About the phase of the fermion determinant in RMT

Jacques Bloch

Collaboration with Robert Lohmayer and Philipp Parzefall

University of Regensburg

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Outline

Investigation of distribution of phase of fermion determinant for RMT model of Osborn with chemical potential

1. Sign problem at nonzero chemical potential
2. Distribution of periodic phase
3. Definition and distribution of extensive phase
4. Gaussian Ansatz
5. Cumulant expansion
6. Quasinormal Ansatz

RMT with chemical potential

Osborn model:

$$Z = \int d\phi_1 d\phi_2 e^{-N\,\mathrm{tr}(\phi_1\phi_1^\dagger + \phi_2\phi_2^\dagger)} \det M$$

where ϕ_1, ϕ_2 are $N \times N$ complex random matrices

Dirac matrix

$$M(m,\mu) = D + m + \mu\Gamma^4$$

with

$$\underbrace{D = \begin{pmatrix} 0 & i\phi_1 \\ i\phi_1^\dagger & 0 \end{pmatrix}}_{\text{antihermitian}} \quad \text{and} \quad \underbrace{\Gamma_4 = \begin{pmatrix} 0 & \phi_2 \\ \phi_2^\dagger & 0 \end{pmatrix}}_{\text{hermitian}}$$

Observables and analytical results

Number density and chiral condensate

$$\Sigma = \frac{1}{2N}\frac{d\log Z}{dm} = \frac{1}{2N}\left\langle \mathrm{tr}[M^{-1}]\right\rangle$$
$$n = \frac{1}{2N}\frac{d\log Z}{d\mu} = \frac{1}{2N}\left\langle \mathrm{tr}\left[M^{-1}\Gamma_4\right]\right\rangle$$

Known analytical results in terms of generalized Laguerre polynomials (Osborn, Splittorff, Verbaarschot):

$$\Sigma = \frac{m}{1-\mu^2}\frac{L^1_{N-1}(q)}{L_N(q)}, \qquad n = -\frac{\mu}{1-\mu^2}\left[1-\frac{m^2}{1-\mu^2}\frac{L^1_{N-1}(q)}{L_N(q)}\right]$$

with $q = -\frac{Nm^2}{1-\mu^2}$.

Computing observables numerically: reweighting 😱

For $\mu \neq 0$: $\det M$ is complex $\Rightarrow$ NO importance sampling

Workaround: Reweighting

$$\langle y \rangle = \frac{\left\langle y e^{i\theta} \right\rangle_{\text{pq}}}{\left\langle e^{i\theta} \right\rangle_{\text{pq}}}, \qquad \text{with } \det M = R e^{i\theta}$$

Sign Problem

Cost grows exponentially with volume

Average phase factor and observables

Write partition function as

$$Z = Z_{\text{pq}} \langle e^{i\theta} \rangle_{\text{pq}}$$

Number density and chiral condensate

$$n = n_{\text{pq}} + \frac{1}{2N} \frac{d \log \langle e^{i\theta} \rangle_{\text{pq}}}{d\mu}, \qquad \Sigma = \Sigma_{\text{pq}} + \frac{1}{2N} \frac{d \log \langle e^{i\theta} \rangle_{\text{pq}}}{dm}$$

- easy: Compute $n_{\text{pq}}, \Sigma_{\text{pq}}$ from phase quenched Monte Carlo simulation
- hard: Dynamical correction? Use information about phase distribution

Phase distribution

Phase distribution of fermion determinant in phase quenched ensemble:
(Gocksch, PRL 61 (1988) 2054)

$$p(\theta) = \frac{1}{Z_{\text{pq}}} \int d\phi_1 d\phi_2 e^{-S_g} |\det M| \, \delta(\theta - \arg\det M)$$

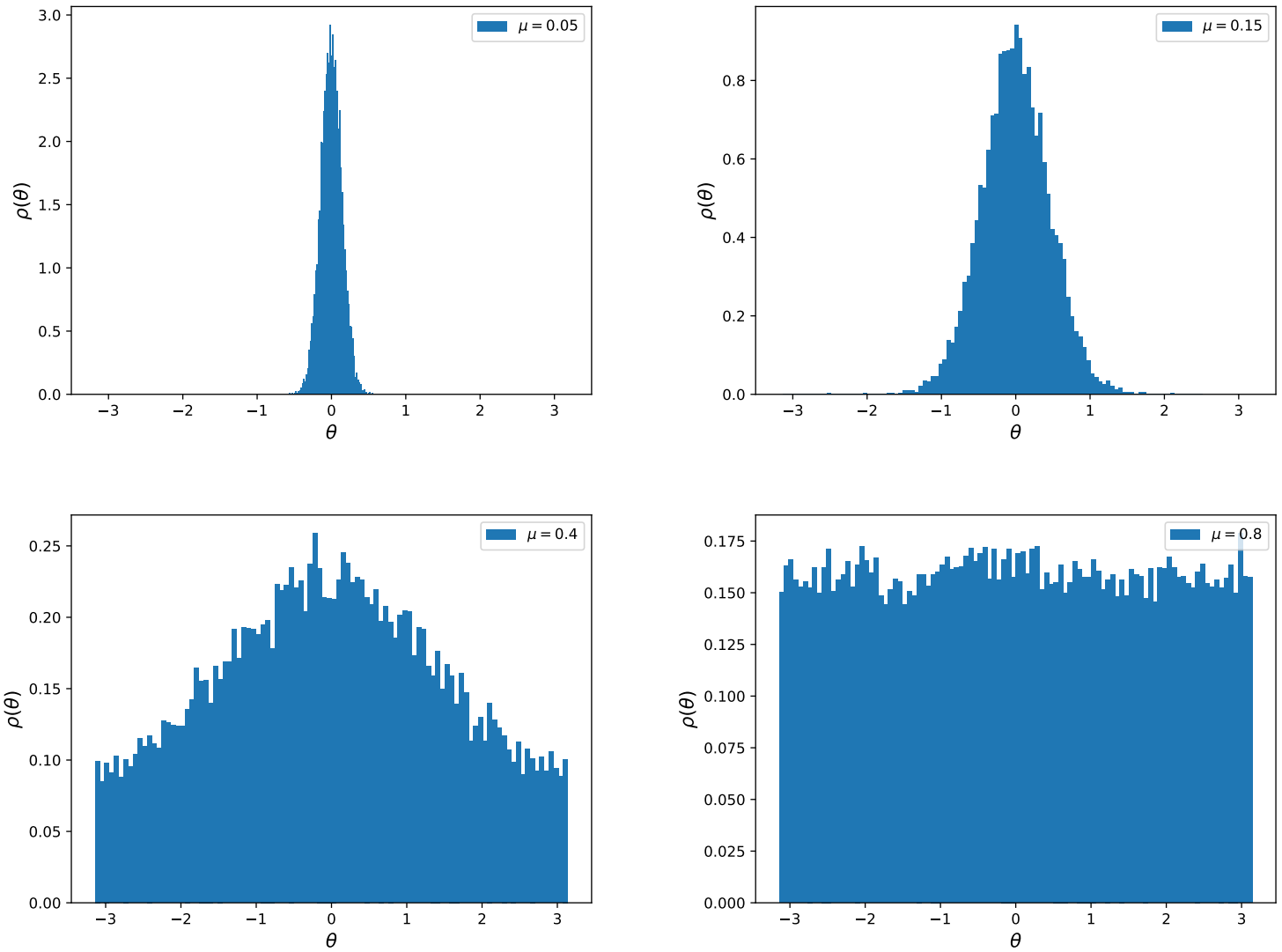
Such that

average phase factor

$$\langle e^{i\theta} \rangle_{\text{pq}} = \int d\theta \, p(\theta) \, e^{i\theta}$$

For periodic phase $\theta \in [-\pi, \pi)$: strong sign problem $\rightarrow$ $p(\theta)$ almost uniform $\rightarrow$ not useful

Distribution of periodic phase for $N = 8$ and $m = 0.1$



Extensive phase

Extensive phase for one configuration (ϕ_1, ϕ_2): (Ejiri et al.)

$$\theta(\mu) = \mathrm{Im} \int_0^\mu d\mu' \, \frac{d \log \det M(m, \mu')}{d\mu'} = \mathrm{Im} \int_0^\mu d\mu' \, \mathrm{tr}\left[M(m, \mu')^{-1} \Gamma_4 \right]$$

pro avoids branch cut discontinuities

con requires M^{-1} along μ-integration

Rewrite kernel

$$\theta(\mu) = \mathrm{Im} \int_0^\mu d\mu' \, \mathrm{tr}[(M_4(m) + \mu')^{-1}]$$

with Γ_4-Dirac matrix $M_4(m)$

$$M_4(m) = \Gamma_4^{-1}(D + m)$$

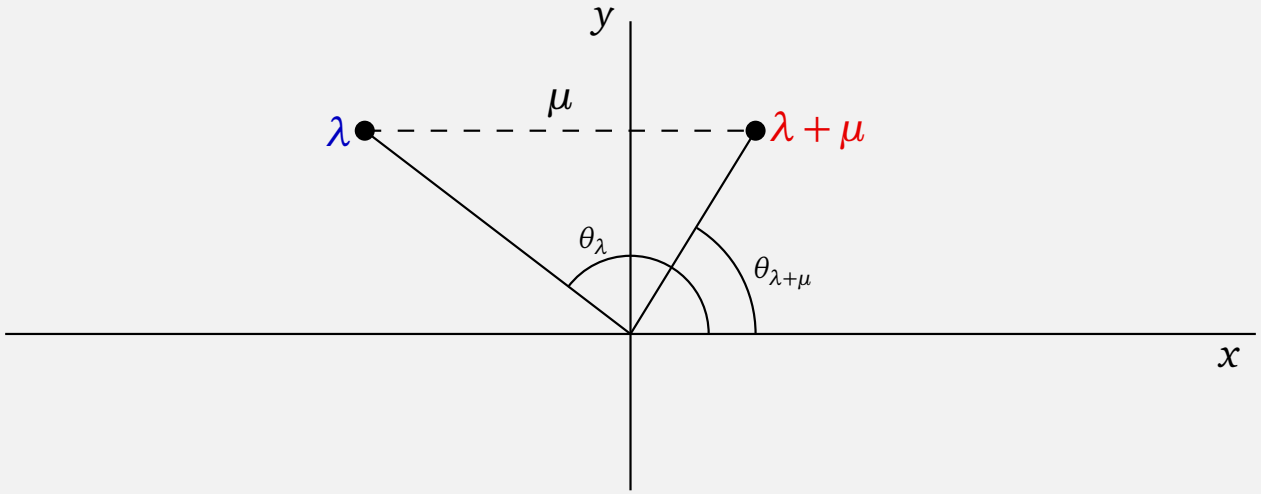
(similar to Ipsen and Splittorff, 2012)

Computing the extensive phase

Assume λ_k are eigenvalues of $M_4(m)$:

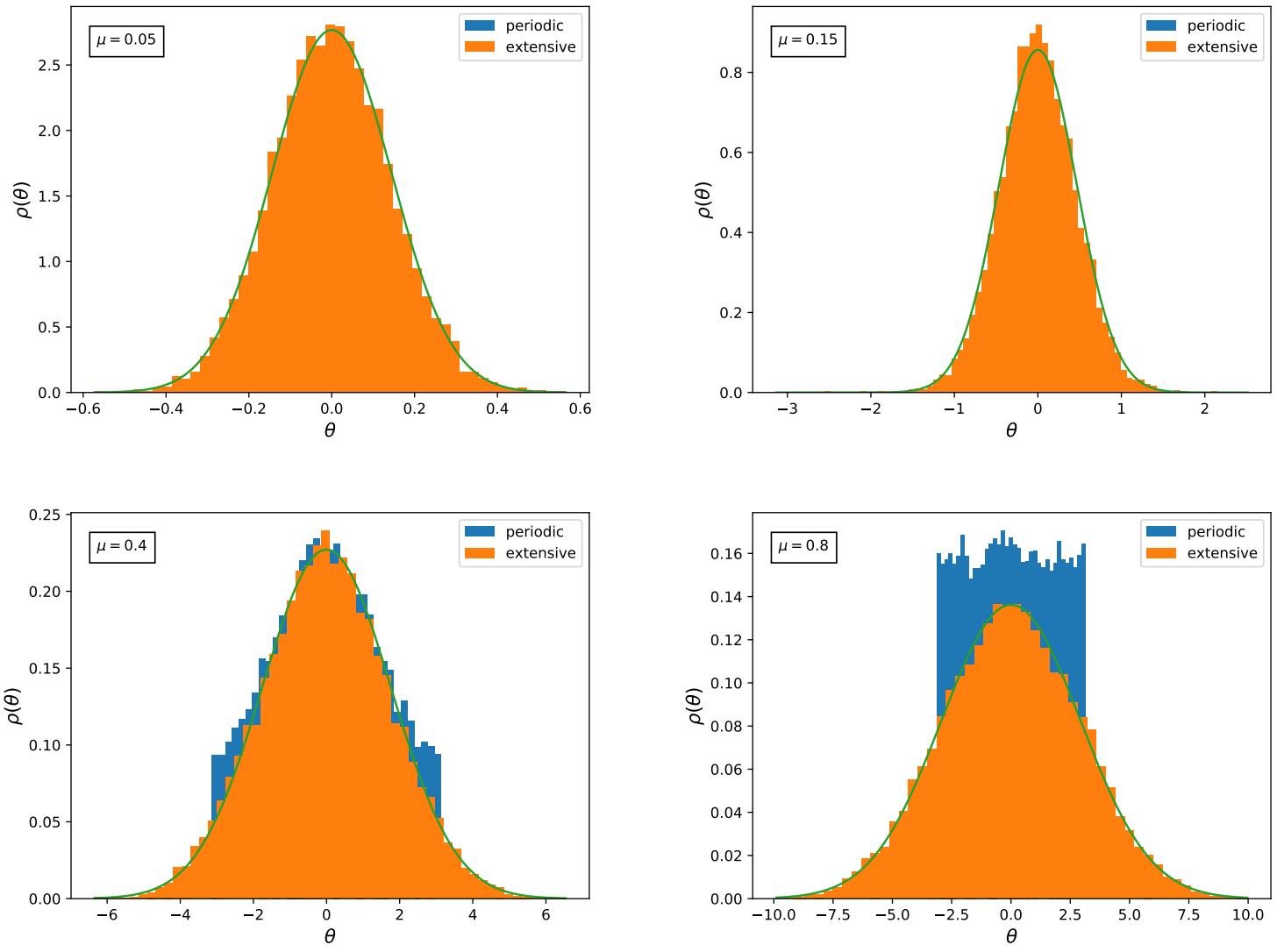
$$\theta(\mu) = \mathrm{Im} \int_0^\mu d\mu' \sum_k \frac{1}{\lambda_k + \mu'} = \sum_k [\arg(\lambda_k + \mu) - \arg(\lambda_k)]$$

μ shifts eigenvalues parallel to real axis $\rightarrow$ no branch cut discontinuities



Note: eigenvalues of M_4 come in pairs $(\lambda, -\lambda^*)$, i.e. mirrored wrt imaginary axis

Distribution of extensive phase for $N = 8$ and $m = 0.1$



How to determine and use phase distribution?

One possibility: LLR approximation (Langfeld, Lucini, Garron)

Accurate piece-wise linear approximation for $\ln p$ → exponential error suppression

- Method very expensive: θ-range subdivided in many intervals; each interval requires several Markov chains
- No clear gain: $\langle e^{i\theta} \rangle_{\text{pq}}$ computed by numerical integration of $p(\theta)\cos\theta$ Integral plagued by strong sign problem → needs very precise knowledge of $p(\theta)$.
- Exponential error suppression → relative error on $p(\theta)$ same for all θ → problem: absolute error in center of distribution $p(\theta)$ is too large.
- Observation: $p(\theta)$ can still be useful when fitted to smooth function

Using the phase distribution

Our approach

Avoid expensive LLR framework → determine $p(\theta)$ directly from phase quenched MC simulations (moments and histogram)

1. Gaussian Ansatz
2. Cumulant expansion
3. Quasinormal fit

Gaussian Ansatz

Gaussian Ansatz

$$p(\theta) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{\theta^2}{2\sigma^2}\right]$$

σ^2 from second moment

$$\langle \theta^2 \rangle_{\text{pq}} = \sigma^2$$

Average phase factor

$$\langle e^{i\theta} \rangle_{\text{pq}} = \exp\left(-\frac{\sigma^2}{2}\right) = \exp\left(-\frac{\langle \theta^2 \rangle_{\text{pq}}}{2}\right)$$

Number density for Gaussian Ansatz

Gaussian Ansatz

$$\log \langle e^{i\theta} \rangle_{\text{pq}} = -\frac{\langle \theta^2 \rangle_{\text{pq}}}{2}$$

Number density

$$n = n_{\text{pq}} + \frac{1}{2N} \frac{d \log \langle e^{i\theta} \rangle_{\text{pq}}}{d\mu}$$

Dynamical correction to particle density

$$\frac{d \log \langle e^{i\theta} \rangle_{\text{pq}}}{d\mu} = -\frac{1}{2} \frac{d \langle \theta^2 \rangle_{\text{pq}}}{d\mu}$$

Dynamical correction for Gaussian Ansatz

Compute derivative using finite differences

$$\frac{d\,\langle\theta^2\rangle_{\text{pq}}}{d\mu} = \frac{\langle\theta(\mu_+)^2\rangle_{\text{pq}+} - \langle\theta(\mu_-)^2\rangle_{\text{pq}-}}{\Delta\mu}$$

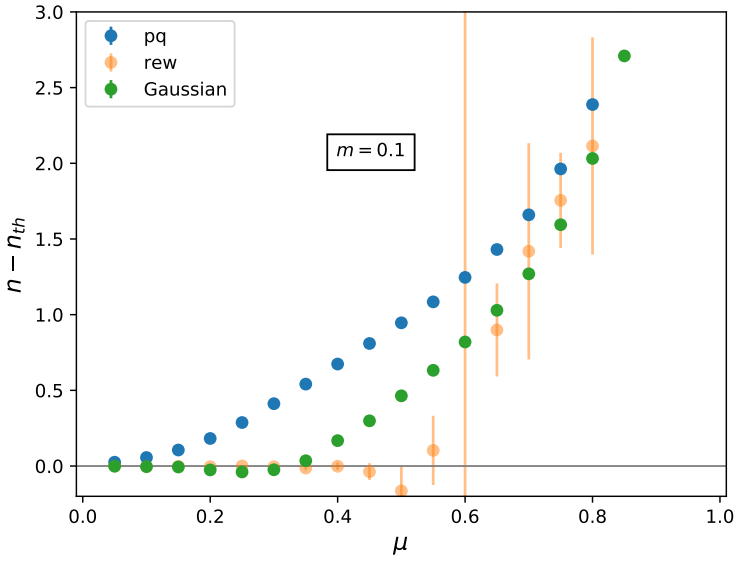
where $\langle\cdots\rangle_{\text{pq}\pm}$ are phase quenched ensemble averages at $\mu_\pm = \mu \pm \frac{\Delta\mu}{2}$

Reduce statistical error on finite difference by using reweighting

$$\langle\theta(\mu_\pm)^2\rangle_{\text{pq}\pm} = \frac{\left\langle \frac{|\det D_\pm|}{|\det D|}\theta(\mu_\pm)^2\right\rangle_{\text{pq}}}{\left\langle \frac{|\det D_\pm|}{|\det D|}\right\rangle_{\text{pq}}}$$

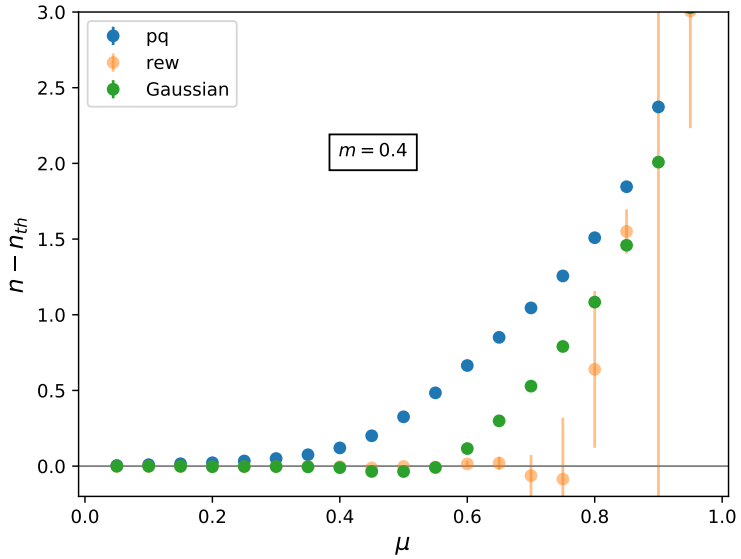
$\rightarrow$ No need for separate Markov chains at $\mu_\pm$
$\rightarrow$ Correlations strongly reduce statistical errors
$\Big\}\rightarrow$ very effficient

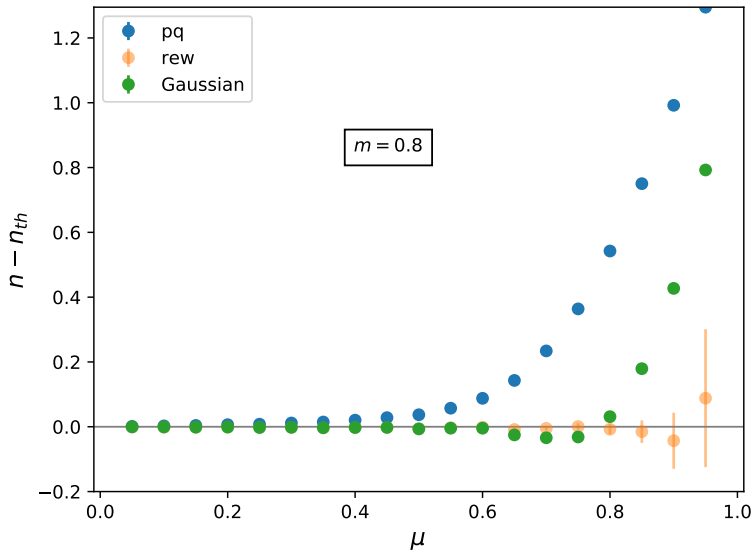
Number density from Gauss Ansatz



Subtract theoretical value:

$$\Delta n = n - n_{\text{th}}$$





Cumulant expansion

Cumulant expansion

$$\log \langle e^{i\theta} \rangle_{\text{pq}} = \sum_{i=1}^{\infty} \frac{(-1)^n}{(2n)!} C_{2n}$$

with cumulants (distribution even in θ):

$$C_2 = \langle \theta^2 \rangle_{\text{pq}}$$

$$C_4 = \langle \theta^4 \rangle_{\text{pq}} - 3 \langle \theta^2 \rangle_{\text{pq}}^2$$

$$C_6 = \left\langle \theta^6 \right\rangle_{\text{pq}} - 15 \left\langle \theta^2 \right\rangle_{\text{pq}} \left\langle \theta^4 \right\rangle_{\text{pq}} + 30 \left\langle \theta^2 \right\rangle_{\text{pq}}^3$$

$$\vdots$$

→ Easy to implement and efficient, elegant way to compute observables

→ BUT, is it any good?

Cumulant expansion: Dynamical correction

Dynamical correction to particle density

$$\frac{\log \langle e^{i\theta} \rangle_{\text{pq}}}{d\mu} = \sum_{n=1}^{\infty} \frac{(-1)^n}{(2n)!} \frac{dC_{2n}}{d\mu}$$

Compute derivative using finite difference with $C_{2n}\left(\langle \theta^2 \rangle_{\text{pq}}, \ldots, \langle \theta^{2n} \rangle_{\text{pq}}\right)$

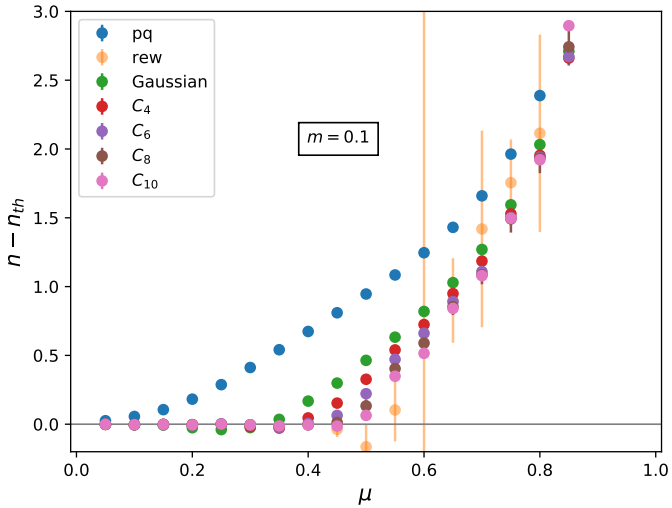
$$\frac{dC_{2n}}{d\mu} = \frac{C_{2n}^{+} - C_{2n}^{-}}{\Delta\mu}$$

where $C_{2n}^{\pm} = C_{2n}\left(\langle \theta(\mu_\pm)^2 \rangle_{\text{pq}\pm}, \ldots, \langle \theta(\mu_\pm)^{2n} \rangle_{\text{pq}\pm}\right)$ with $\mu_\pm = \mu \pm \frac{\Delta\mu}{2}$

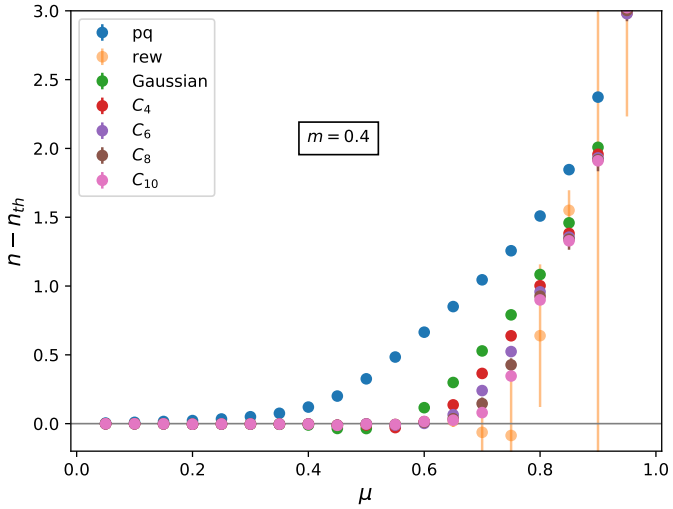
Reduce statistical error on finite difference by using reweighting

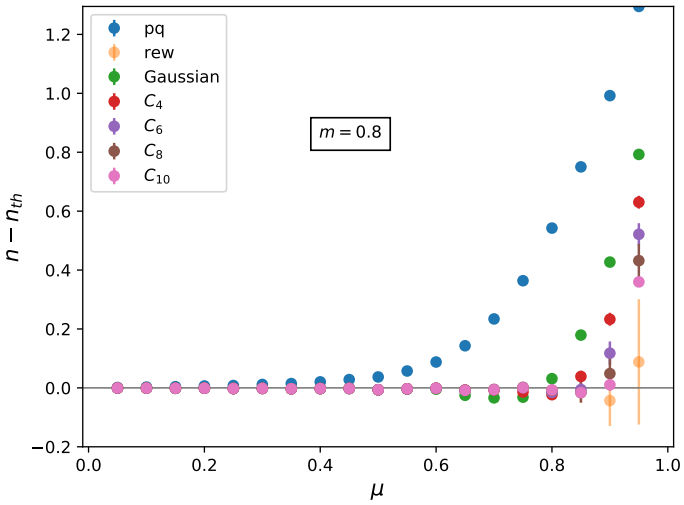
$$\langle \theta(\mu_\pm)^{2k} \rangle_{\text{pq}\pm} = \frac{\left\langle \frac{|\det D_\pm|}{|\det D|} \theta(\mu_\pm)^{2k} \right\rangle_{\text{pq}}}{\left\langle \frac{|\det D_\pm|}{|\det D|} \right\rangle_{\text{pq}}}$$

Number density from cumulant expansion



$$\Delta n = n - n_{\text{th}}$$

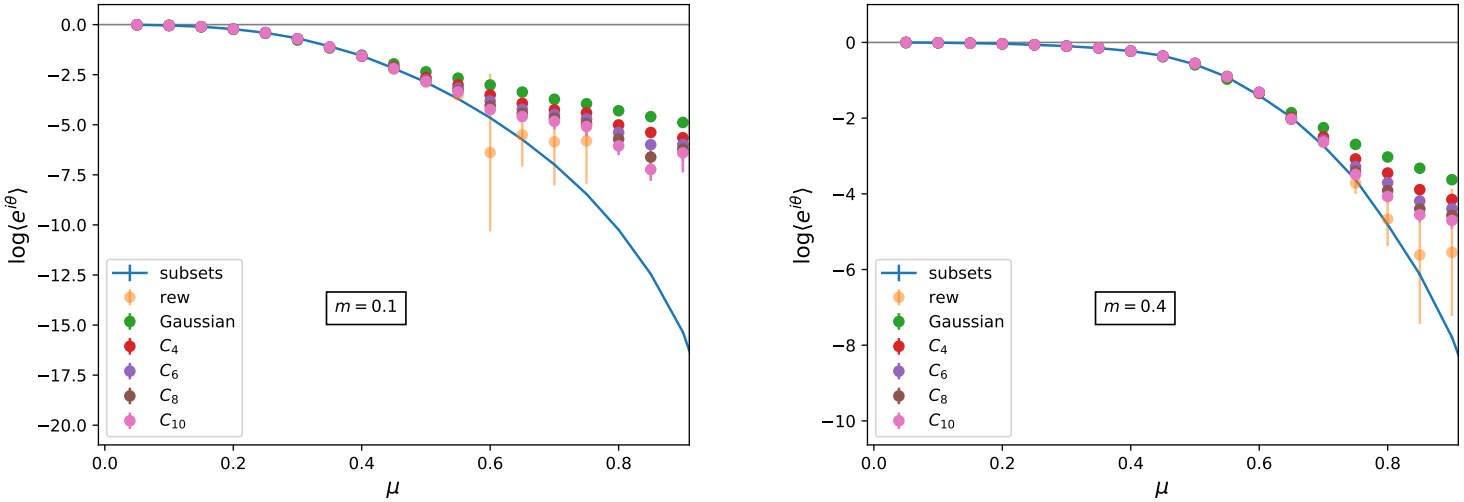




Cumulant expansion on same level as reweighting, but convergence too slow to determine systematical error or allow extrapolation

Cumulant expansion: Average phase factor

- Directly compare $\log \langle e^{i\theta} \rangle_{\text{pq}}$ from cumulant expansion with subset MC results. *Subsets for Osborn RMT is only method available to compute* $\langle e^{i\theta} \rangle_{pq}$ *up to machine precision (JB, 2012)*



→ Gaussian Ansatz: $\langle \theta^2 \rangle_{\text{pq}}$ grows as expected with volume, but insufficiently with μ! → Gaussian Ansatz does not describe the data
→ Cumulant expansion: convergence too slow → method not useful for treatment of sign problem

Alternative: quasinormal Ansatz

Assume distribution $p(\theta)$ of extended phase to be exponential of even polynomial in θ (motivated by Greensite, Myers, Splittorff, 2013)

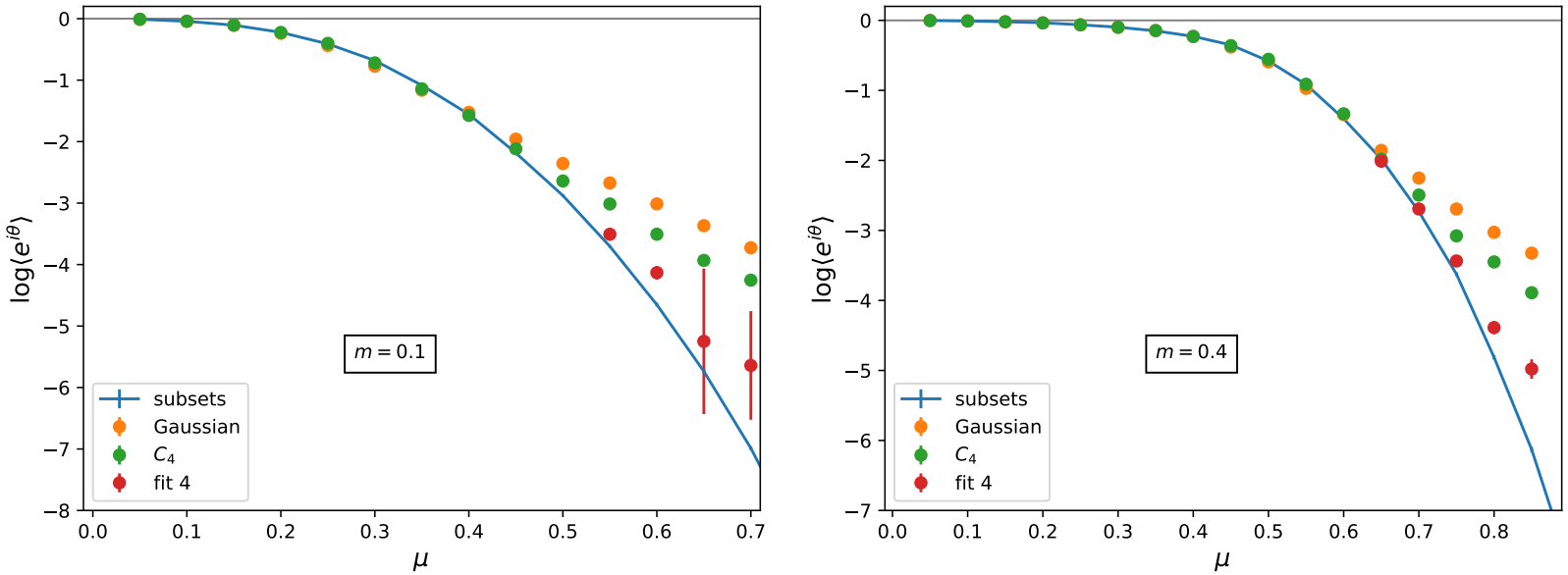
Ansatz: simplest extension of Gaussian distribution

$$p(\theta) = N \exp\left[-\frac{\theta^2}{2\sigma^2}\left(1 + a_4\frac{\theta^2}{\sigma^2} + a_6\frac{\theta^4}{\sigma^4} + \cdots\right)\right]$$

- Ansatz also suggested by our RMT simulations: $p(\theta)$ *almost* Gaussian with small nonzero higher order contributions.
- Parameters: can be fitted to moments $\langle\theta^{2k}\rangle$ or to histogram of $p(\theta)$ measured in phase quenched RMT simulations.

$\langle e^{i\theta} \rangle_{\text{pq}}$ from quasinormal Ansatz

Compare $\log \langle e^{i\theta} \rangle_{\text{pq}}$ computed from quartic Ansatz with NLO cumulant expansion (up to C_4)



$\langle e^{i\theta} \rangle_{\text{pq}}$ from quasinormal Ansatz

Compare $\log \langle e^{i\theta} \rangle_{\text{pq}}$ computed from hexic Ansatz with NNLO cumulant expansion (up to C_6)

