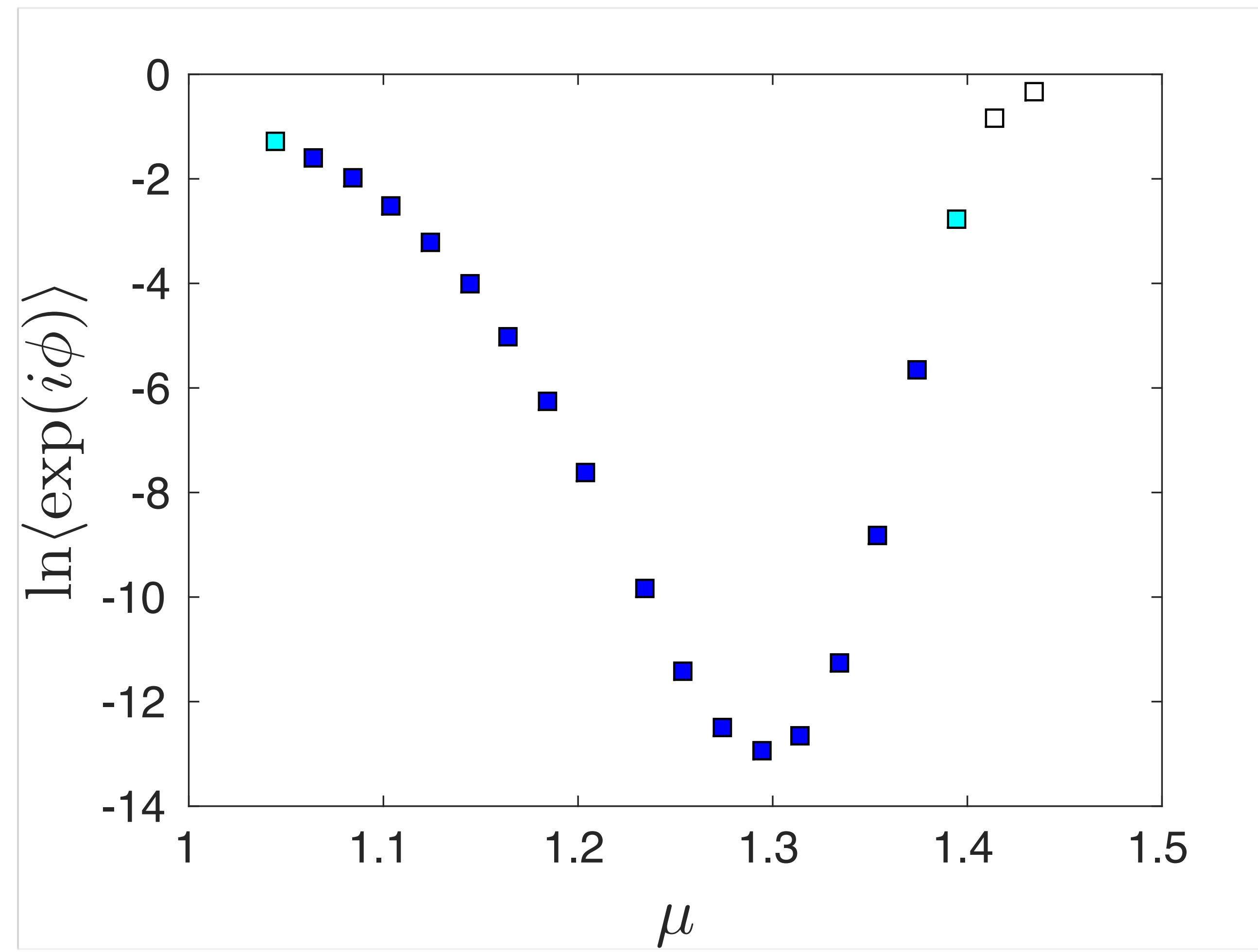
density-of-states

Kurt Langfeld
(Liverpool University)



Lattice 2016 conference,
Southhampton, 24-30 July 2016

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LATTICE 2016

Developments

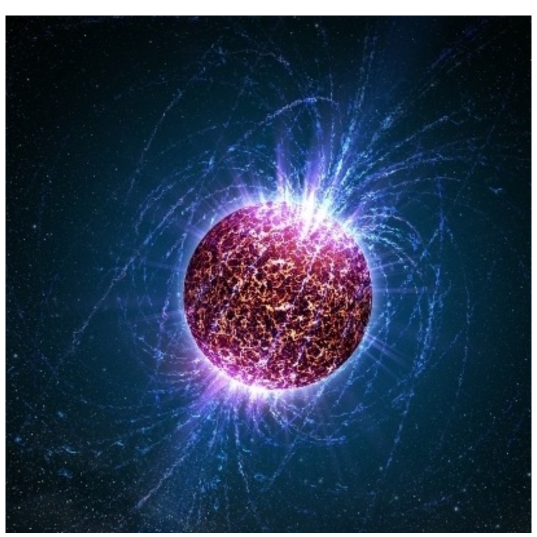
What is the density-of-states method and what is LLR?

- Theoretical & Algorithmic developments
  [ergodicity, exponential error suppression]

Can we simulate slush?

Applications

- Towards the SU(3) latent heat



Finite density QFT

- The HDQCD showcase
- What can we learn for other approaches
  [cumulant, canonical simulations?]

The density-of-states method:

Consider the high dimensional integral:

$$Z \;=\; \int \mathcal{D}\phi \;\exp\{\beta S[\phi]\}$$

The density-of-states:

$$\rho(E) \;=\; \int \mathcal{D}\phi \,\delta\Big(E - S[\phi]\Big)$$

A 1-dimensional integral:

$$Z \;=\; \int dE \; P(E)$$

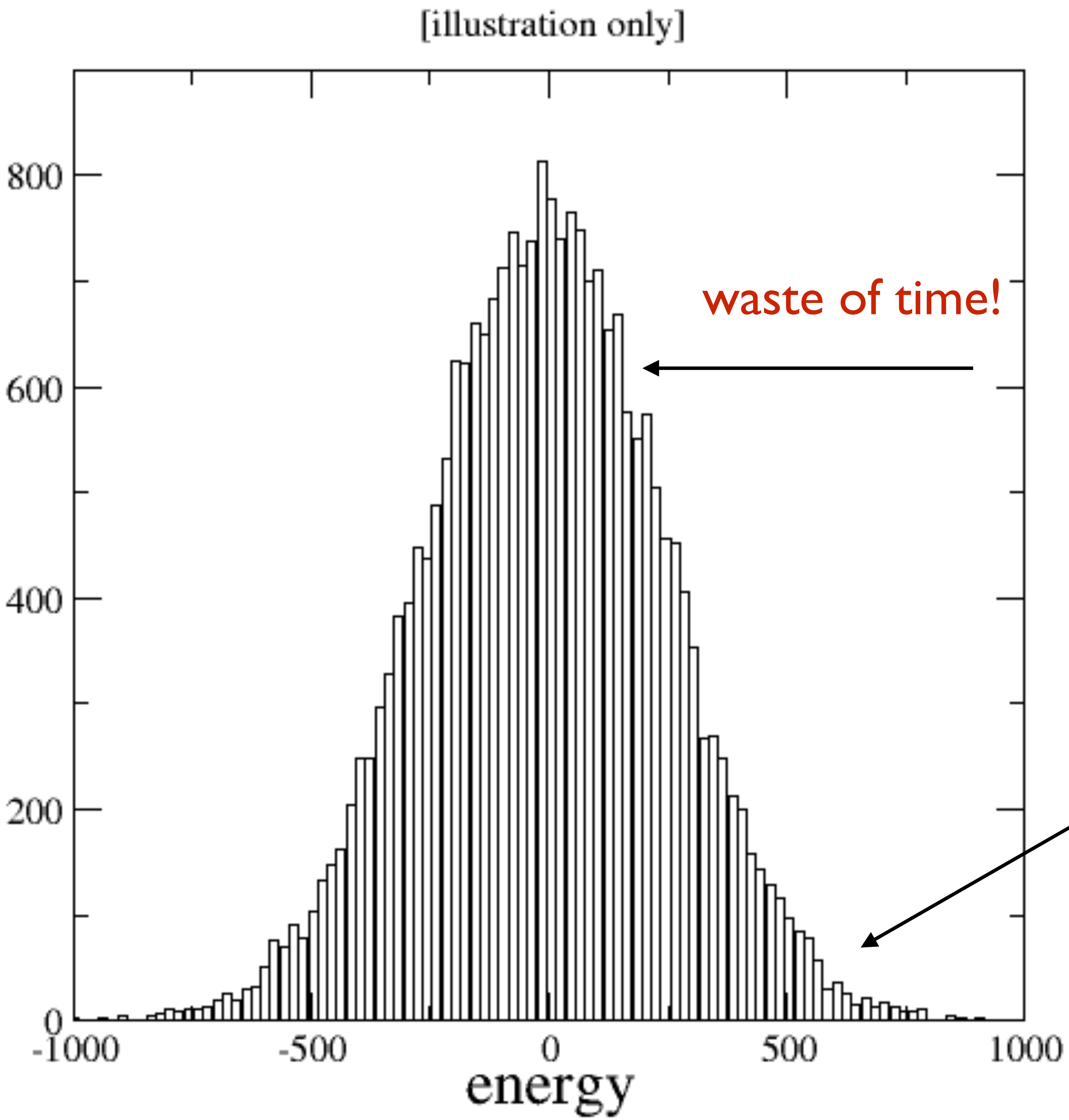
Gibbs factor

entropy

$$P(E) = \rho(E)\; \mathrm{e}^{\beta E}$$

Probabilistic weight

How do I find the density-of-states?



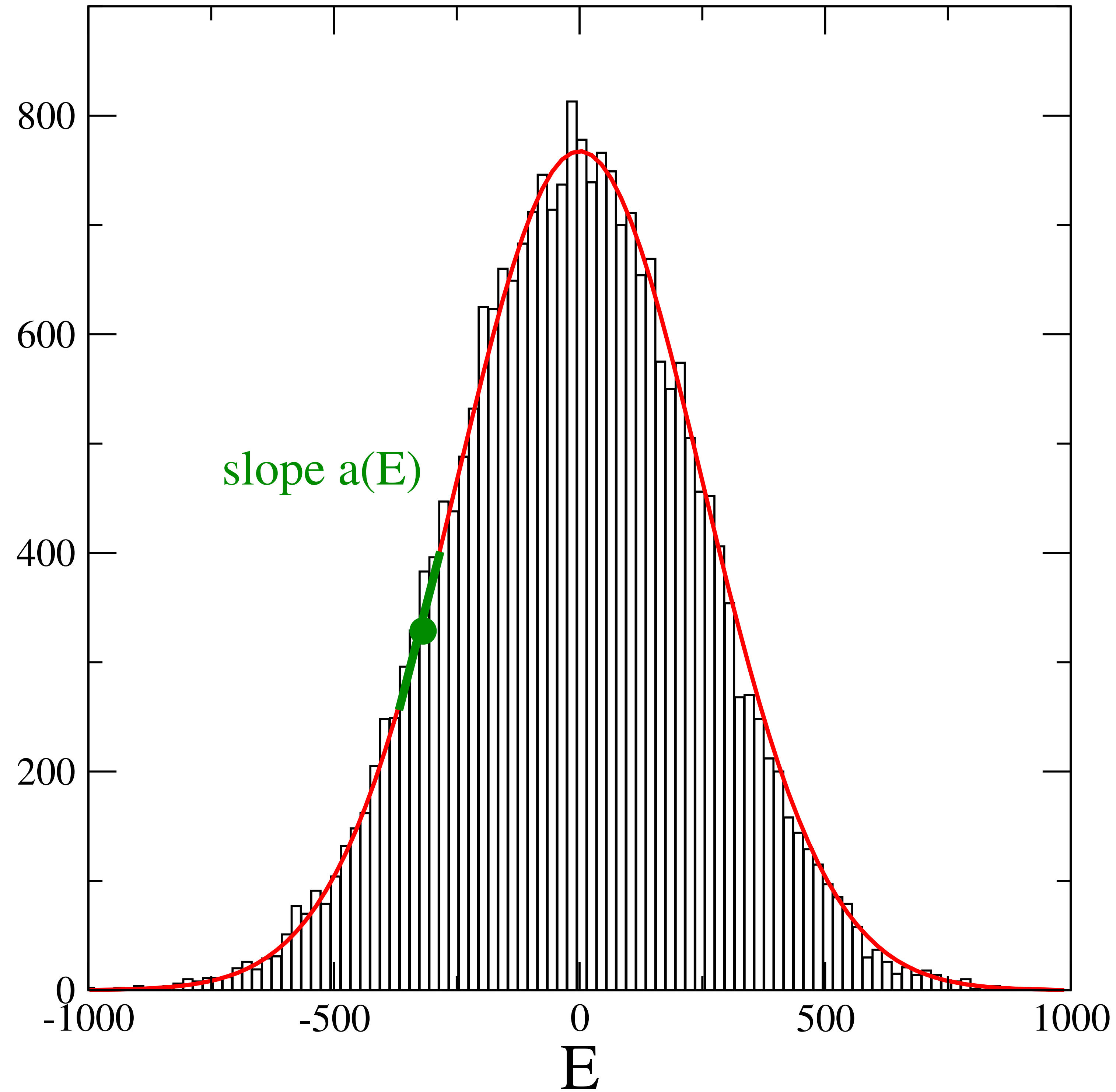
…could use a histogram

bad signal to noise ratio

The LLR approach to the density-of-states:

- calculate instead the slope [of log ρ] a(E) at any point E

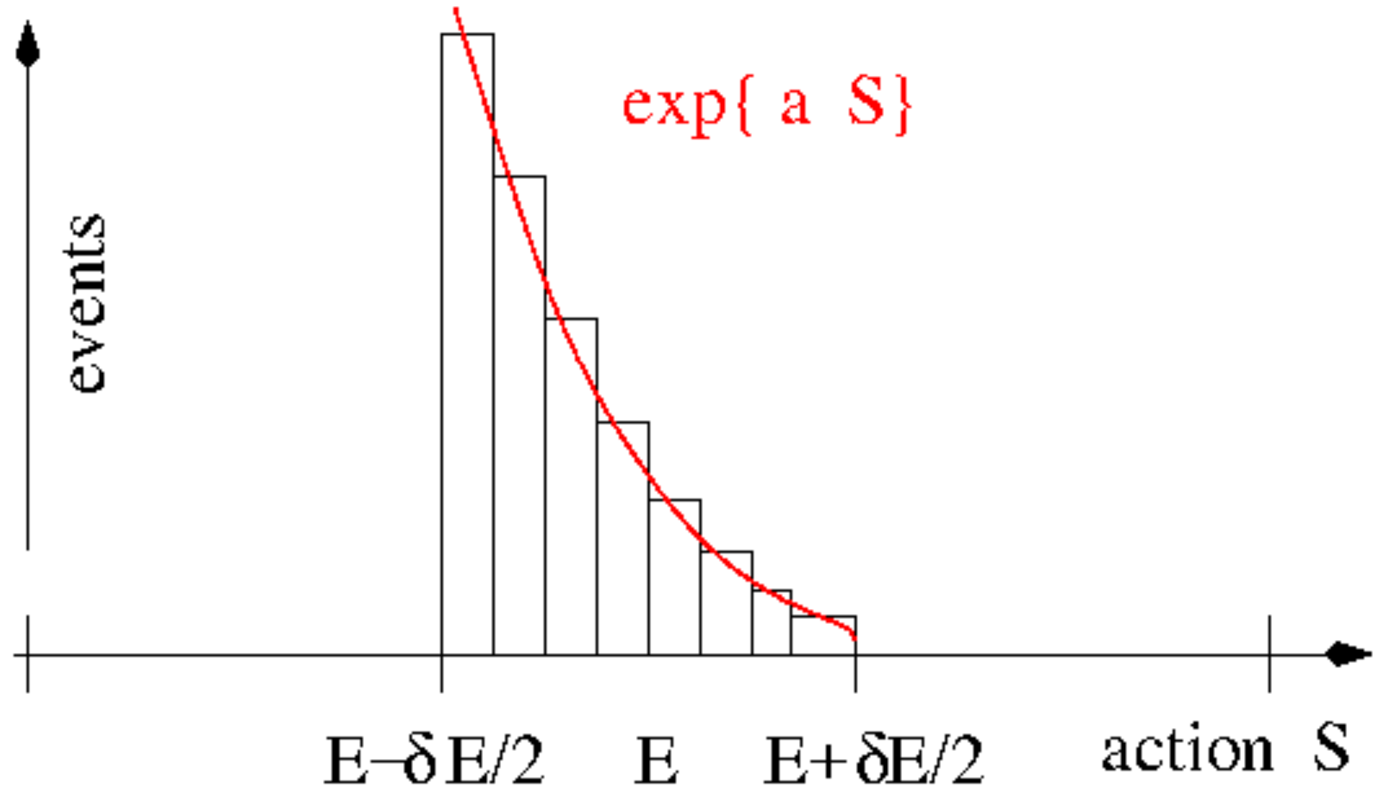
- reconstruct $\rho(E)$



[Langfeld, Lucini, Rago, PRL 109 (2012) 111601]

LLR approach:

- For small enough δE: Poisson distribution



$$\langle\!\langle W[\phi] \rangle\!\rangle (a) = \frac{1}{\mathcal{N}} \int \mathcal{D}\phi \; \Omega_{[E,\delta E]}(S[\phi]) \; W[\phi] \; e^{-a\, S[\phi]}$$

standard MC average

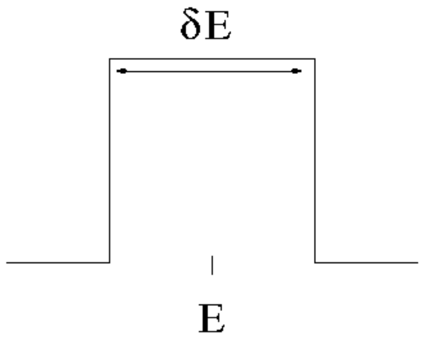
restriction to the action range "window function"

observable

re-weighting factor

need to find "a" !

Window function:



- Needs to be symmetric around E
- Historically [Wang-Landau] $\Omega_{[E,\delta E]}(S) = \theta_{[E,\delta E]}(S)$
- Also: $\Omega_{[E,\delta E]}(S) = \exp\{-(S-E)^2/\delta E^2\}$

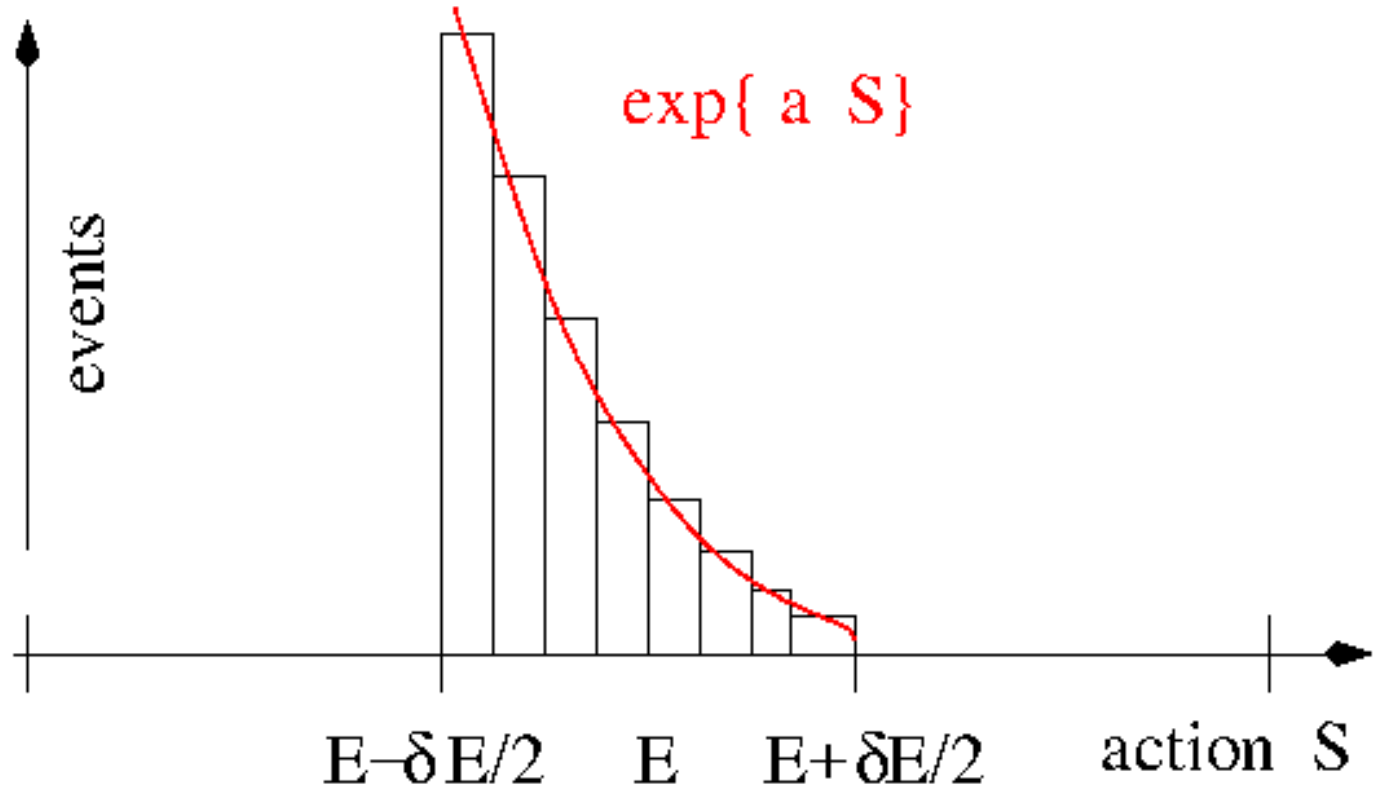
main advantage:
can be used in HMC and LHMC
algorithms to calculate $\langle\langle W[\phi] \rangle\rangle_E$

→ *[see SU(3) latent heat; this talk]*

→ *[see also talk by R Pellegrini: Tuesday, Algorithms]*

LLR approach:

- For small enough δE: Poisson distribution



choose: $W[\phi] = S[\phi] - E$

$$\langle\langle W[\phi] \rangle\rangle (a) = \frac{1}{\mathcal{N}} \int \mathcal{D}\phi \; \Omega_{[E,\delta E]}(S[\phi]) \; W[\phi] \; \mathrm{e}^{-a\, S[\phi]}$$

standard MC average

restriction to the action range

observable

re-weighting factor

For correct a: $\langle\langle S[\phi] - E \rangle\rangle (a) = 0$

Stochastic non-linear equation: $\langle\langle S[\phi] - E \rangle\rangle_E = 0$

[Langfeld, Lucini,Pellegrini, Rago, Eur.Phys.J. C76 (2016) no.6, 306]

- …many possibilities to solve it:

$$a_{n+1} = a_n + \frac{12}{\delta E^2 \, (n+1)} \langle\langle \Delta E \rangle\rangle (a_n)$$

convergence error — statistical error

Do we converge to the correct result?

