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Phase transition of a two-dimensional, multiplicatively coupled XY –Potts model

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Abstract

We investigate the phase transition of a combination of a two-dimensional Potts and an XY model where the coupling is multiplicative. As the XY model has a Kosterlitz–Thouless transition and the Potts variable is constrained to three states (yielding a second order transition), the order of the phase transition and the universality class of the investigated combined model are far from obvious. We find that the transition is shifted to a lower critical temperature while the course of the internal energy is steeper compared to the two constituting models. Still, we find strong indications that the transition is continuous. Our model may serve as a coarse-grained description of surface-attached flexible polymers, e.g. in the context of the extracellular matrix of living cells.

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1. Introduction

Large systems of interacting polymers pose a significant challenge to computational approaches. While one may study with standard Monte Carlo techniques the properties of single polymers in detail (Binder 1996), larger systems are computationally challenging due to their massive increase in the autocorrelation times. Hence, more coarse-grained approaches, e.g. a coupling of well-known models of statistical mechanics, are helpful in elucidating the phase behavior of such complex systems. The phase behavior of coupled models on the other hand is also very interesting from a fundamental point of view, since they may belong to another universality class than the constituting models.

Following this rationale, we defined a new statistical model by multiplicatively coupling the two-dimensional XY model to the 3-state Potts model. This choice is motivated by the

wish to understand the phase behavior of an array of interacting, surface-attached flexible polymer backbones with single rigid side chains (Hellmann *et al* 2007), i.e. a minimal model for the extracellular matrix of living cells. Here, the Potts degree of freedom may reflect the height levels of the polymer backbones while the XY degree may describe the orientation of the side chains. While the Potts model (with $q < 4$ states) undergoes a second-order phase transition (Baxter 1973), the two-dimensional XY model shows a Kosterlitz–Thouless transition (Kosterlitz and Thouless 1973). It is hence far from evident what kind of phase transition will be encountered when multiplicatively coupling these two systems.

One way to approach the problem is to restrict the XY model to a pure two-state (Ising-like) system and then (perturbatively) couple the 3-state Potts model to it. Due to the Ising-nature of the unperturbed system, the resulting 6-state model should have a first-order phase transition. However, taking the Potts model as the unperturbed system, the XY model can be viewed to introduce annealed disorder to the Potts coupling constant which may result in a first-order transition. In general, introducing quenched disorder to systems with a continuous phase transition modifies the critical behavior and also the universality class (Harris 1974, Aharony 1978, Grinstein and Ma 1982, Berker 1984). It has also been suggested that a first-order phase transition can change to second order due to the introduction of quenched disorder (Berker and Hui 1991). Yet, little is known for the case of annealed disorder (which would be the appropriate view in our case). An interesting study in this respect deals with the coupled XY –Ising model (Granato *et al* 1991, Lee *et al* 1991) that shares some features with the system we present here. Computer simulations uncovered a second-order phase transition with critical exponents distinct from the Ising ones. Microscopically, XY disorder is driven by Ising disorder.

Bearing this in mind, the coupled Potts– XY model deserves a close investigation apart from its hypothetical application as a coarse-grained model for the extracellular matrix: it is a random bond model with annealed disorder while, so far, the quenched case has been in the focus (Wu 1982). The nature of its phase transition is far from obvious as it combines a discrete and a continuous degree of freedom both showing different phase behaviors. Basic simulations of a 3-state Potts model coupled to the XY model show that the transition is much steeper and shifted to a lower temperature compared to the two constituting models. However, in a more thorough analysis we find strong indications for a continuous transition and not for a finite jump in the internal energy. The critical exponents γ/ν and $1/\nu$ which we obtain are clearly distinct from those of the genuine Potts model, hence implying a change of the universality class.

2. Model

We start by motivating the construction of our Potts– XY model via a system of surface-attached flexible polymers with a rigid side chain. Such a system forms, for example, the gross structure of the extracellular matrix of living cells. As described previously (Hellmann *et al* 2007), the basic unit of such an extracellular matrix may be reduced to a single flexible, end-grafted backbone with a rigid side chain (figure 1). While a simulation of this unit yields valuable insights into the stiffening of the individual backbone due to the attached rigid side chain (also considered in other studies, as e.g. (Connolly *et al* 2005)), this amount of detailed information may not be necessary to understand the generic behavior of the multi-complex system. The basic quantities describing the interaction of many individual units are the height p of the side chain above the substrate and its orientation θ (with respect to the y -axis). Thus, the individual backbone side-chain complexes are interpreted as mutually interacting rotors aligned on a regular two-dimensional lattice.