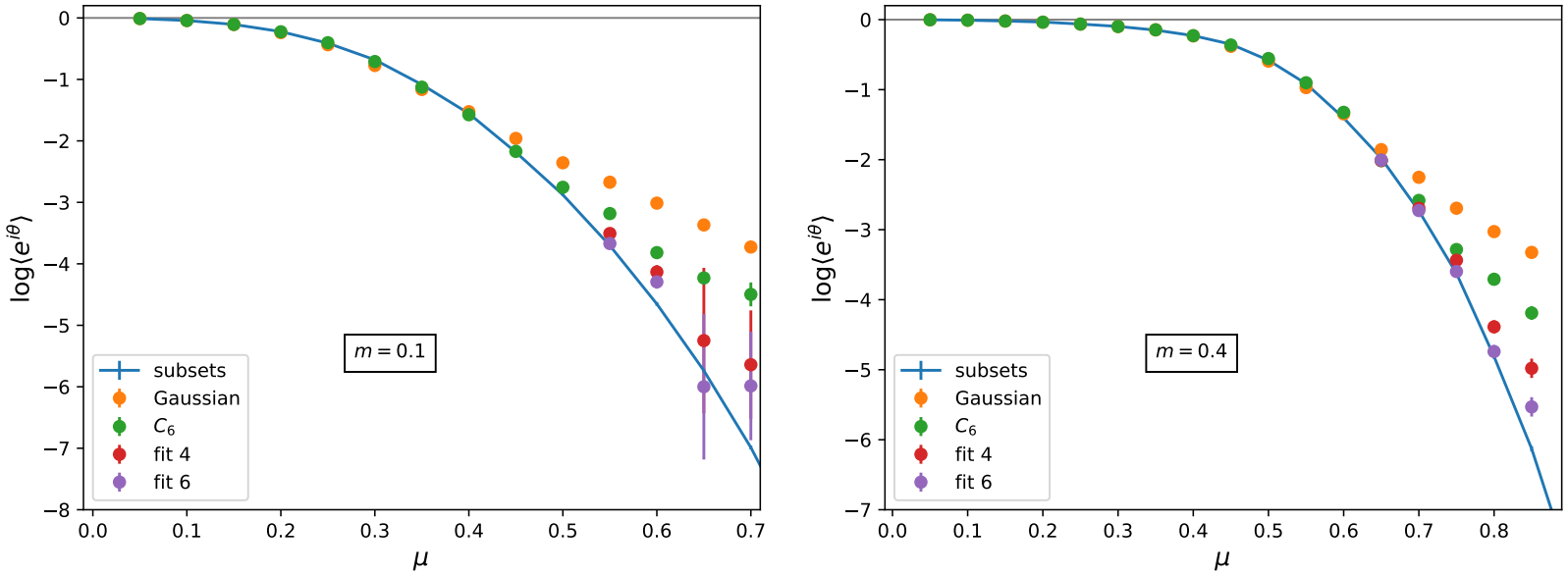
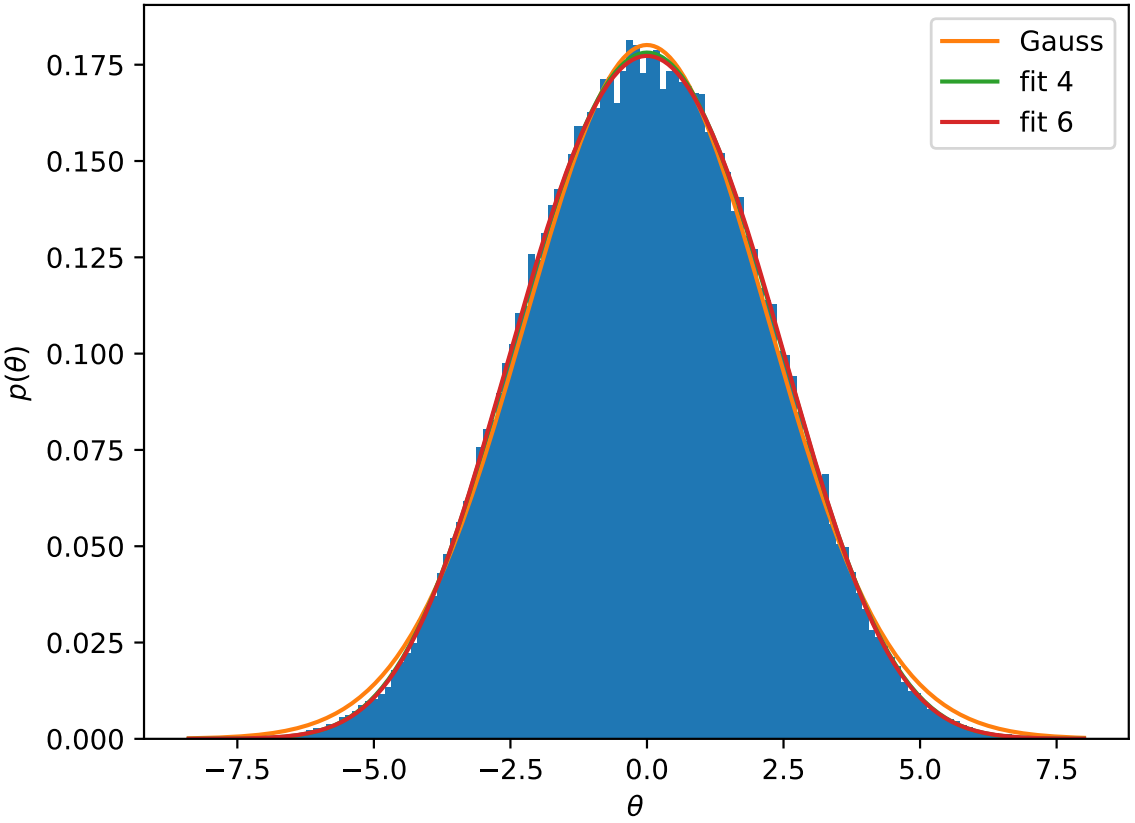


Illustration of fit

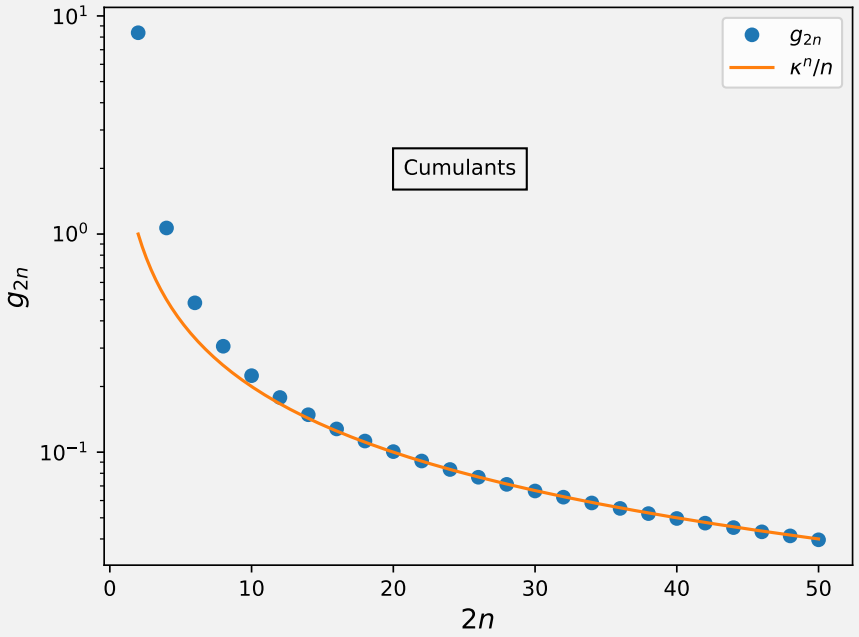
Example of fit for $N = 8, m = 0.4, \mu = 0.7$



