Autocorrelations in Hybrid Monte Carlo Simulations

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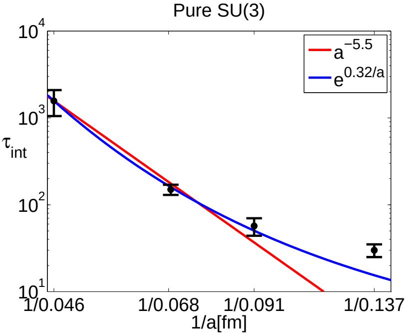
Lattice 2010

Problem



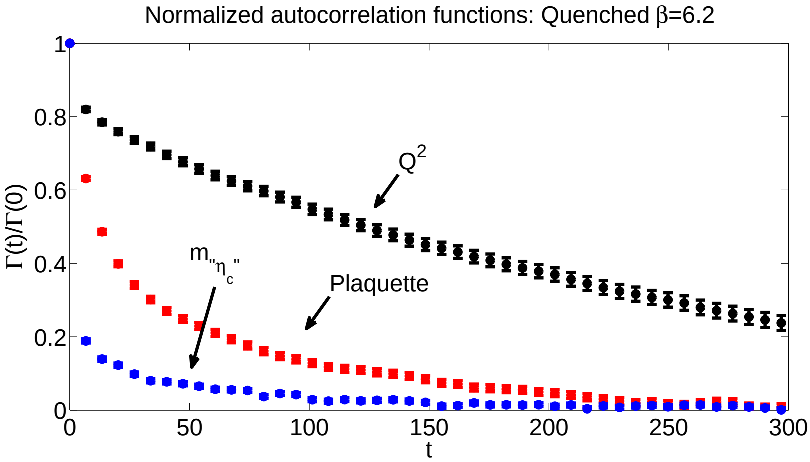
Summary of last year's talk [S.Schaefer]

- Lattice simulations suffer from critical slowing down
- Both in pure gauge and dynamical fermions simulations
- Decoupling for Wilson loops

Here we concentrate on

- How do different observables behave?
- Hadron correlation functions, masses. . .

Autocorrelation for different observables at $a \sim 0.07$fm



- Autocorrelation function $\Gamma_O(t) = \langle (O(t) - \bar{O})(O(0) - \bar{O}) \rangle$
- Observables couple to the slow modes
- Strength of coupling is observable dependent

Autocorrelation functions of Markov Chains

- For algorithms with detailed balance

$$\begin{aligned}\Gamma_O(t) &= \langle (O(t)-\bar{O})(O(0)-\bar{O})\rangle \\ &= \sum_{n\geq 1}(\lambda_n)^t[\eta_n(O)]^2\end{aligned}$$

- O is a primary observable, secondary: [U.Wolff '06]
- λ_n are (real) eigenvalues of

$$\begin{aligned}T(q',q) = [\Pi(q')]^{-1/2}M(q'\leftarrow q)[\Pi(q)]^{1/2} \\ T\chi_n = \lambda_n\chi_n\ , \quad \Pi(q) = \chi_0^2(q)\end{aligned}$$

- $\eta_n(O)$ denotes the "matrix element" for the n-th mode

$$\eta_n(O) = \sum_q \chi_n(q)\sqrt{\Pi(q)}(O(q)-\bar{O})$$

Autocorrelation functions of Markov Chains II

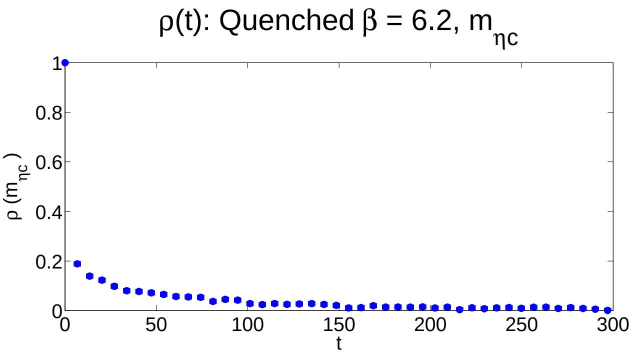
$$\Gamma_O(t) = \sum_{n\geq 1} (\lambda_n)^t [\eta_n(O)]^2$$

- $|\Gamma_O(t)| \leq \text{const.} e^{-t/\tau_{\text{exp}}}$, where $\tau_{\text{exp}}^{-1} = -\log(\lambda_1)$
- In general all modes contribute to Γ
- Symmetries can give selection rules:
  - The slowest mode can be different:

$$\tau_{\text{exp}}(\text{Parity } +) \neq \tau_{\text{exp}}(\text{Parity -})$$

  - In general one sees $\tau_{\text{exp}}(Q^2) \sim \frac{1}{2}\tau_{\text{exp}}(Q)$
  - $\langle O(\text{Parity -})\rangle = 0$, useful for correctness checks
- We restrict ourselves to parity even observables

Setup: Quenched approximation



- Quenched $a = 0.066$fm, $\rho(t) = \Gamma(t)/\Gamma(0)$
- Effective mass of "η_c" averaged over a plateau
- Correlators from noise sources
- Autocorrelation function non-negligible up to large times
- Worries: undetected contributions from very long tail

