Critical Behaviour of Magnetic Polymers

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Abstract

We explore the critical behaviour of two and three dimensional lattice models of polymers in dilute solution where the monomers carry a magnetic moment which interacts ferromagnetically with near-neighbour monomers. Specifically, the model explored consists of a self-avoiding walk on a square or cubic lattice with Ising spins on the visited sites. In three dimensions we confirm and extend previous numerical work and present results for the first time in two dimensions.

Introduction

Garel, Orland and Orlandini[1] looked at 3d SAW with Ising spins on visited sites which interact via standard Ising Hamiltonian. The resulting partition function for the model is The partition function for a walk of length N is

$$Z_N = \sum_{\Omega_N} \sum_{\{\sigma_i = \pm 1\}} \exp\left(\beta J \sum_{\langle i,j\rangle} \sigma_i \sigma_j + \beta h \sum_i \sigma_i\right), \qquad (1)$$

where Ω_N is the set of self-avoiding walks of length N, σ_i are the two-state Ising spins, and as usual $\langle i, j\rangle$ indicates that the sum is over pairs of spins which are nearest-neighbour on the lattice, h is a magnetic field and $\beta = 1/kT$. In what follows we will set J/k=1. Using MFT they found a line of first-order transitions for low h and standard Θ collapse at higher T with a multicritical point. Numerical work tended to confirm this. A fluctuating bond version was studied by Luo[2] found the $h = 0$ transition to be critical with a magnetic exponent β similar to the standard 3d Ising model result.

We look at Ising Self-Avoiding Walk model in 3d using flatPERM[3], proving clear evidence of first order magnetic transition at $h = 0$, but with a geometric exponent $\nu \approx 0.5$. Plotting the phase diagram was difficult in 3d, and we resorted to looking at the scaling of zeros in the complex plane as the best was of determining the critical point for $h \neq 0$.

We examined the 2d case, and found the $h = 0$ transition to be critical with a $\beta \approx 1/8$ as expected for 2d Ising model, and estimated ν for the transition. When $h \neq 0$ the transition seems to be the standard collapse transition.

Finite-Size Scaling

Crossings of the Binder cumulant for different sizes indicates the location of phase transitions. The cumulant is given by

$$U = 1 - \frac{\langle M^4\rangle}{3\langle M^2\rangle^2}. \qquad (2)$$

and define scaling functions:

$$\varphi_m = \frac{\log\left(m_N/m_{N'}\right)}{\log\left(N/N'\right)}; \quad \varphi_{R_g} = \frac{1}{2}\frac{\log\left(r_N/r_{N'}\right)}{\log\left(N/N'\right)} \qquad (3)$$

where $r_N = \langle R_g^2\rangle$ for a walk of length N.

The magnetisation is expected to behave as

$$m \sim (T - T_c)^{-\beta} \qquad (4)$$

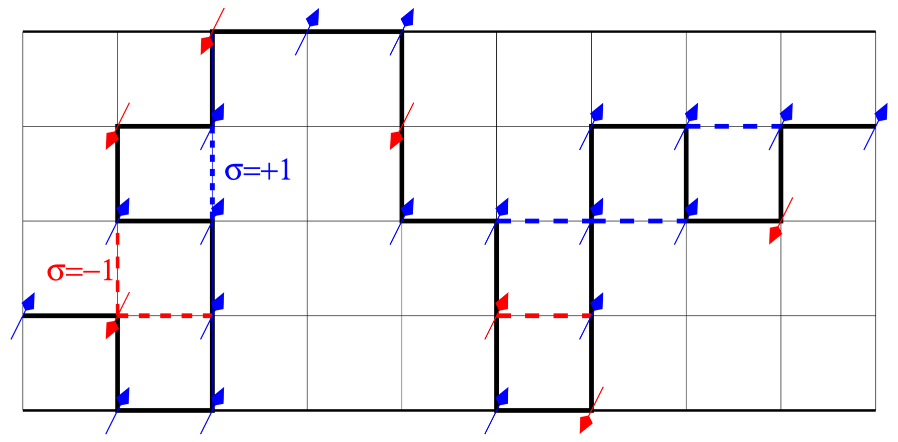
as the temperature is approached and and

$$r(T_c) \sim N^{2\nu}, \qquad (5)$$

then $\varphi_m \to -\beta$ and $\varphi_{R_g} \to \nu$ at T_c as $N \to \infty$, and hence, again crossings can give finite-sized estimates of the transition, as well as estimates of critical exponents.

The Model

Figure 1: Self-Avoiding Walk with Ising Spins. Ferromagnetic interactions between n.n. spins on lattice.



Three Dimensions

Figure 2: Magnetisation and Radius of Gyration as function of T with $h = 0$.

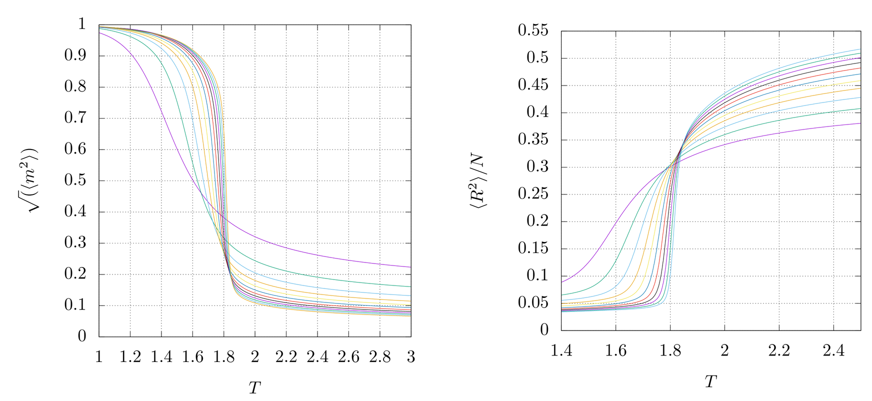
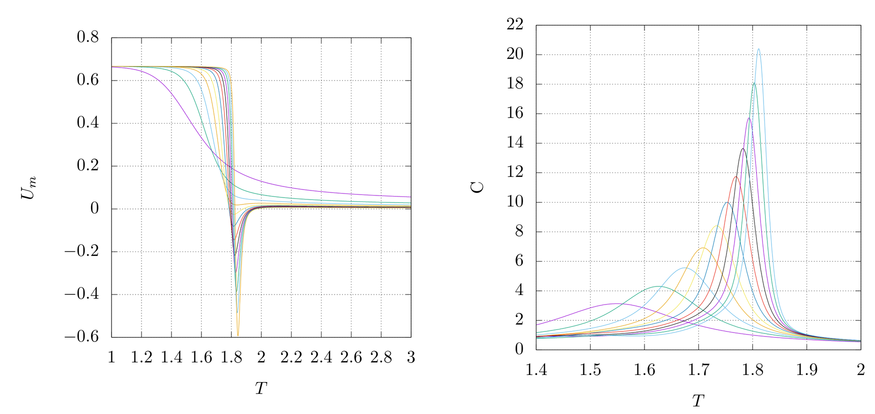
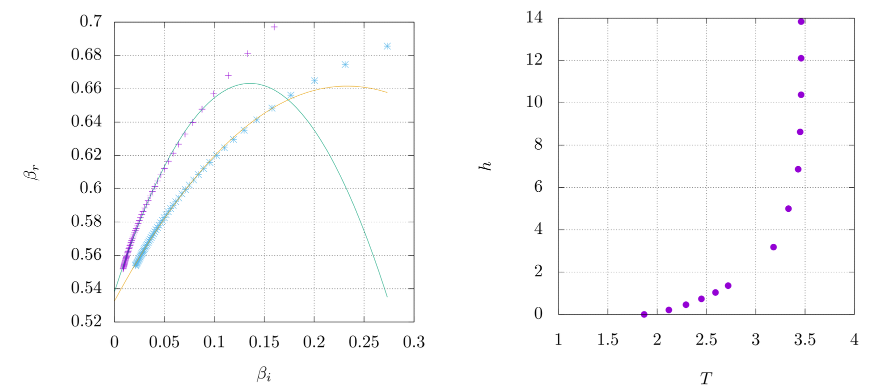


Figure 3: Binder 4th order cumulant and specific heat capacity for $h = 0$.



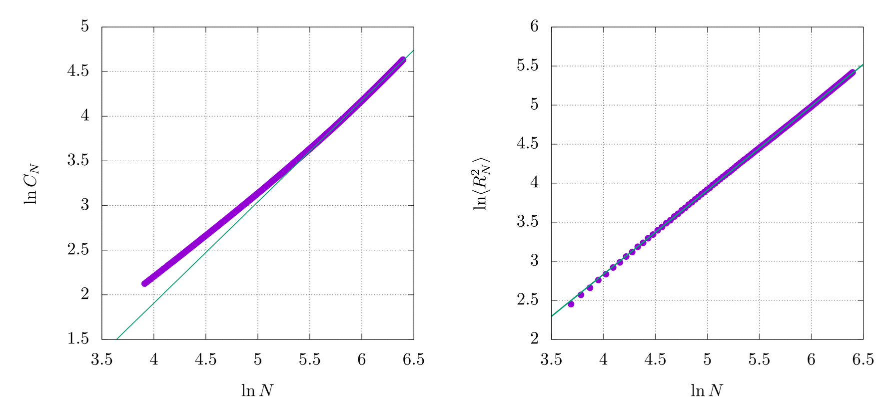
Binder's Cumulant shows characteristic negative spike indicative of a first-order transition.

Figure 4: Locus of first and second most relevant complex zeros of Partition function when $h = 0$ and resulting phase diagram as h is varied



The critical temperature found using locus of zeros, peak of specific heat, Binder Cumulant and scaling functions give transition temperature a little higher than found by Garel *et al*[1]: $T_c(h = 0) = 1.87 \pm 00.01$.

Figure 5: Log/Log plots of specific heat and $\langle R^2\rangle$ against N



The Log-Log plots show almost linear scaling of C_N with N (slope of 1.13), but also a linear scaling of R_g with N (slope 1.075 of shown line). The first is consistent with a first-order transition, but the second gives $\nu = 1/2$ as for a normal collapse transition. U_m measures the magnetic aspect of the transition, which is clearly first order.

Two Dimesions

Figure 6: Magnetisation and Binder Cumulant for $h = 0$ in two-dimensions.

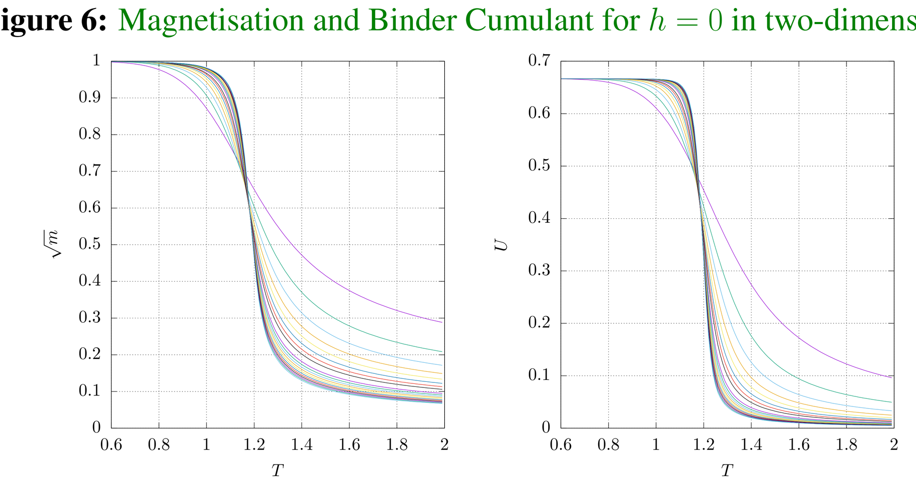


Figure 7: plots of φ_m and φ_{R_g} as a function of T and the critical temperature estimates from different methods

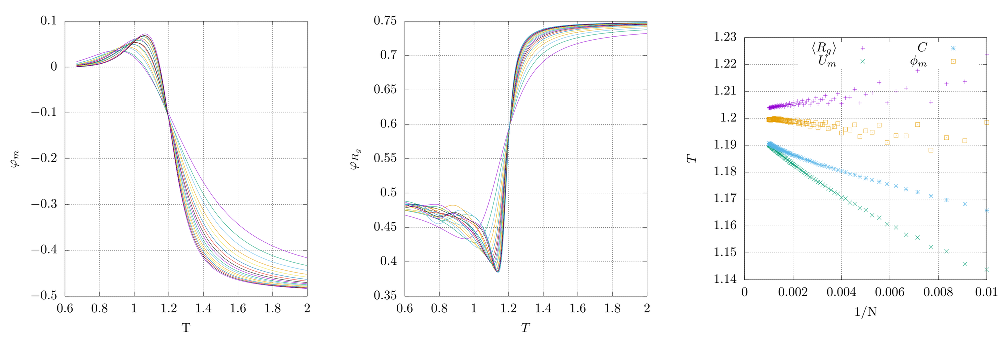
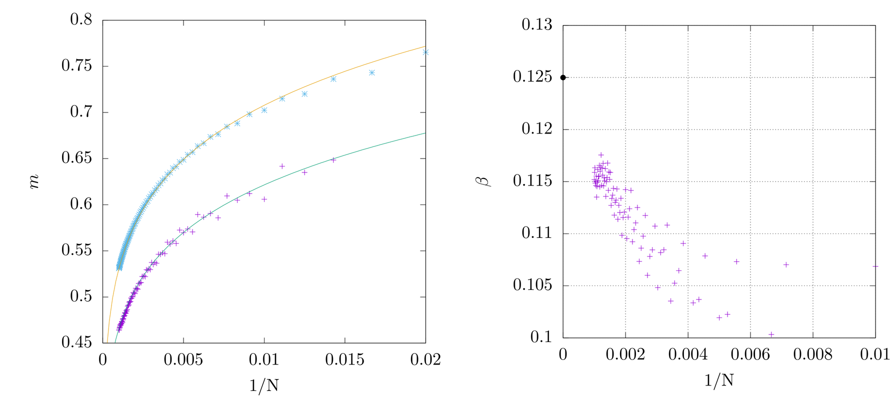
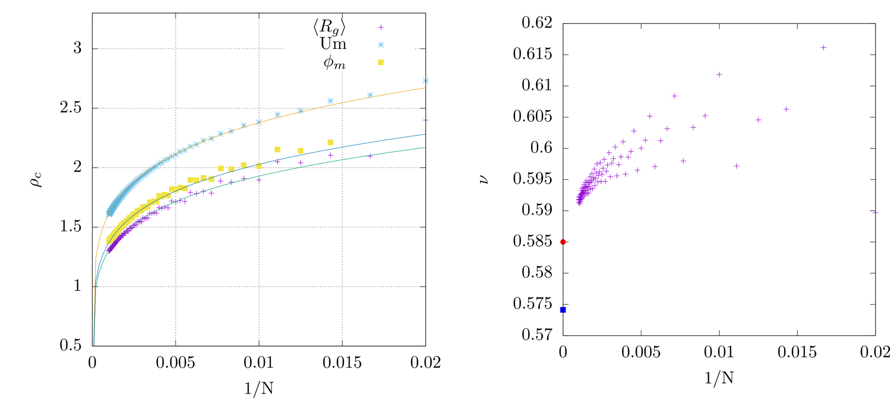


Figure 8: Estimates of magnetisation at finite-sized estimates of critical point ($h = 0$) with fitted curves and finite-size estimates of β as function of $1/N$



Lines fitted with curves $m(T_N) = AN^{1/8}$. Calculation of the exponent from φ_m supports $\beta = 1/8$ as per the standard 2d Ising model.

Figure 9: Estimates of the un-normalised density at finite-sized estimates of critical point ($h = 0$) with fitted curves and finite-size estimates of ν as function of $1/N$



The best fit curves for the density of form $\rho_N(T_N) = AN^{(1-2\nu)}$ give $\nu = 0.585 \pm 0.01$. This is compared to estimates of ν from φ_{R_g} and (black dot) $4/7$ as for the standard collapse (θ) transition.

References

[1] T. Garel, H. Orland, and E. Orlandini. Phase diagram of magnetic polymers. *The European Physical Journal B*, 12(2):261–268, nov 1999.

[2] Meng-Bo Luo. Finite-size scaling analysis on the phase transition of a ferromagnetic polymer chain model. *The Journal of Chemical Physics*, 124(3):034903, jan 2006.

[3] T. Prellberg and J. Krawczyk. Flat histogram version of the pruned and enriched Rosenbluth method. *Physical review letters*, 92(12):120602, 2004.