1) We evaluate the magnetization m, m^2, and the Hamiltonian H_a from the external field $u(x)$.

Writing the Fourier decomposition of the external field, we have:

$$u_l = \sum_{k=1}^{N-1} C_k \sin\left(\frac{k\pi l a}{L}\right)$$

So we have:

(i) $$m = \frac{a}{L} \sum_{i=1}^{N-1} u_i \quad ,$$

$$= \frac{a}{L} \sum_{i=1}^{N-1} \sum_{k=1}^{N-1} C_k \sin\left(\frac{k\pi i a}{L}\right)$$

$$= \sum_{k=1}^{N-1} C_k \frac{a}{L} \sum_{i=1}^{N-1} \sin\left(\frac{k\pi i a}{L}\right)$$

$$= \sum_{k=1}^{N-1} \frac{C_k}{N} \sum_{i=1}^{N-1} \sin\left(\frac{ik\pi}{N}\right)$$

$$= \sum_{k\,\mathrm{odd}} \frac{C_k}{N} \cot\left(\frac{k\pi}{2N}\right) = \frac{1}{N} \sum_{k\,\mathrm{odd}} C_k \cot\left(\frac{k\pi}{2N}\right)$$

$$m^2 = \frac{a}{L} \sum_{i=1}^{N-1} u_i^2 = \frac{a}{L} \sum_{i=1}^{N-1} \left(\sum_{k=1}^{N-1} C_k \sin\left(\frac{k\pi l}{N}\right)\right) \cdot \left(\sum_{q=1}^{N-1} C_q \sin\left(\frac{q\pi l}{N}\right)\right)$$

$$= \frac{1}{N} \left(\sum_{k=1}^{N-1} C_k \sum_{q=1}^{N-1} C_q \left(\sum_{i=1}^{N-1} \sin\left(\frac{k\pi l}{N}\right) \sin\left(\frac{q\pi l}{N}\right) \right)\right)$$

$$= \frac{1}{N} \sum_{k=1}^{N-1} C_k \sum_{q=1}^{N-1} C_q \cdot \frac{N}{2} \delta_{kq}$$

$$= \frac{1}{2} \sum_{k=1}^{N-1} C_k^2$$

$$\cdot\ H_a(u) = \frac{1}{a} \sum_{i=1}^{N} (u_i - u_{i-1})^2$$

$$= N \cdot L \sum_{i=1}^{N} (u_i - u_{i-1})^2$$

$$= N \cdot L \sum_{i=1}^{N} u_i^2 - 2 u_i u_{i-1} + u_{i-1}^2$$

$$= N \cdot L \sum_{i=1}^{N} \left(\left(\sum_k C_k \sin\left(\frac{k\pi i}{N}\right)\right)^2 - 2 \left(\sum_k C_k \sin\left(\frac{k\pi i}{N}\right) \cdot \sum_l C_l \sin\left(\frac{l\pi(i-1)}{N}\right)\right) + \left(\sum_l C_l \sin\left(\frac{l\pi(i-1)}{N}\right)\right)^2 \right)$$

$$= N \cdot L \sum_{i=1}^{N} \left(\sum_k C_k^2 \sin^2\left(\frac{k\pi i}{N}\right) + \sum_k \sum_{k \neq q} \cancel{C_k C_q \sin\left(\frac{k\pi i}{N}\right) \sin\left(\frac{q\pi i}{N}\right)}^{0} \right.$$

$$-2 \sum_k \sum_l C_l C_k \sin\left(\frac{k\pi i}{N}\right) \sin\left(\frac{l\pi(i-1)}{N}\right)$$

$$+ \sum_l C_l^2 \sin\left(\frac{l\pi(i-1)}{N}\right)^2$$

$$\left. + \sum_l \sum_{l \neq p} \cancel{\sin\left(\frac{l\pi(i-1)}{N}\right) \sin\left(\frac{p\pi(i-1)}{N}\right)}^{0} \right)$$

when the cross terms vanish due to orthogonality of $\left\{\sin\left(\frac{n\pi i}{N}\right)\right\}_{n=1}^{\infty}$

$$= N \cdot L \left(\sum_k \sum_i C_k^2 \sin^2\left(\frac{k\pi i}{N}\right) \right.$$

$$-2 \sum_k \sum_l \sum_i \sin\left(\frac{k\pi i}{N}\right) \sin\left(\frac{l\pi(i-1)}{N}\right)$$

$$\left. + \sum_l \sum_i C_l^2 \sin^2\left(\frac{l\pi(i-1)}{N}\right) \right)$$

$$\sin\left(\frac{k\pi i}{N}\right) \sin\left(\frac{l\pi(i-1)}{N}\right) = \sin\left(\frac{k\pi i}{N}\right) \left[\sin\left(\frac{l\pi i}{N}\right) \cos\left(\frac{l\pi}{N}\right) - \cos\left(\frac{l\pi i}{N}\right) \sin\left(\frac{l\pi}{N}\right) \right]$$

$$\Rightarrow \sum_i \sin\left(\frac{k\pi i}{N}\right) \sin\left(\frac{l\pi(i-1)}{N}\right)$$

$$= \frac{N}{2}\delta_{kl}\cos\left(\frac{l\pi}{N}\right) - \sum_i \sum_k \sum_l \sin\left(\frac{k\pi i}{N}\right)\cos\left(\frac{l\pi i}{N}\right)\sin\left(\frac{l\pi}{N}\right)$$

and :

$$\sin^2\left(\frac{l\pi(i-1)}{N}\right) = \left[\sin\left(\frac{l\pi i}{N}\right)\cdot\cos\left(\frac{l\pi}{N}\right) - \cos\left(\frac{l\pi i}{N}\right)\sin\left(\frac{l\pi}{N}\right)\right]^2$$

$$= \sin^2\left(\frac{l\pi i}{N}\right)\cos^2\left(\frac{l\pi}{N}\right) - \frac{1}{2}\sin\left(\frac{2l\pi i}{N}\right)\sin\left(\frac{2l\pi}{N}\right) + \cos^2\left(\frac{l\pi i}{N}\right)\sin^2\left(\frac{l\pi}{N}\right)$$

$$= \sin^2\left(\frac{l\pi i}{N}\right)\cos^2\left(\frac{l\pi}{N}\right) - \frac{1}{2}\sin\left(\frac{2l\pi i}{N}\right)\sin\left(\frac{2l\pi}{N}\right) + \sin^2\left(\frac{l\pi}{N}\right) - \sin^2\left(\frac{l\pi i}{N}\right)\sin^2\left(\frac{l\pi}{N}\right)$$

$$= \sin^2\left(\frac{l\pi i}{N}\right)\cdot\cos\left(\frac{2l\pi}{N}\right) - \frac{1}{2}\sin\left(\frac{2l\pi i}{N}\right)\sin\left(\frac{2l\pi}{N}\right) + \sin^2\left(\frac{l\pi}{N}\right)$$

$$= \frac{1}{2}\cos\left(\frac{2l\pi}{N}\right) - \frac{1}{2}\cos\left(\frac{2l\pi i}{N}\right)\cos\left(\frac{2l\pi}{N}\right) - \frac{1}{2}\sin\left(\frac{2l\pi i}{N}\right)\sin\left(\frac{2l\pi}{N}\right) + \sin^2\left(\frac{l\pi}{N}\right)$$

$$= \frac{1}{2}\cos\left(\frac{2l\pi}{N}\right) - \frac{1}{2}\cos\left(\frac{2l\pi(i+1)}{N}\right) + \sin^2\left(\frac{l\pi}{N}\right)$$

$$\Rightarrow \cdots \Rightarrow \quad H_a(u) = \frac{2N}{a}\sum_{k=1}^{N-1} C_k^2 \sin^2\left(\frac{k\pi}{2N}\right).$$

CompPhys_HW5

November 26, 2021

[10]:
```python
import numpy as np
import matplotlib.pyplot as plt
```

[2]:
```python
def H(a,U):

    ham = 0

    for i in range(len(U)-1):

        ham = ham + (U[i+1]-U[i])**2

    return ham/a

def P(a,U):
    return np.exp(-H(a,U))
```

[3]:
```python
def MH(a,N,du,Ns):

    U_s = np.ones((Ns,N))

    # scale up since O(u) >> O(H)
    U_0 = 100*np.random.random(N)

    for n in range(Ns):

        U_0[0] = 0
        U_0[N-1] = 0

        x = np.random.randint(1,N-1)

        r = np.random.uniform(-1,1)

        U_new = U_0

        U_new[x] = U_0[x] + r*du

        dH = H(a,U_new) - H(a,U_0)
```

```
        dP = np.exp(-dH)

        r_MH = np.random.uniform(0,1)

        if dP>1:
            U_0 = U_new

        if dP > r_MH:
            U_0 = U_new

        U_s[n,:] = U_0

    return U_s
```

[6]:
```
def mag(a,U):

    L = a*len(U)

    ms = 0

    for i in range(len(U)):

        ms = ms + U[i]

    return ms*a/L
```

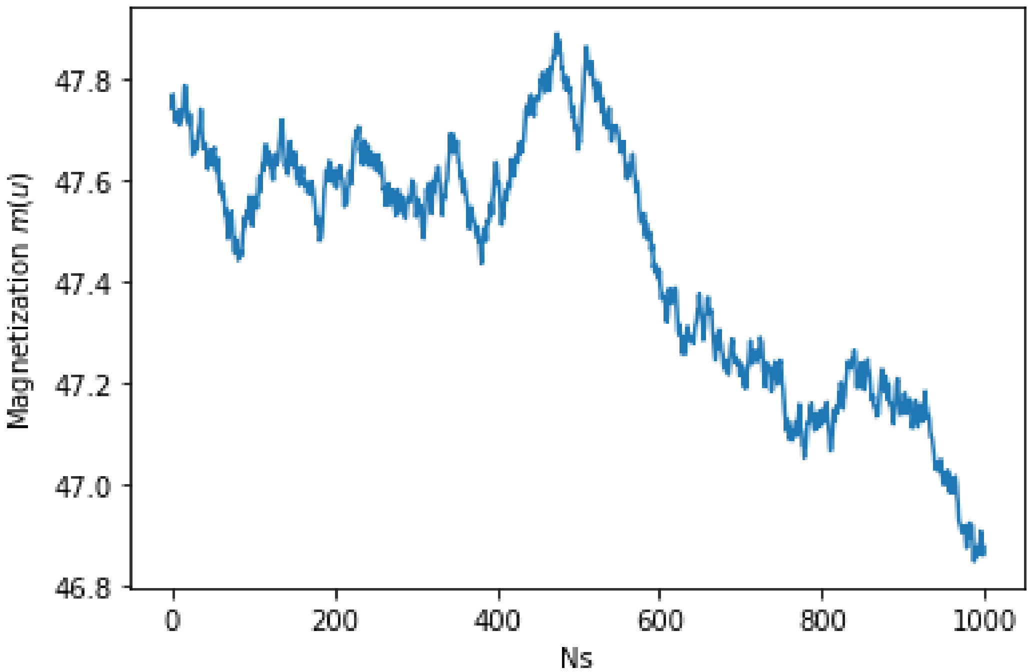
[7]:
```
L = 64
N = 64
a = 1
d = 2.
Ns = 1000

U_S = MH(a,N,d,Ns)
```

[17]:
```
mag_s = np.array([mag(a, U_S[i,:]) for i in range(Ns)])

# plt.plot(U_S[:, 0], mag_s)
plt.plot(mag_s)
plt.xlabel("Ns")
plt.ylabel("Magnetization $m(u)$")
```

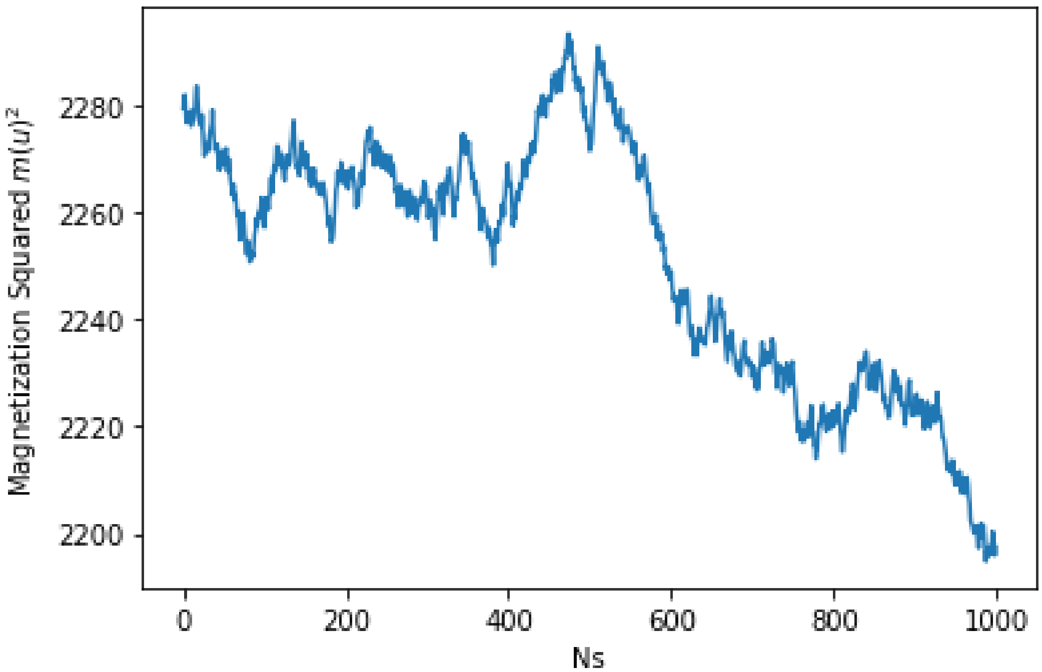
[17]:
```
Text(0, 0.5, 'Magnetization $m(u)$')
```



