Question 1:

Writing the corresponding relation for the average magnetization and average energy per cite we have:

$$\langle m \rangle = \frac{1}{Z} \int \mathcal{D}[\phi] \mathrm{m}[\phi] e^{-\mathrm{S}[\phi]}$$
$$\langle \epsilon \rangle = \frac{1}{Z} \int \mathcal{D}[\phi] \epsilon[\phi] e^{-\mathrm{S}[\phi]}$$

with:

$$\mathcal{D}[\phi] = \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}}$$
$$\mathrm{S}[\phi] = \frac{\phi^2}{2\beta\hat{J}} - \mathrm{N}\log(2\cosh(\beta\mathrm{h} + \phi))$$

to ease the notation. We also have that:

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

The two relations for $\langle m \rangle$ and $\langle \epsilon \rangle$ must be equal, and thus we derive the expressions:

$$\mathrm{m}[\phi] = \tanh(\beta\mathrm{h} + \phi) \qquad \text{and} \qquad \epsilon[\phi] = -\frac{\phi^2}{2\beta^2\hat{J}} - \mathrm{h}\tanh(\beta\mathrm{h} + \phi)$$

Question 2:

By deriving the given Hamiltonian for the respected variables we get:

$$\dot{\phi} = \frac{\partial}{\partial \mathrm{p}} \mathcal{H} = \mathrm{p}$$
$$\dot{\mathrm{p}} = -\frac{\partial}{\partial \phi} \mathcal{H} = -\frac{\phi}{\beta\hat{J}} + N\tanh(\beta\mathrm{h} + \phi)$$

Question 3:

The leapfrog algorithm can be seen on the github repository with its convergence test. A plot for the convergence test can be seen here:

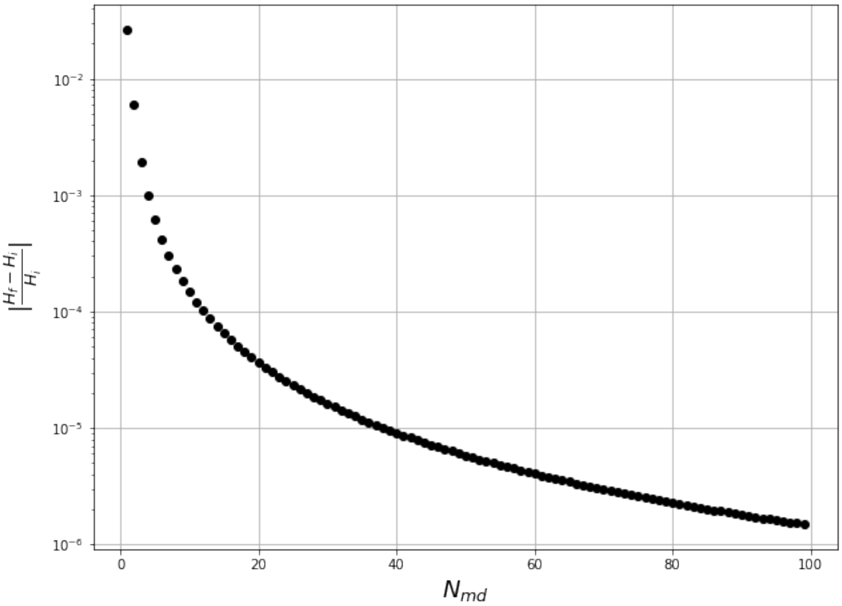


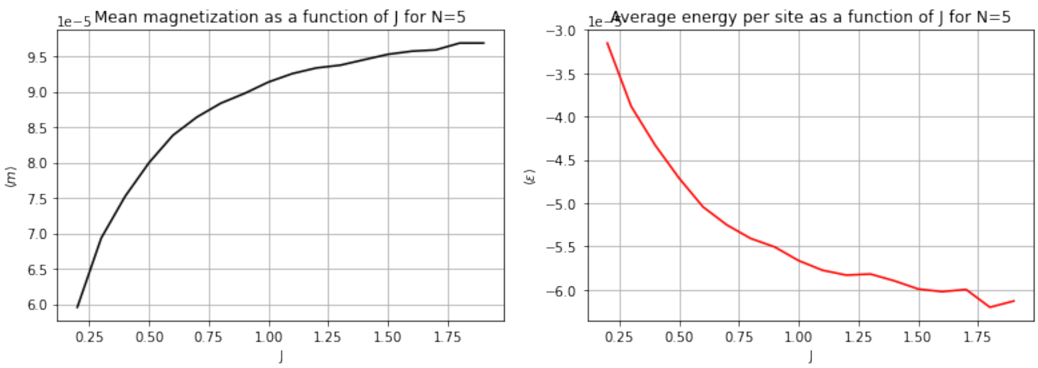
Figure 1: Convergence of leap-frog integrator as a number of integration steps N_{md}.

Question 4:

A working HMC algorithm can be found on github on the respected repository.

Question 5:

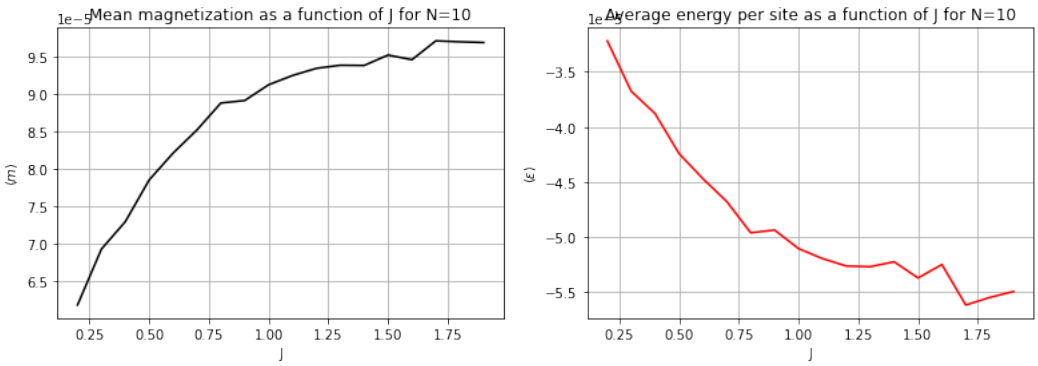
The plots are presented here and the code can again be found on github.



(a)

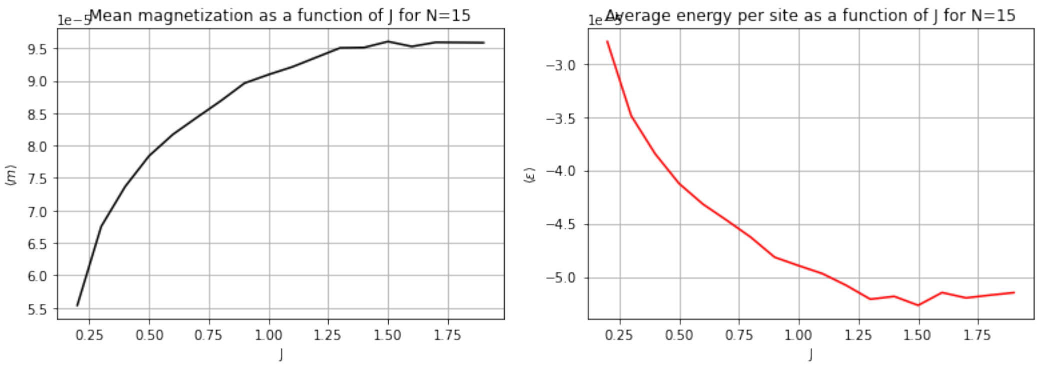
(b)

Figure 2: Mean magnetization for N=5



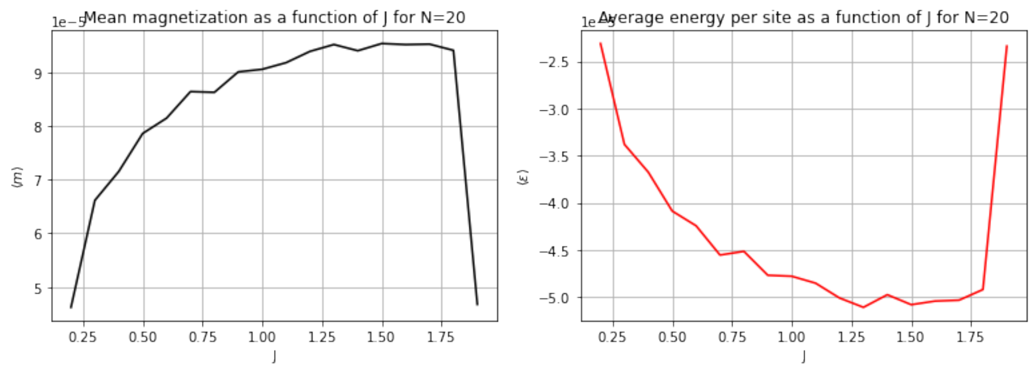
(a) (b)

Figure 3: Mean magnetization for N=10



(a) (b)

Figure 4: Mean magnetization for N=15



(a) (b)

Figure 5: Mean magnetization for N=20