On the changeover in the transition nature of local-interaction Potts models

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A combinatorial approach is used to study the critical behavior of a \( q \)-state Potts model with a round-the-face interaction. Using this approach, it is shown that the transition is of first order for \( q > 3 \). A second order transition is numerically detected for \( q = 2 \). Based on these findings, it is deduced that for some two-dimensional ferromagnetic Potts models with completely local interaction, there is a changeover in the transition order at a critical integer \( q_c \leq 3 \). This stands in contrast to the standard two-spin interaction Potts model where the maximal integer value for which the transition is continuous is \( q_c = 4 \). Under a conceivable assumption, an exact expression for the first order transition critical temperature is additionally derived.

I. INTRODUCTION

The ferromagnetic \( q \)-state Potts model [1, 2] is one of the most widely studied models in statistical physics. At the core of the model is an interacting spin system with each spin possessing one out of \( q \) possible states. The interaction consists of the simple rule that if the spins are monochromatic (have the same state) the energy level is lower than the case where they hold different states. Although the model is very easy to define, it is rich in interesting phenomena. A particular one that has been sparsely studied is the changeover phenomenon or the change in the transition nature, from second to first order, at a critical integer value \( q_c \).

Using an equivalence of the nearest-neighbor interaction model on the square lattice to a staggered ice-type model [3], Baxter [4, 5] obtained an exact nonzero expression for the latent heat when \( q > 4 \). This expression has vanished at \( q = 4 \). A vanishingly small jump in the free energy near \( T_c \) has been found for \( q \leq 4 \). Based on these results, Baxter predicted that the model underwent a continuous (discontinuous) transition for \( q \leq q_c \) \( (q > q_c) \) with \( q_c = 4 \). His findings were believed to be lattice independent [6]. Recently, Duminil-Copin et al [7, 8] have rigorously confirmed Baxter’s predictions using the random cluster representation [9] of the nearest-neighbor interaction model.

Renormalization group (RG) theory has provided a useful framework to detect the changeover in the transition order. Nienhuis et al considered a generalized triangular lattice Potts model with additional lattice-gas variables and corresponding couplings, to control order disorder in the renormalized system. Applying a generalized majority-rule [6, 10] to that model, the authors introduced a RG scheme for continuous values of \( q \) which produced \( q_c \approx 4.7 \). Following [6, 11], Cardy et al [12] proposed a system of differential RG equations describing the scale change of the ordering, thermal, dilution fields in the vicinity of a single multicritical point. The equations were derived based on the assumption that the ordering and thermal fields were relevant while the dilution field was marginal at the multicritical point. Investigating the equations near the multicritical point, the authors have found universal, presumably exact, parameters using previously known results [13, 14].

It is known that some physical properties of all finite-range interaction models with the same dimensionality and symmetries, are universal, that is, independent of the interaction details of one model or another. For instance, universality is manifested in the behavior of physical observables near criticality. One can then ask: do two dimensional local interaction ferromagnetic Potts models defined on various geometries and presenting the usual \( q \)-fold spontaneous symmetry breaking, in general mimic the changeover behavior of the standard pair-interaction model?

Some variants of the pair-interaction Potts model, with long but finite range interactions [15] or with (exponentially) fast decaying infinite-range interactions [16], are known to exhibit a first order transition for \( q \geq 3 \). In another Potts model with the standard nearest-neighbor interaction, \( r \) “invisible” states were added to the usual \( q \) “visible” states [17, 18]. The invisible states affected the entropy but did not alter the internal energy. It has been shown [18] that the transition is of first order for low \( q (q = 2, 3, 4) \), provided that \( r \) is sufficiently large.

Based on Refs. [15–18], the answer to the question raised above is apparently negative. Provided undergoing a continuous transition for some \( q < 3 \), some of the systems [15, 16] display a changeover phenomenon at a critical integer \( q_c < 3 \). It should be noted, however, that the models studied in Refs. [15–18] have a complicated and somewhat “unnatural” interaction content.

A phase transition entails the emergence of monochromatic giant components (macroscopic connected components taking up a positive fraction of the sites, hereby abbreviated as GC) whose existence becomes beneficial once the energy saved by the interactions overcomes the entropy cost. One may then ask what is the typical structure of such monochromatic GC. In [19] some of us used the correspondence between simple (non-fractal) and fractal-like clusters to the topology of ordered phases in first and second order transitions, respectively, to show that for the round-the-face interaction Potts model on the square lattice the changeover in the transition nature occurs at \( q = 4 \). However, Monte-Carlo (MC) simulations [19] of the model with \( q = 4 \) resulting in a pro-
nounced double-peaked shape of the pseudo-critical energy probability-distribution-function [20], hints that a first-order transition is possible then.

