

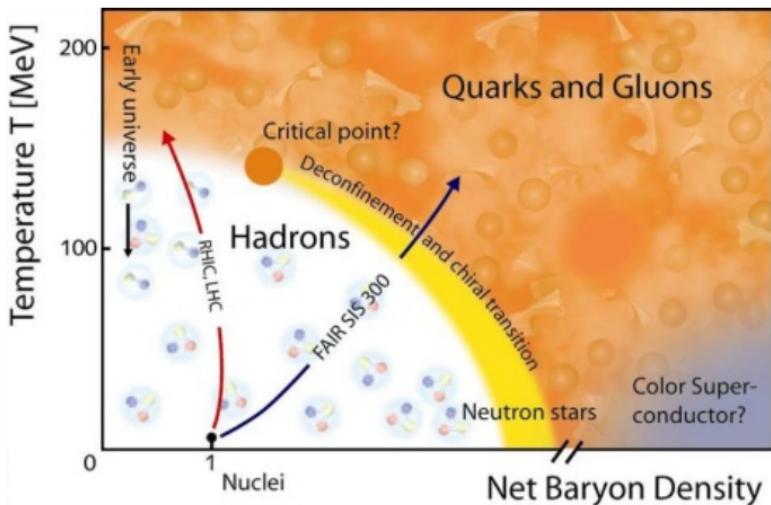
Taylor expansion and the Cauchy Residue Theorem for finite-density QCD

Benjamin Jäger



In collaboration with **Philippe de Forcrand** (ETH Zürich)

Phase diagram for QCD



Taylor Expansion

- Expand around small chemical potentials μ

$$\frac{P(\mu, t)}{T^4} = \sum_k c_k(T) \left(\frac{\mu}{T} \right)^k, \quad k = 0, 2, \dots$$

- The Taylor coefficients can be computed at $\mu = 0$

$$c_k = \frac{1}{n! V T^3} \left. \frac{\partial^k \log Z}{\partial (\mu/T)^k} \right|_{\mu=0}$$

- Typical building blocks

$$\text{Tr} \left(M^{-1} \frac{\partial M}{\partial \mu} \right), \dots, \text{Tr} \left(M^{-1} \frac{\partial^2 M}{\partial \mu^2} M^{-5} \frac{\partial^4 M}{\partial \mu^4} \right)$$

- Use linear chemical potential to reduce to single form

[Gavai & Sharma, 2014]

$$\text{Tr} \left[\left(M^{-1} \frac{\partial M}{\partial \mu} \right)^k \right]$$

- Estimate traces using **many** noise vectors

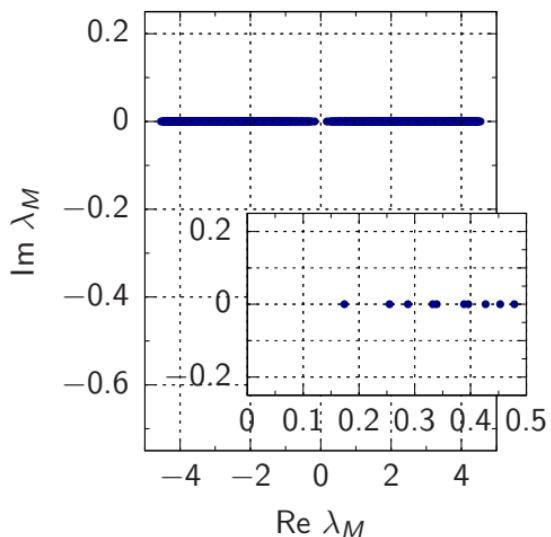
Spectrum

Staggered quarks: $4 \cdot 4^3$, $N_f = 4$, $\beta = 5.05$, $m = 0.07$

Hermitian matrix

$$i\phi$$

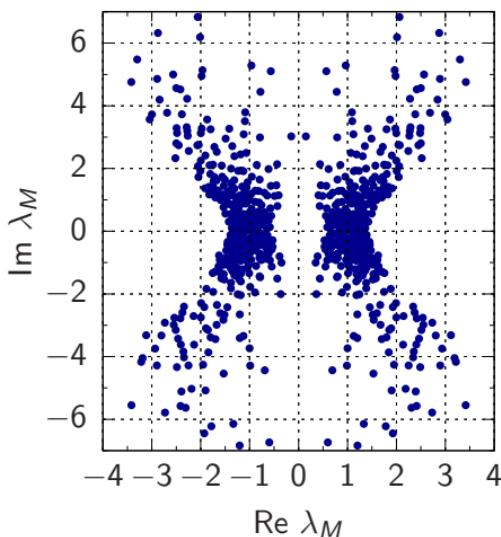
- Real Eigenvalues



Non-Hermitian matrix

$$\phi^{-1} \frac{\partial \phi}{\partial \mu}$$

- Complex Eigenvalues



Chebyshev Polynomials

Chebyshev Polynomials

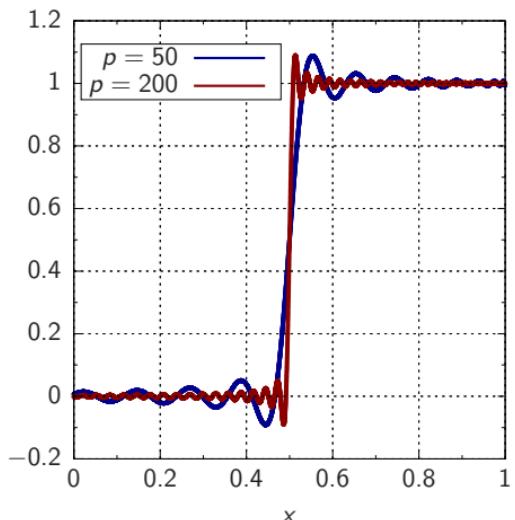
$$T_0(x) = 1, \quad T_1(x) = x$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$$

