Topological Charge and Susceptibility in BSM Lattice Calculations

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Outline

1. Topological charge, instantons, etc.
2. Topological charge in BSM lattice simulations
3. Working in a fixed topological charge sector
4. Maximum Likelihood method
5. Subvolume method
6. Conclusion

* Work done in collaboration with R. Brower, G. Fleming,
M. Lin, E. Neil, D. Schaich to appear soon.

Topological charge

- Topological charge: Field configurations with non-trivial topological winding

$$Q = \frac{1}{32\pi^2} \int d^4x \ \mathrm{tr}\left[F^{\mu\nu}(x)\tilde{F}_{\mu\nu}(x)\right]$$

- Configurations with different Q cannot be smoothly deformed into one another.
- (Anti-)instantons: localized field configuration with Q = ±1
- “Instanton gas” approximation – field configurations with |Q| > 1 can be thought of as a collection of well-separated instantons and anti-instantons.
- Observables receive contributions from all topological sectors.

QCD vacuum

- In principle one can add theta term to QCD Lagrangian.

$$\mathcal{L}_\theta(x) = \frac{i\theta}{32\pi^2}\mathrm{tr}\left[F^{\mu\nu}(x)\tilde{F}_{\mu\nu}(x)\right]$$

- Violates CP unless θ = 0.
- Stringent bounds on CP violation in QCD.
- θ is (apprently) small in QCD – strong CP problem.
- QCD theta vacuum – contributions from all topological sectors.

$$|\theta >= \sum_Q e^{iQ\theta}|Q > \qquad Z(\theta) = \sum_Q Z_Q \exp(i\theta Q)$$

Topology in Lattice simulations

- In the continuum, there is an infinite potential barrier for tunneling between different topological sectors (no smooth joining)
- On the lattice, this barrier is finite, but large.
- HMC methods have problems changing sector → large forces.
- Atiyah-Singer index theorem on the lattice: Topological charge is related to (near-)zero modes of the Dirac operator.

$$Q = n_L - n_R$$

Topology in Lattice simulations

- For LQCD frozen topology is problematic, especially as we move towards continuum.
- Even more severe in BSM simulations of many flavor YM:

$$\det(D + m_q)^{N_f}$$

- In some sense global topology does not matter. QFT is local.
- Fixed topology is a finite volume effect – fluctuation of local topological charge density is important.

P(Q)

- Consider theta-vacuum partition function

$$Z(\theta) = \langle \theta | \theta \rangle = \sum_Q Z_Q \exp(i\theta Q) = \exp(-VE(\theta))$$

- θ=0 is a minimum for E(θ) (Vafa-Witten)
- Expand around this point:

$$< 0|Q^2|0 >= -\frac{d^2 \log Z(\theta)}{d\theta}|_{\theta=0} = V\frac{d^2 E(\theta)}{d\theta} = V\chi_t$$

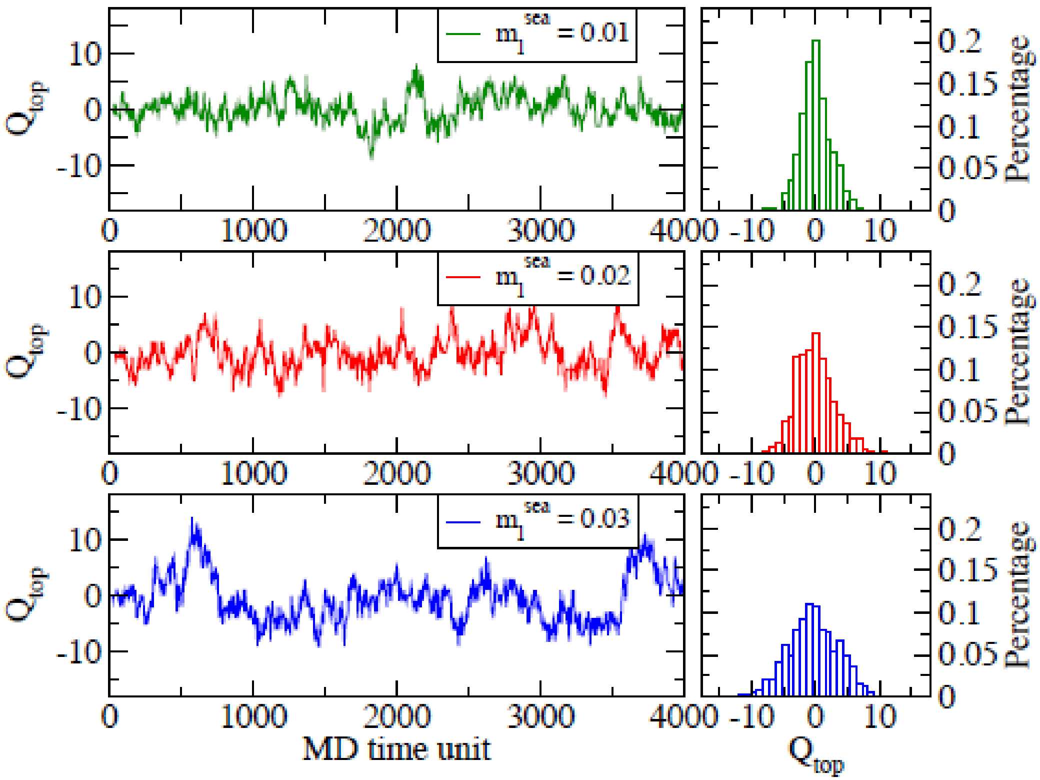
$$E(\theta) = E(\theta = 0) + \chi_t \frac{\theta^2}{2} + \gamma \frac{\theta^4}{4!} + \cdots$$

$$Z_Q = \frac{1}{2\pi} \int_{-\pi}^{\pi} \exp\left(-i\theta Q\right) Z(\theta) \sim \frac{1}{\sqrt{2\pi \chi_t V}} \exp\left[\frac{-Q^2}{2\chi_t V}\right]$$

To leading order, topological charge distribution is Gaussian, with corrections when Q ~ $V\chi_t$

Topological Susceptibility

When topological charge is well-sampled, calculation of susceptibility is straightforward



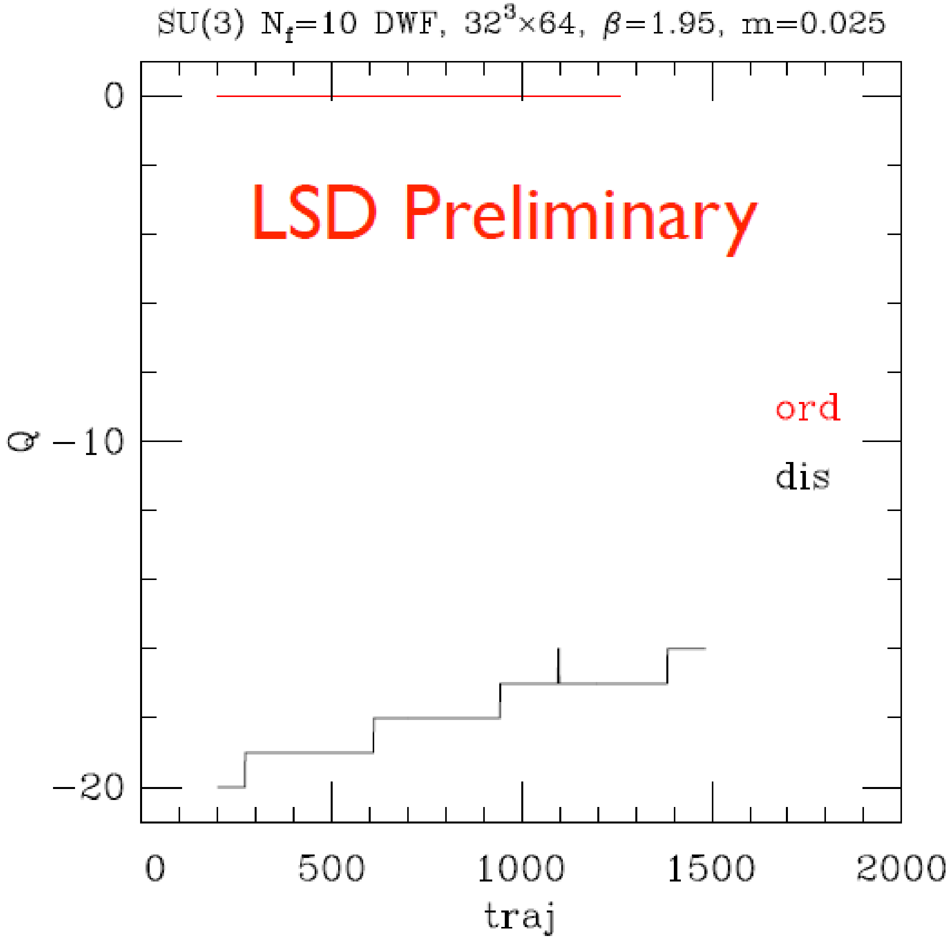
Fit to Gaussian or calculate sample variance:

$$V\chi_t = \langle Q^2 \rangle - \langle Q \rangle^2$$

C. Allton, *et.al.* (RBC-UKQCD)
Phys. Rev. D76 014504 (2007)

10f SU(3)

Unclear what to do when topology is not well-sampled by the HMC evolution.



5LI method
P. de Forcrand,
M. Garcia Perez,
I. Stamatescu
Nucl. Phys. B499, 409 (1997)

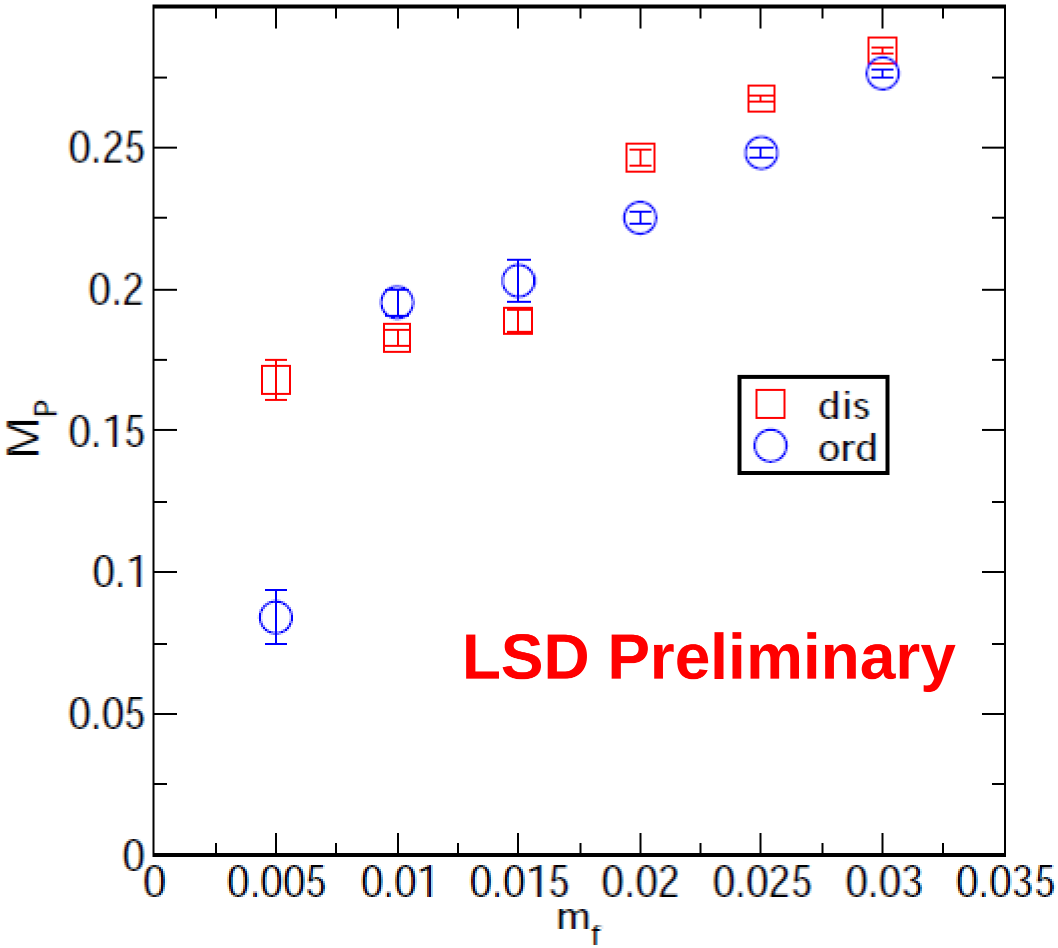
Working at Fixed Q

- Brower, *et. al.* Phys. Lett. B560, 64 (2003) systematically worked out the effect of fixed topological charge in a finite volume V.
- Take some observable such as hadron mass:

$$M(\theta) = M(0) + \frac{1}{2}M''(0)\theta^2 + \cdots$$

$$M_Q = M(\theta = 0) + \frac{1}{2}M''(\theta = 0)\frac{1}{V\chi_t}\left(1 - \frac{Q^2}{V\chi_t}\right)$$