In the present paper we develop a more rigorous approach, based on first principles, to study the phase transition of the round-the-face interaction Potts model. Using this approach, it is demonstrated on a simple "natural" model that satisfies the usual Potts q-fold broken symmetry, that within the class of q-state models with completely local interactions, a changeover phenomenon occurs at an integer value need not equal four. More precisely, we show that the model, defined on the honeycomb lattice, undergoes a first order transition for q > 3. Under a few further conceivable assumptions related to the asymptotic number of hexagonal lattice animals (polyhexes) a first order transition is detected also for q = 3. Extensive MC simulations [21] are performed for different values of q. For q = 2, a second order transition is numerically observed. It follows that the honeycomb lattice model changeovers its transition nature at a critical value q_c ≤ 3. Additional simulations are carried out for the triangular lattice. For the latter, the simulations indicate that q_c = 5.

The rest of the paper is organized as follows. In section II we discuss the role of large scale lattice animals in determining the critical temperature and the changeover in the transition nature of the round-the-face interaction model. In section III we present and analyze in detail the results of Monte Carlo simulations. Our conclusions are drawn in section IV.

II. LATTICE ANIMALS AND THE CHANGEOVER PHENOMENON

Consider a ferromagnetic Potts model where the interaction involves l spins residing at the vertices of an elementary cell (face) of a lattice with N sites (e.g., l = 4 for the square lattice). The model may be described by the Hamiltonian

\[ \mathcal{H} = K \sum_{\text{faces}} \delta_{\sigma_{\text{face}}} , \]

where \( \beta = 1/k_B T \), \( K = \beta J \) and \( J > 0 \) is the ferromagnetic coupling constant (we will take from now on \( k_B = J = 1 \) for convenience). The \( \delta_{\sigma_{\text{face}}} \) symbol assigns 1 if all the spins \( \sigma_{\text{face}} := \{ \sigma_1, \sigma_2, ..., \sigma_l \} \) on a given face simultaneously take one of the q possible Potts states, and 0 otherwise. The partition function of the Hamiltonian (1)

\[ Z = \sum_{\{ \sigma \}} \prod_{\text{faces}} (1 + v \delta_{\sigma_{\text{face}}} ) , \]

where \( v = e^K - 1 \), can take the form [2, 4, 5]

\[ Z = q^N \sum_G q^{\nu(G)} v^{\mu(G)} (1 - 1/q)^{\alpha(G)p(G)} , \]

where \( G \) is a graph made of \( c(G) \) clusters with a total number of \( f(G) \) faces placed on its edges and \( \nu(G) \) nodes. The total number of perimeter nodes is \( p(G) \) and \( \alpha(G) < 1 \) is a positive proportionality factor.

Any cluster is either a lattice animal [22] or a lattice beast, that is, a collection of animals sharing joint nodes such that these animals are left unconnected. Let \( b_{km} \) be the number of beasts with \( k \) faces and \( m \) sites. It is known [23, 24] that the total number of animals of size \( k \) on a two-dimensional periodic lattice takes the asymptotic form \( \sum_m b'_{km} \approx c \lambda^k \) (the prime refers to animal-like clusters), where \( c \) is some constant. The total number of \( k \)-face beasts therefore asymptotically assumes \( \sum_m b'_{km} \sim \lambda^k \) where \( \lambda \geq \lambda \).

Consider a family of beasts such that \( m/k \approx \rho \) where \( \rho \) is the minimal asymptotic number of sites per face (e.g., for a perfect square on the square lattice with \( m = (\sqrt{k} + 1)^2 \), \( \rho = 1 \)). Necessarily, these beasts are simple. Identifying a beast in this family with a boundary of size \( B = o(N) \), its number of sites per face is no larger than \( (m + \Delta m)/k \) with \( m/k \approx \rho \) and \( \Delta m = o(N) \), hence approaches \( \rho \) in the large \( N \) limit. Simple combinatorics shows that the number of simple \( k \)-face beasts is bounded by \( K N^{aB} \) for some constants \( a, K, \) i.e., sub-exponential in (large) \( N \). It follows that for a given \( \delta > 0 \) a family of (quasi) fractal beasts (QF) with \( m/k \approx \rho + \delta \), exponentially-growing at a rate \( \mu = \mu(\delta) \), is established. Making such a family of beasts monochromatic changes the entropy in the amount

\[ \Delta S = \ln \left( \frac{k}{q^m} \right) + \text{perimeter term} + \text{h.o.t.} \]

\[ = k \ln \left( \frac{\mu}{q^{\rho + \delta}} \right) + \theta k \ln (1 - 1/q) + o(N) , \]

where \( \theta k \) is a fraction of \( O(k) \) perimeter sites. Consequently, the change in the free energy \( \Delta F = -k - T \Delta S \) (for large \( k \)) satisfies

\[ \Delta F \geq -k(1 - T \rho \ln q) - Tk \ln \left( \frac{\mu}{q^{\rho}} \right) . \]