Note on cumulant expansion

Mathematica computation of cumulants for quasinormal Ansatz with large sign problem

$$\log \langle e^{i\theta} \rangle_{\text{pq}} = -\sum_{i=1}^{\infty} g_{2n}, \qquad \text{with } g_{2n} = -\frac{(-1)^n}{(2n)!} C_{2n}$$



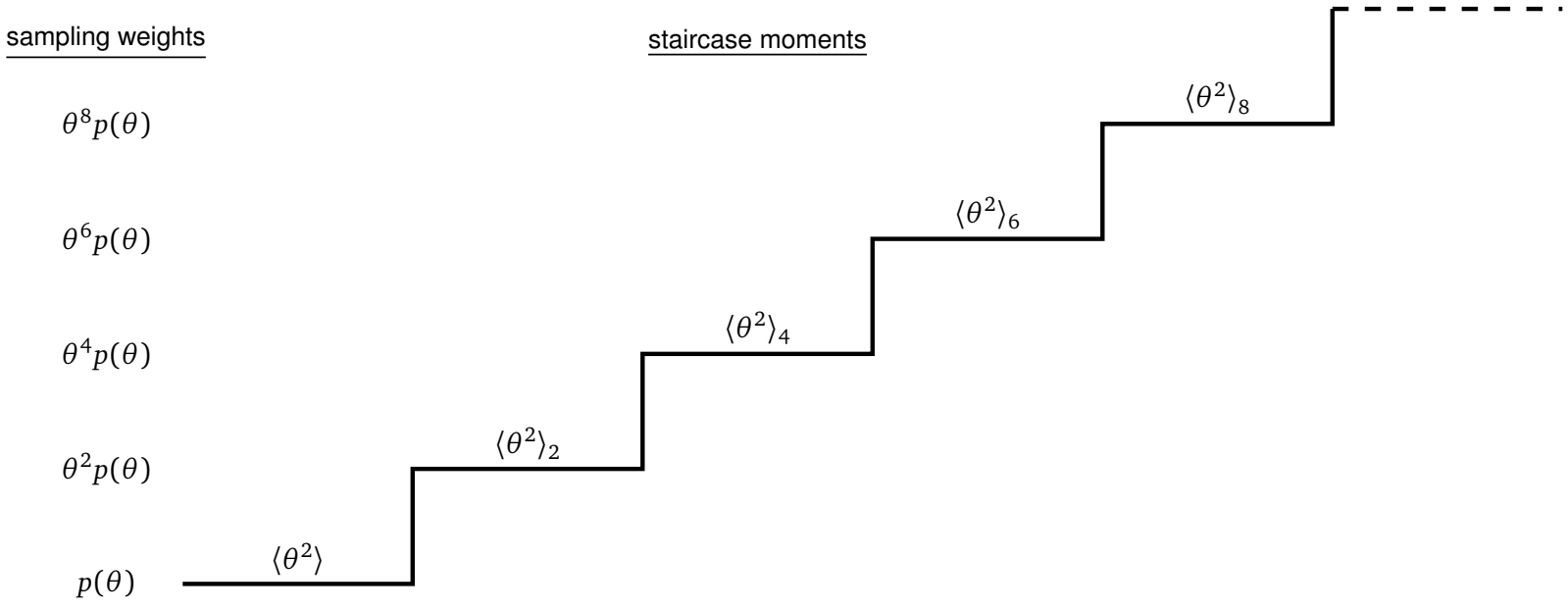
Fit: $f(2n) = \frac{\kappa^n}{n}$ $\rightarrow$ terms of Taylor expansion of $-\log(1-\kappa)$ with $\kappa \approx 1$

Resummation? Requires knowledge of cumulants to exponential accuracy!

Staircase moments

Improve accuracy of parameters of $p(\theta)$ by replacing moments $\langle\theta^{2n}\rangle$ by *staircase moments* $\langle\theta^2\rangle_{2n-2}$ (independent Markov chains)

$$\langle\theta^2\rangle_{2n-2} = \frac{\int d\theta p(\theta)\theta^{2n}}{\int d\theta p(\theta)\theta^{2n-2}}$$



Improved accuracy of moments

Moments of $p(\theta)$ are then given by the recursive formula

$$\langle \theta^{2n} \rangle = \langle \theta^{2n-2} \rangle \, \langle \theta^2 \rangle_{2n-2}$$

→ decrease statistical error on moments due to much better overlap when computing expectation value

Moments and relative standard deviation ϵ for a Gaussian distribution: improvement using the staircase method

Moment	Value	ϵ	ϵ_{sc}	$(\epsilon/\epsilon_{\text{sc}})^2$
$\langle \theta^2 \rangle$	σ^2	1.41	1.41	1.0
$\langle \theta^4 \rangle$	$3\sigma^4$	3.27	1.63	4.0
$\langle \theta^6 \rangle$	$15\sigma^6$	6.72	1.75	14.7
$\langle \theta^8 \rangle$	$105\sigma^8$	13.52	1.83	54.5
$\langle \theta^{10} \rangle$	$945\sigma^{10}$	27.06	1.89	204.8

→ Use staircase moments to determine parameters of $p(\theta)$

Conclusions and Outlook

- Gaussian Ansatz for phase distribution and cumulant expansion $\longrightarrow$ no reliable access to average phase factor
- Higher order fit Ansatz gives useful description of the phase distribution
- Further systematic investigations of statistical error and higher order effects are necessary
- Work on thimbles revealed that average phase can be very sensitive to quartic parameter a_4, but this was not encountered in present work
- Compute number density using fit Ansatz $\longrightarrow$ Requires derivative of parameters wrt μ
- Investigate usefulness of staircase moments