Density of States method for complex action systems

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Introduction

Quantum Field theory at zero density

- Real Action
- Well defined Boltzmann weight
- Importance sampling Monte Carlo

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

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

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Sign Problem

Sign problem "hardness"

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

By dropping the imaginary part of the action $\quad Z_{PQ}(\mu) = \int \mathcal{D}\phi \, e^{-S_R(\phi)}$

We can define the overlap between the full and the phase quenched theory

$$O(\mu) = \frac{Z(\mu)}{Z_{PQ}(\mu)} = \langle \exp\{-i\mu S_I(\phi)\}\rangle \quad \propto \exp\{-\ V\ \Delta F\}$$

Standard reweighting

Simulate the phase quenched system and include the phase in the observables

$$\langle A \rangle = \frac{\langle A \exp\{-i\mu S_I(\phi)\}\rangle}{\langle \exp\{-i\mu S_I(\phi)\}\rangle}$$

An exponential number of Monte Carlo samples is needed.

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

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

The overlap can now be recovered via one simple integral and one oscillatory one

$$\langle e^{i\varphi} \rangle = \frac{\int ds \; \rho(s) \; \cos(\mu s)}{\int ds \; \rho(s)}$$

The DoS must be known to an incredible level of precision

Relativistic Bose Gas

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

Explicit field components: $\phi_x = \phi_{x,1} + i\phi_{x,2}$

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

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

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

LLR – Linear Logarithmic Relaxation [1]

- Restrict the system to a small imaginary action interval of amplitude Δ

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

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

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

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

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

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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 that of solving a stochastic equation to find the appropriate reweighting factor

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

Solving the stochastic equation

Newton Raphson root finding

$$a_{n+1} = a_n + \frac{\langle\langle \Delta S \rangle\rangle_{a_n}}{\langle\langle \Delta S \rangle\rangle'_{a_n}} \simeq \frac{12\ \langle\langle \Delta S \rangle\rangle_{a_n}}{\Delta^2}$$

Not suitable for stochasting equation

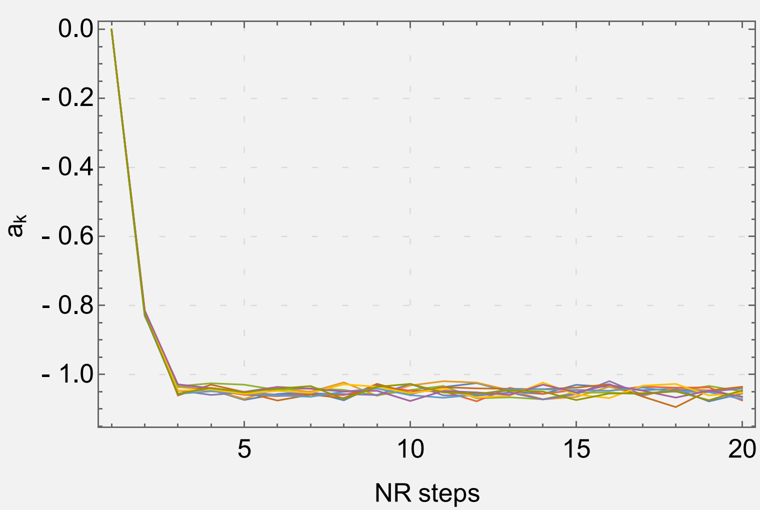
Robbins Monro[2] stochastic root finding

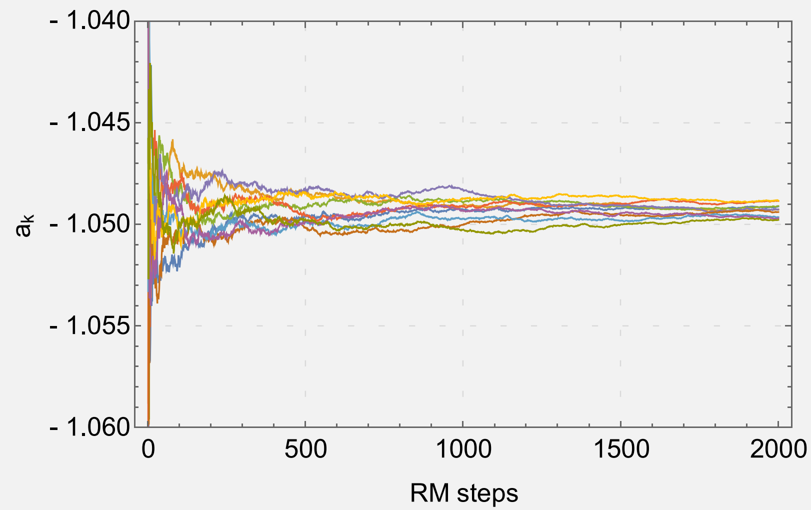
$$a_{n+1} = a_n - c_n \langle\langle \Delta S \rangle\rangle_{a_n}$$

if $$\sum_{n=0}^{\infty} c_n = \infty \qquad \sum_{n=0}^{\infty} c_n^2 < \infty$$ then $$\lim_{n\to\infty} a_n = a$$

