Computing general observables in lattice models with complex actions

Olmo Francesconi *(LPMMC Grenoble, UGA & Swansea University)*

Markus Holzmann *(LPMMC Grenoble)*
Antonio Rago *(University of Plymouth)*

Biagio Lucini *(Swansea University)*
Jarno Rantaharju *(Swansea University)*

Lattice 19
Wuhan·China | June 16-22

Outlook

- **Introduction**
- **Density of states approach**
  - LLR algorithm
  - Bias control
  - DoS rebuilding and integration
- **General Observables in the DoS + LLR framework**
- **Thirring model – DoS of the worldline representation** (Preliminary results)

Introduction

$$Z = \int \mathcal{D}[\phi]\; e^{-S_R[\phi]}\; e^{-i\mu S_I[\phi]}$$

- Relativistic Bose gas at finite density:

$$S = \sum_x \left[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu \delta_{\nu,4}} \phi_x \right) \right]$$

$$\phi_x = \phi_{x,1} + i \phi_{x,2}$$

$$S_R = \sum_x \left[\frac{1}{2} \left(2d + m^2\right) \phi_{a,x}^2 + \frac{\lambda}{4} \left(\phi_{a,x}^2\right)^2 - \sum_{i=1}^{3} \phi_{a,x} \phi_{a,x+\hat{\imath}} - \cosh(\mu) \phi_{a,x} \phi_{a,x+\hat{4}} \right]$$

$$S_I = \sum_x \left[\varepsilon_{ab}\; \phi_{a,x} \phi_{b,x+\hat{4}} \right]$$

$$S = S_R + i \sinh(\mu) S_I$$

Introduction

$$Z = \int \mathcal{D}[\phi] \; e^{-S_R[\phi]} \; e^{-i\mu S_I[\phi]}$$

- Relativistic Bose gas: $S = \sum_x \left[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu \delta_{\nu,4}} \phi_x \right) \right]$

$$\mu > 0 \quad \rightarrow \quad e^{-S[\phi]} \in \mathbb{C}$$

No probability interpretation of the Boltzmann weight, standard Monte Carlo methods fails

Introduction

$$Z = \int \mathcal{D}[\phi] \; e^{-S_R[\phi]} \; e^{-i\mu S_I[\phi]}$$

- Relativistic Bose gas: $S = \sum_x \left[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu\delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu\delta_{\nu,4}} \phi_x\right) \right]$

$$\mu > 0 \quad \rightarrow \quad e^{-S[\phi]} \in \mathbb{C}$$

No probability interpretation of the Boltzmann weight, standard Monte Carlo methods fails

By ignoring the imaginary part of the action we can define the phase-quenched theory

$$Z_{pq} = \int \mathcal{D}[\phi] \; e^{-S_R[\phi]}$$

$$O(\mu) = \frac{Z(\mu)}{Z_{PQ}(\mu)} = \langle e^{i\varphi} \rangle$$

Introduction

$$Z = \int \mathcal{D}[\phi]\ e^{-S_R[\phi]}\ e^{-i\mu S_I[\phi]}$$

- Relativistic Bose gas: $S = \sum_x \left[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu \delta_{\nu,4}} \phi_x \right) \right]$

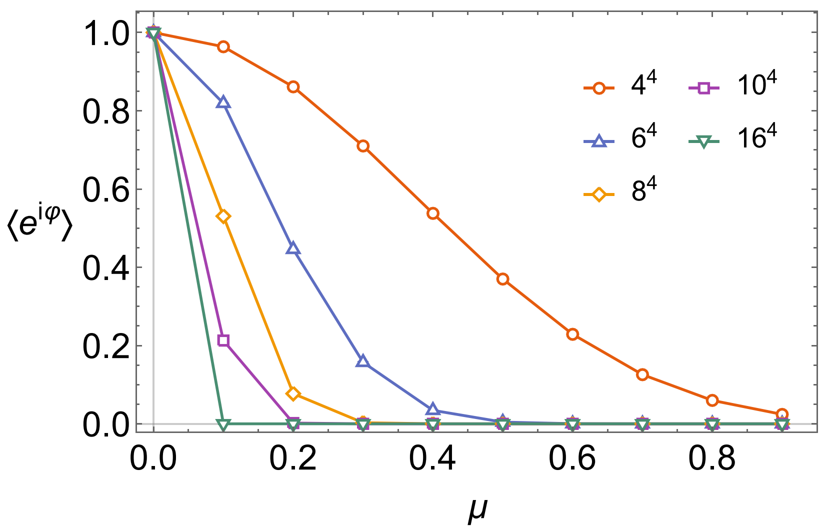
$$\mu > 0 \quad \rightarrow \quad e^{-S[\phi]} \in \mathbb{C}$$

No probability interpretation of the Boltzmann weight, standard Monte Carlo methods fails

By ignoring the imaginary part of the action we can define the phase-quenched theory

$$Z_{pq} = \int \mathcal{D}[\phi]\ e^{-S_R[\phi]}$$

$$O(\mu) = \frac{Z(\mu)}{Z_{PQ}(\mu)} = \langle e^{i\varphi} \rangle$$



Introduction

$$Z = \int \mathcal{D}[\phi]\; e^{-S_R[\phi]}\; e^{-i\mu S_I[\phi]}$$

- Relativistic Bose gas: $S = \sum_x \left[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu \delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu \delta_{\nu,4}} \phi_x \right) \right]$

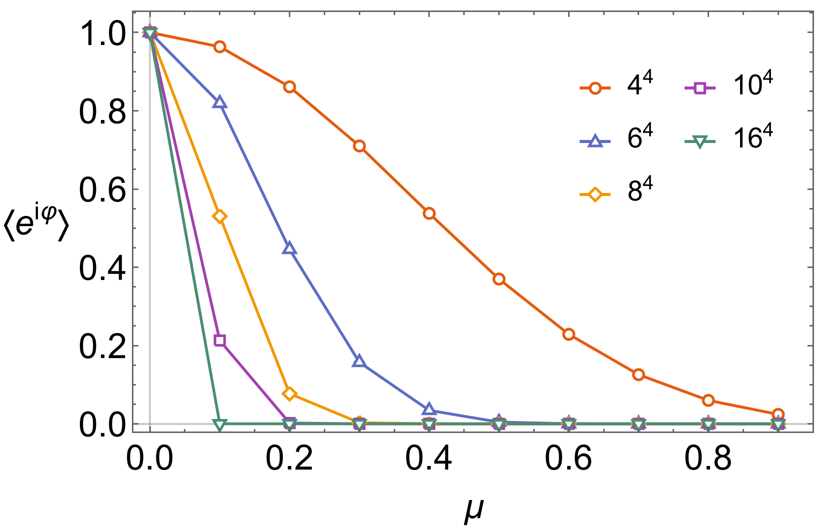
$$\mu > 0 \quad \rightarrow \quad e^{-S[\phi]} \in \mathbb{C}$$

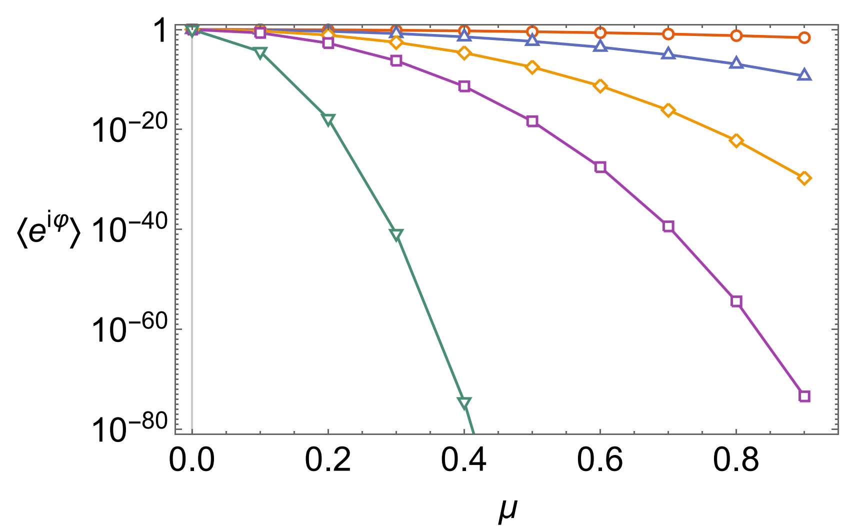
No probability interpretation of the Boltzmann weight, standard Monte Carlo methods fails

By ignoring the imaginary part of the action we can define the phase-quenched theory

$$Z_{pq} = \int \mathcal{D}[\phi]\; e^{-S_R[\phi]}$$

$$O(\mu) = \frac{Z(\mu)}{Z_{PQ}(\mu)} = \langle e^{i\varphi} \rangle$$





Outlook

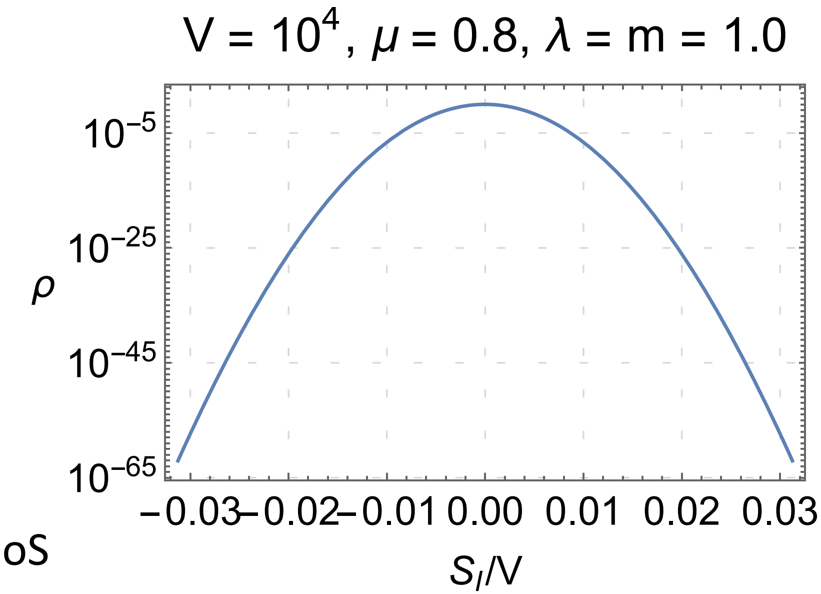
- Introduction
  - Complex action systems
  - Reweighting – Sign problem
- **Density of states approach**
  - LLR algorithm
  - Bias control
  - DoS rebuilding and integration
- General Observables in the DoS + LLR framework
- Fermionic Sign problem – Thirring model (Preliminary results)

Density of States approach

$$Z(\mu) = \int \mathcal{D}\phi \; e^{-S_R(\phi)} \; e^{-i\mu S_I(\phi)}$$

We define the generalized density of states

$$\rho(s) = N \int \mathcal{D}\phi \; \delta(s - S_I(\phi)) \; e^{-S_R(\phi)}$$



The partition function is recovered as a FT of the DoS

$$Z(\mu) = \frac{1}{N} \int ds \; \rho(s) \; e^{-i\mu s} = \frac{1}{N} \int ds \; \rho(s) \; \cos(\mu s)$$

If the DoS in known the phase factor is accessible via a simpler one-dimensional oscillatory integration

$$\langle e^{i\varphi} \rangle = \frac{\int ds \; \rho(s) \; \cos(\mu s)}{\int ds \; \rho(s)} \quad \propto \quad e^{-V\Delta F}$$

The DoS must be defined with great precision over multiple orders of magnitude

LLR – Linear Logarithmic Relaxation [1]

- Restrict the system to a small imaginary action interval of amplitude Δ
- Consider the restricted and reweighted expectation value

$$\langle\langle \mathcal{O}(s) \rangle\rangle_k(a) = \int_{S_k-\Delta/2}^{S_k+\Delta/2} \rho(s)\, \mathcal{O}(s)\, e^{-as}\, ds$$

Idea: Choose *a* to achieve a uniform sampling in the imaginary action interval

$$\rho(s) \exp\{-a\ s\} = constant + \mathcal{O}(\Delta^2)$$

It's easy to see that for $\Delta S = s - S_k$ a uniform sampling leads to

$$\langle\langle \Delta S \rangle\rangle_k(a) = \int_{S_k-\Delta/2}^{S_k+\Delta/2} (s - S_k)\rho(s)\, e^{-as}\, ds = 0 \Leftrightarrow^* a = \left.\frac{d\ \ln(\rho(s))}{d\ s}\right|_{s=S_k}$$

The problem has been translated to solving a stochastic equation to find the appropriate reweighting factor

$^*\ \lim_{\Delta\to 0}$

[1] K. Langfeld, B. Lucini and A. Rago, Phys. Rev. Lett. 109 (2012) 111601

Stochastic root finder

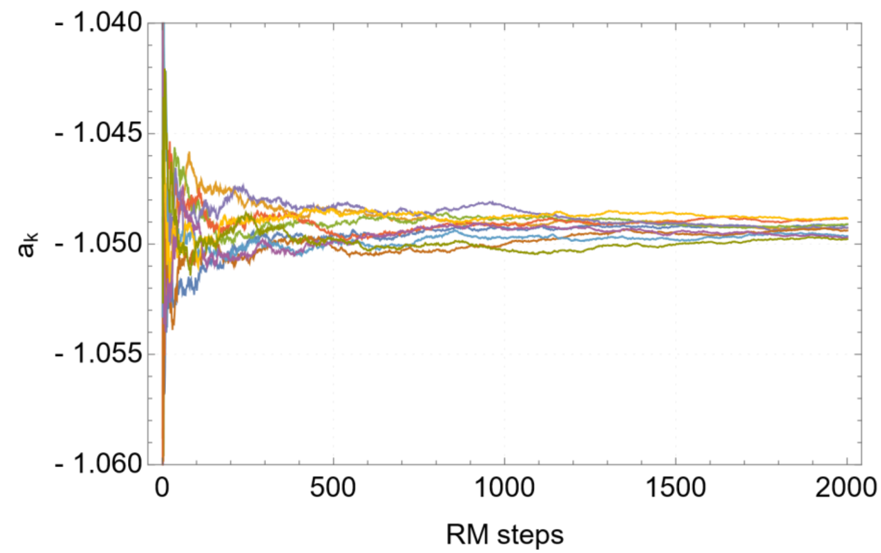
Robbins Monro[2] stochastic root finding

$$a_{n+1} = a_n - c_n \langle\langle \Delta S \rangle\rangle_{a_n}$$

$$a_{n+1} = a_n - \frac{12 \ \langle\langle \Delta S \rangle\rangle_n}{(n+1) \ \Delta^2}$$

$$\sigma_{RM} \propto \sqrt{N_{RM}}/\Delta^2$$

$$\text{LLR exact} \Leftrightarrow \Delta \to 0$$

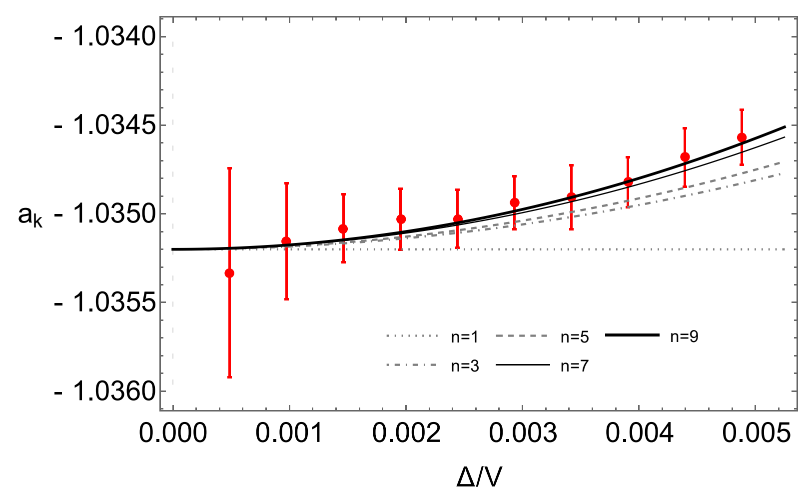


$$\text{Finite } \Delta \quad \to \quad \langle\langle \Delta S \rangle\rangle_k (a \sim a_k) = \frac{\Delta^2}{12} \ (a - a_k) + \frac{f^{(3)}(S_k)}{3!} \frac{\Delta^4}{80} + \mathcal{O}(\Delta^6)$$

Solving this equation for *lhs = 0* gives an estimate of the **bias** as

$$bias = \frac{f^{(3)}(S_k)}{40} \Delta^2 + \mathcal{O}(\Delta^4)$$

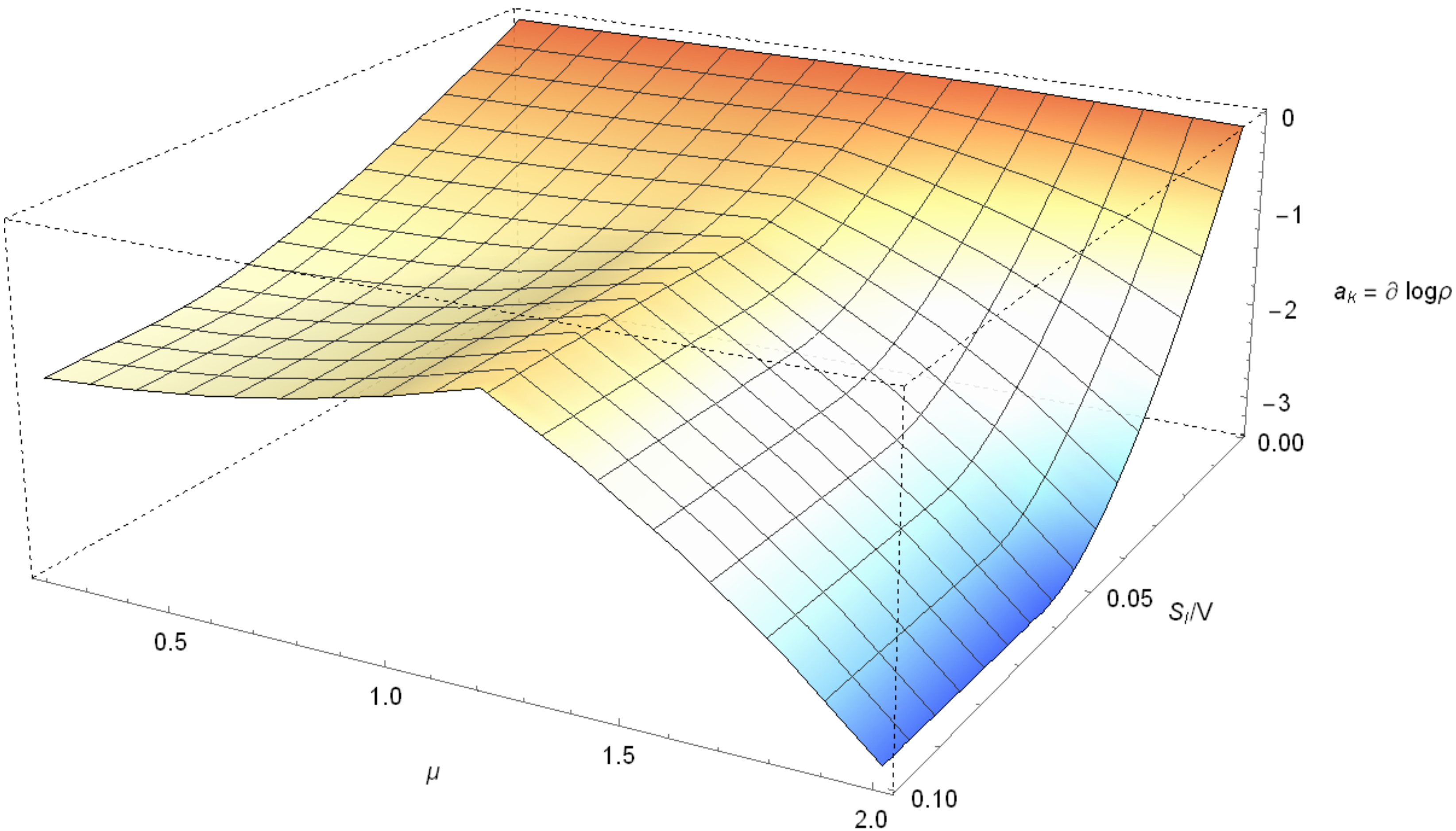
Knowing the scaling of all our simulation parameters we can run **bias-optimized simulations**



[2] Robbins, H.; Monro, The Annals of Mathematical Statistics 22

LLR simulation results

$$V = 8^4,\ \lambda = m = 1,\ \Delta/V = 0.001,\ N_k = 168$$



From this results the DoS can be recovered as $\rho(s) = e^{\int_0^s p_n(x)\ \mathrm{d}x}$
Where pn is a polynomial fit of the reweighting parameters.

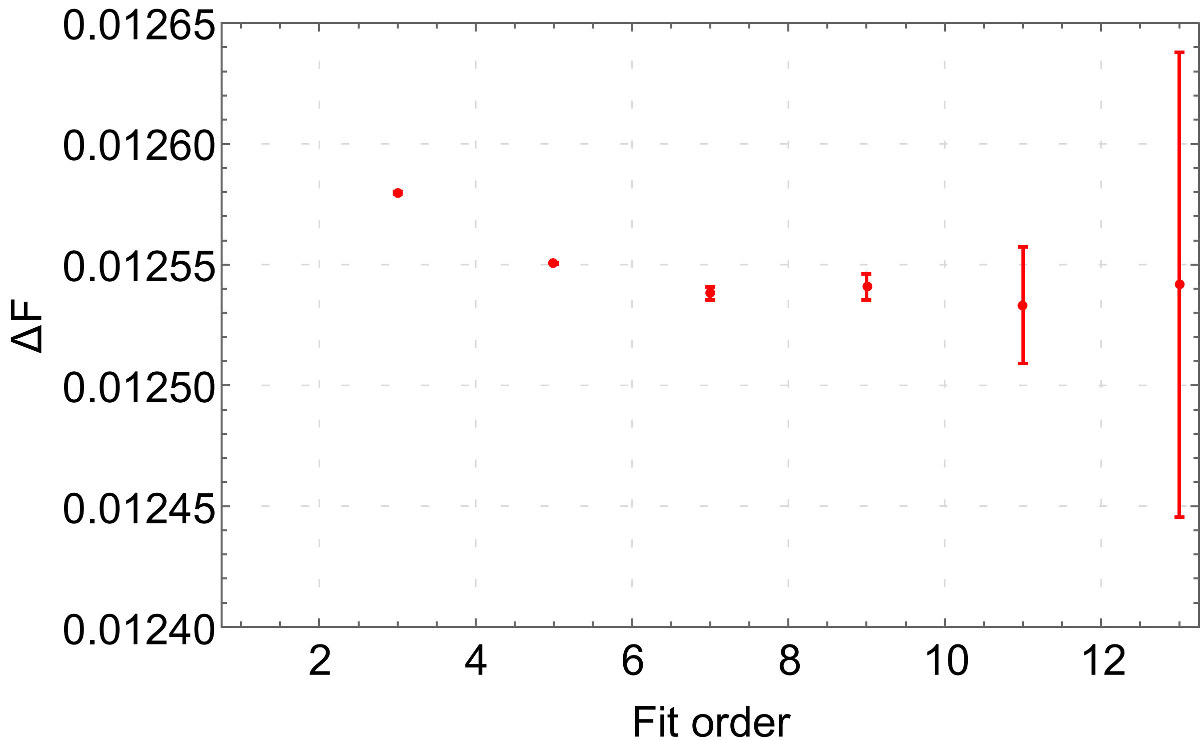
Phase factor integration

$$\langle e^{i\varphi} \rangle = \frac{\int ds\ \rho(s)\ \cos(\mu s)}{\int ds\ \rho(s)} \quad \propto \quad e^{-V \Delta F}$$

$$\Delta F = -\frac{1}{V} \log(\langle e^{i\varphi} \rangle)$$

$$\langle e^{i\varphi} \rangle \sim \mathcal{O}(10^{-360})$$

$$V = 16^4,\ \lambda = m = 1,\ \mu = 0.8$$



Phase factor integration

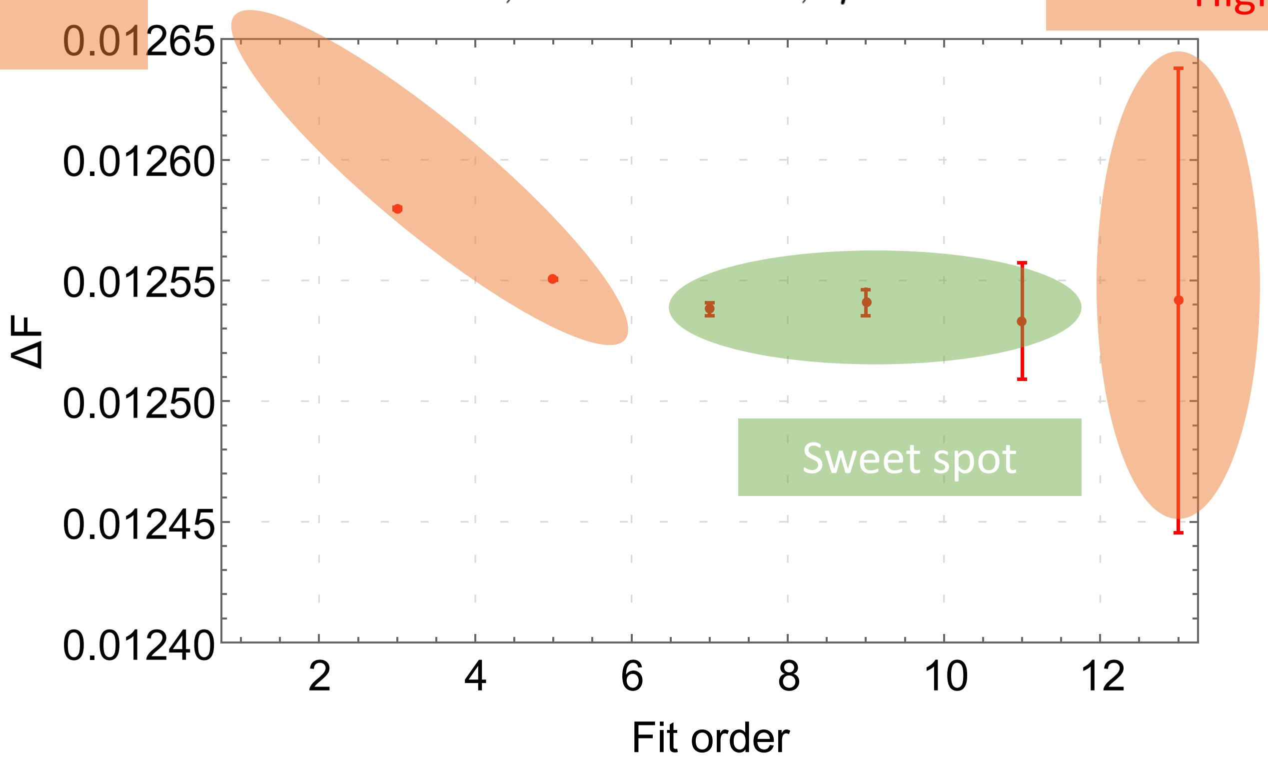
$$\langle e^{i\varphi}\rangle = \frac{\int ds\ \rho(s)\ \cos(\mu s)}{\int ds\ \rho(s)} \quad \propto \quad e^{-V\Delta F}$$

$$\Delta F = -\frac{1}{V}\log(\langle e^{i\varphi}\rangle)$$

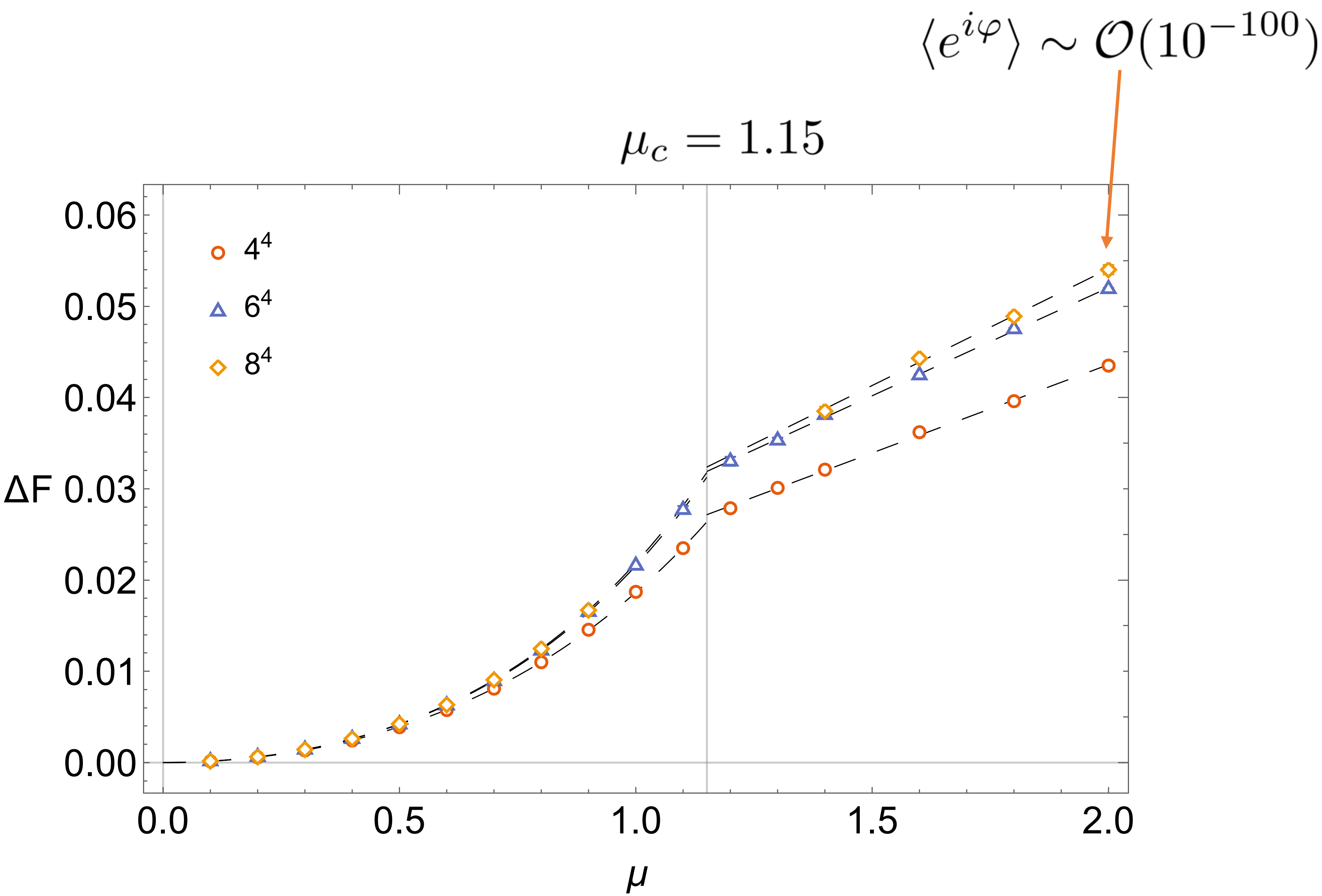
Low order polynomials
Small error
High Bias

