

```

1  # -*- coding: utf-8 -*-
2  """
3  Created on Sat Nov 16 16:12:36 2019
4
5  @author: Alexm
6  """
7  #PART 2: VARIATION OF THE MAGNETIC FIELD WITH CONSTANT J=1
8  from __future__ import division
9  import numpy as np
10 from numpy.random import rand
11 import matplotlib.pyplot as plt
12
13 print('Alexandra Mulholland 17336557')
14 J=-1
15 T=1
16 print('Part 2: varying the external magnetic field for constant J equal to %d'%J)
17 print('T=%d'%T)
18 nt=1
19 nbs=60
20 N=10
21 stepsequil=1000
22 stepsmoncar=1000
23 Bfield=np.linspace(0.0,25.0,nbs)
24
25 #we now define temperature as a constant value rather than a range of values
26 #we can change this value to test the effect it has on the magnetic field
27 #The magnetic field is expected to increase the value of the Curie or Neel temp
28 #as it keeps the system in equilibrium for longer
29 E= np.zeros(nt)
30 M= np.zeros(nt)
31 C= np.zeros(nt)
32 X = np.zeros(nt)
33 T=1
34
35 E,M,C,X = np.zeros(nbs), np.zeros(nbs), np.zeros(nbs), np.zeros(nbs)
36
37 n1= 1.0/(stepsmoncar*N*N)
38 n2=1.0/(stepsmoncar*stepsmoncar*N*N)
39 #again, used later to find X and C
40
41 def randomstate(N):
42     state = 2*np.random.randint(2, size=(N,N))-1
43     return state
44 #now the magf is not zero, but a range of values
45 J=-1
46 #same monte carlo code as explained in part 1 code
47 def moncar(config, beta, magf):
48     for i in range(N):
49         for j in range(N):
50             a = np.random.randint(0, N)
51             b = np.random.randint(0, N)
52             s = config[a, b]
53             spinmag=s*magf
54             naybor = config[(a+1)%N,b] + config[a,(b+1)%N] + config[(a-1)%N,b] + config[a,(b-1)%N]
55             EC = 2*J*s*naybor+2*spinmag
56             if EC < 0:
57                 s *= -1
58             elif rand() < np.exp(-EC*beta):
59                 s *= -1
60             config[a, b] = s
61     return config
62
63 #now factoring in the effect of an external magnetic field into the energy
64 def TotEnergy(config, magf):
65     energy = 0
66     for i in range(len(config)):
67         for j in range(len(config)):
68             S = config[i,j]
69             spinmag =S*magf
70             naybor = config[(i+1)%N, j] + config[i,(j+1)%N] + config[(i-1)%N, j] + config[i,(j-1)%N]
71             energy += -naybor*J*S/4 -spinmag
72     return energy

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73
74
75 def TotSpin(config, MAGFIELD):
76     mag = np.sum(config)
77     return mag
78
79 for bt in range(nbs):
80     avE = avM = avE2 = avM2 = 0
81     config = randomstate(N)
82     BT=1.0/T
83     BT2=BT*BT
84     MAGFIELD=1.0*Bfield[bt] #mirroring the technique used for the temp
85
86     for i in range(stepsequil):
87         moncar(config, BT, bt)
88
89     for i in range(stepsmoncar):
90         moncar(config, BT, MAGFIELD)
91         Ene = TotEnergy(config, MAGFIELD)
92         Mag = TotSpin(config, MAGFIELD)
93
94     avE = avE + Ene
95     avM = avM + Mag
96     avM2 = avM2 + Mag*Mag
97     avE2 = avE2 + Ene*Ene
98
99     E[bt] = n1*avE #finding the average energy over the magnetic field range
100    M[bt] = n1*avM #average magnetisation over mf range
101    C[bt] = (n1*avE2 - n2*avE*avE)*BT2 #heat capacity over mf range
102    X[bt] = (n1*avM2 - n2*avM*avM)*BT #susceptibility over mf range
103
104
105
106 plt.figure(1)
107 plt.plot(Bfield, E, 'p', color='k',
108     markersize=10,
109     markerfacecolor='white',markeredgecolor='k',
110     markeredgewidth=1)
111 plt.suptitle('Plot of the average energy versus magnetic field')
112 plt.title('T=1K and J=%d'%J, fontsize=10)
113 plt.xlabel("Magnetic Field, B / T", fontsize=12);
114 plt.ylabel("Energy/J ", fontsize=12); plt.axis('tight');
115
116
117
118 plt.figure(2)
119 #plotting the absolute value of the magnetisation as this can be negative (1 or -1)
120 plt.plot(Bfield, 1000*M, '-p', color='grey',
121     markersize=10,
122     markerfacecolor='white',markeredgecolor='grey',
123     markeredgewidth=1)
124 plt.suptitle('Plot of the average magnetisation versus magnetic field')
125 plt.title('T=1K and J=%d'%J, fontsize=10)
126 plt.xlabel("Magnetic Field, B / T", fontsize=12);
127 plt.ylabel("Magnetisation / Am-1", fontsize=12);
128
129
130 #specific heat
131 plt.figure(3)
132 plt.plot(Bfield, C, 'p', color='c',
133     markersize=10,
134     markerfacecolor='white',markeredgecolor='c',
135     markeredgewidth=1)
136 plt.suptitle('Plot of the specific heat versus magnetic field', fontsize=13)
137 plt.title('T=1K and J=%d'%J, fontsize=10)
138 plt.xlabel("Magnetic Field, B / T", fontsize=12);
139 plt.ylabel("Heat capacity C / JK-1 ", fontsize=12); plt.axis('tight');
140
141
142 #suscpetibility- measure of the error in the magnetisation
143 plt.figure(4)
144 plt.plot(Bfield, X, 'p',color='blue',

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145     markersize=10,  
146     markerfacecolor='white',markeredgecolor='blue',  
147     markeredgewidth=1)  
148 plt.suptitle('Plot of the susceptibility versus magnetic field', fontsize=13)  
149 plt.title('T=1K and J=%d'%J, fontsize=10)  
150 plt.xlabel("Magnetic Field, B / T", fontsize=12);  
151 plt.ylabel("susceptibility ", fontsize=12); plt.axis('tight');
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