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Computational Physics – Exercise 3

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1 Expectation values of operators

The partition function takes the form,

$$Z[J] = \begin{cases} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))}, & \text{if } J > 0 \\ \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{-\frac{\phi^2}{2\beta|\hat{J}|} + N\log(2\cosh(\beta h \pm i\phi))}, & \text{if } J < 0 \end{cases} \tag{1}$$

Where ϕ is the auxiliary field we introduce by Hubbard-Stratanovich transformation and $\hat{J} = J/N$. We are told that an arbitrary observable takes the form

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

We now have the observables:

$$\langle m \rangle = \frac{1}{N\beta} \frac{\partial}{\partial h} \log(Z) \tag{3}$$

$$\langle \epsilon \rangle = -\frac{1}{N} \frac{\partial}{\partial \beta} \log(Z) \tag{4}$$

We can then write them in the form of equation (2) as follows, we shall split it into the two cases:

1.1 For $J > 0$

$$\frac{\partial}{\partial h} \log(Z[J]) = \frac{1}{Z[J]} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))} .(N\beta) \tanh(\beta h \pm \phi)$$

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

Where we set,

$$e^{-S[\phi]} = e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))} \tag{5}$$

Thus we have,

$$\langle m \rangle = \frac{1}{Z[J]}\int_{-\infty}^{\infty}\frac{d\phi}{\sqrt{2\pi\beta\hat{J}}}\tanh\left(\beta h \pm \phi\right).e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h \pm \phi))} \tag{6}$$

$$\langle \epsilon \rangle = \frac{1}{Z[J]}\int_{-\infty}^{\infty}\frac{d\phi}{\sqrt{2\pi\beta\hat{J}}}e^{-S[\phi]}\left[\frac{1}{N\beta} - \frac{\phi^2}{2N\beta^2\hat{J}} - h.\tanh\left(\beta h \pm \phi\right)\right] \tag{7}$$

Note that these take the form that we expect from equation (2).

1.2 For $J < 0$

For this case, we define:

$$e^{-S[\phi]} = e^{-\frac{\phi^2}{2\beta|\hat{J}|} + N\log(2\cosh(\beta h \pm i\phi))} \tag{8}$$

Thus we have,

$$\langle m \rangle = \frac{1}{Z[J]}\int_{-\infty}^{\infty}\frac{d\phi}{\sqrt{2\pi\beta\left|\hat{J}\right|}}\tanh\left(\beta h \pm i\phi\right).e^{-S[\phi]} \tag{9}$$

$$\langle \epsilon \rangle = \frac{1}{Z[J]}\int_{-\infty}^{\infty}\frac{d\phi}{\sqrt{2\pi\beta\left|\hat{J}\right|}}e^{-S[\phi]}\left[\frac{1}{N\beta} + -\frac{\phi^2}{2N\beta^2\left|\hat{J}\right|} - h.\tanh\left(\beta h \pm i\phi\right)\right] \tag{10}$$

Note that these take the form we expect from equation (2).

2 Determining the Equations of Motion

We define our artificial Hamiltonian to be

$$\mathcal{H}(p,\phi) = \frac{p^2}{2} + \frac{\phi^2}{2\beta\hat{J}} - N\log(2\cosh(\beta h + \phi)) \tag{11}$$

Now we want to find the equations of motion for the auxiliary field and it's conjugate momentum, for that we will use Hamilton's equations

$$\dot{\phi} = \frac{\partial}{\partial p}\mathcal{H} \tag{12}$$

$$\dot{p} = -\frac{\partial}{\partial \phi}\mathcal{H} \tag{13}$$

Inserting equation (11) in (12) and (12), we get

$$\dot{\phi} = p \tag{14}$$

$$\dot{p} = -\frac{\phi}{\beta \hat{J}} + N \tanh\left(\beta h + \phi\right) \tag{15}$$

3 Leapfrog integration of the equations of motion

We now implement the leapfrog algorithm as sketched in the exercise and lecture in order to integrate equations (12) and (13), the code for this can be found at [1].

To verify the convergence of the algorithm we shall plot against for as shown in figure 1.

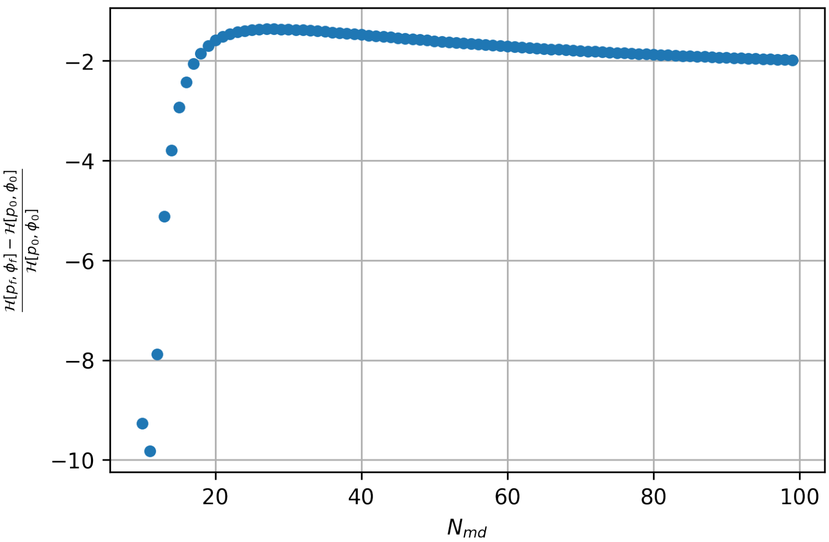

Figure 1: We implement the Leapfrog algorithm. We observe a convergence as N_{md} approaches 100.

4 Hybrid Monte Carlo

We implement the hybrid Monte-Carlo algorithm as sketched in the lecture, the code for it can be found at [1].

5 Calculating the observables numerically

We shall now compute the observables numerically now. For reference we have the following analytical results which we shall plot along the numerical results to verify their correctness:

$$Z = \sum_{n=0}^{N} \binom{N}{n} f(\beta\hat{J}, \beta h, N-2n) \tag{16}$$

$$\langle \beta\varepsilon \rangle = -\frac{1}{NZ} \sum_{n=0}^{N} \binom{N}{n} \left[\frac{1}{2}\beta\hat{J}(N-2n)^2 + \beta h(N-2n)\right] f(\beta\hat{J}, \beta h, N-2n) \tag{17}$$

$$\langle m \rangle = \frac{1}{NZ} \sum_{n=0}^{N} \binom{N}{n} (N-2n) f(\beta\hat{J}, \beta h, N-2n). \tag{18}$$

$$f(\beta\hat{J}, \beta h, x) \equiv e^{\frac{1}{2}\beta\hat{J}x^2 + \beta h x} \tag{19}$$

First we shall find out the best acceptance rate, the plot for this can be seen in figure 2.

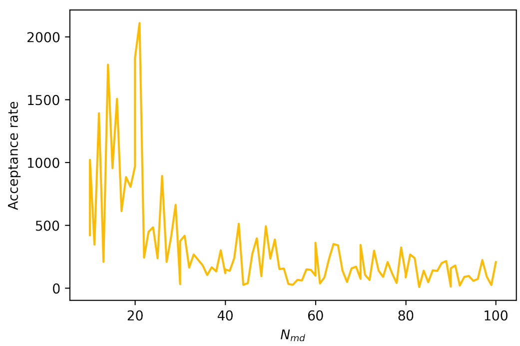

Figure 2: A plot of the acceptance rate versus N_{md}

We find that $N_{md} = 21$, has the highest acceptance rate of 40 percent. Now we turn to simulating the observables:

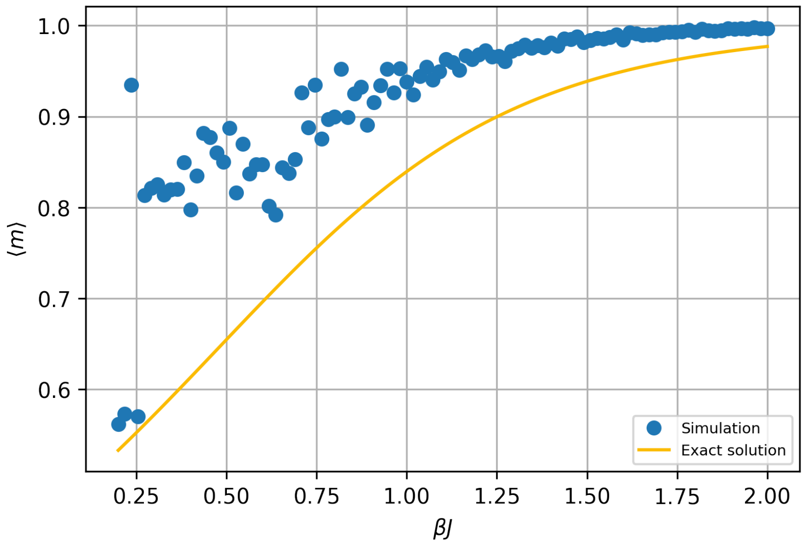

Figure 3: A plot of the mean magnetization per site versus βJ

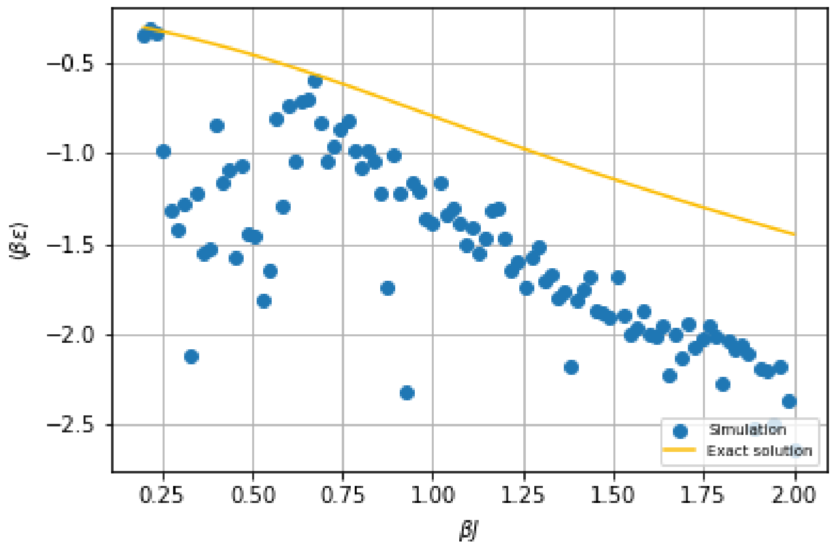

Figure 4: A plot of the mean energy per site versus βJ

References

[1] P. Anancia Devaneyan and R. K. Senthilkumar. Exercises for the Physics 760: Computational Phyics course during the WS 22/23 Term.