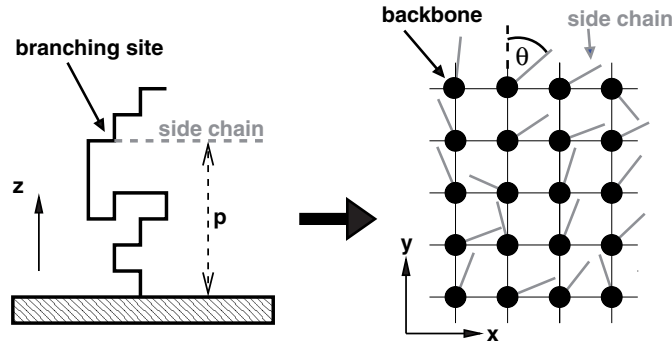


Figure 1. On the left the model for the self-avoiding backbone side chain complex as described in Hellmann *et al* (2007). To study a system of mutually interacting complexes another coarse-graining step is taken, leading to a system of rotors on a two-dimensional lattice. The internal degrees of freedom of each complex are reduced to the height p of the side chain above the substrate and its orientation angle θ .

We assume here that the sites at which the backbones are attached to the substrate are sufficiently far apart from each other so that any interaction between the complexes is mediated by the side chains only. This also necessitates that side chains only interact when they have the same height p . This aspect can be modeled by a Potts-type interaction (Potts 1952, Wu 1982):

$$\mathcal{H}_P = -J_P \sum_{\langle i, j \rangle} \delta_{p_i p_j}; \quad p_i \in \{0, 1, \dots, q-1\}. \quad (1)$$

Here, p_i denotes the height of the side chain i above the substrate, q is the total number of allowed heights, and $J_P > 0$ is the coupling constant.

The interaction between side chains having equal p will be considered as a nearest-neighbor ferromagnetic interaction leading to a preferred parallel alignment of the side chains. This kind of interaction seems plausible as a first approach since it mimics the repulsive forces between side chains that may be due to steric or short-ranged electrostatic potentials. Consequently, we use for this part of the interaction the two-dimensional XY model Hamiltonian

$$\mathcal{H}_{XY} = -J_{XY} \sum_{\langle i, j \rangle} \mathbf{S}_i \mathbf{S}_j = -J_{XY} \sum_{\langle i, j \rangle} S_i S_j \cos \theta_{ij}, \quad (2)$$

where the coupling constant $J_{XY} > 0$ and $\langle i, j \rangle$ denotes a summation over nearest neighbors. For simplicity, the length of the rotors (= side chains) $S_i = |\mathbf{S}_i|$ is set to unity while the angle θ_{ij} denotes the relative orientation of the side chains i and j .

Combining the above model equations (1) and (2) yields the Potts- XY model:

$$\mathcal{H} = -J \sum_{\langle i, j \rangle} \delta_{p_i p_j} \cdot \cos \theta_{ij}; \quad p_i \in \{0, 1, \dots, q-1\}. \quad (3)$$

The two-dimensional Potts model is known to undergo a second-order phase transition for $q < 4$ (Baxter 1973) while the XY model experiences a Kosterlitz-Thouless (KT) transition (Kosterlitz and Thouless 1973, Kosterlitz 1974). For $q = 3$ our model equation (3) can be interpreted as a 3-state Potts model with a randomly varying coupling strength $J_{ij} = J \cos \theta_{ij}$ between neighboring Potts spins i and j . As this local coupling may become very small and even zero, the nature of the phase transition of the hybrid model may be characterized by

effectively vacant bonds that are known to drive the transition of the ($q < 4$)-state Potts model toward first order (Nienhuis *et al* 1979). Given this variety of phase behaviors, it appears difficult to make predictions with respect to the coupled Potts– XY model *a priori*.

A system closely related to the model presented here is the coupled XY –Ising model that has been studied previously (Granato *et al* 1991, Lee *et al* 1991). The central result was that the Ising disorder induces disorder in the XY degrees of freedom. It is tempting to speculate that this feature is also present in the Potts– XY model studied here since the special coupling between the discrete and continuous degrees of freedom is the same. As a result, one would expect that a domain wall in the Potts variable locally decouples the XY spins, i.e. the Potts degree of freedom is supposed to be the driving factor of criticality.

3. Simulation method

For simulations of the hybrid model equation (3), we relied on the Monte Carlo (MC) method (see, e.g., Binder and Heermann (2002) for an introduction). The first preliminary simulations were based on the Metropolis MC algorithm (Metropolis *et al* 1953). In each step, a change of the Potts level (height) as well as a rotation of the rotor (side chain) by some angle $\Delta\theta$ were proposed and this combined move was accepted or rejected according to the Metropolis criterion.

Close to the critical temperature, the standard Metropolis MC suffers from critical slowing down, i.e. it becomes difficult to generate enough statistically independent configurations for a reliable statistics as autocorrelation times increase. To overcome this problem, we used a cluster MC approach (Swendson and Wang 1987), in particular a modification of Wolff’s cluster algorithm (Wolff 1989). Here, one deals with two degrees of freedom, one discrete (Potts state p) and one continuous (orientation angle θ). Thus, two different kinds of clusters are grown and flipped in each step—one with respect to p (embedded in an ensemble of fixed θ_i ’s) and the other with respect to θ (embedded in an ensemble of fixed p_i ’s).

The treatment of the Potts degree of freedom has to be carried out carefully as ferromagnetic and anti-ferromagnetic bonds can occur between neighboring rotors. In the beginning, a pair of values for p is chosen randomly, i.e. (0,1), (0,2), or (1,2), respectively. Rotors in the remaining Potts state are considered as vacancies in the ongoing cluster growing step. The effective (local) coupling between rotors i and j is $K_{\text{eff}} = J \cdot \cos \theta_{i,j}$. For $K_{\text{eff}} > 0$ an ferromagnetic bond is established with probability $P = 1 - \exp(-K_{\text{eff}} \delta_{p_i=p_j})$ between rotors on the same Potts level. If $K_{\text{eff}} < 0$, an anti-ferromagnetic bond is formed with probability $P = 1 - \exp(K_{\text{eff}} \delta_{p_i \neq p_j})$ between rotors on different Potts levels. When the cluster is grown, all Potts levels of the constituting rotors are switched according to the initially chosen pair of p -values (e.g., $0 \leftrightarrow 1$).

Following Wolff’s embedding trick for growing and flipping clusters in the XY model (Wolff 1989) the rotors are projected onto the x -axis. This results in an Ising model of the x -components S_i^x with random couplings. These ‘effective’ spins are connected by a bond with probability $P = 1 - \exp(\delta_{p_i, p_j} \cdot \min[0, 2K \cdot S_i^x \cdot S_j^x])$. Note that the Potts states of the rotors are accounted for by δ_{p_i, p_j} meaning that bonds are only formed between rotors in the same Potts state. Finally, when the cluster is grown, all x -components of the constituting rotors are inverted.

4. Results

To study the thermodynamic properties of the Potts– XY model (equation (3)) with $q = 3$ we conducted extensive MC simulations. The linear system size L (L^2 is the total number of

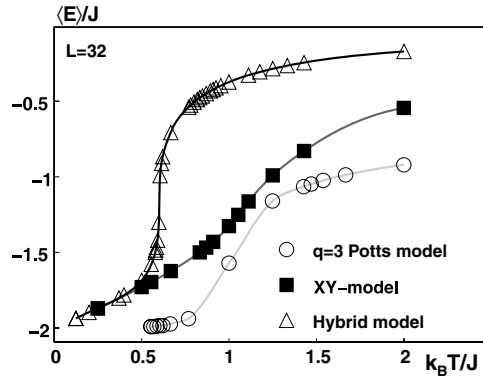


Figure 2. Mean value of the internal energy $\langle E \rangle$ as a function of temperature T (in natural units) for the pure 3-state Potts model (equation (1)); the pure XY model (equation (2)), and the Potts–XY model (equation (3)). Numerical data obtained by Metropolis Monte Carlo are shown with symbols, the full lines are guides to the eye. The critical temperature T_c of the Potts–XY model is shifted to a lower value as compared to the pure models; also an increased slope in the transition region is observed. For low temperatures, the behavior of the XY model is reproduced.

rotors) was varied in a wide range ($16 \leq L \leq 512$) in order to apply a finite size scaling analysis (Binder and Heermann 2002).