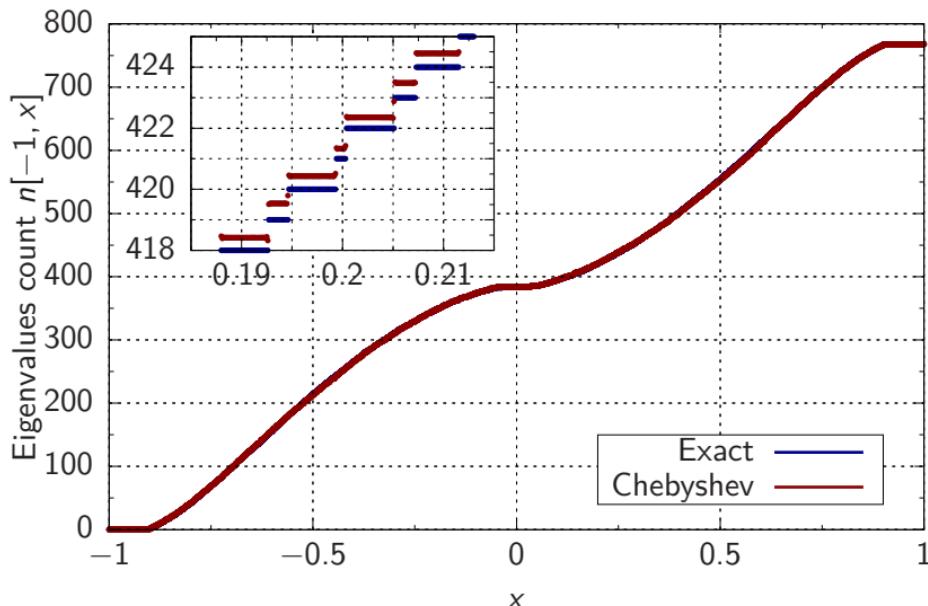
- Construct arbitrary function

$$f(x) = \sum_{p=0}^n \gamma_p T_p(x)$$

- Can be extended to matrix func.
- $x \in [-1, 1]$



Chebyshev Polynomials

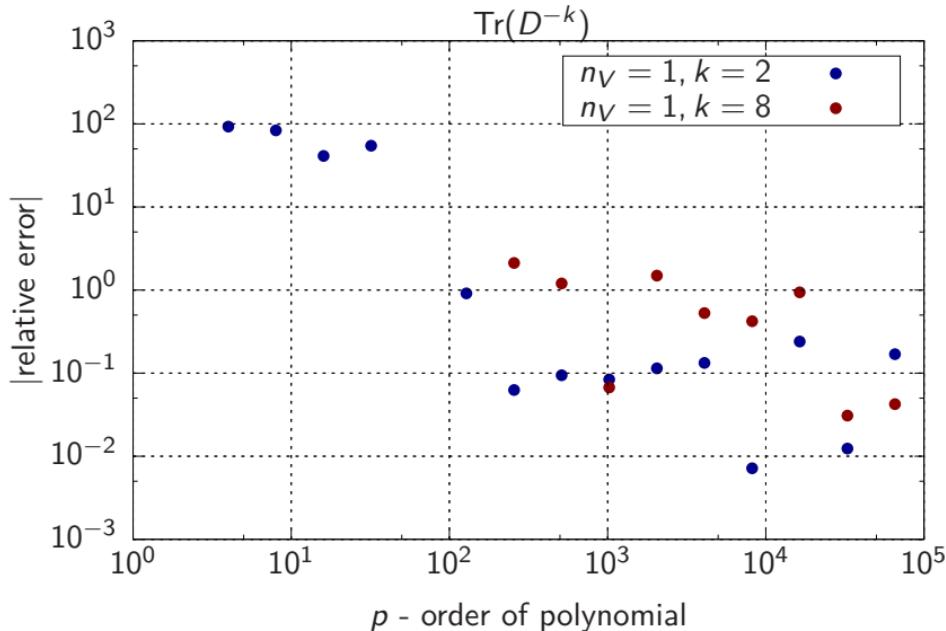


- Number of eigenvalues in the interval $n[-1, x]$

$$n[a, b] = \frac{1}{n} \sum_{i=1}^{n_V} \sum_{p=0}^{p_{max}} g_p(a, b) \langle \eta_i^\dagger T_p(A) \eta_i \rangle$$

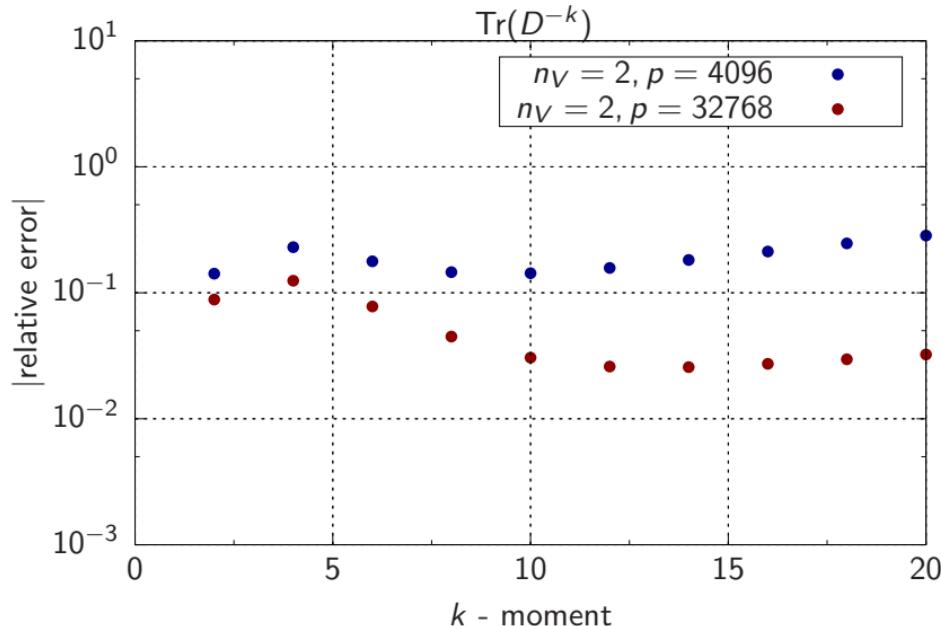
Giusti & Lüscher 2008,
Fodor et. al. 2016,
Cossu et. al. 2016

Chebyshev Polynomials



- Absolute relative error, i.e. $\left| \frac{\text{exact} - \text{approx.}}{\text{exact}} \right|$

Chebyshev Polynomials

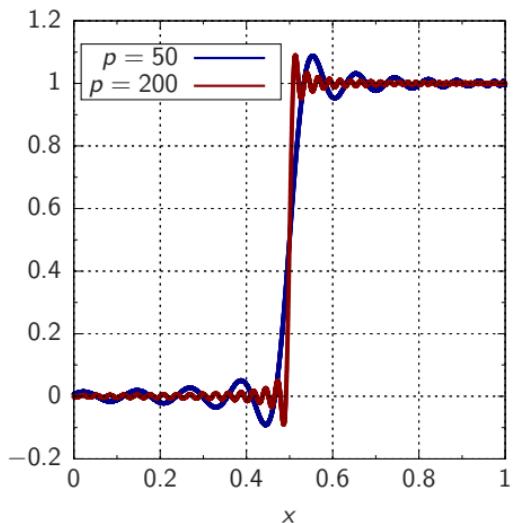


- Accuracy of $\text{Tr} [\mathcal{D}^{-k}]$ for larger moments (or cumulants)

Chebyshev Polynomials

Chebyshev Polynomials

- **Advantages**
 - No inversion necessary
 - Good accuracy on eigenvalues
- **Disadvantages**
 - Only works for Hermitian matrix
 - Limited applicability

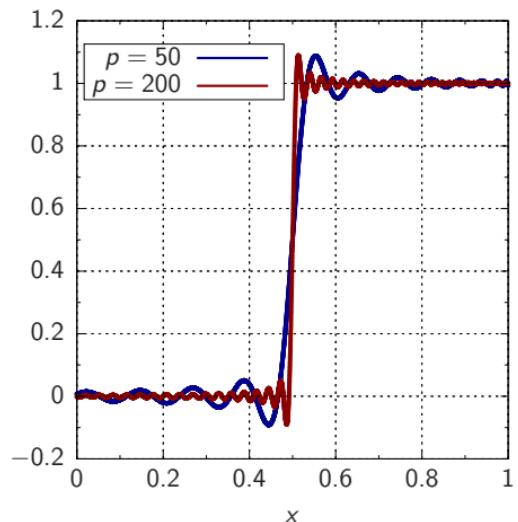


Chebyshev Polynomials

Chebyshev Polynomials

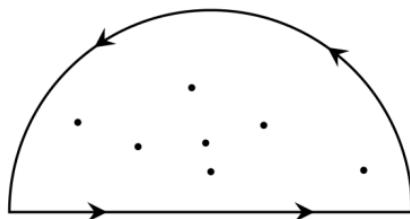
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Can we do better?



Cauchy Residue Theorem

$$\frac{1}{2\pi i} \oint_{\Gamma} f(z) dz = \text{Res}[f(z)]$$



- Number of eigenvalues in the contour $\mu(\Gamma)$

$$\mu(\Gamma) = \frac{1}{2\pi i} \oint_{\Gamma} \text{Tr} [(A - z\mathbb{1})^{-1}] dz$$

- Use inverse matrix (spacewise sparse) and shifted solver

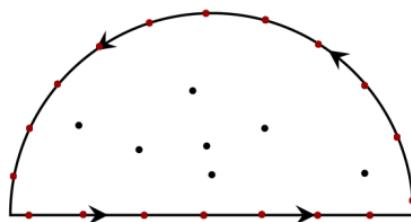
$$M = \mathcal{D}^{-1} \frac{\partial \mathcal{D}}{\partial \mu} \quad A = M^{-1} = \mathcal{D} \left(\frac{\partial \mathcal{D}}{\partial \mu} \right)^{-1}$$

- Start with larger box: Compute contour and refine ($\#\lambda > 1$)



Cauchy Residue Theorem

$$\frac{1}{2\pi i} \oint_{\Gamma} f(z) dz = \text{Res}[f(z)]$$



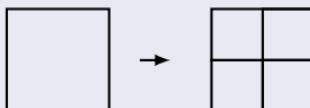
- Number of eigenvalues in **discrete** contour $\mu(\Gamma)$

$$\mu(\Gamma) \sim \frac{1}{n_Q} \sum_{k=0}^{n_Q} z_k \text{Tr} \left[(A - z_k \mathbb{1})^{-1} \right]$$

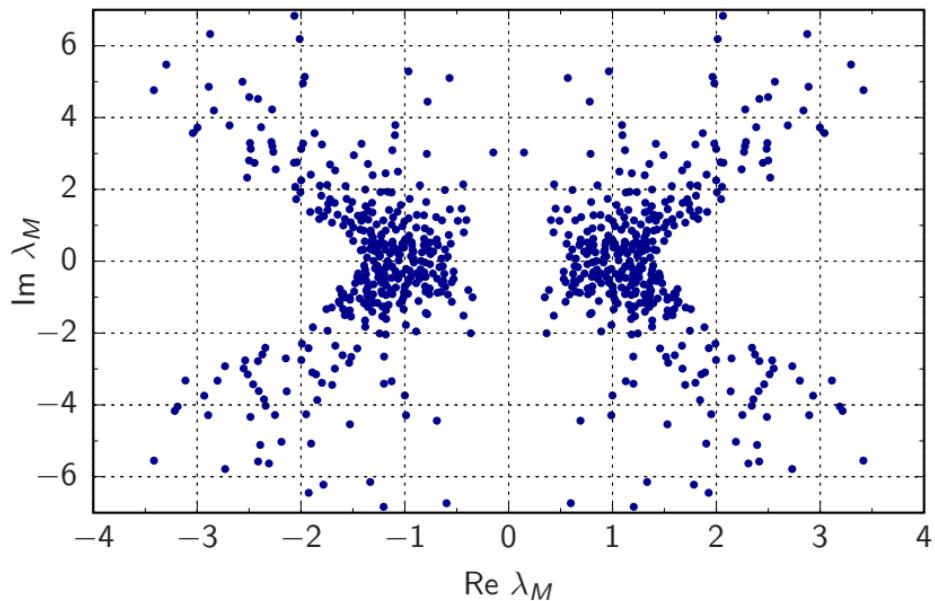
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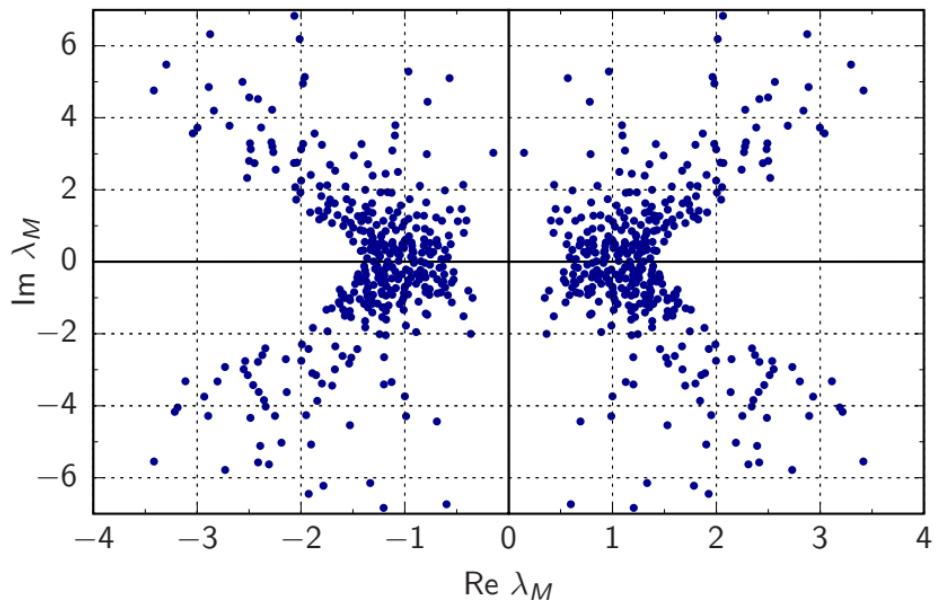
- Start with larger box: Discretize contour and refine ($\#\lambda > 1$)



