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Homework 2

2-D Ising model simulation

Answer 1

```
# Necessary modules

%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import random as r
from random import choice

# We now work to generalize the Ising model to 2-Dimensions and or
that the lattice size becomes (N_x) X (N_y) where we
# assume periodic boundary conditions in both, x and y, directions. It
is given that we use the same coupling constant in
# both directions.

# To calculate change in energy after one spin flips at position (x,y)
def energy_flip(s,J,h,x,y,n):
#     Here, the s is the spin, x and y are th positions of the 2 D
lattice, J,n, and h are the same variables as defined before
#     The function calculates the energy after the spin at one site is
flipped.
    return 2 * s[x][y]*(J*(s[((x+1)%n)][y] + s[((x-1)%n)][y] + s[x]
[((y+1)%n)] + s[x][((y-1)%n)]) + h)

# Number of sweeps for thermalization for every value of J,h
n_therm = 100
# Number of measurements for each J,h
n_meas = 100

def energy(s,J,h,x,y,n):
    return -J*((s[((x+1)%n)][y] + s[((x-1)%n)][y] + s[x][((y+1)%n)] +
s[x][((y-1)%n)])*s[x][y])-h*s[x][y]


def variables(n,J,h,obs):

# Defining local arrays

    m = np.array([])  # Magnetization
    E = np.array([])  # Energy
    m_absolute = np.array([]) # Absolute value of magnetization
```

```
    prob = np.array([]) # Probability information

#   Now we need to assign spins to the site and because this is a 2D
lattice, we have to keep in mind the dimensions
#   x and y and do that. This has been done as follows:
#   The variable (s) is the spin here and n is some random integer

    s = [[choice((+1,-1)) for x in range(n)] for y in range(n)]

    for j in range(n_therm):
#         Assigning a random integer value to x and y
        x = np.random.randint(n)
        y = np.random.randint(n)

#   We need to define the change of energy after flipping the lattice
site (x,y) picked randomly. We call the defined function
#   energy_flip to calculate that.

        delta_energy = energy_flip(s,J,h,x,y,n)
        if delta_energy < 0:
            s[x][y] *= -1         # Condition to accept the spin flip
        else:
            if np.random.uniform(0,1) <= np.exp(-delta_energy):
                s[x][y] *= -1

    for i in range(n_meas):
        for j in range(n**2):  #sweeping the lattice
            x = j % n
            y = j // n
            delta_energy = energy_flip(s,J,h,x,y,n)
            if delta_energy < 0:
                s[x][y] *= -1         # Condition to accept the spin
flip
            else:
                if np.random.uniform(0,1) <= np.exp(-delta_energy):
                    s[x][y] *= -1
                    prob = np.append(prob,1.)   # Accept.
                else:
                    prob = np.append(prob,0.)    # We reject the other
values.

#         Measurements

        if obs == "m":
            m=np.append(m,np.mean(s))
            obs=np.mean(m)
        if obs == "E":
            temp = np.array([])
            for x in range(n):
                for y in range(n):
```

```
                temp = np.append(temp,energy(s,J,h,x,y,n))
            E=np.append(E,np.mean(temp))
            obs=np.mean(E)
        if obs == "m_absolute":
            m_absolute=np.append(m_absolute,np.absolute(np.mean(s)))
            obs=np.mean(m_absolute)

    return obs
```

Answer 2

The system size , Λ, we have to iterate over all lattice sites and every time keep the number of nearest neighbours constant.

Answer 3

We consider the site and the four neighbours to find the difference in energy because O(Λ) is constant.

Answer 4

The significance of critical coupling J_c is that it helps us to see when the phase transition will happen because the system starts behaving in an ordered manner with couplings greater than J_c

