Computational Physics
Exercise 3

Yashasvee Goel
Anushka Menon

4] Applying HMC to the long rang Ising model

1. $$\langle O \rangle = \frac{1}{Z} \int \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} O[\phi] e^{-S[\phi]}$$

$$\langle m \rangle = \frac{1}{N\beta} \frac{\partial}{\partial h} \log(Z) = \frac{1}{N\beta} \frac{1}{Z} \frac{\partial Z}{\partial h}$$

$$= \frac{1}{Z} \int \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} m[\phi] e^{-S[\phi]}$$

$$\therefore m[\phi] = \cancel{\frac{\sqrt{2\pi\beta\hat{J}}}{N\beta}} e^{S[\phi]} \frac{\partial^2 Z}{\partial\phi\partial h}$$

$$\frac{\partial^2 Z}{\partial\phi\partial h} = \frac{1}{\cancel{\sqrt{2\pi\beta\hat{J}}}} \left(\frac{\cancel{N}}{\cancel{2}\cosh(\beta h \pm \phi)} \right) \cancel{2}\beta\sinh(\beta h \pm \phi)$$
$$\exp\left(-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))\right)$$

$$\Longrightarrow m[\phi] = \tanh(\beta h \pm \phi) \cdot \exp\left(-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi)) + S[\phi]\right)$$

Similarly,

$$\langle E \rangle = -\frac{1}{N} \frac{\partial}{\partial\beta} \log Z = -\frac{1}{N} \cdot \frac{1}{Z} \frac{\partial Z}{\partial\beta}$$

$$= \frac{1}{\cancel{Z}} \int \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} \; \mathcal{E}[\phi] e^{-S[\phi]}$$

$$\therefore \mathcal{E}[\phi] = -\frac{\cancel{\sqrt{2\pi\beta\hat{J}}}}{N} e^{S[\phi]} \frac{\partial^2 Z}{\partial\phi\partial\beta}$$

$$\frac{\partial^2 Z}{\partial\phi\partial\beta} = \frac{-3}{2\sqrt{2\pi\beta^3\hat{J}}} \exp\left(\frac{-\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))\right)$$

$$+ \frac{1}{\sqrt{2\pi\beta\hat{J}}} \exp\left(\frac{-\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))\right)$$

$$\left(\frac{\phi^2}{2\beta^2\hat{J}} + \frac{N}{\cancel{2}\cosh(\beta h \pm \phi)} (\cancel{2} h \sinh(\beta h \pm \phi))\right)$$

$$= \frac{-1}{\cancel{\sqrt{2\pi\beta\hat{J}}}} \exp\left(\frac{-\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))\right)$$

$$\left(\frac{3}{2\beta} - \frac{\phi^2}{2\beta^2\hat{J}} - Nh\tanh(\beta h \pm \phi)\right)$$

$$\Rightarrow \mathcal{E}[\phi] = \left(\frac{3}{2\beta N} - \frac{\phi^2}{2\beta^2\hat{J}N} - h\tanh(\beta h \pm \phi)\right)$$
$$\exp\left(-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi)) + S[\phi]\right)$$

2. $$\mathcal{H}(p,\phi) = \frac{p^2}{2} + \frac{\phi^2}{2\beta\hat{J}} - N\log(2\cosh(\beta h + \phi))$$

$$\dot{\phi} = \frac{\partial}{\partial p}\mathcal{H} = p$$

$$\dot{p} = -\frac{\partial}{\partial\phi}\mathcal{H} = -\left[\frac{\phi}{\beta\hat{J}} - \frac{N\,\cancel{2}\sinh(\beta h+\phi)}{\cancel{2}\cosh(\beta h+\phi)}\right]$$

$$\therefore \dot{p} = -\frac{\phi}{\beta\hat{J}} + N\tan(\beta h+\phi)$$

Homework 3

November 18, 2022

1 Long range Ising model

1.0.1 Submitted by: Anushka and Yashasvee

1.0.2 Answer 3 : Leap frog Algorithm

[1]:
```
%matplotlib inline

import numpy as np
import matplotlib.pyplot as plt
import scipy.special as sp
import math
```

[2]:
```
def leapfrog(N_md, p_0, phi_0, J, beta, h, N):
    product_pi= p_0
    capital_phi = phi_0

#     The formulas have been defined as given in the sheet.

#    The beginning
    capital_phi += product_pi/(2*N_md)

#    The middle
    for i in range(N_md-1):
        product_pi -= (capital_phi/(beta*J/N)-N*np.tanh(beta*h+capital_phi))/
 ↪N_md
        capital_phi += product_pi/N_md

#     The end
    product_pi -= (capital_phi/(beta*J/N)-N*np.tanh(beta*h+capital_phi))/N_md
    capital_phi += product_pi/(2*N_md)

    return (product_pi,capital_phi)
```

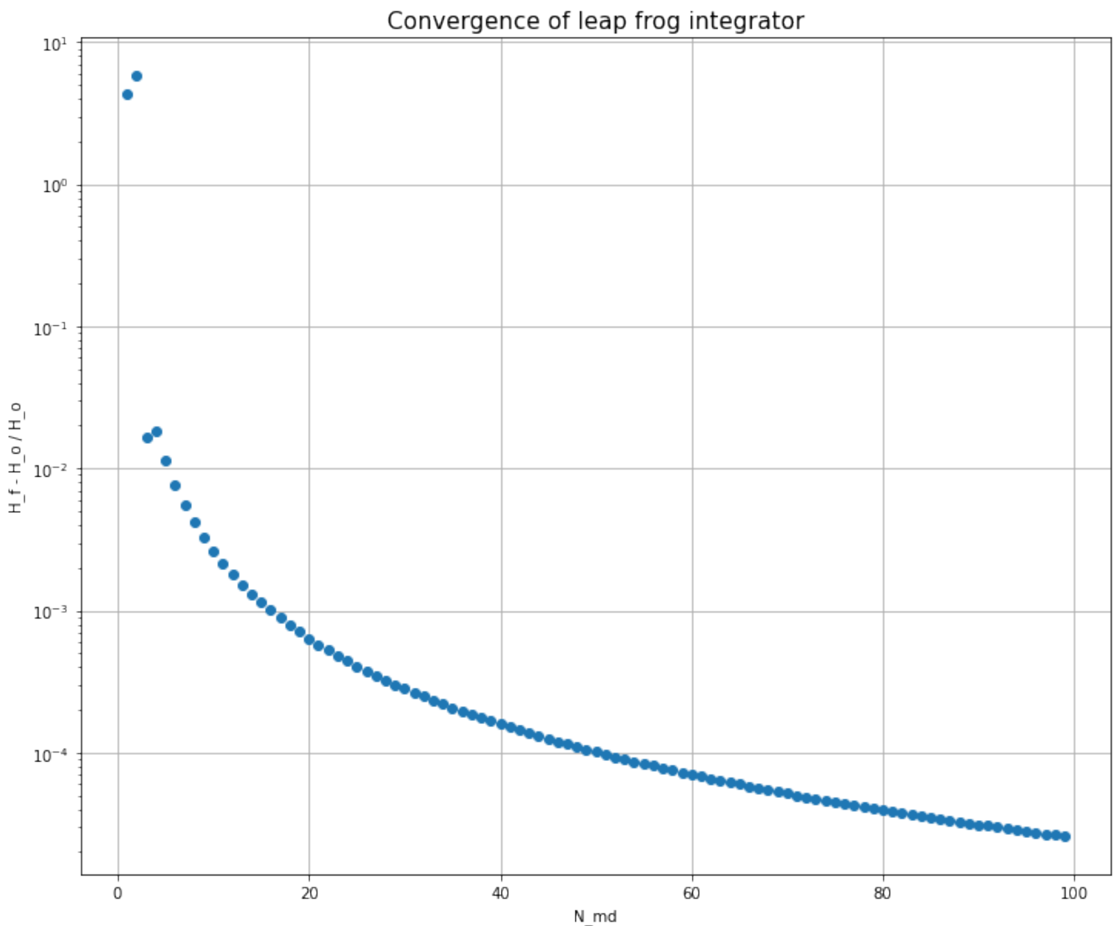
[3]:
```
# Using the artificial Hamiltonian

def hamiltonian(p, phi, J, beta, h, N):
    return p**2/2+phi**2/(2*beta*(J/N))-N*np.log(2*np.cosh(beta*h+phi))
```

[4]:
```
# Defining initial values

p_0 = 0.1
phi_0 = 0.1
J = 0.5       # J should be greater than 0
beta = 1
h = 0.5       # Given
N = 15        # N range is given between 5 to 20
```

[5]:
```
diff = []
range_1 = range(1,100)

for N_md in range_1:
    arr = leapfrog(N_md, p_0, phi_0, J, beta, h, N)
    p_f = arr[0]           # We need final values of p_f and phi_f to calculate␣
 ↪H_f
    phi_f = arr[1]
    H_f = hamiltonian(p_f, phi_f, J, beta, h, N)
    H_0 = hamiltonian(p_0, phi_0, J, beta, h, N)

#     The following is the quantity we want on y-axis
    diff.append(abs((H_f-H_0)/H_0))
```

[6]:
```
plt.figure(figsize=(12,10))
plt.yscale('log')
plt.grid()
plt.xlabel("N_md")
plt.ylabel("H_f - H_o / H_o")
plt.title("Convergence of leap frog integrator", fontsize =15)
plt.plot(range_1, diff,'o')
```

