

Work in progress on analytic continuation from imaginary chemical potential

Marco Aliberti^{1,2}

In collaboration with F. Di Renzo, P. Dimopoulos (Parma)
and the Bielefeld-Parma collaboration

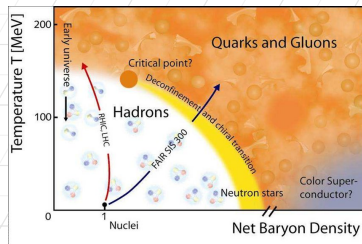
Spetember 13, 2024

¹Università degli Studi di Parma

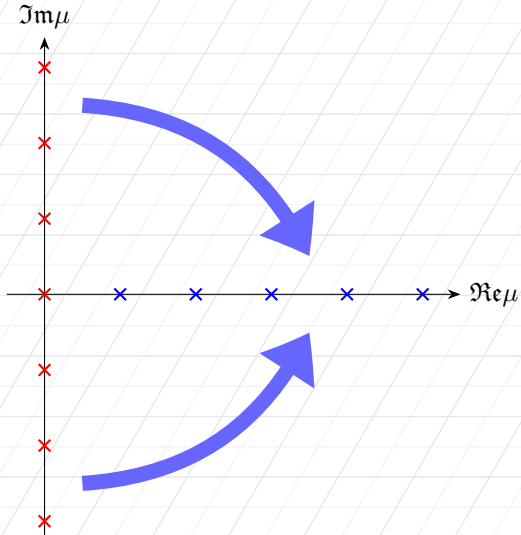
²INFN - Sezione di Milano Bicocca
Gruppo Collegato di Parma

The Sign Problem

- ▶ The study of the phase diagram requires finite baryon number density
- ▶ Finite density lattice simulations \Rightarrow 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

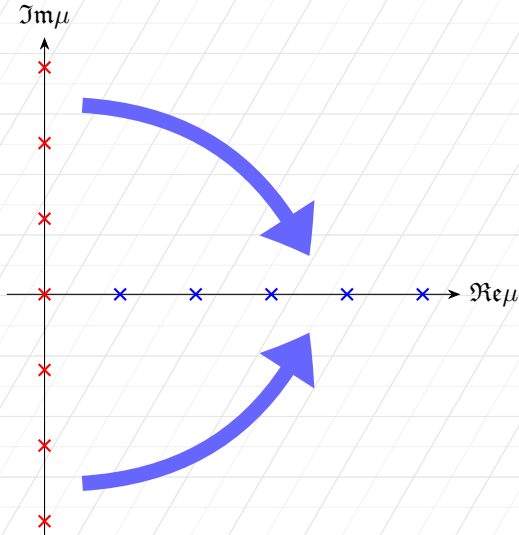


Imaginary μ



- ▶ Data from simulations at imaginary μ
- ▶ Analytic continuation to real μ
- ▶ Propagation of the statistical uncertainty?
- ▶ Radius of convergence?

Imaginary μ



- ▶ Data from simulations at imaginary μ
- ▶ Analytic continuation to real μ
- ▶ Propagation of the statistical uncertainty?
- ▶ Radius of convergence?

Various different methods for analytic continuation

The Methods

- ▶ Taylor Expansion: $P_n(\mu) = \sum_{k=0}^n c_k \mu^k$
- ▶ Padé analysis¹: $R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j}$
- ▶ Cauchy's Theorem integrated numerically²
- ▶ Power series of μ^2 , from $\mu^2 < 0$ to $\mu^2 > 0$

¹Explained in detail by C. Schmidt on Monday

²Explained in detail by F. Di Renzo on Tuesday

The Methods

▶ Taylor Expansion: $P_n(\mu) = \sum_{k=0}^n c_k \mu^k$ $\chi_n(T, V, \mu_B) = \left(\frac{\partial}{\partial \mu_B} \right)^n \frac{\ln Z(T, V, \mu_B)}{VT^3}$

▶ Padé analysis¹: $R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j}$ $\mu \equiv \mu_B/T$

▶ Cauchy's Theorem integrated numerically²

▶ Power series of μ^2 , from $\mu^2 < 0$ to $\mu^2 > 0$

¹Explained in detail by C. Schmidt on Monday

²Explained in detail by F. Di Renzo on Tuesday

The Methods

▶ Taylor Expansion: $P_n(\mu) = \sum_{k=0}^n c_k \mu^k$ $\chi_n(T, V, \mu_B) = \left(\frac{\partial}{\partial \mu_B} \right)^n \frac{\ln Z(T, V, \mu_B)}{VT^3}$

▶ Padé analysis¹: $R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j}$ $\mu \equiv \mu_B/T$

▶ Cauchy's Theorem integrated numerically²

▶ Power series of μ^2 , from $\mu^2 < 0$ to $\mu^2 > 0$

HISQ $N_f = 2 + 1$, $N_\tau = 6$,
 $T = 157.5 \text{ MeV}$

Physical pion mass

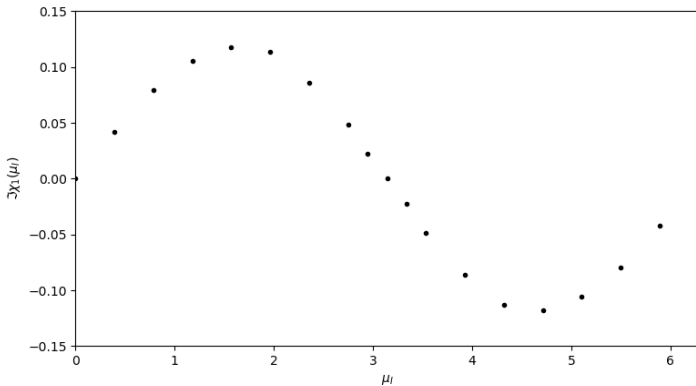
From the Bielefeld-Parma
 collaboration

Disclaimer: For now, only the central values will be shown (without errors).

¹Explained in detail by C. Schmidt on Monday

²Explained in detail by F. Di Renzo on Tuesday

Input Data



Taylor Expansion

Dataset

$$\{\chi_1(\mu_0), \dots, \chi_1(\mu_{N-1})\}$$

$$\chi_1(\mu_i) = \sum_{k=0}^{N-1} \frac{1}{k!} \chi_{1+k}(0) \mu_i^k + O(\mu^N)$$

Taylor Expansion

Dataset

$$\{\chi_1(\mu_0), \dots, \chi_1(\mu_{N-1})\}, \quad \{\chi_2(\mu_N), \dots, \chi_2(\mu_{N+M-1})\}$$

$$\begin{cases} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{k!} \chi_{1+k}(0) \mu_i^k + O(\mu^{N+M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{k}{k!} \chi_{1+k}(0) \mu_j^{k-1} + O(\mu^{N+M-1}) \end{cases}$$

Taylor Expansion

Dataset

$$\{\chi_1(\mu_0), \dots, \chi_1(\mu_{N-1})\}, \quad \{\chi_2(\mu_N), \dots, \chi_2(\mu_{N+M-1})\}$$

- Straightforward to implement

$$\begin{cases} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{k!} \chi_{1+k}(0) \mu_i^k + O(\mu^{N+M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{k}{k!} \chi_{1+k}(0) \mu_j^{k-1} + O(\mu^{N+M-1}) \end{cases}$$

Taylor Expansion

Dataset

$$\{\chi_1(\mu_0), \dots, \chi_1(\mu_{N-1})\}, \quad \{\chi_2(\mu_N), \dots, \chi_2(\mu_{N+M-1})\}$$

$$\begin{cases} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{k!} \chi_{1+k}(0) \mu_i^k + O(\mu^{N+M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{k}{k!} \chi_{1+k}(0) \mu_j^{k-1} + O(\mu^{N+M-1}) \end{cases}$$

- ▶ Straightforward to implement
- ▶ Radius of convergence: (way before) nearest singularity

Taylor Expansion

Dataset

$$\{\chi_1(\mu_0), \dots, \chi_1(\mu_{N-1})\}, \quad \{\chi_2(\mu_N), \dots, \chi_2(\mu_{N+M-1})\}$$

$$\begin{cases} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{k!} \chi_{1+k}(0) \mu_i^k + O(\mu^{N+M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{k}{k!} \chi_{1+k}(0) \mu_j^{k-1} + O(\mu^{N+M-1}) \end{cases}$$

- ▶ Straightforward to implement
- ▶ Radius of convergence: (way before) nearest singularity
- ▶ No singularity structure (polynomial)

Taylor Expansion - Fixed Parity

Charge conjugation symmetry $\implies \chi_1(-\mu) = -\chi_1(\mu)$

Taylor Expansion - Fixed Parity

Charge conjugation symmetry $\implies \chi_1(-\mu) = -\chi_1(\mu)$

$$\left\{ \begin{array}{l} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} \chi_{2+2k}(0) \mu_i^{2k+1} + O(\mu^{2N+2M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{2k+1}{(2k+1)!} \chi_{2+2k}(0) \mu_j^{2k} + O(\mu^{2N+2M-1}) \end{array} \right.$$

Taylor Expansion - Fixed Parity

Charge conjugation symmetry $\implies \chi_1(-\mu) = -\chi_1(\mu)$

$$\left\{ \begin{array}{l} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} \chi_{2+2k}(0) \mu_i^{2k+1} + O(\mu^{2N+2M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{2k+1}{(2k+1)!} \chi_{2+2k}(0) \mu_j^{2k} + O(\mu^{2N+2M-1}) \end{array} \right.$$

- Higher number of *significant* derivatives (with same input data)

Taylor Expansion - Fixed Parity

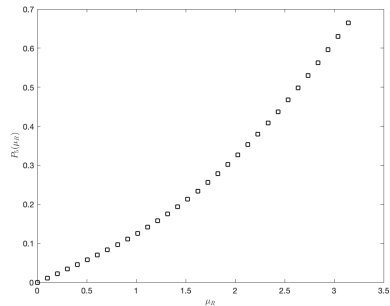
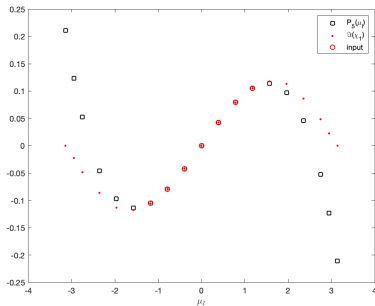
Charge conjugation symmetry $\implies \chi_1(-\mu) = -\chi_1(\mu)$

$$\left\{ \begin{array}{l} \chi_1(\mu_i) = \sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} \chi_{2+2k}(0) \mu_i^{2k+1} + O(\mu^{2N+2M}) \\ \chi_2(\mu_j) = \sum_{k=1}^{N+M-1} \frac{2k+1}{(2k+1)!} \chi_{2+2k}(0) \mu_j^{2k} + O(\mu^{2N+2M-1}) \end{array} \right.$$

► Higher number of *significant* derivatives (with same input data)

► Worse condition number

Taylor Plots



Padé Analysis

- ▶ Rational function
- ▶ Interpolates singularities
- ▶ Can have only poles
- ▶ Branch cuts are represented as a series of poles and zeros

$$R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j}$$

Single-Point Padé

Dataset

$$\chi_1(0), \chi_2(0), \dots, \chi_N(0)$$

$$R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j} \quad \text{with} \quad n + m = N$$

$$\text{Conditions: } R(0) = \chi_1(0), R'(0) = \chi_2(0), \dots, R^{(N-1)}(0) = \chi_N(0)$$

Single-Point Padé

Dataset

$$\chi_1(0), \chi_2(0), \dots, \chi_N(0)$$

$$R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j} \quad \text{with} \quad n + m = N$$

Conditions: $R(0) = \chi_1(0), R'(0) = \chi_2(0), \dots, R^{(N-1)}(0) = \chi_N(0)$

Problem: Noisy high derivatives \implies Few parameters

Multi-Point Padé

Dataset

$$\chi_1(\mu_1), \chi_1(\mu_2), \dots, \chi_1(\mu_N), \quad \chi_2(\mu_{N+1}), \chi_2(\mu_{N+2}), \dots, \chi_2(\mu_{N+M})$$

$$R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j} \quad \text{with} \quad n + m = N + M$$

Conditions:

$$R(\mu_1) = \chi_1(\mu_1), R(\mu_2) = \chi_1(\mu_2), \dots, R(\mu_N) = \chi_1(\mu_N)$$

$$R'(\mu_{N+1}) = \chi_2(\mu_{N+1}), \dots, R'(\mu_{N+M}) = \chi_2(\mu_{N+M})$$

Multi-Point Padé

Dataset

$$\chi_1(\mu_1), \chi_1(\mu_2), \dots, \chi_1(\mu_N), \quad \chi_2(\mu_{N+1}), \chi_2(\mu_{N+2}), \dots, \chi_2(\mu_{N+M})$$

$$R_m^n(\mu) = \frac{\sum_{k=0}^n p_k \mu^k}{1 + \sum_{j=1}^m q_j \mu^j} \quad \text{with} \quad n + m = N + M$$