Now, at \( T^* = 1/\rho \ln q \), the temperature at which the energy gain balances the entropy loss due to the formation of a simple GC (effectively associated with \( \delta = 0, \mu = 1 \) and \( \theta = 0 \) in (4),(5)), \( \Delta F \geq 0 \) if \( \mu/q^\rho \leq 1 \). This means that for \( q \geq q_* \), where

\[ q_* = \sup_{\delta} \mu^{1/\delta} , \]

it is disadvantageous for the system to occupy QF at \( T^* \). Instead, the system possesses a simple GC at that temperature, and a first order transition is exhibited. Conversely, if the system undergoes a second order transition then for some \( q < q_* \) and some \( 0 < \delta \leq 2\rho \) there exist an exponential family \( \mu \) such that

\[ \mu/q^\delta > 1 . \]
\( \langle E \rangle - TS \), where the entropy is bounded by \( N \ln q \), and the mean energy is approximated by \( \langle E \rangle \approx -\partial N p_s \) where \( \partial N \) is the total number of faces of the small clusters and

\[
p_s = \frac{q e^K}{q e^K + q^\ell - q}, \tag{8}
\]

is the probability for a single face to be monochromatic with \( \ell = 2\rho + 2 \) being the number of spins in an interaction (e.g., \( \ell = 6 \) for the honeycomb lattice). In evaluating \( \langle E \rangle \) one can consider additional terms accounting also for monochromatic pairs of faces etc. However, these can be seen to give smaller contributions. Adding \( \langle E \rangle \), where \( p_s \) is computed at \( T^* \), or, at \( c^K = q^\ell \), to the RHS of (5) results (assuming \( \partial N = k \)) in the approximated first order critical temperature

\[
T_c \approx \frac{1 - p_s}{\rho \ln q} \sim T^* - \frac{1}{q^{\rho+1}}. \tag{9}
\]

In App. A it is shown that the exact first order transition critical temperature is

\[
T_c = \frac{1}{\ln(q^\rho + 1)}. \tag{10}
\]

Indeed, \( |T^* - T_c| \geq q^{-\rho-1} \) already for small \( q \).

We focus now on the honeycomb lattice since for this lattice only “pure” animals survive (there are no beasts made of animals with joint nodes). Consider a simply connected animal. Let \( n_1, n_2 \) and \( n_3 \) be the number of sites belonging to one, two and three faces, respectively. The total number of boundary sites is \( b \). A simple counting gives

\[
\begin{align*}
n_1 + 2n_2 + 3n_3 &= 6k, \\
n_1 + n_2 + n_3 &= m, \\
n_1 + n_2 &= b.
\end{align*} \tag{11}
\]

One can easily verify that the minimal asymptotic number of sites per face is \( \rho = 2 \). Expressing \( b/k \) and \( \delta + o(1) = m/k - 2 \) in terms of \( n_1, n_2, n_3 \) and noticing that \( n_1 = n_2 + 6 \) \cite{25} result in

\[
b/k \leq 2\delta + o(1). \tag{12}
\]

It is known \cite{26,27} that the connective constant of self-avoiding walks (SAW) on the honeycomb lattice is \( \mu_c = \sqrt{2 + \sqrt{2}} \). The exponential number of animals of size \( k \) in a family with a growth constant \( \mu \) is bounded by the number of SAW of length \( b = \text{sup}_{n_1} b \), i.e., \( \mu^k \leq \mu_c^b \). With the help of (12) we thus obtain

\[
\mu \leq \mu_c^{2\delta + o(1)}. \tag{13}
\]

Combining (6) and (13) together it follows that \( q_s \leq \mu_c^2 \approx 3.4 \). Consequently, the system undergoes a first order transition for \( q > 3 \).