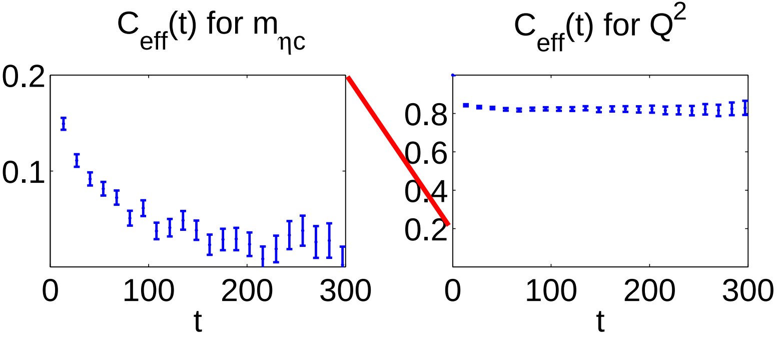
Normalized amplitude of the slow mode

- The contribution of the slow mode to ρ_O

$$\rho_O(t) \sim e^{-t/\tau_{\rm exp}}[\eta_1(O)]^2 \text{ as } t \longrightarrow \infty$$

- An effective amplitude can be extracted ⇒ "Matrix element"

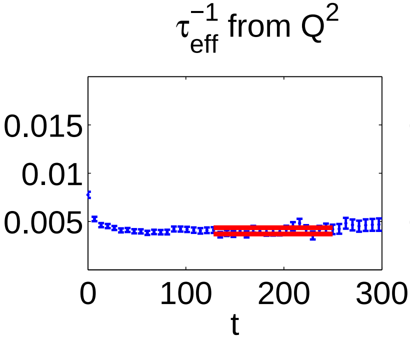
$$C_{\rm eff}(t) = \rho(t)e^{t/\tau_{\rm eff}(t)} \underset{t\to\infty}{\sim} [\eta_1(O)]^2$$



Extracting τ_{eff} from a plateau

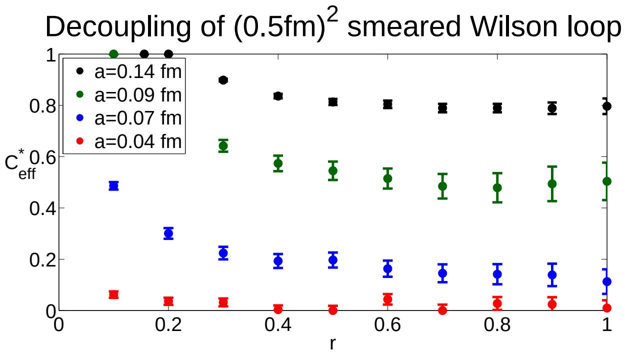
- An effective τ_{exp} is needed $\Rightarrow$ "Effective mass"

$$\tau_{\text{eff}}(t) = 1/\log\left(\frac{\Gamma(t+1)}{\Gamma(t)}\right)$$



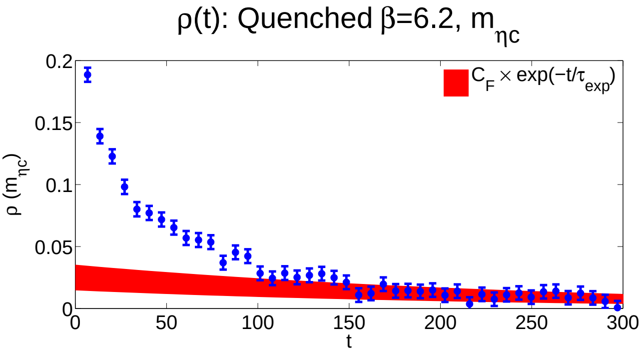
- Slowing down most prominent for the topological charge
- Other observables could be used: need much longer history

a dependence of C_{eff} and decoupling of Wilson loops



- Define $C^*_{\text{eff}}(r) = C_{\text{eff}}(r\tau_{\text{exp}})$

Small contribution from the slow mode?



- $\tau_{\text{int}}(O, W) = \frac{1}{2}\rho_O(0) + \sum_{t=1}^{W} \rho_O(t)$
- With $W = 250$ bias from neglecting the tail up to $\sim 15\%$
- Worst case scenario from various quenched correlators (D_s, "η_c", Φ) at this β value
- Total contribution of slow mode to τ_{int} is $\sim 50\%$

