PROPERTIES OF MAGNETIC MODELS ON

ENSEMBLES OF CONFORMATIONS

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***Abstract* – Ising model is a relatively new model used to determine magnetic properties of materials and objects. In this work we study properties of Ising model on ensembles of conformations. Conformation is a random walk on a regular grid witch can represent a molecule. Structure of the conformation depends on the temperature. And other studies has shown that conformations have a geometric phase transition. Two states of conformation at low and high temperatures are called globule and coil respectively. Geometrically globule and coil conformations are similar to one and two dimensional grids. As most vertexes in globules have 4 neighbors and in coils they mostly have 2. It was proven that on one-dimensional grid Ising model has no magnetic phase transition. Our hypothesis is that globular conformations have magnetic phase transition. But on two-dimensional grid it phase transition exists. The goal of this research is to determine the magnetic phase transition point in globular conformations and compare it to the point of geometric phase transition in conformations.**

***Keywords – Monte Carlo; Ising model; polymer; self-avoiding walk***

# INTRODUCTION

Ising model is a well established physical model. It has found applications in many fields from genetics to social science. But originally it was introduced by Wilhelm Lenz and later solved for one-dimensional grid by Ising in [1]. Since exact solution for the model was found for many other grids such as two and three dimensional [2]. In our research we specifically interested in solutions for one and two-dimensional grids. As those solutions show that on one-dimensional grid Ising model does not have magnetic phase transition, one-dimensional model does not become magnetic at any temperature other than absolute zero. But on two-dimensional grid model has a phase transition. At low temperature two-dimensional grid becomes magnetic.

Other model that we use in this research is SAW

# LITERATURE REVIEW

# METHODS

*In our model we use SAW algorithm to generate pack of conformations and Monte-Carlo algorithm to simulate Ising model on them.*

Algorithm we are using was suggested by Wolf in this paper []. This algorithm based on constructing a cluster of spins and updating the whole cluster simultaneously. This approach has multiple advantages against regular one-spin update. Firstly it works without rejections: after the cluster is built, its update is guaranteed. Where in single-spin update we can spend multiple attempts updating value of the spin due to the possibility of rejection. Secondly updating multiple spins at once gives us more diverse samples. For these reasons, this algorithm converges faster than single-spin algorithm.

*В. Conformation generation*

To generate conformations we also use Monte Сarlo methods

*B. Magnetic susceptibility*

# ANTICIPATED RESULTS

Using described methods we expect to accurately determine the magnetic transition point for globular conformations, describe magnetic properties of conformations near the geometric transition point.

# CONCLUSION

# REFERENCES

[1] Ernst Ising, Contribution to the Theory of Ferromagnetism, 1925

[2] Baxter, Rodney J - Exactly Solved Models in Statistical Mechanics-Dover Publications\_Academic Press (1982)

[3] Reference

Word Count: