Chapter 1

Universality away from critical points in a thermostatistical model

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Nature uses phase transitions as powerful regulators of processes ranging from climate to the alteration of phase behavior of cell membranes to protect cells from cold, building on the fact that thermodynamic properties of a solid, liquid, or gas are sensitive fingerprints of intermolecular interactions. The only known exceptions from this sensitivity are critical points. At a critical point, two phases become indistinguishable and thermodynamic properties exhibit universal behavior: systems with widely different intermolecular interactions behave identically. Here we report a major counterexample. We show that different members of a family of two-dimensional systems -the discrete p-state clock model- with different Hamiltonians describing different microscopic interactions between molecules or spins, may exhibit identical thermodynamic behavior over a wide range of temperatures. The results generate a comprehensive map of the phase diagram of the model and, by virtue of the discrete rotors behaving like continuous rotors, an emergent symmetry, not present in the Hamiltonian. This symmetry, or many-to-one map of intermolecular interactions onto thermodynamic states, demonstrates previously unknown limits for macroscopic distinguishability of different microscopic interactions.

1.1 Introduction

A far-reaching result in the study of phase transitions is the concept of universality, stating that entire families of systems behave identically in the neighborhood of a critical point, such as the liquid-gas critical point in a fluid, or the Curie point in a ferromagnet, at which two phases become indistinguishable. Near the critical point, thermodynamic observables, such as magnetization or susceptibility, do not depend on the detailed form of the interactions between individual particles, and the critical exponents, which describe how observables go to zero or infinity at the transition, depend only on the range of interactions, symmetries of the Hamiltonian, and dimensionality of the system. The origin of this universality is that the system exhibits long-range correlated fluctuations near the critical point, which wash out the microscopic details of the interactions [1, 2, 3, 4].

In this paper, we report a different type of strong universality. We present the surprising result that, in a specific family of systems, different members behave identically both near and *away from critical points*—we refer to this as extended universality, if the temperature and a parameter p, describing the interaction between neighboring molecules, exceed a certain value. In this regime, the thermodynamic observables collapse, in the sense that *their values are identical for different values of* p. No thermodynamic measurements in this regime reveal the details of the microscopic interaction in the Hamiltonian. This demonstrates intrinsic limits to how much information about the microscopic structure of matter can be obtained from macroscopic measurements. As the collapse maps Hamiltonians with different symmetries onto one and the same thermodynamic state, the system exhibits a symmetry not present in the microscopic Hamiltonian. The added symmetry at high temperature is the counterpart of broken symmetry at low temperature. To the best of our knowledge, no such collapse of thermodynamic observables and added symmetry have been observed before.

The family under consideration is the p-state clock model, also known as p-state vector Potts model or Z_p model [5], in two dimensions, with Hamiltonian

$$H_p = -J_0 \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j = -J_0 \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \qquad (1.1)$$

where the spins, $\mathbf{s}_i$, can make any of p angles $\theta_i = 2\pi n_i/p$, $(n_i = 1, \ldots, p)$, with respect to a reference direction; the sum is over nearest neighbors of a square lattice; and the interaction is ferromagnetic, $J_0 > 0$. (In what follows we set $J_0 = k_{\mathrm{B}} = 1$.) The number of directions, p, may be thought of as discrete orientations imposed on each spin by an underlying crystallographic lattice. The model interpolates between the binary spin up/down of the Ising model [6] and the continuum of directions in the planar rotor, or XY, model [7, 8]. The model is of interest to study how the ferromagnetic phase transition in the Ising model, with spontaneously broken symmetry in the ferromagnetic phase, gives way to the Berezinskii-Kosterlitz-Thouless (BKT) transition, without broken symmetry, in the rotor model. For any p, neighboring spins in low- and high-energy configurations are parallel, $\mathbf{s}_i \cdot \mathbf{s}_j \simeq 1$ and antiparallel, $\mathbf{s}_i \cdot \mathbf{s}_j \simeq -1$, respectively.

