Exercises for Computational Physics (physics760)
WS 2020 / 21

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Exercise 3 (20 pts. total)

Homework (due Nov.25 at 18:00)

Please note the due date of this homework. Submission of homework *requires* submitting your solutions (e.g. answers to questions, graphs, results in tabular form) in the form of a brief report (please no 100 page submissions!) **AND** a copy of your code that you used to do the simulations. Please address all questions and requirements written below in *italics* and red font in your homework report.

4 Applying HMC to the long-range Ising model

The goal of this homework is the apply the HMC algorithm to a variant of the Ising model: the *long-range* Ising model. The Hamiltonian for this model is

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

where N is the number of sites. This Hamiltonian should look very familiar to you. But note that in the coupling term on the RHS the sum over sites i, j is *unrestricted*. This means that the spin at any site can interact with the spin at any other site (including itself!). This is what is meant by a *long range* interaction. And because the sum is unrestricted, there is a factor of 1/2 to avoid double counting. Finally, because of the long-range nature of these interactions, we must scale ('renormalize') the interaction by N^{-1} to ensure that we calculate sensible quantities. This really just means that we want to avoid solutions that blow up. This is the reason for introducing $\hat{J} = J/N$.

Some of you might question whether or not applying HMC to the Ising model is possible. Indeed, the HMC algorithm, as discussed in the lectures, works on *continuous* spaces, whereas the Ising model lives in a *discrete* space. Thus to apply the HMC algorithm we have to first transform our Ising model to a continuous space. To do this, we employ a well known numerical "trick" known as the Hubbard-Stratonovich transformation. You will undoubtedly encounter this transformation again in your future studies.

We'll walk you through the transformation of the model to the point where you can apply the HMC algorithm. We start off by considering the partition function

$$Z = \sum_{\{s_i\}=\pm 1} e^{-\beta H(s,h)} = \sum_{\{s_i\}=\pm 1} e^{\beta J\left(\frac{1}{2N}\sum_{i,j} s_i s_j + \frac{h}{J}\sum_i s_i\right)} \ . \tag{2}$$

Now recognize that

$$\sum_{i,j} s_i s_j = \left(\sum_i s_i\right)^2 = s^2 \ , \tag{3}$$

where $s = \sum_i s_i$ is the total spin of the system. Therefore the partition function can be written as

$$Z = \sum_{\{s_i\}=\pm 1} e^{\beta J\left(\frac{1}{2N}s^2 + \frac{h}{J}s\right)} \ . \tag{4}$$

We now apply the Hubbard-Stratonovich (HS) transformation so that the argument of the exponential is 'linearized-in-s'. The HS transformation relies on the following expressions:

$$e^{-\frac{1}{2}|U|s^2} = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi|U|}} e^{-\frac{\phi^2}{2|U|} \pm i\phi s} \tag{5}$$

$$e^{\frac{1}{2}|U|s^2} = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi|U|}} e^{-\frac{\phi^2}{2|U|} \pm \phi s} \ . \tag{6}$$

One can choose either $\pm$ sign. If you apply these expressions to Eq. (4), you get (convince yourself of this)

$$Z = \begin{cases} \sum_{\{s_i\}=\pm 1} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}} + (\beta h \pm \phi)s} & (J > 0) \\ \sum_{\{s_i\}=\pm 1} \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{-\frac{\phi^2}{2\beta|\hat{J}|} + (\beta h \pm i\phi)s} & (J < 0) \end{cases} \tag{7}$$

So here comes something very cool. After application of the HS transformation, we can directly do the sum, $\sum_{s_i=\pm 1}$, over the spins! That is, we *integrate out the spins*. For example, when $J > 0$, we interchange the order of sums over the spin and the integral over the HS variable to get

$$Z[J>0] = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \sum_{\{s_i\}=\pm 1} e^{(\beta h \pm \phi)s} \tag{8}$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \prod_{i=1}^{N} \sum_{s_i=\pm 1} e^{(\beta h \pm \phi)s_j} \tag{9}$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \prod_{i=1}^{N} 2\cosh\left(\beta h \pm \phi\right) \tag{10}$$

$$= \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}} \left[2\cosh\left(\beta h \pm \phi\right)\right]^N \ . \tag{11}$$

[1] For $J < 0$, a similar calculation gives

$$Z[J<0] = \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{-\frac{\phi^2}{2\beta|\hat{J}|}} \left[2\cosh\left(\beta h \pm i\phi\right)\right]^N \ . \tag{12}$$

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[1] Some of you might notice that the term $2\cosh(\beta h \pm \phi)$ is the partition function for a *single* spin in the presence of an external magnetic field, but here with an 'effective field' given by $h \pm \phi/\beta$. Equation (11) can be interpreted as the product of N individual spin partition functions, but coupled via an overall effective magnetic field $h \pm \phi/\beta$.

You can simplify the expression further by bringing the cosh term into the argument of the exponential:

$$Z[J>0] \;=\; \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta\hat{J}}} e^{-\frac{\phi^2}{2\beta\hat{J}}+N\log(2\cosh(\beta h\pm\phi))} \tag{13}$$

$$Z[J<0] \;=\; \int_{-\infty}^{\infty} \frac{d\phi}{\sqrt{2\pi\beta|\hat{J}|}} e^{-\frac{\phi^2}{2\beta|\hat{J}|}+N\log(2\cosh(\beta h\pm i\phi))} \;. \tag{14}$$

Ok, from now on, assume that $J>0$ in all your calculations.

1: 1pt. *The expectation value of some operator O is given by*

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

Use the expression above and the fact that the mean magnetization (per site) and energy (per site) are given by

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

$$\langle\epsilon\rangle = -\frac{1}{N}\frac{\partial}{\partial\beta}\log\left(Z\right) \;,$$

to derive corresponding expressions for $O[\phi]$ for these quantities.

You should now notice that there are no more discrete degrees of freedom in our partition function and that ϕ is a *continuous* variable. So now we can apply the HMC algorithm. We'll walk you through a few more steps.

Recall from the lecture that the first step is to introduce conjugate momenta for each degree of freedom. In this case there is only one degree of freedom, ϕ, and thus only one conjugate momentum is required, which we label as p. We then define the *artificial* Hamiltonian

$$\mathcal{H}(p,\phi) = \frac{p^2}{2} + \frac{\phi^2}{2\beta\hat{J}} - N\log\left(2\cosh\left(\beta h+\phi\right)\right) \;. \tag{15}$$

2: 1pt. *Determine the equations of motion (EoMs) for this Hamiltonian by applying the Hamilton equations*

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

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

Integrating these EoMs allows us to determine trajectories of (p,ϕ) that keep $\mathcal{H}$ constant. In other words, given some initial (p_0,ϕ_0), the EoMs tell us how to evolve these points $(p_0,\phi_0)\rightarrow(p_f,\phi_f)$ such that $\mathcal{H}(p_0,\phi_0)=\mathcal{H}(p_f,\phi_f)$. We will use a numerical integration method called the *leapfrog* algorithm, commonly used in molecular dynamics (MD) simulations, to perform the numerical integration of the EoMs. We assume our total MD trajectory length is $\mathbf{1}$. We split this trajectory up into N_{md} small pieces $\epsilon=1/N_{md}$. The *leapfrog* algorithm (for N_{md} MD steps) is

- Set $(\Pi, \Phi) := (p_0, \phi_0)$
- First (half) step of leapfrog:

$$\Phi := \Phi + \frac{\epsilon}{2}\Pi$$

- $N_{md} - 1$ steps (repeat $N_{md} - 1$ times):

$$\begin{aligned}\Pi &:= \Pi - \epsilon\left(\frac{\Phi}{\beta\hat{J}} - N\tanh(\beta h + \Phi)\right)\\ \Phi &:= \Phi + \epsilon\Pi\end{aligned}$$

- Last step of leapfrog:

$$\begin{aligned}\Pi &:= \Pi - \epsilon\left(\frac{\Phi}{\beta\hat{J}} - N\tanh(\beta h + \Phi)\right)\\ \Phi &:= \Phi + \frac{\epsilon}{2}\Pi\end{aligned}$$

- Set $(p_f, \phi_f) := (\Pi, \Phi)$

Since this is a numerical integrator, we do not have exact constants of motions but should find that $\mathcal{H}(p_f, \phi_f) = \mathcal{H}(p_0, \phi_0) + \mathcal{O}(\epsilon^2)$, which can be improved by increasing N_{md} while keeping the overall trajectory length constant.

3: 3 pts. *Code up the leapfrog algorithm to evolve $(p_0, \phi_0) \to (p_f, \phi_f)$. Verify the convergence claim $\mathcal{H}(p_f, \phi_f) = \mathcal{H}(p_0, \phi_0) + \mathcal{O}(\epsilon^2)$. You should find something similar to Figure 1 (especially for large N_{md}).*

With a working version of the leapfrog algorithm, we are now ready for HMC. Assuming we start with some initial ϕ, the HMC algorithm is as follows:

- Sample $p \in \mathcal{N}_{0,1}$
- Integrate the EoMs using leapfrog to obtain a trial (p', ϕ')
- Accept ϕ' with probability (Metropolis accept/reject)

$$P_{acc.} = \min\{1, e^{\mathcal{H}(p,\phi) - \mathcal{H}(p',\phi')}\}$$

- Repeat

Note that after every Metropolis accept/reject, we store ϕ, *regardless* of whether the proposal was accepted or not![2] In this manner, we generate a whole string of ϕs (our Markov Chain!) that constitutes our ensemble $\{\phi\}$. As stated in the lectures, this ensemble $\{\phi\}$, after an initial *thermalization period*, has the correct probability distribution

$$d\phi\ P[\phi]\ \propto\ d\phi\ e^{-\frac{\phi^2}{2\beta\hat{J}} + N\log(2\cosh(\beta h + \phi))}\ .$$

[2] In case the new ϕ' was rejected, we store the *previous* ϕ again.

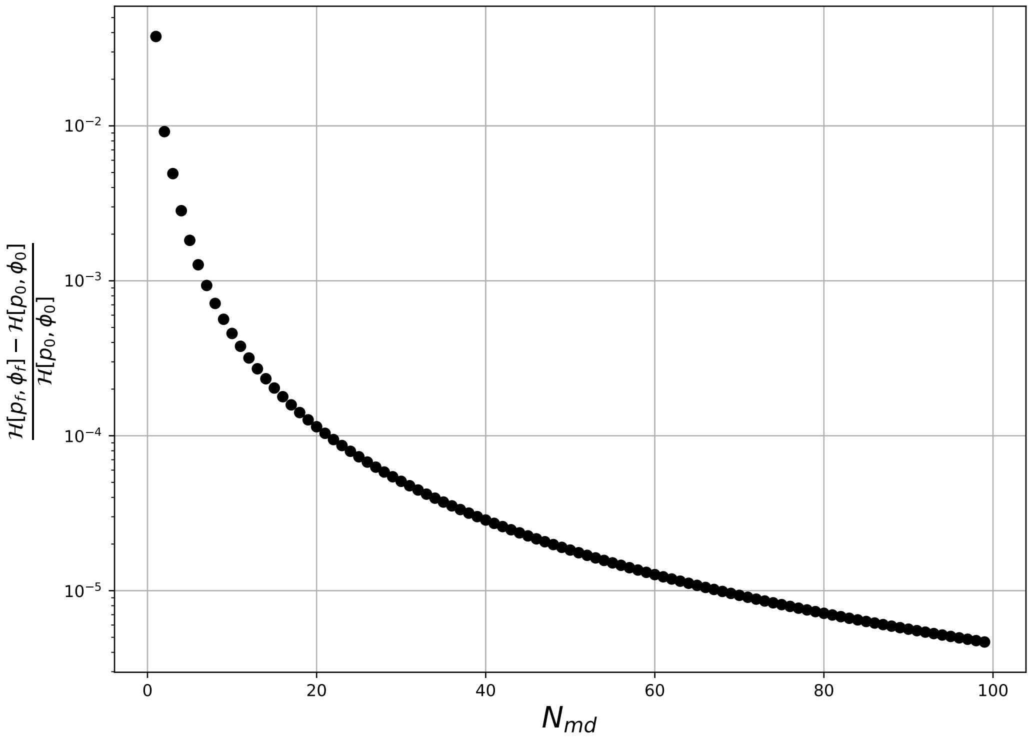

Figure 1: Convergence of leap-frog integrator as a number of integration steps N_{md}.

Any observable is now estimated as

$$\langle O \rangle = \frac{1}{N_{cfg}} \sum_{\phi \in \{\phi\}} O[\phi] \ , \tag{16}$$

where N_{cfg} is the size of our ensemble.

4: 10 pts. *With your working leapfrog integrator, code up the HMC algorithm for the long-range Ising model.*

5: 5 pts. *Setting $h = (\beta h) = .5$ and using some values of N ranging from 5 to 20, calculate the average energy per site and mean magnetization per site as a function of $J = (\beta J) \in [.2, 2]$. Tune N_{md} such that the acceptance rate is above 50%.*

As you might imagine, there are *exact* results for this system. I state the analytic results here without derivation[3] so as to help you gauge whether or not your calculations are correct.

[3]If you are interested in the derivation, please let me know and I'll provide them for you.

$$Z = \sum_{n=0}^{N} \binom{N}{n} f(\beta\hat{J}, \beta h, N-2n) \tag{17}$$

$$\langle \beta\varepsilon \rangle = -\frac{1}{NZ} \sum_{n=0}^{N} \binom{N}{n} \left[\frac{1}{2}\beta\hat{J}(N-2n)^2 + \beta h(N-2n) \right] f(\beta\hat{J}, \beta h, N-2n) \tag{18}$$

$$\langle m \rangle = \frac{1}{NZ} \sum_{n=0}^{N} \binom{N}{n} (N-2n)\, f(\beta\hat{J}, \beta h, N-2n)\ . \tag{19}$$

where

$$f(\beta\hat{J}, \beta h, x) \equiv e^{\frac{1}{2}\beta\hat{J}x^2 + \beta h x}\ . \tag{20}$$