We studied three observables as a function of the interaction strength K between the spins and the lateral system size L : The internal energy per spin

$$E = \frac{1}{2L^2} \sum_i \mathcal{H}(i), \tag{4}$$

the squared XY magnetization

$$m_{XY}^2 = \frac{(\sum_i m_x^i)^2 + (\sum_i m_y^i)^2}{L^4}, \tag{5}$$

and the squared Potts order parameter

$$m_p^2 = \frac{(n_0 - n_1)^2 + (n_0 - n_2)^2 + (n_1 - n_2)^2}{2L^4}.$$

Here, m_x^i and m_y^i denote the components of the XY spin with index i , while n_p counts the number of spins in Potts state p . It is convenient to sample the squared magnetizations as symmetry provides $\langle m_p \rangle = \langle m_{XY} \rangle = 0$. In fact, we analyzed m_{XY}^2 and m_p^2 since we were unable to find a proper unified order parameter that allows one to follow the phase behavior of the combined Potts–XY model. Metropolis MC simulations of small systems revealed significant differences between the Potts–XY model and the two constituting models (figure 2). The course of the internal energy per spin, E for the Potts–XY model shows a significantly smaller transition temperature T_c as compared to the pure Potts or XY model. Furthermore, the transition region is much steeper. From these data, however, it cannot be determined if the internal energy is continuous at T_c or if there is a finite jump. If the latter was the case, the phase behavior of the Potts–XY model would be qualitatively different from that of the constituting models. A close look at figure 2 furthermore shows that for $T < T_c$ the course of E resembles essentially that of the pure XY model. Thus, the Potts degree of freedom seems to be ‘frozen’ in this regime while all excitations occur with respect to the XY-degree of freedom. For more thorough investigations on larger systems, we used the cluster algorithm

