

PROPERTIES OF MAGNETIC MODELS ON ENSEMBLES OF CONFORMATIONS

Moskalenko R.

National Research University Higher School of Economics

`rbmoskalenko@edu.hse.ru`

Conformation is a self-avoiding random walk on a two-dimensional square grid of fixed length. Shape of the conformation depends on the temperature. There is a geometric transition between two phases: coil and globule at high and low temperatures, respectively. Looking at the examples of globule and coil conformations we can see that coils are structurally similar to one-dimensional grid and globules are similar to two-dimensional grid. From studies of the Ising model we know that magnetic phase transition appears on two-dimensional grid and does not appear on one-dimensional. So, our hypothesis is that there is a magnetic transition on globules and no transitions on coils.

In this model, we observe sets of conformations of equal length generated at the same temperature. Each conformations generated independently as a random walk on two-dimensional grid. On each conformation we calculate Ising model, by placing a spin in each vertex of the conformation. We calculate magnetic properties of Ising model using Wolf algorithm with cluster update. Then we average the values over all conformations.

During the work it turned out that not all conformations generated at low temperature can become magnetic. Because of that high variance of magnetization from conformation to conformation we could not use Binder cumulant right away to determine the transition point. To make result clearer we tried to separate nonmagnetic conformations from conformations that we generate. Looking at generated conformations we have noticed that some conformations consist of several domains connected by one-dimensional segments. With probability close to $\frac{1}{2}$ these domains will have different directions, and total magnetization will be close to 0. So, we decided to use the size of domains as a parameter for separation of nonmagnetic conformations. This method proved to be quite effective in separating nonmagnetic conformations, but even when considering the remaining conformations, the error in calculating the cumulant turned out to be too large to determine the transition point.

In this work we can see that magnetization is directly related to the structure of magnetic domains in the conformation. And our results suggest that we should use an alternative method to determine transition point, rather than Binder cumulant.