Lattice field theories
Exercise sheet 1 – Hybrid Monte Carlo and scalar fields

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In this exercise sheet we work on a $1+1$ dimensional square lattice with spacing a and extent $N_t \times N_x$. Consider the action for a real scalar field with a ϕ^4 interaction living on this lattice,

$$S = \sum_{n_t,n_x} \left\{ -\frac{1}{2}\phi_{n_t,n_x}\left[\phi_{n_t+1,n_x} + \phi_{n_t-1,n_x} + \phi_{n_t,n_x+1} + \phi_{n_t,n_x-1} - 4\phi_{n_t,n_x}\right] + \frac{m^2}{2}\phi^2_{n_t,n_x} + \frac{g}{4!}\phi^4_{n_t,n_x} \right\}, \tag{1}$$

where $0 \leq n_t < N_t$ and $0 \leq n_x < N_x$, and $N_t, N_x \in \mathbb{Z}$. The field has periodic boundary conditions, $\phi_{n_t+N_t,n_x} = \phi_{n_t,n_x} = \phi_{n_t,n_x+N_x}$, m is the mass, g is the coupling, and all dimensionful parameters have already been rescaled by appropriate powers of the lattice spacing such that all terms in eq. (1) are dimensionless.

Exercise 1: Area preservation property of the leapfrog algorithm

Show that the leapfrog algorithm preserves the area of the integration measure.

Exercise 2: Reversibility property of the leapfrog algorithm

Show that the leapfrog algorithm is reversible.

Exercise 3: HMC for 1+1 dimensional scalar lattice theory

Write down an expression for the HMC drift,

$$K_{n_t,n_x} = -\frac{\delta S}{\delta \phi_{n_t,n_x}}, \tag{2}$$

for the action of eq. (1).

Exercise 4: HMC for 1+1 dimensional scalar lattice theory

Use the drift from the previous exercise and the Hybrid Monte Carlo algorithm given in the lecture to run a simulation of the ϕ^4 theory in $1+1$ dimensions.

The field is evolved over N_{steps} Monte Carlo steps, where after each the observable O is computed and stored. At the end of execution the ensemble average is computed and may then be printed to a file or the screen. In the HMC algorithm, each Monte Carlo step consists of the Molecular Dynamics evolution followed by the accept/reject step. Note also that for the MD evolution the fields are augmented with the "molecular dynamics" time τ,

$$\phi_{n_t,n_x} \to \phi_{n_t,n_x}(\tau)\,. \tag{3}$$

It is customary to "throw away" the first few configurations generated by any Monte Carlo method. This is because we start from some arbitrary initial condition and the Markov chain has not reached its equilibrium distribution yet (it has not "thermalised", in common parlance). Typically, one runs the Markov chain for $0 < N_{\text{therm}} < N_{\text{steps}}$ steps *without* updating the observable, so that the chain thermalises, and then runs it for N_{steps} collecting statistic for the observable(s).

Another important aspect is that with our choice of updating procedure two subsequent field configurations are correlated, and correlations tend to cause statistical errors to be *underestimated*. In order to avoid that, one can compute ensemble averages using only one configuration for every N_{skip} Monte Carlo steps, with the other configurations being discarded.

Perform the simulation using the algorithm above in a lattice of size 32×32, and compute the "magnetisation"

$$M = \left\langle \frac{1}{N_t N_x} \sum_{n_t,n_x} \phi_{n_t,n_x} \right\rangle , \tag{4}$$

i.e., the expectation value of the volume average field for the following parameters in units of the lattice distance,

- $m^2 = 0.173913$, $g = 2.26843$
- $m^2 = -0.307692$, $g = 1.77515$
- $m^2 = -0.571429$, $g = 1.53061$

Classically, one would expect the $\mathbb{Z}_2$ symmetry of the theory to be broken for $m^2 < 0$, i.e., the "magnetisation" to have a non-zero value. What do you observe for each case in the Monte Carlo simuations?