^{N_L} z^n P_L(n) \,, \tag{79}$$

that is a polynomial of degree N_L in the fugacity z. If the system is SOC, the zeros of this polynomial in the complex-z plane should have an accumulation point on the real positive semi-axis in the thermodynamic limit $L \to \infty$ for any parameters of the system. This reasoning was verified in the above-cited references for various finite-size scaling forms of $P_L(n)$ encountered in the literature on SOC: the zeros pinch the real axis at $z = 1$ as the system size goes to infinity. A scaling theory for the Yang–Lee zeros is proposed in this setting, that shows, under specific conditions, a violation of the scaling usually observed in equilibrium critical phenomena.

Note, however, that the remark we made in Sec. 16.2 with respect to Ref. 249 applies here, too, namely that considering the generating function $\Xi_L(z)$ amounts actually at analysing an equilibrium problem in a grand-canonical statistical ensemble.

20. Connection with Equilibrium Systems with Long-Range Interactions

The examples in the above sections show a surprising analogy between the equilibrium and the noneqilibrium steady-state phase transitions, as far as the behaviour of the zeros of the respective partition function in the plane of the complex control parameter is concerned. The question that arises is then whether or not this analogy can be pushed further, e.g., if one can find a kind of (general rule for a) correspondence between nonequilibrium steady-state and an equilibrium systems.

As discussed in Sec. 14, a nonequilibrium system is characterized by a breaking

of detailed balance in the configuration space, which corresponds to the appearance of macroscopic flows throughout the system. This generates *effective long-range interactions* and correlations in the system, as well as the emergence of an effective criticality in nonequilibrium steady-states, and, in this logic, of universal distribution functions for macroscopic quantities, of the corresponding classes of universality, critical exponents, etc. (see Refs. 8, 255, 266 and 267 for a discussion of these fundamental issues).

Therefore, if one is searching for a kind of correspondence between nonequilibrium steady-states and equilibrium systems, the latter ones have to have long-range interaction Hamiltonians. The history of searching for these effective Hamiltonians (and related problems like, e.g., definitions of an effective nonequilibrium temperature) is long and tortuous and will not be discussed here. In particular, trying to write down an explicit expression of this Hamiltonian does not seem to be a very fruitful approach.

Here we will briefly present a few recent results in this direction (see Refs. 247, 268–270). These studies refer to ASEP-like systems, but in our opinion, in view of their generality, these ideas carry an important potential for further applications. The adopted strategy relies on two key-elements as discussed below.

(A) The formal definition of "particle numbers" and associated "fugacities". Let us consider a Markovian system as described in Secs. 14 and 15, and the corresponding steady-state normalization factor $Z_n(\{\mathcal{W}(\omega \to \omega')\})$ (here n designates the number of configurations ω accessible to the system; it is also explicitly indicated that the normalization factor is a function of the transition rates). A first point discussed in Ref. 268 is that the normalization factor is a *polynomial in the transition rates $\mathcal{W}(\omega \to \omega')$, with positive coefficients*, of degree $n - 1$, i.e., it has the form of a *generating function*. By the Cauchy–Schwartz inequality it follows that its negative logarithm (that we would like to assimilate with a free energy of the system),

$$F_n = -\ln(Z_n), \tag{80}$$

is a *convex function* in all its arguments $\mathcal{W}(\omega \to \omega')$. One is then tempted, by analogy with equilibrium situations, to identify *formally* the transition rates with "fugacities", and to consider the corresponding "particle numbers"

$$N_{\omega,\omega'} = -[\mathcal{W}(\omega \to \omega')] \frac{\partial Z_n}{\partial [\mathcal{W}(\omega \to \omega')]}. \tag{81}$$

These are well-behaved thermodynamic quantities, in the sense that they are positive and increasing functions of the fugacities for any size n of the system. They are, however, linearly-dependent, and some of them may even coincide (because some of the transition rates may be zero or may be equal between them). In the thermodynamic limit of large n

$$N_{\omega,\omega'} = V(n)\rho_{\omega,\omega'}, \tag{82}$$

where $V(n)$ is the "volume" (as defined by the leading asymptotic behaviour of the normalization factor) and $\rho_{\omega,\omega'}$ are the "densities".

One has now all the *formal* ingredients to discuss a nonequilibrium steady-state phase transition by analogy with the equilibrium situations. For example, a first-order phase transition would correspond to a discontinuity of the fugacity as a function of the density. It is not clear, however, in general, that all the known characteristics of the phase transitions (e.g. diverging correlation length for continuous phase transitions) are recovered within this formalism.