Answer 5 : ¿m>¿ vs h

```
# Now plotting the required variables

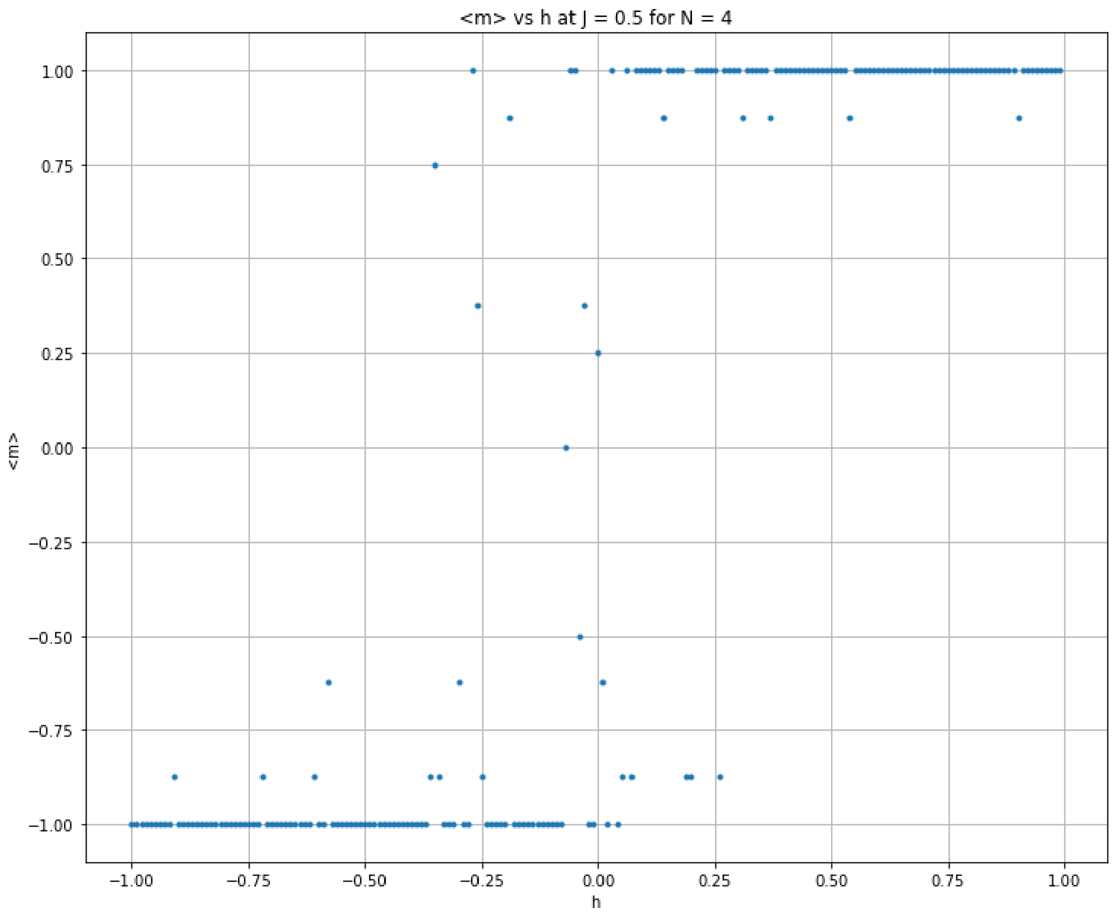
J = 0.5     # Keeping J fixed at a certain value
h_range = np.arange(-1,1,0.01)

# We are supposed to take different values of N (N_x = N_y), so we
define as follows:

mag_4  = [variables(4,J,h,"m") for h in h_range]
mag_8  = [variables(8,J,h,"m") for h in h_range]
mag_12 = [variables(12,J,h,"m") for h in h_range]
mag_16 = [variables(16,J,h,"m") for h in h_range]
mag_20 = [variables(20,J,h,"m") for h in h_range]

plt.figure(figsize=(12,10))
plt.title("<m> vs h at J = 0.5 for N = 4",fontsize=12)
plt.grid()
plt.xlabel("h")
plt.ylabel("<m>")
plt.plot(h_range,mag_4,'.',label="N=4")
plt.legend()
```

```
[<matplotlib.lines.Line2D at 0x7f523ec793d0>]
```




```
# For different values of N:

plt.figure(figsize=(12,10))
plt.title("<m> vs h at J = 0.5 for various N",fontsize=12)
plt.grid()
# plt.plot(h_range,mag_4)
plt.xlabel("h")
plt.ylabel("<m>")
plt.plot(h_range,mag_8,'.',h_range,mag_12,'.',h_range,mag_16,'.',h_ran
ge,mag_20,'.')
plt.legend(("N = 8", "N = 12","N = 16","N = 20"))
```

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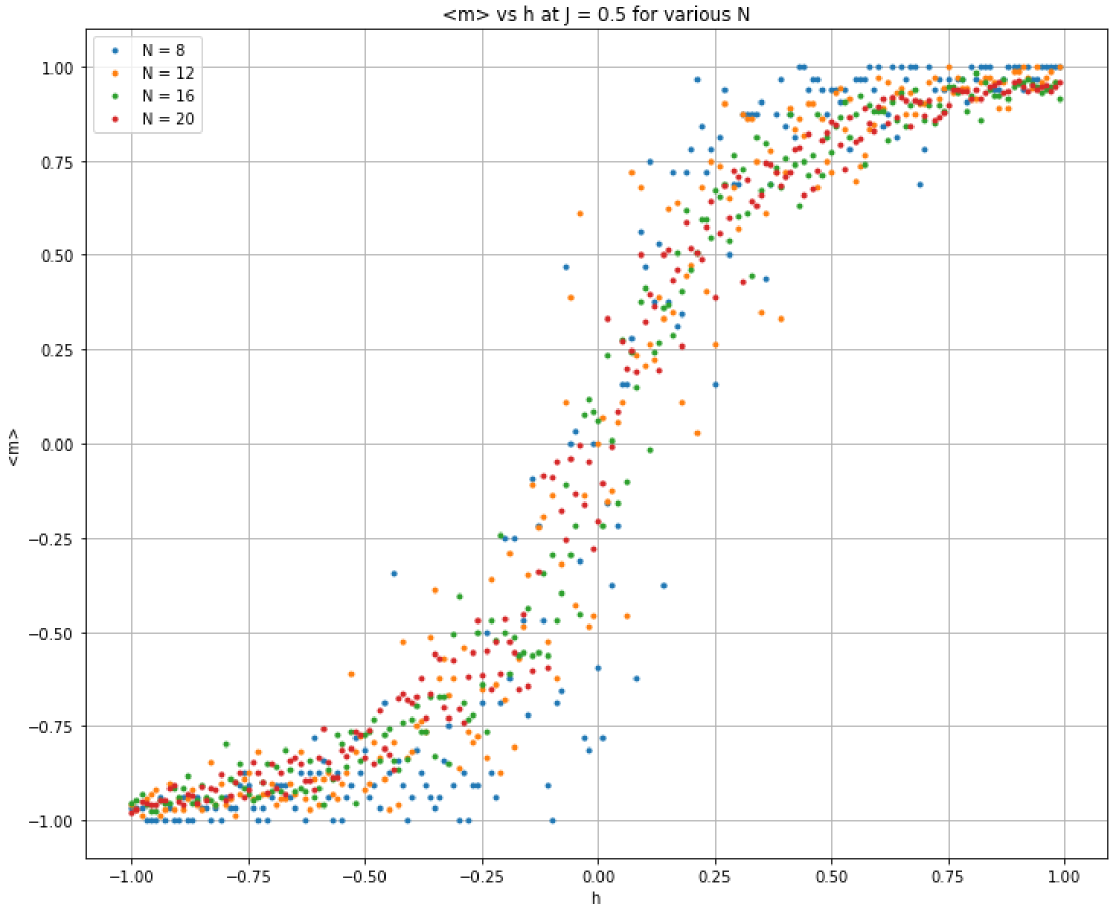
<matplotlib.legend.Legend at 0x7f523e706850>
```



Answer 6 : ϵ vs J at h = 0

```
# Now

import scipy.special as s

h = 0
J_range = np.linspace(0.25,2,100)

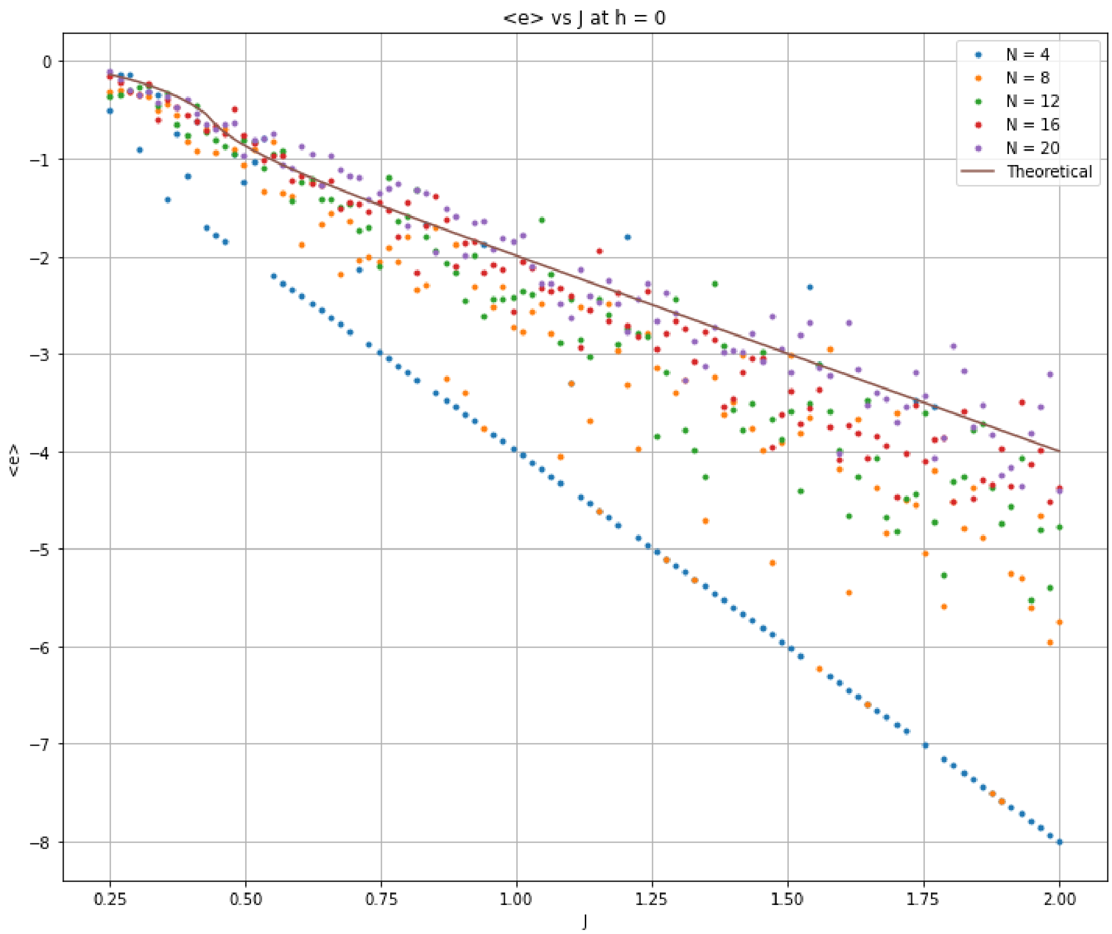
# Given average energy epsilon function is defined as follows:
Eps_th=-J_range*(1/np.tanh(2*J_range))*(1+(2/np.pi)*(2*(np.tanh(2*J_ra
nge))**2-1)*s.ellipk(4*(1/
np.cosh(2*J_range))**2*(np.tanh(2*J_range))**2))

avg_4  = [variables(4,J,h,"E") for J in J_range]
avg_8  = [variables(8,J,h,"E") for J in J_range]
avg_12 = [variables(12,J,h,"E") for J in J_range]
avg_16 = [variables(16,J,h,"E") for J in J_range]
avg_20 = [variables(20,J,h,"E") for J in J_range]

plt.figure(figsize=(12,10))
plt.title("<e> vs J at h = 0",fontsize=12)
plt.grid()
```

```python
plt.xlabel("J")
plt.ylabel("<e>")
# plt.plot(J_range, avg_4)
plt.plot(J_range,avg_4,'.',J_range,avg_8,'.',J_range,avg_12,'.',J_range,avg_16,'.',J_range,avg_20,'.')
plt.plot(J_range,Eps_th,label="Theoretical")
plt.legend(("N = 4", "N = 8", "N = 12","N = 16","N = 20",
"Theoretical"))
```