This model has been extensively studied since its conception [5]. Elitzur *et al.* [9] showed that it presents a rich phase diagram with varying critical properties: for $p \leq 4$ it belongs to the Ising universality class, with a low-temperature ferromagnetic phase and a high-temperature paramagnetic phase; for $p > 4$ three phases exist: a low-temperature ordered and a high-temperature disordered phase, like in the Ising model, and a quasi-liquid intermediate phase. Duality transformations [9, 10] and RG theory gave much insight into the phases in terms of a closely related, self-dual model, the generalized Villain model [11],

$$H_{\mathrm{V}} = \sum_{\langle i,j \rangle} [1 - \cos(\theta_i - \theta_j)] + \sum_i \sum_p h_p \cos(p\,\theta_i)\,, \tag{1.2}$$

where the θ_i's are now continuous and the h_p's are p-fold symmetry-breaking fields, similar to the crystal fields that limit the spins to p directions in the clock model. José *et al.* [12] have shown, via RG analysis, that for $p < 4$ the fields were relevant and the low-temperature phase was ordered, and that the fields were irrelevant for $p > 4$. While the p-state clock model is obtained in the limit of an infinite symmetry-breaking field, $h_p \to \infty$, some properties of Eq. (1.2) for finite fields are still valid for its discrete counterpart, Eq. (1.1) [12, 9]. But (1.1) is no longer self-dual for $p > 4$, and RG approximations regarding the influence of the discreteness of the angular variables are delicate near $p = 6$. As a result, the transition points of (1.1) in the three-phase region are not precisely known.

The collapse of thermodynamic observables, or extended universality, sets in at temperature T_{eu}, at which the system switches from a discrete-symmetry, p-sensitive state to a continuous-symmetry, p-insensitive state, indistinguishable from $p = \infty$, as the temperature increases and crosses T_{eu}, for $p > 4$. For $p \leq 4$, there is no collapse and the system retains its discreteness at arbitrarily high temperatures. The collapse (non-collapse) is responsible for the BKT (non-BKT) behavior of the transitions that lie above (below) T_{eu}. In what follows, we focus on the determination of the phase diagram, including the curve $T_{\mathrm{eu}}(p)$, the characterization of each phase, and the critical properties of the two transitions present at $p > 4$.

1.2 The Phase Diagram

We performed MC simulations on a square 2D lattice of size $N = L \times L$ with periodic boundary conditions. Lattice sizes ranged from $L = 8$ to 72, and averages for the computed quantities involved sampling of 10^5–10^6 independent configurations, with equilibration runs varying from $p \times (1{,}000$–$5{,}000)$ MC steps (a MC step is one attempt to change, on average, *every* lattice element).

Figure 1.1 shows a summary of our results. The Ising model ($p = 2$) shows a single second order phase transition at $T_c^{\mathrm{Ising}} = 2/\ln[1 + \sqrt{2}] \simeq 2.27$, in units of J_0/k_{B}. The $p = 4$ case also shows a single transition (in the Ising universality class) at $T_c = T_c^{\mathrm{Ising}}/2 \simeq 1.13$. Most interesting is the case for $p > 4$, which exhibits a low-temperature ordered phase (Ising-like), which turns into a phase with quasi-long-range order at T_1, and finally disorders at T_2. For $T > T_{\mathrm{eu}}$ the identity of the original symmetry of the problem is lost, and all systems behave strictly like the planar rotor model ($p = \infty$), with a BKT transition at $T_{\mathrm{BKT}} \simeq 0.89$ [8].

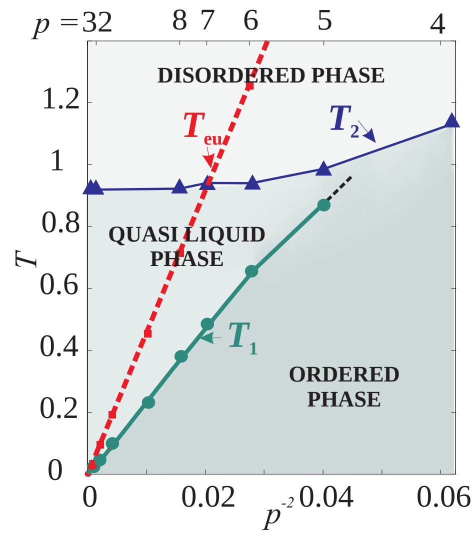

Figure 1.1: Phase diagram of the p-state clock model. The Ising model, $p = 2$, exhibits a single second-order phase transition, as does the $p = 4$ case which is also in the Ising universality class. For $p \geq 6$ a quasi-liquid phase appears, and the transitions at T_1 and T_2 are second-order. The line $T_{\rm eu}$ separates the phase diagram into a region where the thermodynamic observables do depend on p, below $T_{\rm eu}$; and a region where their values are p-independent, above $T_{\rm eu}$ (collapse of observables, extended universality). Thus for $p \geq 8$, we observe $T_{\rm eu} < T_2 = T_{\rm BKT}$.

The transition temperatures are determined from our MC simulations as follows (for details see Ref. [13]). For the high-temperature transition T_2 we use Binder's fourth order cumulants [14] in magnetization, $U_L \equiv 1-\langle m^4\rangle/3\langle m^2\rangle^2$, and energy $V_L \equiv 1-\langle e^4\rangle/3\langle e^2\rangle^2$. The fixed point for U_L is used to determine the critical temperature T_2, whereas the latent heat is proportional to $\lim_{L\to\infty}[(2/3)-\min_T V_L]$ (in all cases $\min_T V_L \to 2/3$, signaling a second-order phase transition).

The transition between the ordered and the quasi-liquid phases, T_1, is analyzed via the temperature derivatives of the magnetization, $\partial\langle|\mathbf{m}|\rangle/\partial T$, and $\partial U_L/\partial T$, both of which diverge in the thermodynamic limit [13]. Finite size scaling (FSS) applied to the location of the minima of these quantities yields $T_1 = \lim_{L\to\infty} T_1(L)$. We find $T_1 = 4\pi^2/(\tilde{T}_2 p^2)$, with $\tilde{T}_2 \simeq 1.67 \pm 0.02$, whereas for the Villain model, in the limit of an infinite h_p and large p, José *et al.* [12] found $T_1^{\rm (JKKN)} \simeq 4\pi^2/(1.7p^2)$. The ordered phase vanishes rapidly as $p \to \infty$, see Fig. 1.1.

Figure 1.2 shows thermodynamic properties of the clock model as obtained from our MC simulations: the the heat capacity per spin at zero external field $c_F \equiv (\langle H^2\rangle - \langle H\rangle^2)/(L^2T^2)$, and the magnetization per spin defined as $\langle \mathbf{m}\rangle \equiv \langle \mathbf{M}\rangle/L^2 = \langle(|\sum_{i=1}^N \cos\theta_i|, |\sum_{i=1}^N \sin\theta_i|)\rangle/L^2$. The Ising-like behavior for $p=4$, and the three-phase behavior for $p \geq 6$ are evident. Figure 1.2 proves the collapse

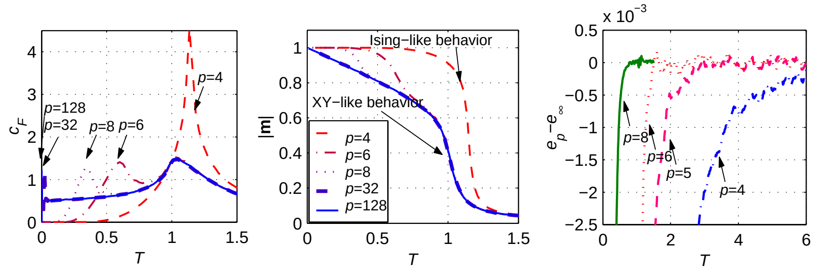

Figure 1.2: Heat capacity (left panel), magnetization (center panel) and difference of internal energy per spin relative to XY model (right panel). The data corresponds to a system size $L=72$ ($N=5,184$ spins). Note that all curves approach each other above some $T_{\rm eu}$ (for $p\geq 5$).