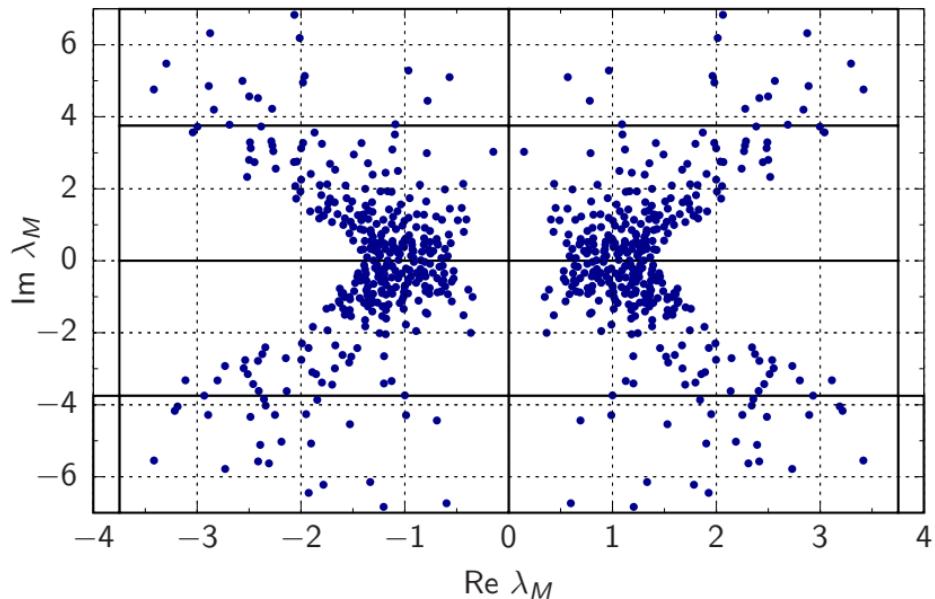
Eigenvalues & Refinement



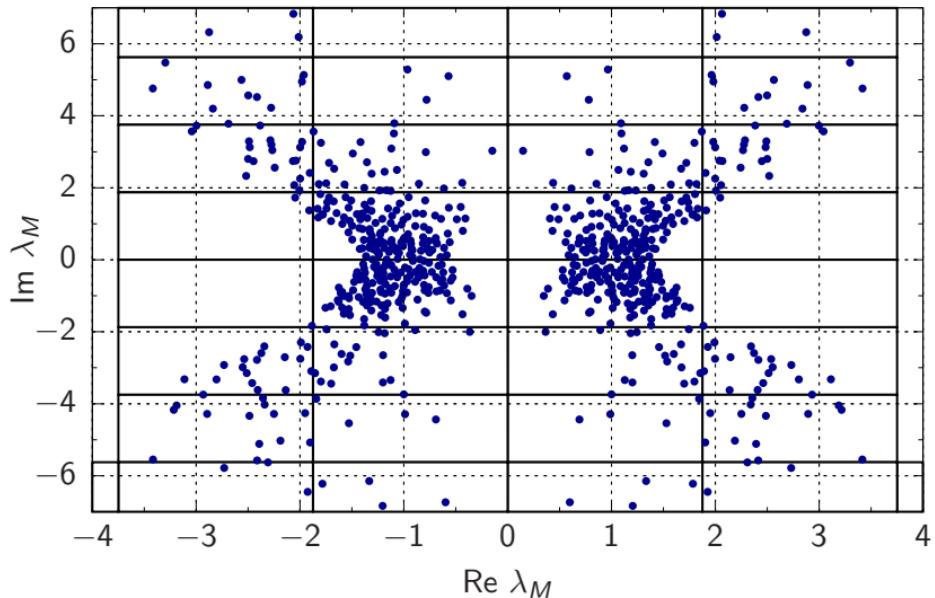
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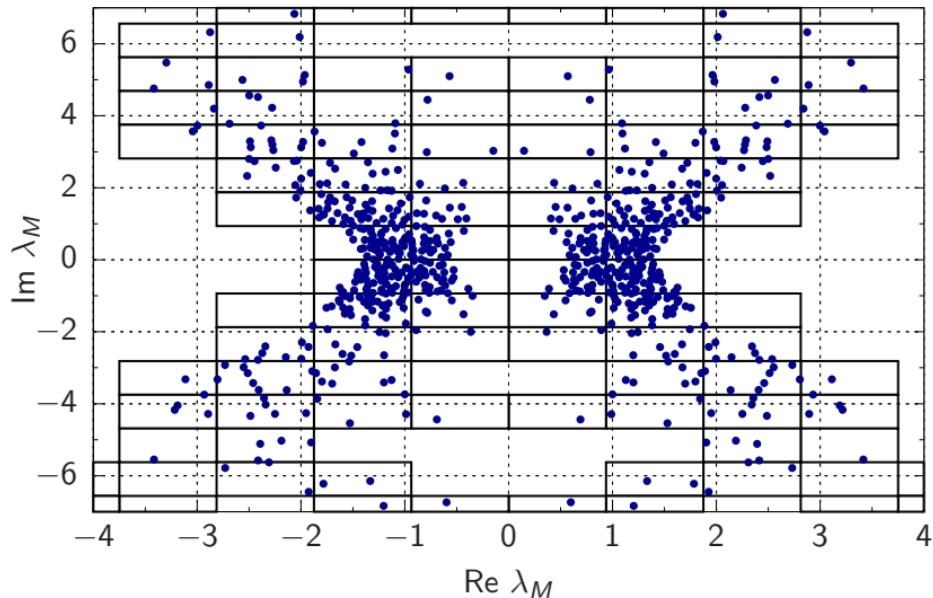
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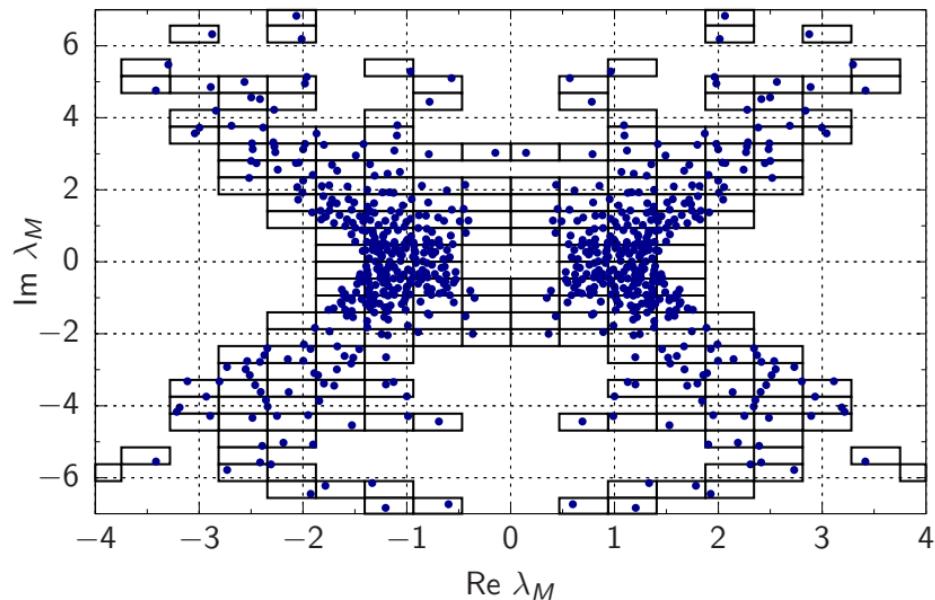
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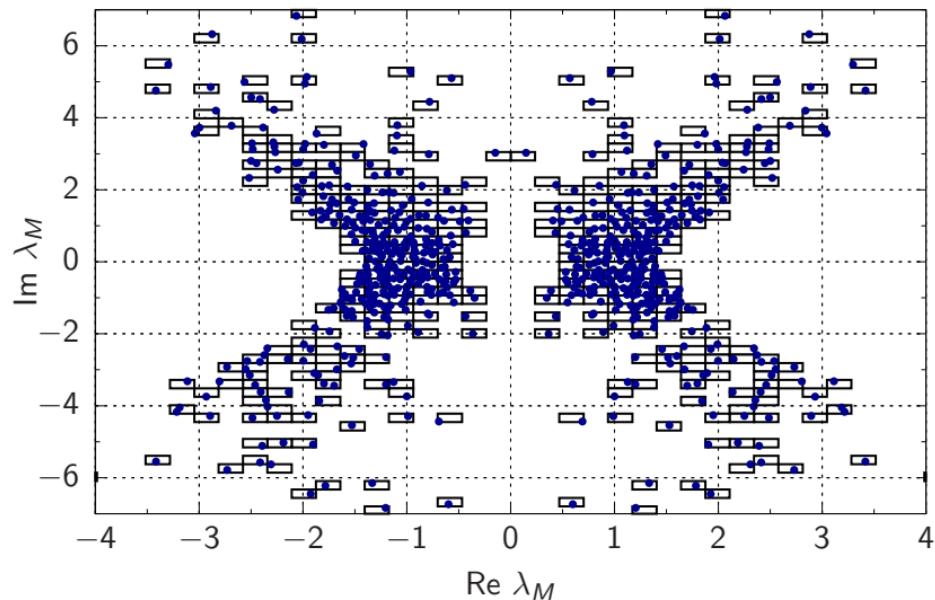
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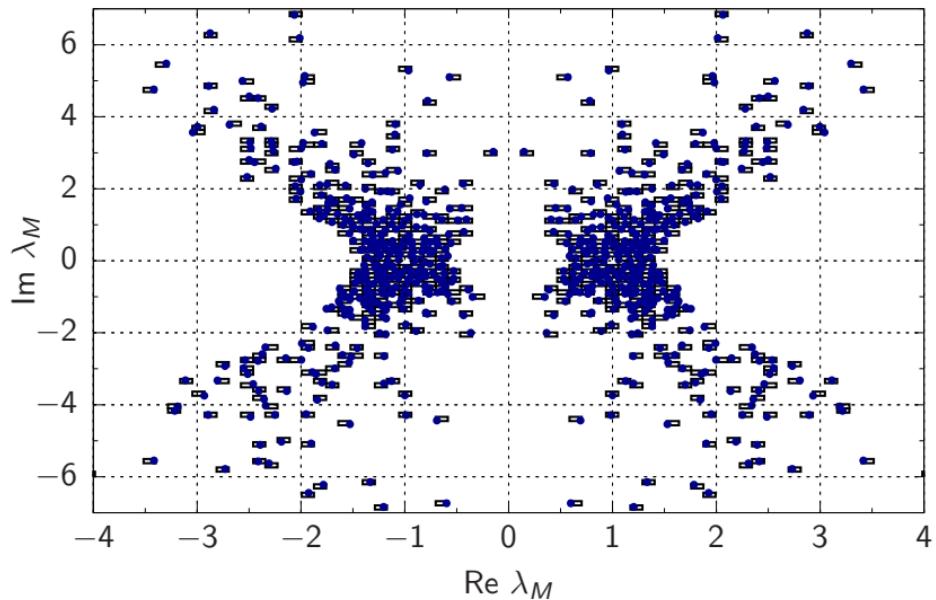
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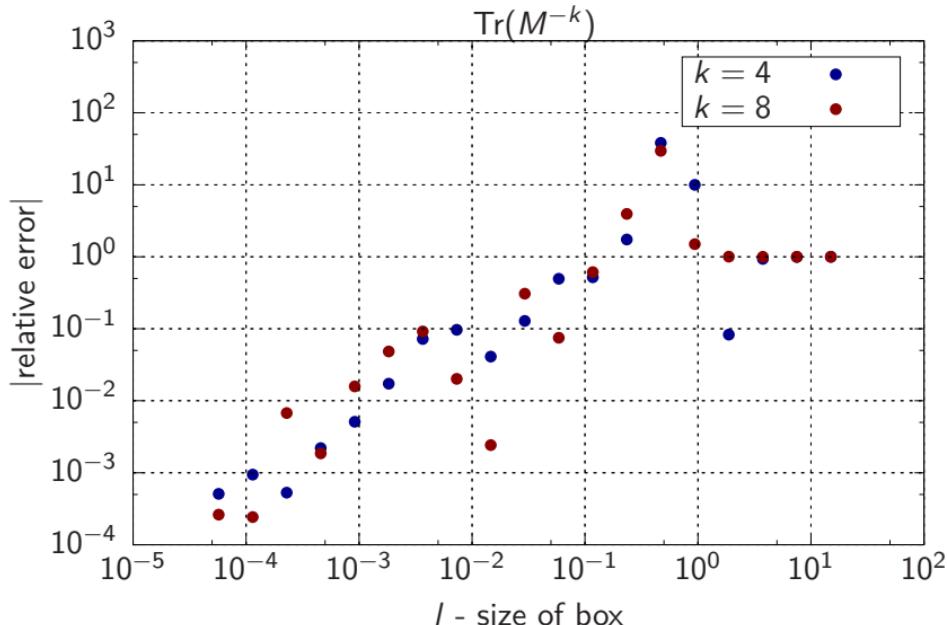
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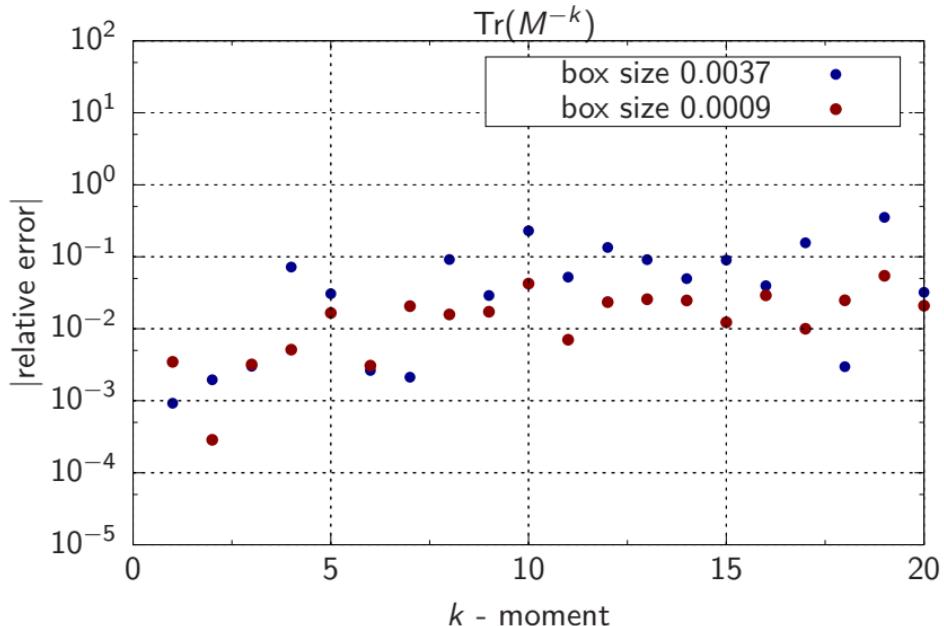


