Computational Physics
Exercise 3

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1 Intro

In this exercise we study the long range Ising model. Its Hamiltonian is:

$$\mathcal{H}(s) = -\frac{1}{2}\frac{J}{N}\sum_{i,j} s_i s_j - h\sum_i s_i \tag{1}$$

The the second sum is over all spin sites and the first over all possible pairs of spin sites. This means that every spin interacts with every other spin. The factor of $\frac{1}{2}$ accounts for the double counting. We use a Hubbard-Stratonovich transformation to transform our problem from a discrete space into a continuous space. Then we can implement a HMC algorithm to vary the whole ensemble at once, instead of just single spins, when producing the desired distribution via a Markov chain. The detailed derivation can be found on exercise sheet 3.

2 Task 1 & 2

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(1)

$$Z = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|J|}}\, e^{-S(\phi)} \quad \text{with} \quad S(\phi) = \frac{\phi^2}{2\beta J} - N \cdot \ln\left(2\cosh(\beta h \pm \phi)\right)$$

$J > 0$

$$\langle O \rangle = \frac{1}{Z} \int \frac{d\phi}{\sqrt{2\pi\beta J}}\, O(\phi)\, e^{-S(\phi)}$$

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

$$= \frac{1}{N\beta} \frac{1}{Z} \frac{\partial}{\partial h} Z$$

$$= \frac{1}{N\beta} \frac{1}{Z} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta J}} \underbrace{\frac{\partial}{\partial h} e^{-S(\phi)}}_{-e^{-S(\phi)} \frac{\partial}{\partial h} S(\phi)}$$

$$= \frac{1}{Z} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta J}} \underbrace{\left(-\frac{1}{N\beta} \frac{\partial}{\partial h} S(\phi)\right)}_{m(\phi)} e^{-S(\phi)}$$

$$\Rightarrow \quad m(\phi) = \tanh(\beta h \pm \phi)$$

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

$$= -\frac{1}{N} \frac{1}{Z} \frac{\partial}{\partial \beta} Z$$

$$= \frac{1}{Z} \int_{-\infty}^{\infty} d\phi \left(-\frac{1}{N}\right) \underbrace{\frac{\partial}{\partial \beta} \frac{1}{\sqrt{2\pi\beta J}}\, e^{-S(\phi,\beta)}}$$

$$-\frac{J}{2\sqrt{2\pi\beta J}\,\beta J}\, e^{-S(\phi,\beta)} + \frac{1}{\sqrt{2\pi\beta J}} \left(-e^{S(\phi,\beta)}\right) \underbrace{\frac{\partial}{\partial \beta} S(\phi,\beta)}_{-\frac{\phi^2}{2\beta^2 J} - hN \underbrace{\tanh(\beta h + \phi)}_{m(\phi)}}$$

$$= \frac{1}{Z} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta J}} \left(-\frac{1}{N} \left(\frac{\phi^2}{2\beta^2 J} + hN\, m(\phi) - \frac{J}{2\beta J}\right) e^{-S(\phi)}\right.$$

$$\Rightarrow \quad \varepsilon(\phi) = -\left(\frac{\phi^2}{2N\beta^2 J} + h\, m(\phi) - \frac{1}{2N\beta}\right)$$

(2)

$$\mathcal{H}(p,\phi) := \frac{p^2}{H} + S(\phi) = \frac{p^2}{2} + \frac{\phi^2}{2\beta J} - N \ln\left(2\cosh(\beta h + \phi)\right)$$

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

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

Exercises Seite 2

Figure 1: Calculations for Tasks 1 and 2

3 Task 3

We code up the leapfrog algorithm as detailed on the exercise sheet. To verify that $\mathcal{H}(p_f, \phi_f) = \mathcal{H}(p_0, \phi_0) + \mathcal{O}(\epsilon^2)$ we plot the dependence of the relative difference $\frac{\mathcal{H}(p_f,\phi_f)-\mathcal{H}(p_0,\phi_0)}{\mathcal{H}(p_0,\phi_0)}$ on $N_{md} \propto \frac{1}{\epsilon}$. The resulting plot is indeed as expected.

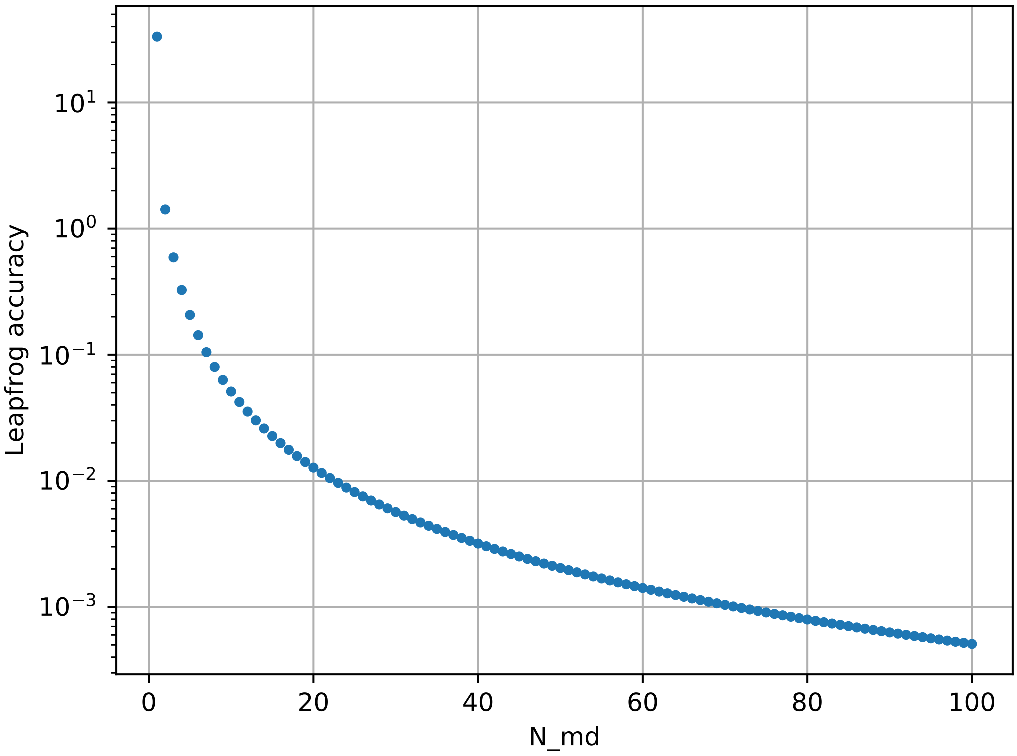

Figure 2: Convergence of leap-frog integrator as number of integration steps N_{md} increases

4 Task 4 and 5

We have implemented the HMC algorithm plus bootstrap errors.

For the following calculations we use 1000 thermalization and 2000 measurement steps. We start with $\phi = 5$, $h = 0.5$ and $\beta = 1$. For each number of spin sites N and for each value of J we run our algorithm with an increasing number of leapfrog steps N_{MD}. We start with $N_{\text{MD}} = 1$ and stop when our acceptance is larger than 50 %. In all plots the orange line is the exact solution, the blue points are the Monte Carlo simulations. One can see a systematic deviation in both the $\langle m \rangle$ plot and the $\langle e \rangle$ $(= \langle \epsilon \rangle)$ plot. One of the main problems is the large acceptance. Even for $N_{md} = 1$ the acceptance is above 95% and thus too high to have an efficient Markov chain.

4.1 Number of spin sites $N = 5$

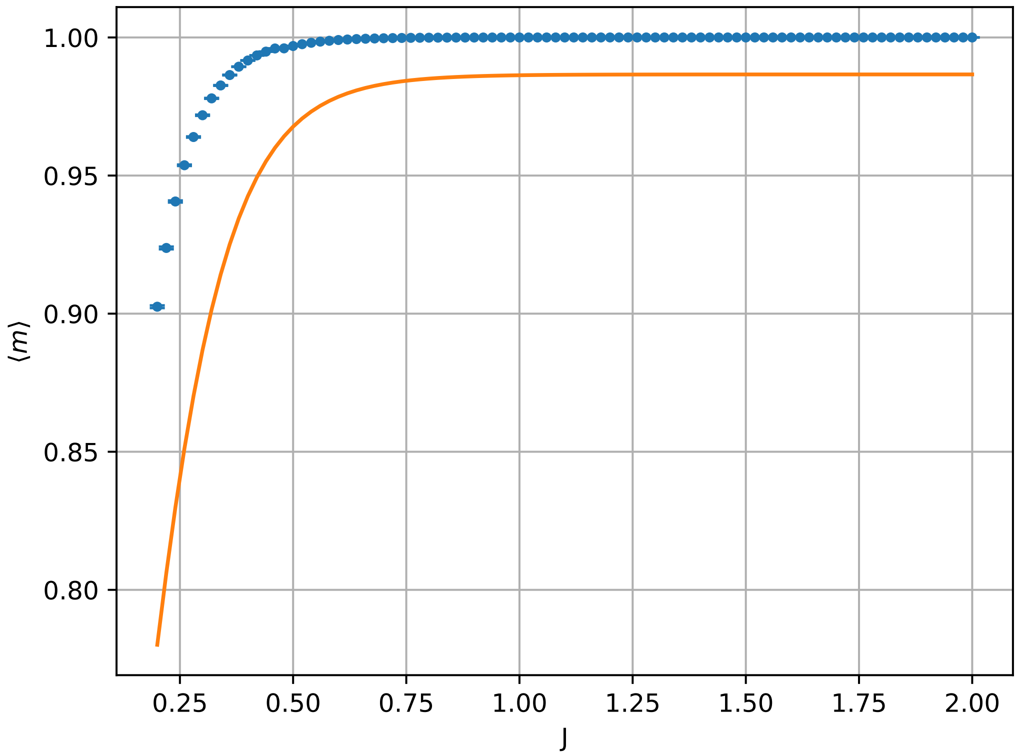

Figure 3: $\langle m \rangle$ in dependence of J for $N = 5$.

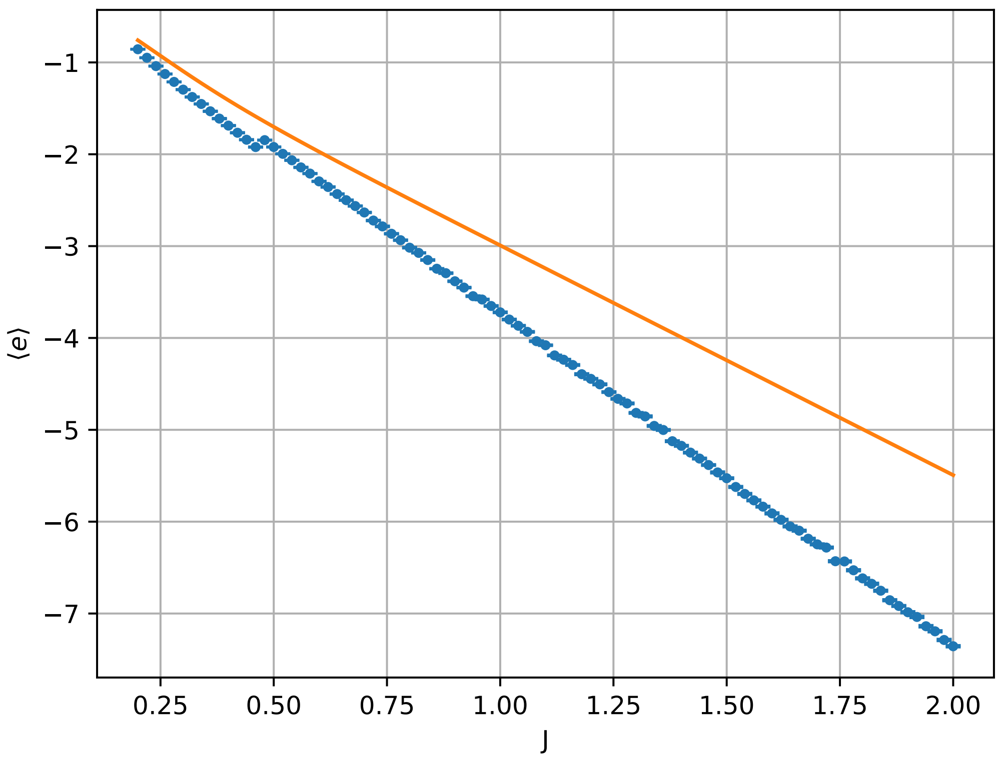

Figure 4: $\langle e \rangle$ in dependence of J for $N = 5$.

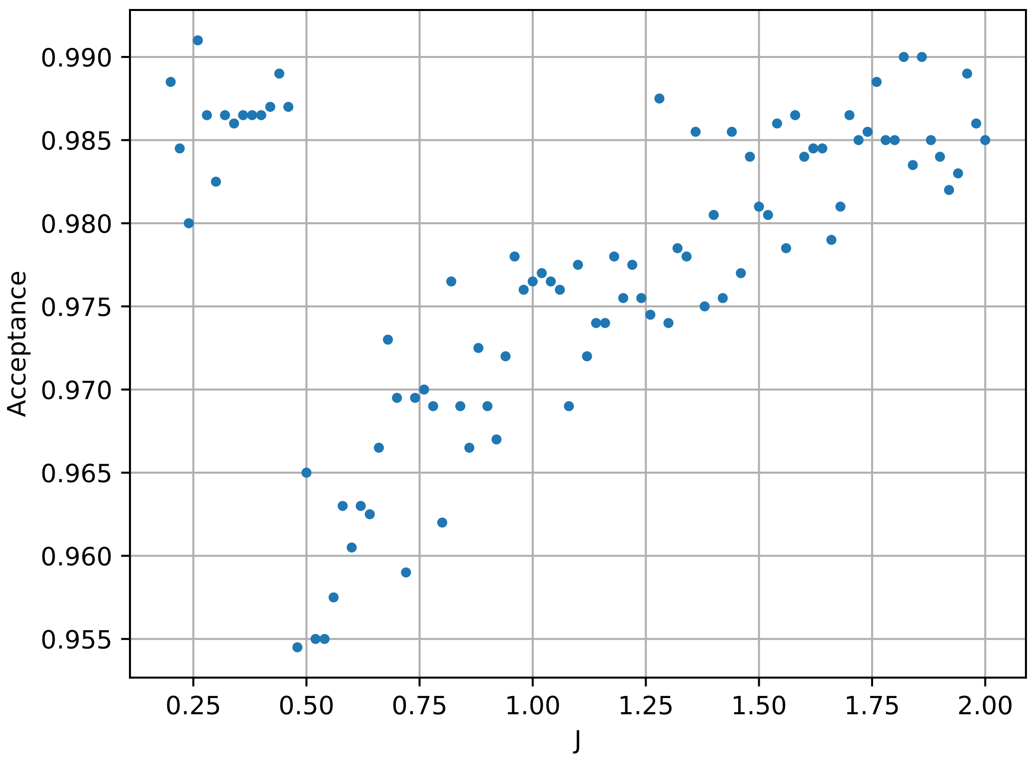

Figure 5: Final acceptance in dependence of J for $N = 5$.

4.2 Number of spin sites $N = 12$

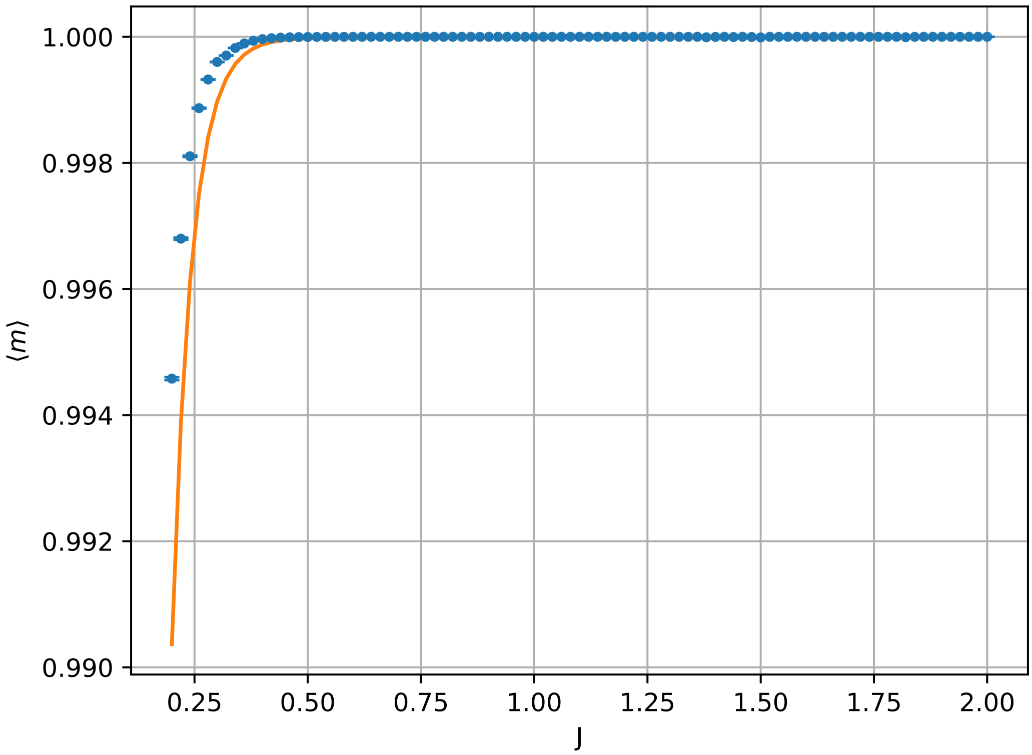

Figure 6: $\langle m \rangle$ in dependence of J for $N = 12$.

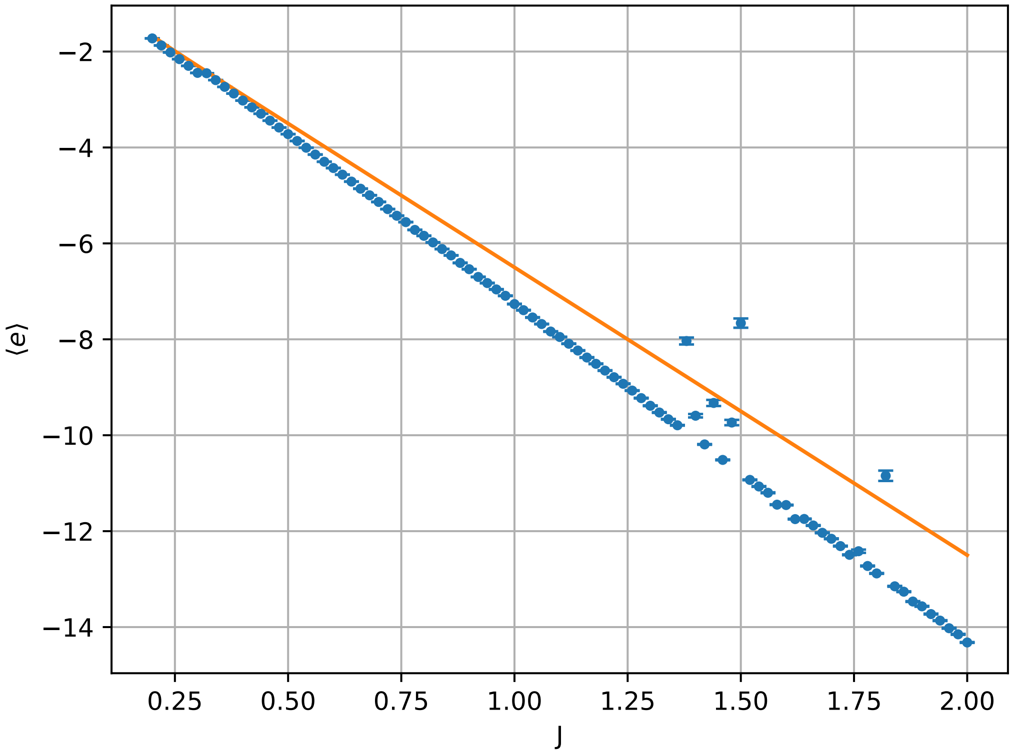

Figure 7: $\langle e \rangle$ in dependence of J for $N = 12$.

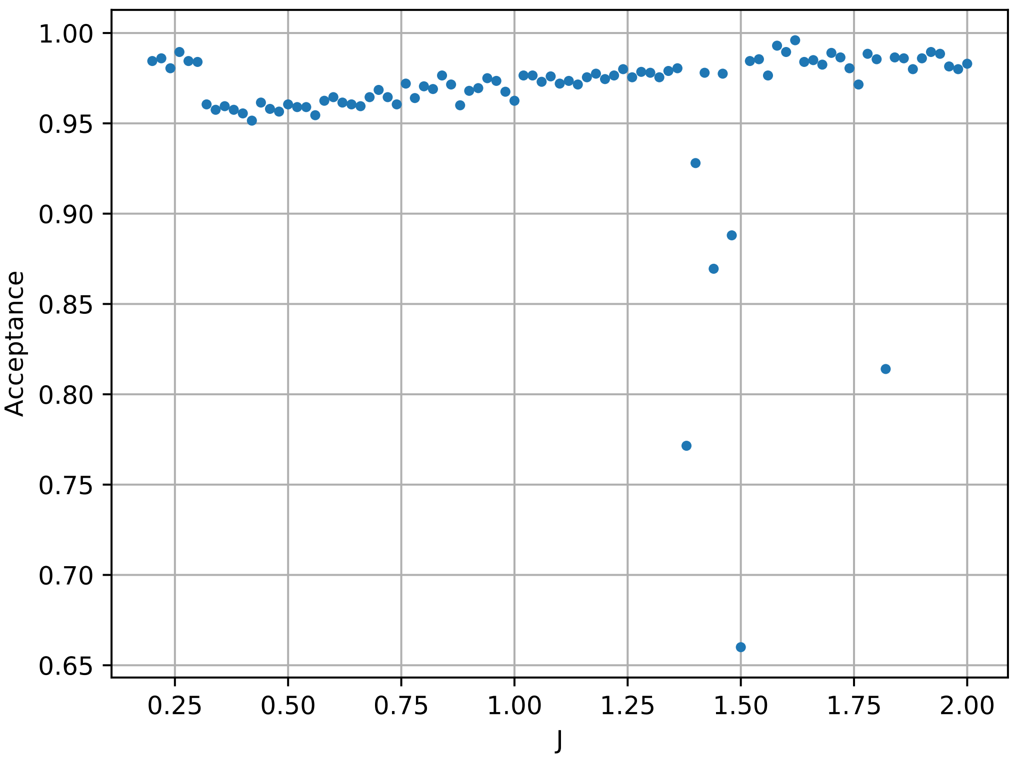

Figure 8: Final acceptance in dependence of J for $N = 12$.

4.3 Number of spin sites $N = 20$

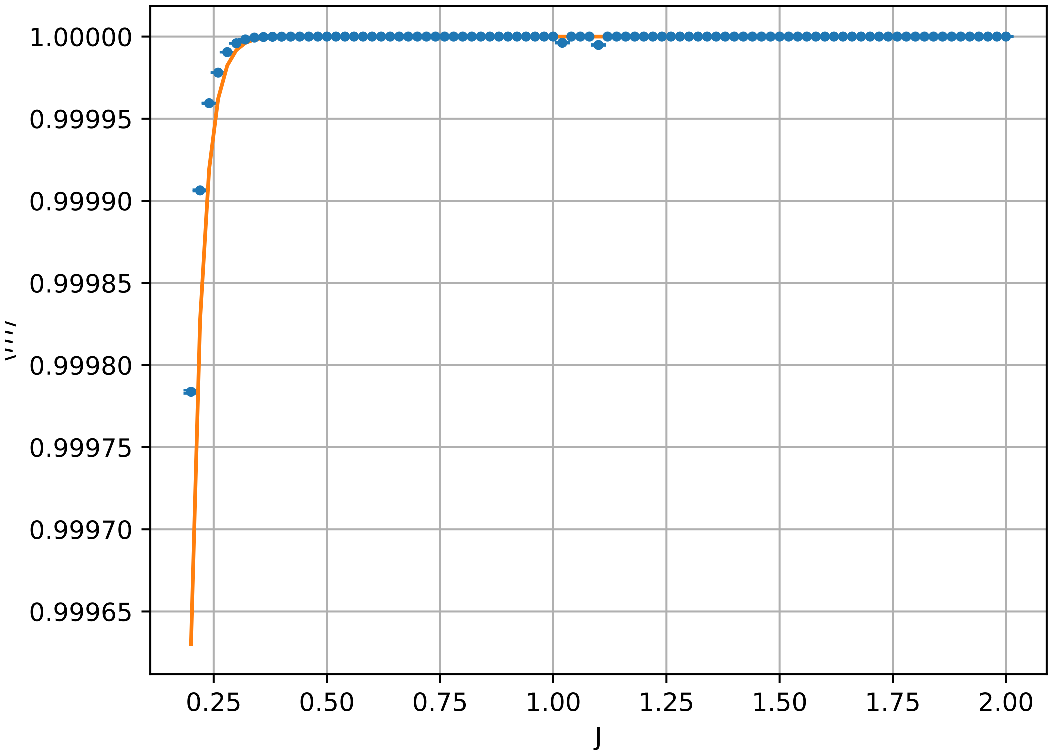

Figure 9: $\langle m \rangle$ in dependence of J for $N = 20$.

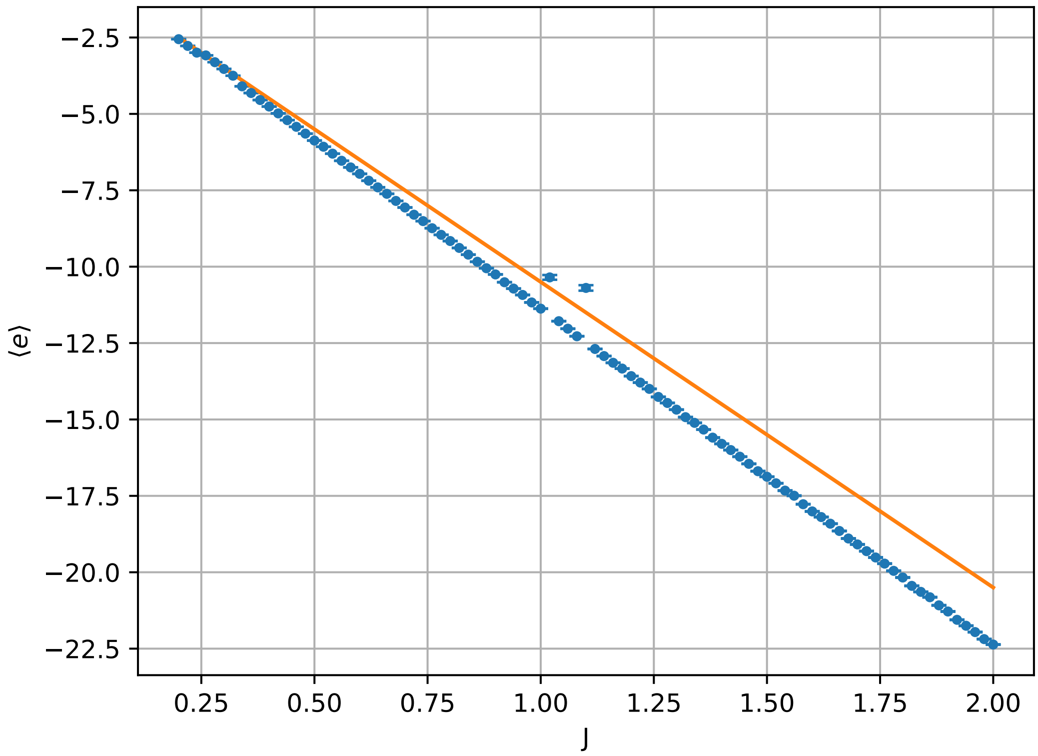

Figure 10: $\langle e \rangle$ in dependence of J for $N = 20$.

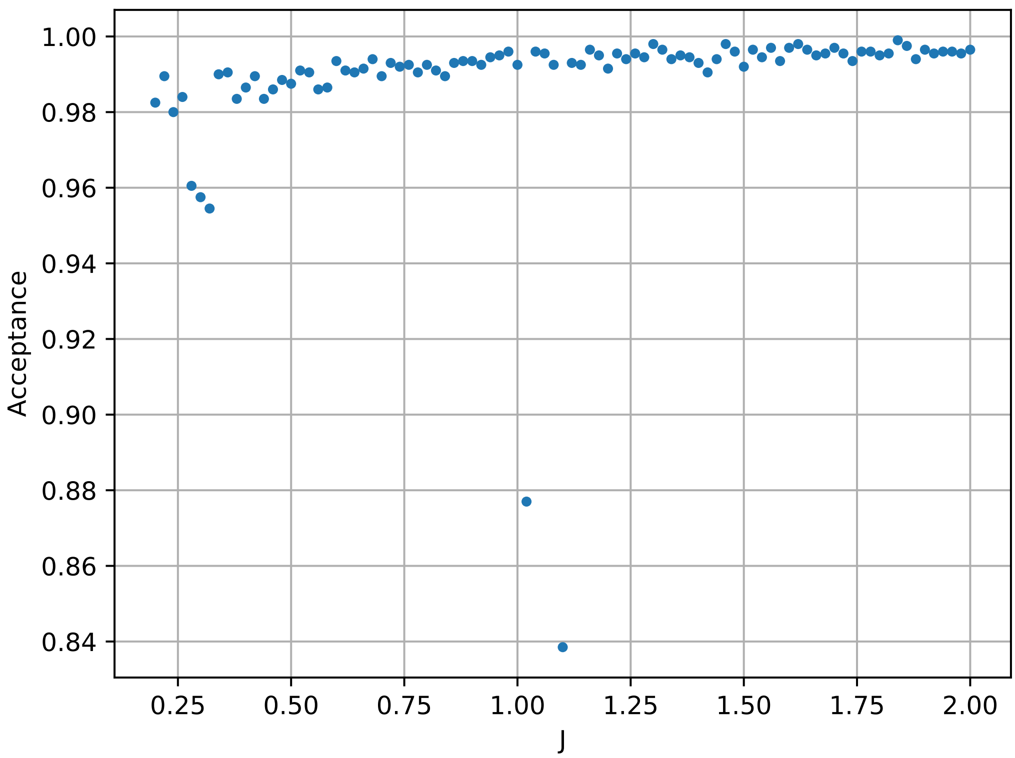

Figure 11: Final acceptance in dependence of J for $N = 20$.