High order polynomials
Small Bias
High errors

$V = 16^4,\ \lambda = m = 1,\ \mu = 0.8$

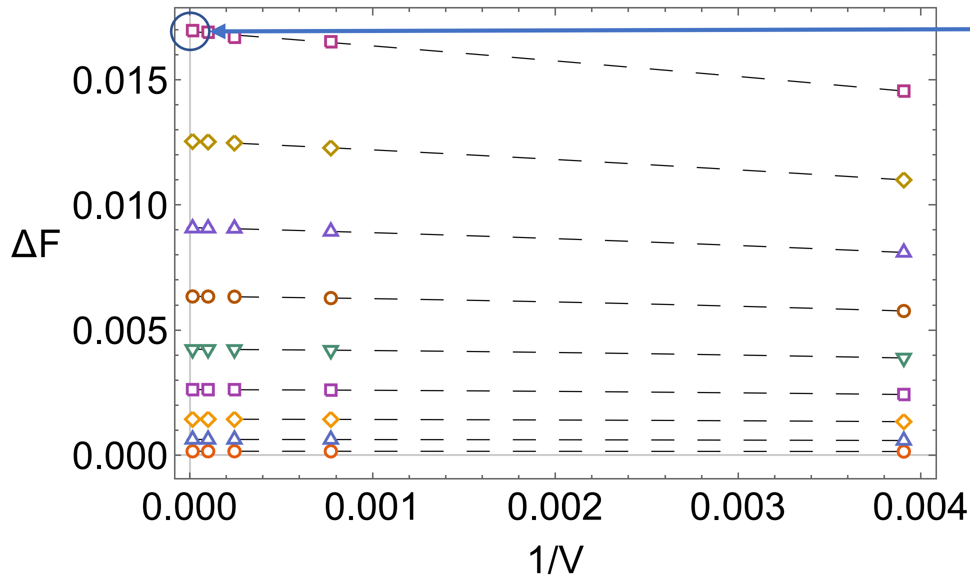


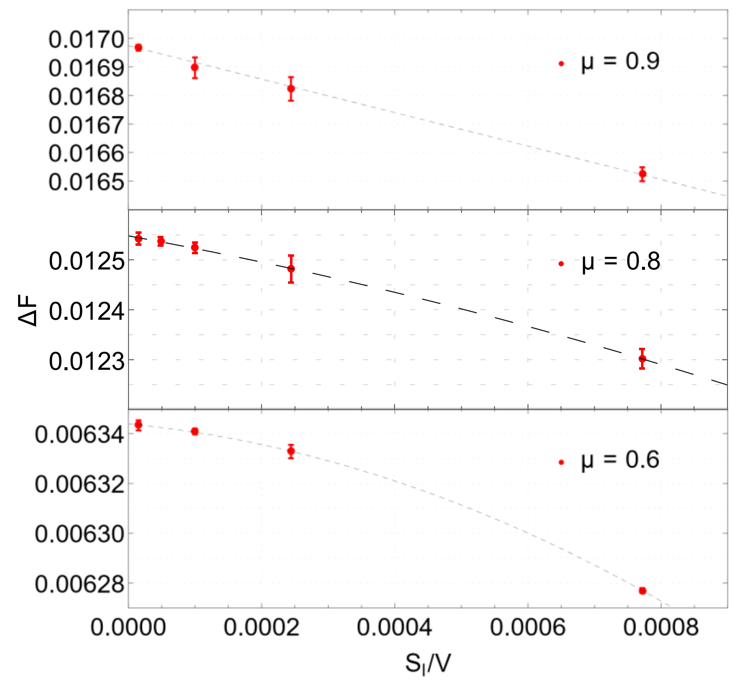
Free energy difference vs chemical potential

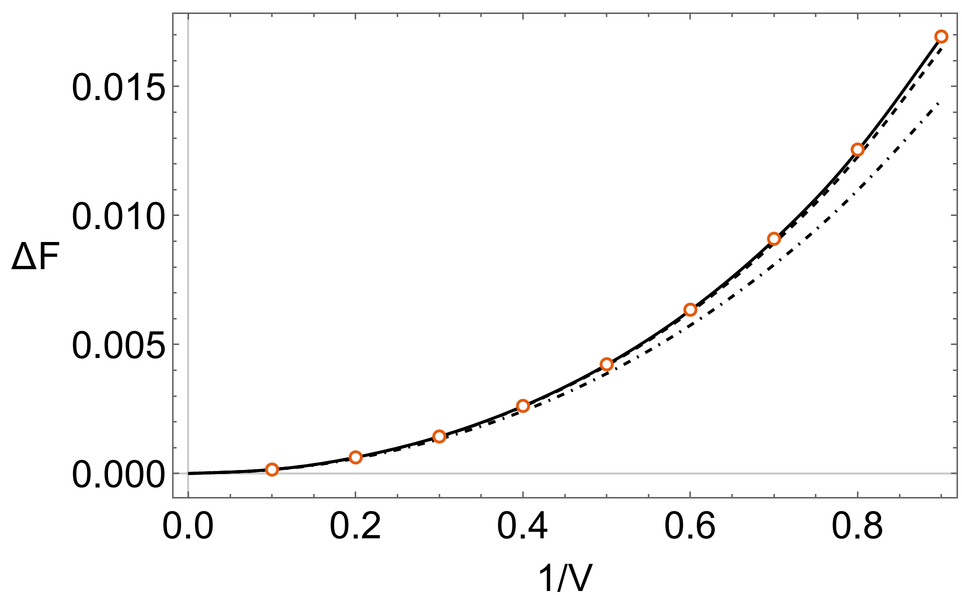


Continuum/Thermodynamic limit

$$\langle e^{i\varphi} \rangle \sim \mathcal{O}(10^{-480})$$







Outlook

- Introduction
  - Complex action systems
  - Reweighting – Sign problem
- Density of states approach
  - LLR algorithm
  - Bias control
  - DoS rebuilding and integration
- General Observables in the DoS + LLR framework
- Fermionic Sign problem – Thirring model (Preliminary results)

General Observables in the Dos + LLR formalism

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}\phi \; \mathcal{O}[\phi] \; e^{-S_R[\phi]} \; e^{-iS_I[\phi]}}{\int \mathcal{D}\phi \; e^{-S_R[\phi]} \; e^{-iS_I[\phi]}} = \frac{\langle \mathcal{O}[\phi] \; e^{-iS_I[\phi]} \rangle}{\langle e^{-iS_I[\phi]} \rangle}$$

Using the definition of the DoS $\quad \rho(s) = N \int \mathcal{D}\phi \; \delta(s - S_I[\phi]) \; e^{-S_R[\phi]}$

We can write the expectation values as the ratio of two one-dimensional oscillatory integrals

$$\langle \mathcal{O} \rangle = \frac{\int \mathrm{d}s \; \rho(s) \; \tilde{\mathcal{O}}(s) \; \exp\{is\}}{\int \mathrm{d}s \; \rho(s) \; \exp\{is\}}$$

Where we have defined a new function that describes the expectation value of the observable restricted to configurations with fixed imaginary action.

$$\tilde{\mathcal{O}}(s) = \frac{\int \mathcal{D}\phi \; \delta(s - S_I[\phi]) \; \mathcal{O}[\phi] \; e^{-S_R[\phi]}}{\int \mathcal{D}\phi \; \delta(s - S_I[\phi]) \; e^{-S_R[\phi]}}$$

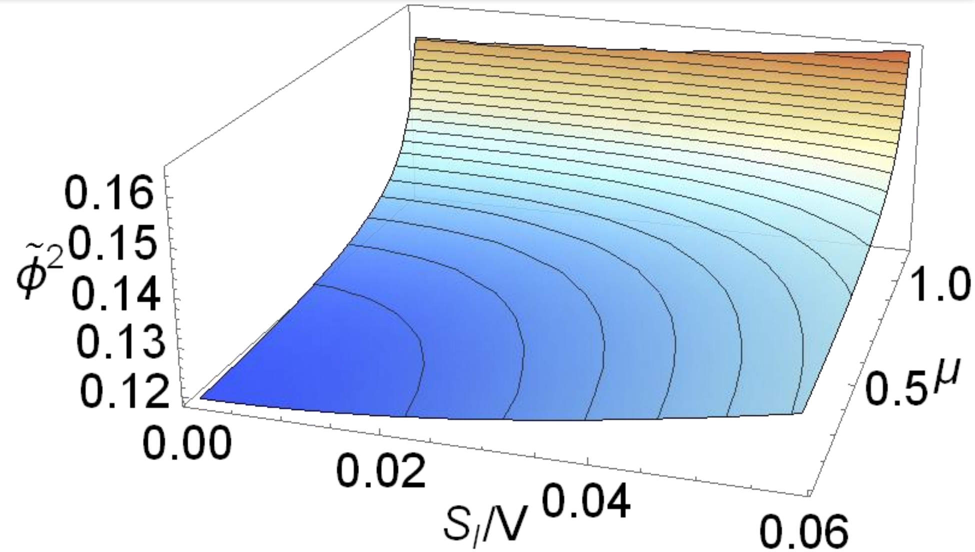
This new quantity can be evaluated as the restricted and reweighted expectation value defined in the LLR method, thus it is easily implemented in our simulations.

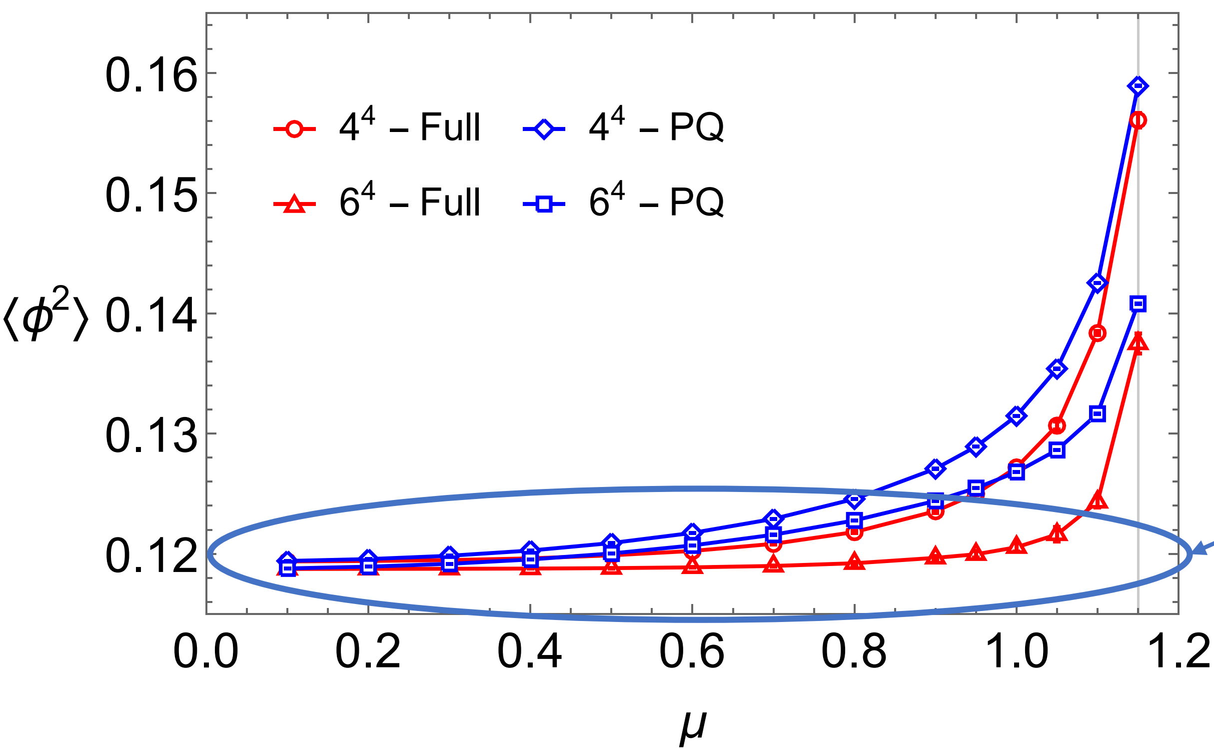
$$\tilde{\mathcal{O}}(S_k) = \langle \langle \mathcal{O} \rangle \rangle_{S_k}(a = a_k) + \mathcal{O}(\Delta^2)$$

Relativistic Bose gas $\langle \phi^2 \rangle$

$$\langle \phi^2 \rangle = \frac{\int \mathrm{d}s\ \tilde{\phi}^2(s)\ \rho(s)\ \cos(\sinh(\mu)\ s)}{\int \mathrm{d}s\ \rho(s)\ \cos(\sinh(\mu)\ s)}$$

$$\langle \phi^2 \rangle_{pq} = \frac{\int \mathrm{d}s\ \tilde{\phi}^2(s)\ \rho(s)}{\int \mathrm{d}s\ \rho(s)}$$





Silver Blazing

Relativistic Bose Gas $\langle n \rangle$

The density of the relativistic Bose gas is defined as

$$n = \frac{1}{\Omega}\frac{\partial \ln Z}{\partial \mu} = \frac{1}{\Omega}\sum_x n_x = \sinh(\mu)\; n_R - i\cosh(\mu)\; n_I$$

$$n_x = (\delta_{ab}\sinh(\mu) - i\epsilon_{ab}\cosh(\mu))\;\phi_{a,x}\;\phi_{b,x+\hat{4}}$$

Using the definition of the imaginary part of the action

$$\sum_x \left[\epsilon_{ab}\;\phi_{a,x}\;\phi_{b,x+\hat{4}}\right] = S_I \rightarrow n_I = s$$

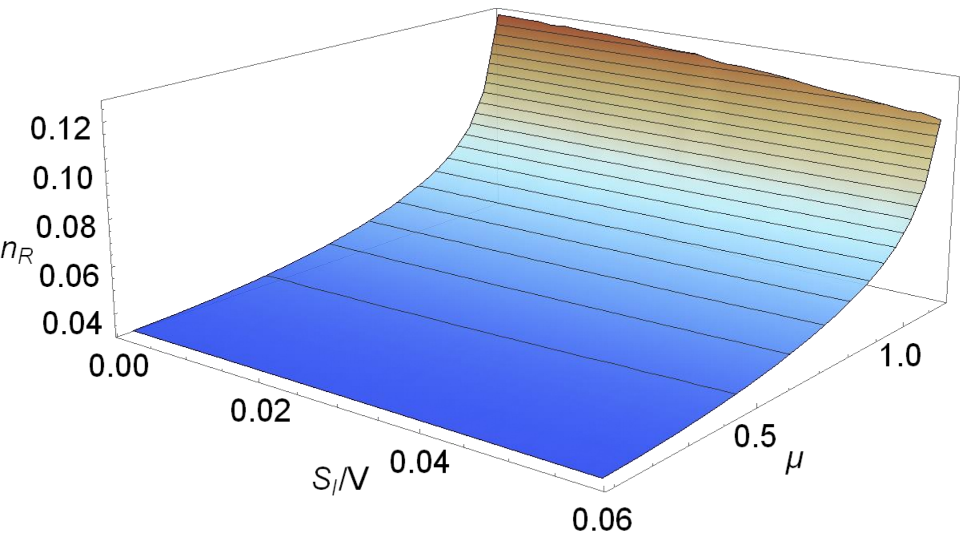
The density can be recovered as

$$\langle n \rangle = \frac{1}{Z}\int \mathrm{d}s\,\rho(s)\;\left[\sinh(\mu) n_R(s)\cos(\sinh(\mu) s) + \cosh(\mu)\;s\;\sin(-\sinh(\mu) s)\right]$$

The density of the system is then given by the sum of these two contributions

$$\langle n \rangle = \langle n_R \rangle + n_{\mathrm{corr}}$$

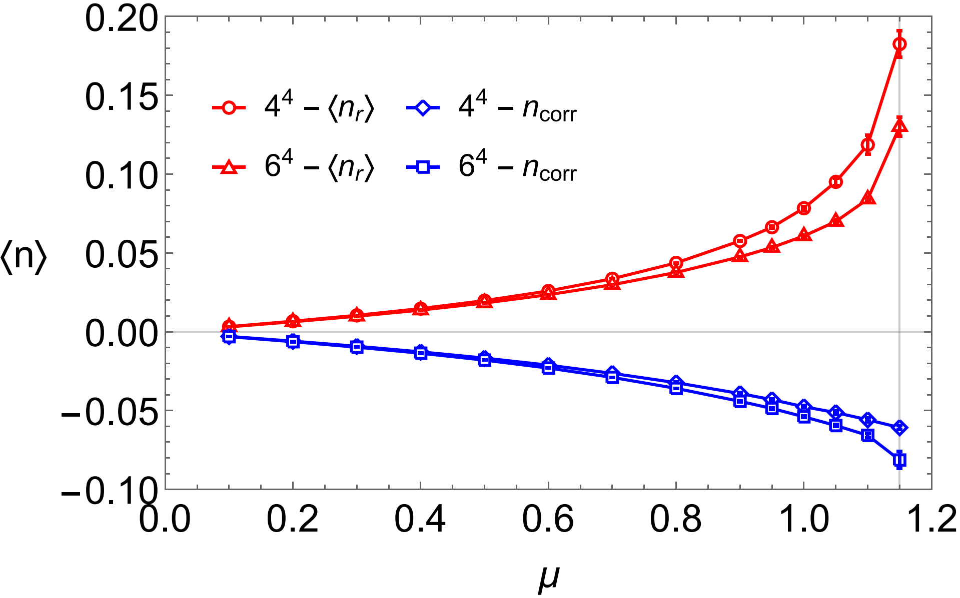
Relativistic Bose Gas $\langle n \rangle$

