Lattice field theories

Exercise sheet 2
- Lattice simulations: 1+1 dim. scalar theory

Lectures: Jan Pawlowski j.pawlowski@thphys.uni-heidelberg.de
Felipe Attanasio pyfelipe@thphys.uni-heidelberg.de

Tutorials: Felipe Attanasio pyfelipe@thphys.uni-heidelberg.de

Institut für Theoretische Physik, Uni Heidelberg

Exercise 4: Detailed balance

In the lecture of 2nd of November the *detailed balance* condition was introduced. It is a sufficient condition for the solution of the balance equation that allows the Markov chain to have an equilibrium distribution.

Prove that the total transition probability $T = T_0 T_A$ of the Metropolis algorithm,

$$T_A(\phi' \leftarrow \phi) = \min\left(1, \frac{T_0(\phi \leftarrow \phi')\exp(-S[\phi'])}{T_0(\phi' \leftarrow \phi)\exp(-S[\phi])}\right), \tag{1}$$

satisfies the detailed balance equation

$$T(\phi' \leftarrow \phi)P(\phi) = T(\phi \leftarrow \phi')P(\phi'), \tag{2}$$

where $P(\phi) = \exp(-S[\phi])/Z$.

Exercise 5: Simulation of a 1+1 dimensional scalar lattice theory

Below, we provide a pseudo-code implementation of the Metropolis algorithm for the $1+1$ dimensional scalar field. The lattice has cubic elementary cells with both lattice distances being a, and its extend is given by $N_t \times N_x$. We also assume the implementation of a function S, that computes the action of a given field configuration. In this example we shall use the following lattice action ,

$$S = \sum_{n_t, n_x}\Bigg\{-\frac{1}{2}\phi(n_t,n_x)\Big(\phi(n_t+1,n_x)+\phi(n_t-1,n_x)+\phi(n_t,n_x+1)+\phi(n_t,n_x-1) - 4\phi(n_t,n_x)\Big] + \frac{m^2}{2}\phi(n_t,n_x)^2 + \frac{g}{4!}\phi(n_t,n_x)^4\Bigg\}, \tag{3}$$

where $0 \leq n_t < N_t$ and $0 \leq n_x < N_x$. The field has periodic boundary conditions, $\phi(n_t + N_t, n_x) = \phi(n_t, n_x) = (n_t, n_x + N_x)$. It is dimensionless in two dimensions. In turn, the dimensionless couplings are measure in the lattice distance a.

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.

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.

```
double phi[Nt][Nx];
for n ← 0 to N_steps do
    for 0 ≤ t < N_t and 0 ≤ x < N_x do          // sweep over the lattice
        oldAction ← S(phi) ;                          // save old action
        oldValue ←phi[t][x] ;                          // save old φ(x)
        phi[t][x] ← phi[t][x] + N(0,1) ;       // random change to φ(x)
        ΔS = S(phi) - oldAction;
        if ΔS > 0 then
            r ← UniformReal(0,1);
            if r > exp(−ΔS) then
                phi[t][x] ← oldValue ;                 // reject proposal
            end
        end
    end
    Obs ← Obs + O(phi) ;          // update computation of observable
end
Obs ← Obs / N_steps;
```

- How would you change the algorithm above to use discard N_{skip} configurations between those that are used to compute ensemble averages?
- 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?

Exercise 6: A convenient (re)parametrisation

When dealing with scalar fields it is very common to apply the following re-scaling of the variables:

$$a^{\frac{d-2}{2}}\phi \to (2\kappa)^{1/2}\varphi\,, \tag{5}$$

$$(am)^2 \to \frac{1-2\lambda}{\kappa} - 2d\,, \tag{6}$$

$$a^{-d+4}g \to \frac{6\lambda}{\kappa^2}\,, \tag{7}$$

where d is the number of spacetime dimensions, and we have introduced the dimensionless field φ and the *hopping parameter* κ. Note that all variables in the new formulation are dimensionless.

- Using the transformation above, rewrite the action in eq. (3) using the new, dimensionless, variables.
- Perform lattice simulations, again on a 32×32 lattice, with $\lambda = 0.02$ and $0.22 \leq \kappa \leq 0.30$. The system should be in different phases for $\kappa = 0.22$ and $\kappa = 0.30$ and undergoes a second order phase transition at a certain value of κ. The different phases are indicated by a (non-)zero value of the "magnetisation"

$$M = \left\langle \frac{1}{N_t N_x} \sum_{n_t, n_x} \varphi(n_t, n_x) \right\rangle . \tag{8}$$

At second order phase transitions the susceptibility,

$$\chi_2 = N_t N_x \left(\left\langle \left(\frac{1}{N_t N_x} \sum_{n_t, n_x} \varphi(n_t, n_x) \right)^2 \right\rangle - \left\langle \frac{1}{N_t N_x} \sum_{n_t, n_x} \varphi(n_t, n_x) \right\rangle^2 \right) , \tag{9}$$

has a peak when in a finite volume, and should diverge in the thermodynamic limit. For which value of κ do you observe the phase transition, i.e., where does M change behaviour and χ_2 diverge?

Note: computing the susceptibility may require more statistics (i.e., longer runs) than the magnetisation.