[6]: [<matplotlib.lines.Line2D at 0x7ff2ae7047f0>]



1.0.3 Answer 4 : HMC Algorithm

[7]:
```
# Now we code the HMC algorithm

# Understanding: We sample from N space and integrate the EOM's using leapfrog
↪to get p' and phi'
# Then we accept the value of phi' with the Metropolis accept/reject (with the
↪given prob.) and repeat the process
# To keep in mind: We store every value of phi regardless to generate our
↪Markov chain. If the algorithm rejcts phi' we
# store phi

# So we need to accept and reject according to the probability distribution
↪given in the sheet which is basically exp(H)

# Size of ensemble is given as N_cfg

def markov_chain(phi_i,N_cfg,N_md,beta,J,h,N):
```

```
    chain = []
    chain.append(phi_i)
    for i in range(N_cfg):
        p = np.random.normal(0,1)  # Random sample
        new = leapfrog(N_md, p, chain[-1], J, beta, h, N) # Integrating␣
 ↪leapfrog algorithm
        prob = np.exp(hamiltonian(p,chain[-1], J, beta, h,␣
 ↪N)-hamiltonian(new[0], new[1], J, beta, h, N))
#  Given probability distribution function defined above
        if prob > np.random.uniform(0,1):   # Accept/reject
            chain.append(new[1])
        else:
            chain.append(chain[-1])
    return chain
```

[8]:
```
#  Now we need to define observables(m and E), that will be similar to the one␣
 ↪done in Homework 2

def variables(phi_i, N_cfg, N_md, J, beta, h, N, obs):
    chain = markov_chain(phi_i,N_cfg,N_md,beta,J,h,N)
#     From Part 1 we have the equations foe <m> and E so we use them here:
    m = 0.0
    E = 0.0
    for i in range(len(chain)):
        m+= np.tanh(beta*h + chain[i])
        E+= -((chain[i]**2)/(2*(J/N)*(beta**2))+(N*h*np.tanh(beta*h +␣
 ↪chain[i])))/N
    m = m/N_cfg
    E = E/N_cfg
    if obs == "m":
        var = m
    if obs == "E":
        var = E

    return var
```

1.0.4 Answer 5 : Average energy per site, ϵ, as a function of J

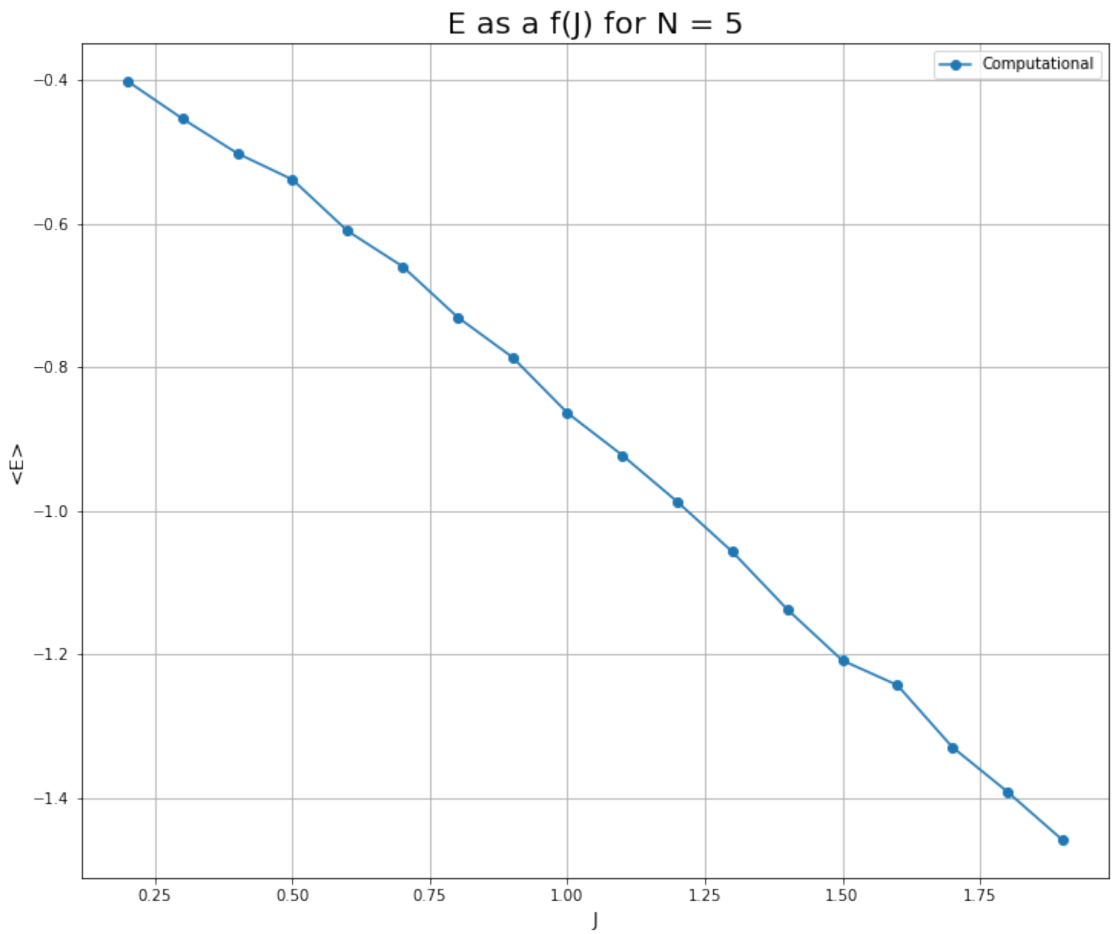
[17]:
```
# We have to also plot the th. functions (the last 3 equations in the sheet),␣
 ↪therefore, we define them as follows:

# import math
# T=1
# def func(j,x):
#     return(np.exp(0.5*j*x**2/T + h*x/T))
```

```
# # The math.comb() method returns the number of ways picking k unordered␣
↪outcomes from n possibilities,
# # without repetition, also known as combinations.

# def z_17(J,beta,h,N):
#     for n in range(N):
#         z+=math.comb(N,n)*func(J/N,N-2*n)
#     return z

# def E_18(J, beta, h, N):
#     Energy = 0.0
#     for n in range(N):
#         Energy += math.comb(N, n) * (0.5*beta*J/N*(N-2*n)**2+beta*h*(N-2*n))␣
↪*func(J,N-2*n)
#     return Energy
```

