

Potts And XY, Together At Last

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We investigate the behavior of an XY model coupled multiplicatively to a Potts model. In addition to the analytic one dimensional results, we use numerics to find the transition behavior on a two dimensional lattice. Extending this model to one with Potts variable dependent coupling, we find that the nature of the transition is similar while the exact transition point has moved to higher temperature. These two models can be interpreted as a rough description of polymers attached to a surface.

INTRODUCTION

The critical behavior of the Potts and XY models is well understood (see [1] and [2]). However, studying a hybrid system that couples these two models presents a new challenge. The critical behavior is not at all obvious when an amalgamated model is considered. As the behavior is expected to be quite complicated, the most natural approach to understanding how these coupled models act is simulations. In particular a simple Monte Carlo simulation on a fairly small lattice size suffices to understand qualitatively how various quantities (e.g. the critical temperature) will shift between models.

A simple multiplicatively coupled XY-Potts model was studied thoroughly in [3]. In order to expand on that work, we add another layer of complication, letting the coupling strength vary with the Potts variable. While at first it may seem like either of these models is merely of mathematical interest, we will see that both can describe physical systems of polymers attached to a surface. Motivated by this analogy, we can think of these models as being applicable to some biological processes.

MODELS

Original Hybrid Model

The most obvious way to couple the XY and Potts models is simple multiplication, given by the following Hamiltonian,

$$-\beta\mathcal{H} = J \sum_{\langle i,j \rangle} \delta_{p_i,p_j} \cos(\theta_i - \theta_j). \quad (1)$$

Here θ is a continuous angle and p_i can take any of q values, where q is an integer. As discussed in [3], this model can describe a lattice of polymer backbones with rigid side chains. The Potts variable describes the height where the side chain branches from the backbone while the XY variable gives the angle of the side chain relative to the lattice. Only when the side chains are at the same height do they interact, which leads to behavior inherently distinct from either model separately. In

particular, they found a lower critical temperature and a sharper transition in the Hybrid model than for the constituent models.

Adjusted Hybrid Model

It is interesting to expand on [3] to a more complicated model. We can adjust the Hamiltonian by adding a factor of the Potts variable, given by

$$-\beta\mathcal{H}' = J \sum_{\langle i,j \rangle} p_i \delta_{p_i,p_j} \cos(\theta_i - \theta_j). \quad (2)$$

There is also a physical analogue of this system. We can imagine this Hamiltonian arising from a lattice of polymers that are free to bend. If we expect them to bend at most in one spot, the fixed length of the polymer means that the height of the bending will be directly related to the length of the effective side chain.

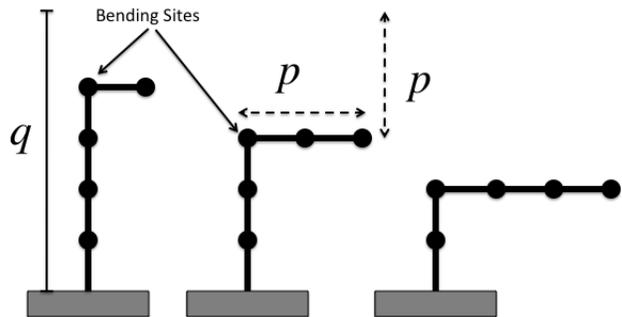


FIG. 1. Schematic picture of bending polymer interpretation of \mathcal{H}' from a side view. The farther down the polymers bend, the longer the side chain is and the stronger we expect the interaction to be.