Indeed, our simulations indicate that a first order transition already occurs at \( q = 3 \). Under a few plausible assumptions, this result can be analytically derived. First, define a snake to be an animal with boundary sites only, such that any of its faces (excluding the head and the tail) has two neighboring faces. Next, consider constrained SAW tracing animals in a way that allows these animals to share three edges at most with any face of the appropriate walks. Consider all the faces with edges mutual to a given constrained walk and placed, say, to its left. It may occur that these faces construct a snake. Conversely, the single side boundary of any snake can be traced by a trajectory overlapping with no more than three edges per face. Thus, the number of snakes \cite{28} is no larger than the number of constrained walks. Noticing that snakes are animals associated with (maximal) \( \delta = 2 \), we may write

\[
\mu \leq \mu_c^{\epsilon \delta/2}, \quad \delta \approx 2, \tag{14}
\]

with \( \epsilon \leq 3 \). Assuming that (6) is governed by quasi-snakes satisfying (14) and substituting \( q_s = 3 \) in (14) imply \( q_s < 3 \) hence a first order transition for \( q \geq 3 \).

\[
\text{FIG. 1. Energy pseudo-critical PDF and FSS of related observables for the honeycomb lattice. The PDF (computed for } L = 45) \text{, FSS of the specific heat maxima and FSS of the specific heat per site maxima are presented from left to right, respectively. The quantities described above are associated (from top to bottom) with } q = 4, 3, 2. \text{ The red symbols in } (h),(i) \text{ represent the large sample } (L = 75) \text{ Metropolis based observables.}
\]

\[
\text{III. MONTE CARLO SIMULATIONS}
\]

In order to numerically support our predictions for the honeycomb lattice and to estimate \( q_s \) for the triangular lattice, we perform Monte-Carlo simulations using the Wang-Landau \cite{21} entropic sampling method. According to this method one hops between successive spin configurations with energies \( E_i \) and \( E_j \), respectively, with a transition probability \( T_{i \to j} = \min\{1, \Omega(E_i)/\Omega(E_j)\} \) where \( \Omega(E_i) \) is an approximation to the density of states with
energy $E_i$. At each visit to a state with energy $E_i$ the corresponding quantity $\ln \Omega(E_i)$ is modified. We use lattices with linear sizes $4 \leq L \leq 60$ and periodic boundary conditions are imposed. First, we measure for each $L$ the specific heat maximum $C^\text{max}_L$ and perform finite size scaling (FSS) analysis to these quantities. The location (temperature, $T_L$) of $C^\text{max}_L$ serves as a definition to the pseudo-critical transition point. Next, the pseudo-critical energy probability-distribution-function at $T_L$ (PDF) is computed. The shape of the PDF can roughly distinguish between second and first order transitions. While for the continuous transition it is expected that the PDF will be single peaked, a double peaked shape is conventional in the discontinuous case [20].

We start with the honeycomb lattice, focusing on $q = 2, 3, 4$. In Fig. 1 we display the PDF for the three models. For $q = 3, 4$ we fit the specific heat maxima $C^\text{max}_L$ with a power-law $C^\text{max}_L \sim L^q$. In order to prune out finite size effects and systematically detect the FSS of large samples, we consider the maxima of the specific heat per site $C^\text{max}_L / N = L^q$ and fit this observable with a power-law $C^\text{max}_L / N \sim L^{-\nu}$ where $\nu = d - \gamma$. Fig. 1(a) shows the PDF at $q = 4$ which displays a strong first-order performance for a rather small sample ($L = 45$). In Fig. 1(b) $C^\text{max}_L \sim L^2$ apparently obey the expected first order $C^\text{max}_L \approx L^d$ scaling law, suggesting that we use sample sizes $L$ comparable with the correlation length. The first order nature is supported by a slowly varying $C^\text{max}_L / N$ (Fig. 1(c)), indicating an expected first order asymptotic non-vanishing behavior. Continuing with $q = 3$ and Fig. 1(d), the typical pronounced double peaked scenario for the PDF is clearly observed, although this quantity apparently suffers from finite size effects, depicted mainly in the width of the peaks. Fitting $C^\text{max}_L$ with $L^2$ as shown in Fig. 1(f), provides an indication for a first order behavior in the case of $q = 3$. Similarly to the $q = 4$ model, the nice fit with a zero-slope straight line observed in Fig. 1(f), suggests for an expected first order asymptotic constant term. The picture is substantially different for $q = 2$. Unlike the dual peak shape characterizing the PDF of the former two models, the current model shows (Fig. 1(g)) a pronounced single peak, indicating a continuous transition. Motivated by this qualitative difference it seems natural to expect for an Ising-like behavior when $q = 2$, i.e., a logarithmic divergence of the specific heat, as captured by Fig. 1(h). Finally, as seen in Fig. 1(i), the pseudo-singularity of the specific heat per site decays with $L$, as expected from second order systems. Furthermore, the rapid decay hints that the $L^{-d}$ Ising scenario is likely to take place for larger samples.