Improved error estimates and upper bound

- The uncertainty of $\bar{O}$ from N measurements is

$$(\delta\bar{O})^2 = \frac{\sigma_O^2}{N} 2\tau_{\rm int}(O)$$

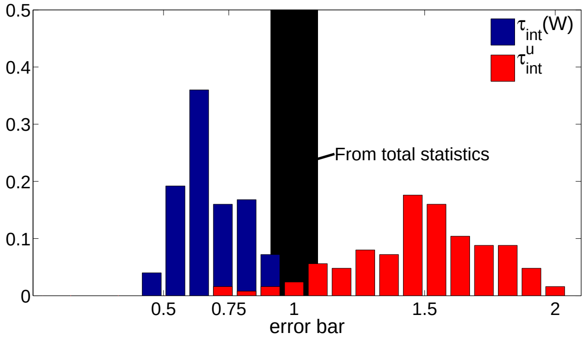
- Upper bound for $\tau_{\rm int}$

$$\tau_{\rm int}^u(O) = \tau_{\rm int}(O, W_u) + \rho_O(W_u)\tau_{\rm exp}$$

- W_u chosen such that $\rho(W_u) > 2.5\ \delta\rho(W_u)$
- $\tau_{\rm exp}$ either measured or given by model
- $\tau_{\rm int}(O) \leq \tau_{\rm int}^u(O)$, for algo. with detailed balance

Our proposal: use $\tau_{\rm int}^u$ for a safe error estimate

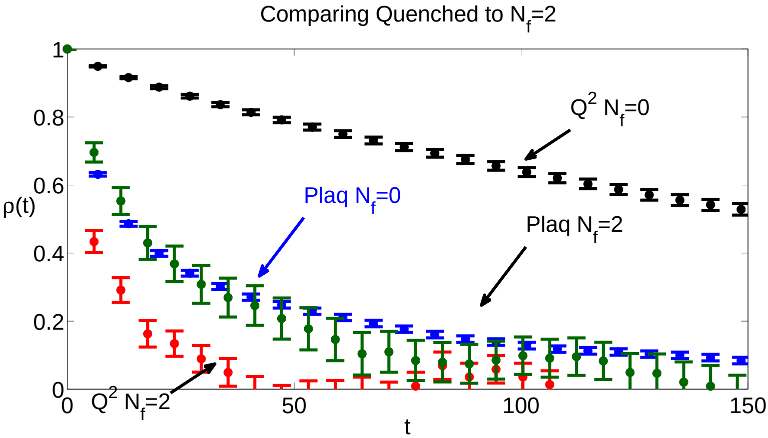
Upper Bound: works with limited statistics?



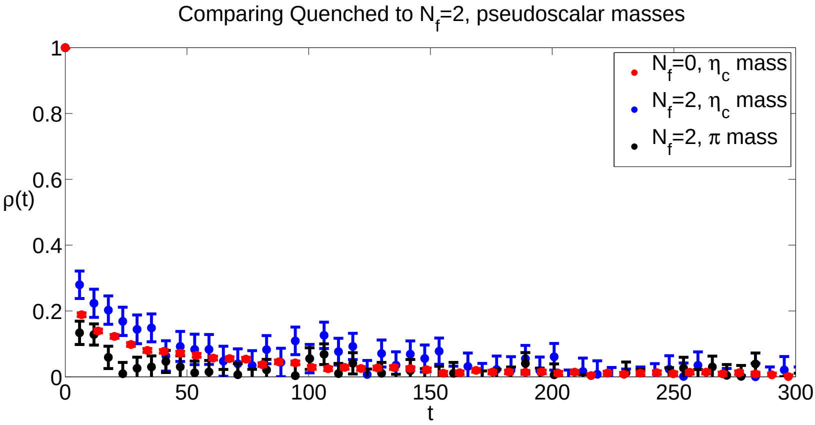
- Many replicae from a single chain (each $\approx 2500 MD$)
- The upper bound works
- Safer than standard method
- In this case study error bars at worst doubled

Results: $N_f = 2$

- Quenched: $r_0/a = 7.38$
- $N_f = 2$ from CLS dataset: ~ 5000 MDR
- $N_f = 2$ we have $r_0/a = 7.05$ [B.Leder, Lattice10]

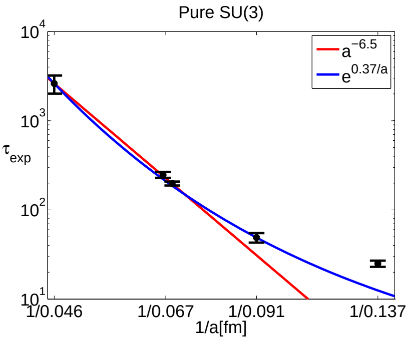


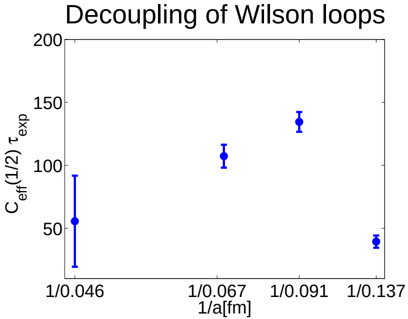
Results: $N_f = 2$ II



- "η_c" mass from noise sources (5 in quenched and 10 in $N_f = 2$)

Conclusions





- The slowing down is an issue that still needs a cure
- Needs careful error estimate, taking into account slow modes
- At $a \approx 0.07$ fm there is a $\sim 1/50$ suppression for hadronic observables
- The brick wall presently somewhere at $a \sim 0.04$ fm