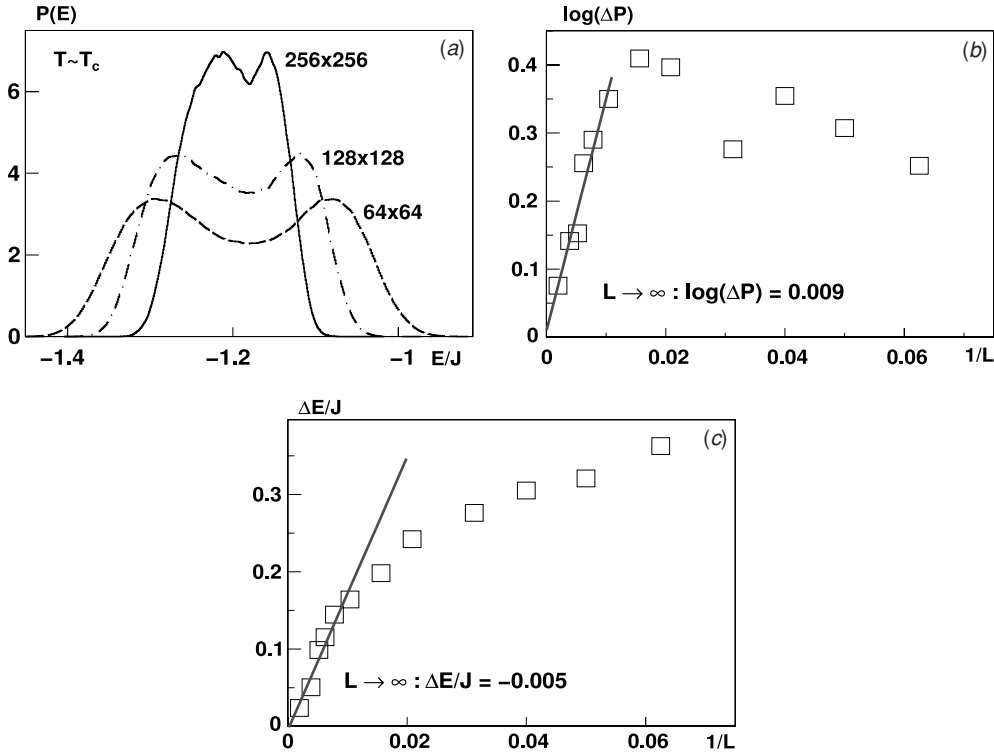


Figure 3. (a) Histogram of the internal energy E per spin at T_c for different system sizes. The double-peak structure indicates two coexisting phases. (b) The logarithm of the relative gap depth ΔP (equation (6)) in the double-peaked energy histogram decays to zero as the system size increases ($L \rightarrow \infty$). (c) Also, the energy difference ΔE between the two phases (i.e., the positions of the two peaks) appears to vanish in the thermodynamic limit. Solid lines in (b) and (c) indicate linear fits to the data for the largest system sizes.

described in the preceding section. In contrast to the standard Metropolis MC method this approach allowed us to study large systems close to T_c due to a reduced dynamic exponent. Nevertheless, the effects of critical slowing down were just reduced and not diminished. In figure 3(a), the distribution $P(E)$ of the internal energy is shown for three different system sizes at $T \approx T_c$. The distributions were obtained by *reweighting* (Ferrenberg and Swendsen 1988) of distributions close to T_c . Apparently, a double-peak structure evolves, indicating the coexistence of two phases. We considered the logarithm of the relative gap depth

$$\Delta P = P(\langle E \rangle)_{\max} / P(\langle E \rangle)_{\min} \quad (6)$$

at T_c as an indicator for the double-peak structure. This quantity furthermore provides a measure for the height of the free energy barrier between the coexisting phases. If the infinite system undergoes a first-order phase transition, this quantity grows with system size (Lee and Kosterlitz 1990, Lee and Kosterlitz 1991). In the Potts-XY model it appears, however, that the gap vanishes for $L \rightarrow \infty$ (figure 3(b)). In addition, the energy difference between the two phases, i.e. the distance of the peaks of $P(E)$, approaches zero in the thermodynamic limit (figure 3(c)). In other words, the distribution at T_c becomes actually a Gaussian, hence suggesting a second-order phase transition with a single phase existing in the system at T_c .