Working at Fixed Q



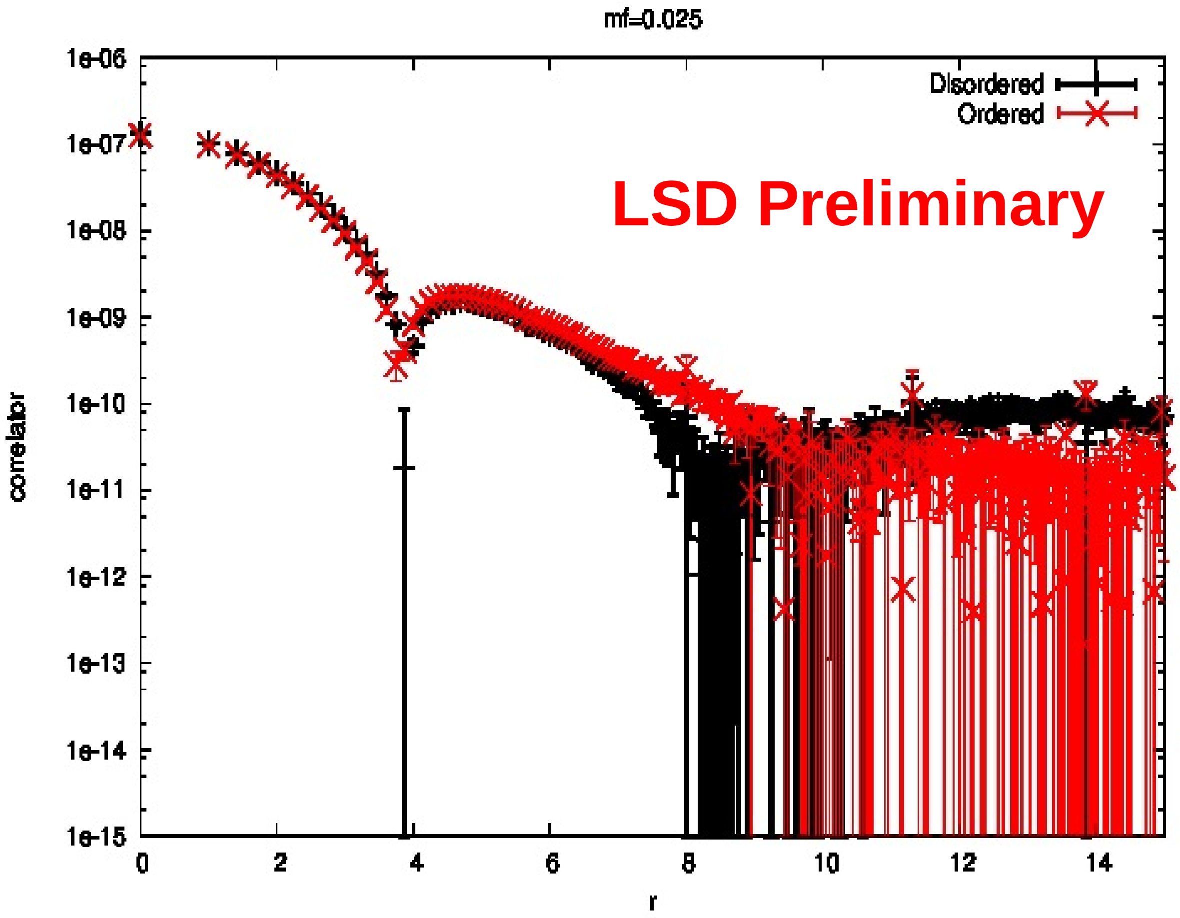
- M_{PS} for 10f SU(3)
- ord: Q = 0
- dis: Q ≠ 0

- Can determine M(θ=0) from several values of M_Q
- Still need χ_t

Topological charge correlator?

$$\lim_{x\to\infty}\langle q(x)q(0)\rangle = \frac{1}{V}\left(\frac{Q^2}{V} - \chi_t - \frac{c_4}{2V\chi_t}\right) + O\left(V^{-3}\right) + O\left(e^{-m_{\eta'}}\right)$$

S. Aoki, *et. al.*, Phys. Rev. D76 054508 (2007)



Long-distance behavior of top. charge correlator too noisy to reliably extract χ_t

Time series method

- Tunneling rate between topological sectors depends on lattice action, algorithm, etc...
- Although the full distribution is not sampled, relative rate of tunneling between sectors gives some information.
- Ornstein-Uhlenbeck Model[Phys. Rev. 36, 823 (1930)] describes Brownian motion with linear friction.
- Only non-trivial Markov process with stationary distribution that is a Gaussian [Doob, Ann. Math. 43, 351 (1942)] (up to linear transformations)

Ornstein-Uhlenbeck Model

$$\frac{d}{dt}x(t) = -\eta(x(t) - \overline{x}) + \sigma \frac{d}{dt}W(t)$$

Mean-restoring friction

Continuous random walk

$$\mathrm{E}[x(t)] = \overline{x} + (x(0) - \overline{x})e^{-\eta t}$$

$$\mathrm{Var}[x(t)] = \frac{\sigma^2}{2\eta}\left(1 - e^{-2\eta t}\right)$$

Discretize OU to get Markov chain:

$$P(Q_i|Q_{i-1}) = (2\pi)^{-1/2}\left[\frac{\sigma^2}{2\eta}\left(1 - e^{-2\eta(n_i - n_{i-1})}\right)\right]^{-1/2} \times \exp\left(-\frac{\eta\left[Q_i - Q_{i-1}e^{-\eta(n_i - n_{i-1})}\right]^2}{\sigma^2\left[1 - e^{-2\eta(n_i - n_{i-1})}\right]}\right)$$

Ornstein Uhlenbeck Process

- For Gaussian distributions, we have:

$$\overline{x} =< Q >= 0 \qquad \frac{\sigma^2}{2\eta} =< Q^2 >= V\chi_t$$

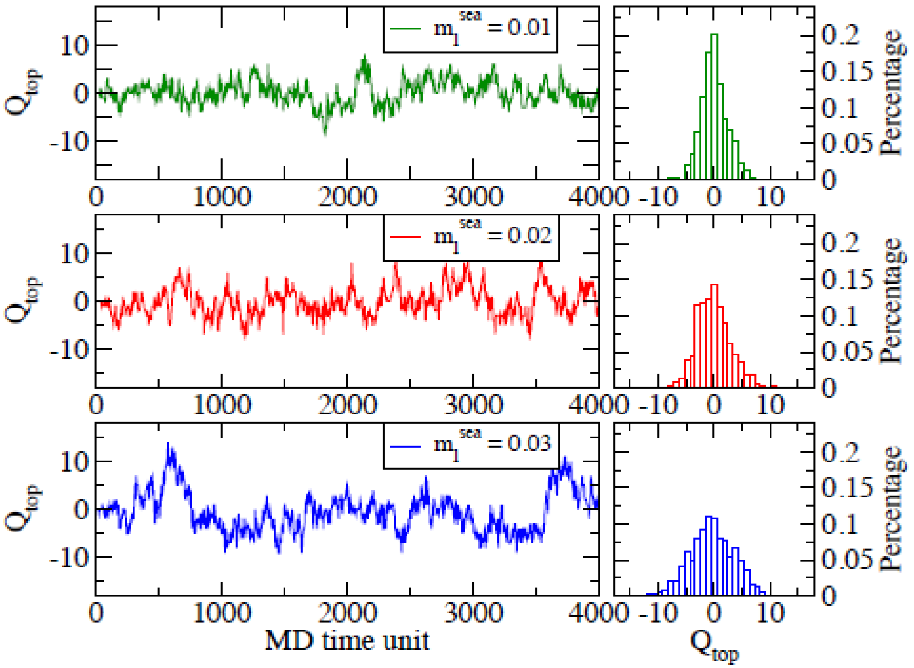
- Maximize log likelihood on time series.

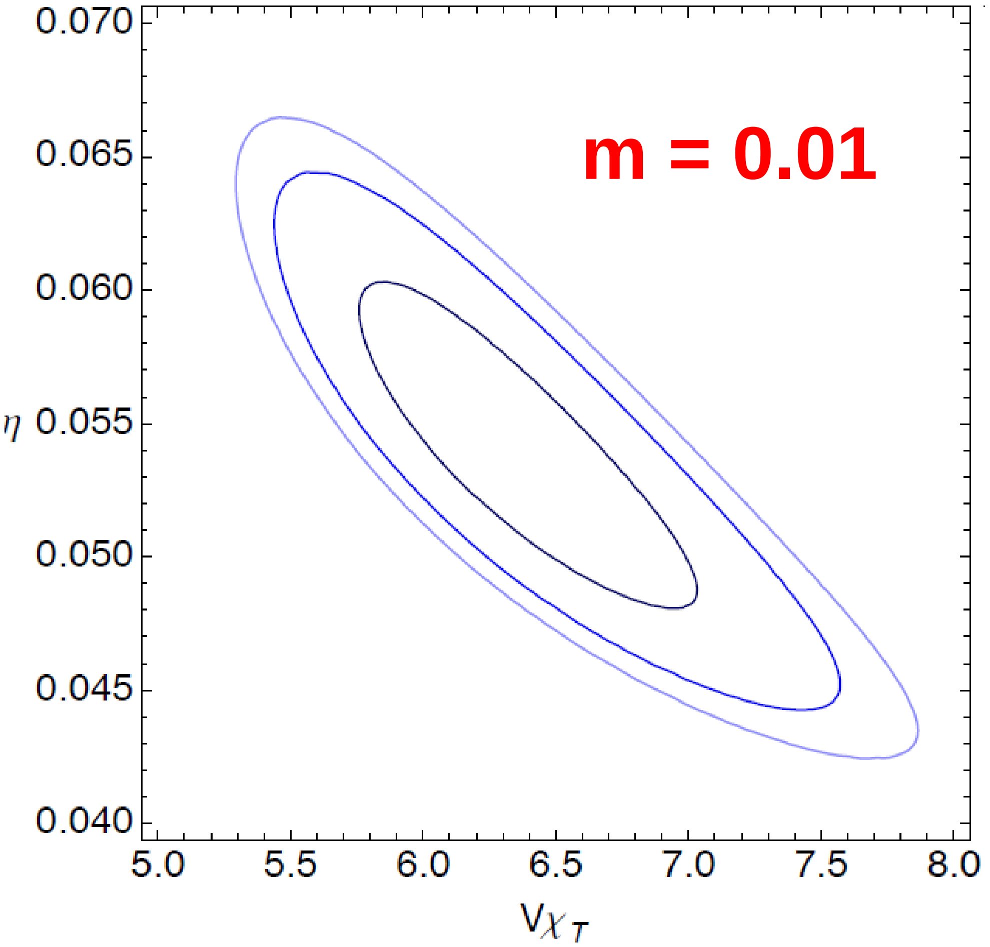
$$-L(\eta, V\chi_t) = \frac{N}{2}\log V\chi_t + \frac{1}{2V\chi_t}S(\eta) + \frac{1}{2}\sum_{i=1} N\log\left[1 - e^{-2\eta(n_i - n_{i-1})}\right]$$

$$S(\eta) = \sum_{i=1}^{N} \frac{\left[Q_i - Q_{i-1}e^{-\eta(n_i - n_{i-1})}\right]^2}{1 - e^{-2\eta(n_i - n_{i-1})}}$$

- Obtain maximum likelihood values for η, $V\chi_t$
- 1/η ~ autocorrelation time of observable.

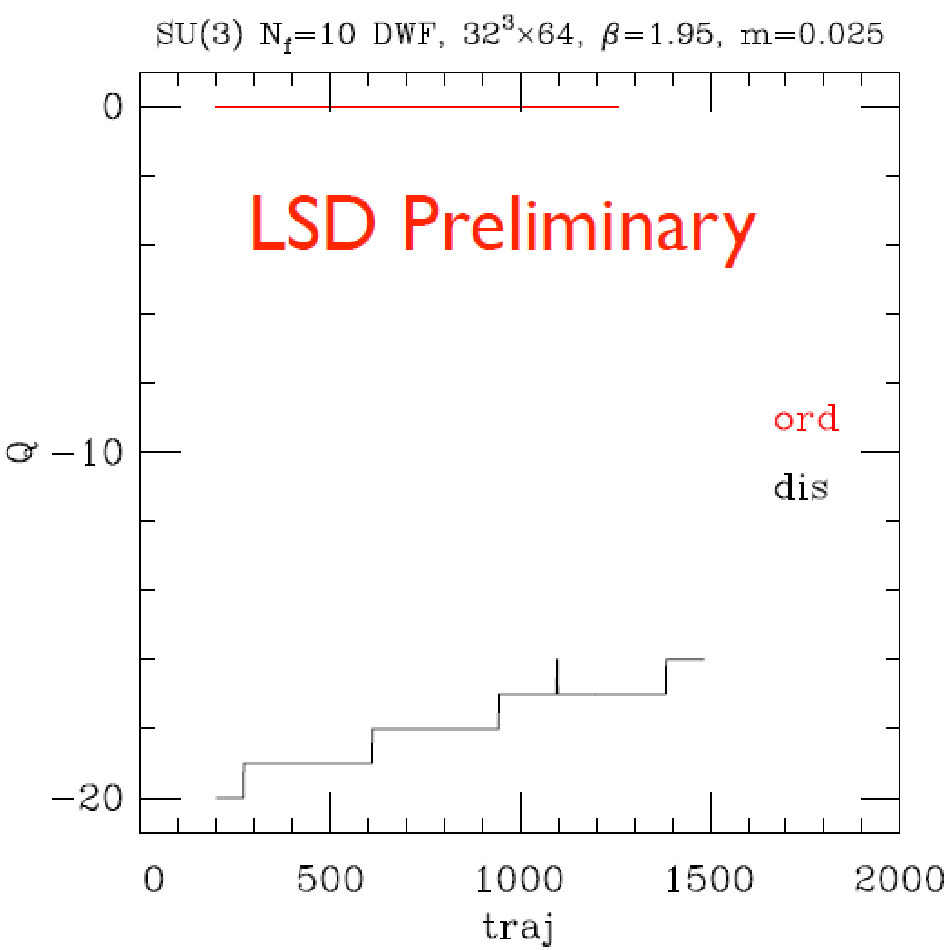
MLE Results

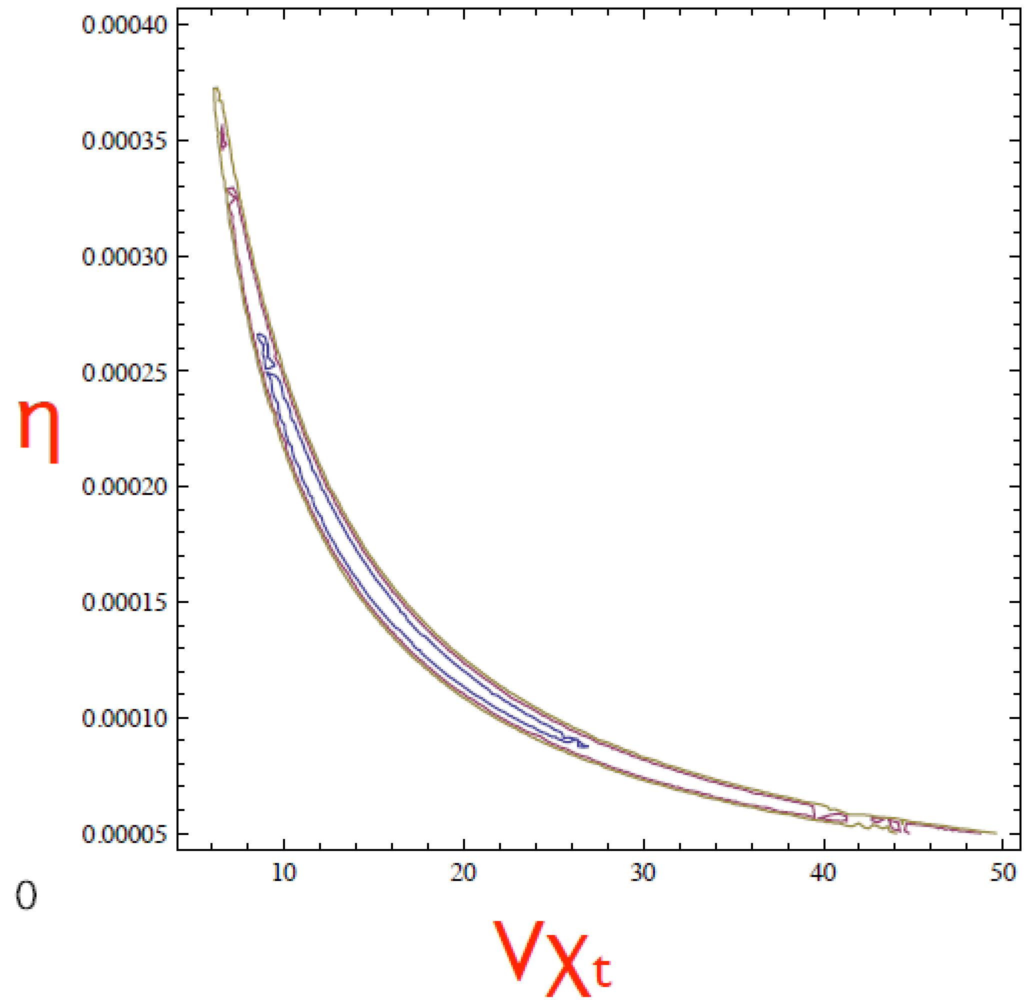




1/η ~ 15-25

MLE Results





1/η ~ 500-1000

Non-Gaussianities

- What if P(Q) is not exactly Gaussian?
- Use Edgeworth series to look at leading-order correction to Gaussian.

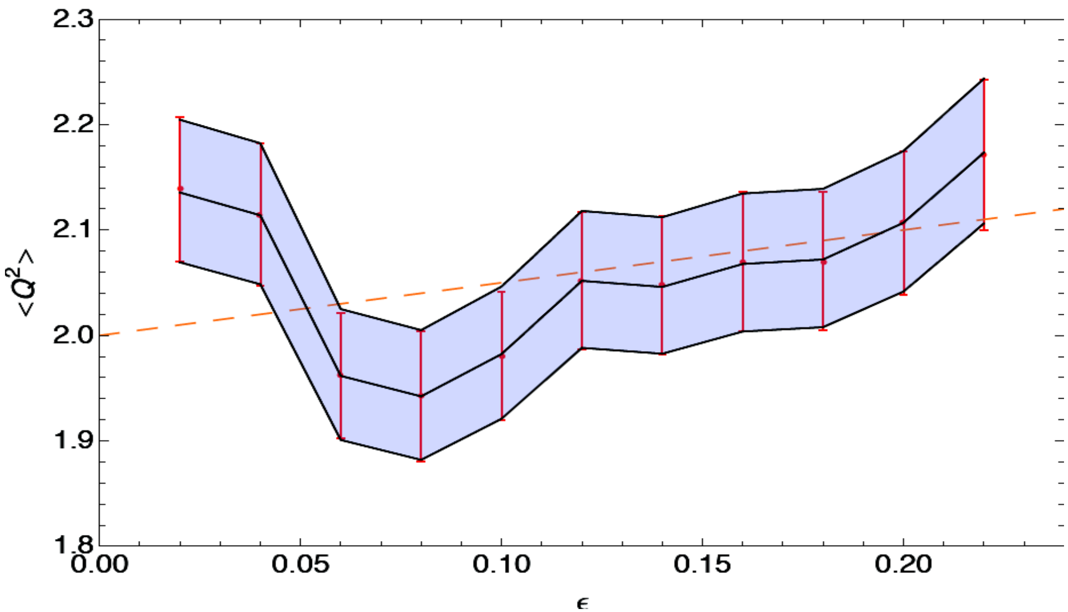
$$P(Q) = \frac{32}{32+\epsilon} \exp\left(-\frac{Q^2}{2V\chi_t}\right) \left[1 + \frac{\epsilon}{4!} \mathrm{He}_4\left(\frac{Q}{\sqrt{V\chi_t}}\right)\right]$$

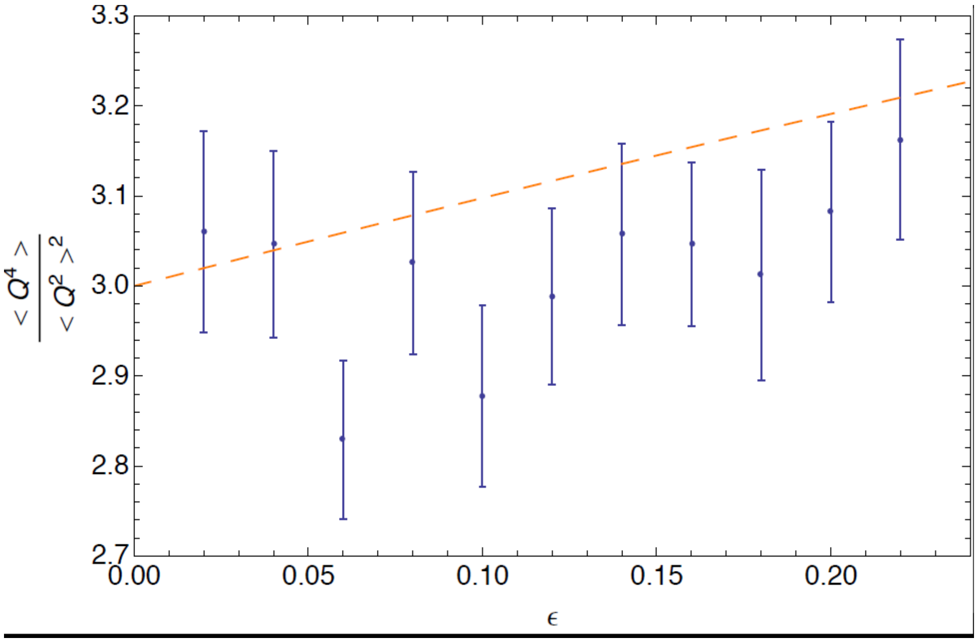
$$\kappa_2 = V\chi_t \left(1 + \frac{\epsilon}{4} - \frac{\epsilon^2}{128} + \cdots\right) \qquad \kappa_4 = < Q^4 > -3 < Q^2 >^2 = \epsilon - \frac{23}{32}\epsilon^2$$

- Giusti, *et. al.* Phys. Rev. D76, 094510 (2007) found ε ~ 0.2 for pure SU(3).
- Large N_c suggests $\kappa_{2n} \sim N_c^{2-2n}$

OU Process with non-Gaussian

- Draw 4096 points from truncated Edgeworth series
- Run OU MLE as well as standard sample calculation of cumulants.





- MLE (black), sample calculation(red), analytic (dashed)

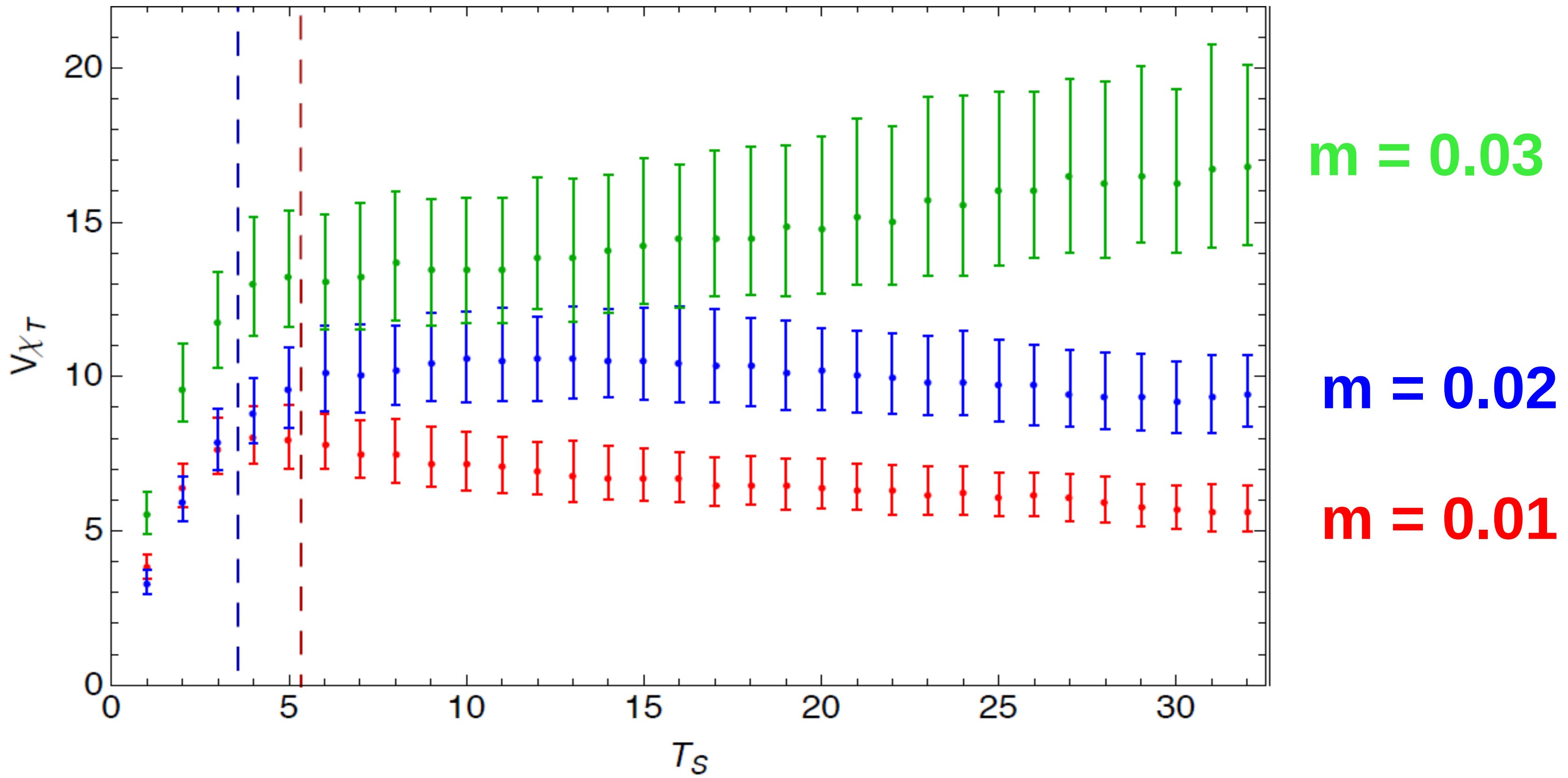
Fixed Q

- MLE works well if we don't have a good sample of P(Q), but must have at least a few transitions.
- Fails if we have no transitions, *i.e.* charge is completely frozen. What to do in this case?
- Lüscher and Schaefer [JHEP07 036 (2011)] propose open boundary conditions to allow topological charge to diffuse in and out of the volume.
- Can use same idea on subvolume.
- Consider dividing up volume into two pieces, V_s, V_r
- V_s = slab of timeslices = $L^3 x T_s$
- Calculate susceptibility as normal using sample variance or MLE on subvolume.

Subvolume Method

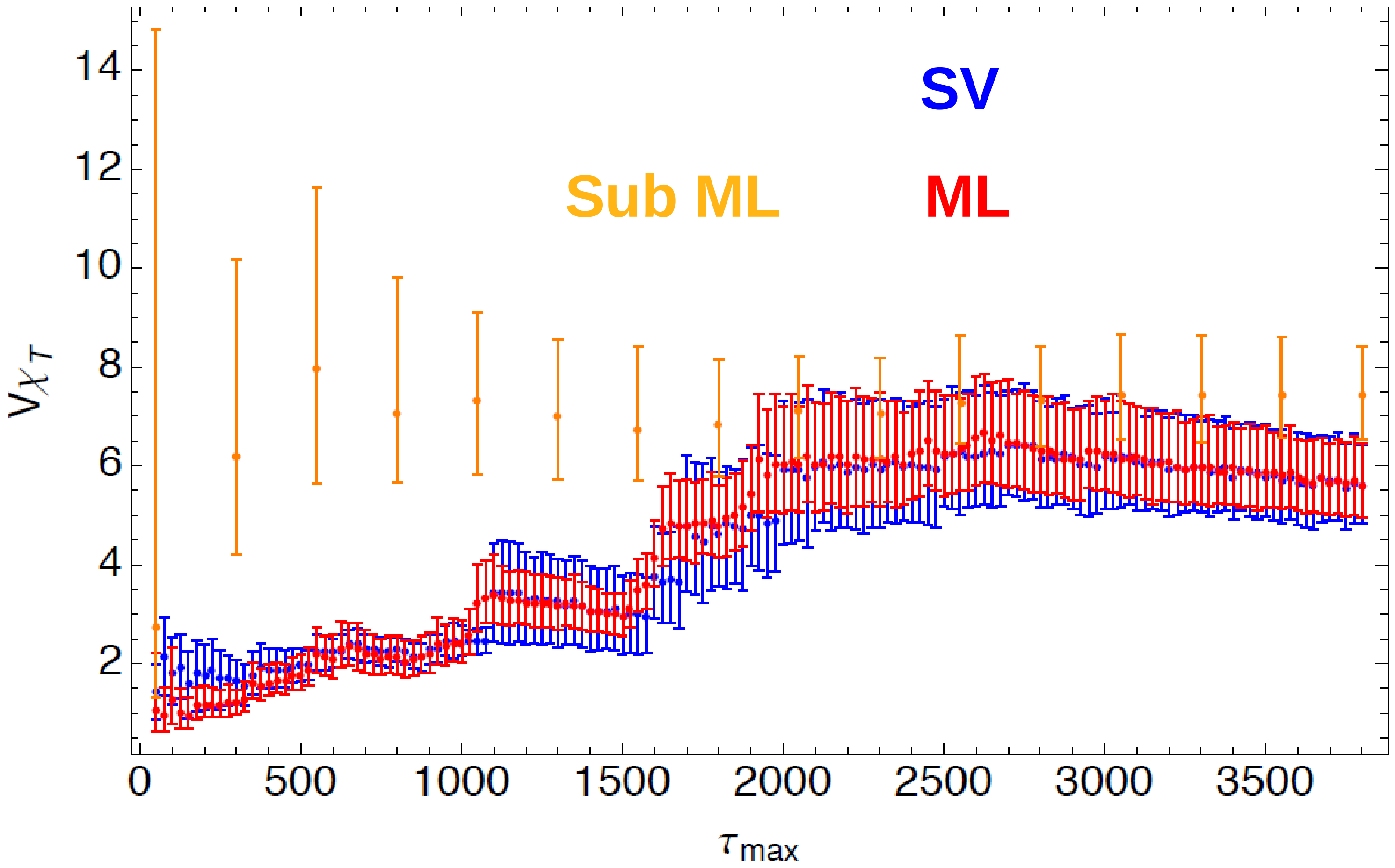
- Has been explored in the past: de Forcrand, *et. al.* Nucl.Phys.Proc.Suppl. 73 (1999) 578-580
- Works well if global topology is changing and is well-sampled.
- Optimal in the case where:
  - Local topological charge fluctuates and is sampled well, but evolution algorithm makes instanton creation/annihilation difficult, *i.e.* fast instanton diffusion through the volume.
  - $V \sim V_r >> V_s >> \chi_t^{-1}$
- Caveat: Since Q is fixed, will suffer same finite volume corrections, which depend on χ_t.

Subvolume Method

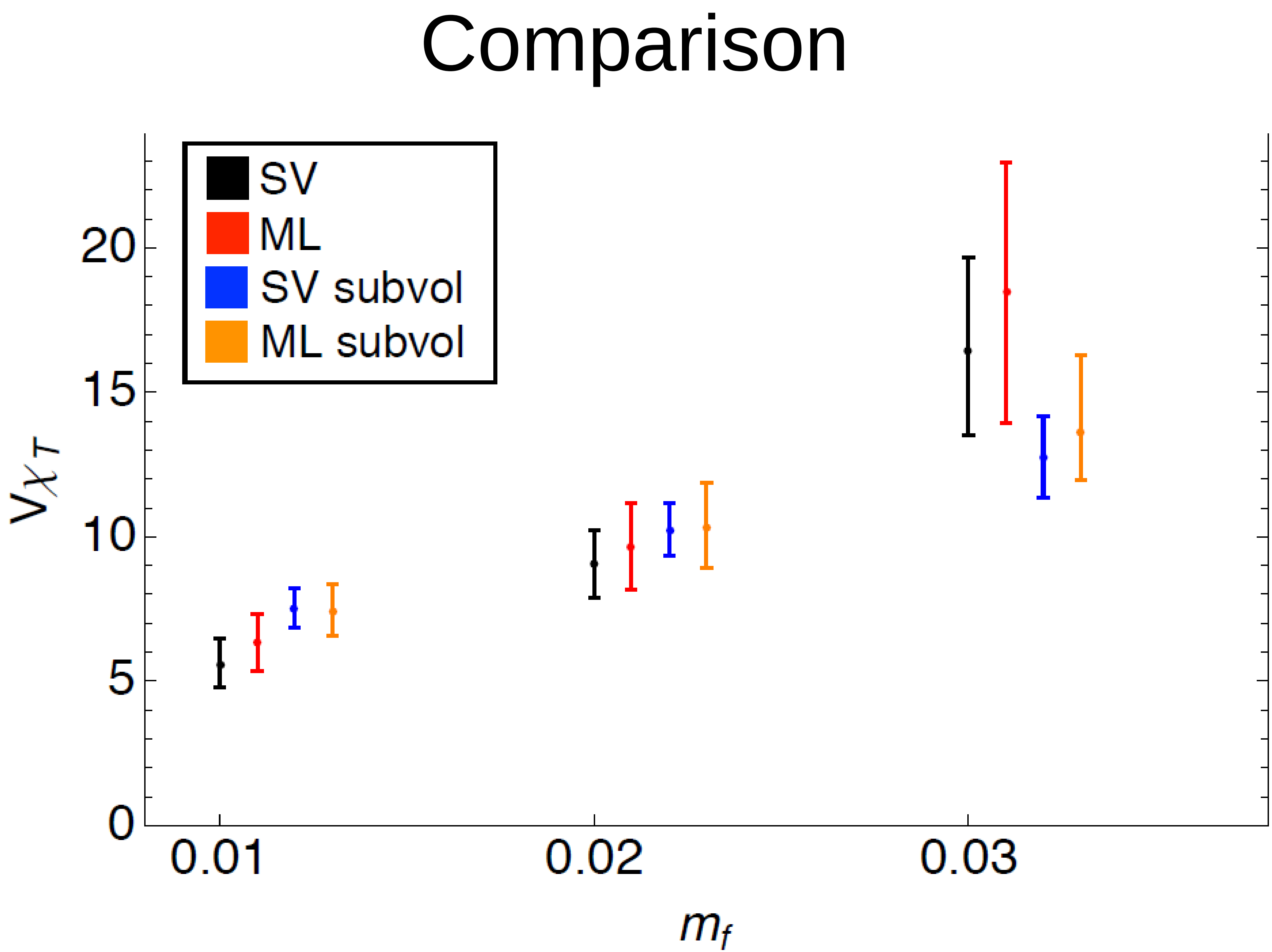


- ML method applied to subvolumes as a function of T_s.
- Look for plateau in T_s.

Subvolume Method



Convergence of different methods as a function of number of configurations used in analysis.



Comparison
SV
ML
SV subvol
ML subvol
v_{χ_T}
0
5
10
15
20
0.01
0.02
0.03
m_f

Conclusion

- Sampling of topological charge is difficult problem in LGT calculations, particularly for BSM as one moves to continuum limit.
- Some observables can depend strongly on topological sector.
- Effects of fixed topological sector known (finite volume corrections).
- Need way to estimate χ_t
- Ornstein-Uhlenbeck method allows one to get estimate of χ_t from a few topological charge transitions, even if one does not have a good sample of the distribution.
- Dividing lattice into a sub-volume and a “reservoir” also allows one to calculate χ_t.
- Different methods show good agreement on RBC-UKQCD lattices.