```
<matplotlib.legend.Legend at 0x7f523c0b40d0>
```

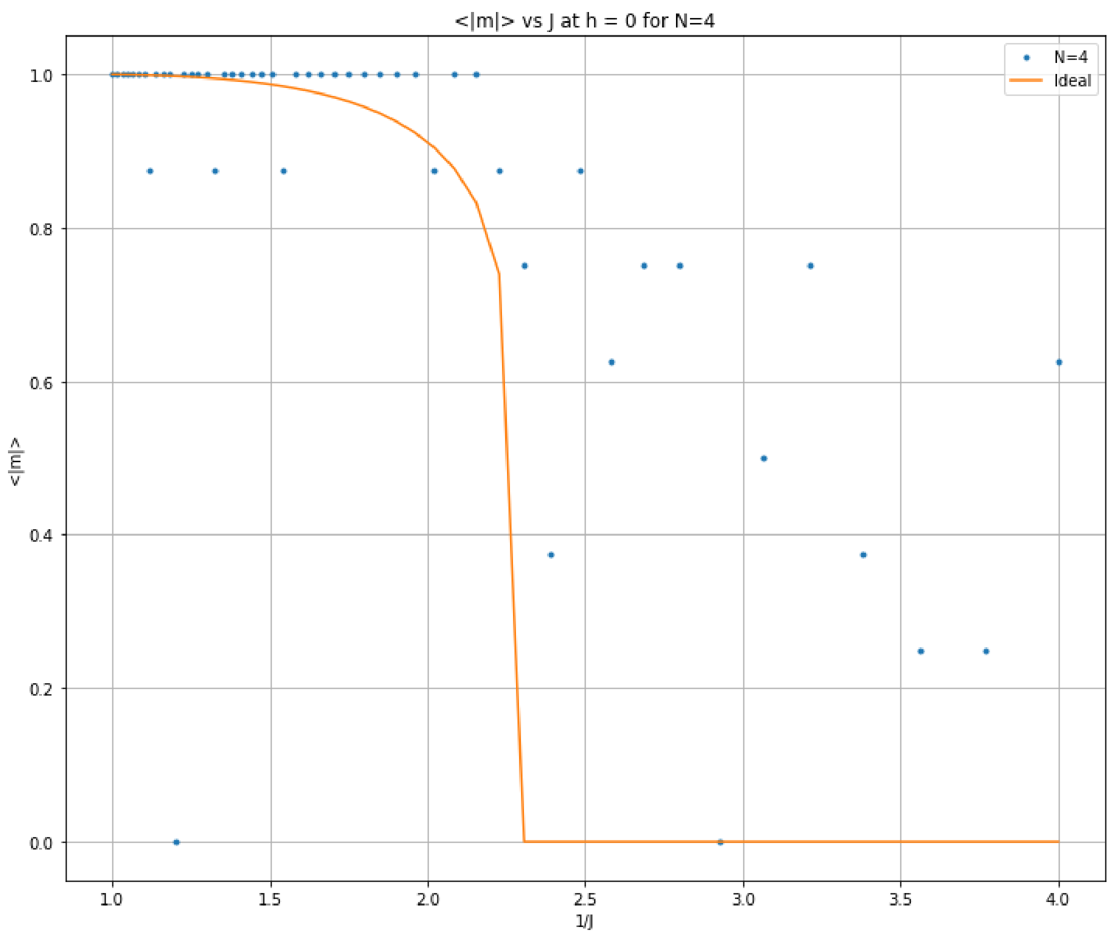


Answer 7 : ¿|m|>¿ vs J at h = 0

```python
J_new = np.linspace(0.25,1,50)
new = np.zeros(len(J_new))

for i in range(len(J_new)):
    if(J_new[i]> 0.440686793):
        new[i] = (1 - 1/(np.sinh(2*J_new[i]))**4)**0.125

# Again

h = 0
```

```python
mabs_4  = [variables(4,J,h,"m_absolute") for J in J_new]
mabs_8  = [variables(8,J,h,"m_absolute") for J in J_new]
mabs_12 = [variables(12,J,h,"m_absolute") for J in J_new]
mabs_16 = [variables(16,J,h,"m_absolute") for J in J_new]
mabs_20 = [variables(20,J,h,"m_absolute") for J in J_new]