To minimize the variance of the results one choses $$a_{n+1} = a_n - \frac{12\ \langle\langle \Delta S \rangle\rangle_n}{(n+1)\ \Delta^2}$$

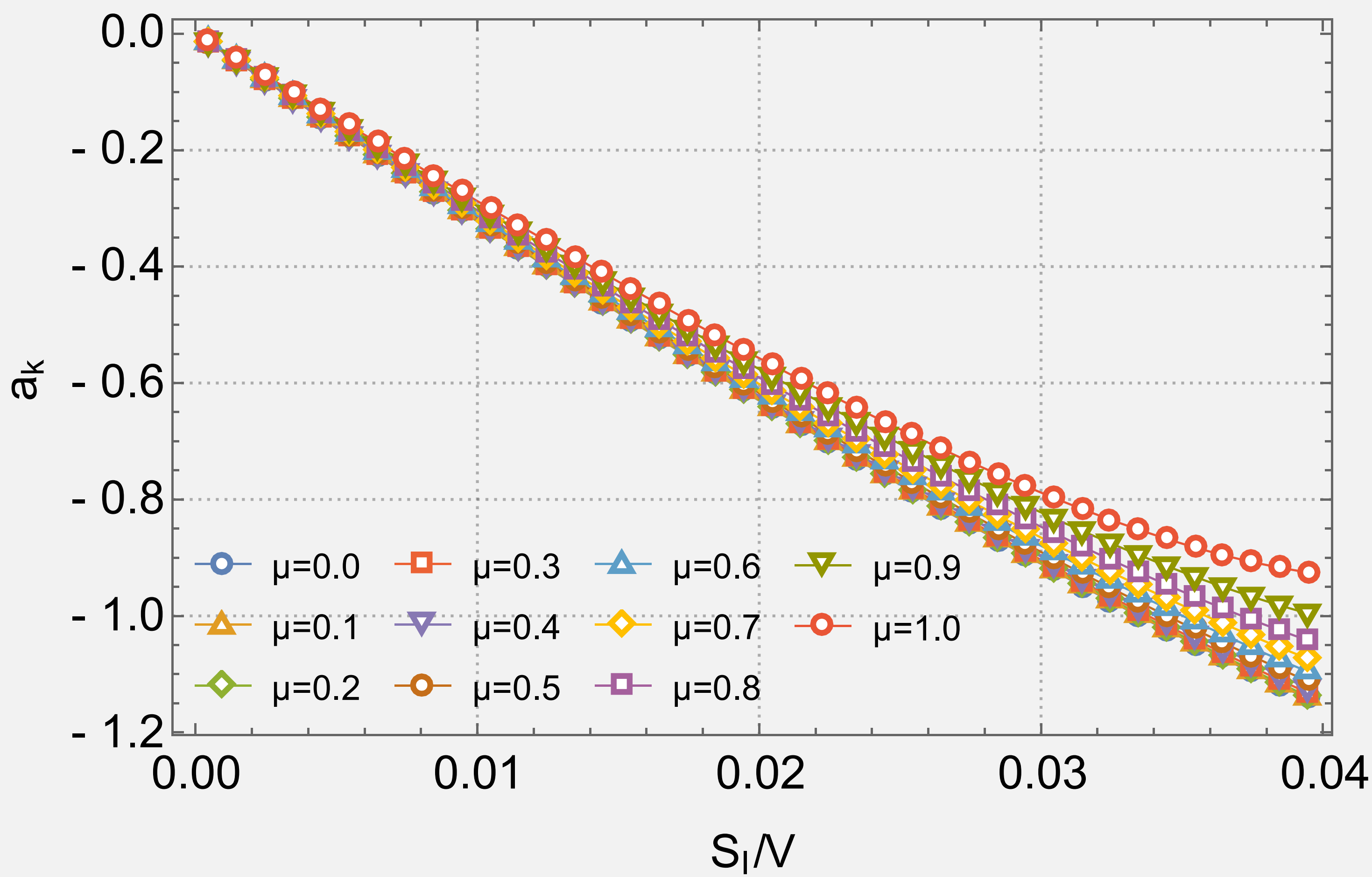
[2] Robbins, H.; Monro, The Annals of Mathematical Statistics 22