Accuracy



- Absolute relative error, i.e. $\left| \frac{\text{exact} - \text{approx.}}{\text{exact}} \right|$

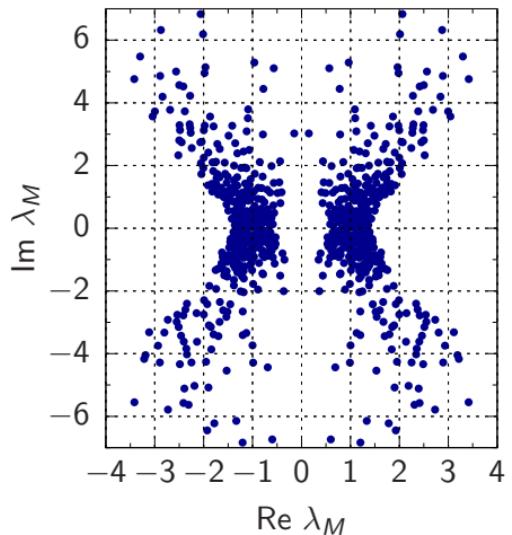
Accuracy



Cauchy Residue Theorem I

Refinement procedure

- **Advantages**
 - Very good accuracy
 - Even for larger moments
- **Disadvantages**
 - A lot of shifted inversions necessary

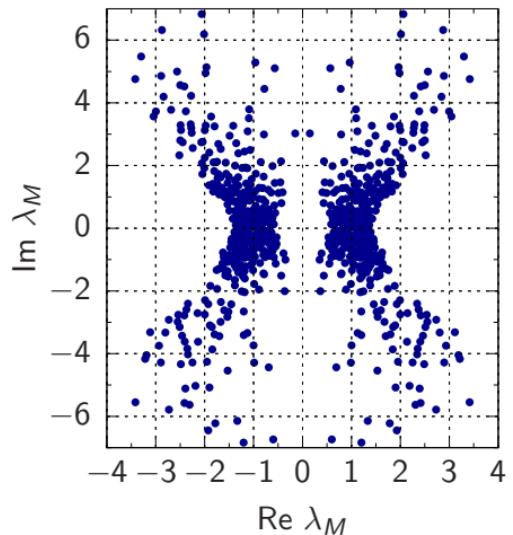


Cauchy Residue Theorem I

Refinement procedure

- **Advantages**
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- **Disadvantages**
 - A lot of shifted inversions necessary

Can we do better?



Cauchy Residue Theorem II

Use a single discrete circular contour

- Number of eigenvalues

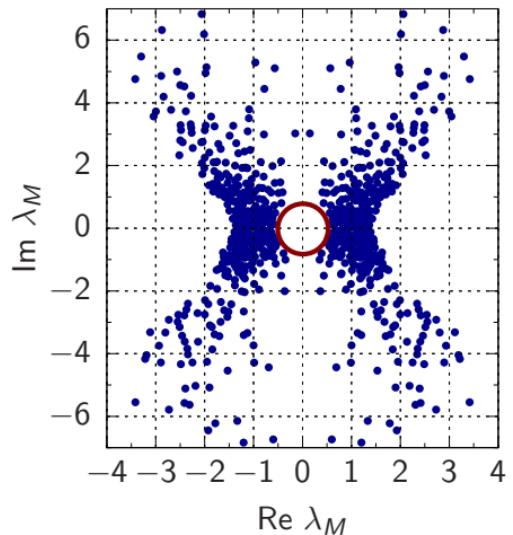
$$\mu(\Gamma) \sim \frac{1}{n_Q} \sum_{k=0}^{n_Q} z_k \operatorname{Tr} [(M - z_k \mathbb{1})^{-1}]$$

- Γ : Circle containing **no** eigenvalues

$$z_k = r e^{\frac{2\pi i}{N} k}$$

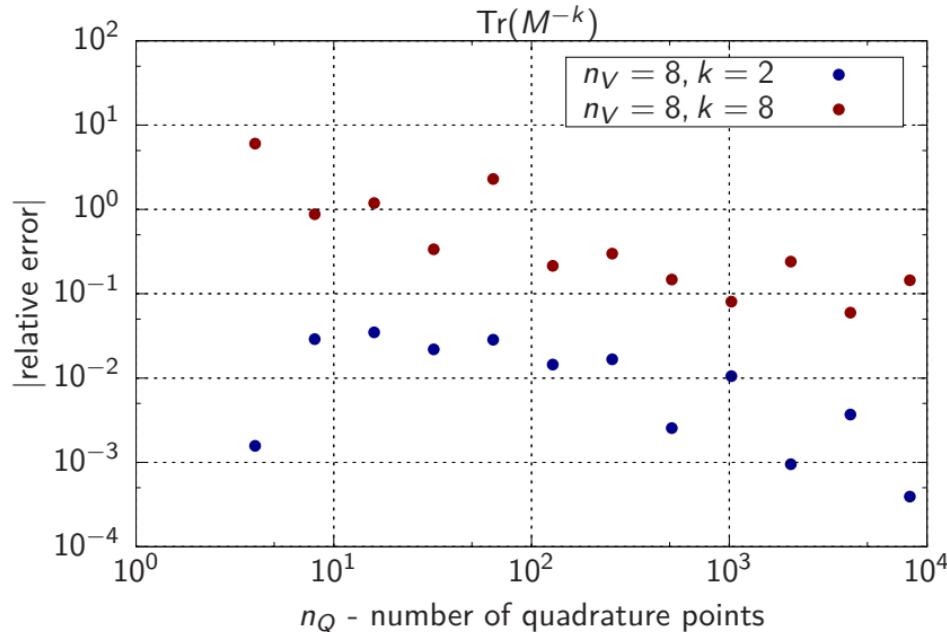
- Use **inverse** moments

$$\operatorname{Tr} [(\mathcal{D}' \mathcal{D}^{-1})^k] = \operatorname{Tr} [(\mathcal{D} \mathcal{D}'^{-1})^{-k}]$$



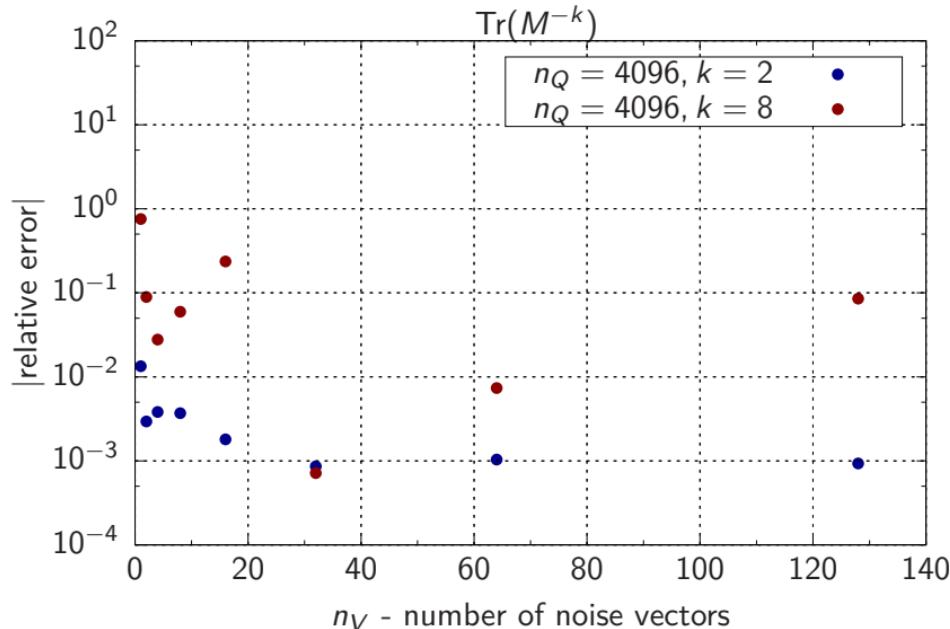
$$\operatorname{Tr} [(\mathcal{D} \mathcal{D}'^{-1})^{-k}] \sim \frac{1}{N} \sum_{i=1}^N z_i^{-k} \operatorname{Tr} [(z_i \mathbb{1} - \mathcal{D} \mathcal{D}'^{-1})^{-1}]$$

Accuracy

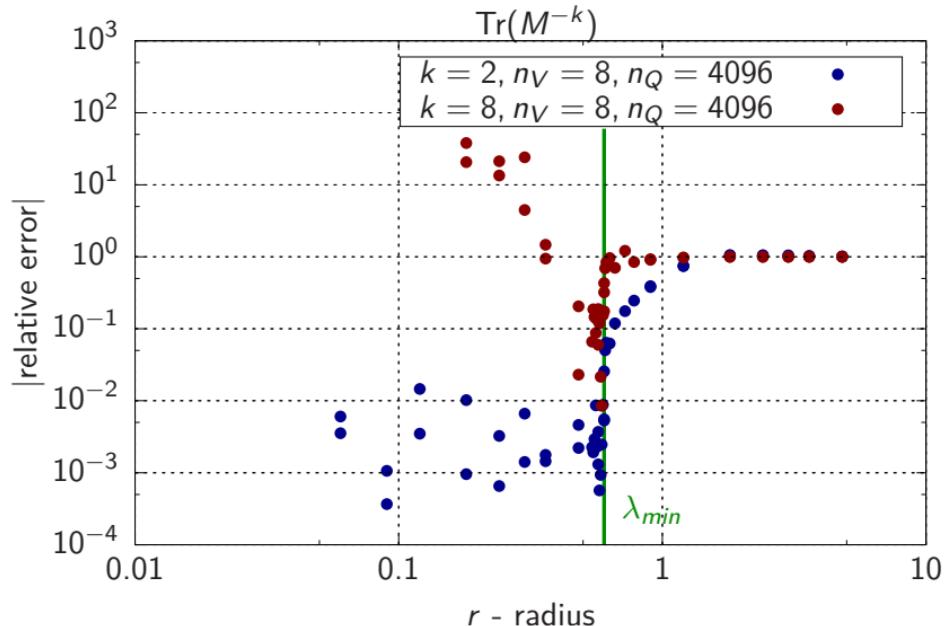


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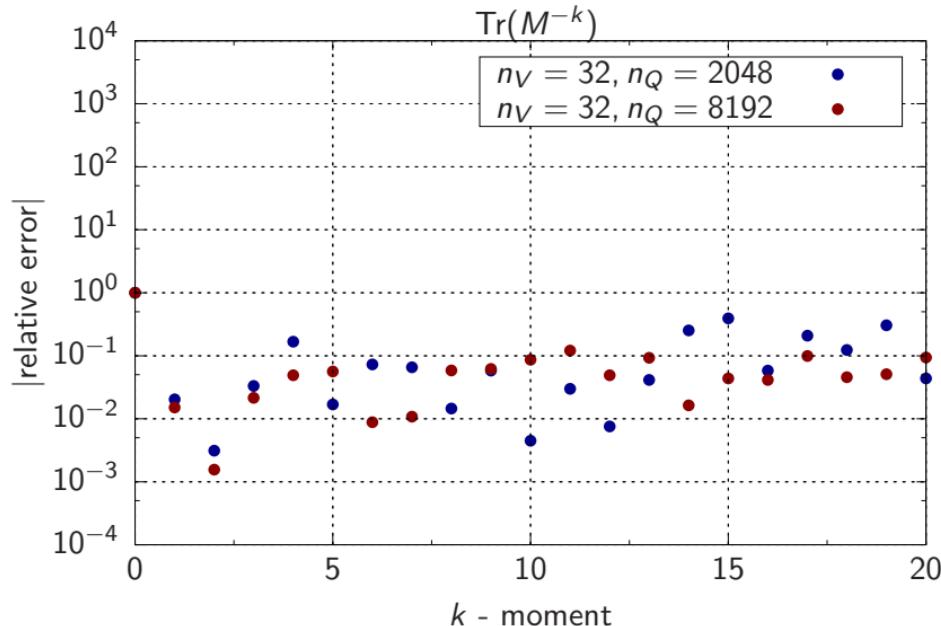
Accuracy



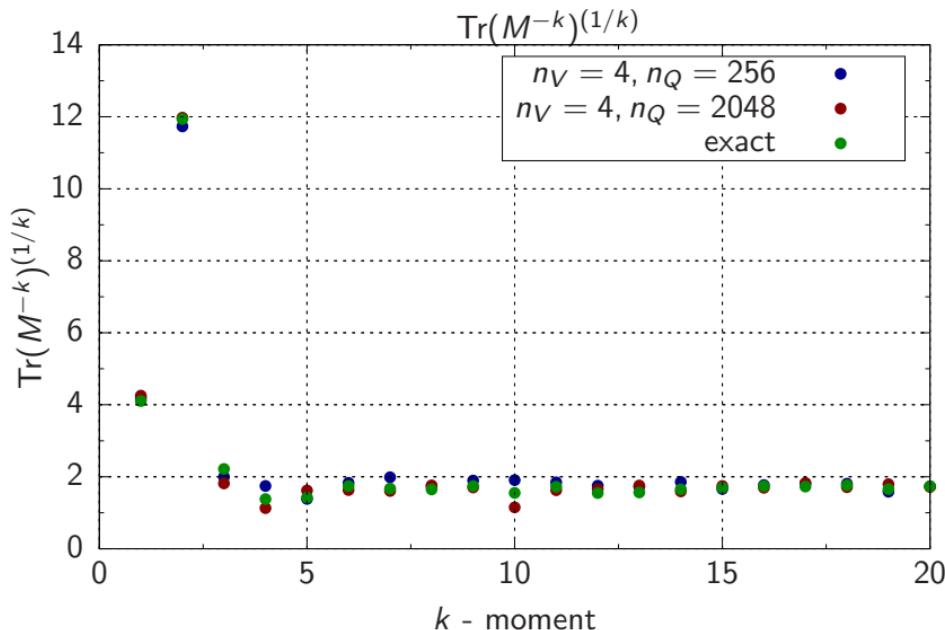
Accuracy



Accuracy

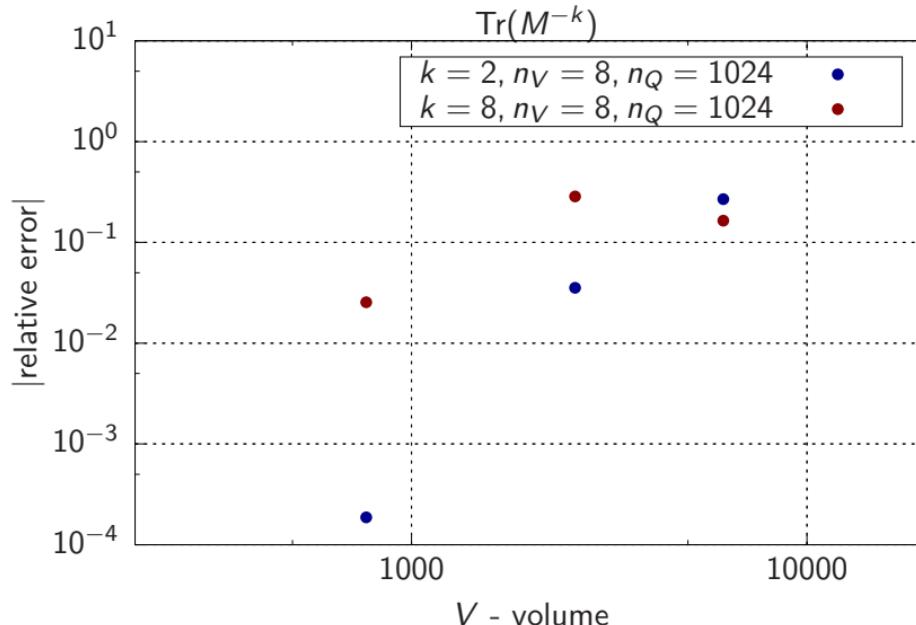


Accuracy



- $\text{Tr}\left[(\mathcal{D}' \mathcal{D}^{-1})^k\right]$ scaled by k -th root - relative size

Accuracy

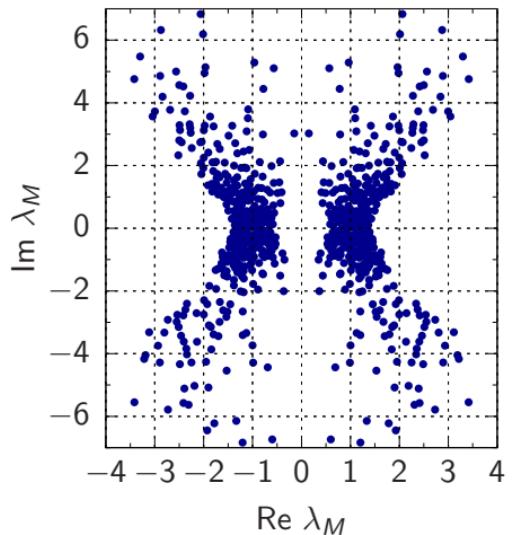


Cauchy Residue Theorem II

Single contour approach

- **Advantages**

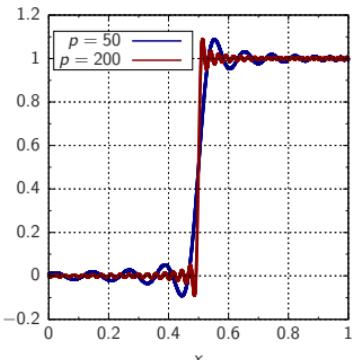
- Good accuracy
- Even for larger moments
- Moderate effort



Conclusion

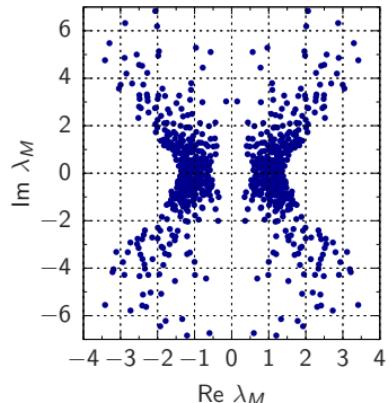
Conclusion

- Based on Cauchy Residue Theorem
- Good accuracy for large moments
- Moderate effort



Future Work

- Truncated solvers or all-mode averaging
- Block solvers
- Multishift block solvers [de Forcrand & Keegan]



Questions?

