The density-of-states approach for dense matter Monte-Carlo simulations

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with:

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Roberto Pellegrini, Turin — *Jan Pawlowski, Heidelberg*

Overlap and Sign Problems

- Consider a theory with complex action:

$$Z(\mu) \;=\; \int \mathcal{D}\phi \, \exp\{i\mu S_I[\phi]\} \; \exp\{S_R[\phi,\mu]\}$$

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- Let us *drop* it:

$$Z_{\rm mod}(\mu) \;=\; \int \mathcal{D}\phi \;\exp\{S_R[\phi,\mu]\}$$

- How big is the error?
  $\Rightarrow$ apparently small for small chemical potential μ

Overlap and Sign Problems

- Quantifying the problem:

  We have: $Z(\mu), \; Z_{\rm mod}(\mu) \; > \; 0$

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- Density:

$$\rho(\mu) \; = \; \Delta\rho(\mu) \; + \; \rho_{\rm mod}(\mu) \; ,$$

$\rho \; = \; \frac{1}{V} \, \frac{d}{d\mu} \, \ln Z(\mu)$: full density

$\Delta\rho \; = \; \frac{1}{V} \, \frac{d}{d\mu} \, \ln O(\mu)$: overlap contribution

$\rho_{\rm mod} \; = \; \frac{1}{V} \, \frac{d}{d\mu} \, \ln \, Z_{\rm mod}(\mu)$: easy to calculate

Overlap and Sign Problems

- How important is the overlap $O(\mu)$? [physics grounds]
  $|\det_\mu[U]|^2 = \det_\mu[U] \det_{-\mu}[U]$
  acts like a isospin chemical potential! $\Rightarrow$ π-condensate

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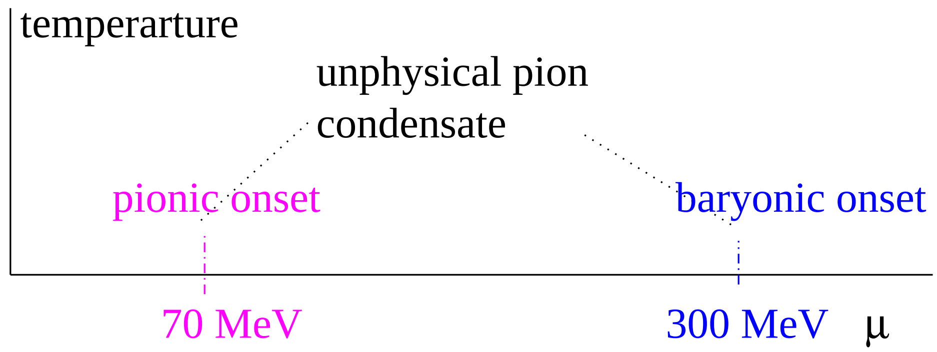
- **Impact -**
  Pions condense for $\mu \approx 70$ MeV
  $O(\mu)$ needs to remove pion condensation
  and provide a density of baryons for
  $\mu \approx 300$ MeV



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  $O(\mu) \to 1$ for $\mu \to 0$

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  F : free energy, Δf : difference in free energy density

$$O(\mu) = \exp\{-[F(\mu) - F_{\text{mod}}(\mu)]\} = \exp\{-\Delta f \; V\} \ll 1$$

V : volume

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- The density-of-states approach (LLR-algorithm)
  [Langfeld, Lucini, Rago, PRL 109 (2012) 111601]

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  [aiming at a *universal* solution]

- Cons: $\triangle$ does it work?
  [need an *exponential* error suppression]

- LLR-algorithm has all prerequisites...
  [Langfeld, Lucini, Rago, PRL 109 (2012) 111601]
  $\Rightarrow$ generically solves overlap problems
  but is it good enough? [potentially theory dependent]

The density of states - SU(3) versus SU(2)

- Definition:

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

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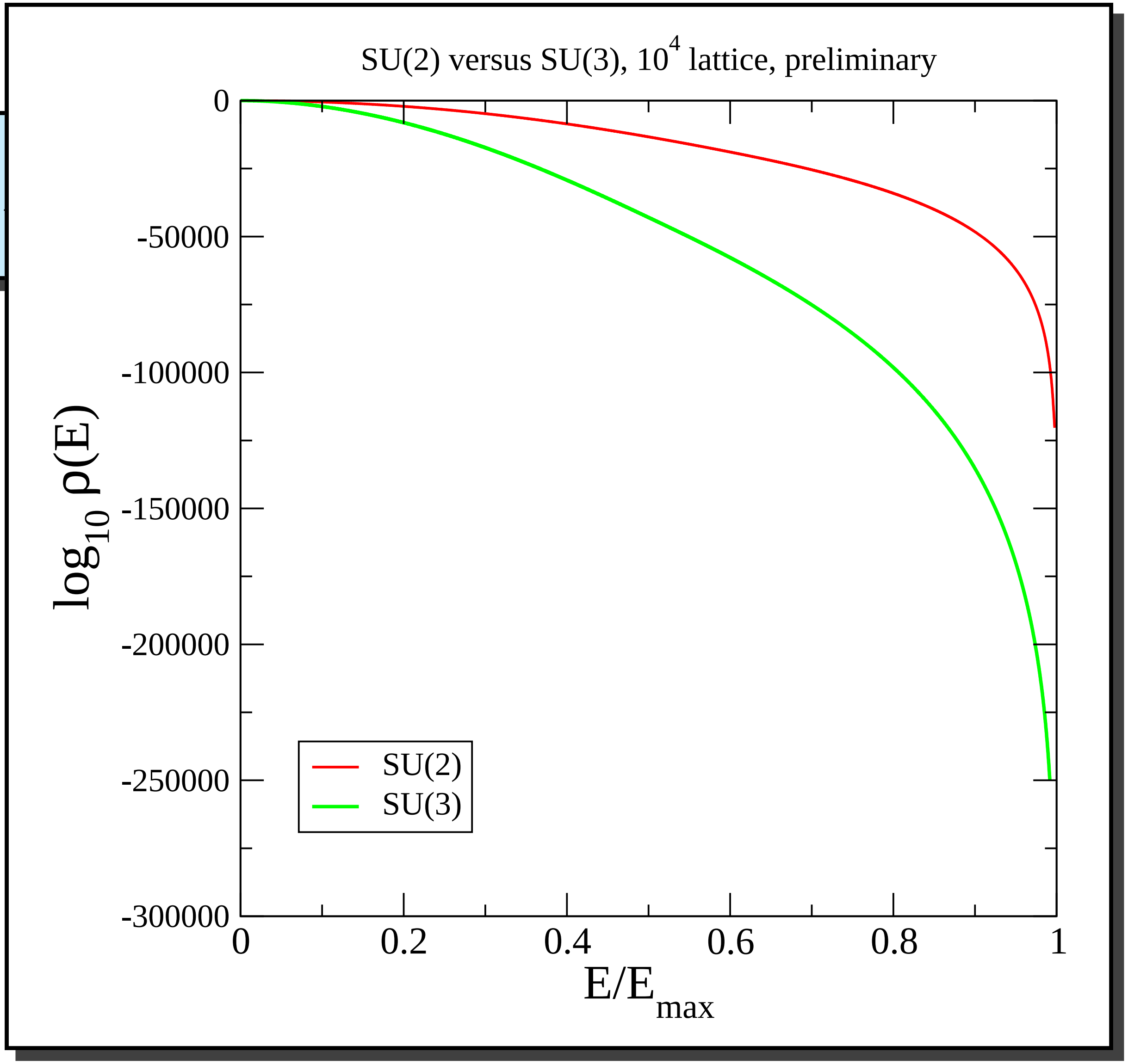

