Autocorrelation studies in two-flavour Wilson Lattice QCD using DD-HMC algorithm

Abhishek Chowdhury, Asit K. De, Sangita De Sarkar, A. Harindranath, Jyotirmoy Maiti, Santanu Mondal, Anwesa Sarkar

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- Dynamical Wilson fermion simulations at smaller quark masses, smaller lattice spacings and and larger lattice volumes on currently available computers have become feasible with recent developments such as DD-HMC algorithm (Luscher).
- Measurements of autocorrelation times help us to evaluate the performance of an algorithm in overcoming critical slowing down.
- In addition, an accurate determination of the uncertainty associated with the measurement of an observable requires a realistic estimation of the autocorrelation of the observable.
- In this work we study autocorrelations of several observables measured with DD-HMC algorithm using naive Wilson fermion and gauge action.

Definitions

The normalized autocorrelation function for an observable $\mathcal{O}$ is defined as, $\Gamma^{\mathcal{O}}(t) = C^{\mathcal{O}}(t) / C^{\mathcal{O}}(0)$ where

$$C^{\mathcal{O}}(t) = \frac{1}{N-t} \sum_{r=1}^{N-t} (\mathcal{O}_r - \langle \mathcal{O} \rangle)(\mathcal{O}_{r+t} - \langle \mathcal{O} \rangle) \ , \quad \langle \mathcal{O} \rangle = \frac{1}{N} \sum_{t=1}^{N} \mathcal{O}_t .$$

The integrated autocorrelation time is,

$$\tau_{\text{int}}^{\mathcal{O}} = \frac{1}{2} + \sum_{t=1}^{\text{window}} \Gamma^{\mathcal{O}}(t)$$

The error ,

$$\delta\langle\mathscr{O}\rangle = \sqrt{\frac{2\tau_{int}(\mathscr{O})var[\mathscr{O}]}{N}}$$

For any stationary Markov chain satisfiying ergodicity and detailed balance,

$$\Gamma^{\mathscr{O}}(t) = \sum_{n\geq 1} e^{-t/\tau_n} \mid \eta_n(\mathscr{O}) \mid^2$$

where $\tau_n = -\frac{1}{\ln\lambda_n}$. λ_n's are real eigenvalues of symmetrized probability transition matrix with $\lambda_0 = 1$ and $|\lambda_n| < 1$ for $n \geq 1$. $\tau_1 = -\frac{1}{\ln\lambda_1} \rightarrow$ exponential autocorrelation time (τ_{exp}).

- Different obsevables couples differently to the eigenmodes.
- $\Gamma^{\mathscr{O}}(t)$ cannot be negative.

Simulation Details

$\beta = 5.6$

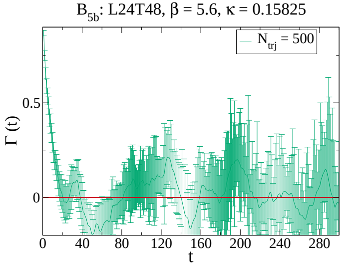
tag	lattice	κ	block	N_2	N_{trj}	τ
B_{1b}	$24^3 \times 48$	0.1575	$12^2 \times 6^2$	18	13128	0.5
B_{3a}	,,	0.158	$6^3 \times 8$	6	7200	0.5
B_{3b}	,,	0.158	$12^2 \times 6^2$	18	13646	0.5
B_{4a}	,,	0.158125	$6^3 \times 8$	8	9360	0.5
B_{4b}	,,	0.158125	$12^2 \times 6^2$	18	11328	0.5
B_{5a}	,,	0.15825	$6^3 \times 8$	8	6960	0.5
B_{5b}	,,	0.15825	$12^2 \times 6^2$	18	12820	0.5
C_2	$32^3 \times 64$	0.158	$8^3 \times 16$	8	7576	0.5
C_3	,,	0.15815	$8^3 \times 16$	8	9556	0.5
C_4	,,	0.15825	$8^3 \times 16$	8	4992	0.25

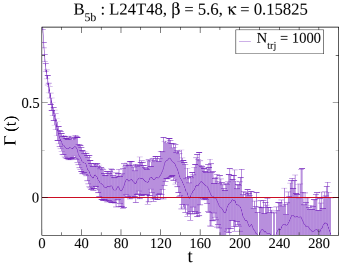
$\beta = 5.8$

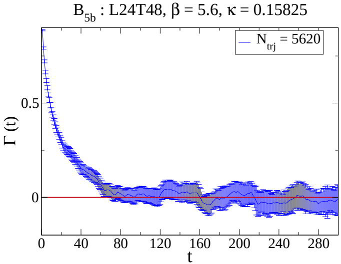
tag	lattice	κ	block	N_2	N_{trj}	τ
D_1	$32^3 \times 64$	0.1543	$8^3 \times 16$	8	9600	0.5
D_5	,,	0.15475	$8^3 \times 16$	8	6820	0.25

Table: Here *block*, N_2, N_{trj}, τ refers to HMC block, step number for the force F_2, number of HMC trajectories and the Molecular Dynamics trajectory length respectively.

Negativity of autocorrelation function for plaquette







Improved Estimation of τ_{int}:
Let τ_* be the best estimate of dominant time constant. If for an observable $\mathcal{O}$ all relevant time scales are smaller or of the same order of τ_* then the upper bound of τ_{int},

$$\tau_{int}^{u} = \frac{1}{2} + \sum_{t=1}^{W_u} \Gamma^{\mathcal{O}}(W_u) + A_{\mathcal{O}}(W_u)\tau_* \text{ where } A_{\mathcal{O}} = max(\Gamma^{\mathcal{O}}(W_u), 2\delta\Gamma^{\mathcal{O}}(W_u)),$$

W_u chosen where autocorrelation function is still significant.

Estimate of τ_*:

$$\tau_{eff} = \frac{t}{2\ln\frac{\Gamma^{\mathcal{O}}(t/2)}{\Gamma^{\mathcal{O}}(t)}}$$

$$\tau_{eff}^{exp} = Max_{\mathcal{O}}\left[\frac{t}{2\ln\frac{\Gamma^{\mathcal{O}}(t/2)}{\Gamma^{\mathcal{O}}(t)}}\right]$$

S. Schaefer *et al.* [ALPHA Collaboration], Nucl. Phys. B **845**, 93 (2011);
S. Schaefer and F. Virotta, PoS LATTICE **2010**, 042 (2010).

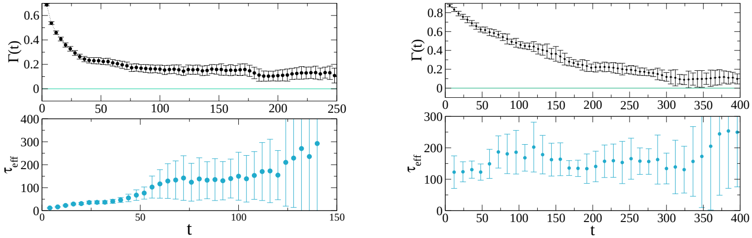


Figure: Normalized autocorrelation function and effective autocorrelation time for P_0 (left) Q_{20}^2 (right) for the ensemble B_{3b}.

Autocorrelations for topological susceptibility (Q_{20}^2)

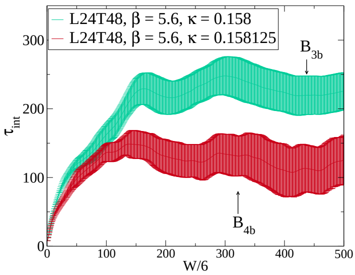


Figure: Integrated autocorrelation times for topological suceptibilities (Q_{20}^2) at $\beta = 5.6$ ($a = 0.069$ fm) (left) and at $\beta = 5.8$ (right) ($a = 0.053$ fm).