- **Solved by Robbins Monroe [1951]:**

➡ converges to the correct result a_∞

➡ truncation at n=N: $P(a_N)$ normal distributed around a_∞

⟶ *bootstrap error analysis!*

Stochastic non-linear equation: $\langle\langle S[\phi] - E \rangle\rangle_E = 0$

more results:

- monotonic function in a: $\langle\langle S[\phi] - E \rangle\rangle_E (a)$

[Langfeld, Lucini,Pellegrini, Rago, Eur.Phys.J. C76 (2016) no.6, 306]

- other iterations possible [let alone Newton Raphson]

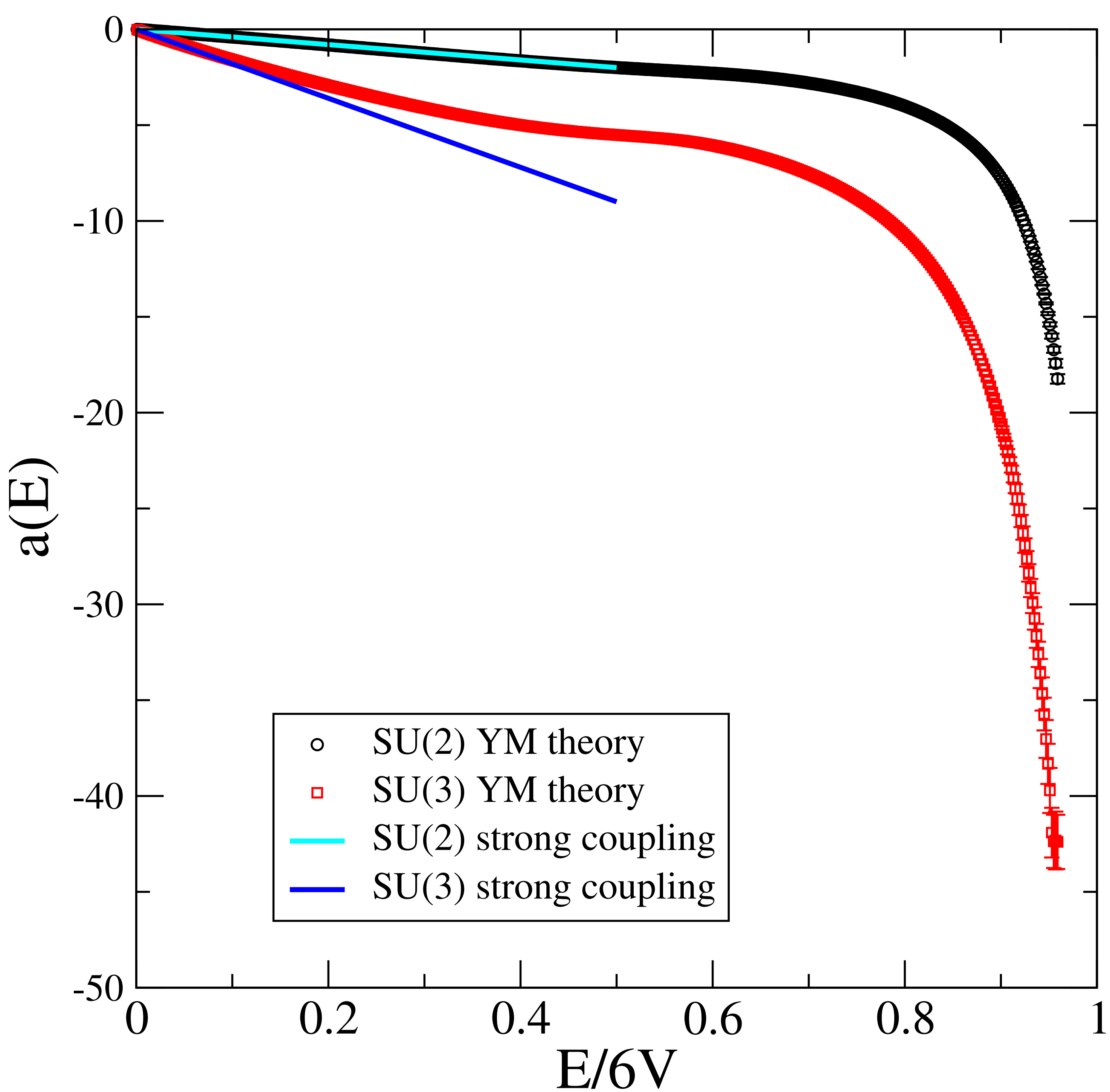
see the *Functional Fit Approach* (FFA)

$\longrightarrow$ talk by Mario Gulliani, Tuesday, Nonzero T and Density

$\longrightarrow$ [Gattringer, Toerek, PLB 747 (2015) 545]

Showcase: SU(2) and SU(3) Yang-Mills theory

[from Gatringer, Langfeld, arXiv:1603.09517]



- Gaussian Window function $\Omega_{[E,\delta E]}$
- LHMC update
- 20 bootstrap samples

Reconstructing the density-of states:

Remember: $a(E) = \frac{d \ln \rho(E)}{dE}$ $\Rightarrow$ $\tilde{\rho}(E)$

discrete set:

Central result:

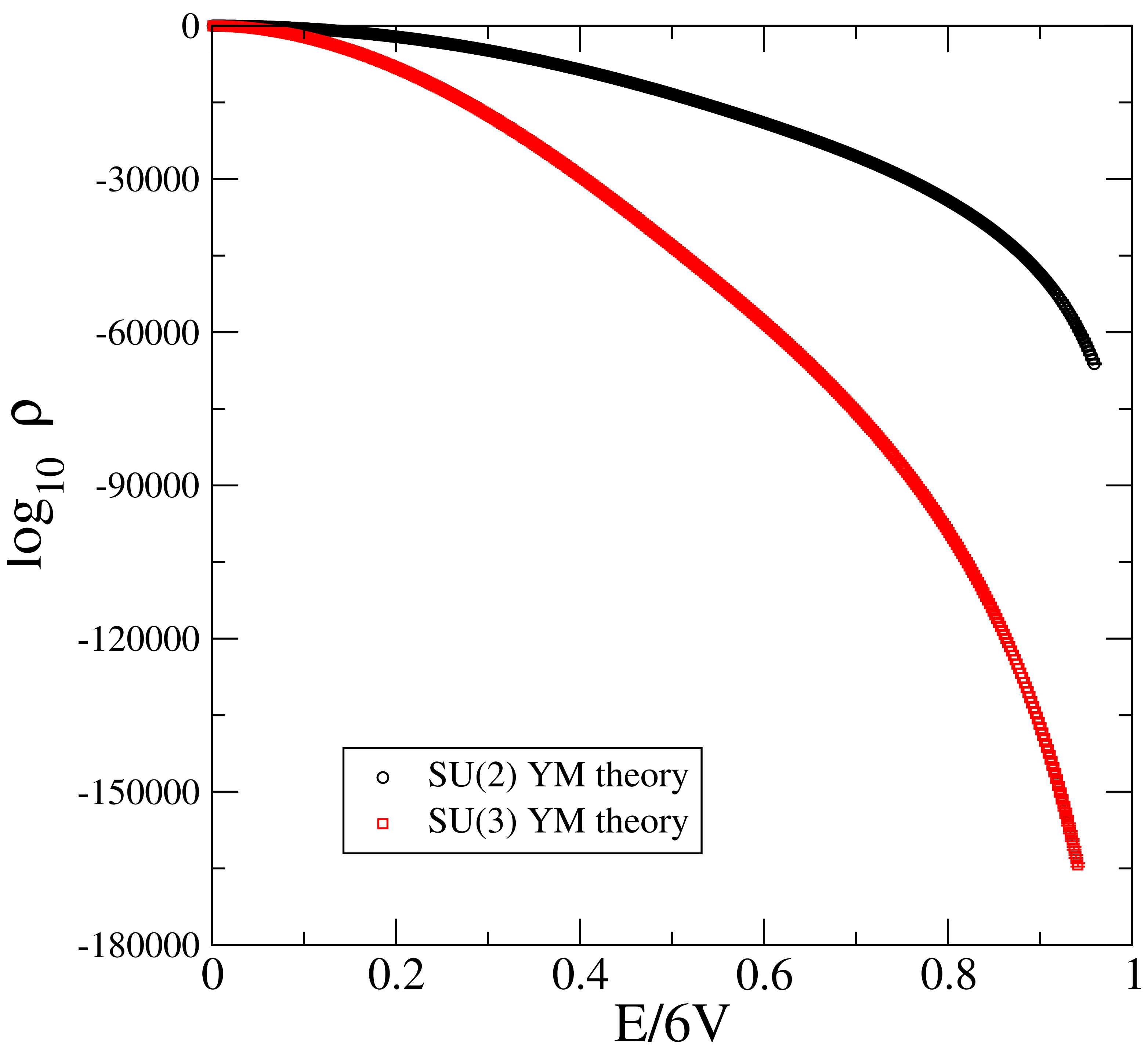
$$\rho(E) = \tilde{\rho}(E) \exp\{\mathrm{trunc.} + \mathrm{stats.\ error}\}$$

relative error

"exponential error suppression"

[Langfeld, Lucini, Pellegrini, Rago, Eur.Phys.J. C76 (2016) no.6, 306]

Showcase: SU(2) and SU(3) Yang-Mills theory



Density of states over 100,000 orders of magnitude!

Early objection: [2012]

Ergodicity could be an issue….

(we confine configurations to action intervals)

use (extended) replica exchange method

proposed in

[Langfeld, Lucini, Pellegrini, Rago, Eur.Phys.J. C76 (2016) no.6, 306]

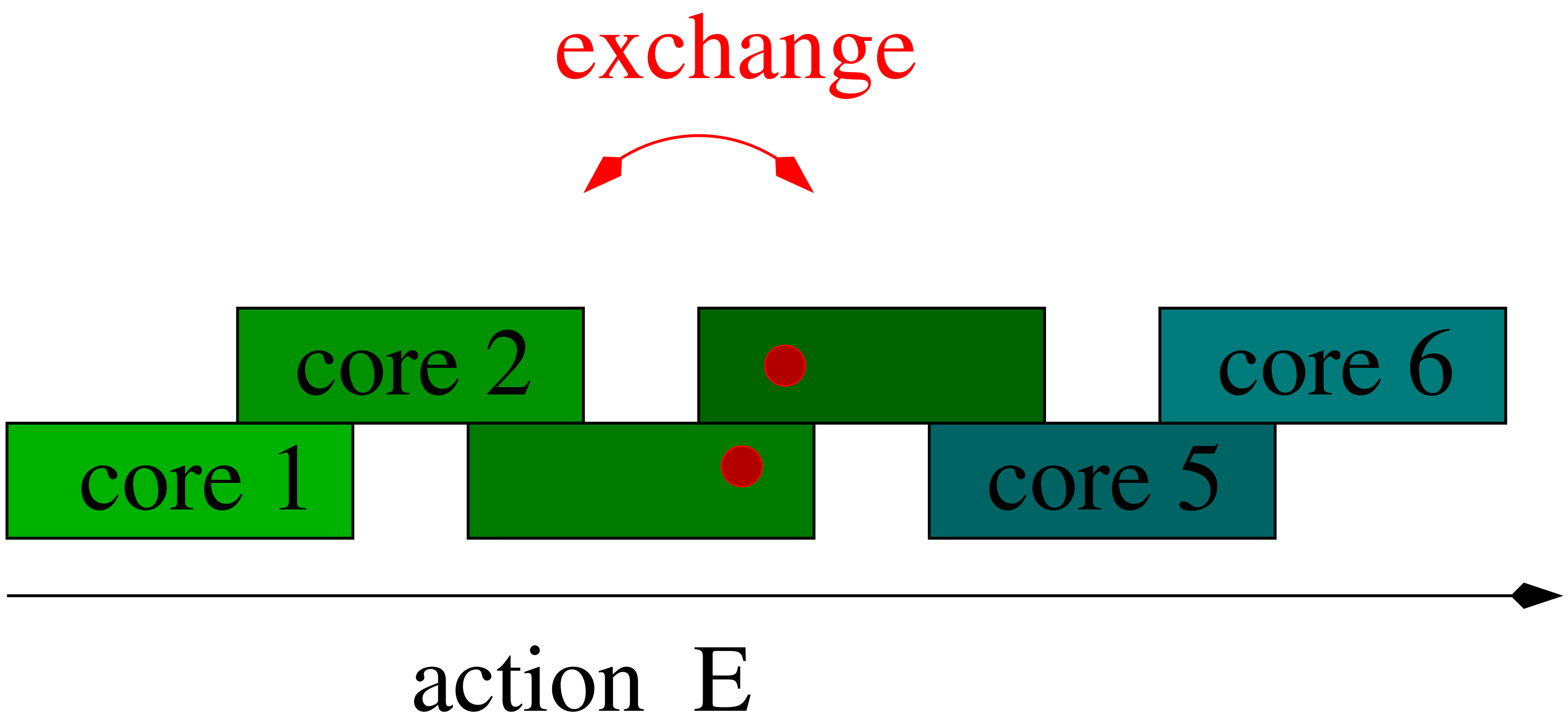
we studied the issue in the Potts model

[see talk by B Lucini, Tuesday, 17:50, Algorithms]

(extended) Replica Exchange method:

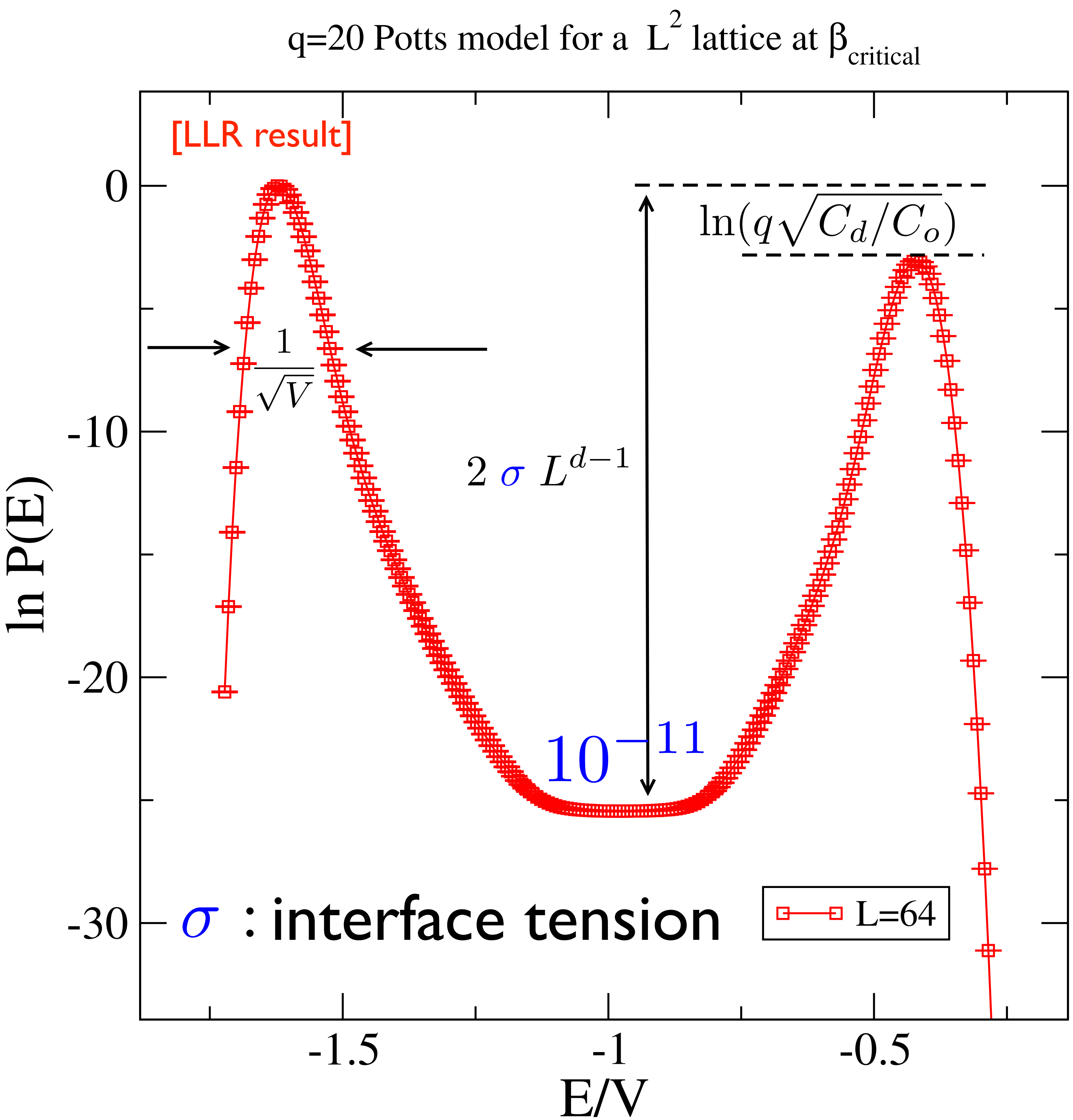
[Swendsen, Wang, PRL 57 (1986) 2607]

Calculate LLR coefficients in parallel



If a(E) is converged: random walk in configuration space

Showcase: q-state Potts model in 2d



σ : interface tension

Exact solution:

R.J. Baxter, J. Phys. C6 (1973) L445

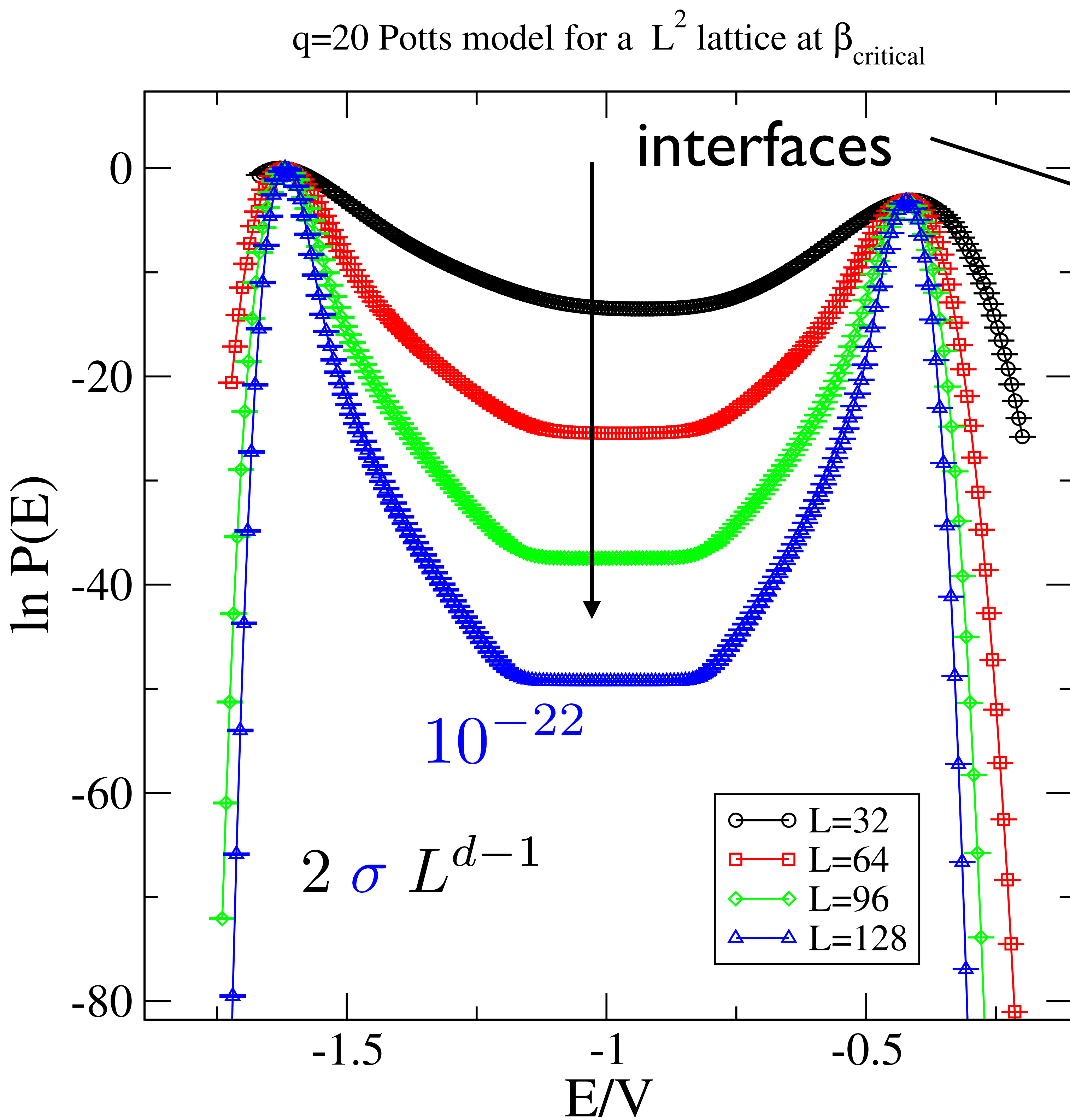
$$\beta_{\text{critical}} = \frac{1}{2}\ln(1+\sqrt{q})$$

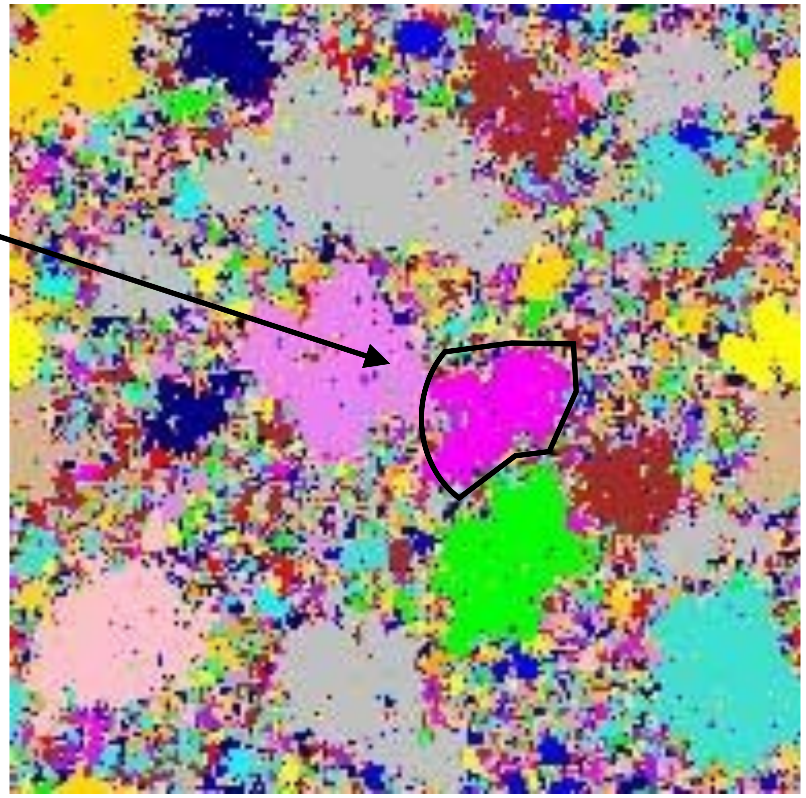
First MC q=20 simulation:

Multi-canonical approach

[Berg, Neuhaus, PRL 68 (1992) 9]
[Billoire, Neuhaus, Berg, NPB (1994) 795]

Showcase: q-state Potts model in 2d





LLR result:

216 energy intervals

replica method

Showcase: q-state Potts model in 2d

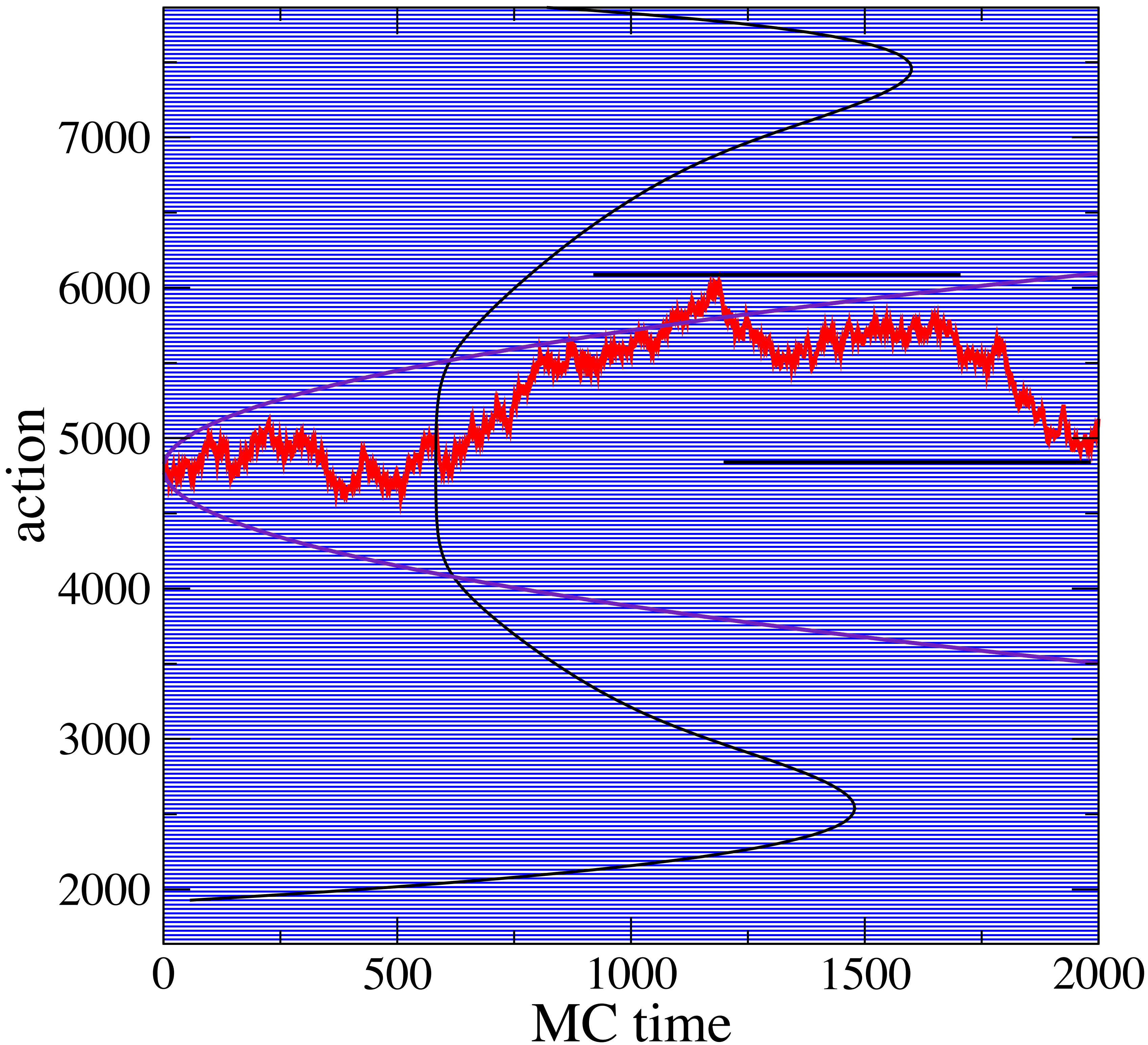
[q=20, L=64]

Tunnelling between LLR action intervals:

Interval size: 29

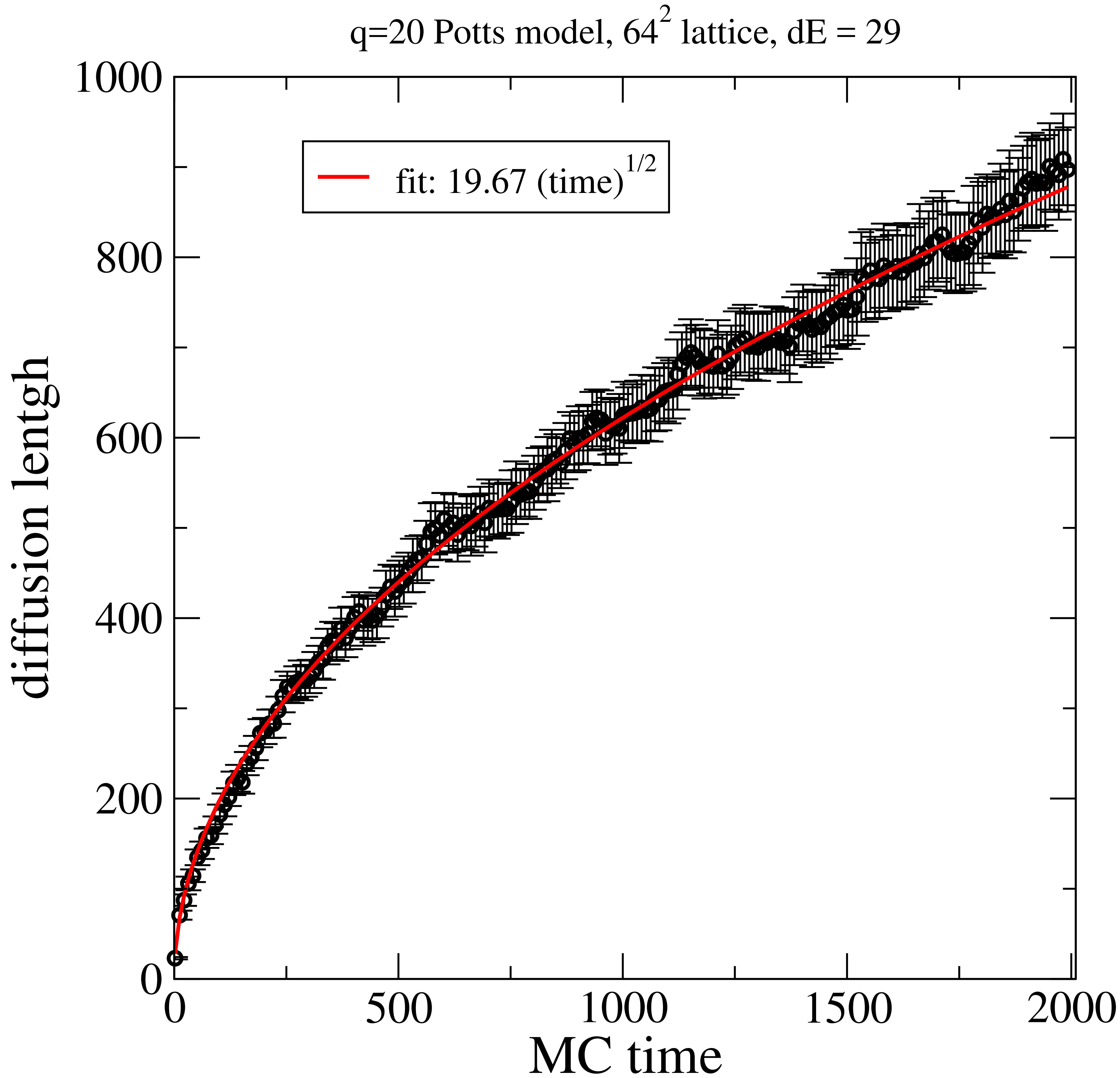
bridged 42 intervals within 750 sweeps

$$\left[\sqrt{750} = 27.38\ldots\right]$$



Showcase: q-state Potts model in 2d

[q=20, L=64]



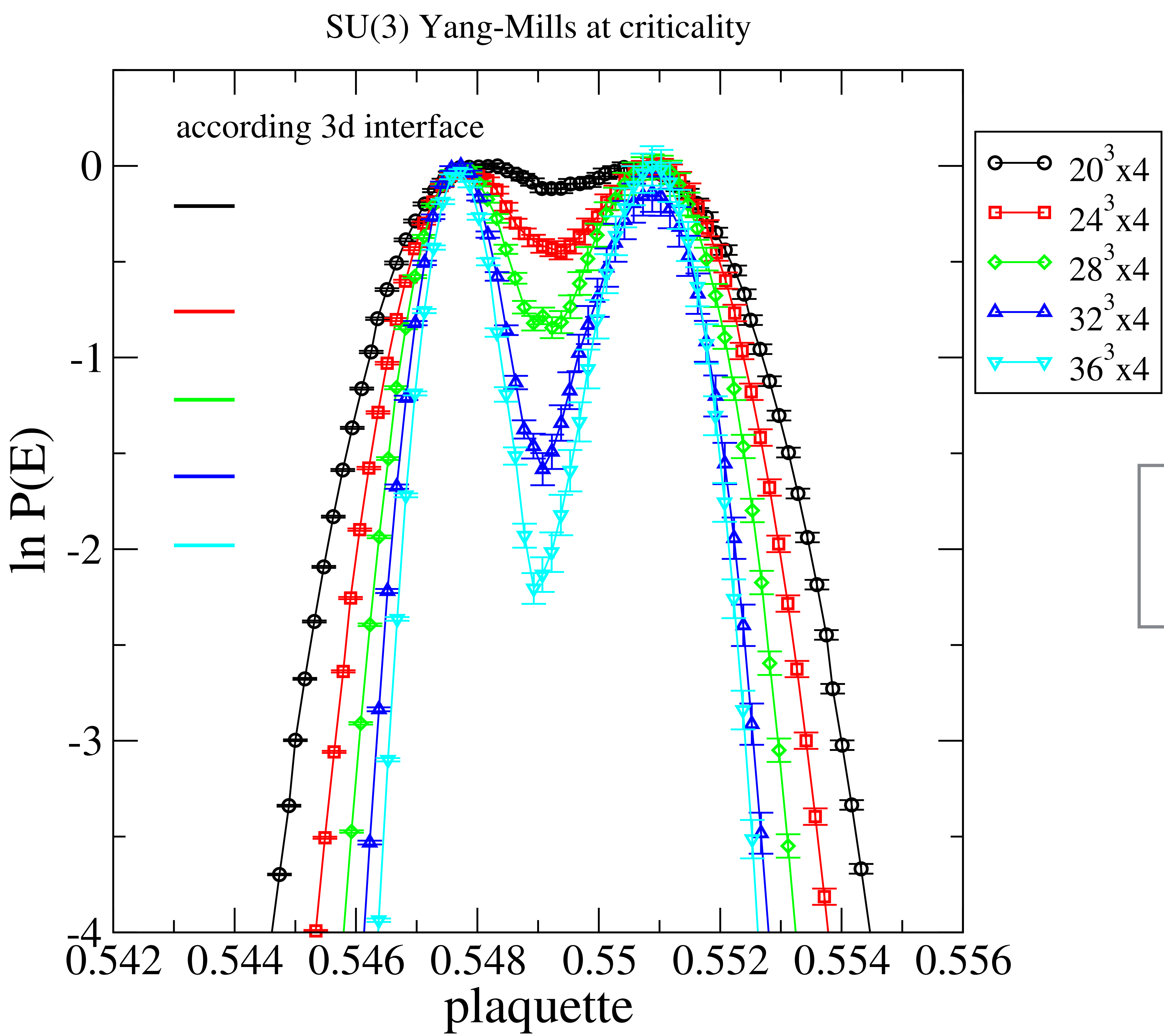
Enough theory.

We want to see results!

Applications

Towards the latent heat in SU(3) YM theory:

- Partition function: $Z(T) = \int dE \; P(E)$
- At criticality: double-peak structure of $P(E)$
- Define β_{crit} by equal height of peaks
- Temperature: $4 \times N_s$, $N_s = 20, \; 24, \; 28, \; 32, \; 36$



Towards:

latent heat

specific heats

order-disorder

interface tension

for $N_s < N_s^{\mathrm{crit}}$:

cross-over!

[KL in preparation]

Applications

What can the LLR approach do for QFT at finite densities?

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The density-of-states approach for complex theories:

- Recall: theory with complex action

$$Z = \int \mathcal{D}\phi \; \exp\{\beta S_R[\phi] + i\mu S_I[\phi]\}$$

- Define the generalised density-of-states:

$$P_\beta(s) = \int \mathcal{D}\phi \; \delta\Big(s - S_I[\phi]\Big) \; \exp\{\beta S_R[\phi]\}$$

Could get it by histogramming

- Partition function emerges from a FT:

$$Z \;=\; \int ds \; P_\beta(s) \; \exp\{i\,\mu\, s\}$$

What is the scale of the problem?

- Indicative result: $P_\beta(s) = \exp\left\{-\frac{s^2}{V}\right\}$

action volume

$$\boxed{Z = \int ds\, \mathrm{e}^{-s^2/V} \exp\{i\,\mu s\} \propto \exp\{-\frac{\mu^2}{4}V\}}$$

statistical errors exponentially small

Need exponential error suppression over the whole action range

LLR approach:

[Langfeld, Lucini, PRD 90 (2014) 094502]

[Langfeld, Lucini, Rago, PRL 109 (2012) 111601]

- Define the *overlap* between full and phase quenched theory

$$O(\mu) = \frac{Z(\mu)}{Z_{\rm PQ}(\mu)} = \langle \exp\{i\mu S_I\}\rangle_{\rm PQ}$$

- Trivially:

$$Z(\mu) = \frac{Z(\mu)}{Z_{\rm PQ}(\mu)} Z_{\rm PQ}(\mu) = O(\mu)\, Z_{\rm PQ}(\mu)$$

$$\sigma(\mu) = \frac{T}{V_3}\frac{\partial}{\partial\mu} \ln O(\mu) + \rho_{\rm PQ}(\mu)$$

standard Monte-Carlo

generically dominant!

Anatomy of a sign problem: Heavy-Dense QCD (HDQCD)

[see talk by N Garron, Tuesday, 14:40, Non-zero Temp & Density]

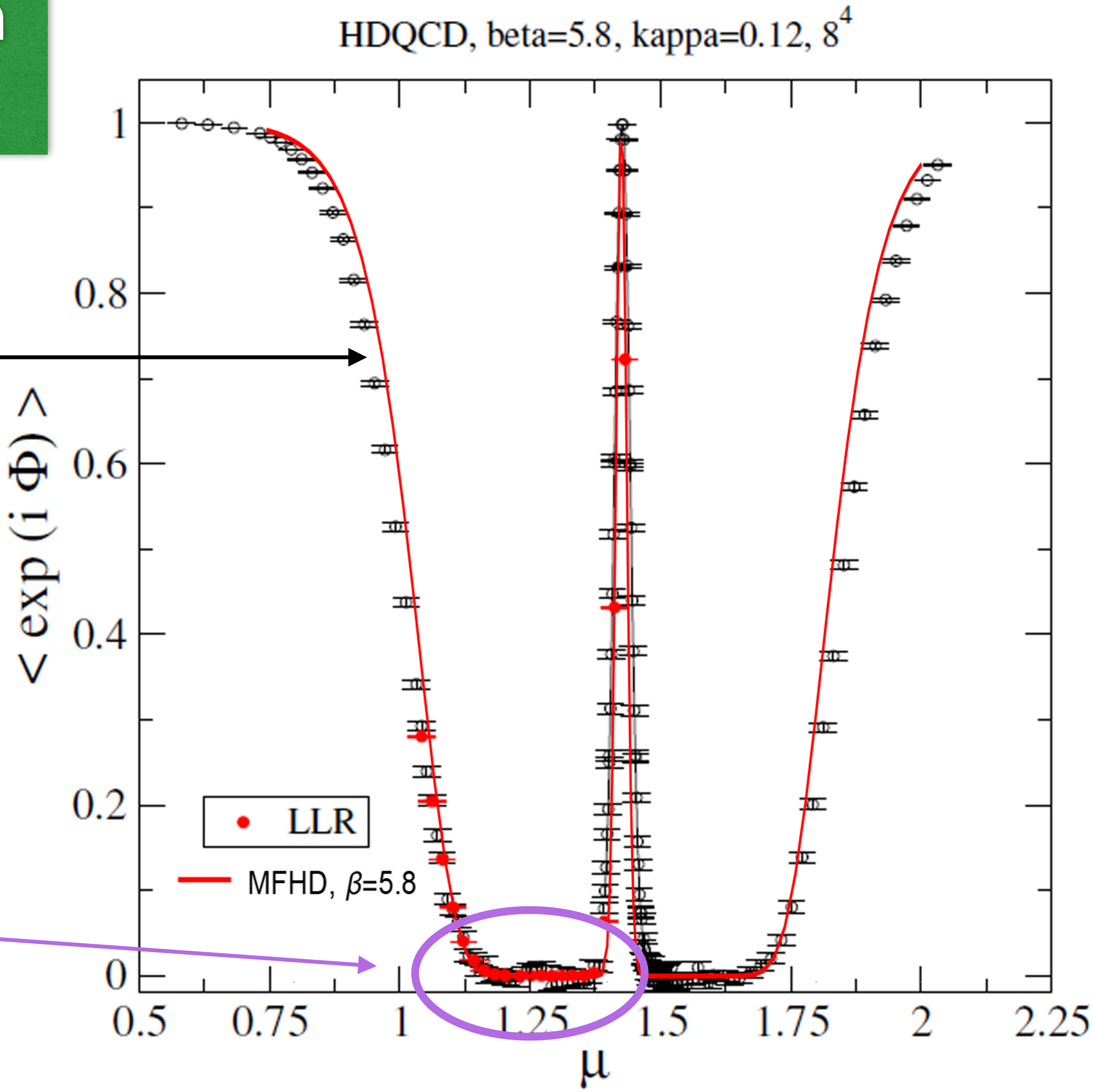
Starting point QCD: $$Z(\mu) = \int \mathcal{D}U_\mu \, \exp\{\beta\, S_{\rm YM}[U]\} \, \mathrm{Det}\, M(\mu)$$

SU(3) gauge theory ↑ quark determinant ↑

Limit quark mass m, μ large, $\mu/m \to \text{finite}$

[Bender, Hashimoto, Karsch, Linke, Nakamura, Plewnia,
Nucl. Phys. Proc. Suppl. 26 (1992) 323]

Here is the result from reweighting (black)



Thanks to Tobias and Philippe for the Mean-Field comparison!

strong sign problem

see also [Rindlisbacher, de Forcrand, JHEP 1602 (2016) 051]

Challenge: How do we carry out a Fourier transform the result of which is 10^{-14} and the integrand of order $\mathcal{O}(1)$ is only known numerically?

Fit a Polynomial: $\ln P(s) = \sum_{i\text{ even}}^{p} c_i\, s^i$, for $p = 2, 4, 6, 8..$

Calculate the Fourier transform semi-analytically

Data Compression essential:

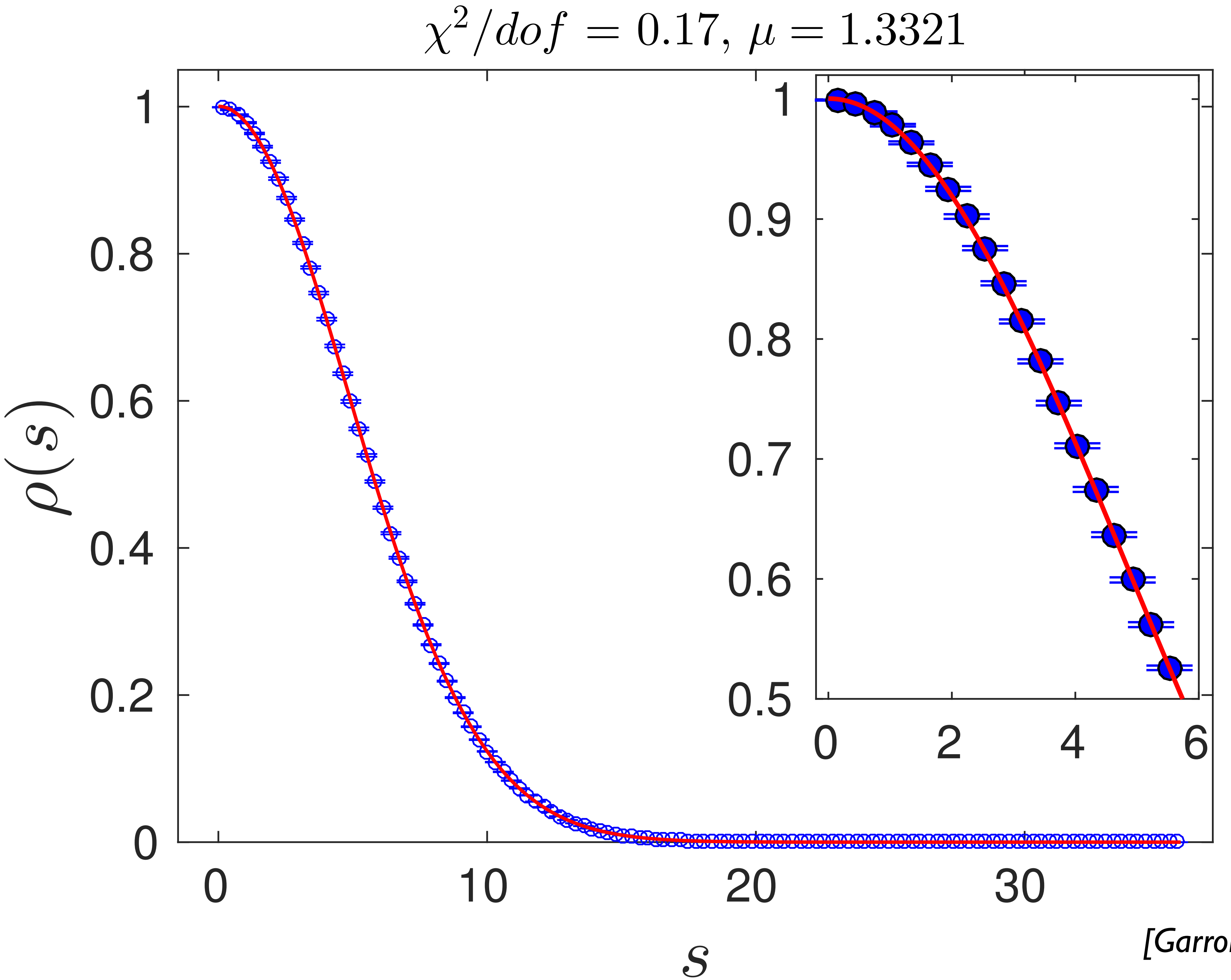
$\ln P(s)$ ~ 1000 data points $\Rightarrow$ c_i ~ 20 coefficients

$\chi^2/\mathrm{dof} = \mathcal{O}(1)$

tested for the Z3 spin model at finite densities!

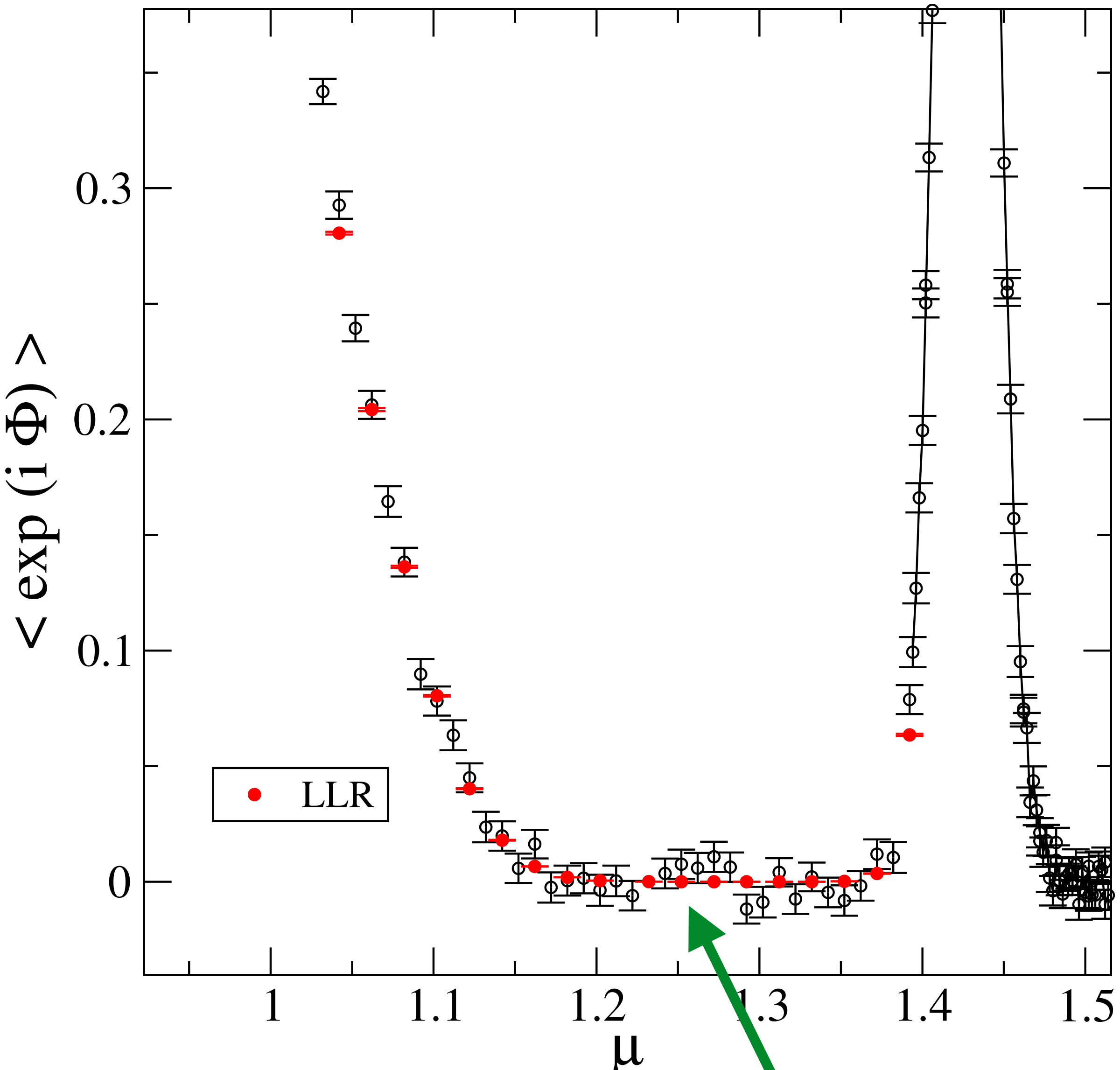
[Langfeld, Lucini, PRD 90 (2014) no.9, 094502]

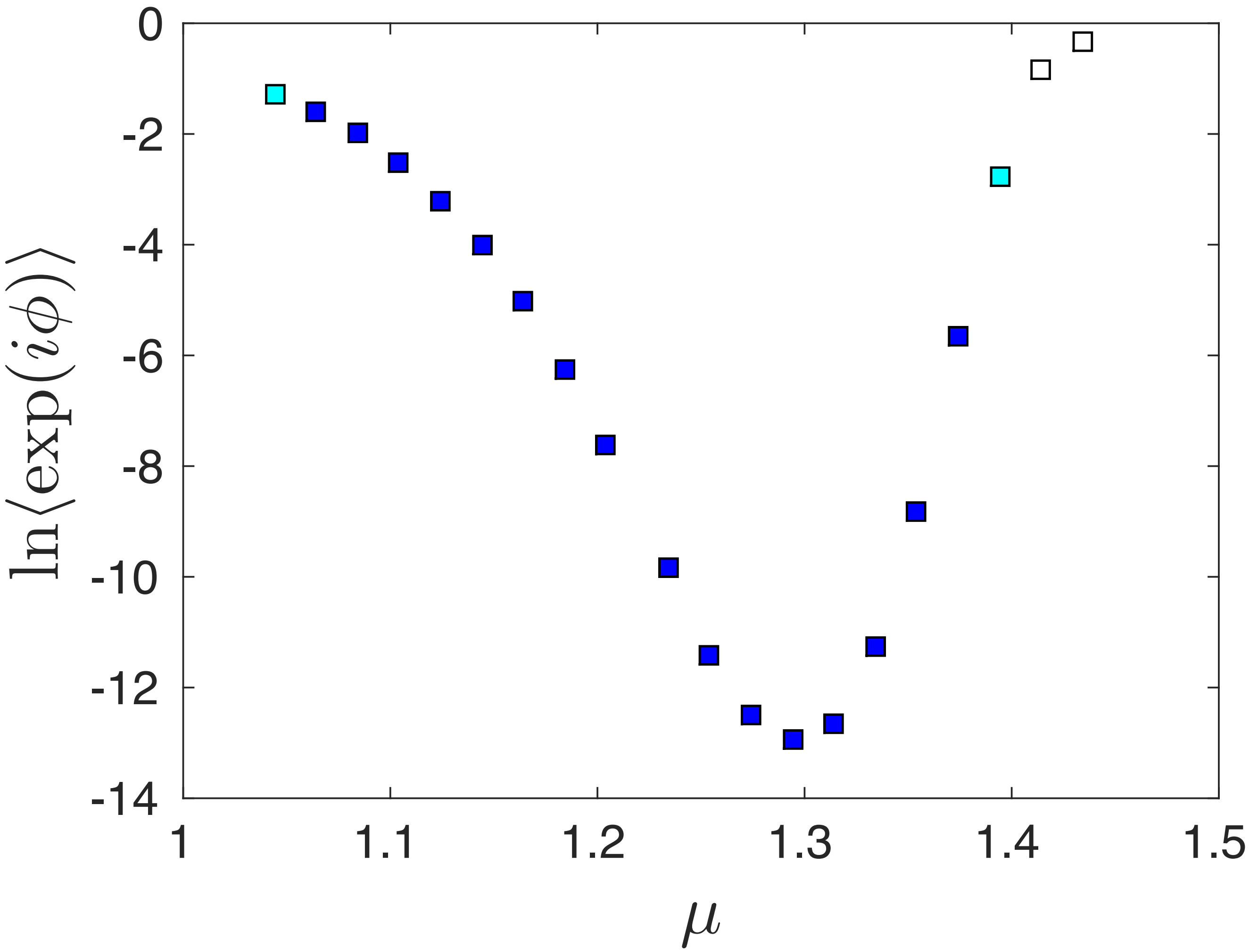
Works very well!



[Garron, Langfeld, arXiv:1605.02709]

What can LLR do for you?





error bars 5 orders of magnitude smaller!

[Garron, Langfeld, arXiv:1605.02709]

Objections:

Fit a Polynomial: $\ln P(s) = \sum_{i\ \mathrm{even}}^{p} c_i\ s^i$, for $p = 2, 4, 6, 8..$

remember: Calculate the Fourier transform semi-analytically

How robust is the approach against the choice of fitting functions?

Extended cumulant approach:

similar to:
[Saito, Ejiri, et al, PRD 89 (2014) no.3, 034507]
see also:
[Greensite, Myers, Splittorff, PoS LATTICE2013 (2014) 023]

Phase of the determinant: ϕ

Probability Distribution very close to "1"

$$P(\phi) = 1 + \epsilon a_1 + \epsilon^2 a_2 + \epsilon^3 a_3 + \ldots$$

suppressed by volume

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Overlap: $\langle \exp\{i\Phi\}\rangle = \frac{1}{N}\int_{-\pi}^{\pi} \mathrm{e}^{i\phi}\, P(\phi)\, d\phi$ $\qquad \langle \phi^n\rangle = \frac{1}{N}\int_{-\pi}^{\pi} \phi^n\, P(\phi)\, d\phi$

Extended cumulant approach:

[see talk by N Garron, Tuesday, 14:40, Non-zero Temp & Density]

$$M_4 = \langle\phi^4\rangle - \frac{3\pi^2}{5}\langle\phi^2\rangle$$

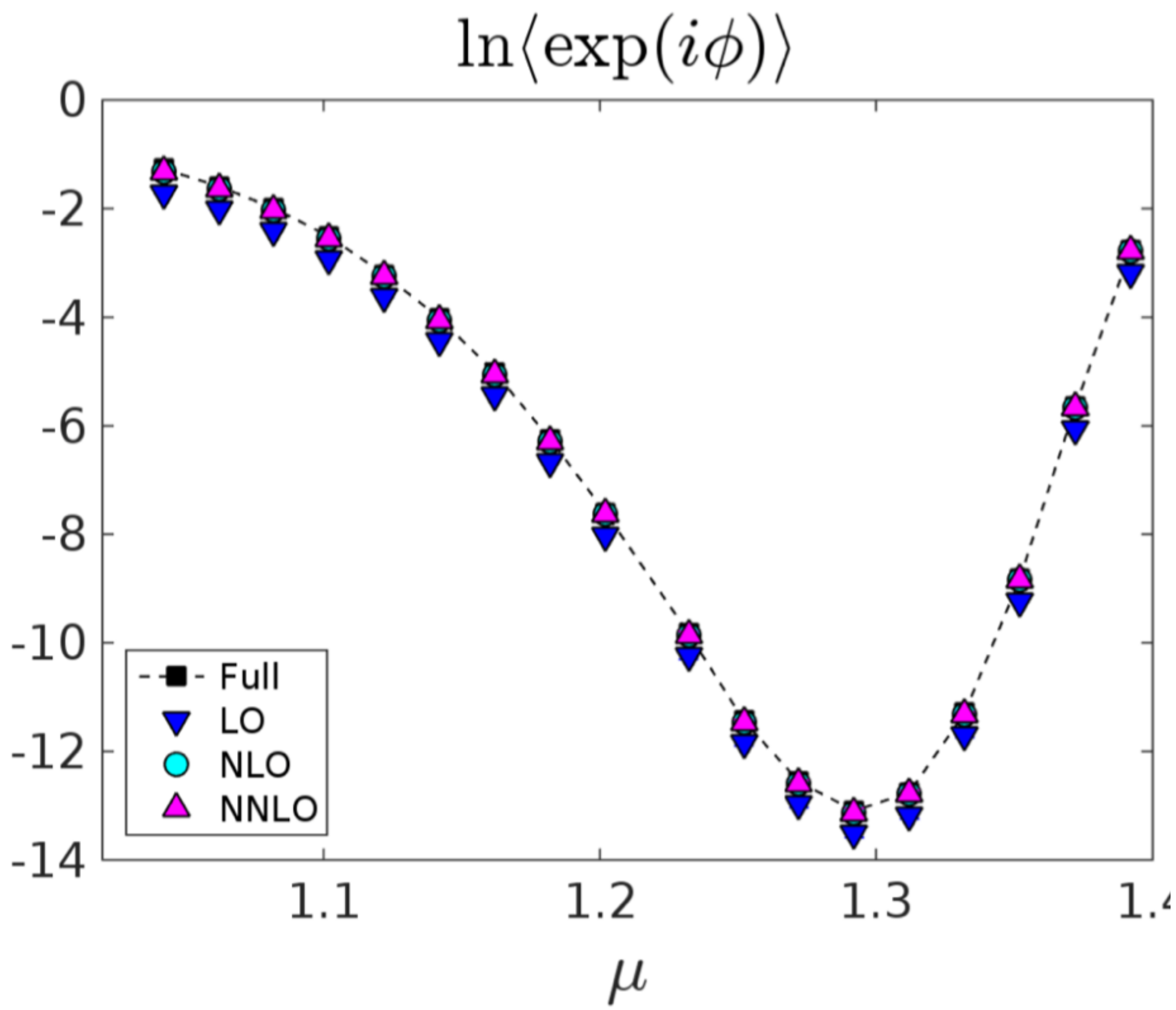
$$M_6 = \langle\phi^6\rangle - \frac{10\pi^2}{9}\langle\phi^4\rangle + \frac{5\pi^4}{21}\langle\phi^2\rangle$$

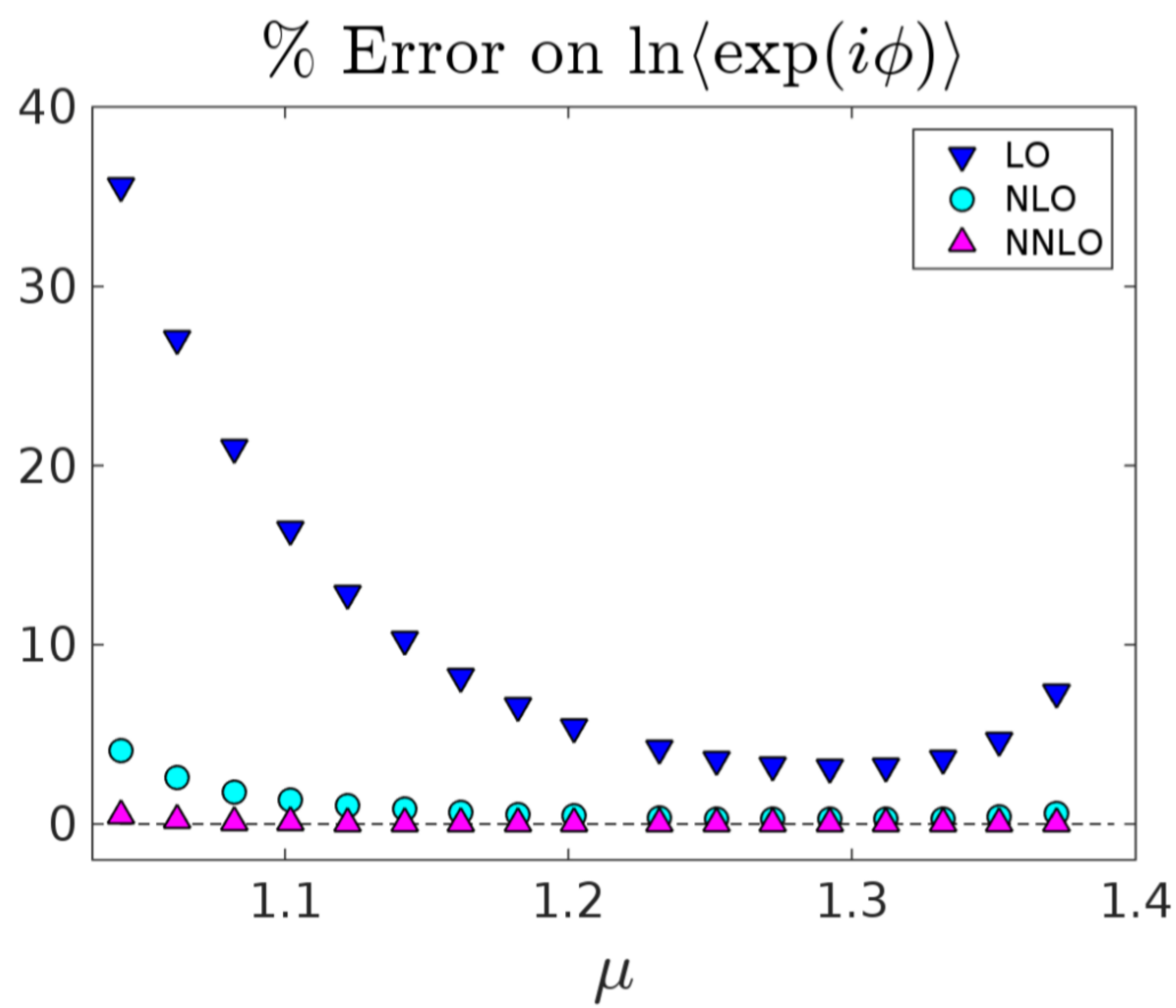
$$M_8 = \langle\phi^8\rangle - \frac{21\pi^2}{13}\langle\phi^6\rangle + \frac{105\pi^4}{143}\langle\phi^4\rangle - \frac{35\pi^6}{429}\langle\phi^2\rangle$$

$$\langle \mathrm{e}^{i\phi}\rangle = -\frac{175}{2\pi^6} M_4 + \frac{4851\,(27-2\pi^2)}{8\pi^{10}} M_6 - \frac{57915\,(3\pi^4-242\pi^2+2145)}{16\pi^{14}} M_8 + \mathcal{O}(\epsilon^4)$$

$$\underset{[\mu = 1.2921]}{\langle \mathrm{e}^{i\phi}\rangle} = 10^{-6}\left[1.45(28) + 0.67(13) + 0.068(13)\right] + \mathcal{O}(\epsilon^4)$$

Extended cumulant approach:



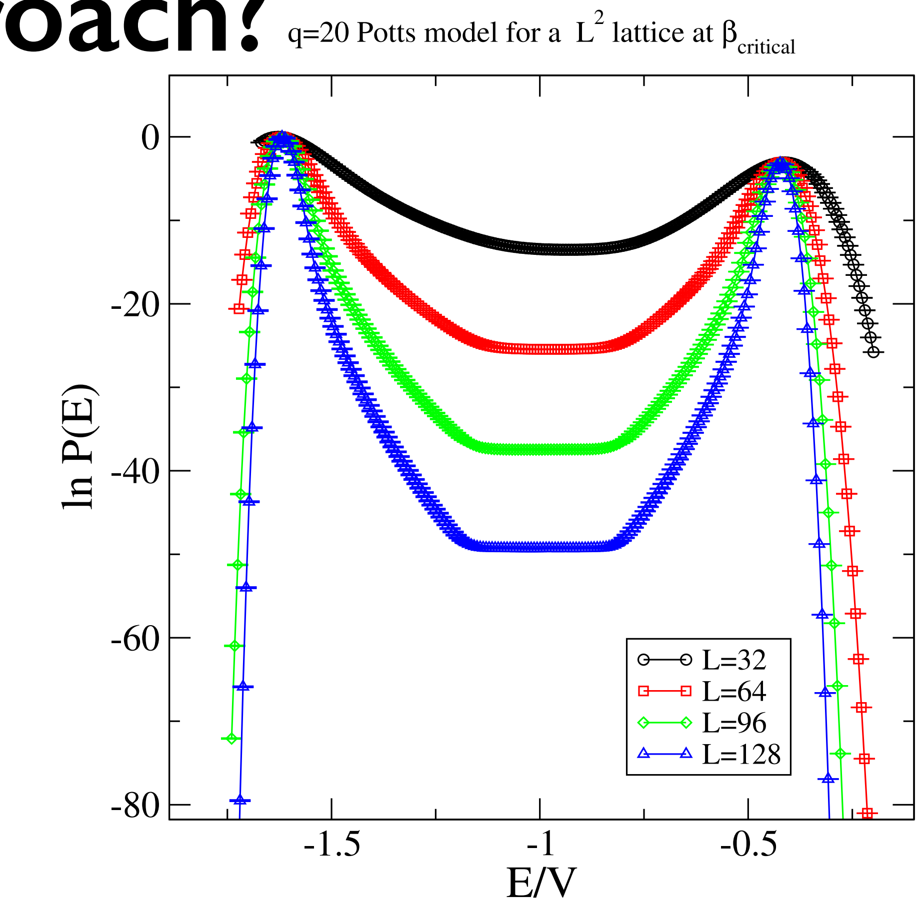


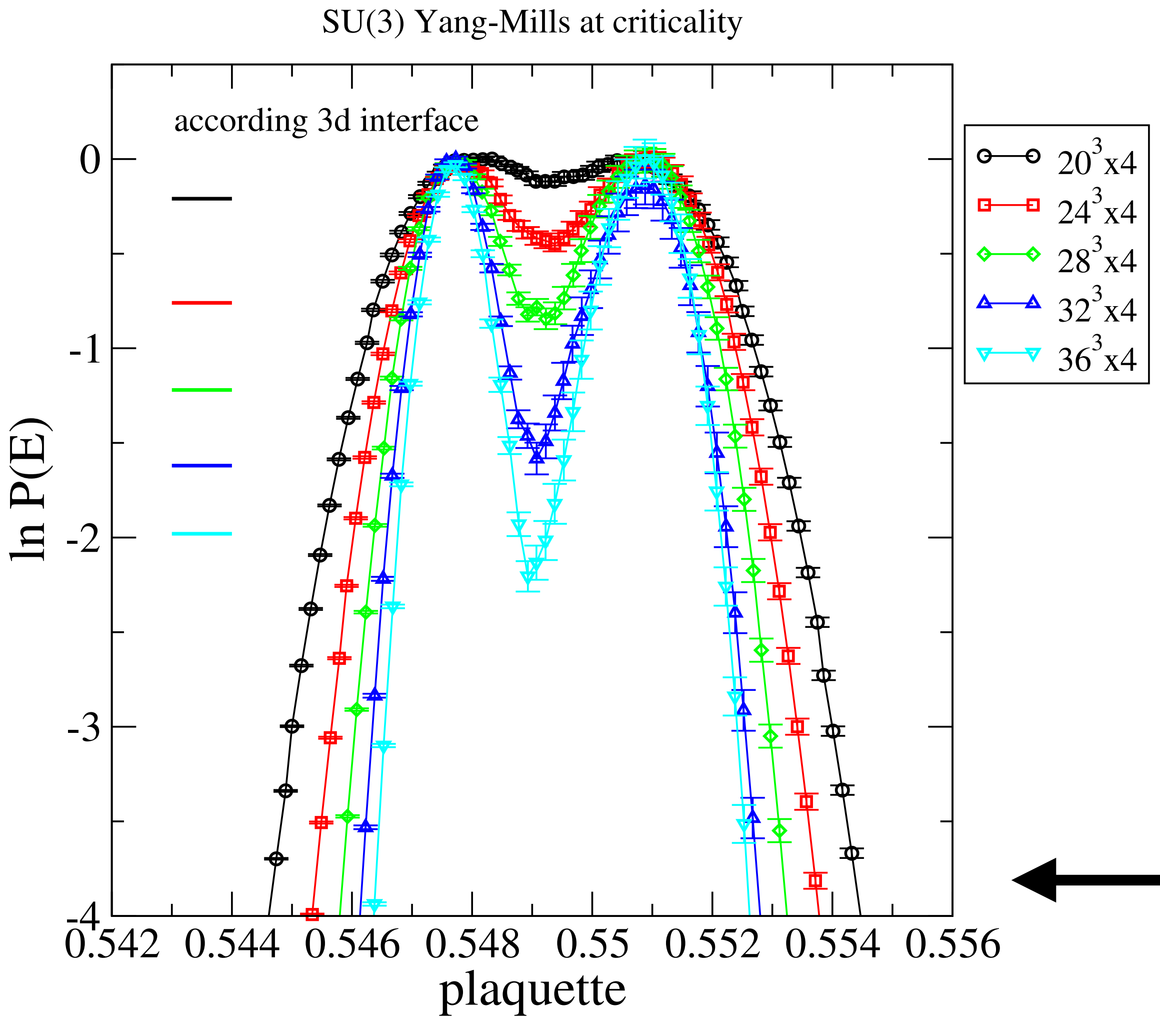
[analysis by N Garron]

Summary: What is the LLR approach?

Non-Markovian Random walk

Calculates the probability distribution of (the imaginary part of) the action with **exponential error suppression**





Technical Progress:

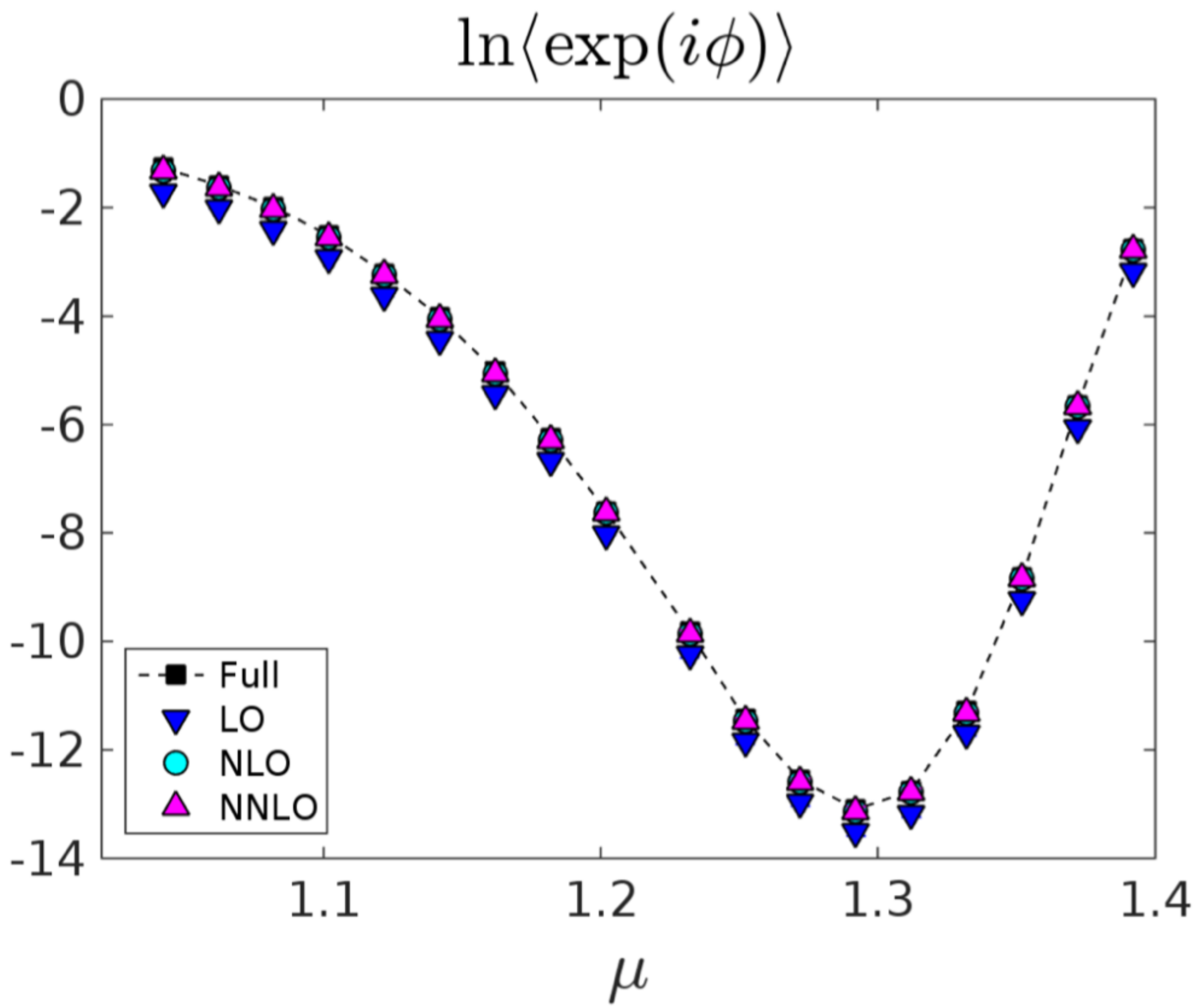
- Ergodicity: Replica Exchange
- Smooth Window function (LHMC & HMC)

[also talk by Pellegrini]

Summary: **Can solve *strong sign problems*:**

Z3 gauge theory at finite densities [Langfeld, Lucini, PRD 90 (2014) no.9, 094502]

HD QCD [Garron, Langfeld, arXiv:1605.02709]



New element:

Extended cumulant approach

Outlook:

[immediate LLR projects very likely to succeed]

- interface tensions in the q=20 Potts model (perfect wetting?) *[Lucini, KL]* talk!
- thermodynamics with shifted BC in SU(2) & …. *[Pellegrini, Rago, Lucini]* talk!
- SU(3) interface tensions, latent heat, etc. *[KL et al.]*

[LLR density projects hopefully to succeed]

- small volume (finite density) QCD *[Garron, KL]*
- Hubbard model, FG model, Graphene *[von Smekal, KL, et al.]* talk!

[other related projects:]

- Topological freezing, CP(n-1): Metadynamics *[Sanfilippo, Martinelli, Laio]* talk!
- Jarzynski's relation *[Nada, Caselle, Panero, Costagliola, Toniato]* talk!