The density of states - compact U(1)

- study phase transition in U(1):

△ weakly first order
[Arnold, Bunk, Lippert, Schilling, Nucl.Proc.Proc.Suppl. 119 (2003) 119]

△ $P_\beta(E) = \rho(E)\exp\{\beta E\}$

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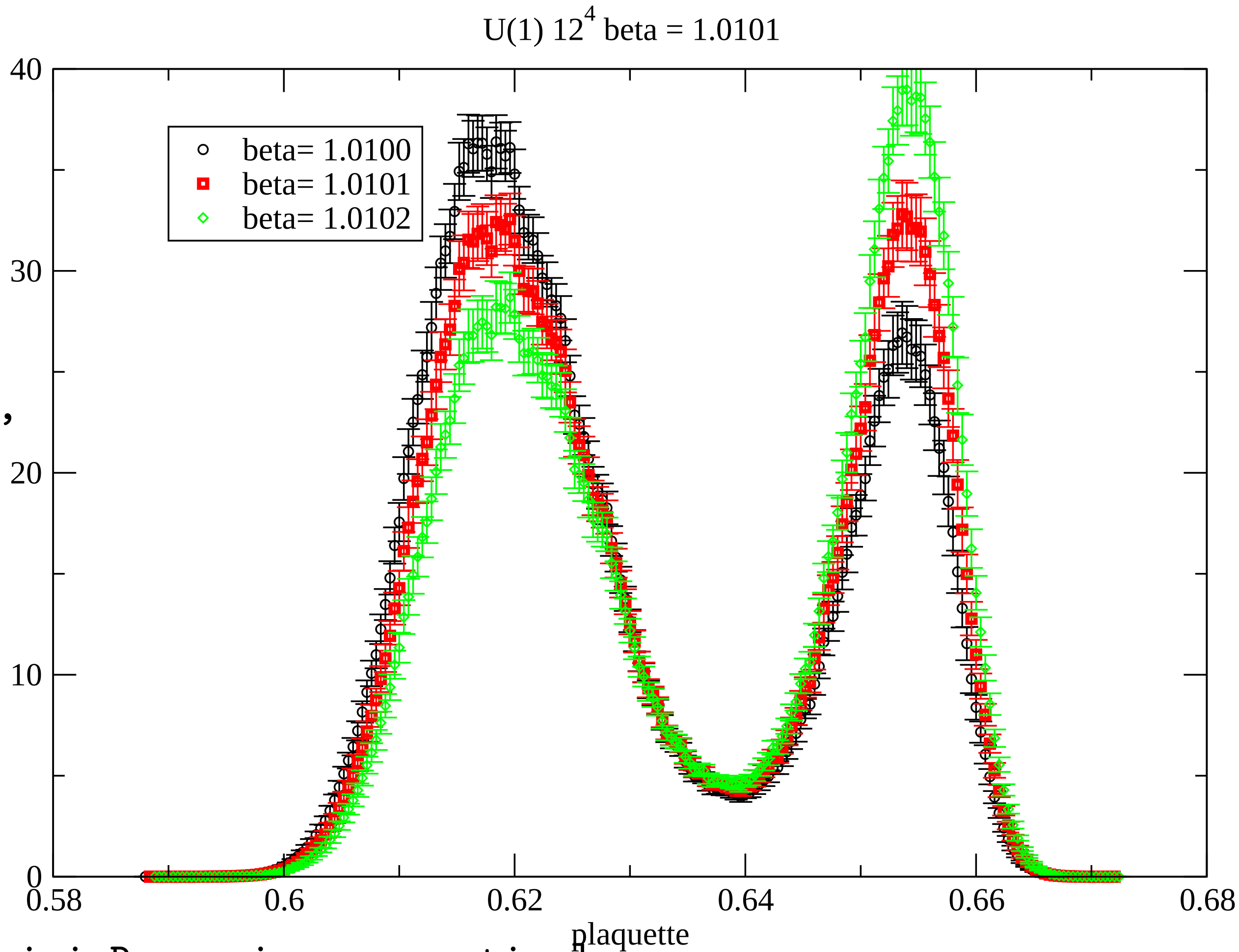

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`[benchmark testing!]`

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⇒ needs to be "solvable" by `standard techniques`

`[benchmark testing!]`

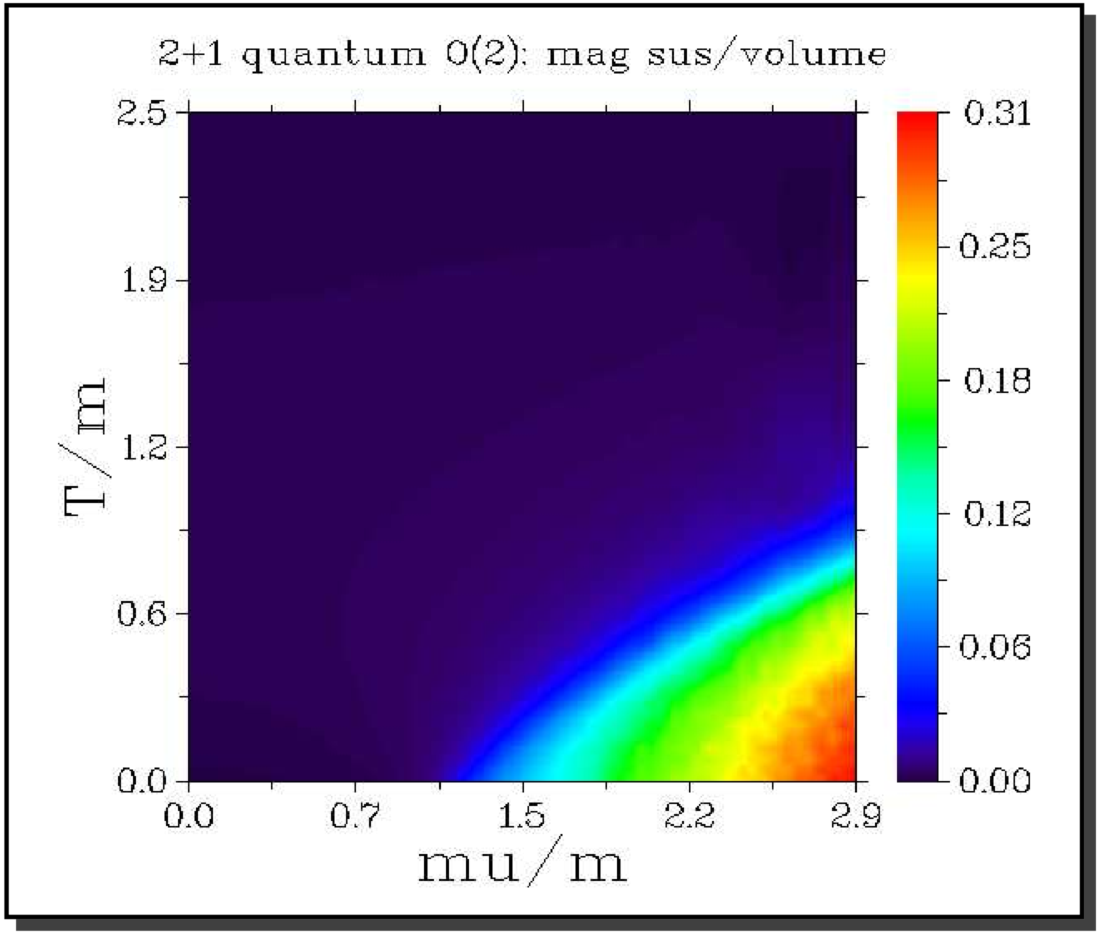
...choose a theory that admits dualisation

`worm algorithm!`

`[Prokof'ev, Svistuno, 2001] [Chandrasekharan 2010] [Gattringer, Evertz, 2011]`

The quantum O(2) model:

Results - phase diagram



quantum : scaling limit of the 2nd order transition

m : mass gap

mu : chemical potential

T : temperature

superfluidity!

in the cold, but dense regime

[KL, PRD D87 (2013) 114504]

The Z(3) Polyakov spin model:

Theory - degrees of freedom: $P(x) \in Z_3$

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

τ : "temperature"

$\eta = \kappa \; \exp(\mu)$

$\bar{\eta} = \kappa \; \exp(-\mu)$

$\Rightarrow$ solvable by a **worm** algorithm

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

The Z(3) Polyakov spin model:

Theory - c

$S[P] =$

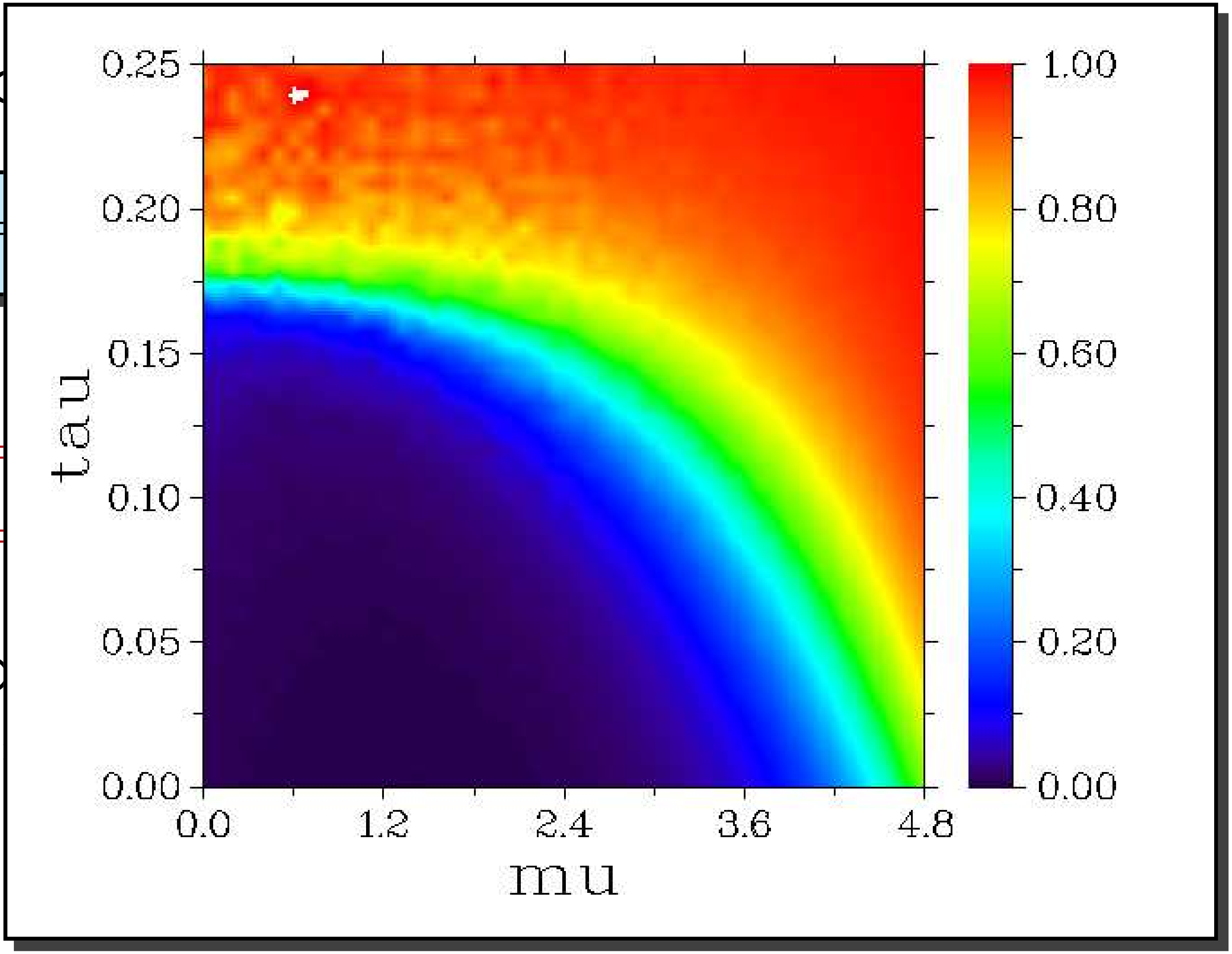
τ :

$\eta =$

$\bar{\eta} =$

$\Rightarrow$ solv

[Delago Me



$\Rightarrow$ **close to QCD, easier: LLR for discrete variables**

$\Rightarrow$ `my choice here!` `...thanks to Ydalia and Christof!`

The Z(3) Polyakov spin model:

- How **strong** is the sign problem?

  Study the overlap factor:

  $$O(\mu) := \frac{Z(\mu)}{Z_{\text{mod}}(\mu)}$$

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- Use the **snake algorithm**:

$$\frac{Z(\mu+\Delta\mu)}{Z(\mu)} = \langle \exp\{S(\mu+\Delta\mu) - S(\mu)\}\rangle_\mu \, .$$

$$Z(5\Delta\mu) = \frac{Z(5\Delta\mu)}{Z(4\Delta\mu)} \frac{Z(4\Delta\mu)}{Z(3\Delta\mu)} \frac{Z(3\Delta\mu)}{Z(2\Delta\mu)} \frac{Z(2\Delta\mu)}{Z(\Delta\mu)} \frac{Z(\Delta\mu)}{Z(0)} Z(0)$$

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- need to caculate $Z(\mu)$ **and** $Z_{\rm mod}(\mu)$

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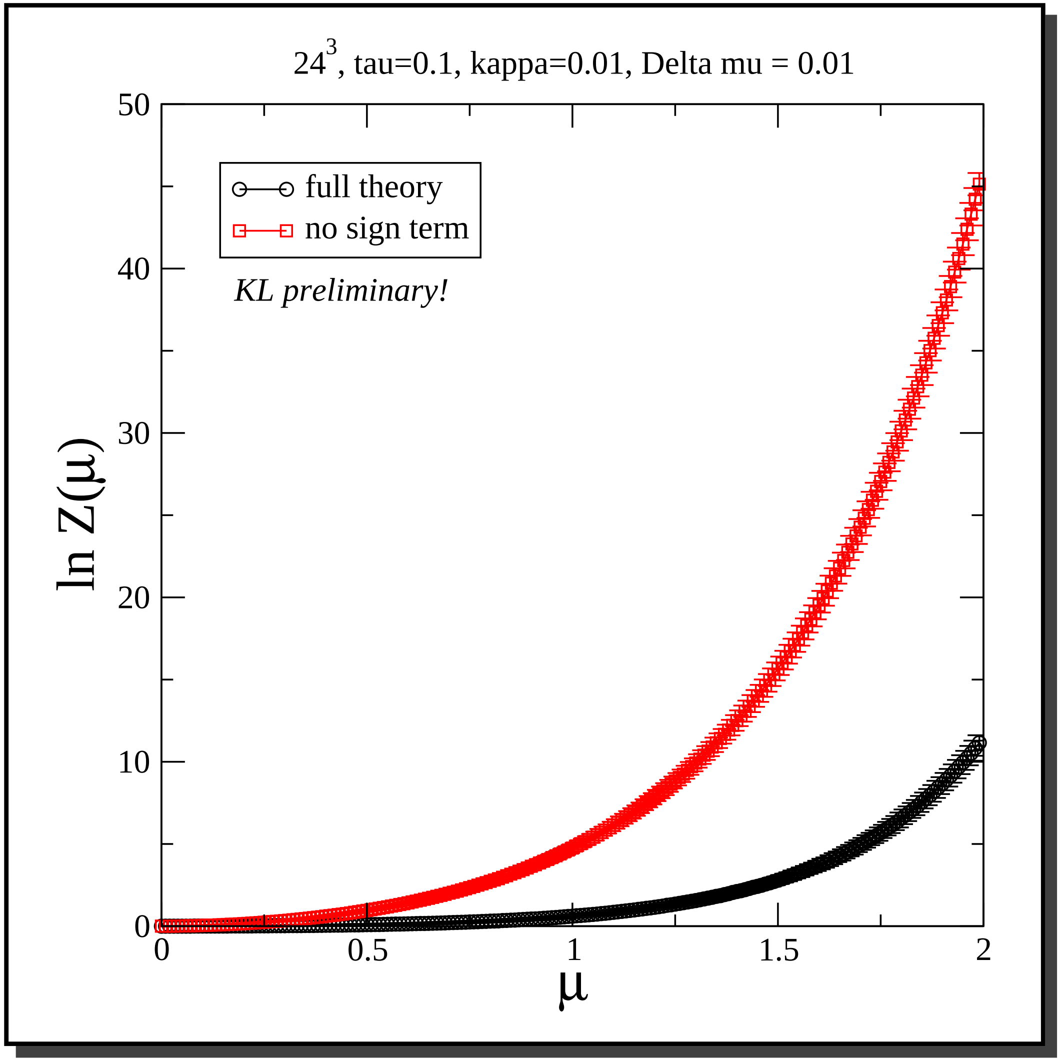

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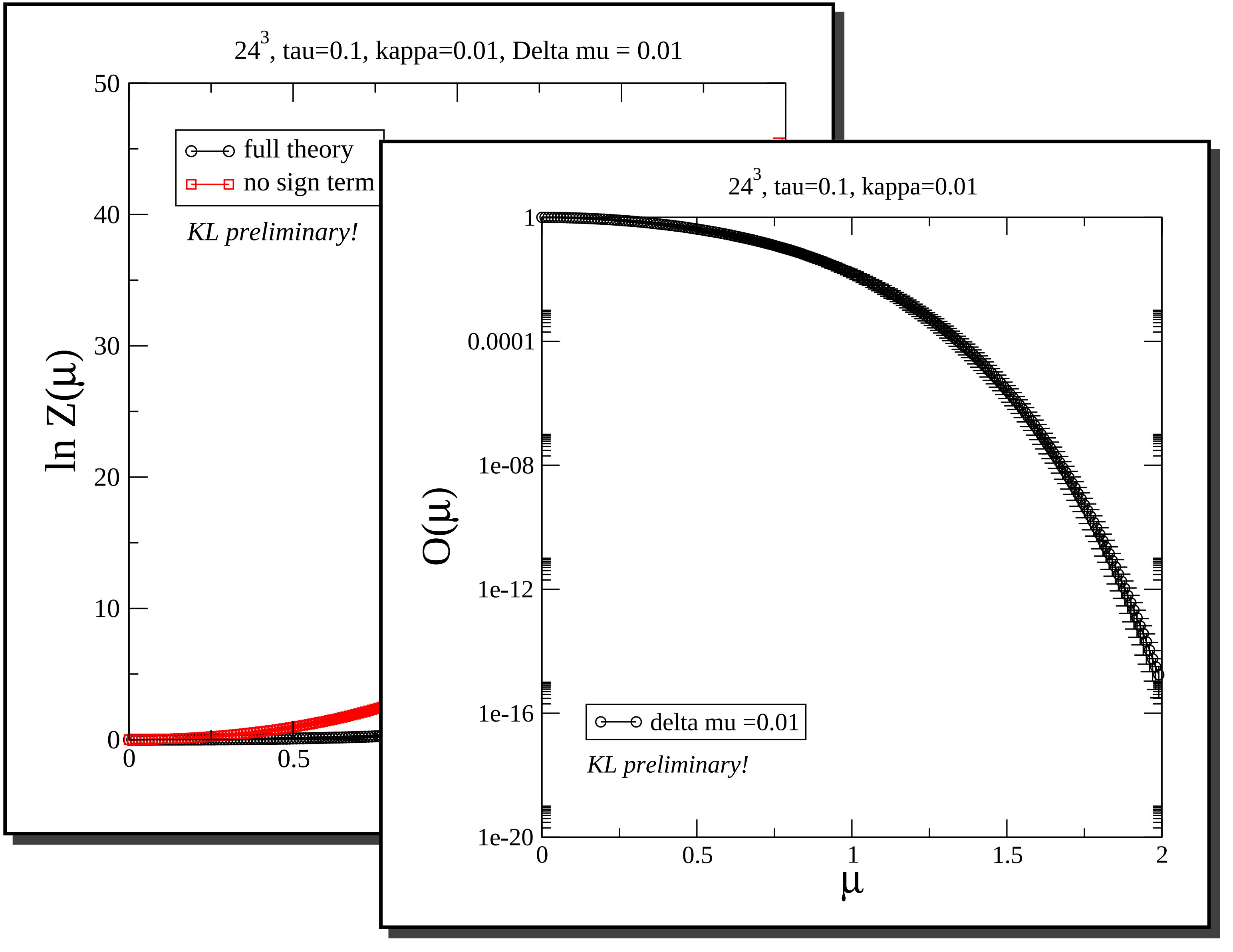

The Z(3) Polyakov spin model:

- A bit of theory:

$$P \in Z_3 : \quad P = \exp\{i \frac{2\pi}{3} m\}$$

$$P \ \in \ \{1, (-1 + i\sqrt{3})/2, (-1 - i\sqrt{3})/2\}.$$

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- The imaginary part of the action:

$$\sum_x \Big(\mathrm{e}^{\mu} P(x) + \mathrm{e}^{-\mu} P^*(x) \Big) \; = \; (3 N_0 - V) \; \cosh(\mu) \; + \; i \, \sqrt{3} \, \sinh(\mu) \, \Delta N$$

N_0 : number with $P = 1$

N_+ : number with $P = (-1 + i\sqrt{3})/2$

N_- : number with $P = (-1 - i\sqrt{3})/2$

$\Delta N = N_+ - N_-$

$V = N_0 + N_+ + N_-$: volume

The Z(3) Polyakov spin model:

- **Introduce -** generalised `density-of-states:`

$$R(s) \;=\; \int \mathcal{D}P \; \delta\Big(s - \Delta N\Big) \; \exp\{S_R[P,\mu]\} \; .$$

symmetries: $R(s) = R(-s)$

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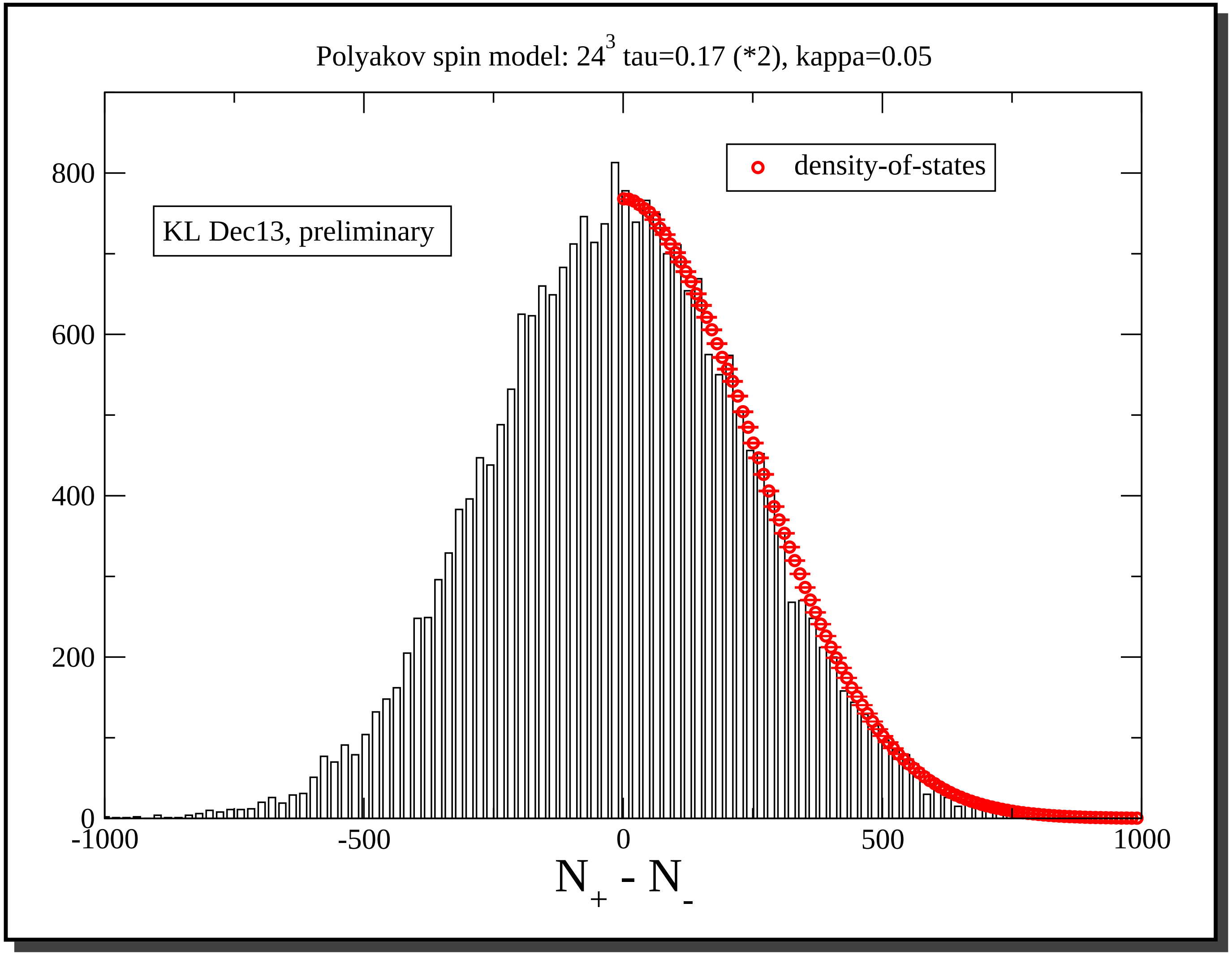
- **Overlap factor:**

$$O(\mu) \;=\; \int ds \; R(s) \; \cos\Big(\sqrt{3}\,\sinh(\mu)\; s\Big) \; / \; \int ds \; R(s)$$

`[no need to calculate the normalisation of` R`]`

The Z(3) Polyakov spin model:

- **Results:** histogram versus `density-of-states` method



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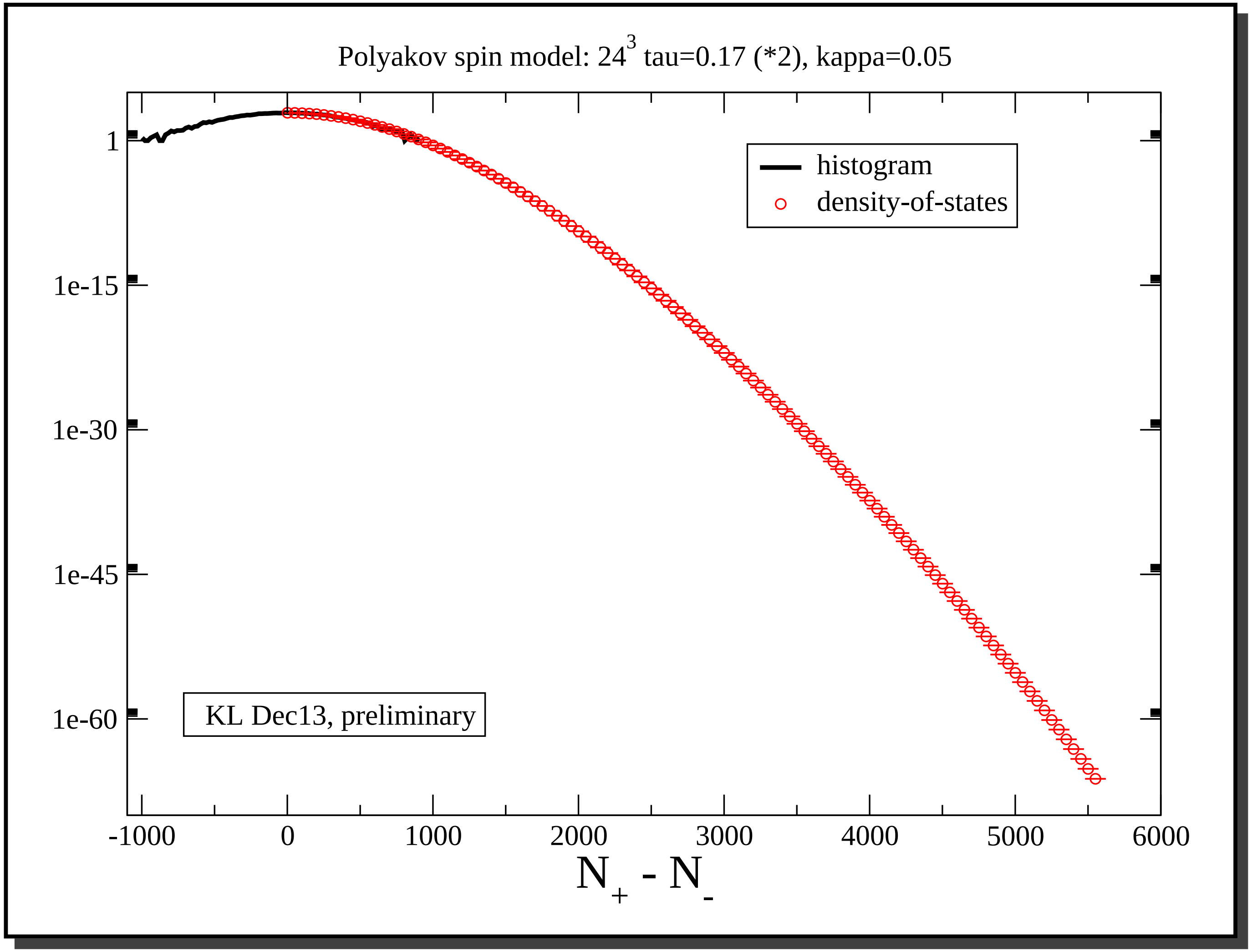

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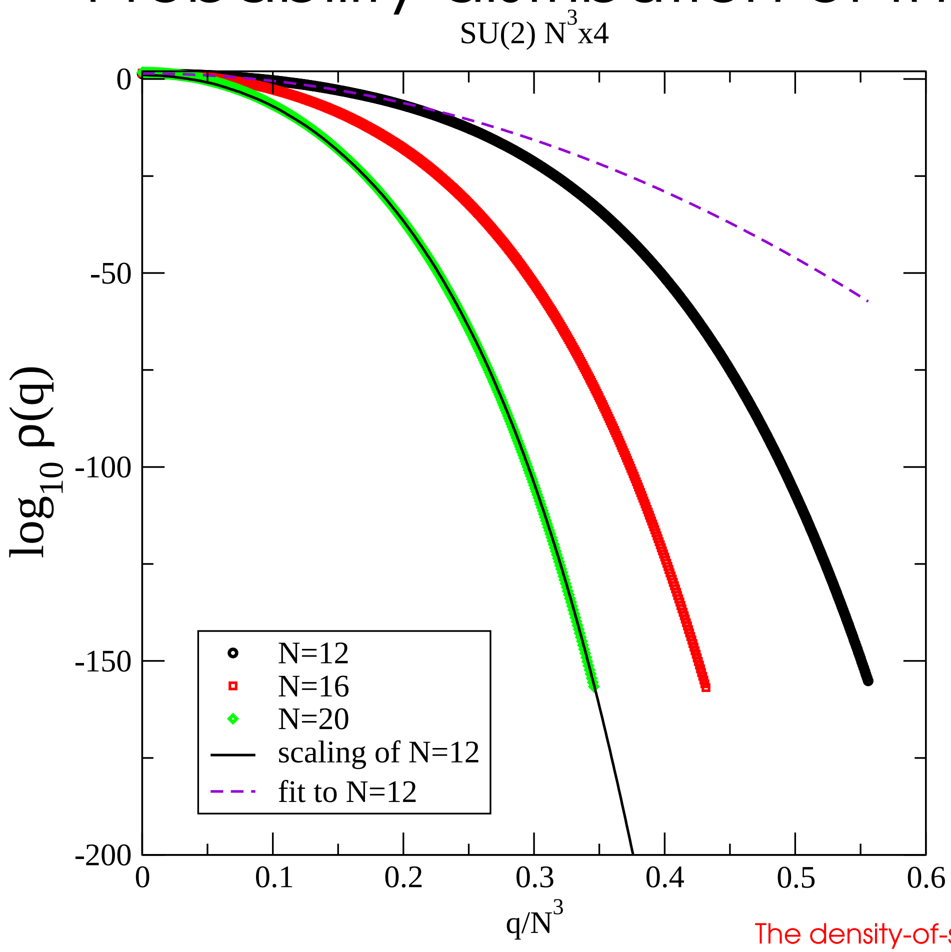

[KL, Pawlowski, PRD 88 (2013) 071502]

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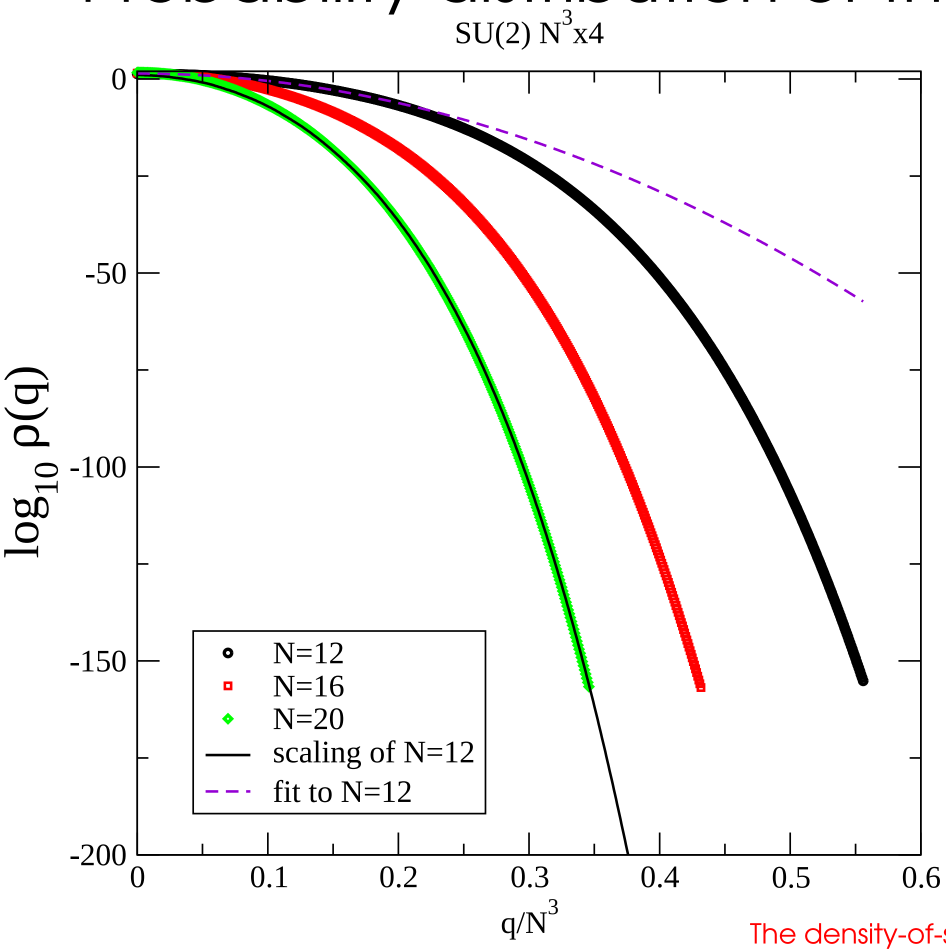

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The Z(3) Polyakov spin model:

- **The overlap $O(\mu)$:**

  Can we do rapidly oscillating integrals?

  $$Z(\mu) \; = \; \int ds \; R(s) \; \cos\Big(\sqrt{3}\,\sinh(\mu)\;s\Big) \; .$$

  $$\mu = 2, \; \Delta N = s = 0 \ldots 5000$$

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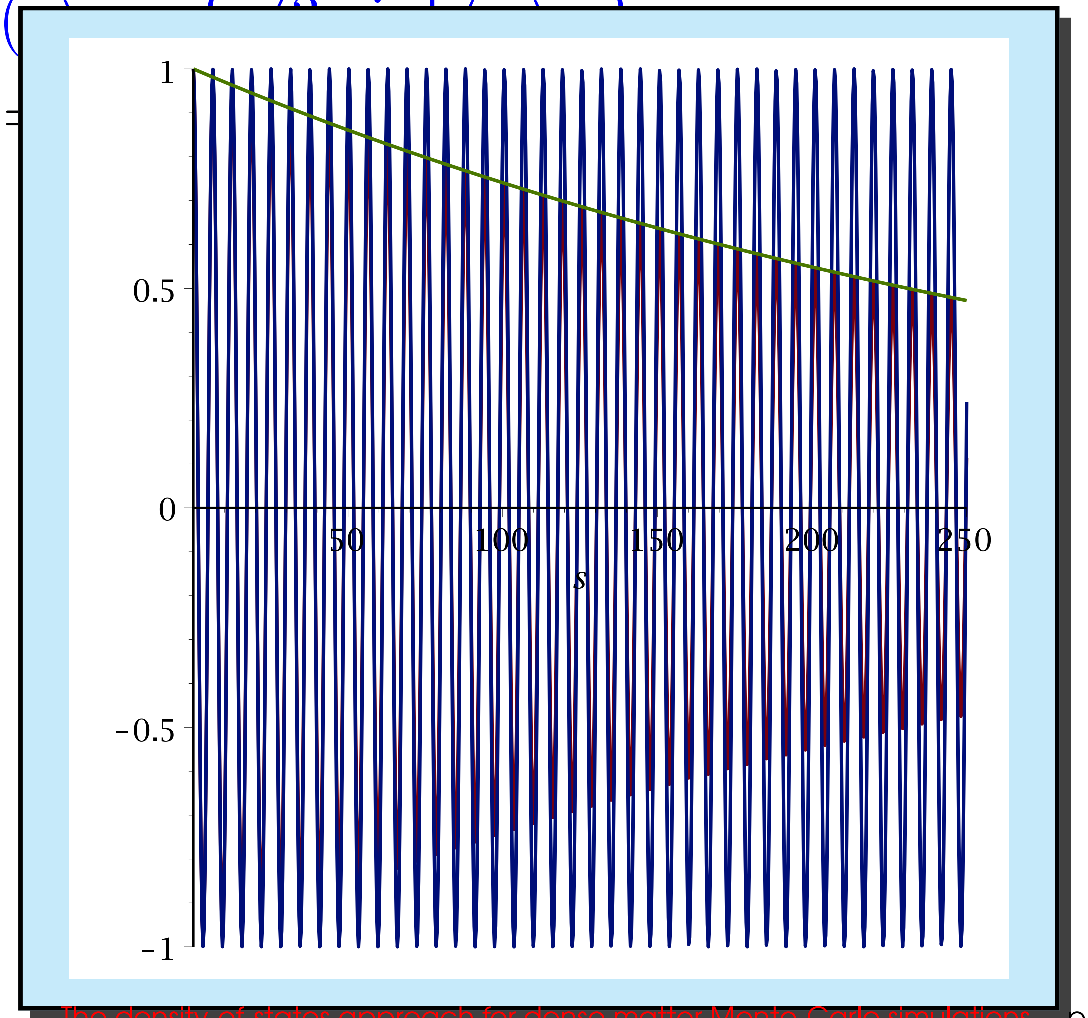
- *yes!*

  `[if the integrand`

  `is boring enough]`



The Z(3) Polyakov spin model:

- **Method and error analysis:**

  key observation: $\ln R(s)$ very smooth function

  $$R(s) \ = \ \prod_{s=1}^{s0} e^{a(s_0)} \ \exp\{a(s0)\,(s-s_0)\}$$ for $s \in [s, s0+1]$

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- **Bootstrap error analysis:**
  1. Choose a set of $a(s_0)$, $s_0 = 1 \ldots s_{max} \approx 5000$
  2. Fit a Polynomial: $\ln R(s) \;=\; \sum_{i\ \mathrm{even}}^{p} c_i\ s^i$, for $p = 2, 4, 6, 8..$
  3. Get an answer for $O(\mu)$

  Repeat steps 1-3 times and produce the boostrap average & standard deviation for $O(\mu)$.

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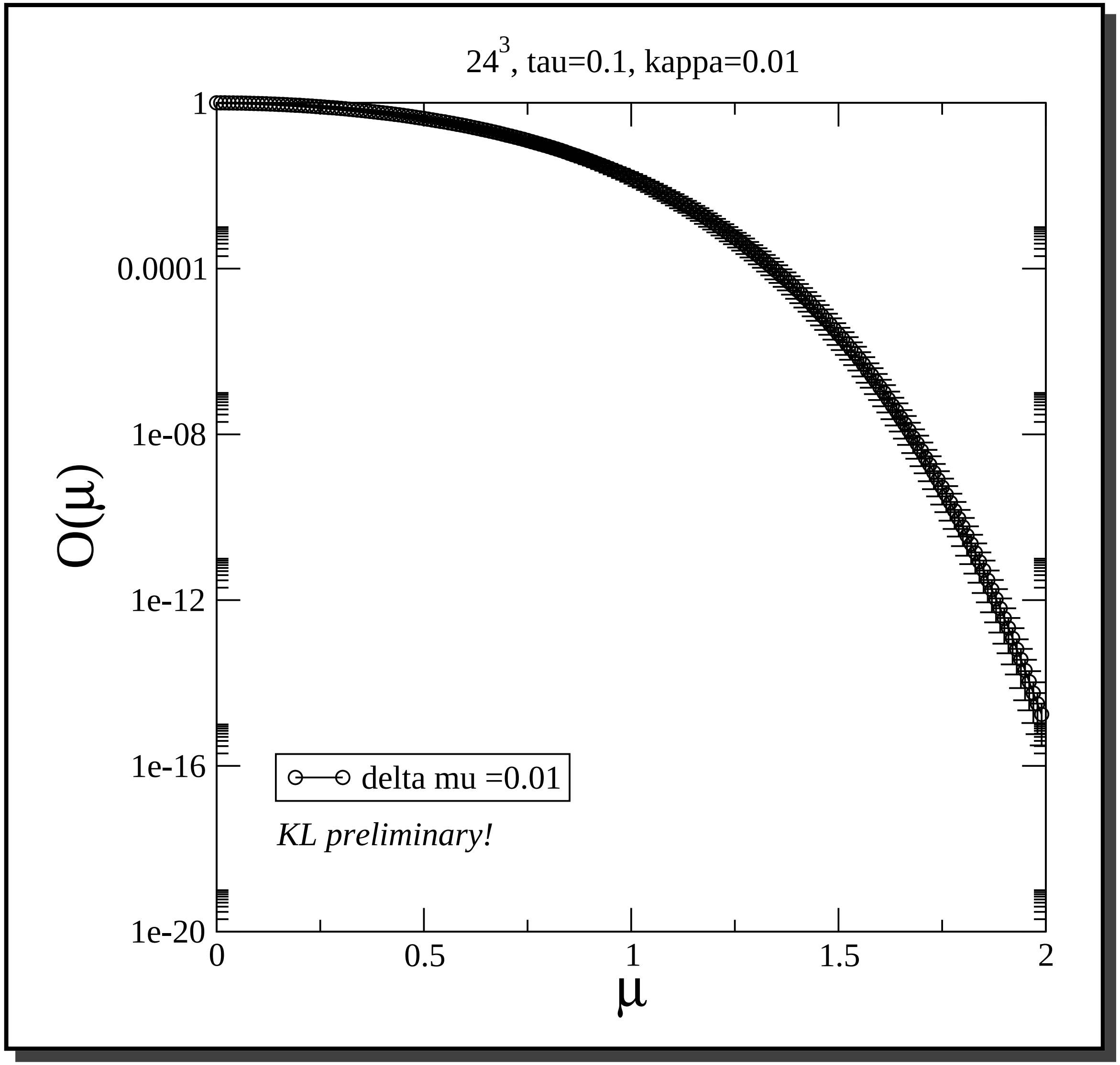
- **Results for the overlap:**



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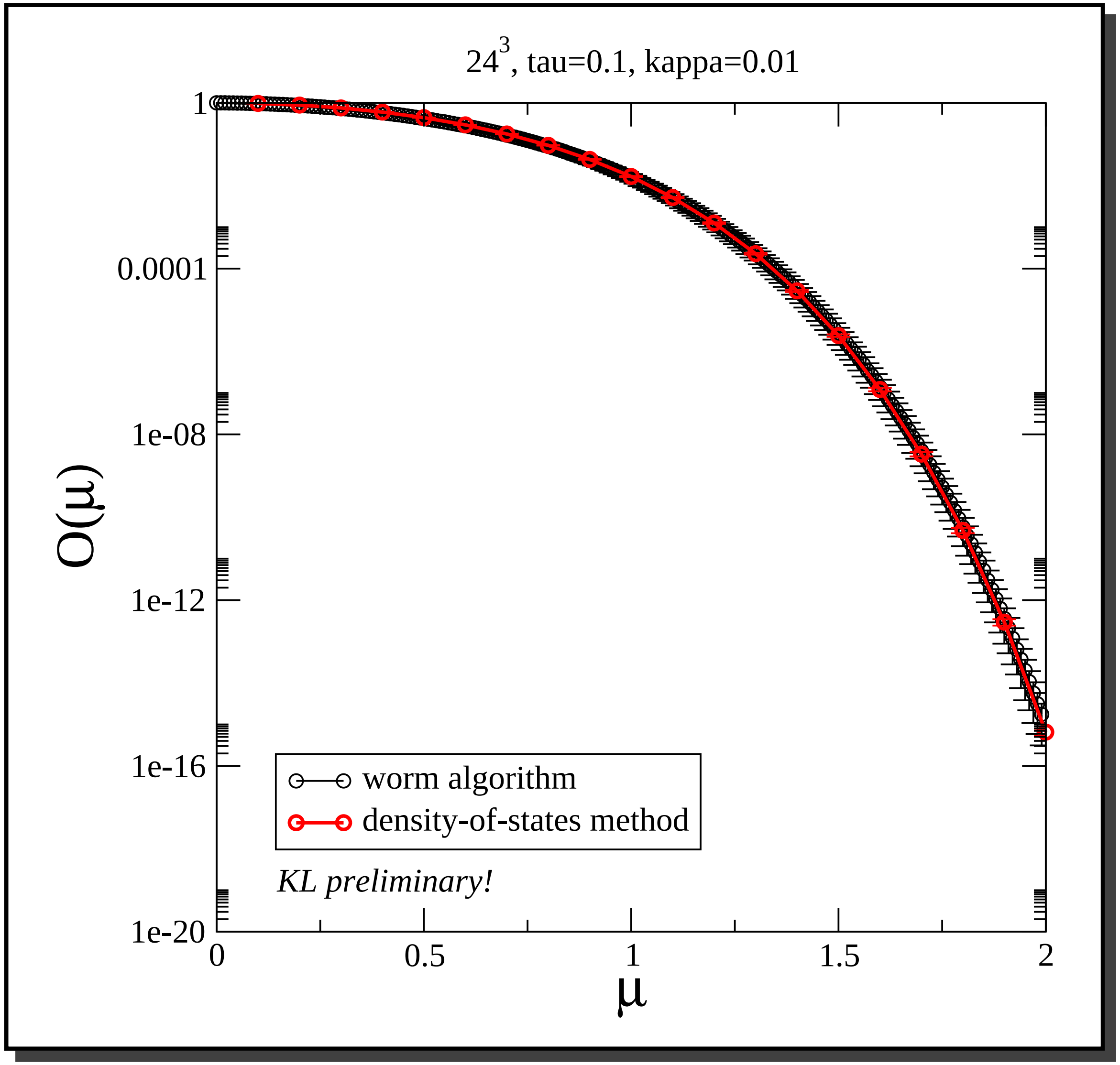

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- Studied the Z(3) Polyakov Spin model
  $\Rightarrow$ standard Solution: worm + snake algorithm
- The density-of-states + LLR approach seems to work well
  $\Rightarrow$ I am carefully optimistic
  $\Rightarrow$ Next test case: quantum O(2) model