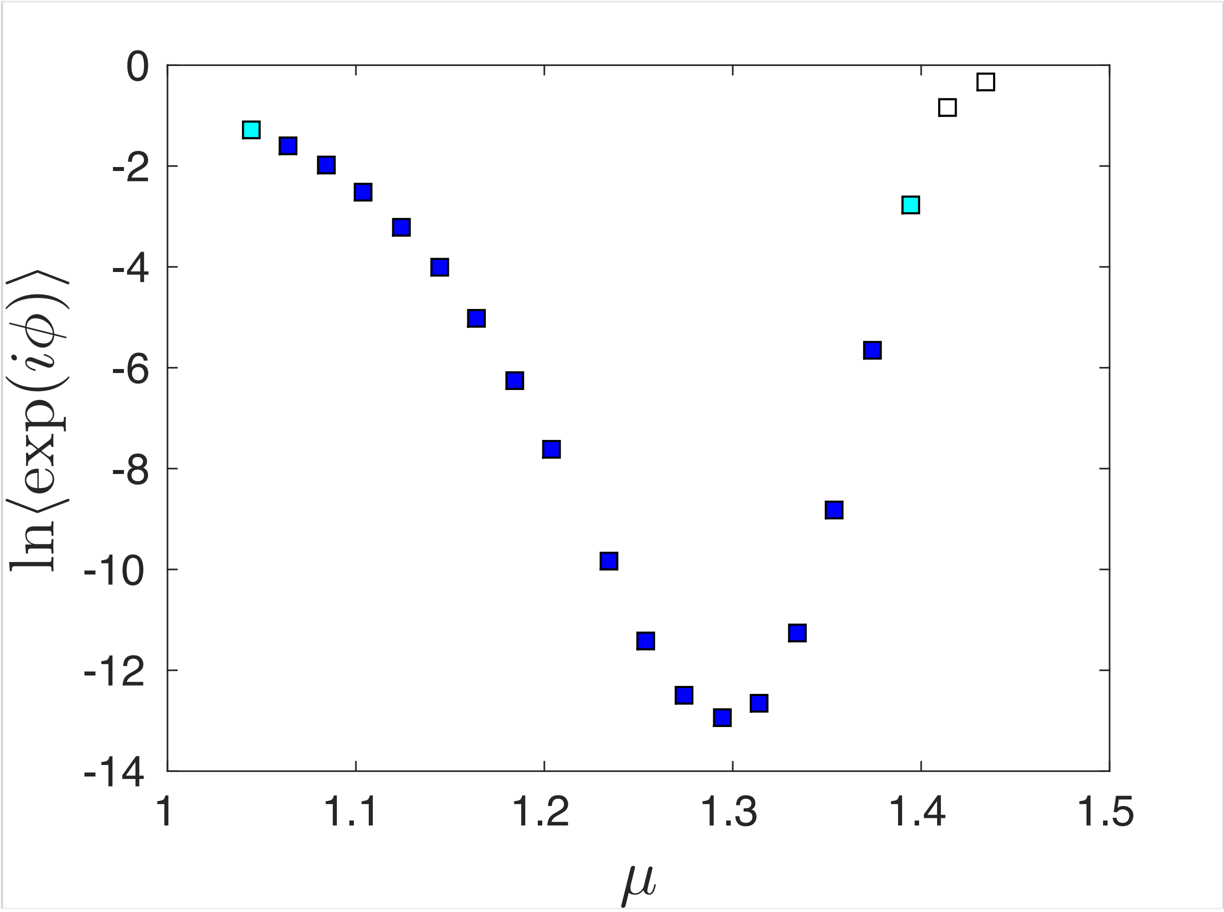
RESEARCH WITH PLYMOUTH UNIVERSITY

Can the density-of-states method solve sign problems ?



Kurt Langfeld (Plymouth & Liverpool)

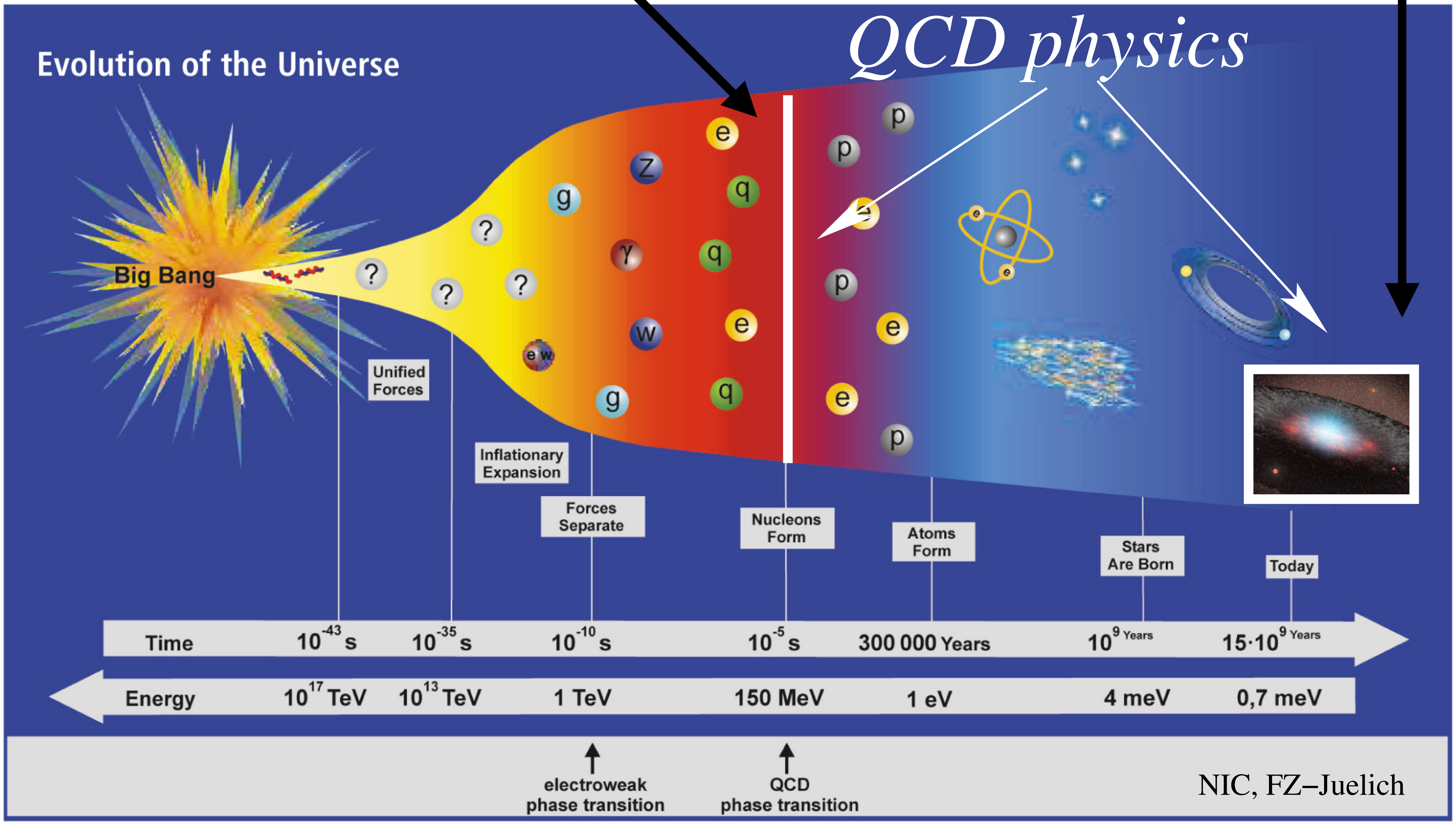
Delta Meeting, Heidelberg, 28-30 April 2016

Biagio Lucini (Swansea)
Antonio Rago, Nicolas Garron (Plymouth)
Roberto Pellegrini (Edinburgh)

low density & high T
Standard LGT: ✓

high density & low T
Standard LGT: ✗

QCD physics



NIC, FZ–Juelich

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

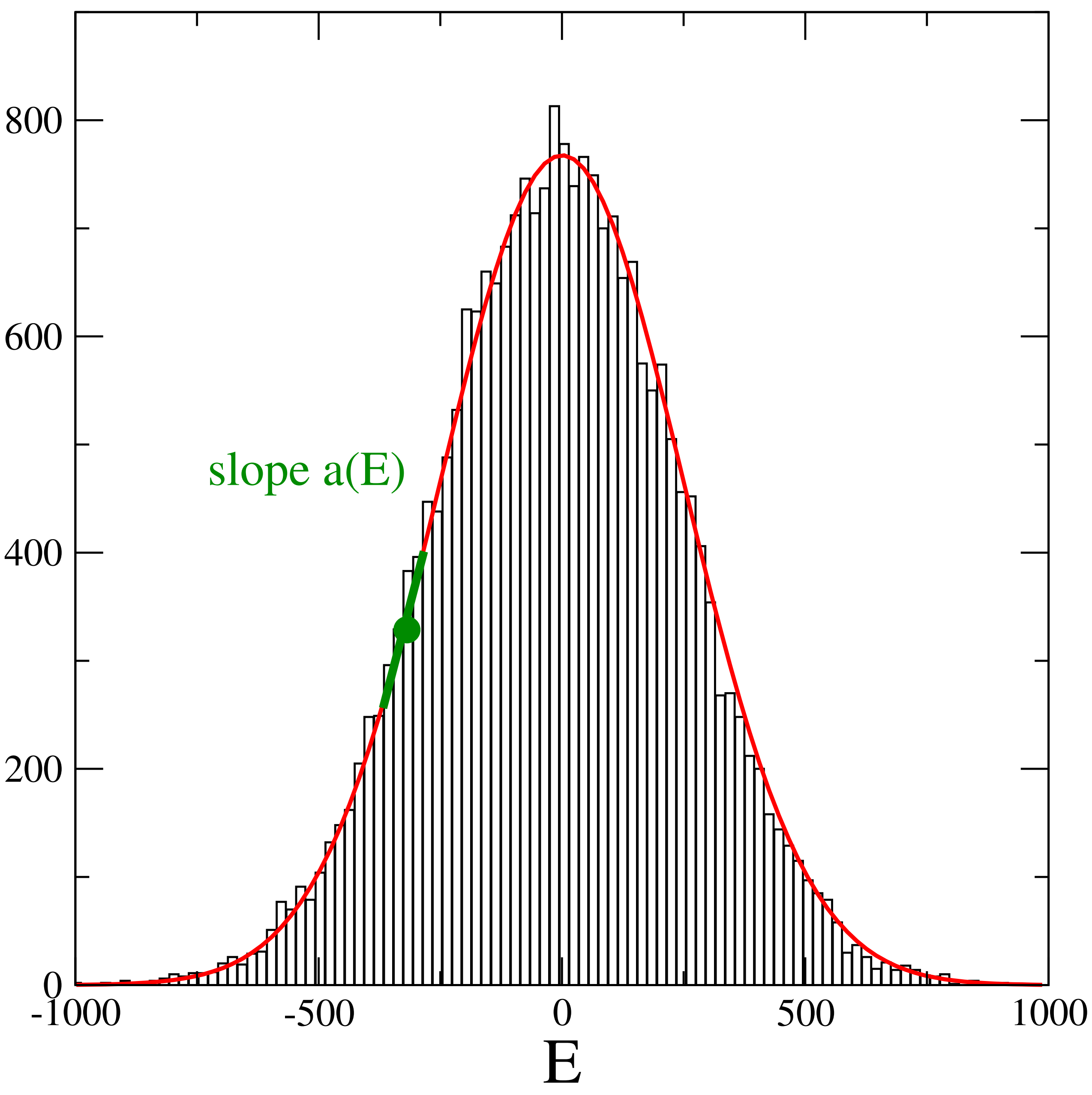
$$P(E) = \rho(E) \ \mathrm{e}^{\beta E}$$

Probabilistic weight

How do I find the density-of-states?

straightforward: Histogram of the action S

The LLR approach to the density-of-states:



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

1. Calculate the slope at E from a stochastic non-linear equation:

$$a(E) = \frac{d \ln \rho(E)}{dE}$$

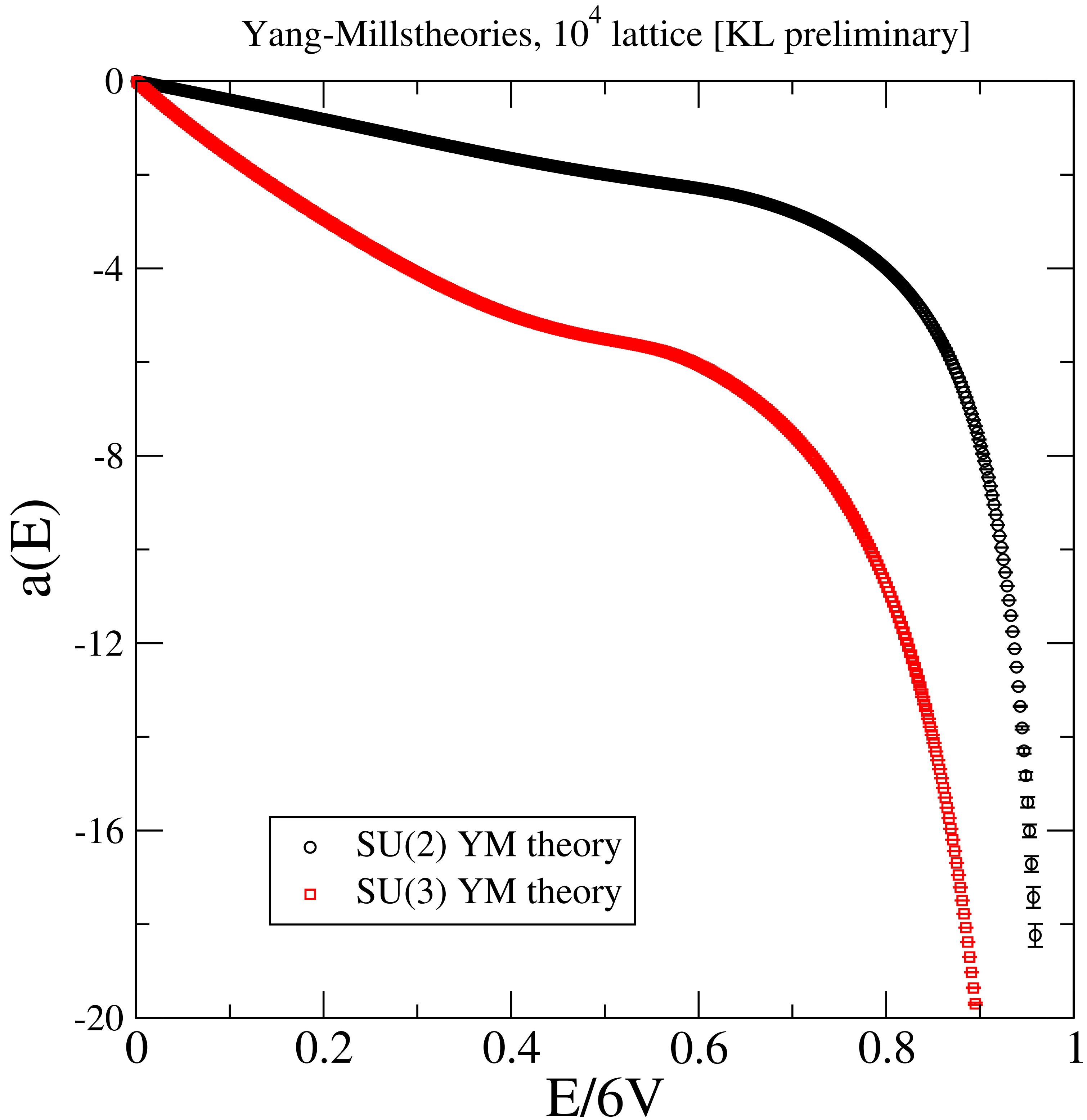
$$\langle\langle S - E \rangle\rangle \, (a) \ = \ 0$$

↑ MC average

2. Reconstruct $\rho(E)$

3. Find: $P(E) = \rho(E) \, \mathrm{e}^{\beta E}$

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

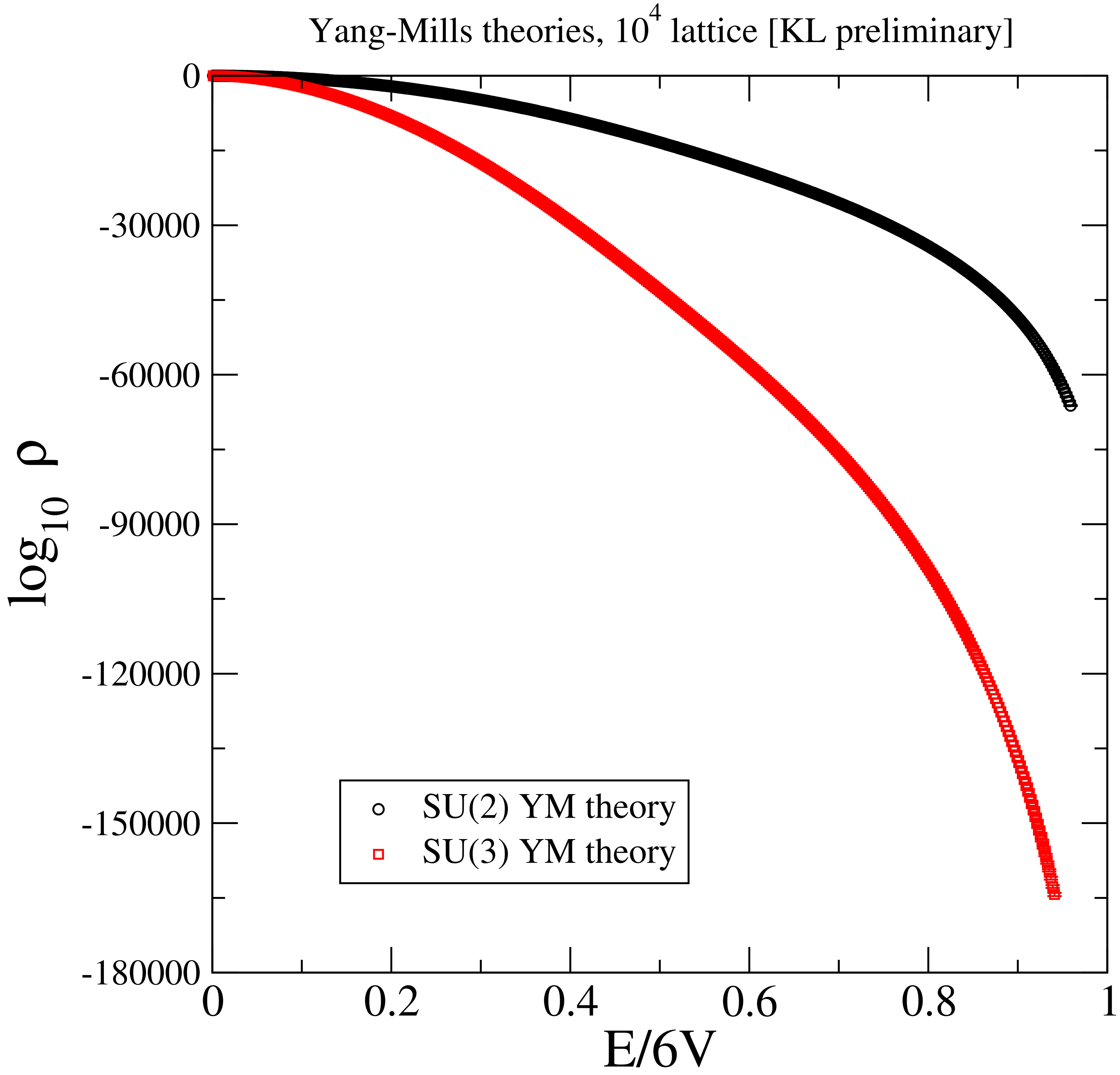


Error bars from bootstrap (20 independent runs per interval)

features an *exponential error suppression*

[Langfeld, Lucini, Pellegrini, Rago, arXiv:1509.08391]

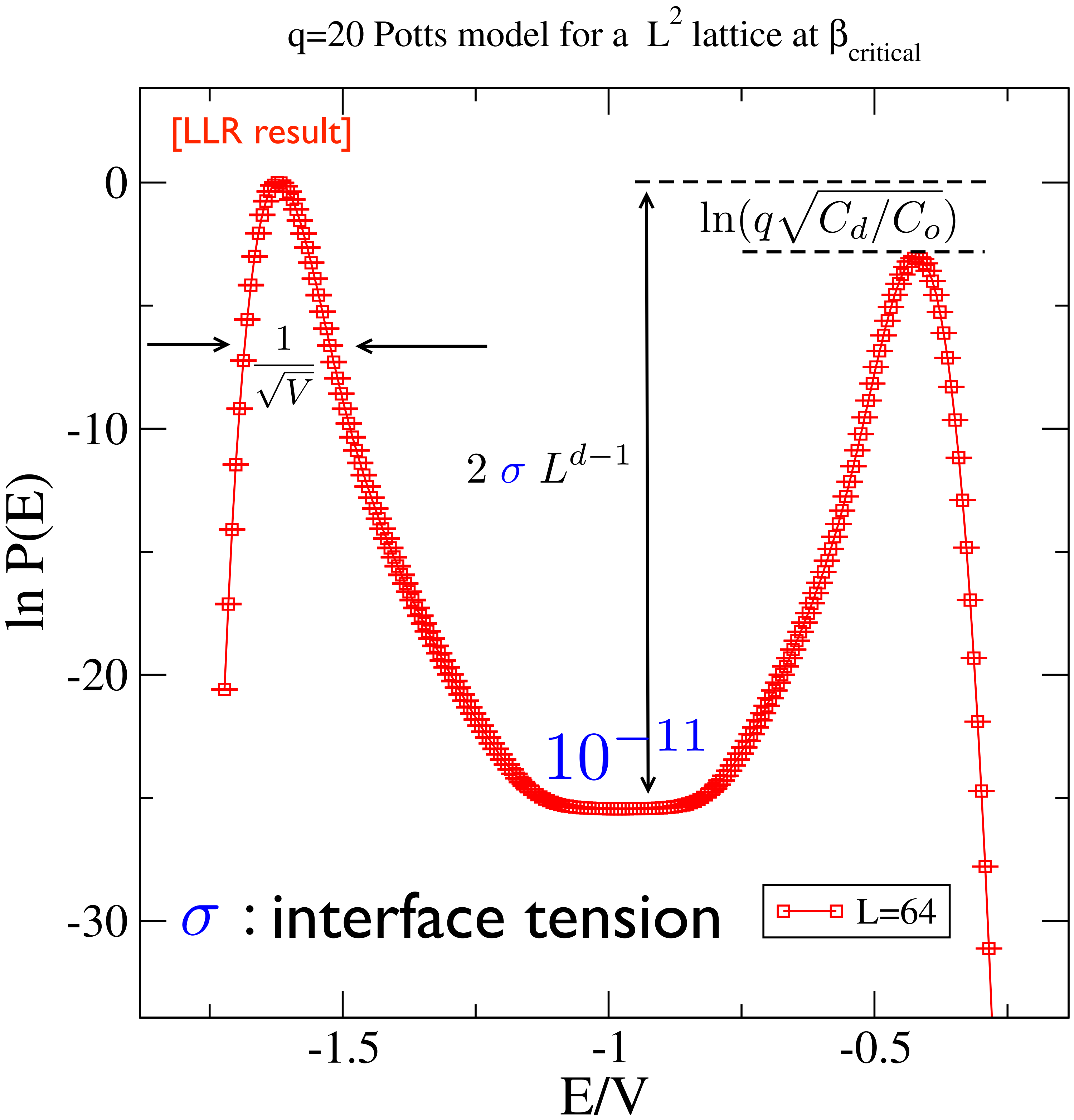
Showcase: SU(2) and SU(3) Yang-Mills theory



Density of states over 100,000 orders of magnitude!

[Gattringer Langfeld, arXiv:1603.09517]

Showcase: q-state Potts model in 2d



LLR solves overlap problems!

Exact solution:

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

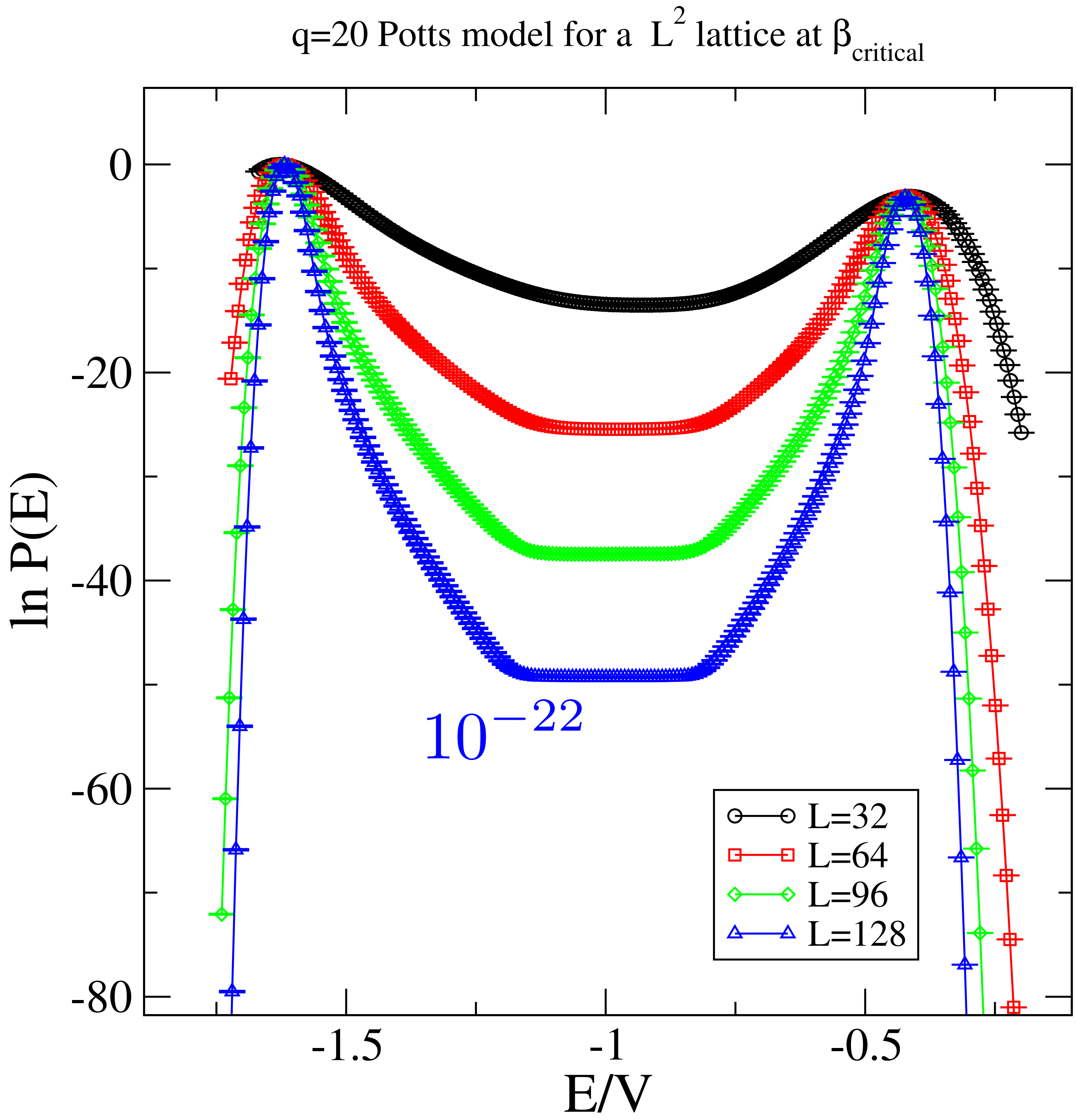
$$\beta_{\text{critical}} = \frac{1}{2}\ln(1+\sqrt{q})$$

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

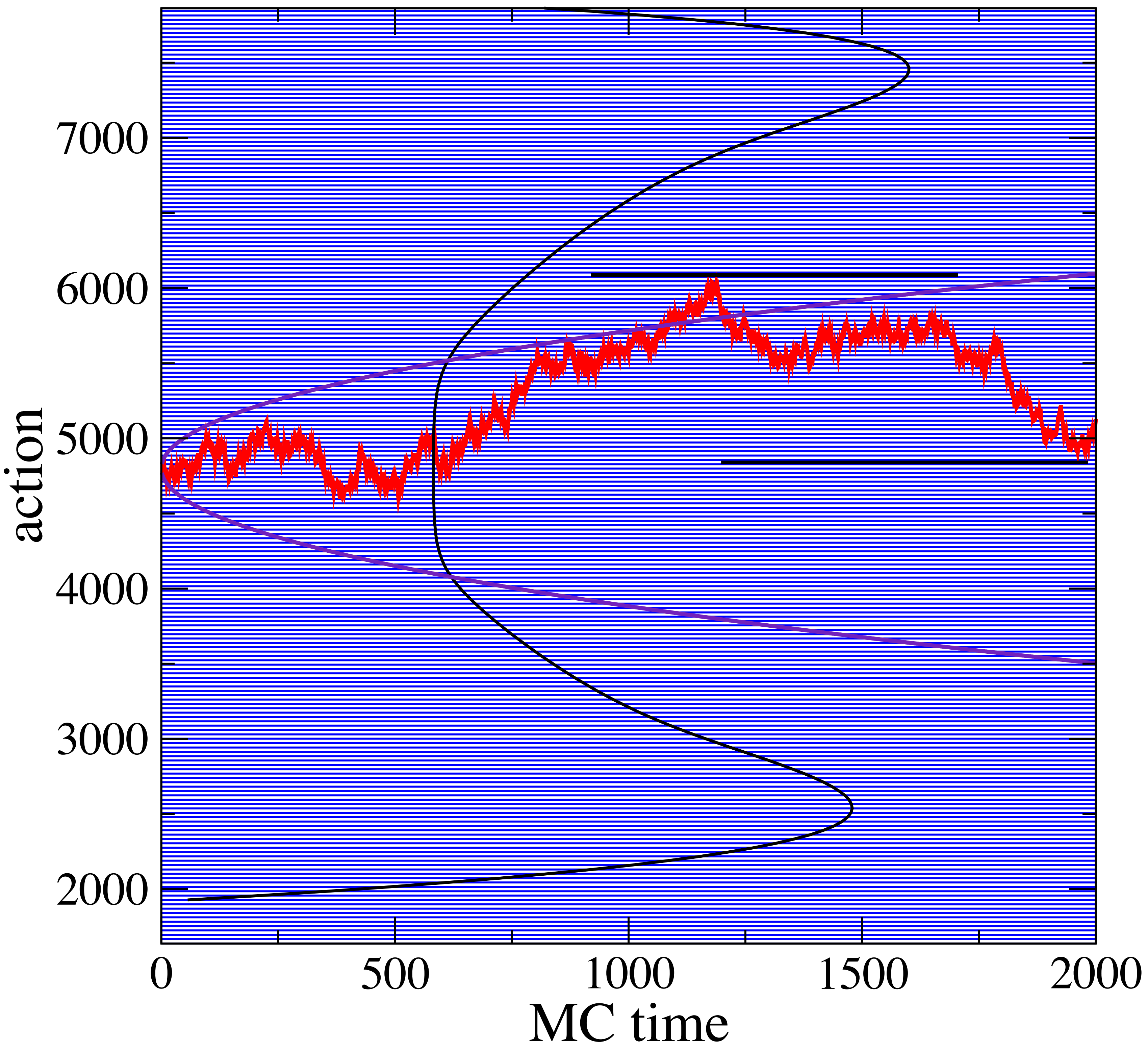
[q=20, L=64]

Tunnelling between LLR action intervals:

Interval size: 29

bridged 42 intervals within 750 sweeps

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



How do we simulate dense matter QFT with the density-of-states method?

- Quantum Field Theory:

$$\boxed{Z = \int \mathcal{D}\phi \ \exp\{\beta S_R[\phi]\}}$$

infinite dimension integral

Monte-Carlo simulation (importance sampling!)

$\exp\{\beta S_R[\phi]\}$: probabilistic weight

- QFT at finite densities:

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

μ: chemical potential

S_I: imaginary part of the action

complex!

How can we quantify the problem?

- If we drop the imaginary part of the action:

$$Z_{\mathrm{PQ}}(\mu) = \int \mathcal{D}\phi \; \exp\{S_R[\phi]\}$$

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

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

Overlap problem:

- Z and $Z_{\rm PQ}$ have different *free energy densities*

$$O(\mu) = \frac{Z(\mu)}{Z_{\rm PQ}(\mu)} = \exp\{-\Delta f \; V\} \quad \Rightarrow$$

can be very small
$(\Delta f > 0)$

re-weighting is inefficient!

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

$$\boxed{\rho(\mu) \;=\; \frac{T}{V_3} \, \frac{\partial}{\partial \mu} O(\mu) \;+\; \rho_{\rm PQ}(\mu)}$$

standard Monte-Carlo

generically dominant!

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:

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

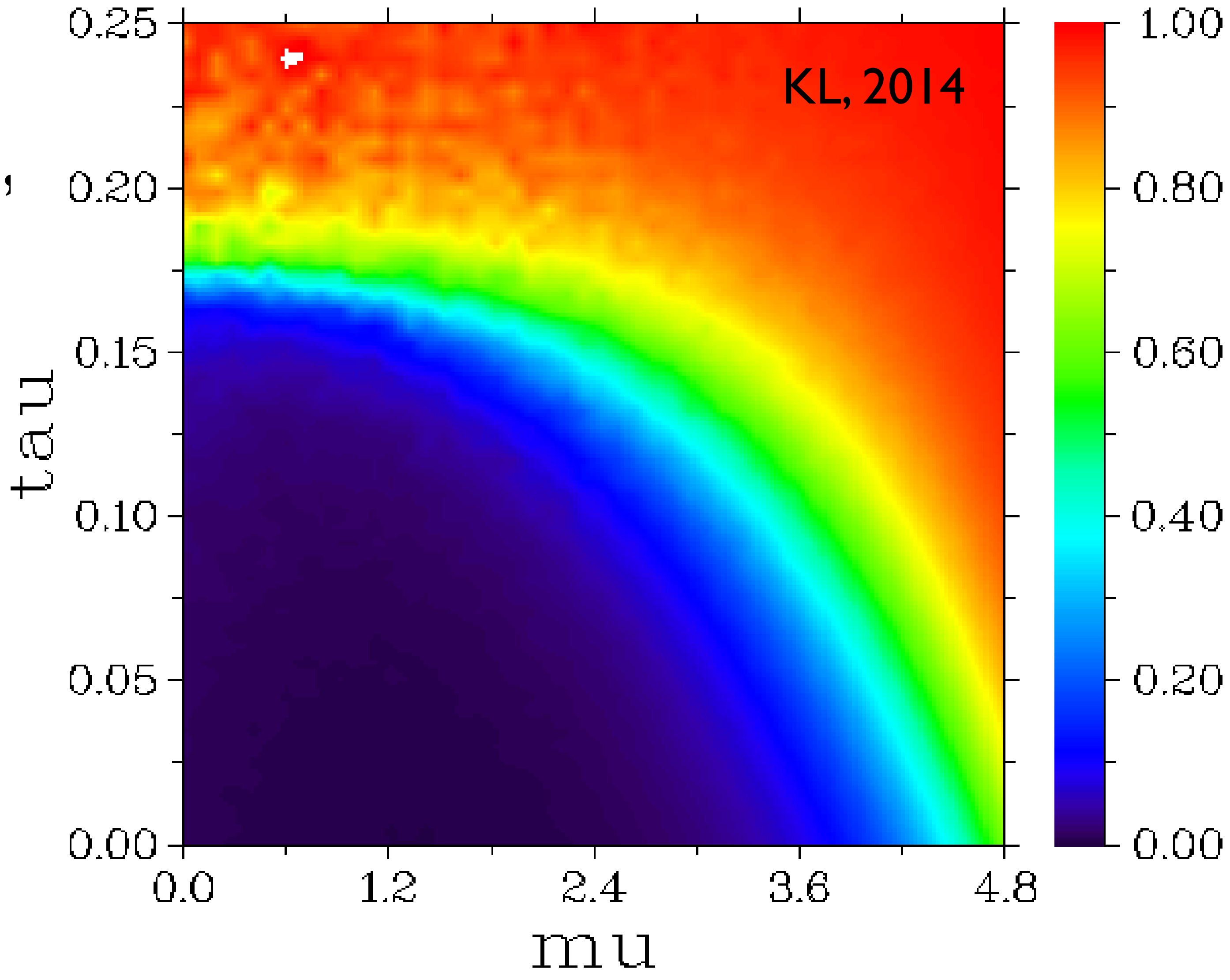
The Z3 showcase:

$$S[z] = \tau \sum_{x,\nu} [z_x z^*_{x+\nu} + cc] \; + \; \sum_x [\eta z_x + \bar{\eta} z^*_x]$$

$\tau \; : \;$ temperature, $\quad \eta = \kappa \, e^{\mu} \;, \quad \bar{\eta} = \kappa \, e^{-\mu} \quad z \in Z_3$

- Solvable: dual theory is real, efficient flux algorithm

[Mercado, Evertz, Gattringer, PRL 106 (2011) 222001]



What is the scale of the problem?

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

action

volume

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

statistical errors

exponentially small

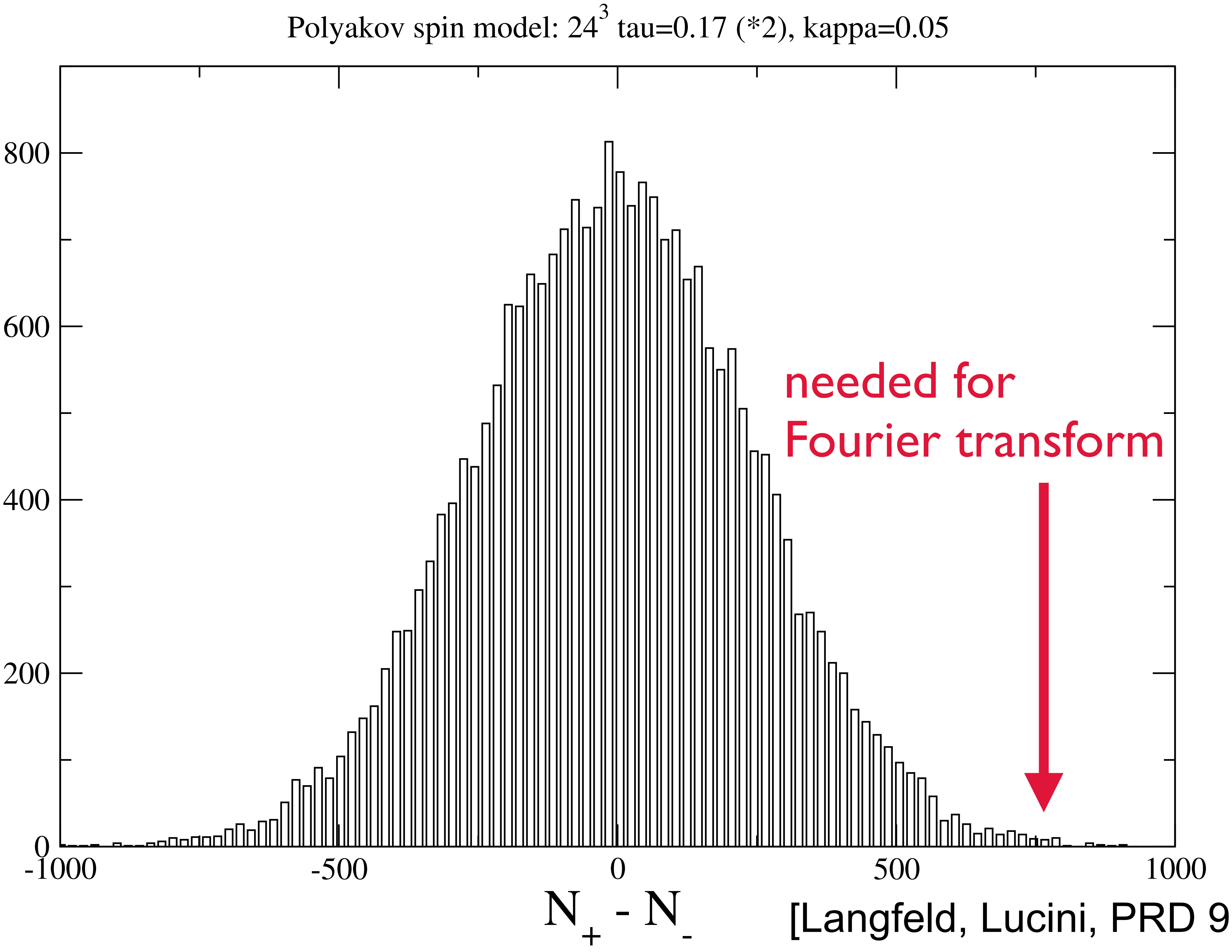
Need exponential error suppression over the whole action range

LLR approach:

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

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

What do we find for P(s)?

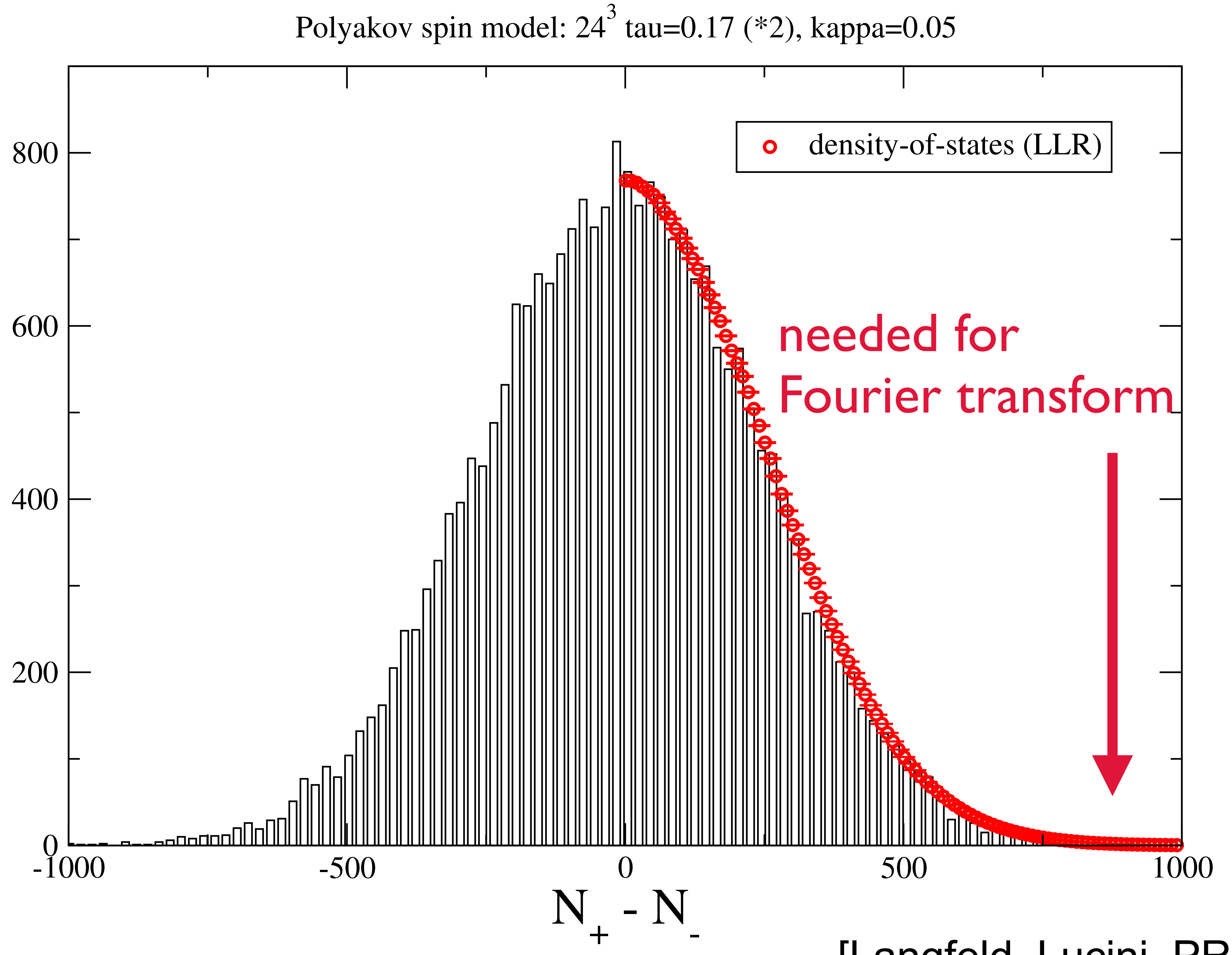


needed for Fourier transform

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

Histogramming is not good enough!

Let's go back to P(imaginary part) of the Z3 theory:

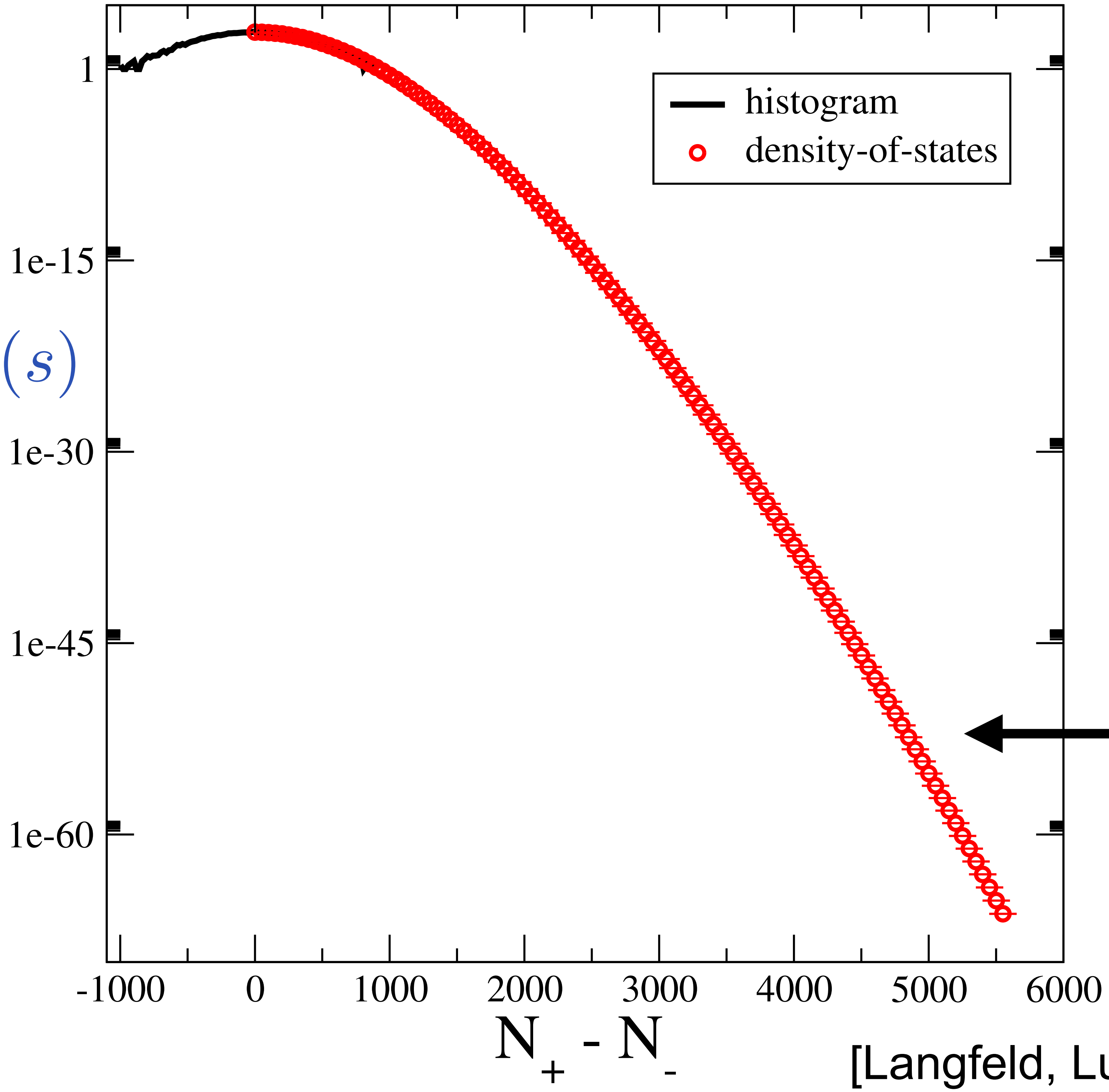


needed for
Fourier transform

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

Let's go back to P(imaginary part) of the Z3 theory:

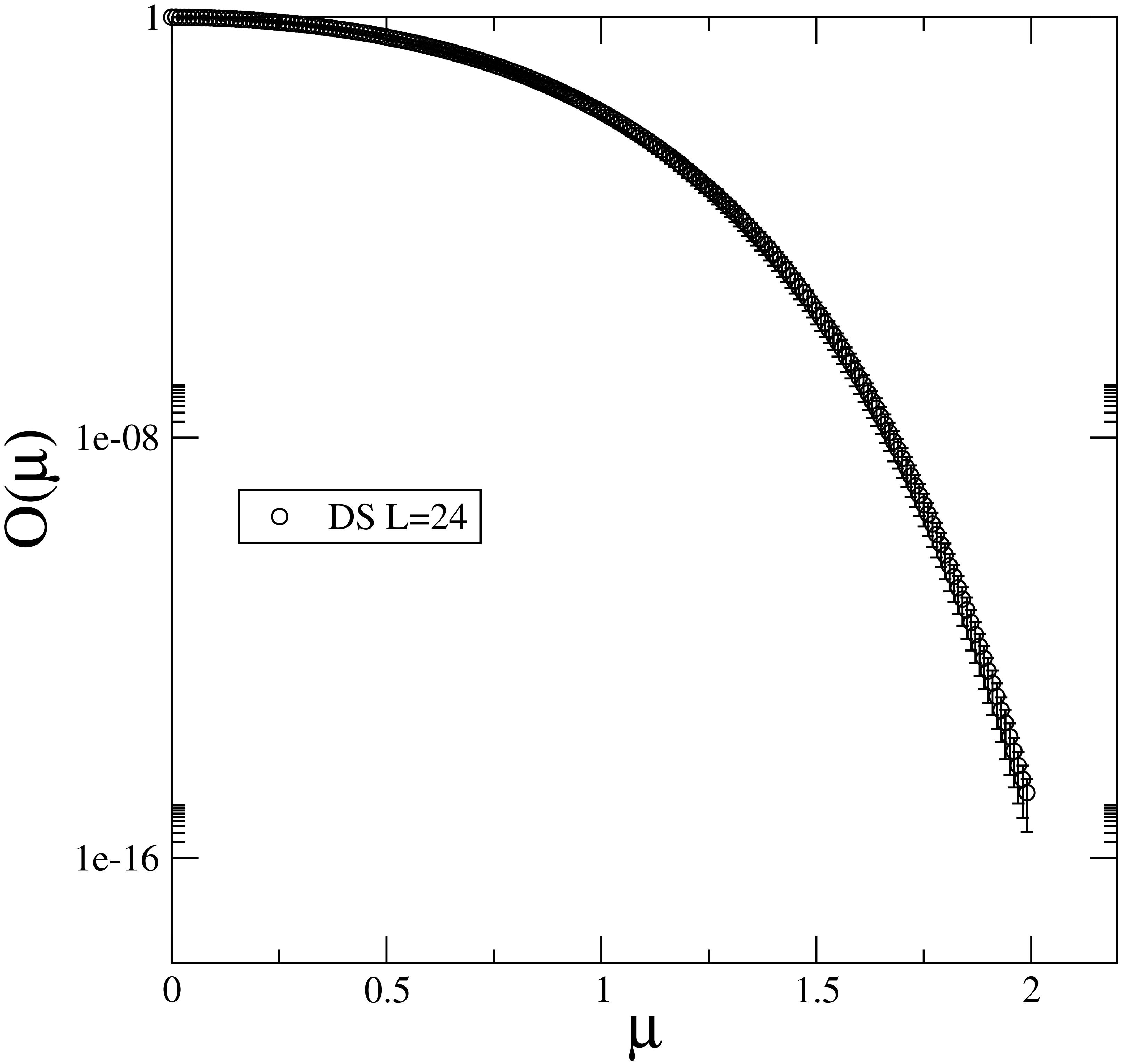
$P_\beta(s)$



Is this now good enough for Fourier transform?

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

Numerical results: Z3 gauge theory

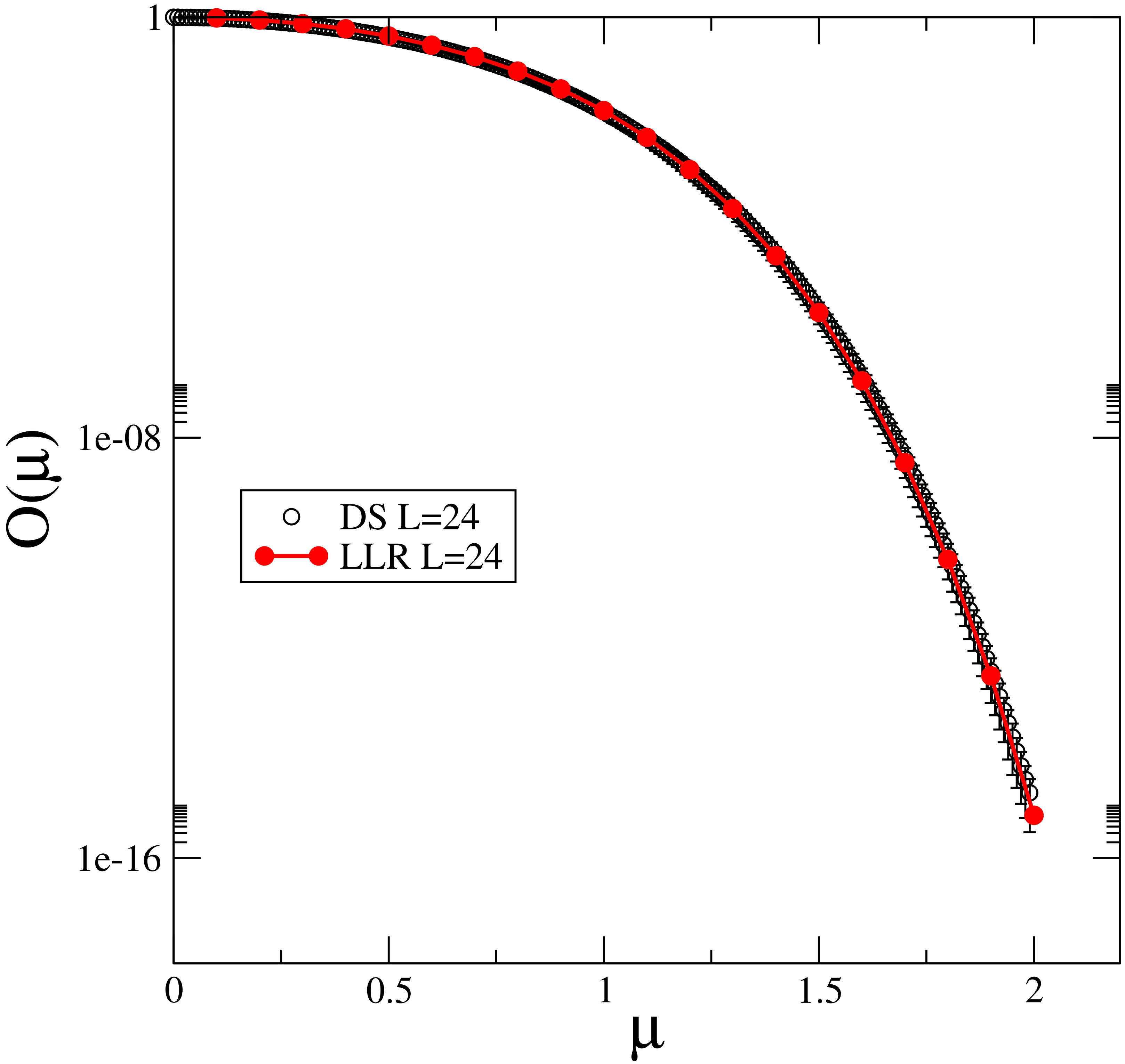


$$O(\mu) \;=\; \langle \mathrm{e}^{i\varphi} \rangle_{\mathrm{PQ}}$$

Result from the (real) dual theory: “snake algorithm”

←

Numerical results: Z3 gauge theory



$$O(\mu) \;=\; \langle \mathrm{e}^{i\varphi} \rangle_{\mathrm{PQ}}$$

Result from the (real) dual theory: “snake algorithm”

Excellent agreement!

First “head on” solution of a sign problem!

[Langfeld, Lucini, PRD9 (2014) 094502]

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

Starting point QCD:

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

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]

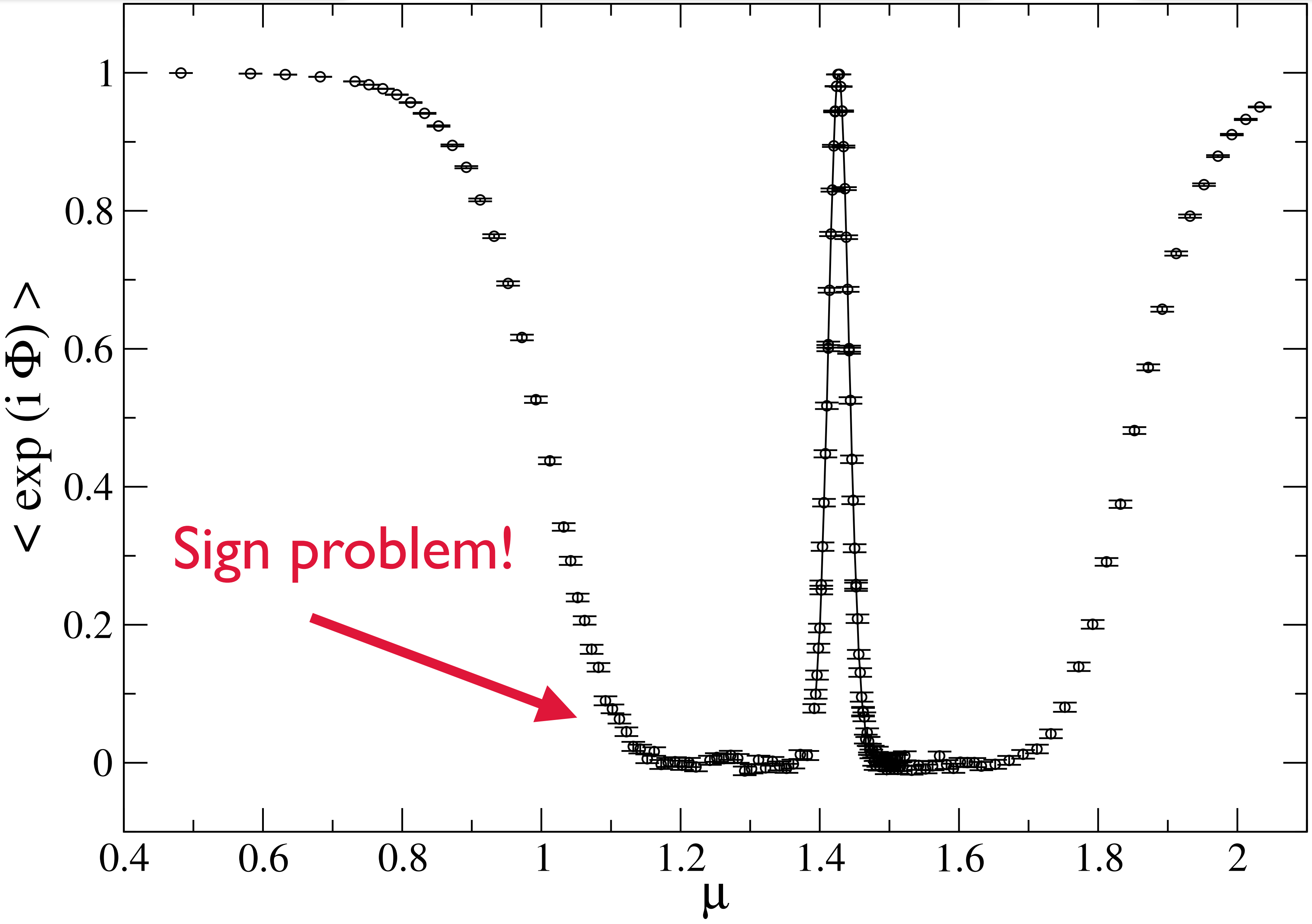
Heavy-dense QCD

[Garron, Langfeld, et al, in preparation]

low density

“half-filling”

saturation



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

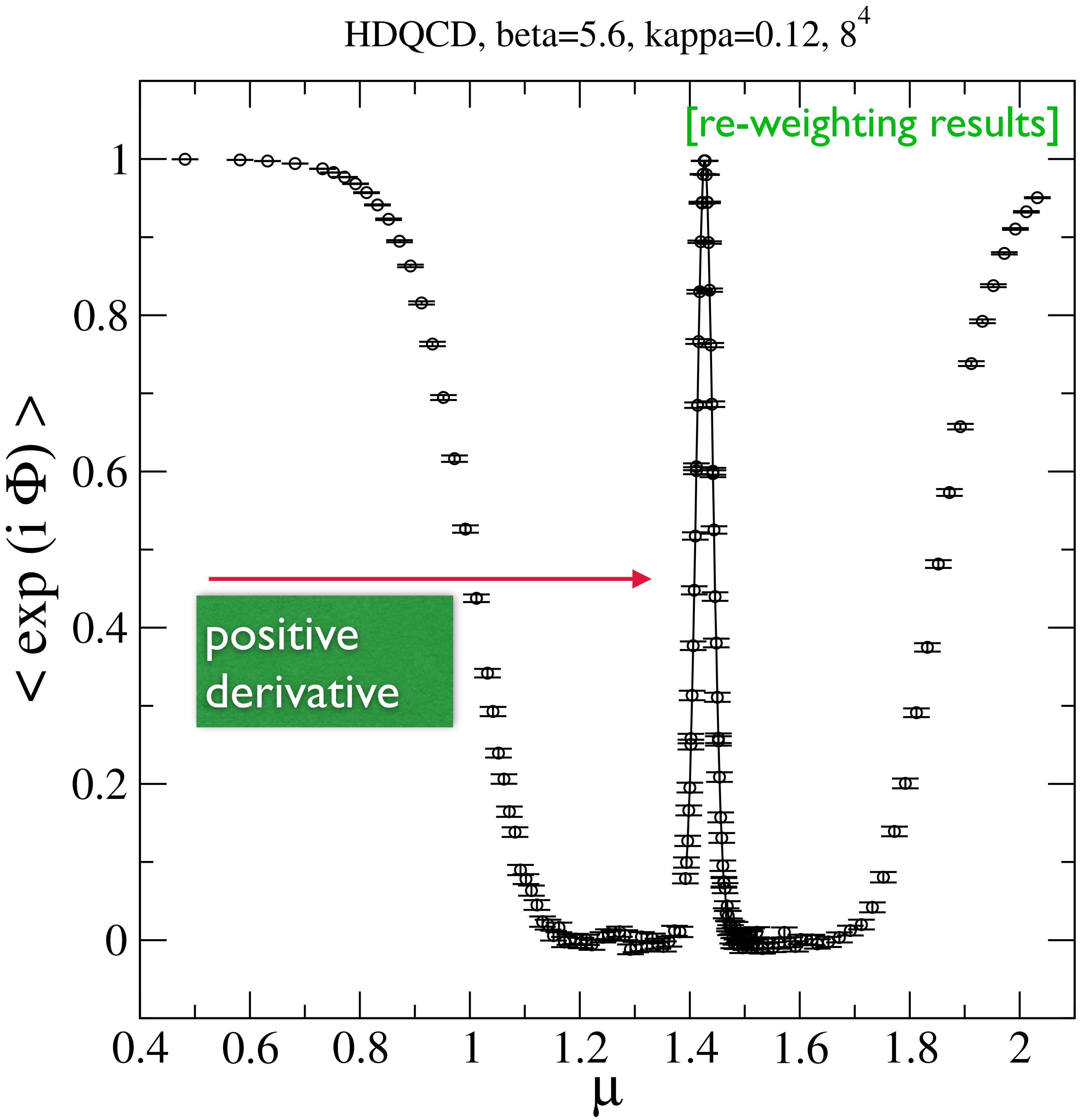
“half-filling”

$''\mu = m''$
(physical)

Is QCD real at threshold $\mu = m_B/3$?

Heavy-dense QCD

Inverse Silver Blaze feature



Recall:

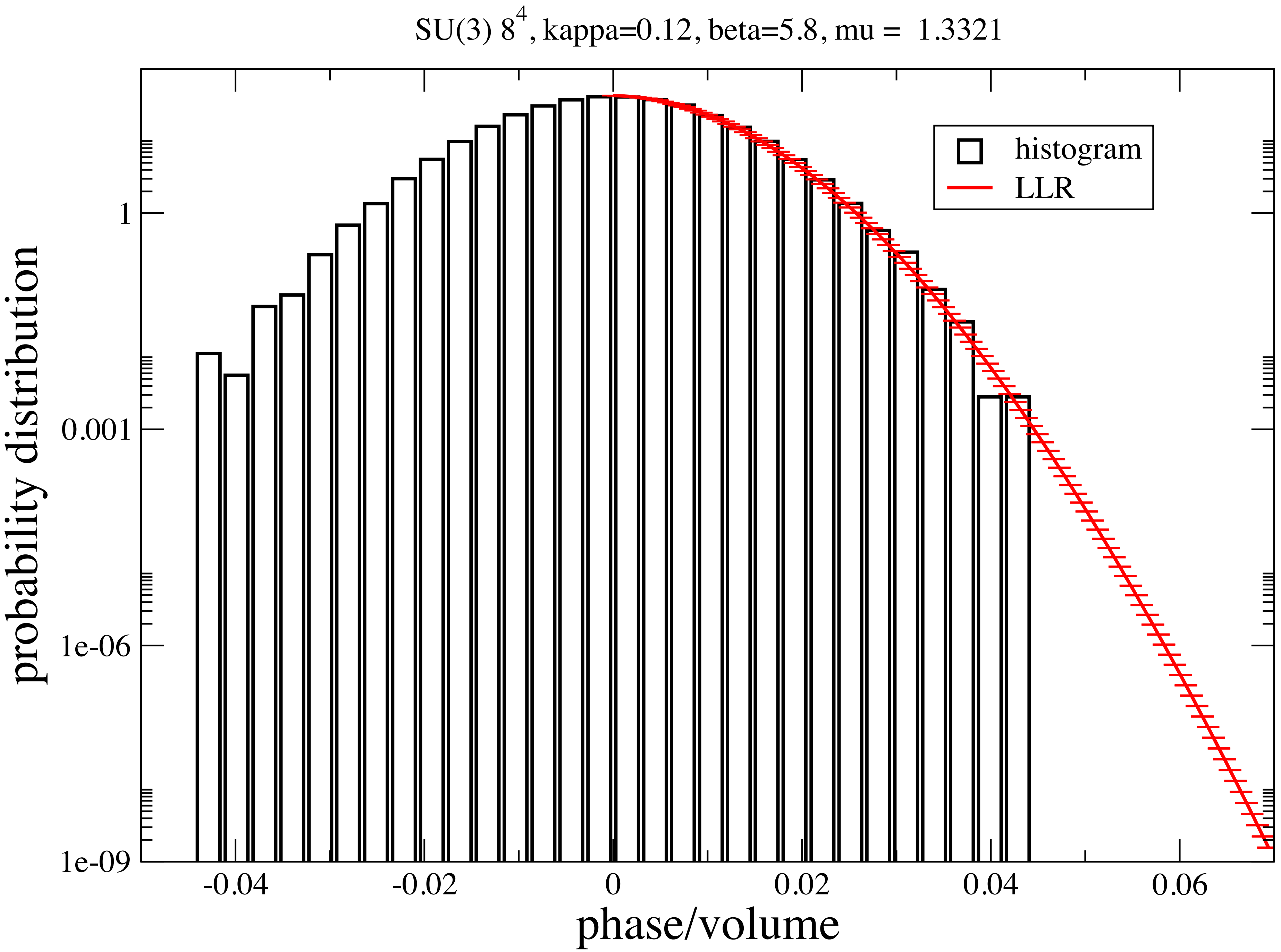
$$\rho(\mu) \;=\; \frac{T}{V_3}\,\frac{\partial}{\partial\mu}O(\mu) \;+\; \rho_{\rm PQ}(\mu)$$

Phase quenching *underestimates* the true density!

[Garron, Langfeld, et al, in preparation]

What can LLR do for you?

$\mu = 1.3321$



$P_\beta(s)$

LLR
exponential
error
suppression !

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 $p = 2, 4, 6, 8..$

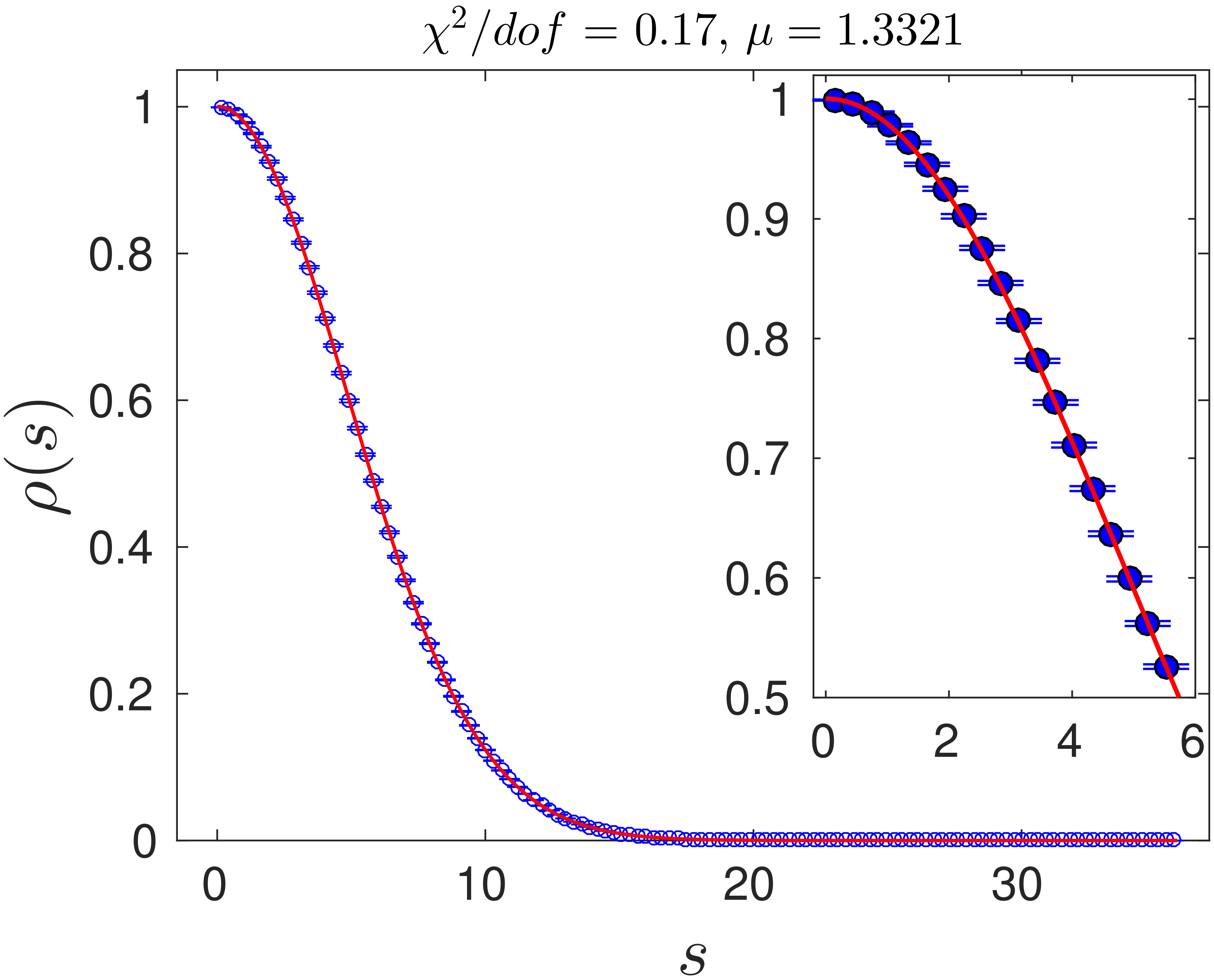
Calculate the Fourier transform semi-analytically

Compressed Sensing:

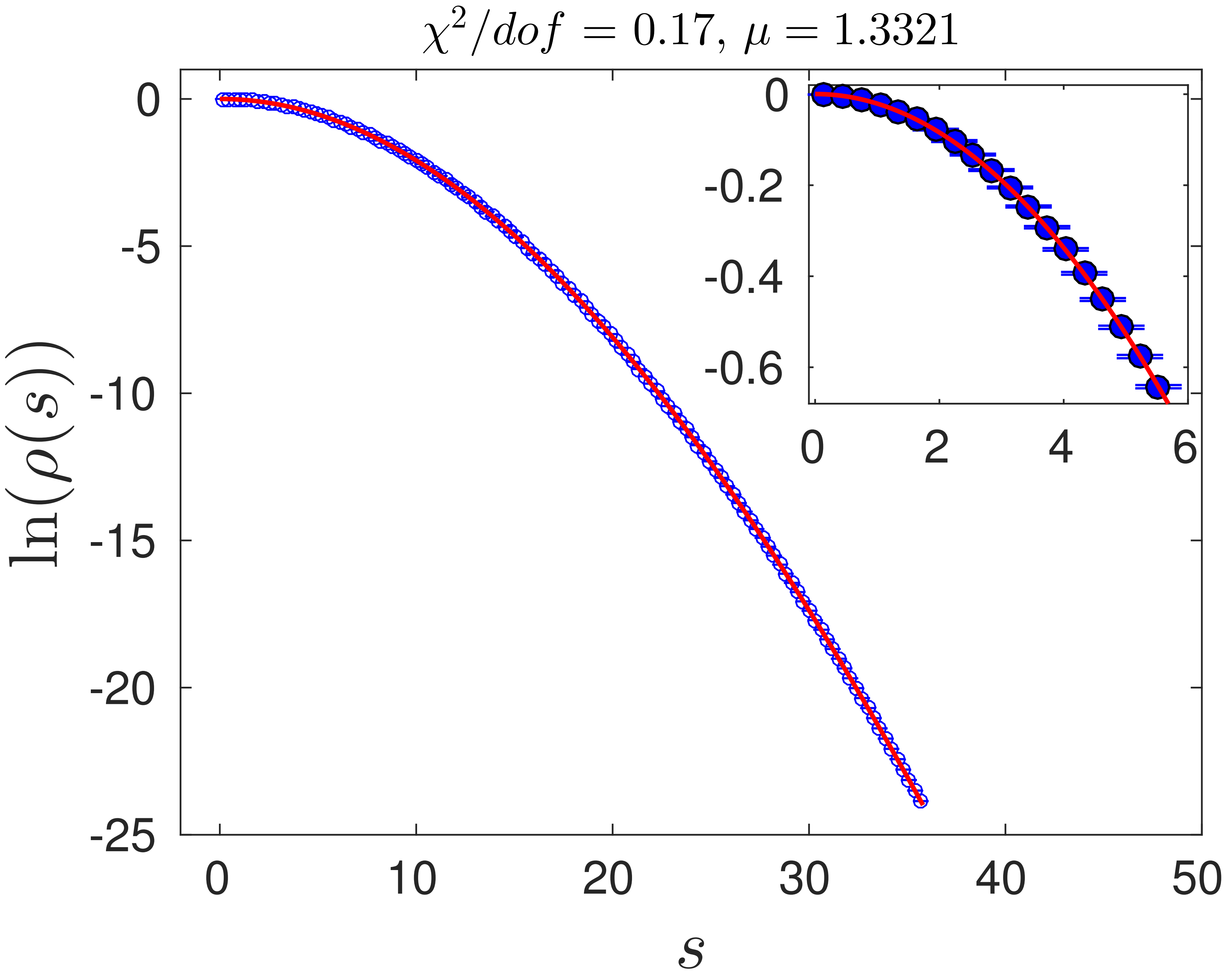
$\ln P(s)$ ~ 1000 data points $\Rightarrow$ c_i ~ 20 coefficients

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

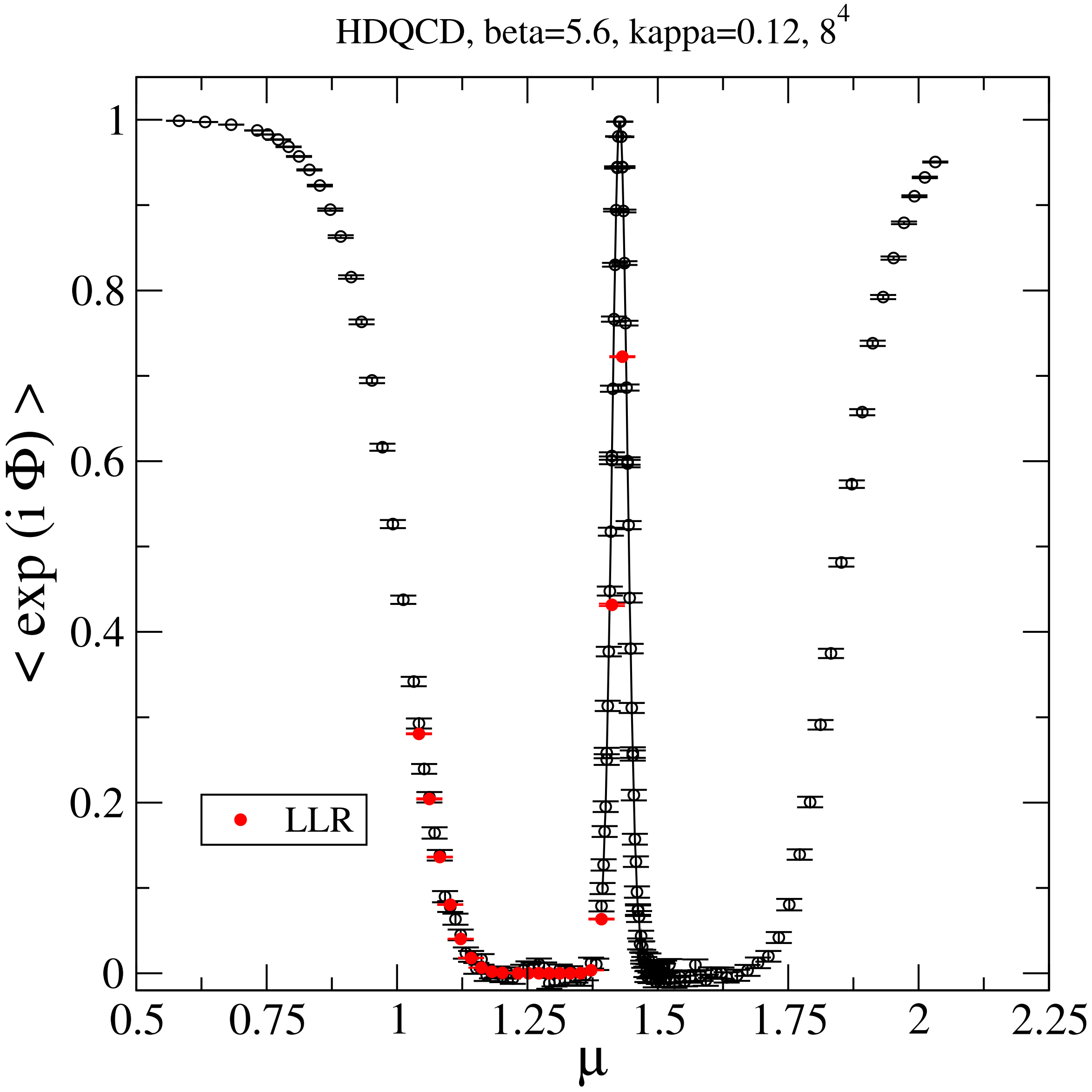
Works very well!

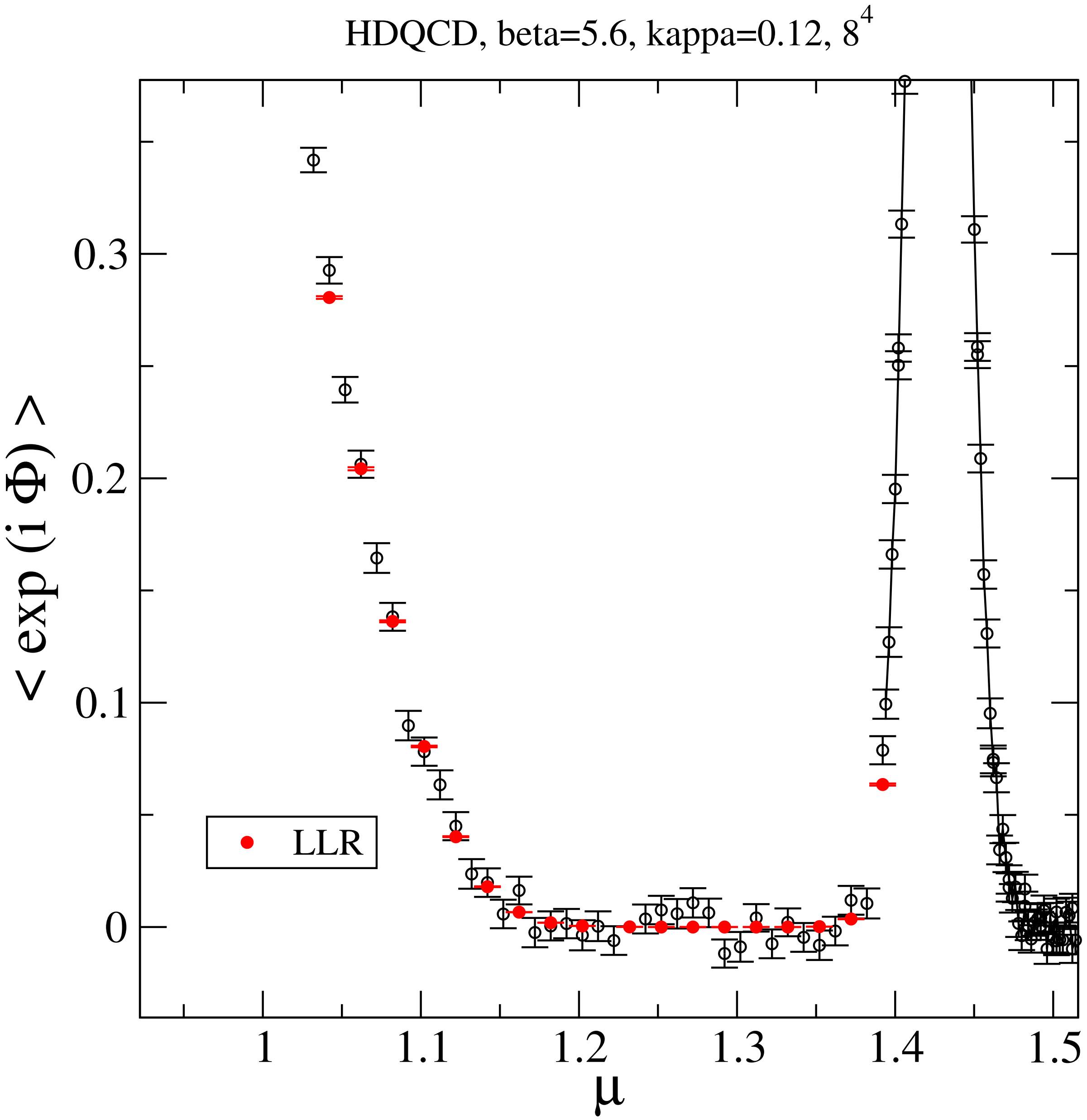


Works very well!



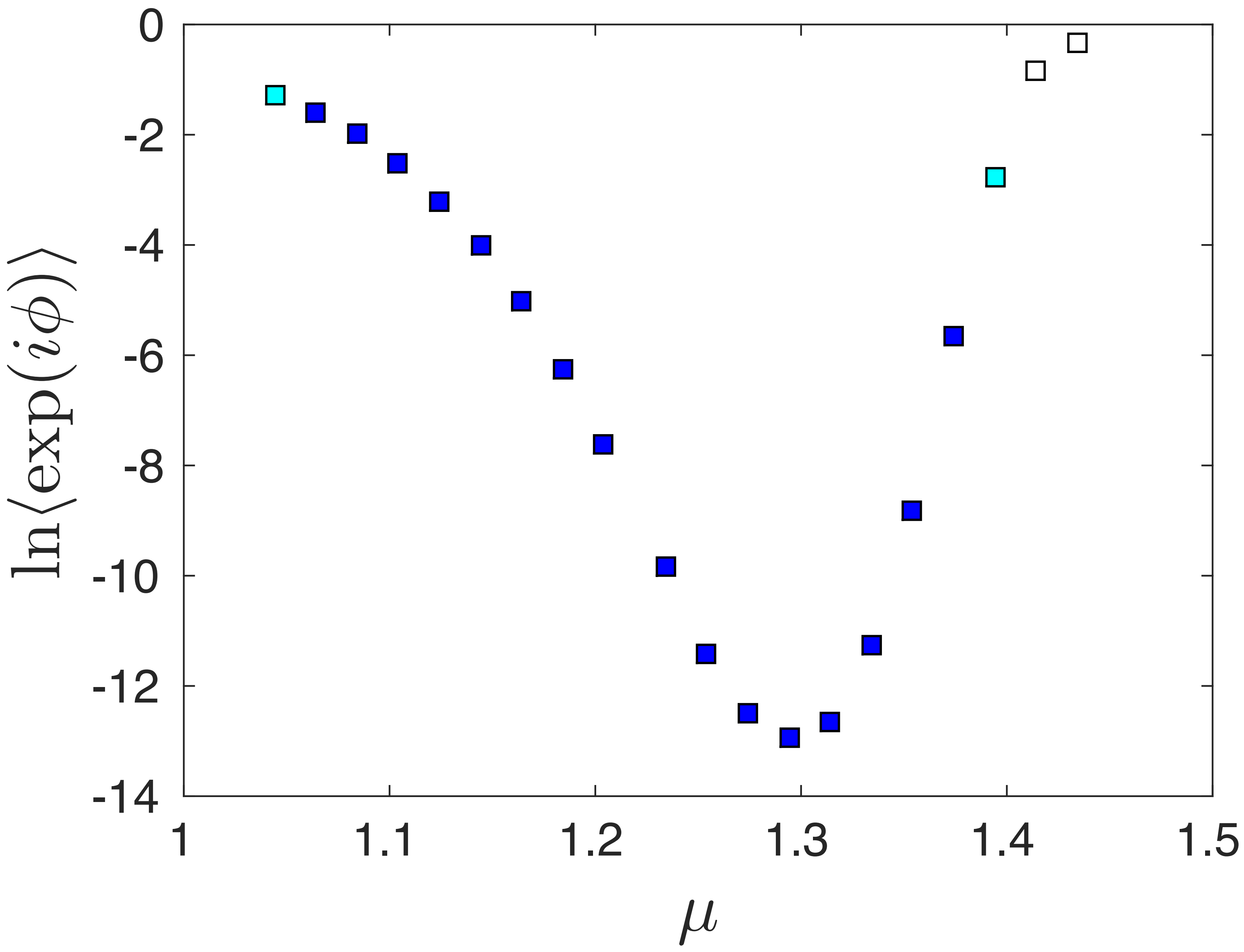
What can LLR do for you?





[Garron, Langfeld, et al, in preparation]

What can LLR do for you?

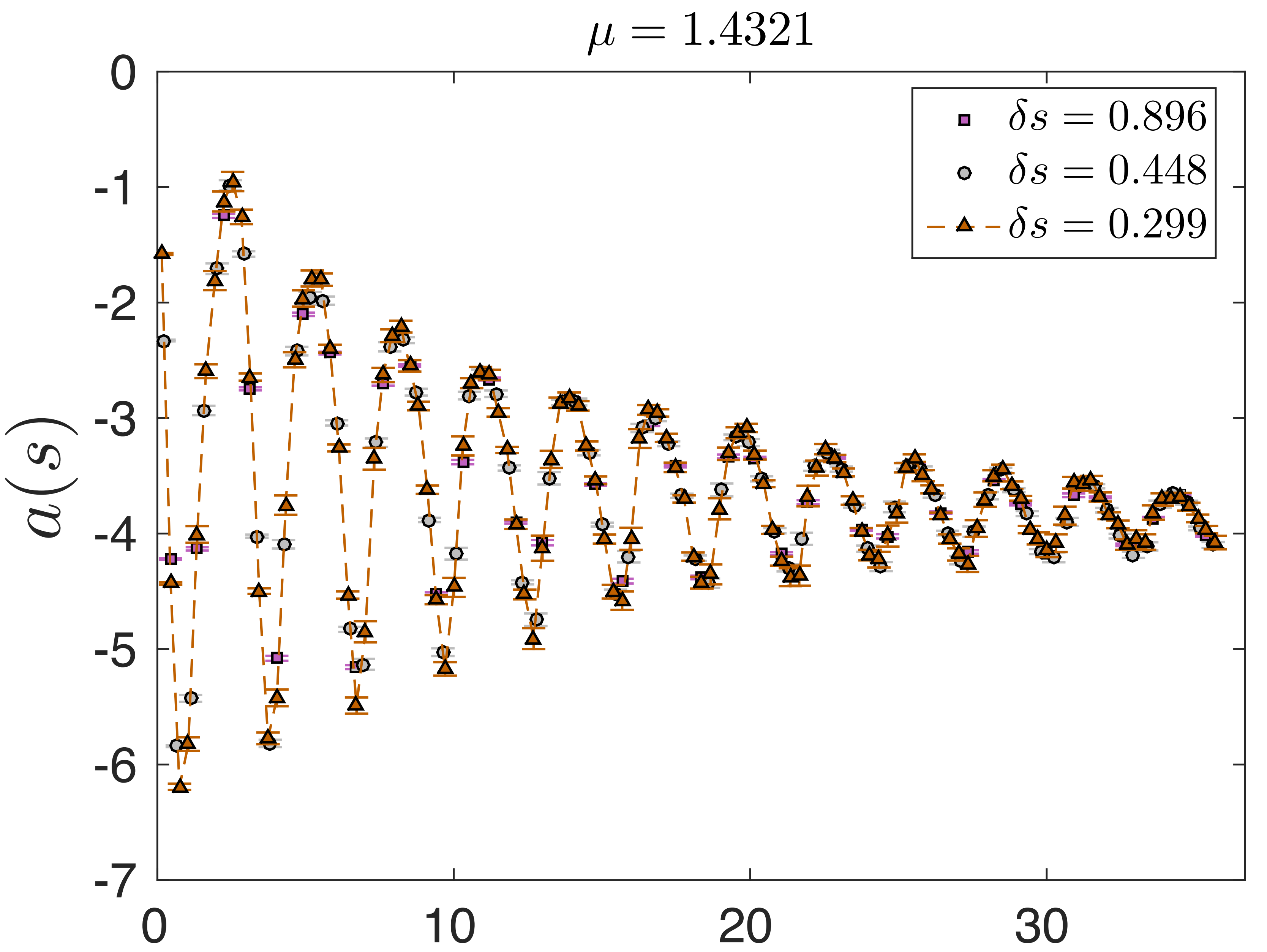


Our final result for the Overlap in HDQCD

[Garron, Langfeld, et al, in preparation]

And some surprises…

…close to onset $\mu \lesssim m$



s imaginary part of Det

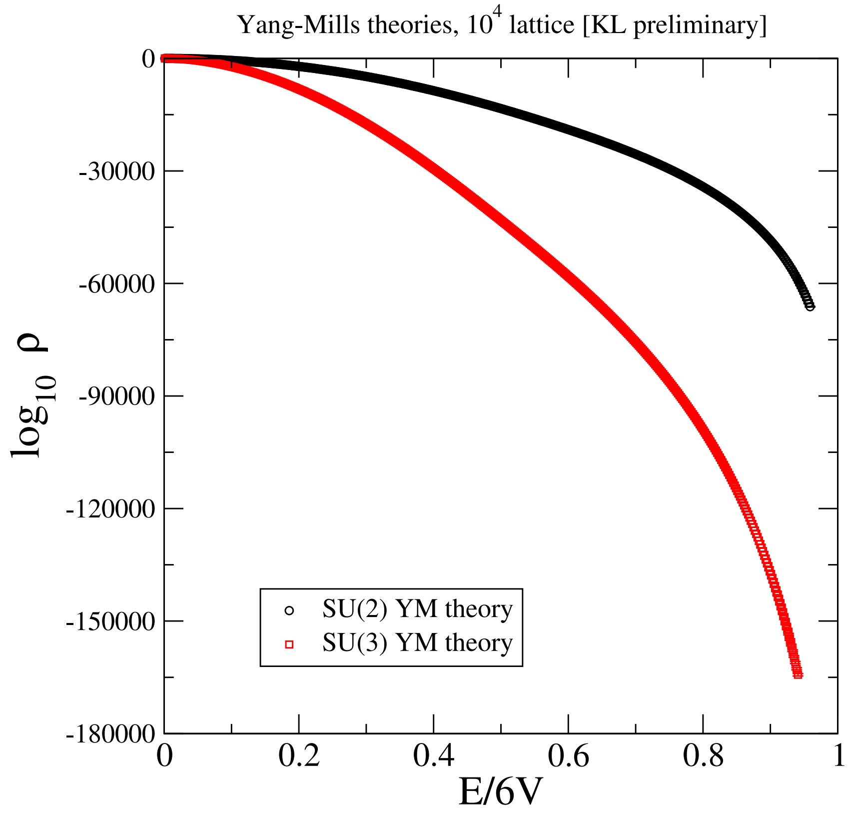
LLR coefficient:

$$a(s) = \frac{d \ln \rho(s)}{ds}$$

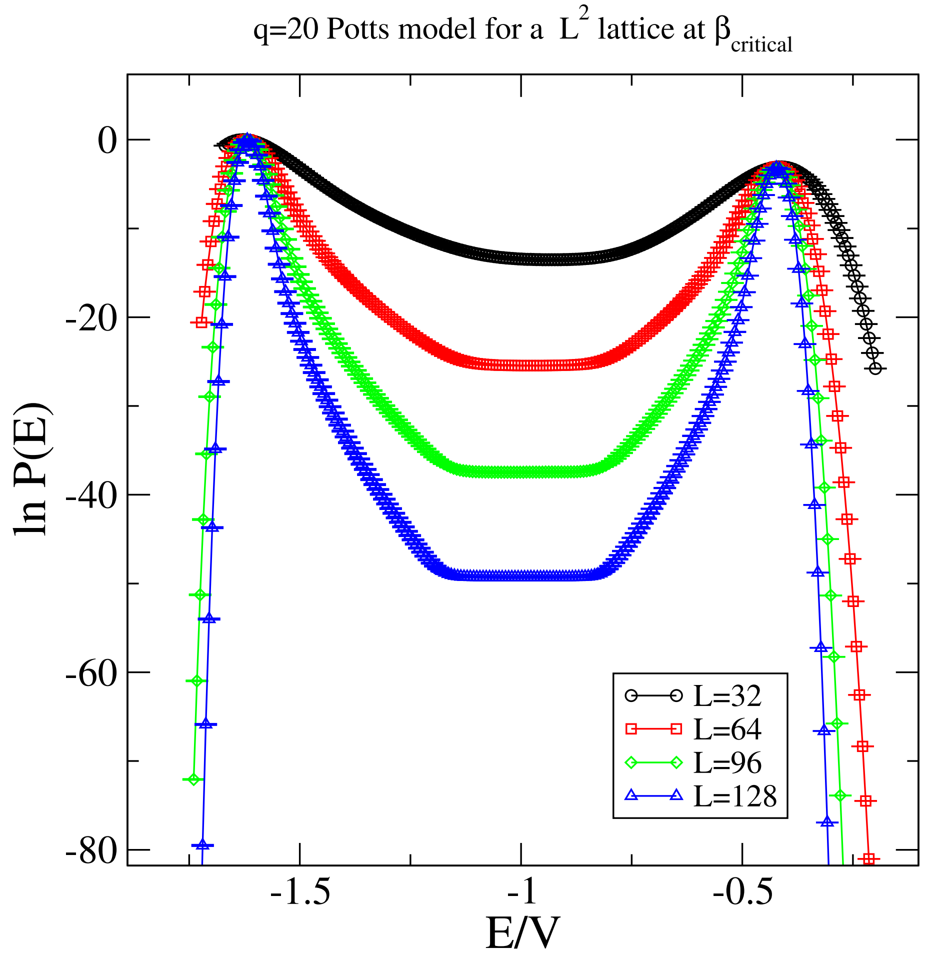
[Garron, Langfeld, et al, in preparation]

Summary:

What is the LLR approach?



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



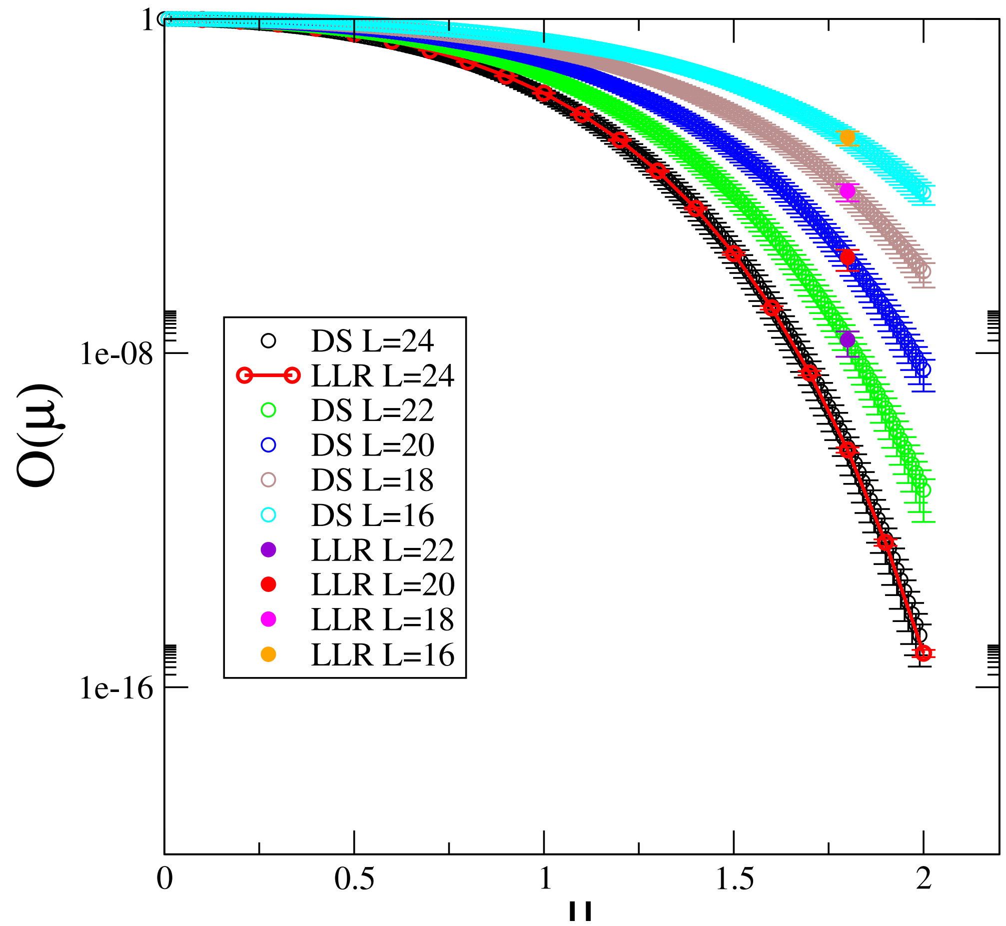
Non-Markovian process (does not rely on importance sampling)

$\Rightarrow$ solves overlap problems

Summary:

Can solve *strong sign problems*:

Z3 gauge theory at finite densities
HD QCD



Open questions:

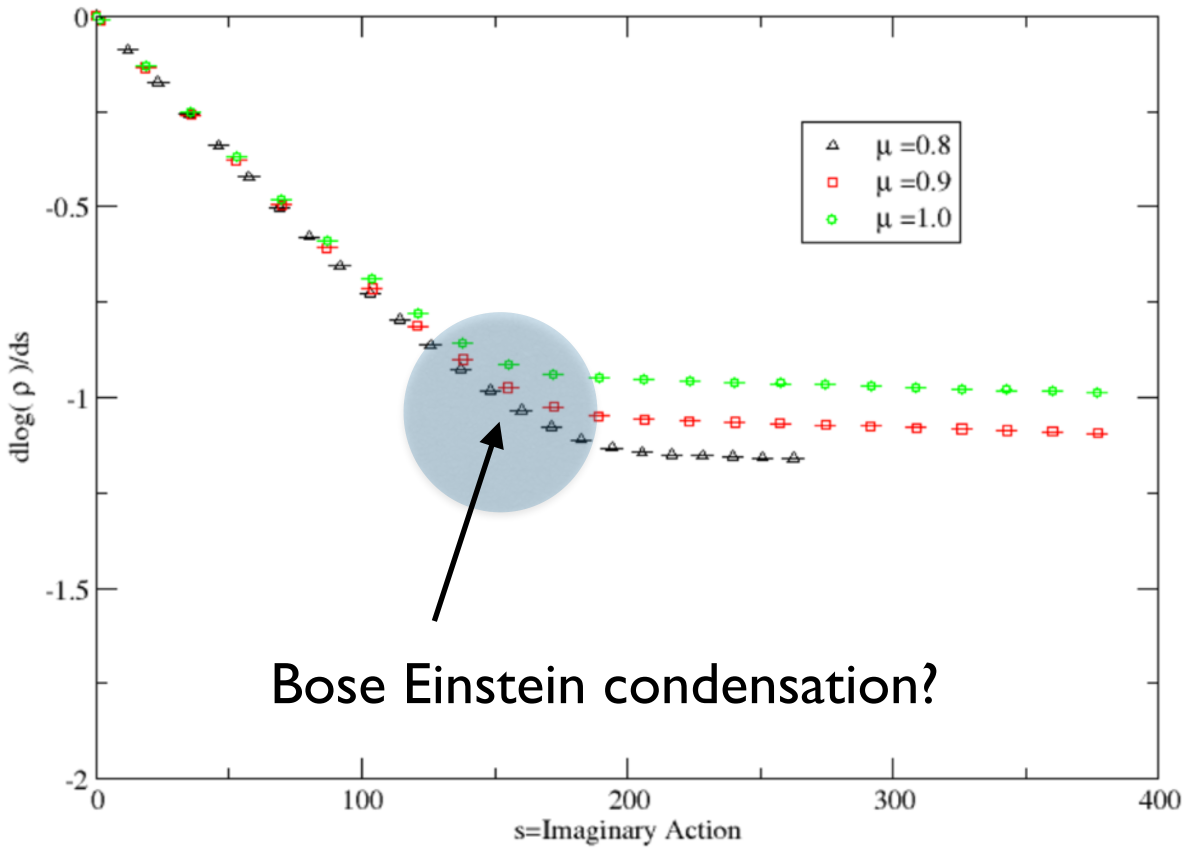
Hinges on the ability to "compress information"

$\ln P(s)$ ~ 1000 data points

$\Rightarrow$ c_i ~ 24 coefficients

difficult for ϕ^4 theory!

[Bongiovanni, Langfeld, Lucini, Pellegrini, Rago, Lattice 2015]



Bose Einstein condensation?

Conclusion:

Promising first results for finite density QFT!

More new ideas for "compressing information" is needed (FT)

Thank you!