Doubt: When I uncomment the code for analytic equations, even my computational graphs change, I do not understand what is happening here. Also, the theoretical curves are not coming out to be right.

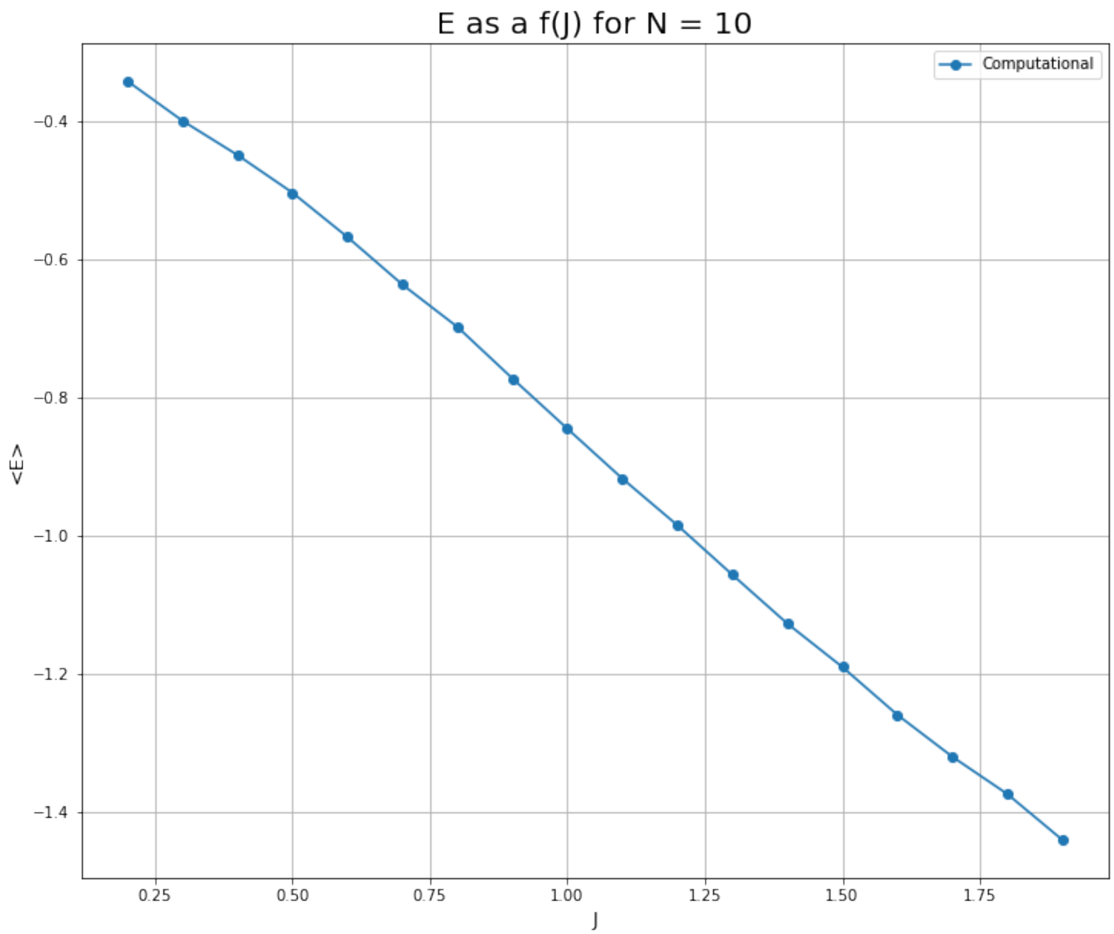
[18]:
```
# Average energy per site for different values of N

h = 0.5
# Given, beta*h = h so beta =1
beta = 1
N_md = 25
N_cfg = 4000
range_2 = np.arange(0.2,2,0.1) # Given
phi_random = np.random.normal(0,1)

energy_5 = [variables(phi_random, N_cfg, N_md, J, beta, h, 5, "E") for J in␣
↪range_2]
# e_18_5 = [E_18(J,beta,h,5) for J in range_2]
plt.figure(figsize = (12,10))
plt.plot(range_2, energy_5, 'o-',label="Computational")
# plt.plot(range_2, e_18_5, 'o-',label="Theoretical")
plt.grid()
plt.xlabel("J", fontsize = 13)
plt.ylabel("<E>", fontsize = 13)
plt.legend()
plt.title("E as a f(J) for N = 5", fontsize = 20 )
```

[18]:
```
Text(0.5, 1.0, 'E as a f(J) for N = 5')
```



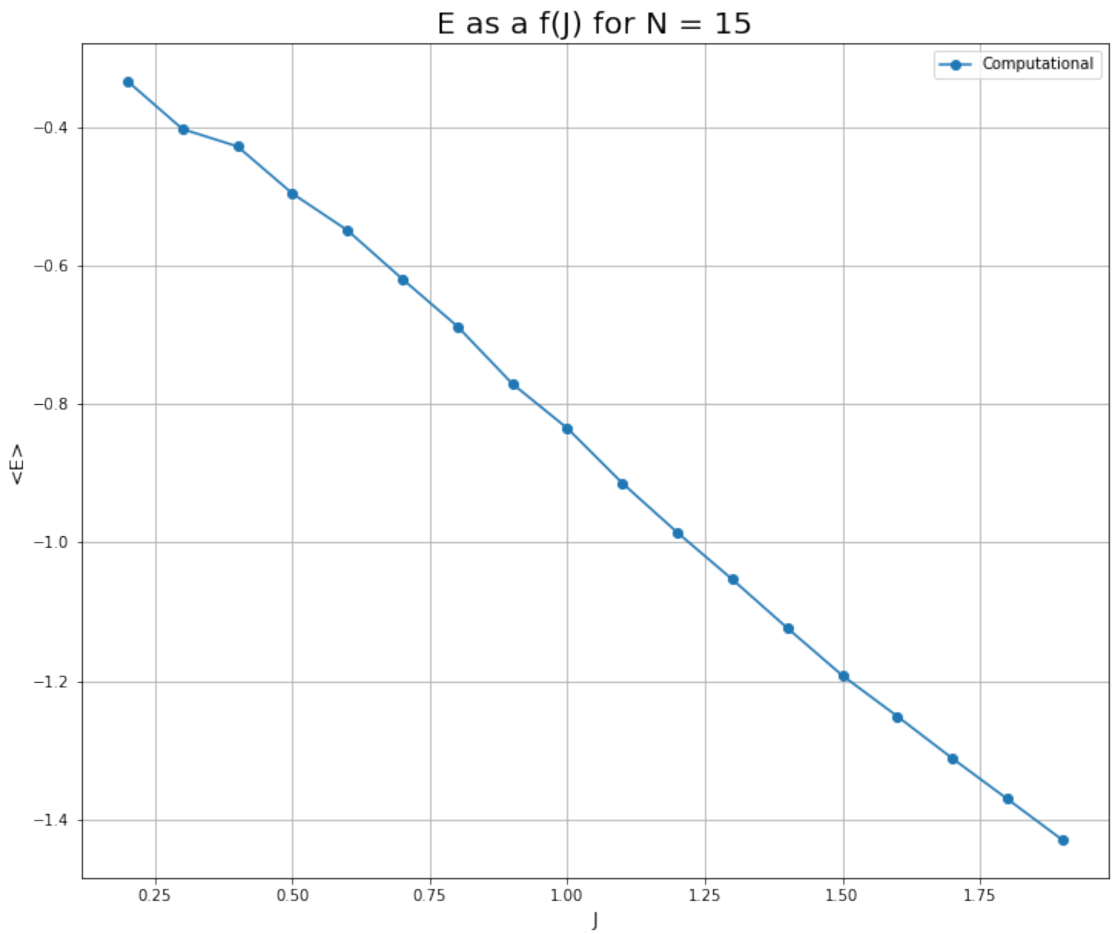
[19]:
```
energy_10 = [variables(phi_random, N_cfg, N_md, J, beta, h, 10, "E") for J in
  range_2]
plt.figure(figsize = (12,10))
plt.plot(range_2, energy_10, 'o-',label="Computational")
plt.grid()
plt.xlabel("J", fontsize = 13)
plt.ylabel("<E>", fontsize = 13)
plt.legend()
plt.title("E as a f(J) for N = 10", fontsize = 20 )
```