LLR simulation results

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



DoS Reconstruction

Piecewise approximation

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

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

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

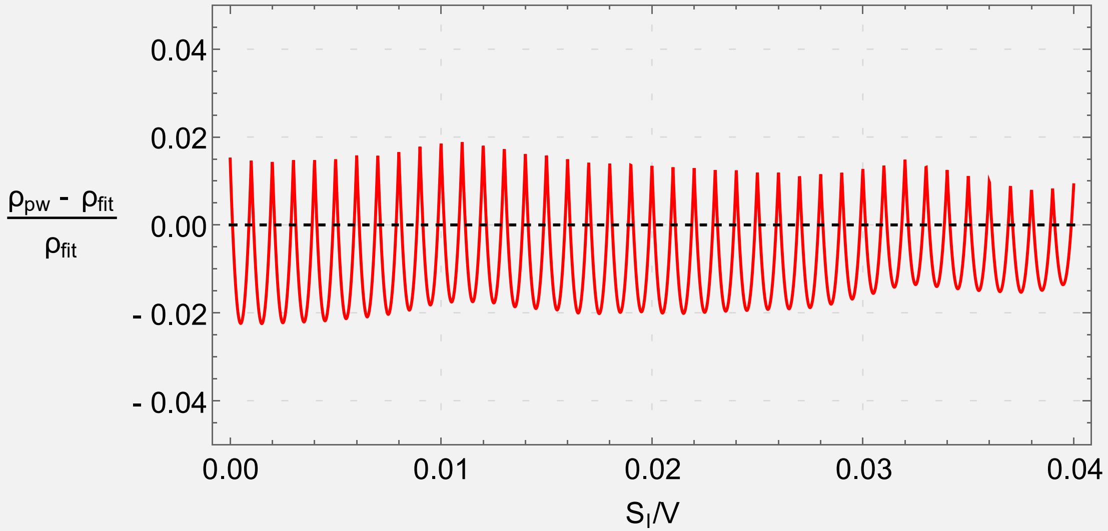
Exponential error suppression

Polynomial fit approximation

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

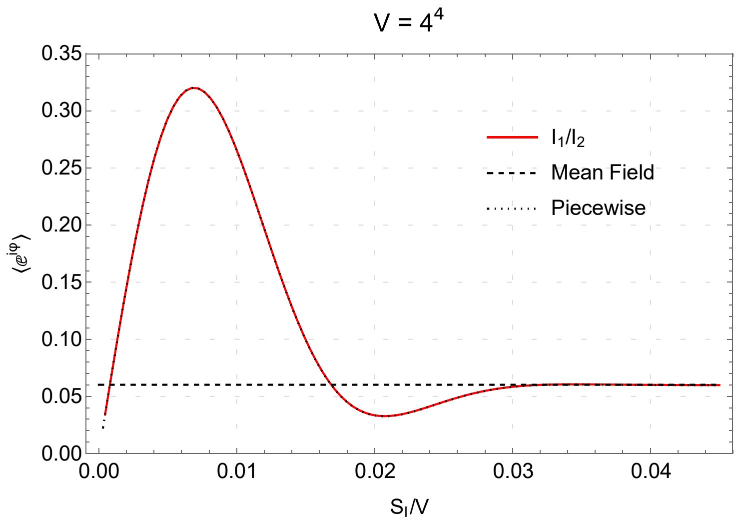
$$\rho_{fit}(s) = e^{\int_0^s p'_n(s') \ ds'}$$