Figure 1 gives a schematic view where we see that polymers that bend farther down should have stronger interactions. Note that polymers that are standing entirely upright have $p = 0$ and do not interact with each other, which makes physical sense when we ignore backbone interactions. The interpretation of the XY degrees of freedom, shown in Figure 2, is not affected by the change

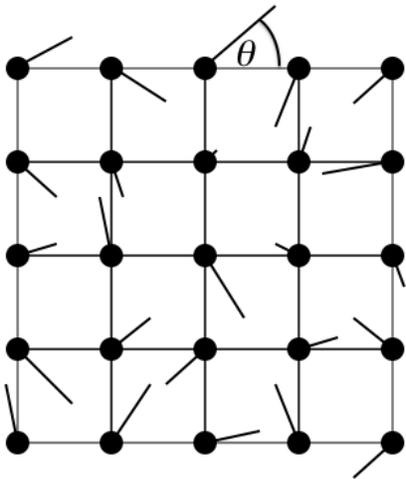


FIG. 2. Top view of our lattice of bending polymers. The angle θ is defined relative to the lattice and our interaction encourages alignment among side chains at the same level.

in the Hamiltonian. Just as coupling the XY and Potts models leads to behavior that is hard to predict from either model individually, this new variable coupling may lead to changes that are not intuitive before running the simulations.

ONE DIMENSIONAL ANALYSIS

We first look at the original Hybrid model in one dimension, solving the system analytically using the transfer matrix method. While we do not expect this system to show any order or interesting long range behavior, it is worth studying in order to get an idea of how the multiplicatively coupled model compares to the original models in a solvable situation. This exercise can give us insight into what to expect for the two dimensional case, which we cannot solve analytically. In order to calculate our partition function and solve this model, we look at the transfer matrix defined as

$$\langle p, \theta | T | p', \theta' \rangle \equiv e^{J \delta_{p,p'} \cos(\theta - \theta')}. \quad (3)$$

We want the eigenvalues of this matrix, so we guess eigenvectors and verify that they work. Following the structure of the Potts and XY models, we expect our eigenvector to be given by some normalized vector in q -space coupled to an integer indicating the Fourier component in θ -space. We define this eigenvector by its overlap with our known states,

$$\langle p, \theta | \vec{a}, m \rangle \equiv a_p e^{im\theta}. \quad (4)$$

For the maximum eigenvalues we expect the eigenvectors to respect the maximum amount of symmetry. This

vector is \vec{a}_s , which has $\sqrt{\frac{1}{q}}$ as every entry. By plugging this value in, we easily find the eigenvalue from

$$\langle p, \theta | T | \vec{a}_s, m \rangle = \langle p, \theta | \vec{a}_s, m \rangle \int_0^{2\pi} (e^{J \cos(\phi)} + q - 1) e^{im\phi} d\phi. \quad (5)$$

The other possibilities for \vec{a} will be vectors where all of the entries sum to zero, which we call \vec{a}_a . Notice that the $q-1$ independent vectors that satisfy this will give an eigenvalue with degeneracy $q-1$. Once again, a simple substitution gives

$$\langle p, \theta | T | \vec{a}_a, m \rangle = \langle p, \theta | \vec{a}_a, m \rangle \int_0^{2\pi} (e^{J \cos(\phi)} - 1) e^{im\phi} d\phi. \quad (6)$$

We notice that for $m > 0$, the terms in the integrands proportional to just $e^{im\phi}$ will integrate to zero. Also, the J dependent integrals just give modified Bessel functions of the first kind. So, we find that the spectrum of eigenvalues is given by

$$\begin{aligned} \lambda_s &= 2\pi(I_0(J) + q - 1) \\ \lambda_a &= 2\pi(I_0(J) - 1) \quad (q - 1 \text{ degenerate}) \\ \lambda_m &= 2\pi I_m(J) \quad (q \text{ degenerate}). \end{aligned} \quad (7)$$

For a given value of q we can plot the largest few eigenvalues.

