PH5730 - Assignment 1 (BONUS)

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Old submission had an error in the code and plot, this is the corrected code and plot.

1 Theory: Triangular Lattice

The energy (restriction) of a lattice system is represented by:

$$E = J \sum_{\langle i,j \rangle} s_i s_j \tag{1}$$

The slight difference between Square and Triangular lattice is that we can transform the triangular lattice into a square lattice with each element of the lattice having 2 more nearest neighbors in the following configuration transformation:

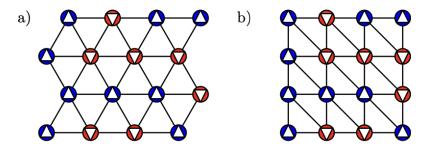


Figure 1: (a) Triangular Lattice (b) Linear transformation of the lattice to a square lattice (ref: Classical Monte Carlo, M-LAB)

2 Anti-Ferromagnetic Triangular Lattice Code (J = +1):

The following Python code simulates the Ising Model for Anti-ferromagnetic Triangular lattice:

```
# Antiferromagnetic
   import numpy as np
   import matplotlib.pyplot as plt
   # Lattice generation
6
   s_{-} = [1, -1]
   N = 10 # Lattice size
   lattice = np.random.choice(s_, size=(N, N))
10
11
   lower\_temp = 0.5
12
   upper_temp = 7
   temp_pts = 200
   t_limit = 2000
   limit = 9000
```

```
17
             # Restriction Calc updated
19
20
             def energyCalc(lattice, N):
                           ener = 0
21
                           for i in range(N):
                                           for j in range(N):
23
                                                           s = lattice[i,j]
                                                            nb = lattice[(i+1)\%N,j] + lattice[i,(j+1)\%N] + lattice[(i-1)\%N,j] + lattice[i,(j+1)\%N] + l
25
                                                                          -1)%N] + lattice[(i+1)%N,(j+1)%N] + lattice[(i-1)%N,(j-1)%N]
                                                           ener += s*nb
26
27
                           return ener
28
             #Magnetization Calculations
29
30
             def magCalc(lattice):
31
                           mag = np.sum(lattice)
32
                           return mag
33
34
             #Monte Carlo Steps - Metropolis Algorithm
35
36
             def mc_steps(lattice, beta):
37
                           for i in range(N):
38
                                           (a,b) = np.random.randint(0, N, size=2)
39
                                           s = lattice[a,b]
40
                                            n_b = lattice[(a+1)\%N,b] + lattice[a,(b+1)\%N] + lattice[(a-1)\%N,b] + lattice[a,(b-1)\%N] + 
                                                          %N] + lattice[(a+1)%N,(b+1)%N] + lattice[(a-1)%N,(b-1)%N]
                                           delta_restriction = -2*s*n_b
42
                                           if delta_restriction < 0:</pre>
43
                                                   s *= -1
44
                                           elif np.random.rand() < np.exp(-delta_restriction*beta):</pre>
45
                                                  s *= -1
46
                                           lattice[a,b] = s
47
48
                           return lattice
49
            Temperatures = np.linspace(lower_temp,upper_temp,temp_pts)
50
            energy_arr = []
            mag_arr = []
53
54
            C_arr = []
            X_arr = []
55
56
            t_limit = 1000
57
            limit = 9000
58
             for temp in Temperatures:
59
                           ener = 0
60
                           magn = 0
61
                           ener2 = 0
62
                           magn2 = 0
63
64
                           l = np.copy(lattice)
65
                           beta = 1/temp
66
67
                           for t in range(t_limit):
                                           mc_steps(1,beta)
68
69
                           for z in range(limit):
                                           mc_steps(1,beta)
70
                                           e = energyCalc(1,N)
71
72
                                           m = magCalc(1)
73
74
                                           ener += e
                                           ener2 += e**2
                                           magn += m
                                           magn2 += m**2
77
78
79
                           energy_arr.append(ener/(N*N*limit))
                           \texttt{C\_arr.append}(((\texttt{ener2}/(\texttt{N*N*limit}) - ((\texttt{ener*ener})/(\texttt{N*N*limit*limit})))*(\texttt{beta**2})))
80
81
                           mag_arr.append(magn/(N*N*limit))
                            X_{arr.append}(((magn2/(N*N*limit) - ((magn*magn)/(N*N*limit*limit)))*(beta))) \\
82
```

```
83
    f = plt.figure(figsize=(18, 10))
85
86
    sp = f.add_subplot(2, 2, 1)
    plt.scatter(Temperatures, energy_arr, s=10, marker='o', color='red')
plt.xlabel("Temperature_u(T)")
plt.ylabel("Energy_")
87
88
89
   plt.axis('tight')
90
91
    sp = f.add_subplot(2, 2, 3 )
92
    plt.scatter(Temperatures, C_arr, s=10, marker='o', color='blue')
plt.xlabel("Temperature_u(T)")
93
94
    plt.ylabel("Specific_heat_")
95
    plt.axis('tight')
97
    sp = f.add_subplot(2, 2, 2)
   plt.scatter(Temperatures, np.abs(mag_arr), s=10, marker='o', color='green')
99
   plt.xlabel("Temperature_(T)")
100
   plt.ylabel("Magnetization")
101
    plt.axis('tight')
102
103
sp = f.add_subplot(2, 2, 4)
plt.scatter(Temperatures, X_arr, s=10, marker='o', color='black')
plt.xlabel("Temperature (T)")
   plt.ylabel("MagneticuSusceptibilityu")
107
    plt.axis('tight')
```