Problem Sheet 9

for the course
“Introduction to Lattice Gauge Theory”
Summer 2019

Lecturer: PD Dr. G. von Hippel

1. *Reading List*

   1. Les Houches Lecture Notes, sections 6.2.2.4 and 6.2.3.1 (p. 355-357), and section 6.2.4 (p. 361-365)
   2. Gattringer/Lang, sections 4.5 (p. 93-100) and 8.2 (p. 190-199)

2. *Molecular Dynamics and HMC Algorithm*

   In Problem Sheet 4 we studied Markov chains over discrete state spaces as a basis for Monte-Carlo algorithms. For lattice gauge theories with continuous gauge groups, however, we require continuous state spaces. In this case the transition probability matrix $T_{s's}$ is replaced by a transition probability density $T(U' \leftarrow U)$ which must be positive,

$$T(U' \leftarrow U) \geq 0 \;\; \forall U', U \in X,$$

   and normalized with regard to the measure μ on X,

$$\int_X \mathrm{d}\mu(U')\, T(U' \leftarrow U) = 1 \;\; \forall U \in X,$$

   in order to be interpretable as a probability density. We will moreover demand that an invariant distribution is given by P,

$$\int_X \mathrm{d}\mu(U)\, T(U' \leftarrow U) P(U) = P(U') \;\; \forall U' \in X,$$

   as well as a condition that corresponds to the aperiodicity and ergodicity conditions of the discrete case, e.g.

$$\forall V \in X \; \exists N \text{ open}, V \in N \; \exists \epsilon > 0 \; \forall U, U' \in N \; T(U' \leftarrow U) \geq \epsilon.$$

   Under these conditions, the results we obtained in the discrete case also hold (although proving this rigorously is hard).

   In the following, we will consider in particular the case $X = \mathrm{SU}(N_c)^{VD}$ with the measure induced by the Haar measure on $\mathrm{SU}(N_c)$.

(a) We denote by $U_\tau(U_0, \pi_0)$ the solution $U(\tau)$ of Hamilton's equations

$$\begin{aligned} \dot{\pi} &= -\left.\frac{\partial S(\mathrm{e}^{\omega} U)}{\partial \omega}\right|_{\omega=0} \\ \dot{U} &= \pi U \end{aligned}$$

for $\pi \in Y = \mathfrak{su}(N_c)^{VD}$ with initial conditions $U(0) = U_0$, $\pi(0) = \pi_0$ at time $t = \tau$. Show (as far as possible) that the transition probability density

$$T(U' \leftarrow U) = \frac{1}{\mathcal{Z}_\pi} \int_Y \mathrm{d}\pi \, \mathrm{e}^{-\frac{1}{2}||\pi||^2} \delta(U' - U_\tau(U, \pi))$$

with $\mathcal{Z}_\pi = \int_Y \mathrm{d}\pi \, \mathrm{e}^{-\frac{1}{2}||\pi||^2}$ satisfies our conditions for $P(U) \propto \mathrm{e}^{-S(U)}$. Which algorithm (MD method) does this correspond to?

(b) In practical applications we cannot solve Hamilton's equations exactly and have to make do with numerical solutions. Show that the *leapfrog method*

$$(U_\tau, \pi_\tau) = V_{\frac{\epsilon}{2}} T_\epsilon V_\epsilon V_\epsilon \cdots V_\epsilon T_\epsilon V_{\frac{\epsilon}{2}} (U_0, \pi_0)$$

for $\tau = N\epsilon$ with N applications of

$$\begin{aligned} T_\epsilon(U, \pi) &= (\mathrm{e}^{\epsilon \pi} U, \pi) \\ V_\epsilon(U, \pi) &= (U, \pi - \epsilon F(U)) \end{aligned}$$

preserves the measure $\mathrm{d}\mu(U) \wedge \mathrm{d}\pi$ on $X \times Y$ as well as the time-reversal invariance of the time evolution.

(c) Since the Hamiltonian function $H(U, \pi) = \frac{1}{2}||\pi||^2 + S(U)$ is not preserved exactly by numerical integration, we have to augment the numerical solution $(\widetilde{U}_\tau, \widetilde{\pi}_\tau)$ of Hamilton's equations by a Metropolis accept-reject step. This gives us the *Hybrid Monte-Carlo* (HMC) Algorithm with transition probability density

$$T(U' \leftarrow U) = \frac{1}{\mathcal{Z}_\pi} \int_Y \mathrm{d}\pi \, \mathrm{e}^{-\frac{1}{2}||\pi||^2} \Big(P_{\mathrm{acc}}(\tau, U, \pi) \delta(U' - \widetilde{U}_\tau) + [1 - P_{\mathrm{acc}}(\tau, U, \pi)] \delta(U' - U) \Big)$$

where $P_{\mathrm{acc}}(\tau, U, \pi) = \min\{1, \mathrm{e}^{-(H(\widetilde{U}_\tau(U,\pi), \widetilde{\pi}_\tau(U,\pi)) - H(U,\pi))}\}$. Convince yourself (as far as possible) that this satisfies our conditions, and spell out the algorithm in terms of computational steps.

3. *Autocorrelations in Markov Chains*

The successive states s_k of a Markov chain are (after a sufficiently long thermalization phase) each drawn from the probability distribution $P(s)$, but in general they are not statistically independent. A measure of correlations along the Markov chain is the autocorrelation function

$$\Gamma_O(t) = \langle\langle O(s_k)O(s_{k+t})\rangle\rangle - \langle\langle O(s_k)\rangle\rangle\langle\langle O(s_{k+t})\rangle\rangle$$

where $\langle\langle\cdots\rangle\rangle$ stands for the expectation value over an ensemble of infinitely many parallel Markov chains.

(a) Show that for $k \gg \tau$ the autocorrelation function is given by

$$\Gamma_O(t) = \sum_{s_k,\ldots,s_{k+t}} O(s_{k+t})T(s_{k+t} \leftarrow s_{k+t-1})\cdots T(s_{k+1} \leftarrow s_k)P(s_k)O(s_k) - \langle O\rangle^2$$

where $\langle O\rangle$ is the expectation value with regard to $P(s)$.

(b) Infer from $P(s)O(s) = P(s)\langle O\rangle + f(s)$, $f \in \mathcal{H}_0$, that $\Gamma(t) \sim \mathrm{e}^{-t/\tau}$ for large t, and conclude that for $|i-j| \gg \tau$ the measured values $O(s_i)$ and $O(s_j)$ become statistically independent.

(c) Show that the statistical estimator

$$\overline{O} = \frac{1}{N}\sum_{k=1}^{N} O(s_k)$$

has the variance

$$\langle\langle(\overline{O} - \langle O\rangle)^2\rangle\rangle = \frac{1}{N^2}\sum_{i,j=1}^{N} \Gamma_O(|i-j|) = \sigma_0^2\frac{2\tau_O}{N} + \mathrm{O}(N^{-2})$$

where the intrinsic variance σ_0^2 and the integrated autocorrelation τ_O are defined by

$$\sigma_0^2 = \Gamma(0) = \langle(O - \langle O\rangle)^2\rangle, \qquad \tau_O = \frac{1}{2} + \sum_{t=1}^{\infty}\frac{\Gamma(t)}{\Gamma(0)}.$$