There is one more very important point to be made, and which represents a major difference between nonequilibrium systems and equilibrium systems with short-range interactions. It is the fact that the "particle numbers" defined above are not necessarily extensive quantities. This implies that in the space of the parameters of the system (which are the transition rates), besides the regions where the "particle densities" are well behaved and finite, there may appear regions where $\rho_{\omega,\omega'}$ may diverge (and one has to change then the definition of $V(n)$). The frontiers between these regions then correspond to phase transitions that do not have a correspondent in the short-ranged interactions equilibrium systems. Note, however, that phase transitions of this type are know in *equilibrium systems with long-range (or nonlocal) interactions*,[268] a remark that goes in the sense of the general statements made in the beginning of this paragraph.

(B) The correspondence with equilibrium systems. Once this formal frame is set-up, comes the most delicate part, which is to find a way (possibly a systematic one) to assign a physical meaning to the normalization factor, "particle densities", etc. in a properly-defined *equilibrium* statistical problem. The general solution proposed in Ref. 268, and illustrated on concrete examples in Refs. 247, 268–270 comes from the combinatorial graph theory, and consists in relating explicitly the normalization of a stationary state to the combinatorial problem of counting weighted spanning trees on graphs; the weights of the configurations depend on parameters which correspond to the transition rates of the nonequilibrium stochastic process. This implies directly an interpretation of the normalization factor as a statistical mechanics partition sum. Of course, establishing the right correspondence is a difficult task, and no general recipe can be given for it.

A first heuristic application of this approach is given in Ref. 271, where a one-dimensional, stochastic, adsorption-desorption nonequilibrium model for interface growth (the raise-and-peel model) was put in correspondence with a two-dimensional ice model with domain-wall boundary conditions (an equilibrium problem with nonlocal interactions). Brak and Essam[269] showed that the matrix representation of the stationary-state algebra of TASEP can be interpreted combinatorially as various weighted lattice paths. The normalization factor of TASEP is identical to the equilibrium configuration sum of a polymer chain having a two-parameter interaction with a surface (the so-called one-transit walk). As shown in Ref. 268, the TASEP current and density are simply related to the equilibrium

densities of the latter model; in particular, the second-order phase transitions of the TASEP (see Sec. 16.1) are related to a special type of surface phase transition encountered in polymer physics. Later on Blythe *et al.*[247] found that the normalization factor of the discrete-time parallel-update TASEP can be expressed as one of several equivalent variants of two-dimensional lattice constrained-path problems. Finally, in Ref. 270 it was shown that the grand-canonical normalization factor of the TASEP (that corresponds to the immersion of the lattice in a reservoir of particles, with fixed fugacity z) can be computed in a closed analytical form, and thus it allows a direct derivation of the asymptotics of the canonical normalization for the various phases, and the immediate correspondence with the one-transit walk mentioned above.

21. Conclusions and Perspectives

In order to explain the origin of singularities of the thermodynamic potentials in some first-order equilibrium phase transitions, Lee and Yang proposed to examine the behaviour of the zeros of the partition function. Such an idea turned out to have far reaching consequences. Indeed, subsequent generalizations of this approach showed that from the analysis of zeros of the partition function one can extract a lot of information about phase transitions in many different systems. When combined with finite-size scaling arguments, this method may be used to calculate the location of the transition point and even critical exponents. An important point is the fact that in this approach we directly refer to the properties of the partition function, which is the most basic quantity of equilibrium statistical mechanics. Thus, one can apply mathematically rigorous techniques to obtain a number of interesting results concerning, e.g., the very existence and the location of phase transitions in various systems.

Recent large interest in the Yang–Lee approach is related, however, to its further extension to nonequilibrium phase transitions. Several examples show that accomplishing such an ambitious task may be feasible in some nonequilibrium systems. But the entire approach is much more problematic than in equilibrium situations. It is not entirely clear what the analogue of the partition function in nonequilibrium situations might be. For the directed percolation, coalescence of zeros was observed for the percolation probability — that is actually the order parameter of the system. For self-organized criticality this effect appears in some generating functions. Perhaps, the most promising are the results obtained for TASEP models. In this case the normalization factor of a steady-state probability distribution seems to play the role of the partition function. In some cases one can even establish much closer relations with equilibrium systems. But it is not known yet whether such an approach can be applied to other classes of nonequilibrium systems. For example, it would be interesting to test this method on systems for which the transition rates are not constant, but state-dependent, like, e.g., the zero-range processes (ZRP).

It seems therefore that, after more than 50 years of generalizations and extensions, the full potential of the Yang–Lee approach is yet to be uncovered. Important developments in its application to the study of nonequilibrium phase transitions are in progress.

Acknowledgments

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