In order to better understand the Ising-like nature of the $q = 2$ model we employ the Metropolis [29] method to calculate $C^\text{max}_L$ and $C^\text{max}_L / N$, using the energy histogram of a sample with $L = 75$. The associated temperature $T_L = 0.6549$ is extrapolated by fitting the WL data with the Ising form $[T_L - T^*] \propto L^{-1}$ where $T_c = 0.6596$ ($L_{\text{min}} = 11$, $x^2$/d.o.f. = 0.04/12, $p$ value = $4 \times 10^{-6}$ [19, 30]). Indeed, as evident from Figs. 1(h),1(i), the FSS based on the WL simulations is preserved. Further analyses of Metropolis simulations on large scale and WL-based energy-dependent observables are provided in App. B.

The counting argument (11) can be generalized to the square and triangular lattices (see App. C). Moreover, it can be shown that (12) holds for these two lattices as well. It follows that since (6) is governed by a family $\mu$ most likely dominated by large animals such that (13) is valid, applying the large connective constant of SAW on the triangular lattice $\mu_c \approx 4.15$ [31] to (13) opens a door to $q_c > 4$. Our next goal is therefore to estimate $q_c$ for the triangular lattice. To this end, we find it plausible to initially take $q = 4$. Indeed, as evident from Fig. 2(a), the PDF has two humps with a small dip between them. However, it is likely to be a finite size effect (see, e.g., Ref. [32]), that eventually vanishes in the large $L$ limit. Figs. 2(b)(c), suggest that the triangular lattice round-the-face interaction $q = 4$ model is in the universality class of the standard $q = 4$ square lattice model. For $q = 5$ the PDF is plotted in Fig. 2(d). Although two peaks are ob-

![FIG. 2. Energy pseudo-critical PDF and FSS of related observables for the triangular lattice. The PDF (computed for $L = 45$), FSS of the specific heat maxima and FSS of the specific heat per site maxima are displayed from left to right, respectively. The quantities described above are associated (from top to bottom) with $q = 4, 5, 6$.](image-url)
the $q = 6$ triangular lattice model undergoes a discontinuous transition.

Our conclusion from the above analysis of the round-the-face interaction model on the triangular lattice is that $q_c = 5$ is plausibly numerically supported for this model.

### IV. CONCLUSIONS

The changeover phenomenon in local-interaction ferromagnetic Potts models is studied. The close link between the round-the-face interaction Potts model and two-dimensional lattice animals, applied to the honeycomb lattice, together with Monte-Carlo simulations, is used to derive $q_c \leq 3$. Our approach can be generalized to other lattices. For instance, when applied to the triangular lattice, it leaves room for $q_c > 4$. Indeed, simulations performed for this lattice provide evidences that $q_c = 5$. An acceptable theory to clarify this result is left for a future study.

Our results for $q_c$, in particular that of the honeycomb lattice, stand in contrast to the well known result $q_c = 4$ of the usual model [4, 5, 7, 8].

Thus, first, by demonstrating on a natural local-interaction model a changeover phenomenon at a critical value $q_c \neq 4$, we provide a deeper insight on this problem strengthening the realization that $q_c = 4$ being universal is a false statement [15–18]. Second, our analytical and numerical analyses propose that the RG framework of Ref. [12] assuming a single multicritical point, does not capture a changeover phenomenon in multiple models. In other words, our study suggests that there may be multiple multicritical points were critical and tricritical branches terminate, keeping the thermal and ordering field relevant and the dilution field marginal at these points. Equivalently, our work may push the boundaries of the conventional ordering field, temperature, dilution picture [6, 12, 33], such that a new scaling field allowing for the variation of $q_c$ is introduced.

### Appendix A: The exact first order transition critical temperature

In the following we show that

$$T_c = \frac{1}{\ln(q^\rho + 1)}. \quad (A1)$$

In general, one can write the partition function as a sum $Z = Z_g + Z_s$ where $Z_g, Z_s$ are associated with the GC and with “small” clusters, respectively. Introducing the variables $f(G) = k$, $\nu(G) = m$ and taking $c(G) = 1$ in (3), $Z_g$ can be written as

$$Z_g \propto q^N \sum_{m} b_{km} q^{-m} v^k \times \text{(perimeter terms)} \quad (A2)$$

Since the number of simple beasts $\sum m b_{km}$ is subexponential, $Z_g$ is governed by the single beast exponential terms, i.e., $Z_g \sim q^{N-m} v^k$.

The partition function of the small (of size $o(N)$) clusters is governed by

$$Z_s \sim \Lambda(t)^k q^{N+\alpha_k(t)k-\zeta_k(t)k}(1-1/q)^{\delta_k(t)k} v^k, \quad (A3)$$

where $t$ is a graph with a total number of $k$ faces. The number of clusters and sites per faces is denoted by $\alpha_k(t)$ and $\zeta_k(t)$, respectively. The variable $\theta_k(t)$ corresponds to a fraction of the total number of perimeter sites per face. The number of ways placing the small clusters in the lattice is $\Lambda(t)^k \leq 2^k$. Note that the leading order term of (A3) refers to finite clusters, whereas $k$-dependent-size clusters (e.g., $\sqrt{k}$ clusters of size $\sqrt{k}$) may result in higher order contributions such that typically, terms of the form $q^k$ are absent. Taking $m = \rho k + o(N)$ and introducing the variables $k^* = k^*(N)$, $\alpha_{k^*}$, $\zeta_{k^*}$, $\theta_{k^*}$ [34] and $\Lambda$ that maximize (A2),(A3) we can write

$$Z_{\max} = \max_{k, \rho} \{Z_g + Z_s\} = q^N (vq^{\rho})^{k^*} \times \left\{ 1 + \left[ \frac{\Lambda(1-1/q)^{\theta_{k^*} k^*}}{q^{\zeta_{k^*}-\alpha_{k^*} k^*}} \right]^{k^*} \right\}. \quad (A4)$$

It follows that the free energy density is

$$\phi = -T \ln \lim_{N \to \infty} Z_{\max}^{1/N} \quad (A5)$$

$$= \left\{ \begin{array}{ll}
-\ln q - T \kappa \ln(vq^{\rho}) & , v > q^\rho \\
-\ln q & , v \leq q^\rho, 
\end{array} \right.$$ 

where $\kappa = \lim_{N \to \infty} k^*/N$, if and only if

$$\zeta_{k^*} - \alpha_{k^*} \geq \rho. \quad (A6)$$

The critical point

$$v_c = q^\rho, \quad (A7)$$

is determined to be the point at which $\phi$ is non-differentiable. Eq. (A1) is the critical temperature associated with (A7).

It remains to prove (A6). In general one can express $\zeta_{k^*} - \alpha_{k^*}$ as a finite sum

$$\zeta_{k^*} - \alpha_{k^*} = \sum_j c_j (\eta_j - 1/j) \quad (A8)$$

where $\eta_j$ is the number of sites per face and $1/j$ is the number of clusters per face, when dividing a total number of $k^*$ faces into small clusters of size $j$ each. The fractions $c_j$ sum up to unity. For instance, for the “trivial” single-faces partition $\alpha_k = j = c_1 = 1$, $\zeta_{k^*} = \eta_1 = 2\rho + 2$ and so $\zeta_{k^*} - \alpha_{k^*} = 2\rho + 1$. 


Now comes the crucial point: it is assumed that the finite small clusters, typically with boundaries minimal in size, are "homogeneous enough", such that

$$ (j + 1)\eta_{j+1} \geq j\eta_j + g(\rho) , $$

where

$$ g(\rho) = \begin{cases} 
2\rho & \text{if } \rho = \frac{1}{3} , \\
2\rho - 1 & \text{if } \rho = \frac{1}{2}, \frac{2}{3} [35] . 
\end{cases} $$

This assumption guaranties that the entropy loss due to the presence of small clusters in general (not necessarily finite) is minimal. By "homogeneous enough" we mean that the mean number of sites per face $\langle \eta_j \rangle$ may be slightly different than $\eta_j$ in the marginal case where all the clusters of size $j$ have the same shape and Eq. (A9) trivially holds. With the help of (A9) it can be easily shown that

$$ \eta_j \geq \rho + \frac{1}{j} , $$

for all $j \geq 1$ (finite). Eq. (A6) now immediately follows.

**Appendix B: Energy-dependent observables and magnetization**

We discuss additional numerical manifestations of the occurrence and nature of phase transitions on the honeycomb lattice. Some of them are remarkably captured by the specific heat and internal energy which are closely related to the first and second moments of the energy PDF. The specific heat per spin is given by

$$ c_L = L^d \beta^2 (\langle x^2 \rangle - \langle x \rangle^2) , $$

and the internal energy is $\langle \epsilon \rangle$. The thermal averages $\langle ... \rangle$ are taken with respect to the PDF [36]

$$ p_L(\epsilon) \propto g_L(\epsilon)e^{-L^q\epsilon} , $$

and $g_L(\epsilon)$ is the density of states with energy $\epsilon$. Plots of the two observables are given in Fig. A.1. Fig. A.1(a) shows the variation of the specific heat with temperature. While a clear sharp and narrow peak is observed at $q = 3$ and $q = 4$ (first order), a broad, two order of magnitude smaller (essentially hardly seen on a uniform scale) peak, is seen when $q = 2$. The latter scenario is indeed typical to second order transitions where large energy fluctuations are present on a relatively large energy scale.

In Fig. A.1(b) we plot the internal energy against the temperature. A latent heat proportional to the ground state energy (per spin) of one-half, is evident for $q = 3, 4$. In the Ising-like case of $q = 2$, however, the internal energy is a moderate monotonically increasing function of the temperature. Note also the nice proximity of the positions of both the peak and the jump in energy, to the approximated critical temperature $T_c \approx 1/\ln(q^d + 1)$ ($\rho = 2$) for $q = 3$ and, in particular, for $q = 4$.

Another observable which presents a typical first order behavior when computed for the $q = 4$ model is the magnetization at time (Monte-Carlo sweep) $t$, given by

$$ m(t) = \frac{x(t) - 1}{q - 1} , $$

where $x(t)$ is the maximal fraction of spins which are simultaneously at the same Potts state. Indeed, since $q^{-1} \leq x(t) \leq 1$, (B3) implies that $0 \leq m(t) \leq 1$. We employ the Metropolis method to measure the magnetization (B3). We also simulate the energy density according to (1) in the main text.

In Fig. A.2(a) we plot the magnetization for a large sample ($L = 100$) in the vicinity of $T^*$ for $q = 4$. Note that $T^* - T_c = (\ln 16)^{-1} - (\ln 17)^{-1} \approx 0.008$ so that the observed metastability at $T^* - \epsilon_1$ reasonably agrees with the expected metastability at $T_L \approx T^* - \epsilon_1 \approx T_c$ satisfying the usual first order relation $|T_e - T_L| \propto L^{-d}$. When distorted in $\epsilon_2 > \epsilon_1$ below (above) $T^*$, or, at temperatures smaller (larger) than $T_c$, the system rapidly relaxes to the ordered (disordered) state, respectively. Since relaxation times for large samples, when approaching $T_c$, are extremely long, we additionally simulate a small sample ($L = 20$) near $T_c$ and plot the time dependent magnetization and energy density, in Fig. A.2(b) and Fig. A.2(c). As clearly observed in these figures, the large fluctuations enable the system to visit coexisting states in a reasonable time.
FIG. A.2. Magnetization and energy density against time for the \( q = 4 \) model on the honeycomb lattice, simulated in the vicinity of \( T^* = (2 \ln 4)^{-1} \). Two different samples with \( L = 100 \) and \( L = 20 \) are used. We let the system equilibrate starting from a totally ordered configuration, and translate the time frame by the equilibration time \( t_0 \). (a) \( L = 100, t_0 = 2000, \epsilon_1 = 0.001, \epsilon_2 = 0.01 \) (b) \( L = 20, t_0 = 1000, T = T^* - 0.025 \) (c) \( L = 20, t_0 = 1000, T = T^* - 0.025 \).

Appendix C: Eq. (10) is lattice independent

We generalize Eq. (12)

\[
\frac{b}{k} \leq 2\delta + o(1) , \tag{C1}
\]

obtained for the honeycomb lattice, to the triangular and square lattices. The notations \( k, m \) and \( b \) refer to the number of faces, sites and boundary sites, respectively, of an arbitrary beast. The derivations are valid for simply connected beasts.

\( a. \) The triangular lattice

The total number of sites of any cluster on the triangular lattice can be decomposed into (non-zero) numbers \( n_1, n_2, n_3, n_4, n_6 \) of sites belonging to one, two, three, four, six faces, respectively (it is impossible to uniformly colour five faces with a joint vertex, as the face-interaction imposes that the sixth face sharing that vertex will have the same colour. Therefore \( n_5 = 0 \)). Similarly to (10) in the main text we write

\[
\begin{align*}
n_1 + 2n_2 + 3n_3 + 4n_4 + 6n_6 &= 3k , \\
n_1 + n_2 + n_3 + n_4 + n_6 &= m , \\
n_1 + n_2 + n_3 + n_4 &= b . \tag{C2}
\end{align*}
\]

Noticing that the minimal asymptotic number of sites per face on the triangular lattice is \( \rho = 1/2 \) and expressing \( b/k \) and \( \delta + o(1) = m/k - 1/2 \) in terms of \( n_1, \ldots, n_6 \), we have that (C1) immediately follows if and only if

\[
2n_1 + n_2 \geq n_4 . \tag{C3}
\]

In order to prove (C3) we first consider a single animal \( a \). We notice that one gains a total curvature of \( 2\pi \) when travelling in six different directions along the animal’s perimeter. This is achieved by crossing \( n_{1a}, n_{2a} \) and \( n_{4a} \) of sites per face for \( 2\pi/3, \pi/3 \) and \(-\pi/3\), respectively. We thus have

\[
2n_{1a} + n_{2a} - n_{4a} = 6 . \tag{C4}
\]

We next observe that a simply connected beast is essentially made of \( s \) animals interacting via \( s - 1 \) vertices. Thus, the total number of sites of the beast, belonging to one, two and four faces is

\[
\begin{align*}
n_1 &= \sum_a n_{1a} - 2s + 2 , \\
n_2 &= \sum_a n_{2a} + s - 1 , \\
n_4 &= \sum_a n_{4a} , \tag{C5}
\end{align*}
\]

respectively. Summing over (C4) and using (C5) lead to

\[
2n_1 + n_2 - n_4 = 3s + 3 , \tag{C6}
\]

which completes the proof.

\( b. \) The square lattice

Let \( n_1, n_2, n_3 \) and \( n_4 \) be the number of sites belonging to one, two, three and four faces, respectively, of a given cluster on the square lattice. Then

\[
\begin{align*}
n_1 + 2n_2 + 3n_3 + 4n_4 &= 4k , \\
n_1 + n_2 + n_3 + n_4 &= m , \\
n_1 + n_2 + n_3 &= b . \tag{C7}
\end{align*}
\]

On the square lattice there are \( \rho = 1 \) sites per face for simple large clusters. Writing \( \delta + o(1) = m/k - 1 \) and \( b/k \) by means of \( n_1, \ldots, n_4 \) results in (C1), iff

\[
n_1 \geq n_3 \tag{C8}
\]

holds. To prove (C8) we, again, first consider a single animal \( a \). We see that any vertex on its perimeter with a non-zero curvature, belongs either to a single face or to three faces. A vertex of each type contributes \( \pi/2 \) and \(-\pi/2\), respectively, to the total curvature of \( 2\pi \). Thus,

\[
n_{1a} - n_{3a} = 4 . \tag{C9}
\]

Next we consider a simply connected beast which can be decomposed into \( s \) animals. Employing procedures
similar to those described for the triangular lattice, we wind up with

\[ n_1 - n_3 = 2s + 2, \quad \text{(C10)} \]

which completes the proof.

As a final remark we point out that since

\[ q_s = \sup_{\delta} \mu^{1/\delta} \quad \text{(C11)} \]

is governed by a family \( \mu \) composed of beasts that most likely have large “animal” components, the number of such beasts is bounded by the number of SAW proportional to the perimeter of these components. Denoting by \( \mu_c \) the connective constant of SAW on any lattice (triangular, square or honeycomb), we have that

\[ q_s \leq \mu_c^2 \quad \text{(C12)} \]

is lattice independent. Eq. (C12) suggests that the changeover in the transition order is a universal property of the face-interaction Potts model.

[25] Travelling along the perimeter, every \( n_1 \) vertex contributes a curvature of \( \pi/3 \) and every \( n_2 \) vertex contributes a negative curvature \( -\pi/3 \). Since the total curvature is \( 2\pi \), we have that \( n_1 \equiv n_2 \equiv 6 \).
[28] Other animals with \( n_3 = 0 \) containing junctions, each branches into three snakes, can be treated as if they were solely snakes, provided the number of junctions is \( o(k) \).
[34] For simplicity, it is assumed that \( Z_q \) is simultaneously maximized by the face variable \( k^* \).
[35] For example, adding a single face to a cluster on the square lattice increases the number of sites in that cluster at least by \( 2 \times 1 - 1 = 1 \).
[36] In practice we calculate moments of the distribution associated with \( \Omega(E) \), \( \sum_{E} k^{a} e^{-\beta E_k} \), with \( E = L^d \epsilon \), and rescale them properly.
[37] The quantities \( n_{1a}, n_{2a}, n_{3a} \) correspond to the number of sites of animal \( a \) belonging to one, two and four faces, respectively.