$\tau_{int}(Q_{20}^2) \downarrow$ as $\kappa \uparrow$

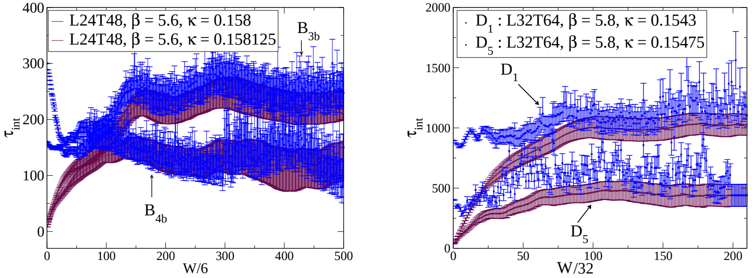
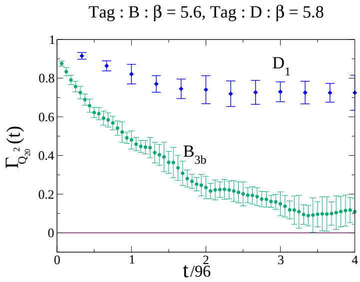


Figure: Integrated autocorrelation times and their upper bounds (τ^{u}_{int}) for topological suceptibilities (Q^2_{20}) at $\beta = 5.6$ ($a = 0.07$ fm) (left) and at $\beta = 5.8$ (right) ($a = 0.055$ fm).

$\tau_{int}(Q^2_{20})$ & $\tau^{u}_{int}(Q^2_{20}) \downarrow$ as $\kappa \uparrow$

Topological Charge Density Correlator (C(r))



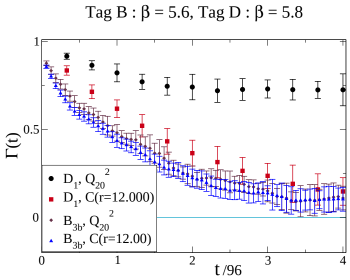


Figure: (left) Comaparison of normalized autocorrelation functions for Q_{20}^2 at $\beta = 5.6$ and 5.8. (right) Comparison of β dependence of normalized autocorrelation functions for Q_{20}^2 and $C(r = 12.0)$.

$C(r)$ is affected only slightly by critical slowing down.

More about the properties of $C(r) \longrightarrow$ talk by SM, Session: Chiral Symmetry

Effect of Size and Smearing

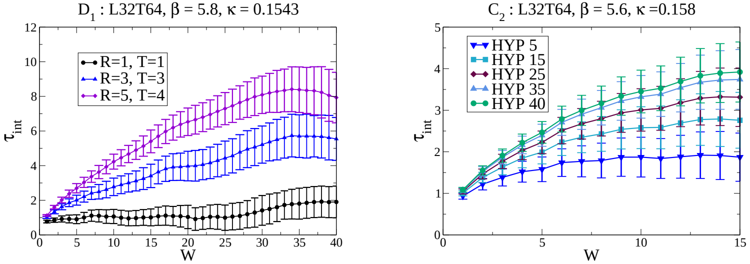


Figure: Integrated autocorrelation times of Wilson loops for different sizes (left) and for different levels of HYP smearing (right).

Autocorrelation increases with increasing size and smearing level.

Pion and Nucleon Propagators

$\beta = 5.6$

tag	κ	τ_{int}^{Pion}	$\tau_{int}^{Nucleon}$
B_{3a}	0.158	99(19)	75(18)
B_{4a}	0.158125	50(9)	34(9)
B_{5a}	0.15825	40(10)	25(9)
C_2	0.158	39(13)	33(17)
C_3	0.15815	31(15)	26(7)
C_4	0.15825	34(11)	18(6)

Table: Integrated autocorrelation times for pion (PP) and nucleon propagators with wall sources.

Autocorrelation decreases with increasing κ.