of the thermodynamic observables: c_F and $\langle|\mathbf{m}|\rangle$ are manifestly p-independent for $p>4$ and $T>T_{\rm eu}$, with

$$T_{\rm eu} = 4\pi/(p^2 T_{\rm BKT})\,, \tag{1.3}$$

where $T_{\rm BKT}\simeq 0.89$; and the internal energy difference sharply drops to zero at $T=T_{\rm eu}$.

The collapse of thermodynamic variables and the specific form of $T_{\rm eu}(p)$ can be understood as follows. *(i)* The large-p, small-$(\theta_i-\theta_j)$ expansion of Eq. (1.1) yields a characteristic temperature $\sim(2\pi/p)^2$ above which the thermodynamic observables become p-independent, as $T/(2\pi/p)^2\gg 1$ [13]. This implies an *asymptotic* collapse of thermodynamic observables. *(ii)* Elitzur *et al.* [9] noted that the discreteness of the angles θ_i in Eq. (1.1) becomes irrelevant for the *critical properties* of the system, for sufficiently large p. This implies a collapse of thermodynamic variables at *critical points* T_2. A similar irrelevance of the discreteness of angles, imposed by one $h_p\to\infty$, had been previously observed in the generalized Villain model, Eq. (1.2) [12]. There it was shown that necessary for the discreteness to become irrelevant is $T>4\pi^2/(p^2T_{\rm k})$, where $T_{\rm k}\simeq 1.35$ is the BKT point of model (1.2). This suggest that a necessary condition for the collapse of thermodynamic observables in the p-state clock model is $T>4\pi^2/(p^2T_{\rm BKT})$. The fit of our numerical data for $T_{\rm eu}(p)$ [13], yielding Eq. (1.3), shows that the condition is satisfied as an equality and is both necessary and sufficient.

The implications of the collapse above $T_{\rm eu}$ are crucial for the understanding of critical properties at the transition point T_2. We observe that $T_2(p\geq 8)>T_{\rm eu}$, which implies that the transition T_2 for $p\geq 8$ *must* be BKT. Previous work focused only on the *plausibility* of such behavior. For the purposes of this discussion, we take the BKT behavior as the following set of properties of the planar rotor model [8]: *(i)* a universal discontinuous jump to zero of the helicity modulus $\Delta\Upsilon|_{T_{BKT}}=2T_{BKT}/\pi$, *(ii)* the exponential divergence of the correlation length as $\xi\sim\exp[c/|T-T_{\rm BKT}|^{1/2}]$, *(iii)* the temperature-dependent power law decay of two point correlation functions with a critical exponent at T_2 given by $\eta(T_{\rm BKT})=1/4$, and *(iv)* an exponent related to the decay of the magnetization given by $\tilde{\beta}=3\pi^2/128$ [16].

In fact, our numerical simulations show these features being satisfied, giving a rotund confirmation of the nature of the high temperature phase transition for $p \geq 8$. To illustrate this, we follow Minnhagen-Kim's elegant arguments [15] and evaluate whether the helicity is discontinuous at T_2. The essence of Minnhagen's idea consists in applying a twist Δ to the spins and evaluating the change in the free energy:

$$f = \frac{\Upsilon}{2}\Delta^2 + \frac{\Upsilon_4}{4!}\Delta^4 + \cdots . \tag{1.4}$$

Although it is evident that Υ vanishes in the high-temperature regime, it is not possible to substantiate its discontinuity in any numerical simulation as predicted by the RG equations. However, at the transition, Υ_4 converges to the negative universal value -0.126 ± 0.005 , implying that an expansion of the free energy is non-analytic, and that the helicity is, indeed, discontinuous. Similar results are observed for all $p \geq 8$ (as expected from the extended universal behavior for $T > T_{\rm eu}$). Further analysis indicates that the discontinuity corresponds to the results of the RG equations [13].