[19]:
```
Text(0.5, 1.0, 'E as a f(J) for N = 10')
```



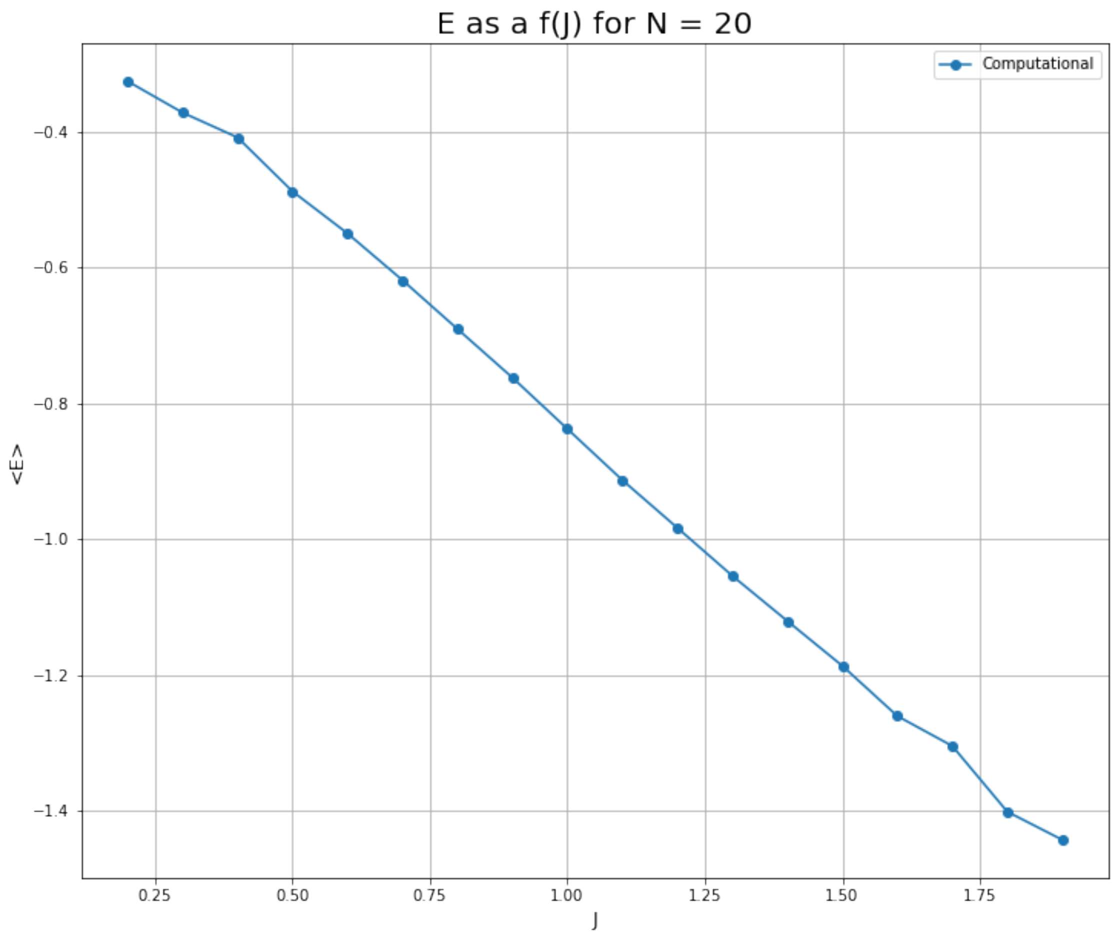
[20]:
```python
energy_15 = [variables(phi_random, N_cfg, N_md, J, beta, h, 15, "E") for J in␣
    ↪range_2]
plt.figure(figsize = (12,10))
plt.plot(range_2, energy_15, 'o-',label="Computational")
plt.grid()
plt.xlabel("J", fontsize = 13)
plt.ylabel("<E>", fontsize = 13)
plt.legend()
plt.title("E as a f(J) for N = 15", fontsize = 20 )
```

