The Les Houches Recitations: Day 2
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1 Hybrid Molecular Dynamics

Today we start to implement the actual updating algorithm. For the moment, we forget about HMC, but start with its inexact precursor, the Hybrid Molecular Dynamics algorithm. For the classic QCD citation see Ref. [1]. It is summarized in Alg. 1.

Algorithm 1 Hybrid Molecular Dynamics

```
Initialize phi[] field
for i=1 to ntraj do
  Momentum heat bath on field mom[]; fill with Gaussian random numbers
  Molecular Dynamics with initial values phi[] and mom[] → new values phi[], mom[]
end for
```

The program so far initializes the fields `phi[]` and `mom[]` and computes the Hamiltonian and the magnetization. Now the second step of the algorithm is to be implemented: the molecular dynamics evolution.

1.1 Molecular Dynamics

Given the starting fields ϕ^0 and π^0, we want to find the solution to the differential equations

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}\phi_x^\tau &= \frac{\partial}{\partial \pi_x} H(\phi^\tau,\pi^\tau)\\ \frac{\mathrm{d}}{\mathrm{d}\tau}\pi_x^\tau &= -\frac{\partial}{\partial \phi_x} H(\phi^\tau,\pi^\tau)\ .\end{aligned}$$

A simple algorithm is the so-called Verlet method, sometimes also called leap-frog. It is based on a decomposition of the Hamiltonian in exactly integrable pieces

$$H(\phi,\pi) = H_1(\pi) + H_2(\phi)$$

with $H_1(\pi) = \sum_x \pi_x^2/2$ and $H_2(\phi) = S(\phi)$. It consists of repeated application of the following elementary step:

$$\phi^{n+1/2} = \phi^n + \frac{\epsilon}{2}\nabla_\pi H_1(\pi^n) \tag{1}$$

$$\pi^{n+1} = \pi^n - \epsilon\nabla_\phi S(\phi^{n+1/2}) \tag{2}$$

$$\phi^{n+1} = \phi^{n+1/2} + \frac{\epsilon}{2}\nabla_\pi H_1(\pi^{n+1}) \tag{3}$$

In an abuse of notation, we labelled the fields at time $n\epsilon$ by n. For the ϕ^4 Hamiltonian the derivatives are easily computed. This moves the fields forward by a step ϵ in the MC time. They are repeated $m = \tau/\epsilon$ times, see Alg. 2.

1.2 Tasks

1. Derive the explicit expressions for the derivatives in Eqs. 1-3.
2. Write routines which perform the two elementary updates in Eq. 2 and Eqs. 1, 3, see Alg. 3.

Algorithm 2 Molecular dynamics

procedure leapfrog(tau, nstep)

    eps ← tau/nstep
    for $j = 1$ to nstep **do**
        move_phi(eps/2)
        move_mom(eps)
        move_phi(eps/2)
    end for

Algorithm 3 Elementary updates

procedure move_phi(eps)

    for all x **do**
        phi(x) ← phi(x) + eps*mom(x)
    end for

procedure move_mom(eps)

    for all x **do**
        mom ← mom - eps*force(x)
    end for

3. Write a routine which repeats the sequence of these three steps m times. This moves the fields to time $\tau = m\epsilon$.

4. Test this routine by measuring the Hamiltonian after each application of the three steps. Since they are supposed to solve the Hamiltonian equations, the energy H should be conserved up to $\mathcal{O}(\epsilon^2)$. Use trajectories of length 1 and test for various ϵ that this is indeed the case. Suggestion: use a 4^4 lattice, $\kappa = 0.18169$ and $\lambda = 1.3282$, starting from a random ϕ field. Do 100 trajectories and measure the energy violation after each.

5. An important property of the integrator is that it is reversible. So if we do a trajectory $(\pi, \phi) \to (\pi', \phi')$ and flip the momentum $\pi' \to -\pi'$, then the trajectory with $(-\pi', \phi')$ as initial values should lead to (π, ϕ). Check that this is the case. What spoils this?

References

[1] S. A. Gottlieb, W. Liu, D. Toussaint, R. L. Renken and R. L. Sugar, "Hybrid Molecular Dynamics Algorithms for the Numerical Simulation of Phys. Rev. D **35** (1987) 2531.