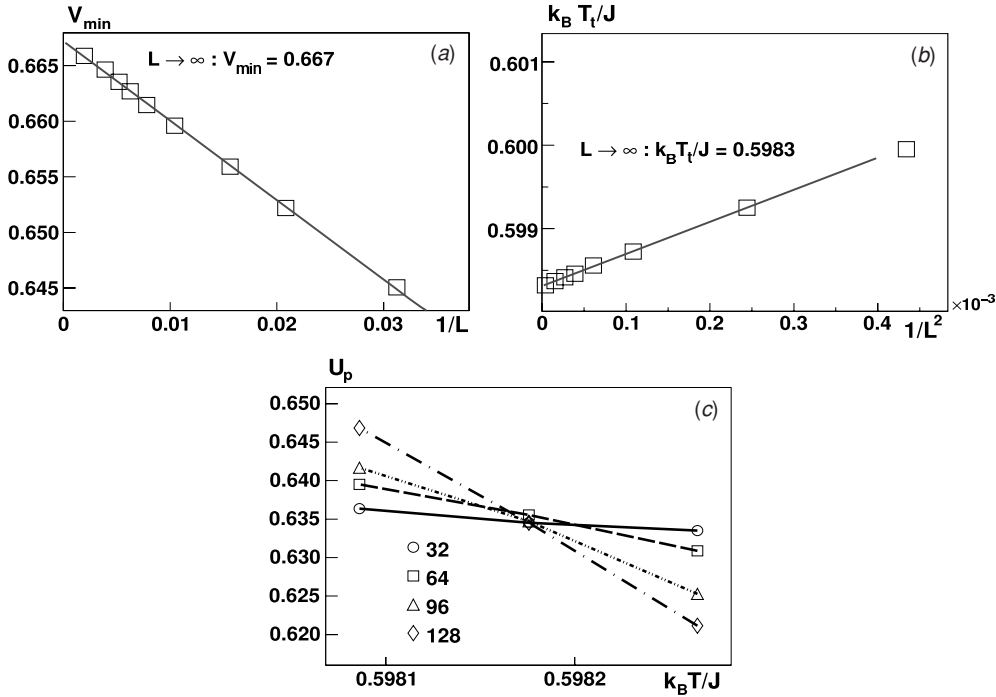


Figure 4. (a) Scaling behavior of the minimum of the cumulant of the internal energy V_{\min} (equation (7)). The cumulant V increases linearly toward an asymptotic value $V = 2/3$ for increasing system size, hence indicating a continuous phase transition. (b) The arithmetic mean of the temperatures at which the specific heat reaches its maximum and V its minimum, T_t , appears to scale with the system volume L^2 . The asymptotic value $k_B T_t / J = 0.5983$ is close to the critical temperature T_c . (c) The reduced fourth-order cumulants of the Potts order parameter for different system sizes cross at $T \approx 0.59818$ (apart from minor corrections for very small systems).

Further evidence for a second-order phase transition comes from the reduced fourth order cumulant (‘Binder cumulant’) of the energy distribution (Binder 1981)

$$V = 1 - \frac{\langle E^4 \rangle}{3 \cdot \langle E^2 \rangle^2}. \quad (7)$$

Far away from a phase transition, $P(E)$ assumes the form of a single Gaussian. In the thermodynamic limit ($L \rightarrow \infty$), this results in a δ -like singularity and hence $\langle E^4 \rangle = \langle E^2 \rangle^2$. This holds true for first- and second-order transitions (Challa *et al* 1986). So, the fourth-order cumulant takes on the (trivial) limit value $V = 2/3$. Distributions with a double-peak structure are characterized by $V \neq 2/3$. To be more precise, they appear as a dip of $V(T)$. Extrapolating the depth V_{\min} of this dip linearly toward infinite system sizes gives an asymptotic value of $V_{\min} = 0.667$ for the Potts-XY model (figure 4(a)), thus supporting the hypothesis of a continuous phase transition. Indeed, for a first-order transition the scaling $V_{\min} \sim L^{-d}$ is expected (Challa *et al* 1986), which appears incompatible with our data.

Furthermore, the temperatures where the specific heat maximum ($T_C(L)$) and the Binder cumulant minimum ($T_V(L)$) are located, both shift proportional to different powers of the system size L in the case of a second- and first-order transitions, respectively: for a first-order transition, $T_{V;C}L \sim L^{-d}$ is found (Challa *et al* 1986), where d denotes the dimension.

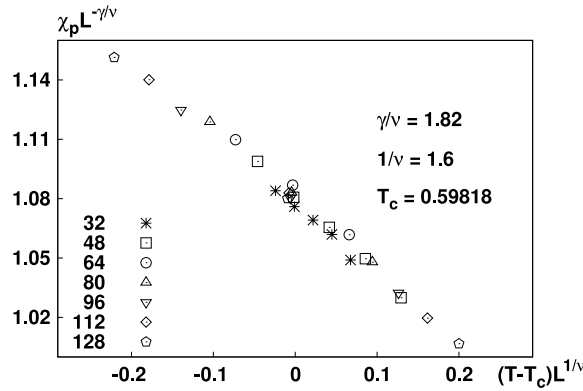


Figure 5. Finite size scaling analysis for the susceptibility χ_p (equation (8)). Using $T_c = 0.59818$ and the exponents $\gamma/\nu = 1.82$ and $1/\nu = 1.6$ the curves for different system sizes collapse nicely. These values differ significantly from those conjectured for the pure Potts model.

In contrast, for a continuous transition $T_{V;C}(L) \sim L^{-1/\nu}$ has been conjectured (Fisher and Nakanishi 1981) with ν being the critical exponent associated with the correlation length.

We also tried to obtain the value of $1/\nu$ by other means but were not able to compute a reliable result (see below). We plotted, however, the arithmetic mean of $T_V(L)$ and $T_C(L)$, called T_t , against the inverse system volume, L^2 , (figure 4(b)) which resulted in an (approximately) linear behavior. Knowing that $T_{V;C}(L) \sim L^{-2}$ would correspond to a first-order transition which is highly improbable due to our above results, we only can conclude that $1/\nu$ has a value closer to but smaller than 2. So we may denote the observed phase transition as ‘strong second order’. In the thermodynamic limit, a temperature $T_t = 0.5983$ is found by linear extrapolation which is slightly above the critical temperature T_c found by a more accurate method (see below).

The distributions of the Potts order parameter and the XY magnetization defined by equations (5) and (6) appear very similar. In the low temperature limit, they resemble Gaussian distributions (i.e. δ -function singularities for $L \rightarrow \infty$) while for high temperatures an exponential decay is observed. The reduced fourth-order cumulants U_{XY} and U_p converge in these limiting cases toward $2/3$ and -1 , respectively. At the critical point, a different, nontrivial value is obtained. As functions of T , the cumulants of an order parameter calculated for different system sizes meet at one point (aside from scaling corrections). This point is a very sensitive measure for T_c . A look at the crossing of the cumulants in figure 4(c) shows that the curves $U_p(T; L)$ very well coincide at $T_c \approx 0.59818$ aside from some minor corrections due to the finite system size.

Based on our data, it cannot be distinguished if there are two different transitions, namely a KT transition followed by a second-order transition, or if the curves for $U_{XY}(T; L)$ will finally meet at T_c for very large system sizes. The second scenario would indicate a simultaneous loss of XY and Potts order. If the first scenario should be true, the KT transition has to occur before the second-order transition because Potts domain walls uncouple the XY spins. The KT transition could thus only be observed when the great majority of the spins are in the same Potts state. The onset of this behavior was already observed in the internal energy (cf figure 2).

To further approach the origin of the phase transition we studied the susceptibility with respect to the Potts degree of freedom

$$\chi_p = L^2 \langle (m_p^2) \rangle. \quad (8)$$

Close to a second-order phase transition the susceptibility of the order parameter scales as $\chi_p \propto L^{\gamma/\nu}$ with the lateral system size L . Here, γ and ν are critical exponents for which we find $\gamma/\nu = 1.82(1)$. This value is significantly different from the value $26/15 \approx 1.73$ that is theoretically conjectured for the 3-state Potts model (Wu 1982). On the other hand, $1/\nu$ could not be obtained with good precision. For the scaling shown in figure 5, 1.6 was chosen but in a wide range between 1.2 and 1.8 similarly good collapsing of the curves can be seen. From the finite size scaling behavior of T_t that was discussed before, we assume the true value being rather close to 2. In all, it appears that the XY–Potts model does not fall into the universality class of the 3-state Potts model.

5. Conclusions

We have investigated the phase transition of a multiplicatively coupled Potts–XY model and our findings are consistent with the results found for the XY–Ising model (Granato *et al* 1991). We also see a continuous temperature-driven transition characterized by critical exponents distinct from those of the constituting models, especially the Potts model. The discrete degree of freedom induces the disorder of the continuous one. On the other hand, we also found that the annealed randomized coupling between the Potts spins due to the XY degree of freedom leads to a reduced critical temperature and a steeper transition region.

As the randomized coupling of the Potts spins includes the existence of vacancies, it is interesting to relate our results to the theoretical findings of Nienhuis *et al* (1979): vacancies are known to drive the transition of the 3-state Potts model from second to first order. Now, the coupling of the Potts with the XY model leads to a certain concentration of vacancies, and indeed, at first glance, the transition appears to change character (steep transition region, double peak energy histogram). Only more thorough investigations revealed the transition to be still continuous. Thus, the vacancies evoked by the annealed random coupling drive the transition toward first order, but do not suffice to fully change its character.

We finally would like to speculate on the impact of our findings on the original biological problem, the dynamics of hyaluron polymers in the extracellular matrix, that inspired the XY–Potts model. The ordering of the system for $T < T_c$ with the very steep transition characteristics indeed may help cells to quickly change the thickness of the protective extracellular matrix. That is, a cell may use the transition to fix the matrix in a more protective homogeneous ordered state by tuning the interactions of aggrecan side chains (hence changing the coupling constant J_{XY}).

Acknowledgments

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