14/20

Submitted by: Anushka and Yashasvee

Homework 2

2-D Ising model simulation

Answer 1

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Seperate Global and local variable! Don't define Global variable in middle of functions!

```
# 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
```

no. of steps too low for monte carlo & thermalization use atleast

```
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
```

Don't make such a huge function it makes the code very inefficient adding a lot of if statement make it inefficient

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

define array of fixed lengths to reduce computation time

```
#   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)]
```

Don't use list it takes long time!

```
    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
```

This doesn't help sweep over entire lattice !! run for ($n^2=4$)

to check

```
    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):
```

if random() ≤ min(1, exp(-ΔE))

s[x][y] *= -1

These two statements can be combined

Bring indent here

Mean has to be performed at indent specified and because of this your curve was in steps

Missing from code!

Sample after every 10-20 sweeps to reduce auto correlation

```
                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.

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Answer 3

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

0.5/1

Calculating ΔS just requires knowing no. of nearest neighbours.

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

1/1

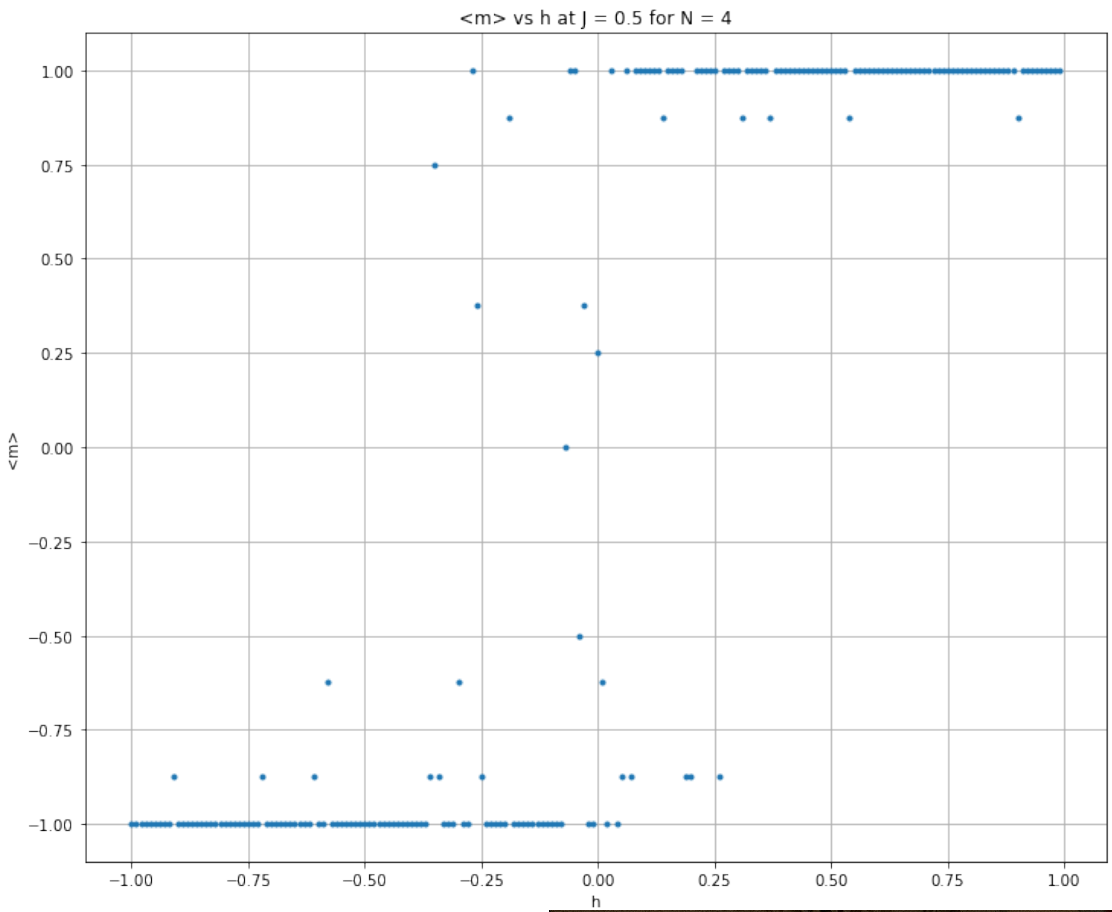
Answer 5 : ¿m>¿ vs h

```
# 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()
```

this precision is not required 0.1 or 0.2 is sufficient

this is increases code time

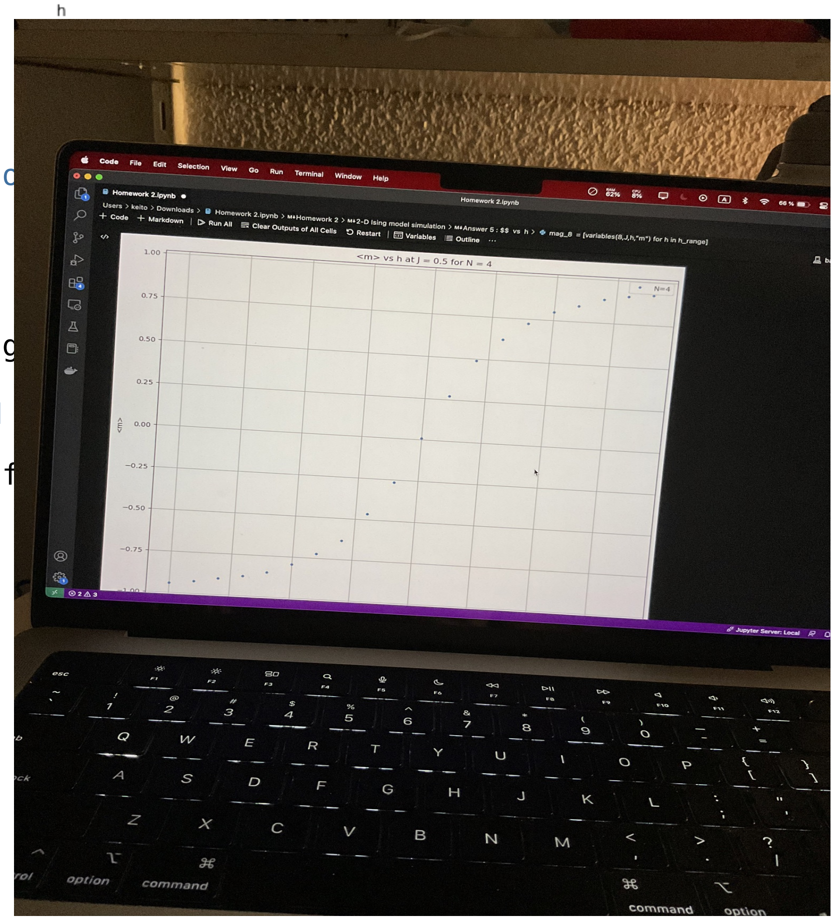
```
[<matplotlib.lines.Line2D at 0x7f523ec793d0>]
```

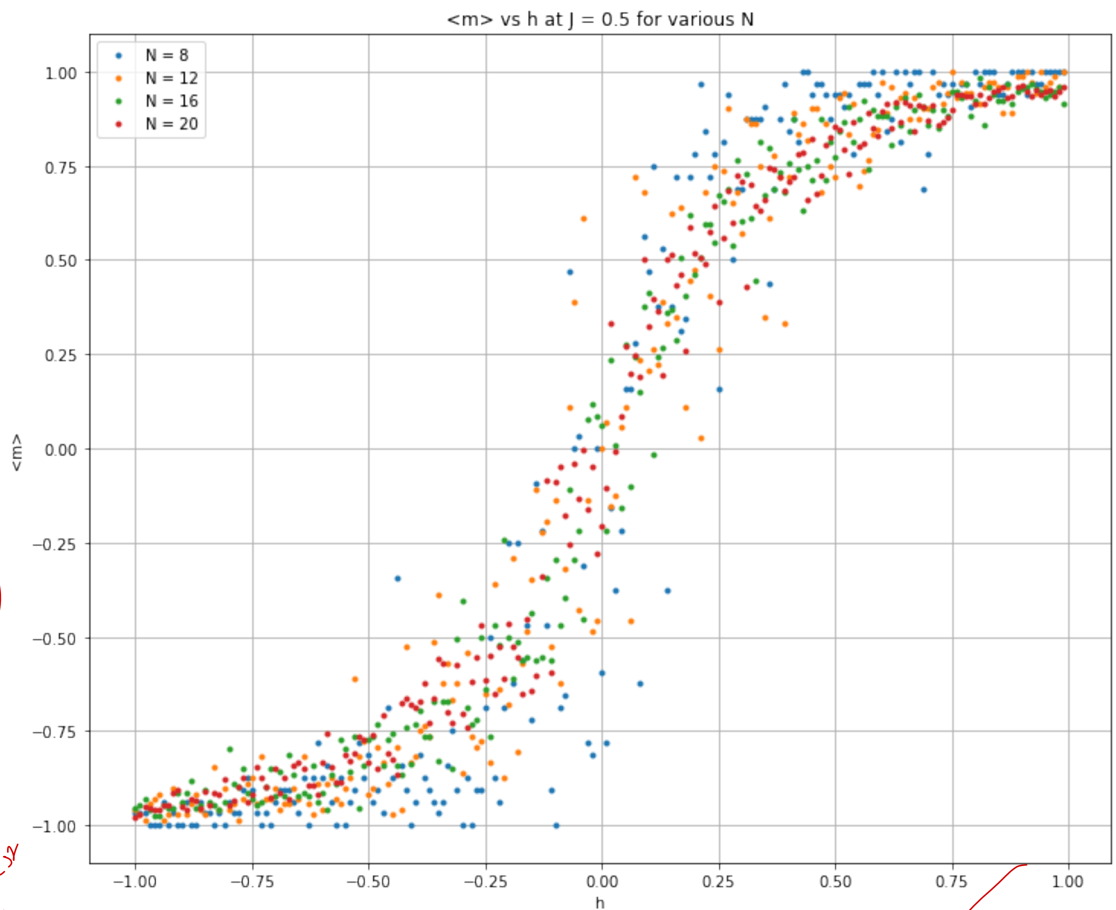


Use the suggested values to get better plots

```python
# For different values of N:

plt.figure(figsize=(12,10))
plt.title("<m> vs h at J = 0.5 fo
plt.grid()
# plt.plot(h_range,mag_4)
plt.xlabel("h")
plt.ylabel("<m>")
plt.plot(h_range,mag_8,'.',h_rang
ge,mag_20,'.')
plt.legend(("N = 8", "N = 12","N
```

```
<matplotlib.legend.Legend at 0x7f
```





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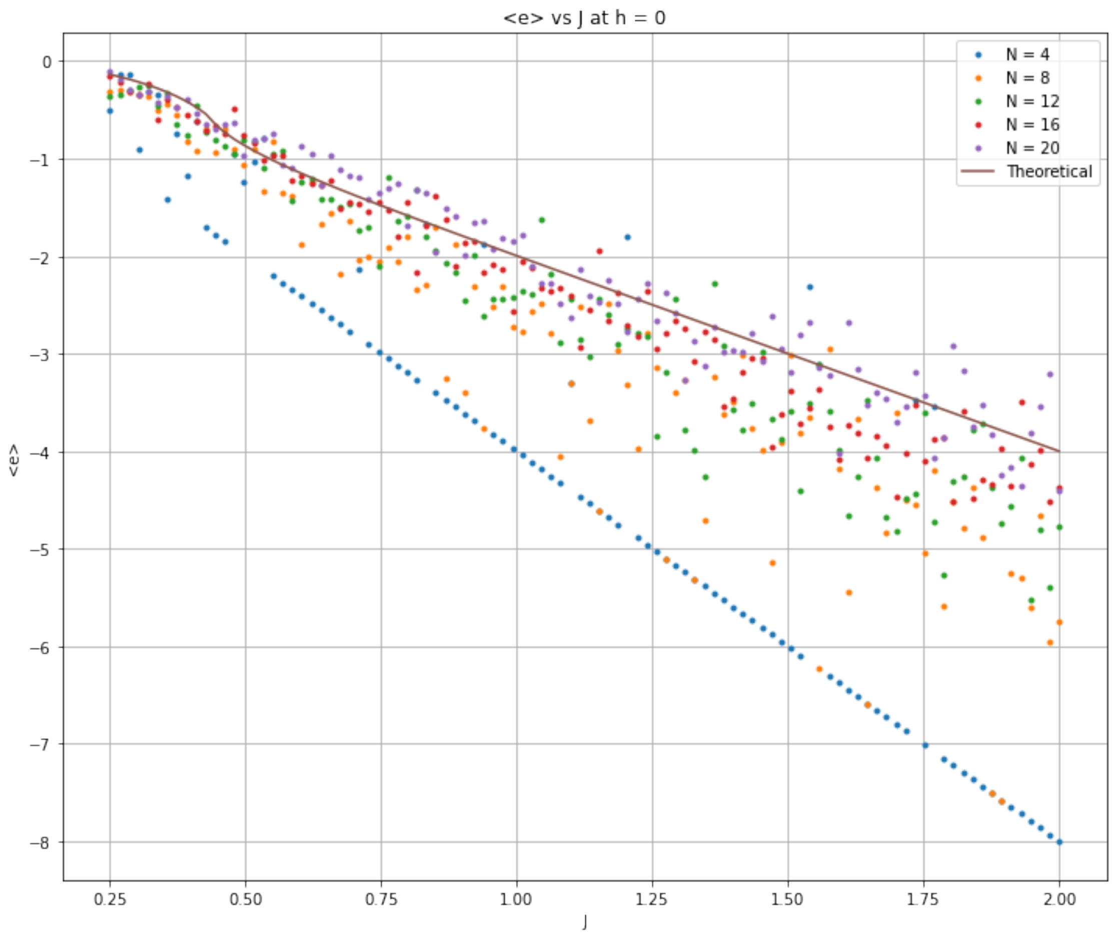
Something to check as <m> goes up in steps

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_rang
e,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>
```



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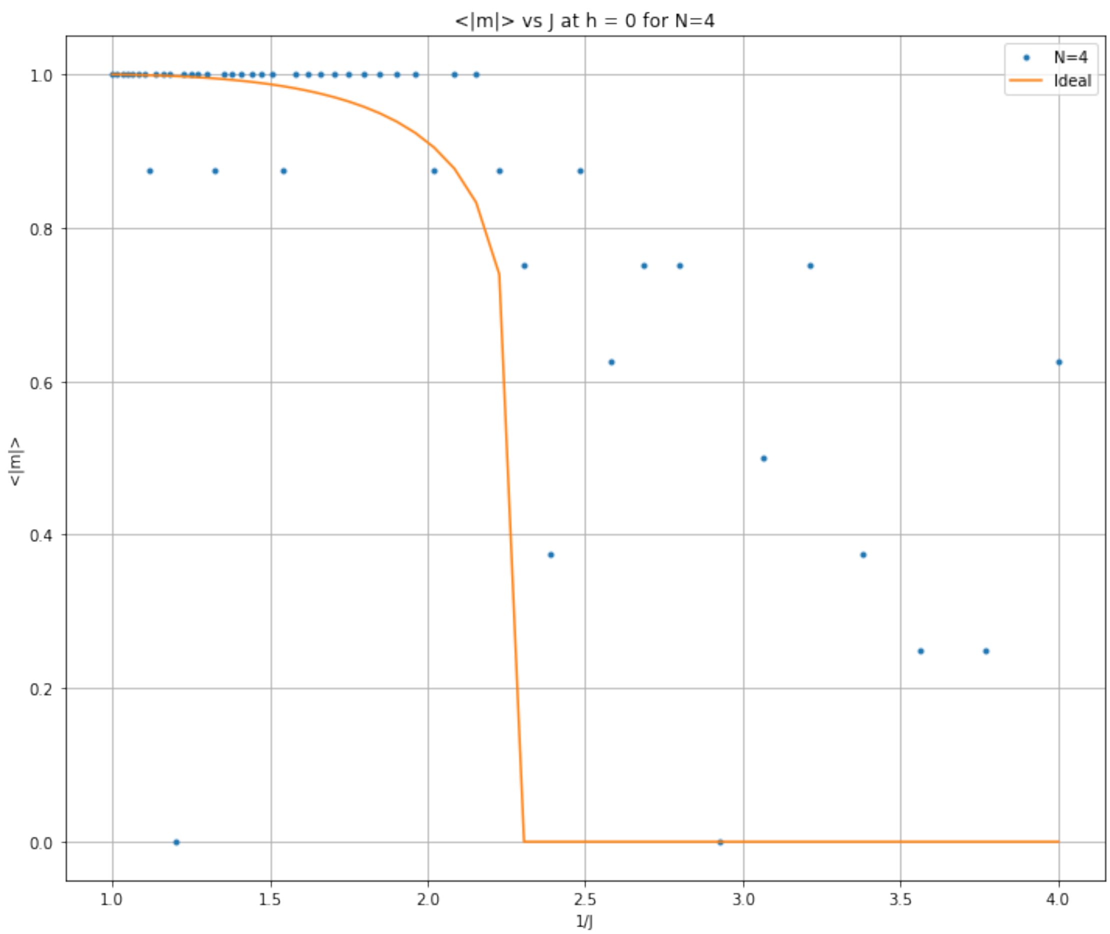
Answer 7 : ¿|m|>¿ vs J at h = 0

```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
```

```
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()
```

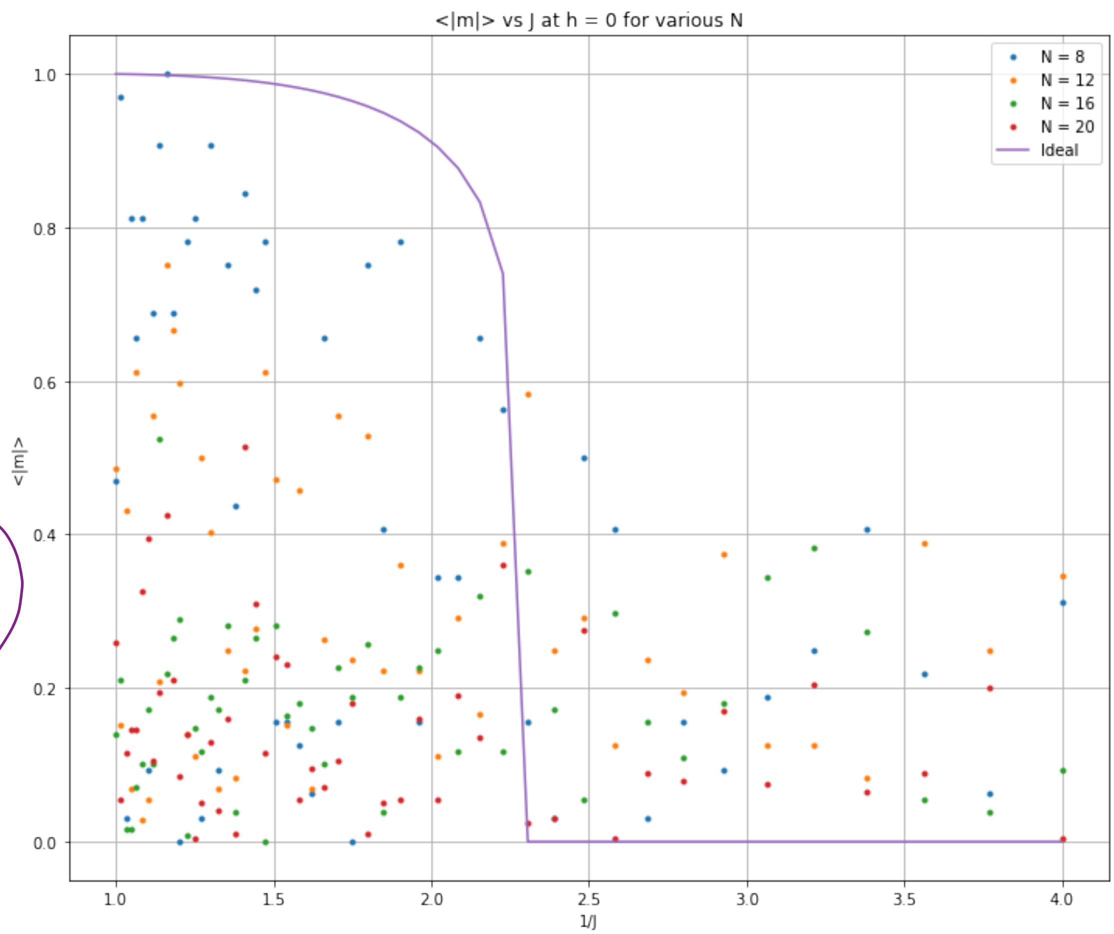
```
<matplotlib.legend.Legend at 0x7f5237f171f0>
```




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

```python
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>
```



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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

Compare $\langle m \rangle$ & $\langle |m| \rangle$ & significance?