The Les Houches Recitations: Day 3
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1 Hybrid Monte Carlo

So far we have implemented the Hybrid Molecular Dynamics algorithm, which is inexact due to the integration errors of $\mathcal{O}(\epsilon^2)$. In a seminal paper on the Hybrid Monte Carlo algorithm [1], Duane, Kennedy, Pendleton and Roweth realized that it can easily be made exact by a Metropolis acceptance step. Basically one measures the value of the Hamiltonian $H_i = H(\pi, \phi)$ at the beginning of the trajectory and saves the field ϕ. Then one performs the molecular dynamics evolution and again measures the Hamiltonian $H_f = H(\pi', \phi')$. This "proposed" new ϕ' is accepted with probability $\min[1, \exp(-(H_f - H_i))]$, else the new field is set to the initial field ϕ. Alg. 1 gives the pseudo-code for the full HMC algorithm and the realization of the accept/reject step.

1.1 Tasks

1. Extend your program to the HMC algorithm: measure H and save the `phi[]` field at the beginning; perform the Metropolis step at the end.
2. We also want to do physics measurements, so measure the magnetization m and the acton S after each trajectory.
3. Detour, if time allows: Computing the energy difference from H_i and H_f is susceptible to round-off errors. It is better to subtract first the energy densities and then perform the sum. Implement this improvement of Alg. 1.

Algorithm 1 Hybrid Monte Carlo

```
procedure hmc()
  Initialize phi[] field
  for i = 1 to ntraj do
    Momentum heat bath on field mom[]
    phiold[] ← phi[]
    H_0 ← hamiltonian()
    Molecular Dynamics with initial values phi[] and mom[]
    dH ← hamiltionian()-H_0
    if not acceptance(dH) then
      phi[] ← phiold[]
    end if
  end for
procedure acceptance(Δ)
  if Δ ≤ 0 then
    return true
  else
    if exp(−Δ) >random() then
      return true
    else
      return false
    end if
  end if
```

2 Thermalization

Given a correct algorithm, i.e. one that is ergodic and stable, one can start the Markov chain from any configuration, or distribution of configurations. Applying the algorithm for a sufficiently large number of iterations will depleat the wrong contributions of this distribution and in the end, one is left with the correct distribution given by the theory one wants to simulate. This decay is exponential but the corresponding decay rates can be very small. The process is called 'thermalization' and once it is over, one is in 'equilibrium'.
In practical simulations, one measures several quantities in regular intervals. During the thermalization, their values show a systematic drift, once equilibrium is reached, they fluctuate around their 'true' average. This can look rather differently for various quantities, but as long as there are these systematic movements in any quantity, equilibrium has not been reached.
If one is uncertain about equilibration, a way to proceed is to start from very different starting configurations and observe whether or not common values for the observables are reached.

2.1 Tasks

We do some initial test using $L = 6$, $\kappa = 0.185825$ and $\lambda = 1.1689$. This is pretty close to the critical line.

1. Perform 5000 trajectories of length 1, $\epsilon = 0.05$, starting from a random initial configuration. Observe how the system thermalizes. Compare with runs at $\kappa = 0.1$ and $\kappa = 0.2$. How long (in MC time) do we have to wait until we can say that we are in equilibrium?

2. Now make a longer run, eg. 10^5 trajectories. Start measuring after the thermalization has been completed. What are the values of the Binder cumulant, the magnetization and the action? To avoid problems with auto-correlations, combine the results from $N_{av} = 1000$ consecutive measurements and then do a naive error analysis on these values. What is the acceptance rate?

3. Verify that $\langle e^{-\Delta H} \rangle = 1$.

4. Convince yourself, that you actually have a correct algorithm. The results should not depend on the step-size. If the steps are too large, only the acceptance rates goes down, the average values of the observables should not be affected. Again, block 1000 measurements.

5. Now change to $\lambda = 1.145$ where the critical point is according to Ref. [2] at $\kappa_c = 0.1864463(4)$. How does $\langle |m| \rangle / V$ change when you cross the phase transition. How does the picture depend on L?

References

[1] S. Duane, A.D. Kennedy, B.J. Pendleton and D. Roweth, Phys. Lett. B **195** (1987) 216.

[2] M. Hasenbusch, J. Phys. A **32** (1999) 4851 [arXiv:hep-lat/9902026].