plt.figure(figsize=(12,10))
plt.title("<|m|> vs J at h = 0 for N=4",fontsize=12)
plt.grid()
plt.xlabel("1/J")
plt.ylabel("<|m|>")
plt.plot(1/J_new,mabs_4,'.',label="N=4")
plt.plot(1/J_new,new,label="Ideal")
plt.legend()
```

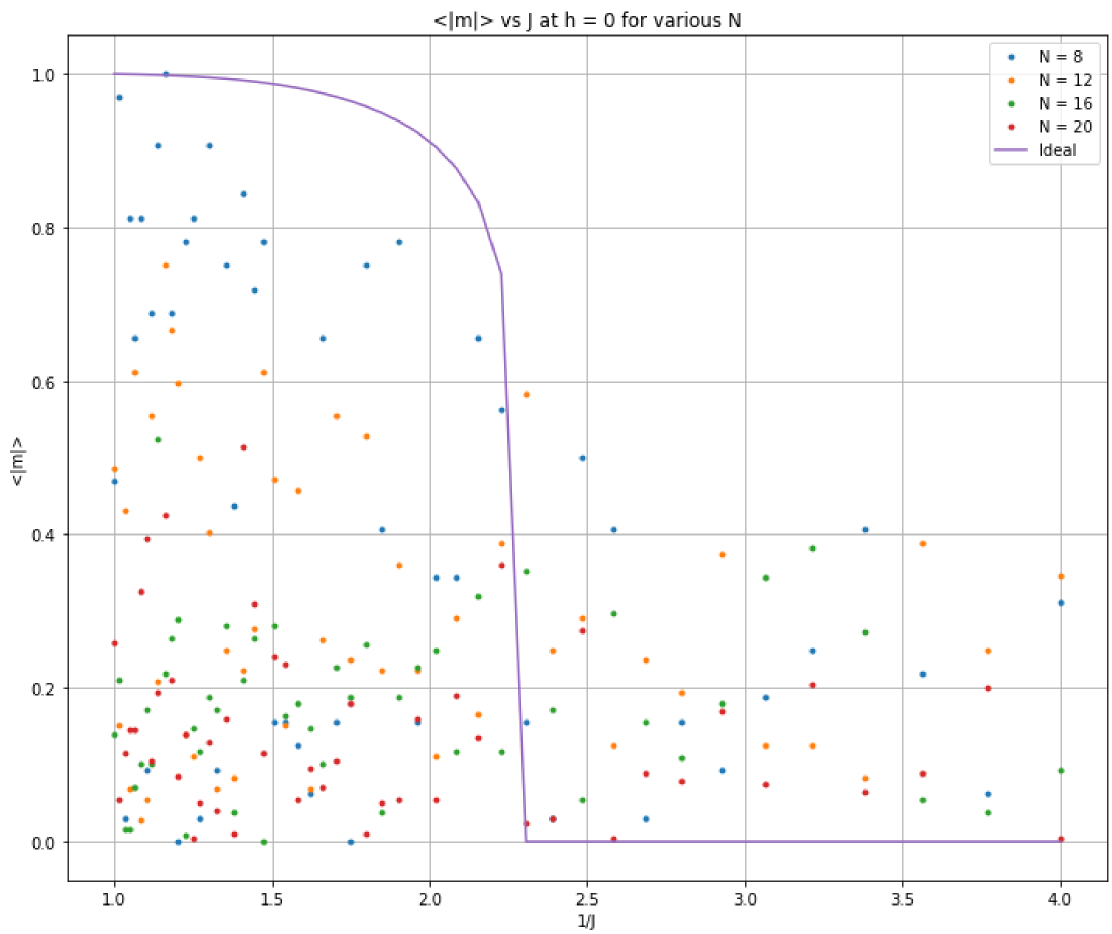
```
<matplotlib.legend.Legend at 0x7f5237f171f0>
```




```python
plt.figure(figsize=(12,10))
plt.title("<|m|> vs J at h = 0 for various N",fontsize=12)
plt.grid()
```

```
plt.xlabel("1/J")
plt.ylabel("<|m|>")
# plt.plot(1/J_new,mabs_4,'.')
plt.plot(1/J_new,mabs_8,'.',1/J_new,mabs_12,'.',1/J_new,mabs_16,'.',1/
J_new,mabs_20,'.')
plt.plot(1/J_new,new,label="Ideal")
plt.legend(("N = 8", "N = 12","N = 16","N = 20","Ideal"))
```

```
<matplotlib.legend.Legend at 0x7f5237e12580>
```



Note: For some reason, the plots for N=4 seem nicer than the others. I have separated the simulations for N=4 and higher N's

Also, I don't understand the difference in the simulation between N=4 and others: In the sense that, for N=4, we have some points at 0 but this is not the case for higher N's