Effect of FTHMC with 2+1 Domain Wall Fermions on Autocorrelation Times via Master-Field Technique I

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Lattice QCD

In lattice QCD, $\langle O \rangle$ is evaluated non-perturbatively.

- Wick-rotated

$$\langle O \rangle = \frac{1}{Z} \int \mathcal{D}\phi O(\phi) e^{-S_{\mathrm{E}}}$$

- Then, we use $e^{-S_{\mathrm{E}}}$ as a Monte-Carlo weight and have

$$\langle O \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{i}^{N} O_i \approx \frac{1}{N} \sum_{i}^{N} O_i .$$

- Configurations are sampled using importance sampling method

Markov Chains

Markov chain: $\{X_n\}_{n=0}^{N}$

- A sequence of random variables with Markov Property:

$$\begin{aligned}&\Pr\{X_n = x_n | X_{n-1} = x_{n-1}, X_{n-2} = x_{n-2}, \cdots, X_0 = x_0\} \\ &\qquad = \Pr\{X_n = x_n | X_{n-1} = x_{n-1}\} = P_n^{x_{n-1}}(x_n) = \frac{P_{X_n \cap X_{n-1}}(x_n, x_{n-1})}{P_{X_{n-1}}(x_{n-1})}\end{aligned}$$

- In words, the probability of a event happening depends only on the outcome of the last outcome and not on the history of events
- Here, $P_n^{x_{n-1}} : E \to [0, 1]$
- P_0 is an initial distribution corresponding to an independent random variable
- Transition Probability, $T_n : E \times E \to [0, 1]$ via $T_n(x_n, x_{n-1}) = P_n^{x_{n-1}}(x_n)$

Markov Chains

In QCD, we consider time-homogeneous Markov Chain, i.e.,

- $\Pr\{X_{n+1} = x_{n+1} | X_n = x_n\} = \Pr\{X_n = x_n | X_{n_1} = x_{n-1}\} \quad \therefore T_n = T$
- Also, $P_n(x_n) = T^n P_0(x_n)$

We assume

- our Markov chains is irreducible
- all states are aperiodic, $(\forall s \in E\, \forall N \in \mathbb{N})\ T^N(s \to s) \neq 0$ and positive recurrent $E[\tau_{\text{recurrence}}] < \infty$

Then, [Rothe, 2012]

- There exists a stationary distribution π, and it is unique
- if the initial distribution is π, it is (wide-sense) stationary (WSS)
- if we further have $E[\tau^2_{\text{recurrence}}] < \infty$,

$$\langle O \rangle = (1/N) \sum_{i=1}^{N} O(x_i) + \mathcal{O}(1/\sqrt{N})$$

How do we find such T with a desired distribution π?

The Acceptance-Rejection Method

$T(i \to j) = T_0(i \to j)P_{acc}(i,j) + \delta_{ij}\sum_k T_0(i \to j)[1 - P_{\mathrm{acc}}(i,j)]$

- T_0: a transition matrix with micro-reversibility,
  $T_0(s \to s') = T_0(s' \to s)$
- $P_{acc}(i,j) = \min\{1, \pi(i)/\pi(j)\}$

Then, the stationary distribution of T is the target distribution π.

Also, it satisfies detailed balance condition:

$$P(i)T(i \to j) = P(j)T(j \to i)$$

$SU(3)$

For QCD,

- $\pi(U) = \frac{1}{Z} e^{-S_G(U)}$
- $Z = \int \mathcal{D}U e^{-S_G(U)}$

Requirement: [Luscher, 2010]

- $T(U \to U') \geq 0$ for all U, U' and $\int \mathcal{D}U' \ T(U \to U') = 1$ for all U.
- $\int \mathcal{D}U \ \pi(U) T(U \to U') = \pi(U')$ for all U'
- $\forall V \ \exists \mathcal{N}_V$, where $\mathcal{N}_V$ is an open neighborhood of V in the space of gauge configurations, s.t.

$$\forall U, U' \in \mathcal{N}_V \ \exists \varepsilon > 0 \text{ s.t. } T(U \to U') \geq \varepsilon$$

The Acceptance-Rejection Method Revisited

Given a link U,

1. Propose a new link U' according to $T_0(U \to U')$
2. Accept U' as the new link in the MC chain with probability $P_{acc} = \min\{1, e^{S_G(U) - S_G(U')}\}$
3. Leave the link variable unchanged if the new value proposed in step (2) is not accepted, i.e., $U' = U$
4. back to (1)

HMC

- HMC = Hybrid Monte Carlo = Molecular Dynamics (MD) + Monte Carlo (MC)
- In MD, a partition function of classical statistical system is approximated by trajectories of the canonical Hamilton system by using ergodicity
- To use the technique of MD,

$$Z = \int \mathcal{D}U\, e^{-S(U)} \propto \int \mathcal{D}U\mathcal{D}P\, e^{-P^2/2} e^{-S(U)} = \int \mathcal{D}U\mathcal{D}P\, e^{-H}$$

- $H = P^2/2 + S(U)$

HMC Steps

1. A momentum field P is generated randomly with probability density proportional to $e^{-P^2/2}$
2. The Hamilton equations are integrated from time $t = 0$ to some later time τ with the initial fields of P and U to obtain a new field U'
3. Apply the Acceptance-Reject step to decide whether to set U_τ to U' or keep U, i.e., $U_\tau = U$
4. Repeat

The above steps correspond to

$$T_0(U \to U') = \frac{1}{\mathcal{Z}_P} \int \mathcal{D}P\, e^{-P^2/2} \prod_{x,\mu} \delta(U'(x,\mu)U(x,\mu))$$

Numerical Integration

Elementary updates for P and U

$$I_P(\varepsilon) : (P, U) \to (P - \varepsilon F, U)$$
$$I_U(\varepsilon) : (P, U) \to (P, e^{\varepsilon P} U)$$

Leap-frog integrator:

$$\mathcal{J}(\varepsilon, N) = \{I_P(\varepsilon/2) I_U(\varepsilon) I_P(\varepsilon/2)\}^N$$

where $\varepsilon = \tau/N$

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Field-Transformation HMC

Consider $U = \mathcal{F}_t(V)$

Under $\mathcal{F}$

$$Z = \int \mathcal{D}U e^{-S(U)} = \int \mathcal{D}V \mathrm{Det}[\mathcal{F}_*(V)]\, e^{-S(\mathcal{F}(V))} = \int \mathcal{D}V\, e^{-S_{FT}(V)}$$

$$S_{FT} = S(\mathcal{F}_t(V)) - \ln \mathrm{Det}\mathcal{F}_*(V)$$

$$\mathcal{F}_*(x,\mu;y,\nu)^{ab}(V) = \theta^a_{x,\mu}(\mathcal{F}_*\hat{\partial}^b_{y,\nu}) = -2\mathrm{tr}\,\left[\left(\hat{\partial}^b_{y,\nu}U(x,\mu)\right)U(x,\mu)^{-1}T^a\right]$$

Notation:

- $T^a \in \mathfrak{su}(3)$: generators of $\mathfrak{su}(3)$
- $\omega_{U(x,\mu)} = dU(x,\mu)U^{-1}(x,\mu)$: Mauler-Cartan form
- $\theta^a_{x,\mu}(v) = (\omega_{U(x,\mu)}(v), T^a) = -2\mathrm{tr}\,[\omega_{U(x,\mu)}(v)T^a] \quad (v \in T_{U(x,\mu)}\mathbb{R}^4 \times SU(3)^4)$
- $\partial^a_{x,\mu}[f]|_U = \frac{d}{dt}f(U_t)|_{t=0}$ where

$$U_t(y,\nu) = \begin{cases} e^{tT^a}U(x,\mu) & \text{if } (y,\nu) = (x,\mu) \\ U(y,\nu) & \text{othersie} \end{cases}$$

Field-Transformation HMC

- originally proposed by Luscher [Lüscher, 2010]
- Perfect trivialization: $S_{FT} = 0$
- Transformation via flow $U \to U + \varepsilon Z(U)U + \mathcal{O}(\varepsilon^2) \longrightarrow \dot{U}_t = Z(U_t)U_t$
- Then,

$$S_{FT} = 0 \iff \int_0^t ds \sum_{x,\mu} \{\partial^a_{x,\mu}[Z_s(U)]^a(x,\mu)\}|_{U=U_s} = tS_G(U_t) + C_t$$

- Perfect trivialization is achieved at $t = 1$

Wilson Flow

- Ansatz:

$$[Z_t(U)]^a(x,\mu) = -\partial^a_{x,\mu}\tilde{S}_t(U)$$

- Insert this to the previous equation:

$$\mathfrak{L}_t\tilde{S}_t = S_G + \dot{C}_t$$
$$\mathfrak{L}_t = \sum_{x,\mu}\{\partial^a_{x,\mu}\partial^a_{x,\mu} + t(\partial^a_{x,\mu}S_G)\partial^a_{x,\mu}\}$$

- Expand: $\tilde{S}_t = \sum_{k=0}^{\infty} t^k \tilde{S}_t^{(k)}$
- Matching t leads to recursive relations

$$\mathfrak{L}_0\tilde{S}^{(0)} = S_G + \dot{C}^{(0)}$$
$$\mathfrak{L}_0\tilde{S}^{(k)} = -\sum_{x,\mu}\partial^a_{x,\mu}S_G\partial^a_{x,\mu}\tilde{S}^{(k-1)} + \dot{C}^{(k)}$$

Wilson Flow

- The solution of the recursion

$$\tilde{S}^{(0)} = \mathfrak{L}_0^{-1} S_G$$
$$\tilde{S}^{(k)} = -\mathfrak{L}_0^{-1} \sum_{x,\mu} \partial^a_{x,\mu} S_G \partial^a_{x,\mu} \tilde{S}^{(k-1)}$$

- Approximation:
  - $\tilde{S} \approx \tilde{S}^{(0)}$
  - $S_G = S_W = -\frac{\beta}{6} \sum_{x,\mu \neq \nu} \mathrm{tr}[P_{\mu\nu}(x)]$
  - Plaquette: $P_{\mu\nu}(x) = U_\mu(x) U_\nu(x+\hat{\mu}) U^\dagger_\mu(x+\hat{\nu}) U^\dagger_\nu(x)$

Wilson Flow

- Then,

$$
\begin{aligned}
Z_t(U_t)(x,\mu) = \mathcal{P}(C(x,\mu)) &\equiv \frac{1}{2}(C(x,\mu) - C(x,\mu)^\dagger) \\
&\quad - \frac{1}{6}\mathrm{tr}\,[C(x,\mu) - C(x,\mu)^\dagger] \\
\mathcal{P}(M) &= \frac{1}{2}(M - M^\dagger) - \frac{1}{6}\mathrm{tr}\,(M - M^\dagger) \\
C(x,\mu) &= \sum_{\nu \neq \pm\mu} \rho_{\mu,\nu} U(x,\nu) U(x+\hat{\nu},\mu) U(x+\hat{\mu},\nu)^\dagger U(x,\mu)^\dagger .
\end{aligned}
$$

- Numerical integration
  - discretize the transformation with step of size $\rho \equiv \rho_{\mu\nu}$
  - ρ includes a expansion parameter ε
  - The number of integration steps for the discretized trivializing map is set to 1

Wilson Flow

- A single Euler step:

$$U(x,\mu) \to \mathcal{E}_{x,\mu}(y,\nu) = \begin{cases} e^{Z_t(U)(x,\mu)} U(x,\mu) & \text{if } (y,\nu) = (x,\mu) \\ U(y,\nu) & \text{otherwise.} \end{cases}$$

- This approximation is cheaper than perfect trivialization yet effective
- The transformation is wavelength-dependent
- Its effect on autocorrelation is also wavelength-dependent

Thank you!

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