[20]: Text(0.5, 1.0, 'E as a f(J) for N = 15')



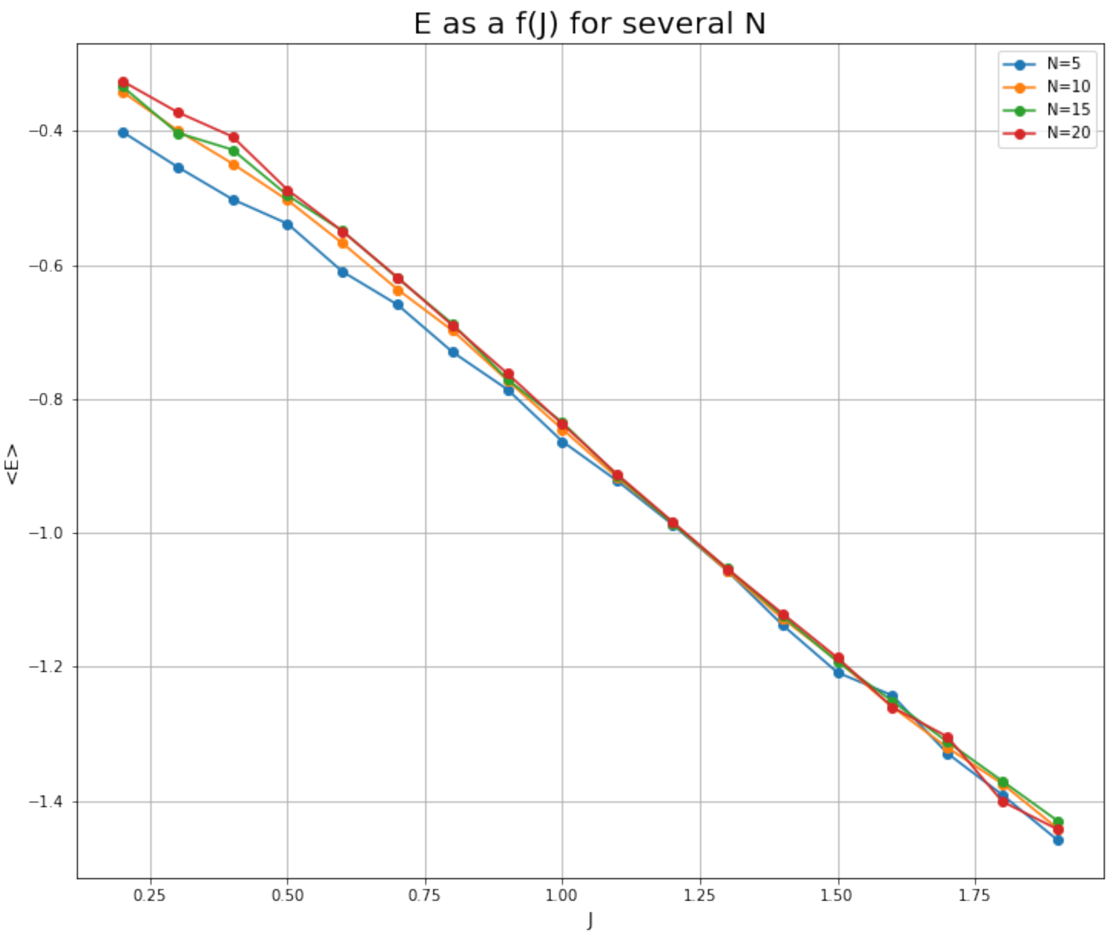
[21]:
```
energy_20 = [variables(phi_random, N_cfg, N_md, J, beta, h, 20, "E") for J in␣
 ↪range_2]
plt.figure(figsize = (12,10))
plt.plot(range_2, energy_20, 'o-', label="Computational")

plt.grid()
plt.xlabel("J", fontsize = 13)
plt.ylabel("<E>", fontsize = 13)
plt.legend()
plt.title("E as a f(J) for N = 20", fontsize = 20 )
```

[21]:
```
Text(0.5, 1.0, 'E as a f(J) for N = 20')
```



[22]:
```
plt.figure(figsize=(12,10))
plt.grid()
plt.plot(range_2, energy_5, 'o-', label = "N=5")
plt.plot(range_2, energy_10, 'o-',label = "N=10")
plt.plot(range_2, energy_15, 'o-',label = "N=15")
plt.plot(range_2, energy_20, 'o-',label = "N=20")
plt.xlabel("J", fontsize = 13)
plt.ylabel("<E>", fontsize = 13)
plt.legend()
plt.title("E as a f(J) for several N", fontsize = 20 )
```

