Analytic continuation from imaginary chemical potential, via a Cauchy formula inverse problem: state of the art

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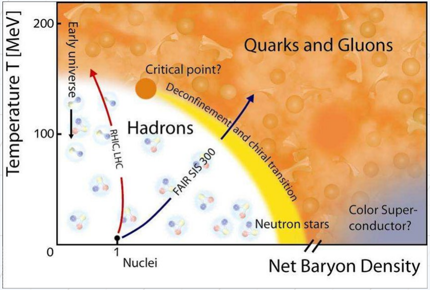
The Sign Problem

$$Z = \int \mathfrak{D}U \det(\mathcal{D}(\mu, U)) e^{-S[U]}$$

$$\mathcal{D} = \not{D} + m + \mu\gamma_0, \quad \gamma_5 \not{D} \gamma_5 = \not{D}^\dagger$$

$$\det(\not{D} + m + \mu\gamma_0) = \det(\not{D} + m - \mu_0^* \gamma_0)^*$$

- The study of the phase diagram requires finite baryon number density
- Finite density lattice simulations need chemical potential $\mu \neq 0$
- Generic $\mu \Rightarrow$ complex Dirac determinant, leads to sign problem
- For purely imaginary values of μ the Dirac determinant remains real
- Methods to extrapolate physical functions of real μ from the imaginary axis are needed



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Cumulants of the Partition Function

$$\chi_n(T,V,\mu_B) = \left(\frac{\partial}{\partial \mu_B}\right)^n \frac{\ln \mathcal{Z}(T,V,\mu_B)}{VT^3}$$

Change of variable

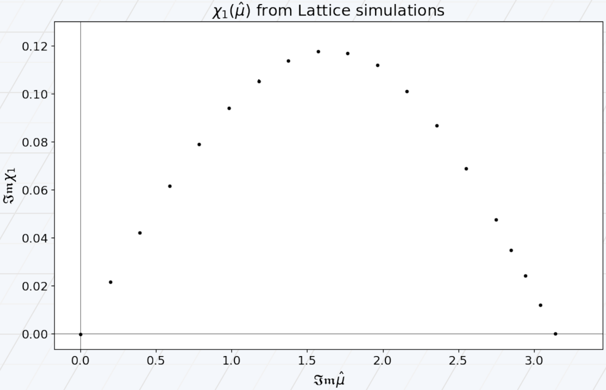
$$\hat{\mu} \equiv \mu_B/T$$

$$\chi_n(T,V,\hat{\mu}) = \left(\frac{\partial}{\partial \hat{\mu}}\right)^n \frac{\ln \mathcal{Z}(T,V,\hat{\mu})}{VT^{3+n}}$$

Charge conjugation symmetry

$$\chi_{2m}(T,V,\hat{\mu}) = \chi_{2m}(T,V,-\hat{\mu})$$

Baryon number density: $\chi_1(\hat{\mu})$



Data from the Bielefeld-Parma collaboration, obtained with $N_f = 2+1$ HISQ, at $N_\tau = 6$, $T = 157.5$ MeV and with physical pion masses.

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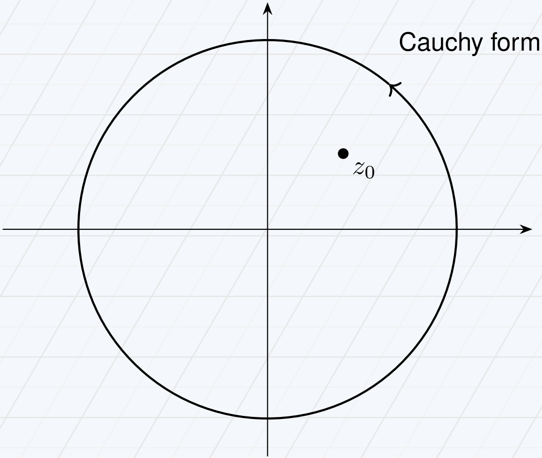
Cauchy Formula as an Inverse Problem



Cauchy formula: $f(z_0) = \frac{1}{2\pi i}\oint_{\mathcal{C}} \frac{f(z)}{z - z_0} dz$

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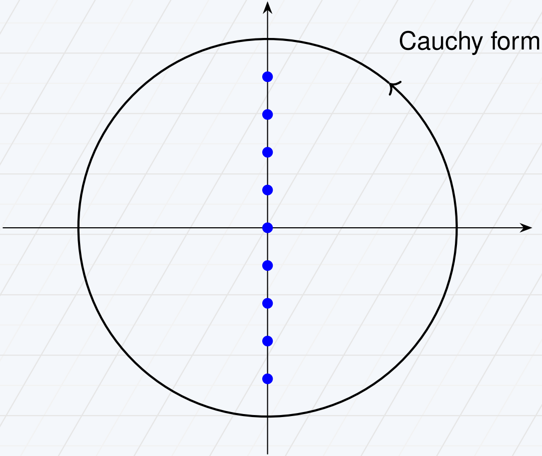
Cauchy Formula as an Inverse Problem



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$$\chi_1(\mu_j) = \frac{1}{2\pi}\int_0^{2\pi} \frac{Re^{i\theta}\chi_1(Re^{i\theta})}{Re^{i\theta} - \mu_j}d\theta$$

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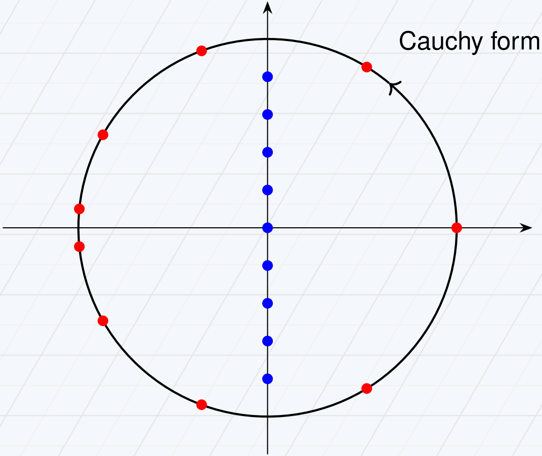
Cauchy Formula as an Inverse Problem



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Gauss-Legendre [Num. Recipes, 2007, Sec. 4.6]

$$\chi_1(\mu_j) \simeq \frac{1}{2\pi}\sum_{k=1}^{N} w_k \frac{Re^{i\theta_k}}{Re^{i\theta_k}-\mu_j}\hat{\chi}_k$$

$$j = 1, \ldots, N$$

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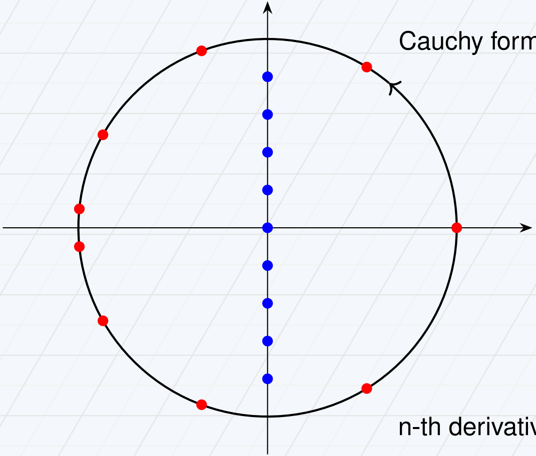

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$$j = 1, \ldots, N$$

n-th derivative: $f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{(z - z_0)^{n+1}} dz$

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Tikhonov Regularization

$$\chi_1(\mu_j) \simeq \frac{1}{2\pi}\sum_{k=1}^{N} w_k \frac{Re^{i\theta_k}}{Re^{i\theta_k}-\mu_j}\hat{\chi}_k \qquad \chi_{1+n}(0) \simeq \frac{n!}{2\pi}\sum_{k=1}^{N} w_k \frac{1}{R^n e^{in\theta_k}}\hat{\chi}_k = 0 \text{ for } n \text{ even}$$

$$\underbrace{\begin{pmatrix} \frac{w_1 Re^{i\theta_1}}{2\pi\left(Re^{i\theta_1}-\mu_1\right)} & \cdots & \frac{w_N Re^{i\theta_N}}{2\pi\left(Re^{i\theta_N}-\mu_1\right)} \\ \vdots & \ddots & \vdots \\ \frac{(2n)!w_1}{2\pi R^{2n}e^{2in\theta_1}} & \cdots & \frac{(2n)!w_N}{2\pi R^{2n}e^{2in\theta_N}} \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} \hat{\chi}_1 \\ \vdots \\ \hat{\chi}_N \end{pmatrix}}_{X} = \underbrace{\begin{pmatrix} \chi_1(\mu_1) \\ \vdots \\ 0 \end{pmatrix}}_{B}$$

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Tikhonov Regularization

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$$\underbrace{\begin{pmatrix} \frac{w_1 Re^{i\theta_1}}{2\pi(Re^{i\theta_1}-\mu_1)} & \cdots & \frac{w_N Re^{i\theta_N}}{2\pi(Re^{i\theta_N}-\mu_1)} \\ \vdots & \ddots & \vdots \\ \frac{(2n)!w_1}{2\pi R^{2n}e^{2in\theta_1}} & \cdots & \frac{(2n)!w_N}{2\pi R^{2n}e^{2in\theta_N}} \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} \hat{\chi}_1 \\ \vdots \\ \hat{\chi}_N \end{pmatrix}}_{X} = \underbrace{\begin{pmatrix} \chi_1(\mu_1) \\ \vdots \\ 0 \end{pmatrix}}_{B}$$

- Matrix A is ill-defined (big condition number, approximate formula, lattice data affected by errors).
- Instead of minimizing $||AX-B||^2$, a regularization parameter is introduced: $||AX-B||^2 + ||\alpha X||^2$ is minimized instead.
- After obtaining the unkowns X, the formula can be applied directly
  - to $\chi_1(\mu)$ for $|\mu| < R$
  - or to $\chi_{1+n}(0)$

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Analytic Continuation

Points on the real axis, $\mu_R \in \mathbb{R}$

$$\chi_1(\mu_R) = \sum_{k=1}^{N} \frac{w_k R e^{i\theta_k}}{2\pi(Re^{i\theta_k} - \mu_R)} \hat{\chi}_k$$

Variability of results depending on:

- Shape and size of the contour of integration
- Closeness of μ_R to the contour
- Interval of integration of θ

Derivatives at the origin ($\mu = 0$)

$$\chi_{1+(2n+1)}(0) = \sum_{k=1}^{N} \frac{(2n+1)! w_k}{2\pi R^{2n+1} e^{i(2n+1)\theta_k}} \hat{\chi}_k$$

- Taylor expansion allows to evaluate the function inside its radius of convergence
- Padé expansion estimates the closest singularity
- Ratios like χ_4/χ_2 or χ_6/χ_2 can be compared with experiments at particle colliders, however there is still debate on how μ_B and $\sqrt{s}$ are realated

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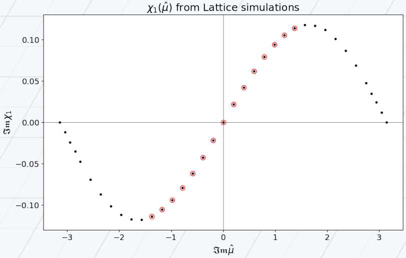
Higher Cumulants Extraction



$$\underbrace{n_{in}}_{\text{number of input points}} + \underbrace{n_D}_{\text{number of even derivatives set to } 0} + \underbrace{1}_{\text{Cauchy Formula}} = \underbrace{24}_{\text{Total conditions}}$$

$$R = \pi$$

Cauchy Formula

$$\oint_{\mathcal{C}} \chi_1(\mu) d\mu = 0$$

- Evaluation of even-order cumulants $\chi_{2k}(0)$
- Taylor expansion $O(\mu^7)$: $T_7 = \sum_{k=1}^{4} \frac{\chi_{2k}(0)}{(2k-1)!}\mu^{2k-1}$
- Taylor expansion $O(\mu^9)$: $T_9 = \sum_{k=1}^{5} \frac{\chi_{2k}(0)}{(2k-1)!}\mu^{2k-1}$

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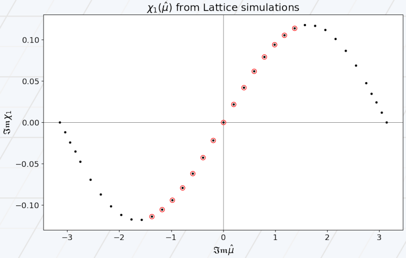

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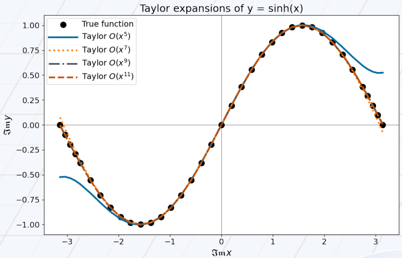

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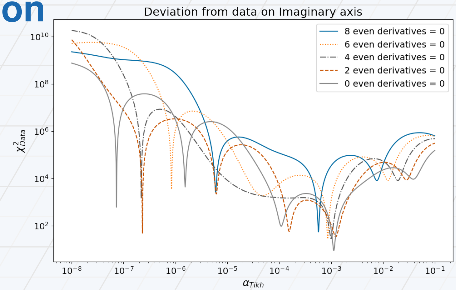
Tikhonov Parameter Selection

$$\chi^2_{Data} = \sum_i \left(\frac{\chi_1^{comp.}(\mu_i) - \chi_1^{Data}(\mu_i)}{\sigma_i} \right)^2$$



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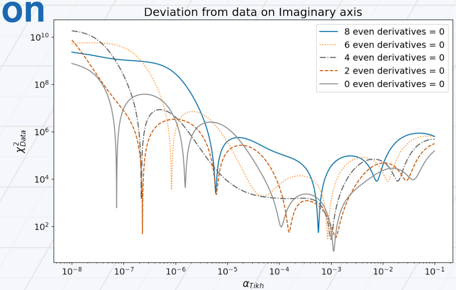
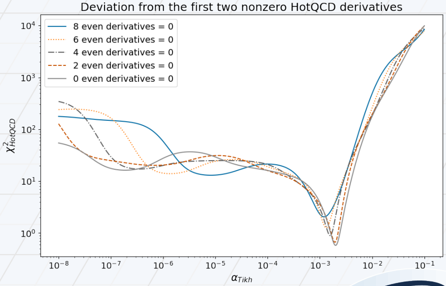
Cumulants from HotQCD collaboration [Bollweg et al., 2022] at $N_\tau = 6$ and $T = 157.5$ MeV:

HotQCD	
$\chi_2(0)$	$1.087(4) \times 10^{-1}$
$\chi_4(0)$	$8.4(4) \times 10^{-2}$

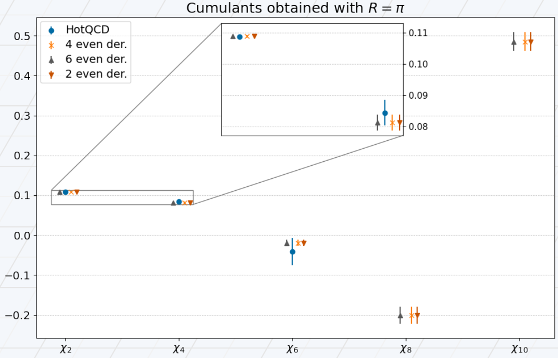
$$\chi^2_{HotQCD} = \sum_{i=2,4} \left(\frac{\chi_i^{comp.}(0) - \chi_i^{HotQCD}(0)}{\sigma_i^{HotQCD}} \right)^2$$





Cumulants at $\mu = 0$

- Results obtained by minimizing the χ^2_{HotQCD} variable
- Statistical errors estimated via a Jackknife analysis



	Cauchy	HotQCD
$\chi_2\ (0)$	$1.088(4) \times 10^{-1}$	$1.087(4) \times 10^{-1}$
$\chi_4\ (0)$	$8.12(25) \times 10^{-2}$	$8.44(41) \times 10^{-2}$
$\chi_6\ (0)$	$-2.1(8) \times 10^{-2}$	$-4(3) \times 10^{-2}$
$\chi_8\ (0)$	$-2.13(22) \times 10^{-1}$	$-7(9) \times 10^{-1}$
$\chi_{10}(0)$	$4.12(15) \times 10^{-1}$	

All measurements at $N_\tau = 6$ and $T = 157.5$ MeV; for HotQCD, χ_6 is obtained at $N_\tau = 8$ and χ_8 at $N_\tau = 8$ and through a different regularization scheme.

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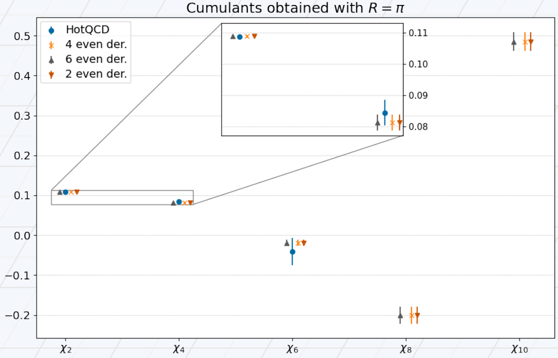
Systematics?

What happens if R changes?



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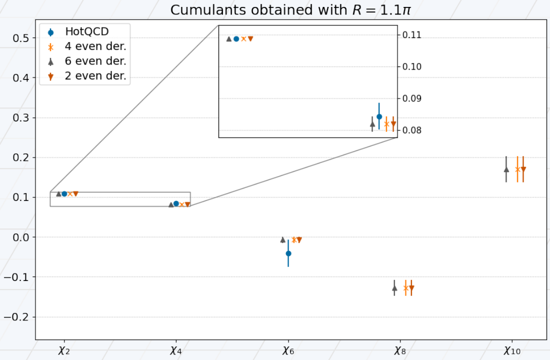
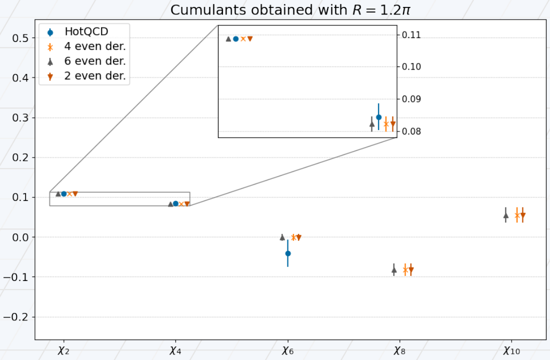
Cumulants at $\mu = 0$ - Systematics

- χ_8 starts to "oscillate"
- χ_{10} is highly unstable





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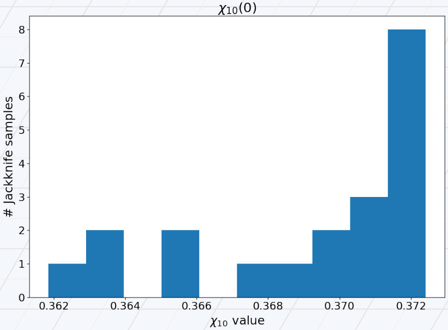
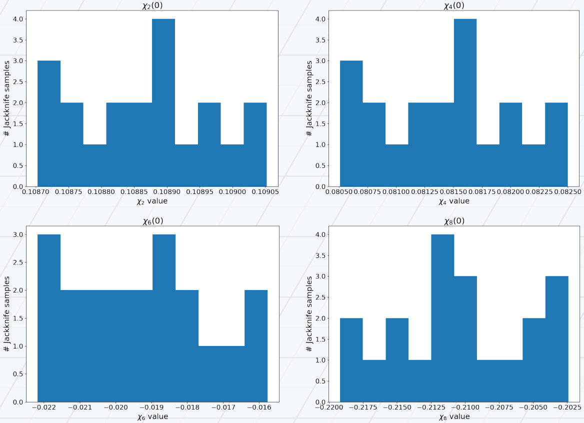
The χ_{10} anomaly

Let's inspect the cumulants computed for each Jackknife sample...





- Highly skewed, non-Gaussian distribution
- The order of derivative may be too high for our statistics to resolve it correctly

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Statistical + Systematic error analysis

	Cauchy	HotQCD
$\chi_2(0)$	$1.088(4)(0) \times 10^{-1}$	$1.087(4) \times 10^{-1}$
$\chi_4(0)$	$8.17(25)(2) \times 10^{-2}$	$8.44(41) \times 10^{-2}$
$\chi_6(0)$	$-1.1(8)(9) \times 10^{-2}$	$-4(3) \times 10^{-2}$
$\chi_8(0)$	$-1.46(22)(63) \times 10^{-1}$	$-7(9) \times 10^{-1}$
$\chi_{10}(0)$	$1.9(0.2)(1.9) \times 10^{-1}$	

- Systematics computed with computations at different values of $\pi \leq R \leq 1.2\pi$
- Closest singularity estimated with Padé: $4.2 < |\hat{\mu}_S| < 5.2$
- Radius up to $1.2\pi \lesssim 3.77$ is justified
- Estimation of χ_{10} is NOT to be trusted

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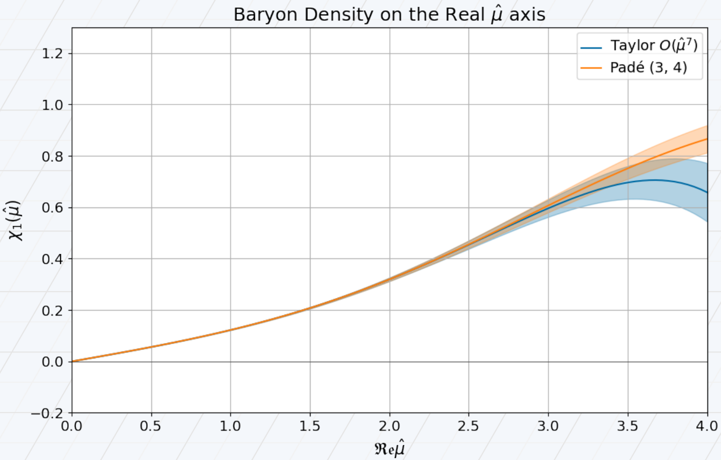
Analytic Continuation

- Obtained with cumulants up to $\chi_8(0)$
- Preliminary statistical analysis; Systematics are yet to be determined



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Conclusions and Future Outlooks

- Discretizing the Cauchy formula allowed a precise estimation of the first 4 nonzero cumulants of the partition function;
- The ill-conditioned system has been regularized with a Tikhonov parameter, that has been tuned by using the direct computation of the χ_2 and the χ_4 present in the literature;
- Overall, the higher order cumulants are obtained with a fairly high accuracy and much lower computational power than the ones obtained by direct evaluation with Monte Carlo simulations;
- The χ_{10} is too unstable for the current statistics we are working with;
- The systematic effects on the analytic continuation of the baryon number density $\chi_1(\hat{\mu}_R)$ are still to be determined...

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Thank you for your attention

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Bibliography

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