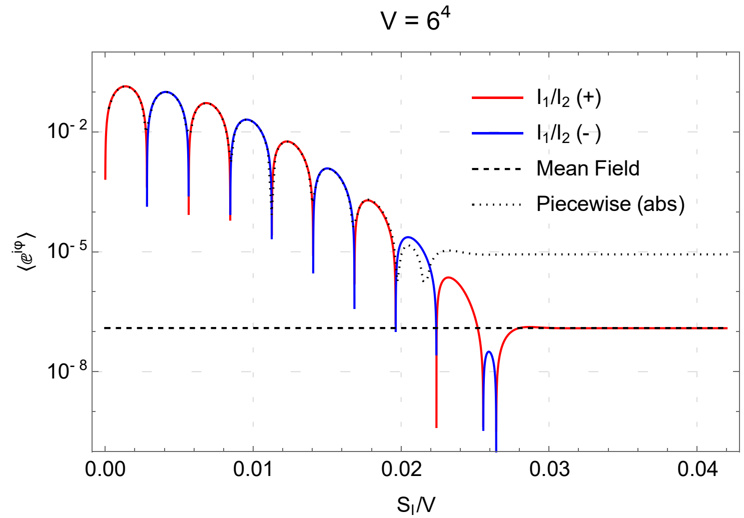
Exponential error suppression
Smooth

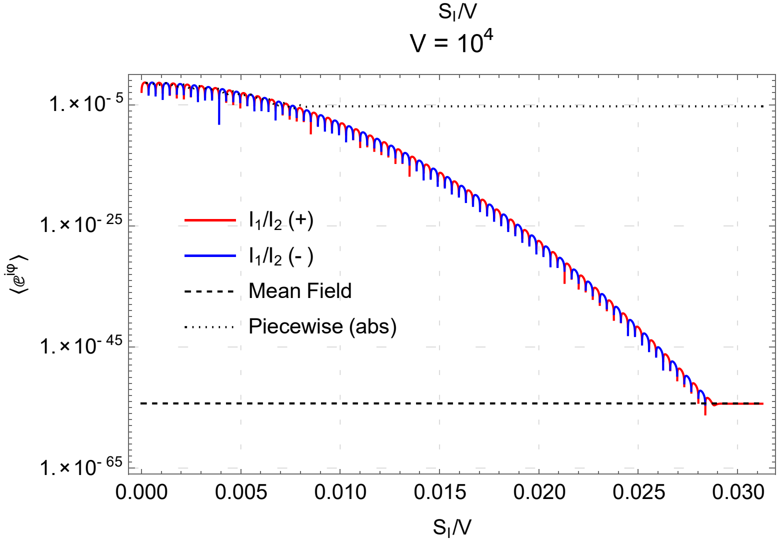


Overlap factor integration comparison

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







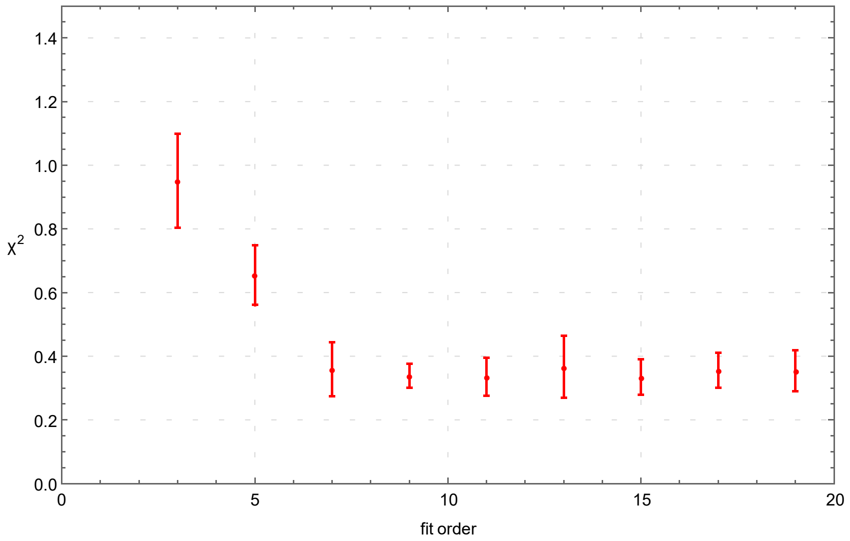
The fitted approximation is able to achieve the desired accuracy

Bias related to the fitting procedure is hard to detect.

What polynomial order should I choose?

Fitting order best choice

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



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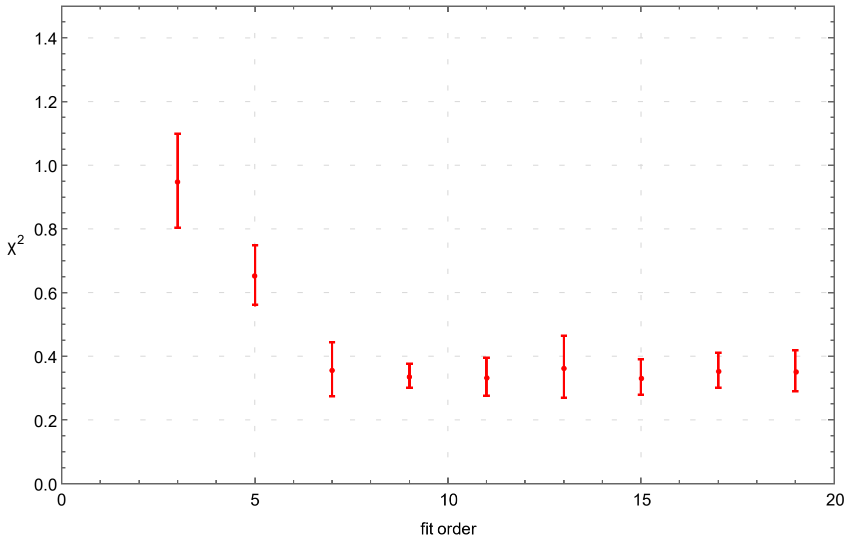


Overfitting

This is generally visible through unwanted oscillation of the interpolation between consecutive data points.

A χ^2 analysis will not detect it no matter how bad the overfitting.

Can we compare our fit to other observables other that the reweighting factor?

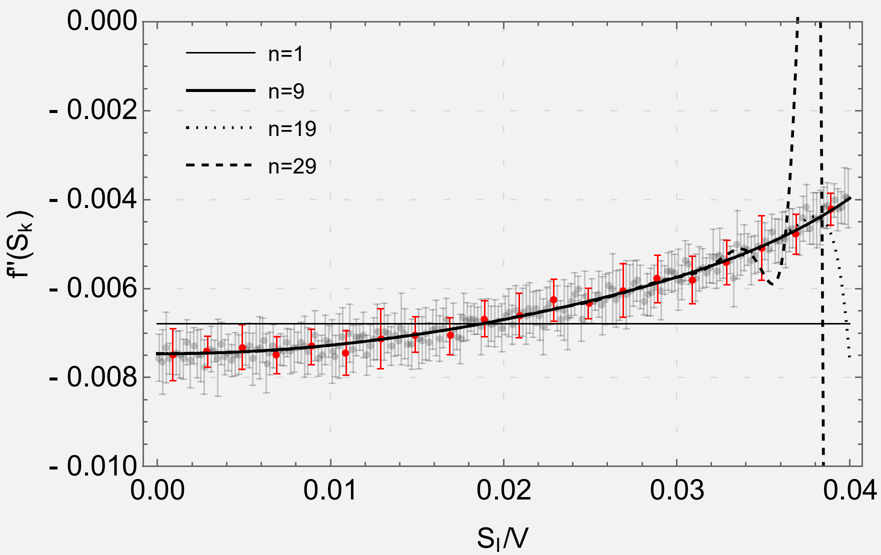
Second derivative fit validation

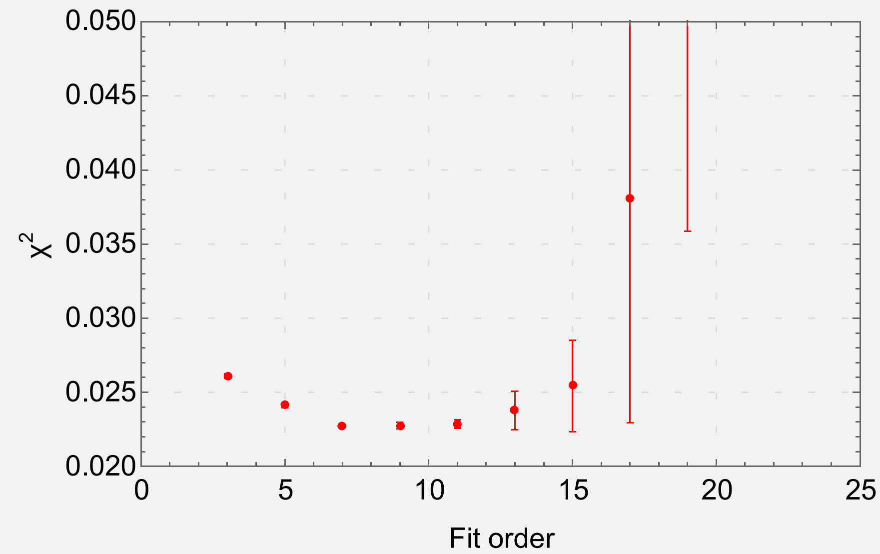
The second order derivative is defined as

$$f''(S_k) = \frac{360}{\Delta^4}\left(\langle\langle \Delta S^2\rangle\rangle_k - \frac{\Delta^2}{12}\right) + \mathcal{O}(\Delta^2)$$

A χ^2 analysis between these values and the derivative of the fit give us a quantitative indication of the overfitting.

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





LLR – Intrinsic Bias

The LLR algorithm converges to the right solution for $\Delta \to 0$

The variance of the Robbins Monro procedure instead goes as $\sigma_{RM} \propto 1/\Delta^2$

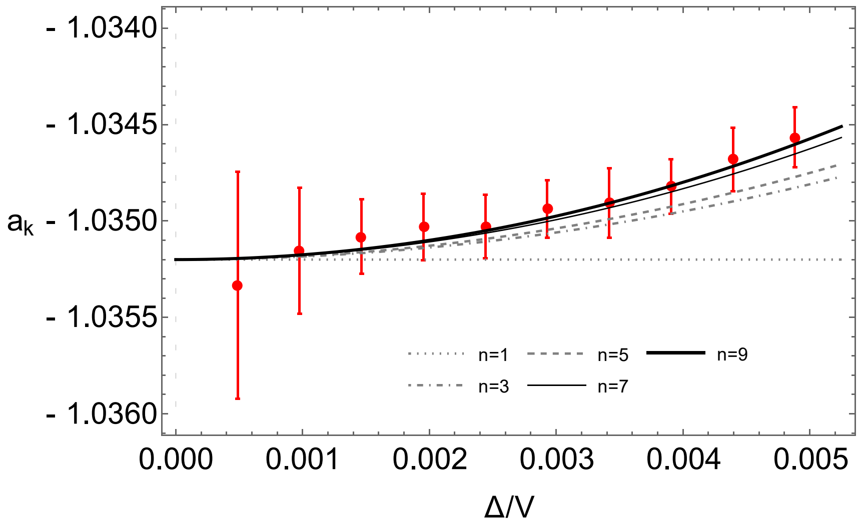
The first non vanishing term in the stochastic equation is

$$\langle\langle \Delta S \rangle\rangle_k (a = a_k) = \frac{f^{(3)}(S_k)}{3!} \frac{\Delta^4}{80} + \mathcal{O}(\Delta^6)$$

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

The solution to the modified equation will give an estimate of the bias

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



Bias optimized simulation

- Run a low precision simulation (fewer Monte Carlo samplings as well as Robbins-Monro steps) with a small and constant interval width for each interval, extract the values of the reweighting factor, and use those to estimate the bias over the complex action range taken into consideration.

- Scale the simulation parameters so that the bias estimate will be lower than the statistical noise.

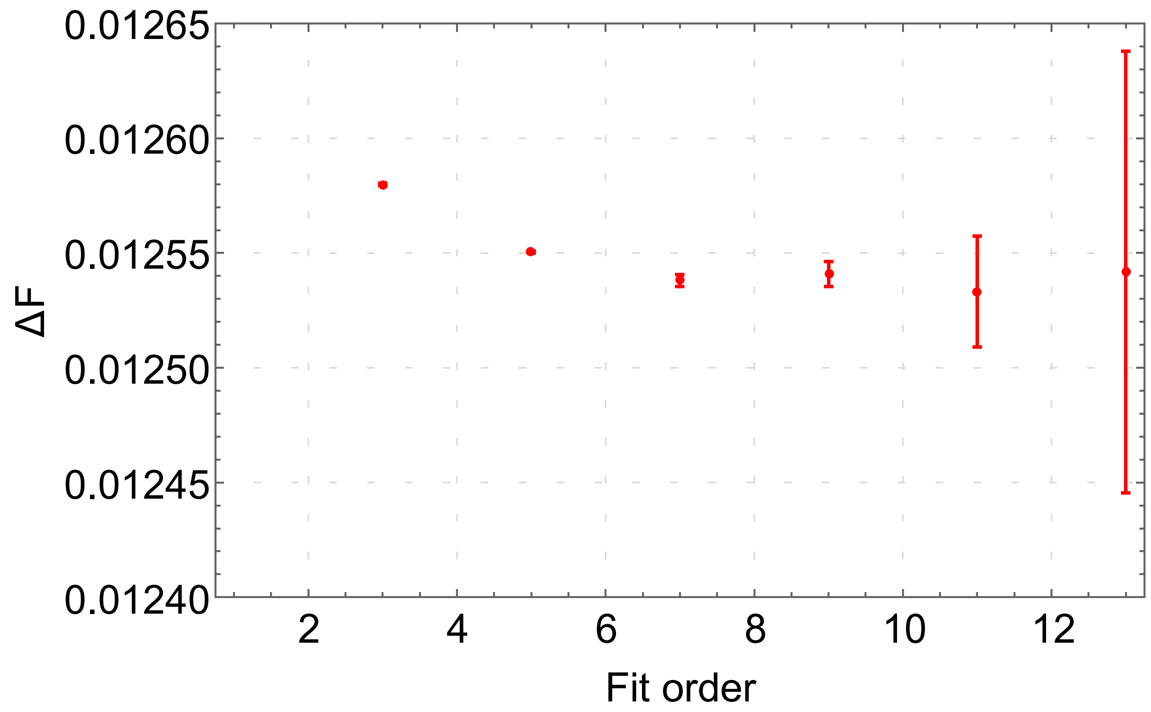
$$bias \propto \Delta^2 \qquad , \qquad \sigma \propto 1/\sqrt{N_{MC} * N_{RM}}$$

- With the scaled parameters run a high precision simulation, the results of which will be used to rebuilt the Dos.

- Lastly, using the high precision results double check that the bias is in fact negligible in comparison to the statistical noise of the results.

Benchmark study result

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



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

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

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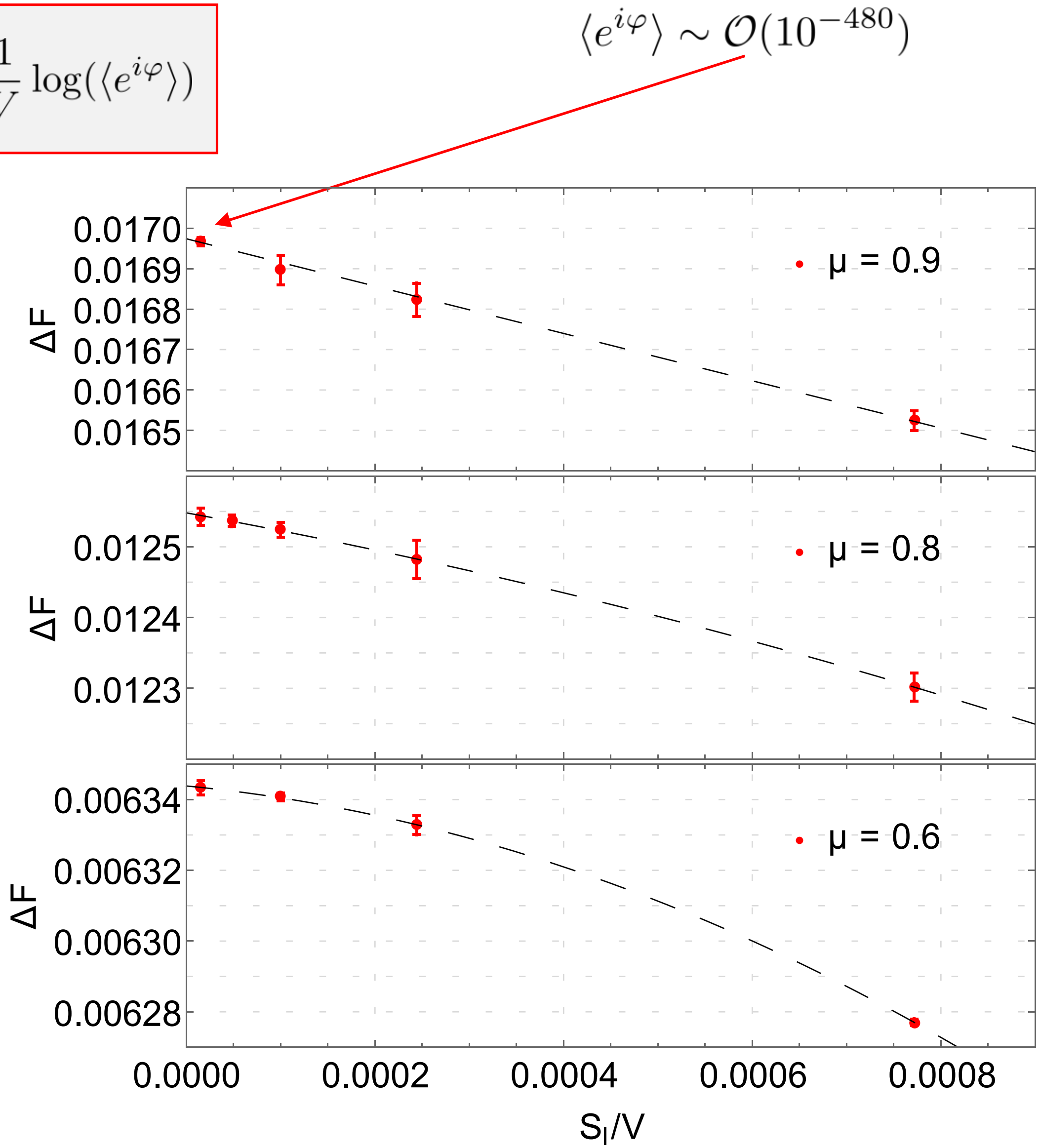

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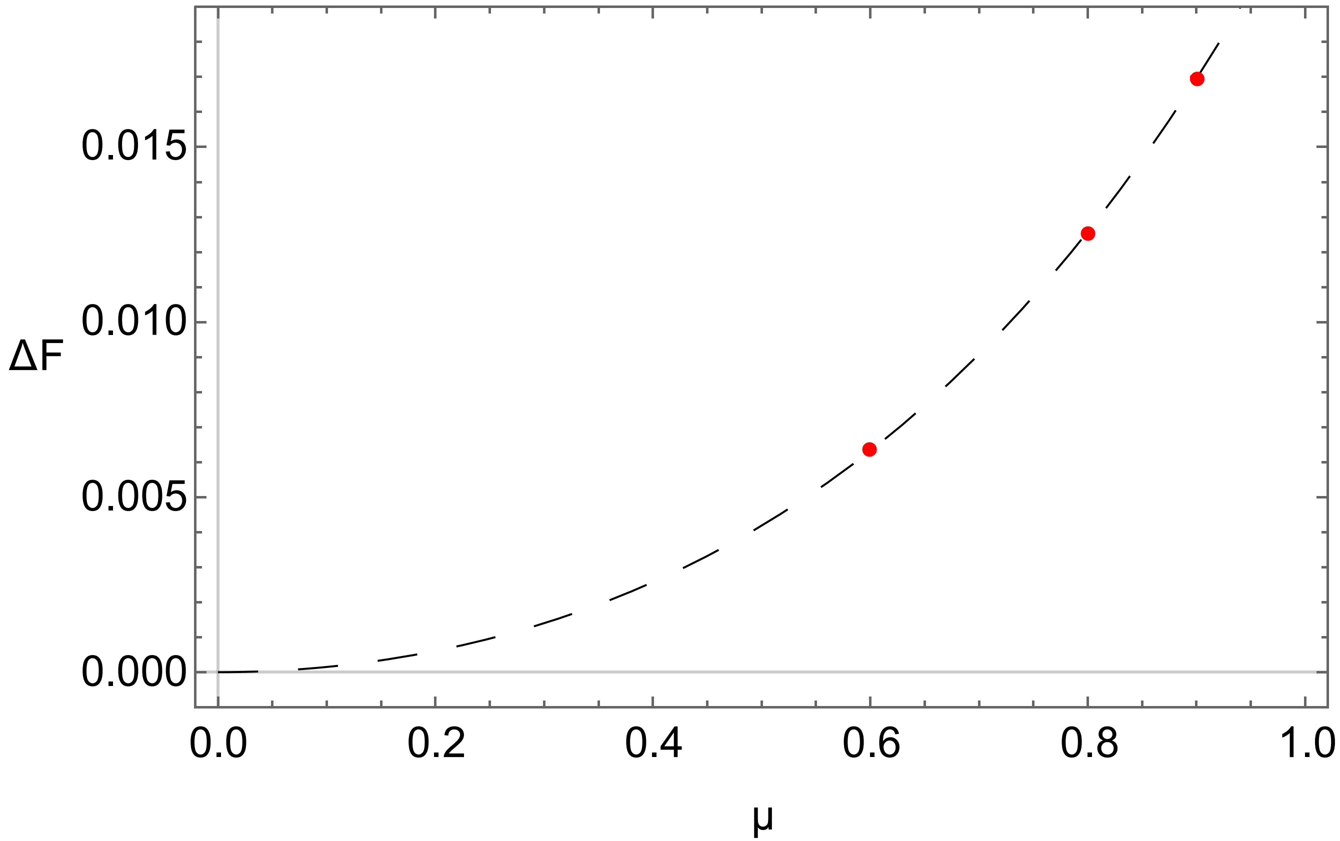

Conclusion and outlooks

- The density of states approach makes the simulation of complex action systems possible
- The LLR algorithm can approximate the DoS of the system over hundreds of orders of magnitude
- A careful fitting procedure enables us to evaluate consistently the oscillatory integral over hundreds orders of magnitudes
- The fitted reconstruction od the DoS enables us to recover information even on the higher derivative of the DoS.

- Implement a way to measure generic observables
- Start to study fermionic systems