[22]:
```
Text(0.5, 1.0, 'E as a f(J) for several N')
```



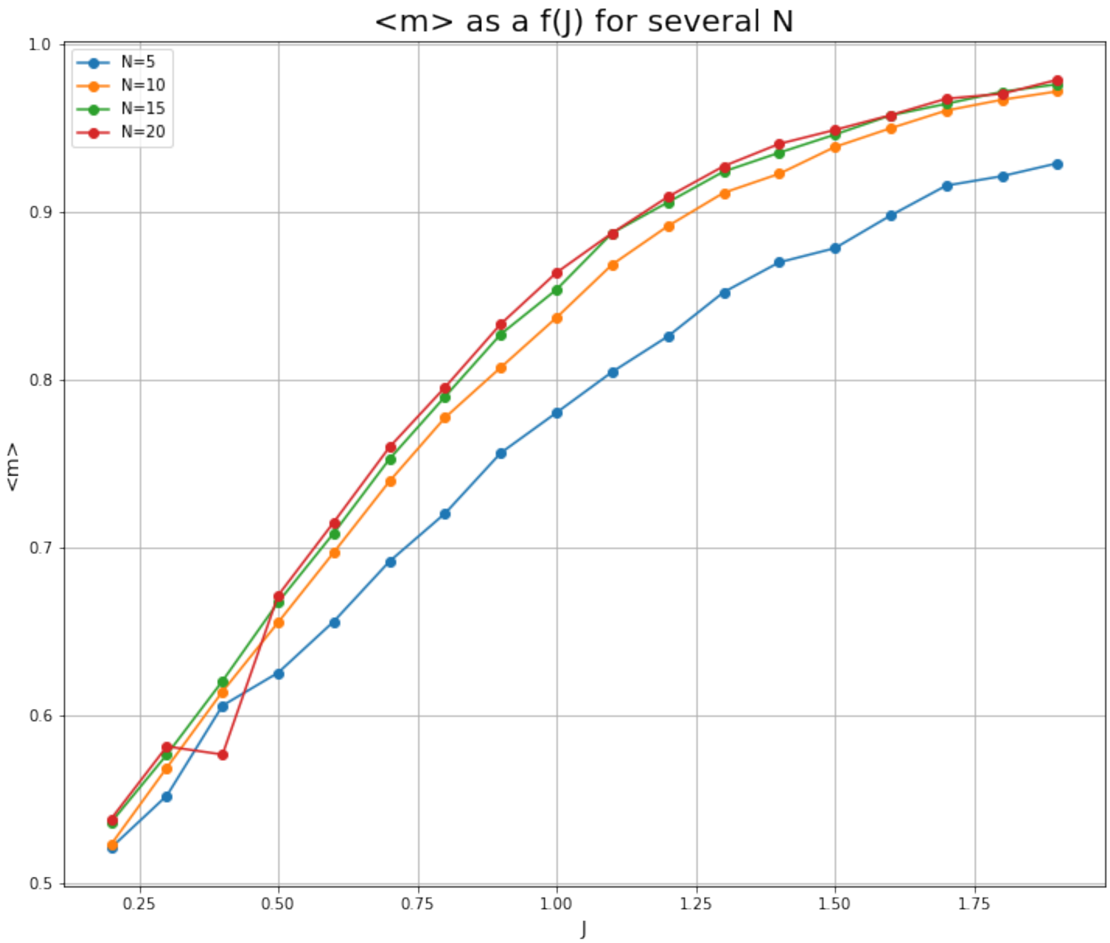
1.0.5 Answer 5 : Magnetization, $< m >$, as a function of J

[23]:
```
m_5 =  [variables(phi_random, N_cfg, N_md, J, beta, h, 5, "m") for J in range_2]
m_10 = [variables(phi_random, N_cfg, N_md, J, beta, h, 10, "m") for J in␣
 ↪range_2]
m_15 = [variables(phi_random, N_cfg, N_md, J, beta, h, 15, "m") for J in␣
 ↪range_2]
m_20 = [variables(phi_random, N_cfg, N_md, J, beta, h, 20, "m") for J in␣
 ↪range_2]
```

[24]:
```
plt.figure(figsize=(12,10))
plt.grid()
plt.plot(range_2, m_5, 'o-', label = "N=5")
plt.plot(range_2, m_10, 'o-',label = "N=10")
plt.plot(range_2, m_15, 'o-',label = "N=15")
plt.plot(range_2, m_20, 'o-',label = "N=20")
plt.xlabel("J", fontsize = 13)
```

```
plt.ylabel("<m>", fontsize = 13)
plt.legend()
plt.title("<m> as a f(J) for several N", fontsize = 20 )
```

[24]: Text(0.5, 1.0, '<m> as a f(J) for several N')



[ ]:

[ ]: