Computational Physics Homework Sheet - 3

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In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
import random as r
from tqdm import tqdm
import math
```

Theoretical Questions

Que-1) Use the expression above and the fact that the mean magnetization (per site) and energy (per site) are given by to derive corresponding expressions for $O[\phi]$ for these quantities

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

Given,

$$Z[J>0] = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\beta\hat{J}|}} e^{\frac{-\phi^2}{2\beta\hat{J}} + Nlog(2cosh(\beta h \pm \phi))}$$

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

$$\frac{\partial Z}{\partial h} = \int \frac{d\phi}{\sqrt{2\pi\beta|\beta\hat{J}|}} e^{\frac{-\phi^2}{2\beta\hat{J}} + Nlog(2cosh(\beta h \pm \phi))} \times N\beta \frac{2sinh(\beta h \pm \phi)}{2cosh(\beta h \pm \phi)} = N\beta \int \frac{d\phi}{\sqrt{2\pi\beta|\beta\hat{J}|}} e^{\frac{-\phi^2}{2\beta\hat{J}} + Nlog(2cosh(\beta h \pm$$

Substituting this in $\langle m \rangle$

$$\langle m \rangle = \frac{1}{Z} \int \frac{d\phi}{2\pi\beta\hat{J}} \; tanh(\beta h \pm \phi) e^{-S[\phi]}$$
$$\therefore O[\phi] = tanh(\beta h \pm \phi)$$

For energy,

$$\langle \epsilon \rangle = -\frac{1}{N} \frac{\partial}{\partial \beta} log(Z) = -\frac{1}{NZ} \frac{\partial Z}{\partial \beta}$$

$$\frac{\partial Z}{\partial \beta} = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{\frac{-\phi^2}{2\beta\hat{J}} + Nlog(2cosh(\beta h \pm \phi))} \left[-\frac{1}{2\beta} + \frac{\phi^2}{2J\beta^2} + Nhtanh(\beta h \pm \phi) \right]$$

$$\langle \epsilon \rangle = -\frac{1}{N} \frac{\partial}{\partial \beta} log(Z) = -\frac{1}{NZ} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{-S[\phi]} \left[-\frac{1}{2\beta} + \frac{\phi^2}{2\hat{J}\beta^2} + Nh\tanh(\beta h \pm \phi) \right]$$

$$\therefore O[\phi] = \left[\frac{1}{2N\beta} - \frac{\phi^2}{2N\hat{J}\beta^2} - h\tanh(\beta h \pm \phi) \right]$$

Que-2) Determine the equations of motion (EoMs) for this Hamiltonian by applying the Hamilton equations.

$$\dot{\phi} = \frac{\partial H}{\partial p} = p$$
$$\dot{p} = -\frac{\partial H}{\partial \phi} = -\frac{\phi}{\beta \hat{J}} + Ntanh(\beta h + \phi)$$

In [2]:

```
N=5
T=0.5
h=1.
j=1/N
```

In [3]:

```
def H(p,phi):
    return 0.5*p**2 + (0.5*T*phi**2)/j -(N)*np.log(2*np.cosh(h/T+phi))
def phidot(p):
    return (p)
def pdot(phi):
    return(-phi*T/j + N*np.tanh(h/T+phi))
```

In [4]:

```
def leapfrog(p,phi,n):
    epsilon=1/n ## if the length if trajectory is 1: $p^2+ phi^2=1$
    P,Phi=p,phi
    P=p+epsilon*0.5*pdot(phi)
    for i in range(n):
        Phi= Phi + epsilon*phidot(P)
        P=P+epsilon*pdot(Phi)

    P=P-0.5*epsilon*pdot(Phi)
    return P,Phi
```

In [5]:

```
def deltaH (p,phi,P,Phi):
    Prob=min([1,np.exp(H(p,phi)-H(P,Phi))])
    #print(np.exp(H(p,phi)-H(P,Phi)))
    if(Prob<1):
        #print(Prob)
        a=np.random.uniform(0,1)
        if(a<Prob):
            Prob=1

    if(Prob==1):
        return Prob,P,Phi
    else:
        return Prob,p,phi
```

In [6]:

```
## Bootstrap error
def bootstrap(marr):
    means = []
    for j in range(8):
        Marr = []
        for i in range(10):
            Marr.append(np.random.choice(marr))
        means.append(np.mean(Marr))

    Me = np.mean(means)
    var = 0
    for i in range(8):
        var += (means[i] - Me)**2

    std = np.sqrt(var/8)
    return std
```

In [7]:

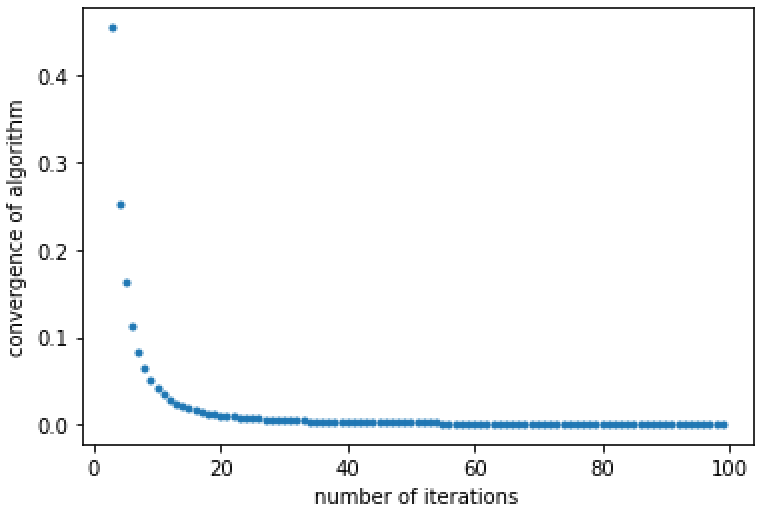
```
po=1.
phio=-2
DH=[]
Nar=[i for i in range(3,100)]
for i in range(3,100):
    Pf,Phif=leapfrog(po,phio,i)
    DH.append(abs((H(Pf,Phif)-H(po,phio))/H(po,phio)))
```

In [8]:

```
plt.plot(Nar,DH,'.')
plt.xlabel("number of iterations")
plt.ylabel("convergence of algorithm")
```

Out[8]:

```
Text(0, 0.5, 'convergence of algorithm')
```



The trend matches the trend shown in Figure 1 given in the exercise sheet 3.

HMC

In [26]:

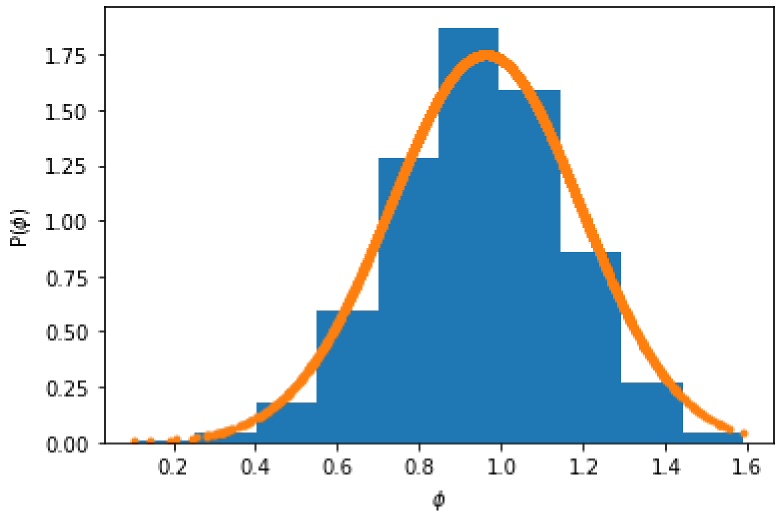
```
phyarr=[]
for i in range(5000):
    p=np.random.normal(0,1)
    phi=1
    pf,phif=leapfrog(p,phi,100) ## Leapfrog convergence is good enough for n=100
    prob,P_f,Phi_f=deltaH(p,phi,pf,phif)
    p,phi=P_f,Phi_f
    if(i>500):
        phyarr.append(phi)
```

In [27]:

```
plt.hist(phyarr,bins=10,density=1)
N=20
T=1
h = 1
j=1/N
phyarr = np.array(phyarr)
p = np.linspace(0,2)
Pth = np.exp(-T*phyarr**2/(2*1*j))*np.exp(N*np.log(2*np.cosh(h/T + phyarr)))
Pth = 1.75*Pth/max(Pth)
plt.plot(phyarr,Pth,'.')
plt.xlabel('$\phi$')
plt.ylabel('P($\phi$)')
```

Out[27]:

```
Text(0, 0.5, 'P($\\phi$)')
```



In [11]:

```
h=0.5
T=1.
J=np.linspace(0.2,2,15)
N=5
earr=[]
marr=[]


for k in tqdm(range(len(J))):
    count = 0
    mavg=0
    eavg=0
    j=J[k]/N
    phyarr=[]
    for i in range(5000):
        p=np.random.normal(0,1)
        phi=1
        pf,phif=leapfrog(p,phi,100) ## Leapfrog convergence is good enough for n=50
        prob,P_f,Phi_f=deltaH(p,phi,pf,phif)
        if(prob==1):
            count += 1

        p,phi=P_f,Phi_f
        if(i>500):
            phyarr.append(phi)
            mavg+=np.tanh(h/T+phyarr[i-501])
            eavg+=(0.5*T/N-0.5*phyarr[i-501]**2*T**2/(N*j)-h*np.tanh(h/T+phyarr[i-501]))
        #print(mavg)
    #print(count/5000)
    mavg=mavg/len(phyarr)
    eavg=eavg/len(phyarr)
    earr.append(eavg)
    marr.append(mavg)
```

```
100%|████████████████████████████████████████████████████████████████████
██████████| 15/15 [00:27<00:00,  1.86s/it]
```

In [12]:

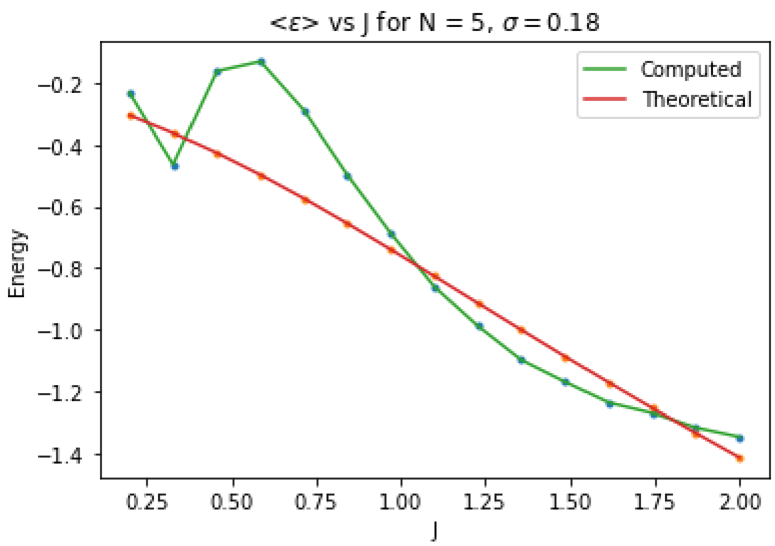
```
def f (j,x):
    return(np.exp(0.5*j*x**2/T + h*x/T))
```

In [13]:

```
Z=np.zeros(len(J))
E=np.zeros(len(J))

for i in range(N+1):
    Z+=math.comb(N,i)*f(J/N,N-2*i)

for i in range(N + 1):
        E+= -(math.comb(N,i)*((0.5*(J/N)*(N - 2*i)**2)/T + h*(N - 2*i)/T)*f(J/(N*T),N-2*i))


std = bootstrap(earr)
plt.title('<$\epsilon$> vs J for N = 5, $\sigma = %s$'%np.round(std,2))
plt.plot(J,earr,".",)
plt.plot(J,E,'.')
plt.plot(J,earr,label = 'Computed')
plt.plot(J,E,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("Energy")
plt.legend()
```

Out[13]:

```
<matplotlib.legend.Legend at 0x1de911cf9a0>
```

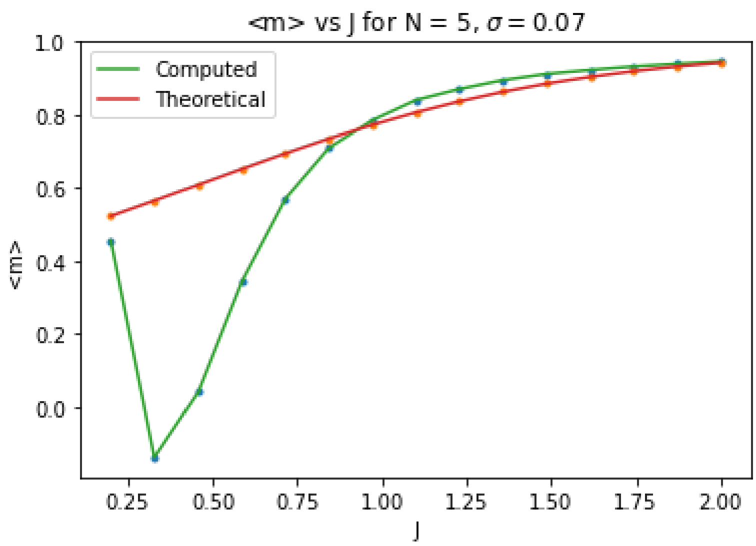


In [14]:

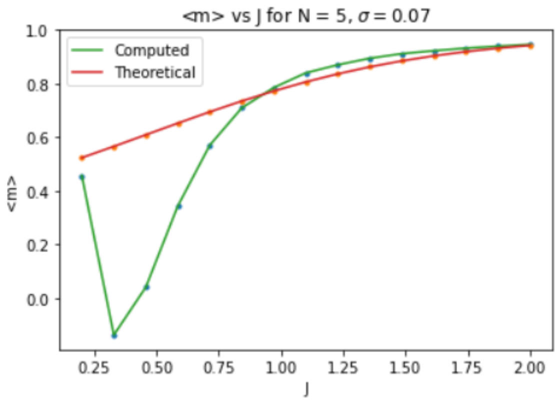
```
M = np.zeros(len(J))

for i in range(N + 1):
        M+= (math.comb(N,i)*((N - 2*i)*f(J/(N*T),N-2*i))/(Z*N))

std = bootstrap(marr)
plt.title('<m> vs J for N = 5, $\sigma = %s$'%np.round(std,2))
plt.plot(J,marr,'.')
plt.plot(J,M,'.')
plt.plot(J,marr,label = 'Computed')
plt.plot(J,M,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("<m>")
plt.legend()
```

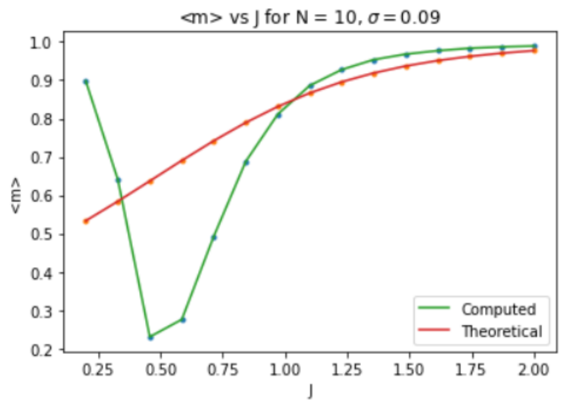
Out[14]:

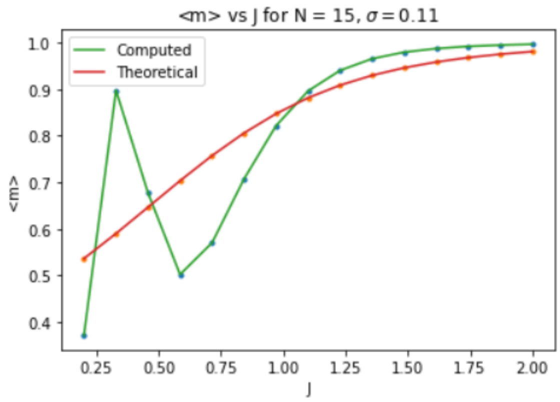
```
<matplotlib.legend.Legend at 0x1de912a1d30>
```

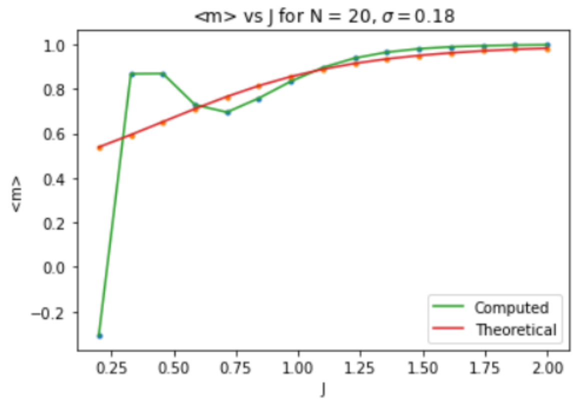


Plots of $< m >$ vs J

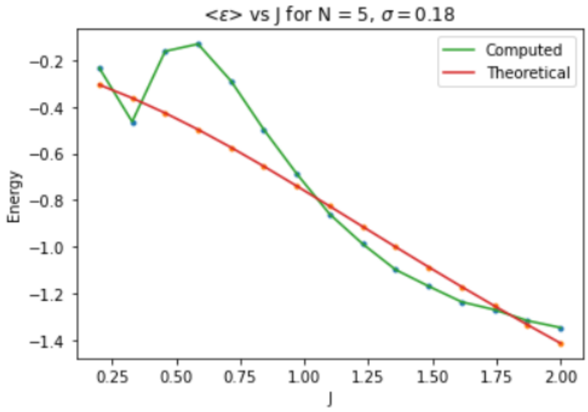


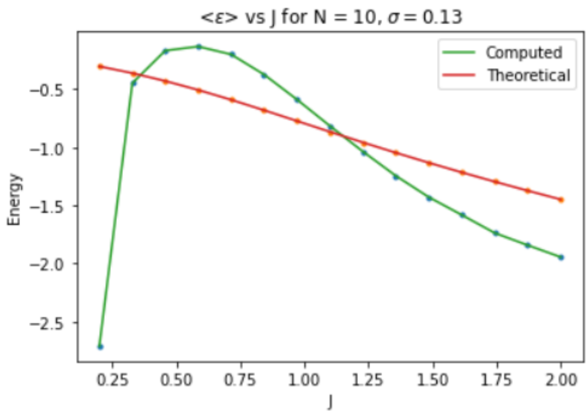


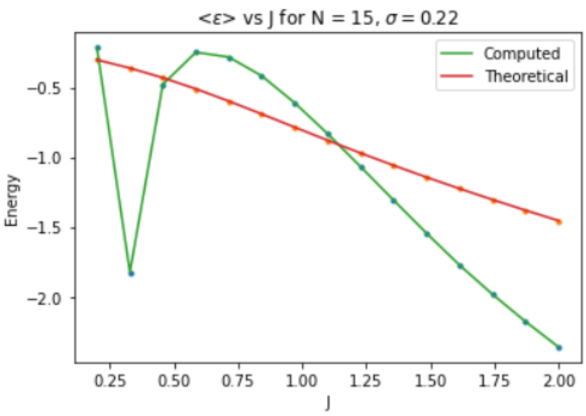


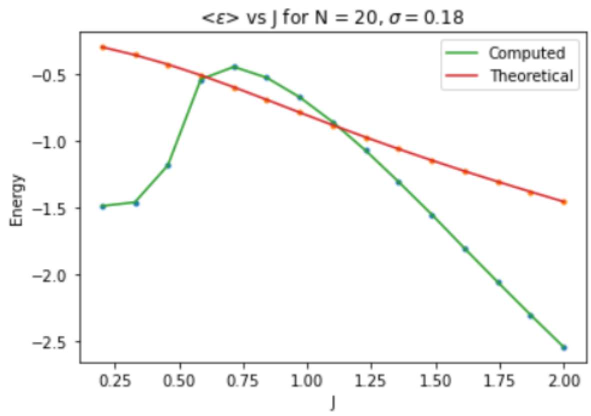


Plots of $< \epsilon >$ vs J









All the plots that we have obtained for different N's have been obtained from the

code written below. We have used the same variables throughout so run the whole code in order.

In [15]:

```
h=0.5
T=1.
J=np.linspace(0.2,2,15)
N=10
earr=[]
marr=[]


for k in tqdm(range(len(J))):
    count = 0
    mavg=0
    eavg=0
    j=J[k]/N
    phyarr=[]
    for i in range(5000):
        p=np.random.normal(0,1)
        phi=1
        pf,phif=leapfrog(p,phi,100) ## Leapfrog convergence is good enough for n=50
        prob,P_f,Phi_f=deltaH(p,phi,pf,phif)
        if(prob==1):
            count += 1

        p,phi=P_f,Phi_f
        if(i>500):
            phyarr.append(phi)
            mavg+=np.tanh(h/T+phyarr[i-501])
            eavg+=(0.5*T/N-0.5*phyarr[i-501]**2*T**2/(N*j)-h*np.tanh(h/T+phyarr[i-501]))
        #print(mavg)
    #print(count/5000)
    mavg=mavg/len(phyarr)
    eavg=eavg/len(phyarr)
    earr.append(eavg)
    marr.append(mavg)
```

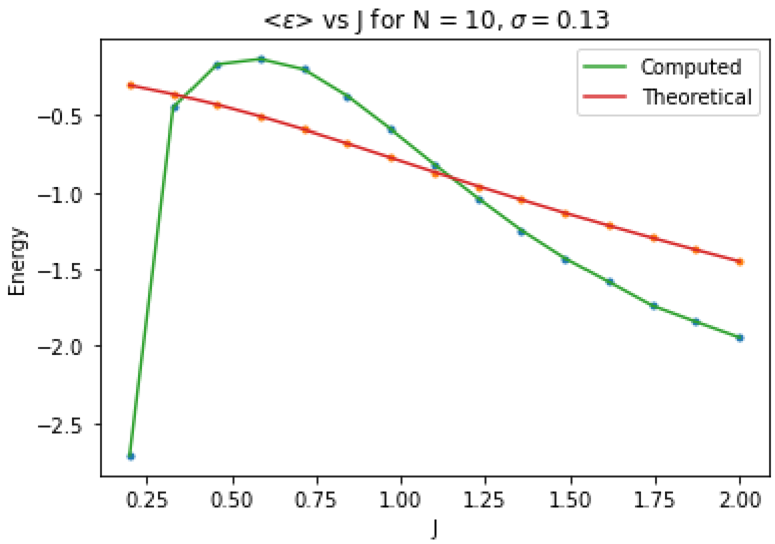
```
100%|██████████████████████████████████████████████████████████████████████████████████████████| 15/15 [00:28<00:00,  1.87s/it]
```

In [16]:

```
Z=np.zeros(len(J))
E=np.zeros(len(J))

for i in range(N+1):
    Z+=math.comb(N,i)*f(J/N,N-2*i)

for i in range(N + 1):
        E+= -(math.comb(N,i)*((0.5*(J/N)*(N - 2*i)**2)/T + h*(N - 2*i)/T)*f(J/(N*T),N-2*i))


std = bootstrap(earr)
plt.title('<$\epsilon$> vs J for N = 10, $\sigma = %s$'%np.round(std,2))
plt.plot(J,earr,".",)
plt.plot(J,E,'.')
plt.plot(J,earr,label = 'Computed')
plt.plot(J,E,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("Energy")
plt.legend()
```

Out[16]:

```
<matplotlib.legend.Legend at 0x1de91302c40>
```

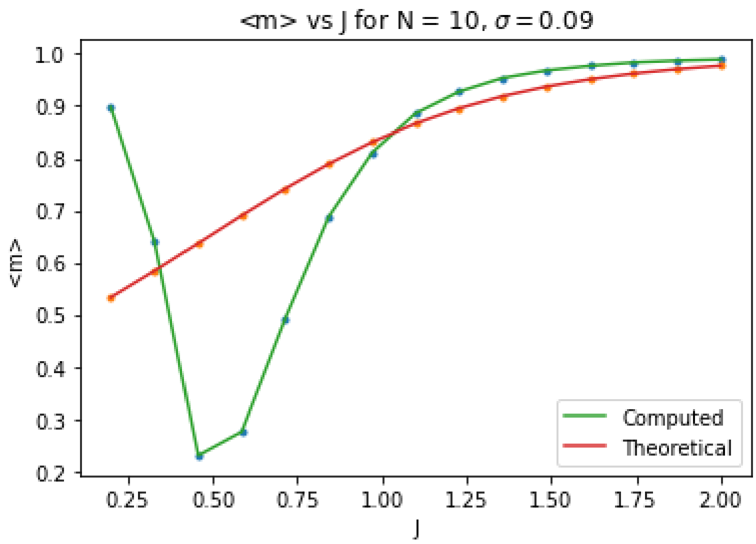


In [17]:

```
M = np.zeros(len(J))

for i in range(N + 1):
        M+= (math.comb(N,i)*((N - 2*i)*f(J/(N*T),N-2*i))/(Z*N))


std = bootstrap(marr)
plt.title('<m> vs J for N = 10, $\sigma = %s$'%np.round(std,2))
plt.plot(J,marr,'.')
plt.plot(J,M,'.')
plt.plot(J,marr,label = 'Computed')
plt.plot(J,M,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("<m>")
plt.legend()
```

Out[17]:

```
<matplotlib.legend.Legend at 0x1de91387c70>
```



In [18]:

```
h=0.5
T=1.
J=np.linspace(0.2,2,15)
N=15
earr=[]
marr=[]


for k in tqdm(range(len(J))):
    count = 0
    mavg=0
    eavg=0
    j=J[k]/N
    phyarr=[]
    for i in range(5000):
        p=np.random.normal(0,1)
        phi=1
        pf,phif=leapfrog(p,phi,100) ## Leapfrog convergence is good enough for n=50
        prob,P_f,Phi_f=deltaH(p,phi,pf,phif)
        if(prob==1):
            count += 1

        p,phi=P_f,Phi_f
        if(i>500):
            phyarr.append(phi)
            mavg+=np.tanh(h/T+phyarr[i-501])
            eavg+=(0.5*T/N-0.5*phyarr[i-501]**2*T**2/(N*j)-h*np.tanh(h/T+phyarr[i-501]))
        #print(mavg)
    #print(count/5000)
    mavg=mavg/len(phyarr)
    eavg=eavg/len(phyarr)
    earr.append(eavg)
    marr.append(mavg)
```

```
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```
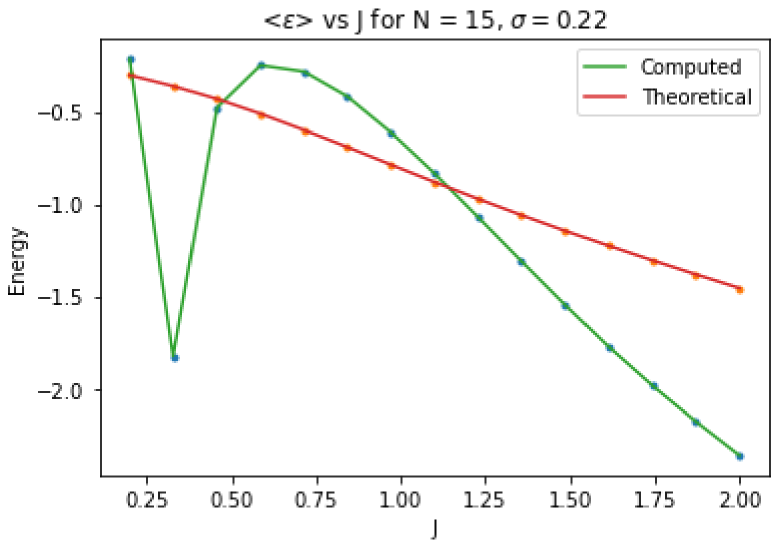

In [19]:

```
Z=np.zeros(len(J))
E=np.zeros(len(J))

for i in range(N+1):
    Z+=math.comb(N,i)*f(J/N,N-2*i)

for i in range(N + 1):
        E+= -(math.comb(N,i)*((0.5*(J/N)*(N - 2*i)**2)/T + h*(N - 2*i)/T)*f(J/(N*T),N-2*i))


std = bootstrap(earr)
plt.title('<$\epsilon$> vs J for N = 15, $\sigma = %s$'%np.round(std,2))
plt.plot(J,earr,".",)
plt.plot(J,E,'.')
plt.plot(J,earr,label = 'Computed')
plt.plot(J,E,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("Energy")
plt.legend()
```

Out[19]:

```
<matplotlib.legend.Legend at 0x1de913cf2e0>
```

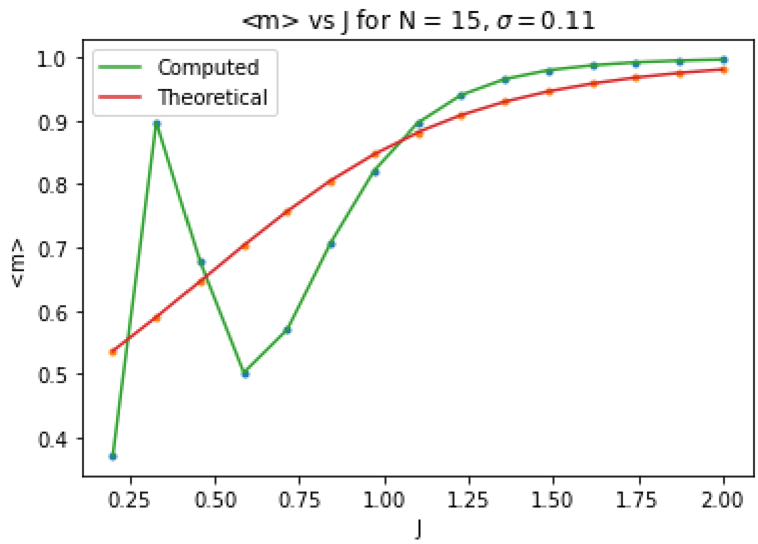


In [20]:

```
M = np.zeros(len(J))

for i in range(N + 1):
        M+= (math.comb(N,i)*((N - 2*i)*f(J/(N*T),N-2*i))/(Z*N))


std = bootstrap(marr)
plt.title('<m> vs J for N = 15, $\sigma = %s$'%np.round(std,2))
plt.plot(J,marr,'.')
plt.plot(J,M,'.')
plt.plot(J,marr,label = 'Computed')
plt.plot(J,M,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("<m>")
plt.legend()
```

Out[20]:

```
<matplotlib.legend.Legend at 0x1de914718b0>
```



In [21]:

```
h=0.5
T=1.
J=np.linspace(0.2,2,15)
N=20
earr=[]
marr=[]


for k in tqdm(range(len(J))):
    count = 0
    mavg=0
    eavg=0
    j=J[k]/N
    phyarr=[]
    for i in range(5000):
        p=np.random.normal(0,1)
        phi=1
        pf,phif=leapfrog(p,phi,100) ## Leapfrog convergence is good enough for n=50
        prob,P_f,Phi_f=deltaH(p,phi,pf,phif)
        if(prob==1):
            count += 1

        p,phi=P_f,Phi_f
        if(i>500):
            phyarr.append(phi)
            mavg+=np.tanh(h/T+phyarr[i-501])
            eavg+=(0.5*T/N-0.5*phyarr[i-501]**2*T**2/(N*j)-h*np.tanh(h/T+phyarr[i-501]))
        #print(mavg)
    #print(count/5000)
    mavg=mavg/len(phyarr)
    eavg=eavg/len(phyarr)
    earr.append(eavg)
    marr.append(mavg)
```

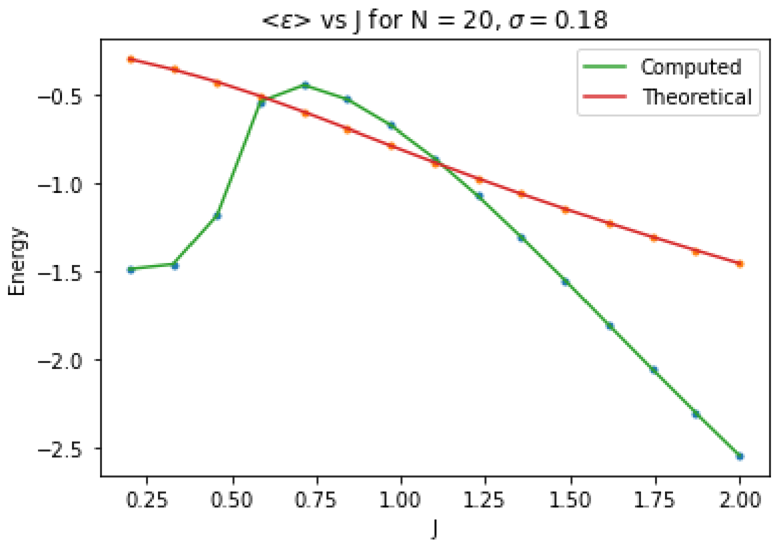
```
100%|██████████████████████████████████████████████████| 15/15 [00:27<00:00,  1.82s/it]
```

In [22]:

```
Z=np.zeros(len(J))
E=np.zeros(len(J))

for i in range(N+1):
    Z+=math.comb(N,i)*f(J/N,N-2*i)

for i in range(N + 1):
        E+= -(math.comb(N,i)*((0.5*(J/N)*(N - 2*i)**2)/T + h*(N - 2*i)/T)*f(J/(N*T),N-2*i))


std = bootstrap(earr)
plt.title('<$\epsilon$> vs J for N = 20, $\sigma = %s$'%np.round(std,2))
plt.plot(J,earr,".",)
plt.plot(J,E,'.')
plt.plot(J,earr,label = 'Computed')
plt.plot(J,E,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("Energy")
plt.legend()
```

Out[22]:

```
<matplotlib.legend.Legend at 0x1de911ec3a0>
```



In [23]:

```
M = np.zeros(len(J))

for i in range(N + 1):
        M+= (math.comb(N,i)*((N - 2*i)*f(J/(N*T),N-2*i))/(Z*N))

std = bootstrap(earr)
plt.title('<m> vs J for N = 20, $\sigma = %s$'%np.round(std,2))
plt.plot(J,marr,'.')
plt.plot(J,M,'.')
plt.plot(J,marr,label = 'Computed')
plt.plot(J,M,label = 'Theoretical')
plt.xlabel("J")
plt.ylabel("<m>")
plt.legend()
```

Out[23]:

```
<matplotlib.legend.Legend at 0x1de9110f070>
```