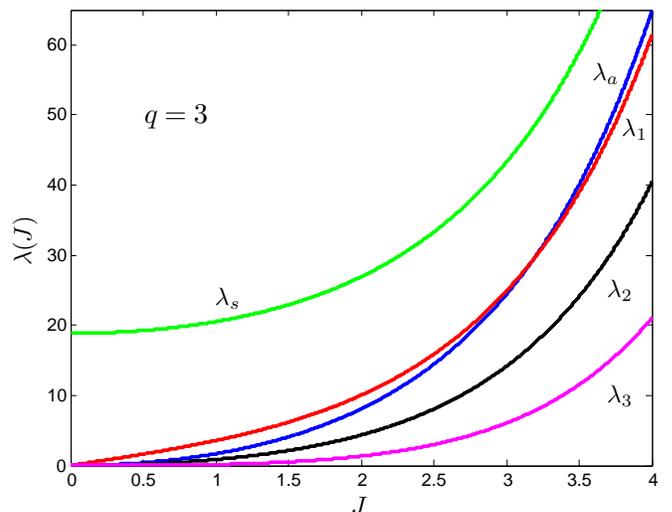


FIG. 3. Plot of eigenvalues of the transfer matrix T

For large J (which corresponds to low temperature) all of these eigenvalues grow exponentially. The eigenvalues with $m \neq 0$ all match exactly the XY behavior, but come in with a degeneracy of q . The $m = 0$ eigenvalues develop in a fashion closer to the Potts model. The most interesting aspect of this plot is that two of the eigenvalues

cross at $J \approx 3.2$. This will lead to a mixed behavior in this regime.

Using these results, we can calculate useful quantities. First we get the partition function $Z = \text{tr}[T^N] \approx \lambda_s^N$. From this, we can find the free energy per particle,

$$-\beta f = \frac{\ln(Z)}{N} = 2\pi(I_0(J) + q - 1). \quad (8)$$

In the XY model we get $-\beta f = 2\pi I_0(J)$ and in the Potts model we have $-\beta f = e^J + q - 1$. So, we can see that the behavior of the free energy is a mixture of the two models. For large J (or low temperatures) we see that the free energy is dominated by the XY contribution. We can interpret this as the freezing out of the Potts degrees of freedom. We'll later see that this behavior carries through to two dimensions.

Finally, we look at the result for the correlation length. From the usual transfer matrix results we get

$$\xi(J) = \left[\ln \left(\frac{\lambda_s}{\max(\lambda_a, \lambda_2)} \right) \right]^{-1}. \quad (9)$$

Looking at figure 3 we see that the correlation length with have a kink at $J \approx 3.2$, where the two relevant eigenvalues cross. At large J , we use equation 7 to find $\xi \propto e^J$. So, we see that in one dimension our coupled XY-Potts model displays behavior influenced by both models. At low temperatures, the Potts degrees of freedom are frozen out and we expect predominantly XY behavior. Next we will see how these phenomena translate to two dimensions.

SIMULATIONS

In order to see the behavior of the coupled models in two dimensions, we must simulate the system on a lattice. For simplicity, we use a square lattice of side length L . In order to get results that are directly comparable to [3], we set $L = 32$, though the qualitative results will not depend on this value. For a lattice this size, it suffices to simply use the Metropolis algorithm Monte Carlo method (for further details, see [4] and [5]). At each step of the simulation, one of the sites is picked at random. We then try to change the Potts variable by a random Δp and the XY variable by a random $\Delta\theta$. Based on the change in energy of the system, the Metropolis criterion then determines whether or not the changes will be applied.

Using this method, we can look at the average value of the internal energy per spin, given by $U = \frac{1}{L^2} \mathcal{H}$. Plots of $\langle U \rangle$ versus temperature should exhibit a transition around the critical temperature, if there is one. For these simulations, we use $q = 3$ and periodic boundary conditions.

Original Hybrid Model Results

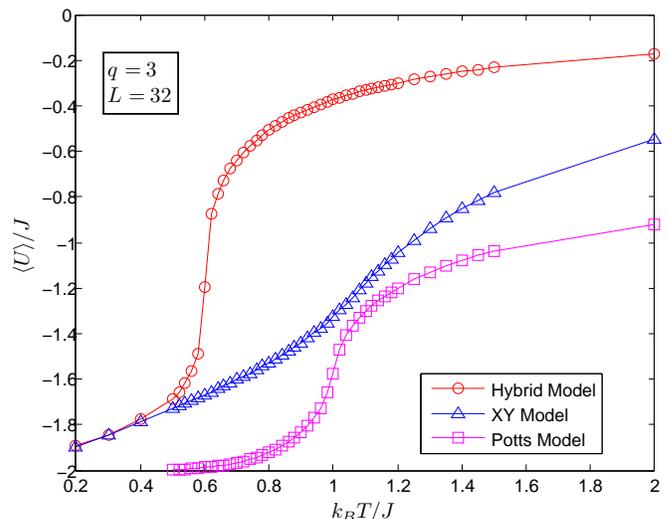


FIG. 4. Plot of simulation results for temperature development of average energy for the Potts Model, XY Model, and Multiplicatively Coupled Hybrid Model. Each point represents one Monte Carlo simulation.

The results of the Monte Carlo simulation for the original Hybrid model, XY model, and Potts model can be seen in figure 4. This plot agrees with a similar one found in [3]. There are many similarities between the behavior of different models. At high temperatures, there will be no order and the average energy will increase towards zero. At low temperatures, all of the models asymptote to $\langle U \rangle / J = -2$. It is easy to see where this value comes from. The minimum energy per bond is given when all of the Potts variables are equal and all the XY angles are aligned, giving a -1 contribution to the energy. As there are two bonds per site, we simply multiply by two to give the energy per site.

There are also several differences between the models. First of all, we can see a clear transition temperature in the Hybrid model, with a value $k_b T_c / J \approx 0.6$. Comparatively, the transition temperatures associated with the Potts model and XY model seem to be almost twice as high (both with a value $k_b T_c / J \approx 1$). Additionally, the transition is sharper for the Hybrid model than the other two. As shown in [3] this transition does not have a distinct character from the Potts transition but merely has a steeper slope.

At low temperatures, the XY and Hybrid models converge to one line. The Potts model curve is distinct down to very low temperatures. This indicates that the Potts degrees of freedom are frozen out at low temperatures. The discrete Potts levels will all align as the temperatures goes below the transition temperature, leaving only the continuous XY angles to determine the behavior of the curve.

Updated Hybrid Model Results

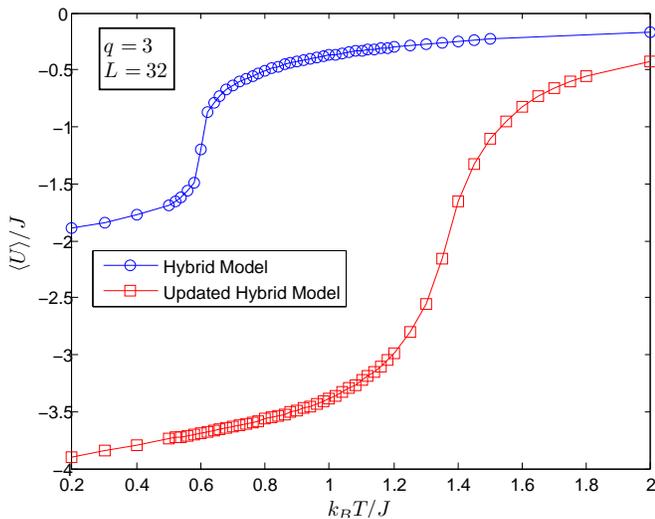


FIG. 5. Plot of simulation results for temperature development of average energy for the Multiplicatively Coupled Hybrid Model and the Updated Hybrid Model. Each point represents one Monte Carlo simulation.

Now that we are confident in the accuracy of our simulations, we can extend them to our new model. The results of the simulations for the original Hybrid model as well as the updated Hybrid model are shown in figure 5. We can see that there are large differences between the two models. The most striking difference is the overall scale. However, this dissimilarity can be explained by looking at the Hamiltonians for the two models. For the original Hybrid model, we have $\beta\mathcal{H}_{min} = -L^2J$ when all of the states are aligned in both the Potts and XY variables. In the updated Hybrid model, we see $\beta\mathcal{H}_{min} = -2L^2J$ when all of the states are aligned in the $p = 2$ position. So, we expect the minimum energy per site to be twice as large in the updated Hybrid model. One interesting result of this is that we have eliminated all Potts degeneracy in the ground state. The q different choices of lowest energy orientation have become one unique ground state. Of course, the continuous XY degeneracy is unaffected when we eliminate symmetry in the Potts variable.

Additionally, we see that the critical temperature has increased in the updated model. In fact, the critical temperature of the updated model is higher than that of the other models. This shift can be explained by the change in overall energy scale. By increasing the scale of the energy of the lattice, we also increase the characteristic temperature that sets $U/k_B T$ to order one. So, we expect the transition temperature to roughly double, which is exactly the behavior observed in simulations. Another way to interpret this effect is to notice that at low temperatures, the alignment of the Potts variables in the $p = 2$

state effectively doubles J . So, we actually want to study $k_B T_c / J'$ between the two models, where $J' = J$ in the original Hybrid model and $J' = 2J$ in the updated Hybrid model. When we look at this temperature variable, the two transitions do occur at pretty much the same point.

Another difference between the two models is that the slope of the transition is less in the updated Hybrid model. The updated model has a transition that more closely resembles the Potts model in overall shape. This is an effect of the variable bond strength in this region of the updated Hybrid model. As the Potts variables are no longer all aligned with $p = 2$, the changing values of the bond strength effectively smooth out this curve.

Physically, the differences between the two models have important effects. In the original model, at low temperatures, all of the polymers aligned in any state where they branch at the same height and align all of their branched angles. In the updated model, we see that the polymers will all bend at the lowest site in order to minimize their energy. So, in this case, as temperature rises, we go from an ordered state with small height to a disordered state with highly variable height. Returning to our biological motivation, we see that biological systems could use exactly this kind of transition to quickly change the width of a polymer wall and allow or disallow passage through it.

FURTHER POSSIBILITIES

While simple Monte Carlo simulations can give a general idea of the behavior for each model, we would have to go farther to get detailed information, particularly near transition in larger lattices. In order to do a more complete analysis, we should follow up our analysis with a cluster Monte Carlo approach (for more, see [6]). Unfortunately, this is simply not feasible with the computational resources we currently have available.

There are also many other parameters that would be interesting to explore. We could test how changing the values of q and L affects the behavior of the updated Hybrid model. Ultimately, it would be ideal to look at the limit $L \rightarrow \infty$. For small lattices, the boundary conditions can have a large impact on the behavior of the model, so it would be worthwhile to test various possibilities along the boundaries. Ultimately, there are many different directions to take the simulations as the parameter space that can be explored is extremely large.

CONCLUSION

We have seen that multiplicatively coupling a Potts and XY model together results in a sharper transition at a lower critical temperature than in the constituent

models. Further adding dependence on the Potts variable changes multiple aspects of the transition. In the updated Hybrid model, we can think of this transition as changing the heights of polymers from their minimum height to a state where polymers are in a highly disordered state between being bent and standing up straight. Further numerical studies are necessary to understand all of the differences between these two models.

[1] R. J. Baxter, *Journal of Physics C: Solid State Physics* **6**, L445 (1973).

- [2] J. M. Kosterlitz and D. J. Thouless, *Journal of Physics C: Solid State Physics* **6**, 1181 (1973).
- [3] M. Hellmann, Y. Deng, M. Weiss, and D. W. Heermann, *Journal of Physics A: Mathematical and Theoretical* **42**, 225001 (2009).
- [4] D. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics* (Cambridge University Press, New York, NY, USA, 2000).
- [5] K. Binder, *Monte Carlo methods in statistical physics*, Topics in current physics (Springer-Verlag, 1986).
- [6] R. H. Swendsen and J.-S. Wang, *Phys. Rev. Lett.* **58**, 86 (1987).