[19]:
```
mag_s2 = np.array([mag(a, U_S[i,:])**2 for i in range(Ns)])

# plt.plot(U_S[:, 0], mag_s)
plt.plot(mag_s2)
plt.xlabel("Ns")
plt.ylabel("Magnetization Squared $m(u)^2$")
```

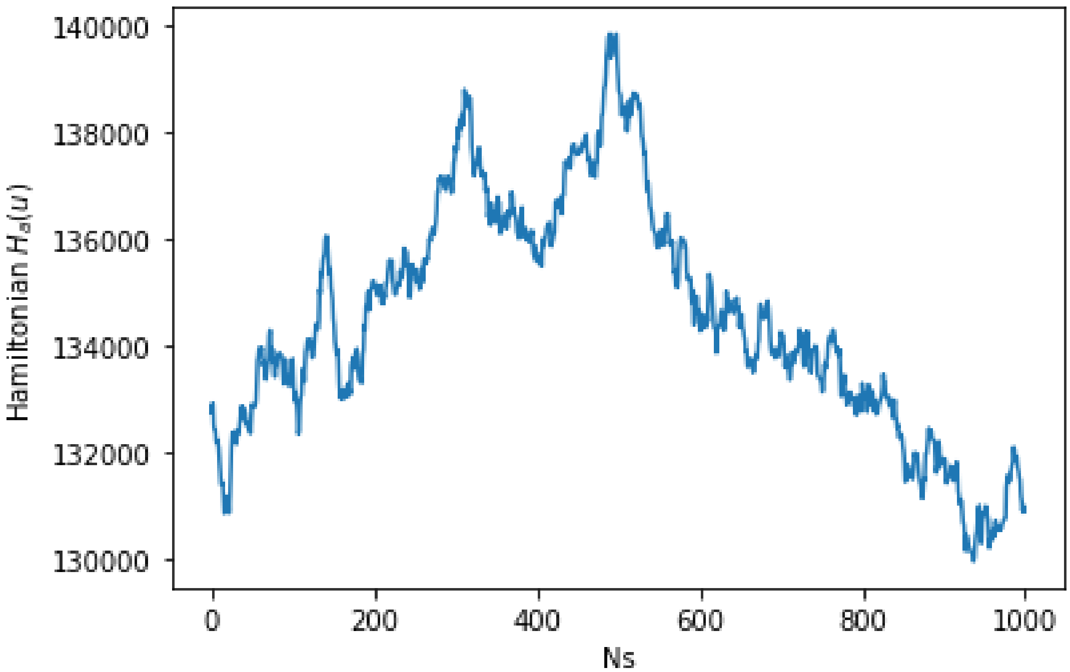
[19]:
```
Text(0, 0.5, 'Magnetization Squared $m(u)^2$')
```



[18]:
```
energy_s = np.array([H(a,U_S[i,:]) for i in range(Ns)])

plt.plot(energy_s)
plt.xlabel("Ns")
plt.ylabel("Hamiltonian $H_a(u)$")
```

[18]:
```
Text(0, 0.5, 'Hamiltonian $H_a(u)$')
```


Hamiltonian $H_a(u)$
140000
138000
136000
134000
132000
130000
0
200
400
600
800
1000
Ns

[ ]: