The Hackthon Project

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(Dated: May 10, 2019)

In this note, we record all the details related with the SSH Hackthon Project. We give several solutions for the questions.

I. INTRODUCTION

The buckyball lattice structure has 60 sites which form 12 regular pentagon and 20 regular hexagon. We study the anti-ferromagnetic Ising model on this buckyball lattice.

Our model Hamiltonian is

$$H = \sum_{<i,j>} \sigma_i \sigma_j. \tag{1}$$

II. ANSWER FOR QUESTION 1

Question1: Obtain $\ln(Z)/N$, where $Z = \sum_{\{\sigma_i\}} \exp\left(-\sum_{<i,j>} \sigma_i \sigma_j\right)$, N is the number of sites.

A. Mean-field theory method

In the *simple* mean-field theory, the free energy per spin is

$$f = -kT \ln Z_1 = -kT \ln\left(2\cosh\left[\frac{Jqm + H}{kT}\right]\right), \tag{2}$$

where H is the magnetic field and q is the number of nearest neighbors of one spin. And the magnetization is

$$m = -\frac{\partial f}{\partial H} = \tanh\left[\frac{Jqm + H}{kT}\right]. \tag{3}$$

The critical temperature Tc is determined by

$$kT_c = Jq. \tag{4}$$

In the *improved* mean-field theory, we do the approximation

$$s_i s_j \approx -m^2 + m(s_i + s_j). \tag{5}$$

The partition function $Z(T, H, Z)$ can be expressed as

$$Z = e^{-NqJm^2/2kT}\left[\left(\frac{2\cosh(qJm + H)}{kT}\right)\right]^N. \tag{6}$$

The free energy per spin is

$$f(T, H) = \frac{1}{2}Jqm^2 - kT \ln\left(2\cosh\left[\frac{Jqm + H}{kT}\right]\right), \tag{7}$$

where H is the magnetic field and q is the number of nearest neighbors of one spin. And the magnetization is

$$m = \tanh\left[\frac{Jqm + H}{kT}\right]. \tag{8}$$

The critical temperature Tc is determined by

$$kT_c = Jq. \tag{9}$$

We use the Newton method to solve the self-consistent equation.

At temperature $T = 1$, we have $m = \pm 0.00494$. We choose the result which minimize the free energy per site. Then we get $m = \pm 0.00494$, $f = -1.5000$.

For the Buckyball lattice, $q = 3$, so we have $\beta_c \equiv \frac{1}{kT_c} = \frac{1}{3}$.

B. Monte Carlo Method

We use the Wang-Landau[1] Monte Calo algorithm to estimate the density of states and obtain the free energy. Then we will get the answoer of question 1.

The code is 95 percent finished till now.

C. Tensor Network Method

The partition function of $2-D$ anti-ferromagnetic Ising model can be written as

$$Z(\beta) = \sum_{\mathbf{s}} \prod_{ij} e^{\beta s_i s_j} = \mathbf{Tr}\left(\mathcal{A}^{(1)} \times \mathcal{A}^{(2)} \times \cdots \times \mathcal{A}^{(\mathcal{L}\times\mathcal{L})}\right). \tag{10}$$

Here the last term denotes tensor contraction of all the tensors, each of which is a tensor given by

$$\mathcal{A}^{(i)} = I \times_1 \sqrt{\mathbf{B}} \times_2 \sqrt{\mathbf{B}} \times_3 \sqrt{\mathbf{B}}, \tag{11}$$

where I is a identity tensor with order equals to the degree of node i, and B_{ij} defines a Boltzmann matrix with

$$\mathbf{B} = \begin{bmatrix} e^{-\beta} & e^{\beta} \\ e^{\beta} & e^{-\beta} \end{bmatrix}. \tag{12}$$

$\sqrt{B}$ indicates square root of matrix B, yileding $\sqrt{B} \times \sqrt{B} = B$.
Given eigen decomposition of the semi-definite symmetric matrix B, $B = V\Sigma V^T$, simple calculation gives

$$\sqrt{B} = V\sqrt{\Sigma}V^T \tag{13}$$

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Our algorithm design:
1. getBuckyball return a 3 order tensor with dimension 2.
2. getIcosahedron return a 5 order tensor with dimension 2.
3. getTetrahedron return a 3 order tensor with dimenison 2^3.
And this is the best contraction policy at present, because we use the geometrical symmetry.

D. Variational Autoregressive Network Method

We use the variational autoregressive networks[2] to solve this statistical mechniacs. It's very convient to use this tool.

E. Quantum Circuit Method

Studying$\cdots$

III. ANSWER FOR QUESTION 2

Question 2: Calculate the ground state degeneracy.

A. Graph Theory

We find its dual problem in graph theory. Using the tools in graph theory, we get the solution.

IV. CONCLUSIONS

The statistical physics will recover vitality thanks to the development of the interdisciplinary sciences related with it.

ACKNOWLEDGEMENTS

We thank all the lecturers (Lei Wang, Pan Zhang, Xiuzhe Luo and Jinguo Liu) for giving us the inspiring classes. Thanks Songshan Lake materials laboratory for giving us this good opportunity to step further to deep learning and quantum programming field.

[1] F. Wang and D. P. Landau, Phys. Rev. Lett. **86**, 2050-2053 (2001)
[2] D. Wu, L. Wang, and P. Zhang, Phys. Rev. Lett. **122**, 080602 (2019).