About low lying hadron hadrons and chiral condensate $\longrightarrow$ talk by Asit De, session: Chiral Symmetry

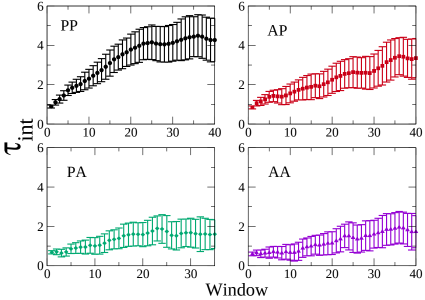


Figure: Integrated autocorrelation times for *PP*, *AP*, *PA* and *AA* correlators with wall source for the ensemble B_{3a}. Measurements are done with a gap of 24 trajectories.

$$\begin{aligned} P &= \bar{q}\gamma_5 q \quad \text{and} \\ A &= \bar{q}\gamma_4\gamma_5 q \end{aligned}$$

$$q = u/d \text{ quark.}$$

Conclusions

- Autocorrelations of topological susceptibility, pion and nucleon propagators decrease with decreasing quark mass.
- The topological charge density correlator is affected only slightly by critical slowing down compared to topological susceptibility.
- Increasing the size and the smearing level increases the autocorrelation of Wilson loop.

$\beta = 5.6$	MeV	
κ	m_q	m_{pi}
0.1575	123	790
0.15755	95	684
0.158	65	562
0.158125	51	499
0.15815	49	483
0.15825	35	416
0.1583	28	378
0.1584	21	315

$\beta = 5.8$, Volume=$32^3 64$	MeV	
κ	m_q	m_{pi}
0.1543	76	600
0.15455	42	453
0.15462	31	400
0.1547	18	317
0.15475	16	275

The statistical variance of the measured value $\langle \mathscr{O} \rangle$ is,

$$\sigma^2 = 2\tau_{int}\sigma_0^2$$

For any stationary Markov chain

$$\Gamma^{\mathscr{O}}(t) = \sum_{n\geq 1} (\lambda_n)^t \; \mid \eta_n(\mathscr{O}) \mid^2 .$$

λ_n, are the eigenvalues of the matrix,

$$\begin{aligned} T_{x,y} &= \pi_x^{\frac{1}{2}} P_{xy} \pi_y^{-\frac{1}{2}} \\ & P_{xy} \;\rightarrow\; \text{probability transition matrix of the Markov chain,} \\ & \pi_x \;\rightarrow \text{is the stationary distribution.} \end{aligned}$$

$\eta_n(\mathscr{O}) = \sum_x \mathscr{O}(x)\chi_n(x)\pi_x^{\frac{1}{2}}$ where $\chi_n(x)$ is the eigenfunction corresponding to λ_n.

$T_{x,y}$ is positive definite. Now if the algorithm satisfies detailed balance $T_{x,y}$ is symmetric.
Then by Perron-Frobenius theorem,
$T_{x,y}$ has real positive eigenvalues λ_n, $n \geq 0$ with $\lambda_0 = 1$ and $|\lambda_n| < 1$ for $n \geq 1$.
Hence,

$$\Gamma^{\mathscr{O}}(t) = \sum_{n \geq 1} e^{-t/\tau_n} \mid \eta_n(\mathscr{O}) \mid^2$$

where $\tau_n = -\frac{1}{\ln \lambda_n}$.
$\tau_1 = -\frac{1}{\ln \lambda_1} \rightarrow$ exponential autocorrelation time (τ_{exp}).

Q_{20}^2

β	κ	τ_{int}	τ_{int}^u
5.6	0.158	247(27)	276(30)
5.8	0.1543	1030(93)	1056(190)

$C(r = 12.0)$

β	κ	τ_{int}	τ_{int}^u
5.6	0.158	264(53)	314(76)
5.8	0.1543	458(83)	850(168)

Table: Integrated autocorrelation times (τ_{int}) and their upper bounds (τ_{int}^u) for Q_{20}^2 and $C(r)$ in two β's.