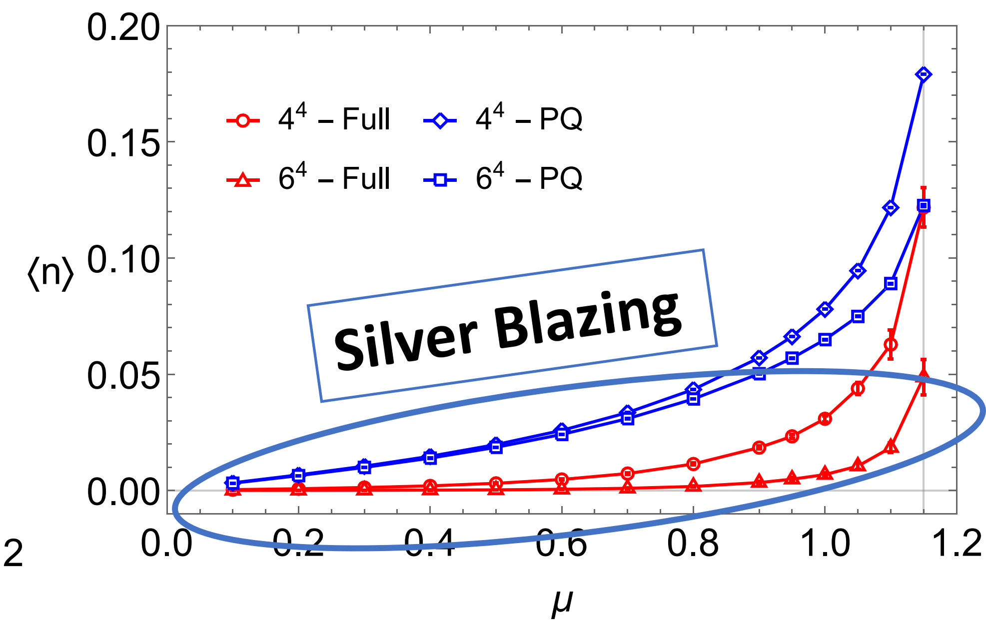


$$\langle n \rangle = \langle n_R \rangle + n_{\text{corr}}$$

$$\langle n \rangle_{pq} = \frac{\int \mathrm{d}s \; \tilde{n}_R(s) \; \rho(s)}{\int \mathrm{d}s \; \rho(s)}$$

Both contribution can be obtained with great precision, leading to a precise evaluation of the density, that shows again the **Silver Blazing** phenomenon.





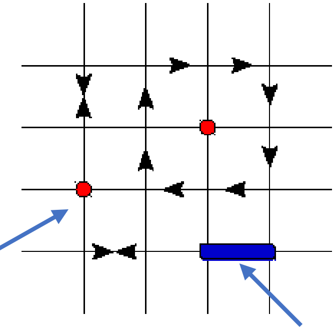
Outlook

- Introduction
  - Complex action systems
  - Reweighting – Sign problem
- Density of states approach
  - LLR algorithm
  - Bias control
  - DoS rebuilding and integration
- General Observables in the DoS + LLR framework
- Fermionic Sign problem – Thirring model (Preliminary results)

Thirring model – Worldline formulation[3]

$$S = \sum_{x,y} \bar{\chi}_x \left(D^{KS}_{x,y}(\mu) - m\delta_{x,y} \right) \chi_y + U \sum_{x,\nu} \bar{\chi}_x \chi_x \bar{\chi}_{x+\nu} \chi_{x+\nu}$$

Staggered Dirac matrix



$$Z = \int d\bar{\chi} d\chi e^{-\sum_{x,y} \bar{\chi}_x D^{KS}_{x,y}(\mu) \chi_y} \times \prod_x (1 + m\bar{\chi}_x \chi_x) \prod_{x,\nu} (1 + U\bar{\chi}_x \chi_x \bar{\chi}_{x+\nu} \chi_{x+\nu})$$

$$Z = \sum_{[d],[n]} m^{N_m} U^{N_d} \det \left(W([f], \mu) \right)$$

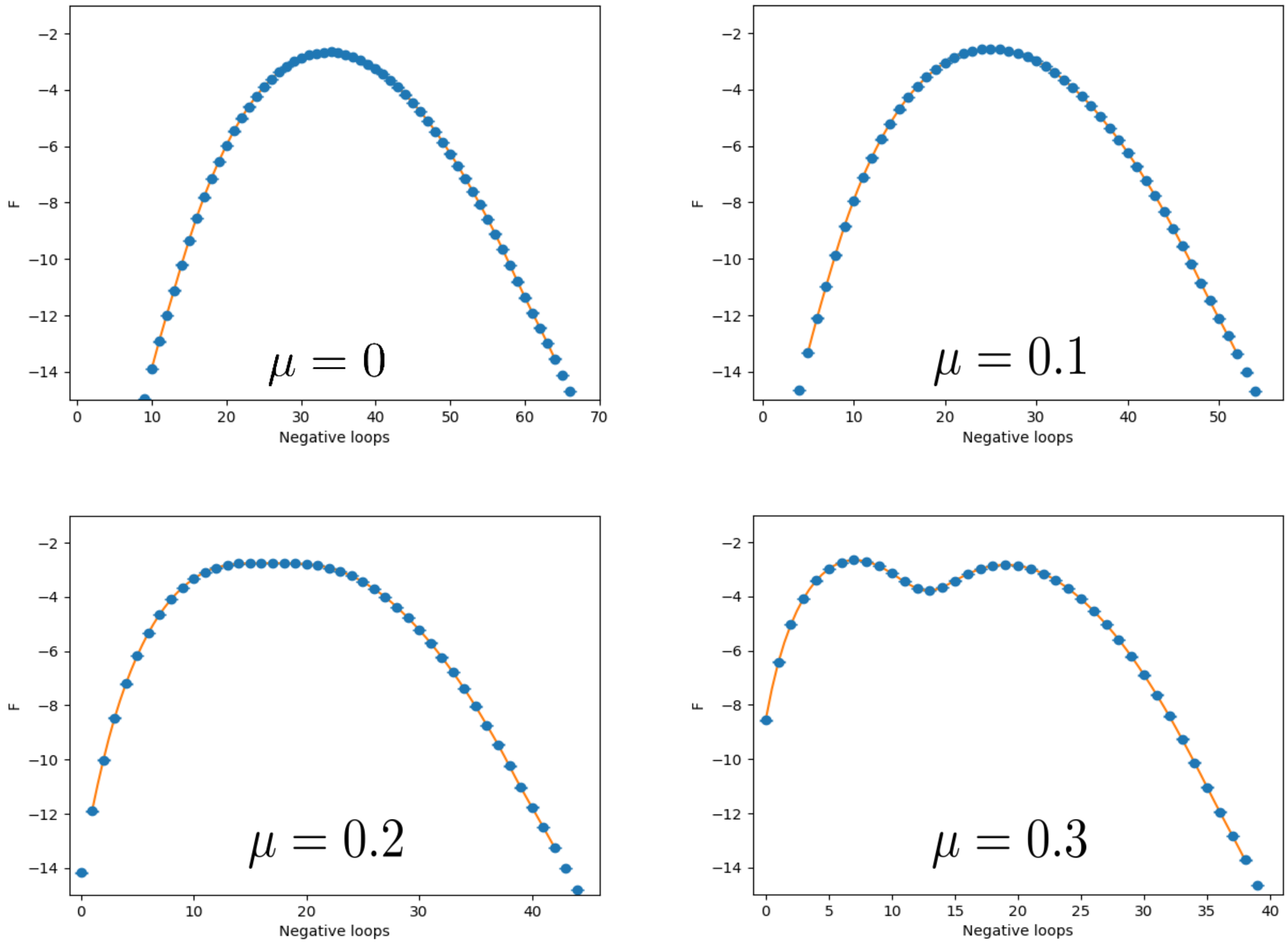
The sign of a configuration is determined by the signs of the closed loops of links.

Idea: Use the number of negative sign loops as the quantity on which we build the density of states of the system.

[3] V. Ayyar, S. Chandrasekharan and J. Rantaharju, Phys. Rev. D 97 (2018) nr.5, [arXiv:1711.07898[hep-lat]]

Thirring model – Preliminary results

Wang-Landau method results for the Thirring model with $U = 0, \ m = 0.1$ on a 128x128 lattice



Conclusion and outlooks

- **DoS + LLR:** precise reconstruction of the DoS over hundreds orders of magnitude
- **Bias control and careful fitting:** consistent evaluation of the Phase factor also in the hard-sign problem region up to $\mathcal{O}\left(10^{-480}\right)$.
- **General observables** evaluation can be implemented in the framework without too much troubles
  - Study on bigger volumes is needed
- Preliminary results for the Thirring model show encouraging levels of precision for the DoS rebuilding, a systematic study on the error for the discrete DoS is still needed.

DoS Reconstruction

Piecewise approximation

$$\hat{\rho}_k(s) = C_k \ \exp\left(a_k(s - S_k)\right)$$

$$C_k = \prod_{i=0}^{i<k} \exp\{a_i \Delta\}$$

$$\hat{\rho}(s) = \rho_{exact}(s) \ e^{c\Delta^2}$$

Exponential error suppression

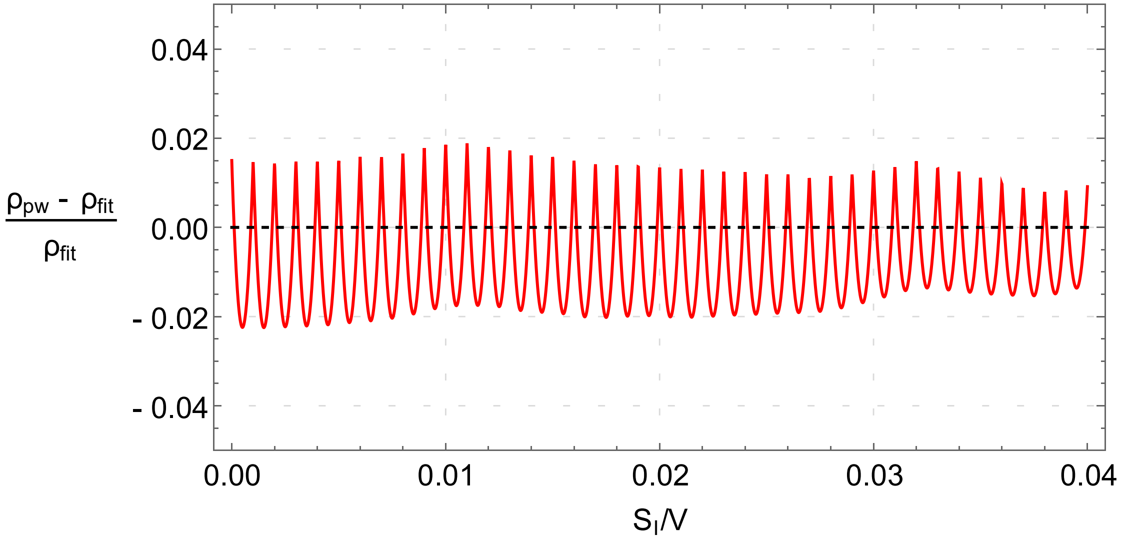
Polynomial fit approximation

$$p'_n(s) = \sum_{i=1}^{n} c_i \ s^{2i-1}$$

$$\rho_{fit}(s) = e^{\int_0^s p'_n(s') \ ds'}$$

Exponential error suppression

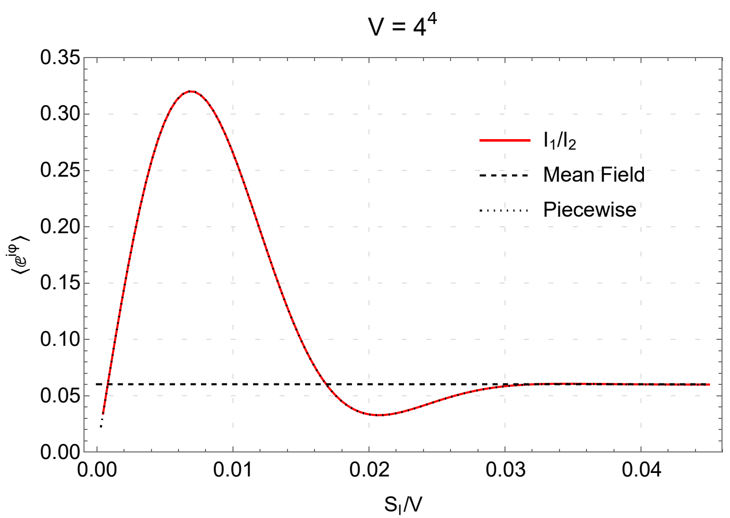
Smooth

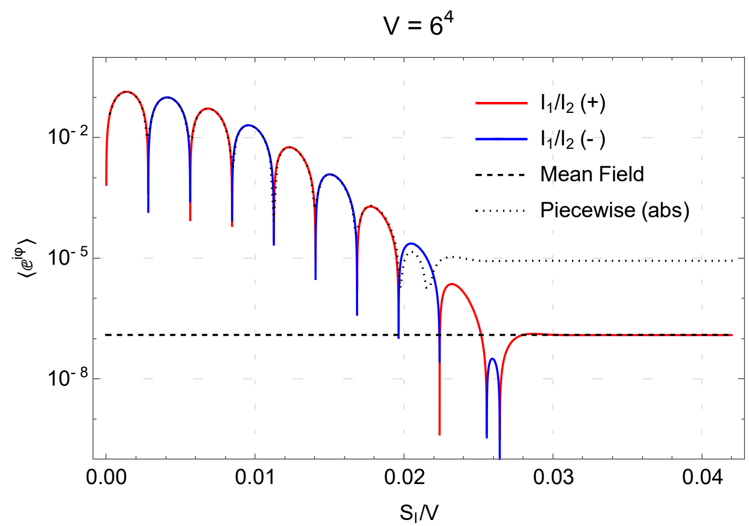


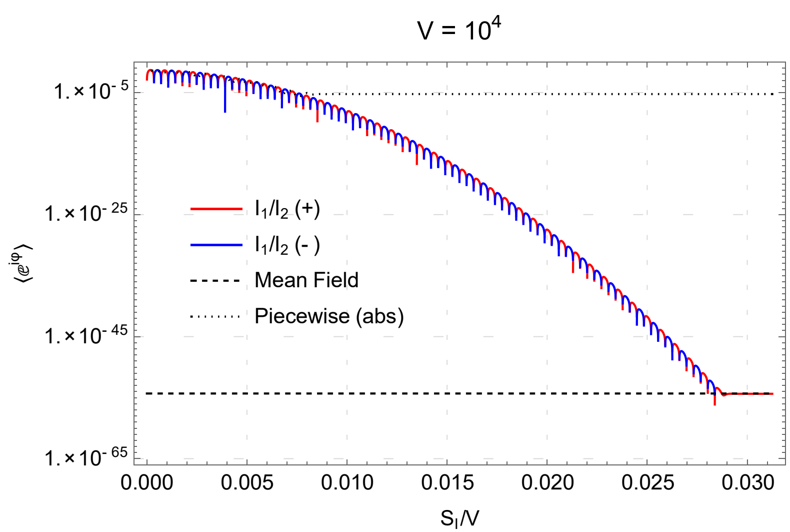
$\mathcal{O}(\Delta^2)$ error in the integration in each interval for the piecewise approximation, this would require an exponential number of intervals to integrate the phase factor as the sign problem gets harder.

Overlap factor integration comparison

$$\langle e^{i\varphi}\rangle(s_{max}) = \frac{\int_0^{s_{max}} ds\ \rho(s)\ \cos(\mu s)}{\int ds\ \rho(s)} = \frac{I_1(s_{max})}{I_2}$$





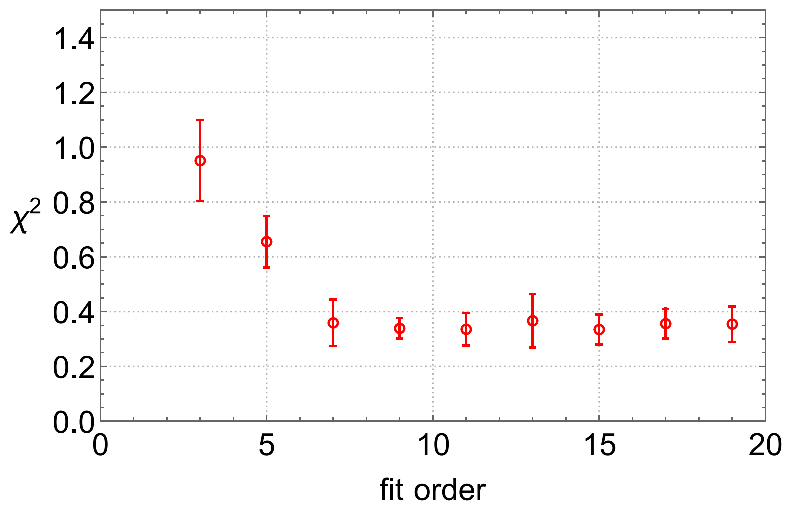


The fitted approach has a clear advantage, but

What polynomial order should we choose?

Optimal fitting order

Underfitting: a χ^2analysis is enough to determine if the functional form is adequate to describe the data.



Overfitting: if the polynomial order is too large we risk to introduce unwanted oscillations in the DoS.
We compare the Derivative of the fit with the second derivative of the DoS logarithm obtained via independent simulations.

$$\chi^2_{f''}(n) = \frac{1}{N}\sqrt{\sum_{i=1}^{N}\frac{\left(p'_n(s_i) - f''(s_i)\right)^2}{\sigma^2(f''(s_i))}}$$