On the other hand, since $T_2(p < 8) < T_{\rm eu}$, it is possible that the nature of the phase transition for $p = 6$ could be significantly different. Indeed, Υ does not appear to vanish as $L \to \infty$, while Υ_4 converges to zero

It is also evident from numerical data [13] that the high temperature phase transition $T_2(p < 8)$is *not* completely BKT-like. These facts highlight the importance of *where* the extended universality ($T > T_{\rm eu}$) occurs (see Fig. 1.1).

1.3 Summary, Implications, and Open Questions

In our study we obtained valuable evidence from the macroscopic properties of the Z_p model, a model that, although completely discrete, shows regimes with continuous-like thermodynamic behavior. We have presented the phase diagram for the Z_p model analyzing its critical properties. The 3-phase regime was observed for $p > 4$ in agreement with earlier predictions. Of particular interest is the surprising *extended universal* behavior above some temperature $T_{\rm eu}$, where the identity of the Z_p model is completely lost as all observables become indistinguishable from those of the XY model. In fact, the presence of an "exact" BKT transition at the point T_2 for $p \geq 8$ is now firmly established as a consequence of the existence of this temperature line $T_{\rm eu}$, which divides the phase diagram in two regions: with and without a collapse of the thermodynamic observables. This extended universal behavior is not present at $T_2(p < 8)$, since $T_2(p < 8) > T_{\rm eu}$. These conclusions were confirmed by studying the critical properties at T_2 (indeed, for $p < 8$ critical exponents and the helicity do not behave as expected from the BKT RG equations).

Our studies raise important questions: If observables below T_1 show ferromagnetic ordering with a significant p-dependence, and for $T > T_{\rm eu}$ all information about p is lost, what is the nature of the region $T_1 < T < T_{\rm eu}$? What are the collective excitations that make the system thermodynamically indistinguishable above $T_{\rm eu}$? Why is the extended universal behavior approached so rapidly (for $p > 4$), and what is *qualitatively* different for smaller p since *no temperature* exists that makes this degeneracy be achieved?

A very broad variety of systems from confined turbulent flows to statistical ecology models show collapsing probability distribution functions in finite-sized systems, suggesting that scaling is independent of various systems attributes such as symmetry, state (equilibrium/not equilibrium), etc [17]. We present a *stronger result* in the sense that *all observables* become identical for $T > T_{\rm eu}$: the critical properties' collapse is a *consequence* of the *extended universality*.

The existence of this *collapse of the thermodynamic observables* implies that, experimentally, *any* observable $\langle\mathcal{O}\rangle$ of the system measured at temperatures above $T_{\rm eu}$ will fail to show *any* signature of the underlying discreteness, i.e. $\langle\mathcal{O}\rangle_p = \langle\mathcal{O}\rangle_\infty$. The corollary is that in the presence of this *extended universality*, lower-temperature measurements are necessary if a complete characterization of the symmetry of a system is desired, as may be expected in a wide range of experimental situations where the XY-like behavior is observed [18]. Experiments in a wide variety of physical systems—from ultra-thin magnetic films, to linear polymers adsorbed on a substrate—may show signatures of these effects. It may imply, e.g., that the critical properties at the melting transition of certain adsorbed polymer films may be unaffected by the symmetry of the substrate.

Further details about the results presented in this letter and additional properties, plus some ideas on how to address the questions posed above will be published elsewhere [13].

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