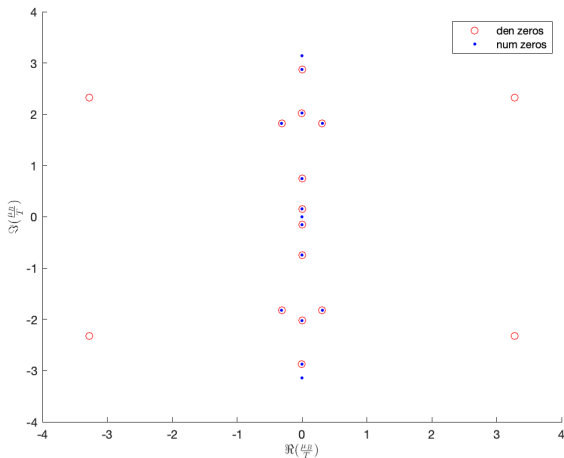
Conditions:

$$R(\mu_1) = \chi_1(\mu_1), R(\mu_2) = \chi_1(\mu_2), \dots, R(\mu_N) = \chi_1(\mu_N)$$

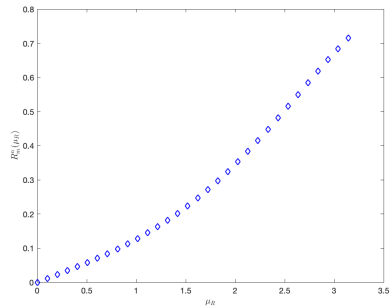
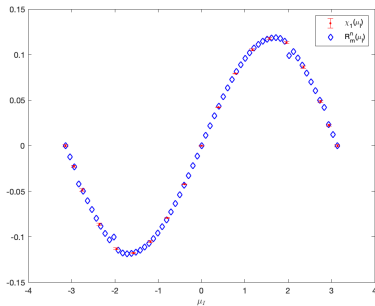
$$R'(\mu_{N+1}) = \chi_2(\mu_{N+1}), \dots, R'(\mu_{N+M}) = \chi_2(\mu_{N+M})$$

Problem: Convergence not rigorously defined

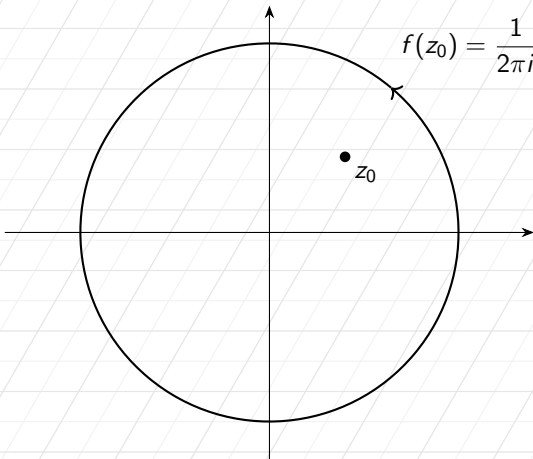
"Simplified" Multi-Point Padé



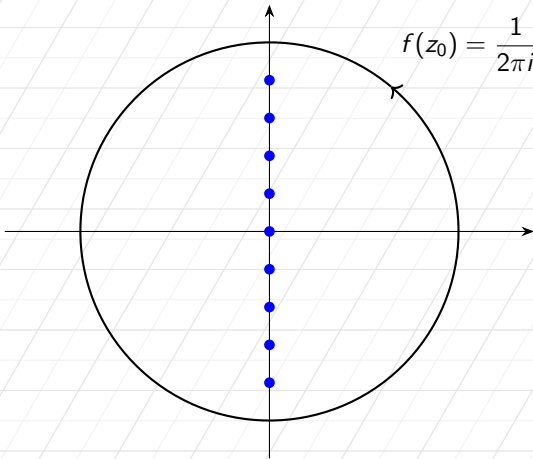
Padé Plots



Inverse Problem



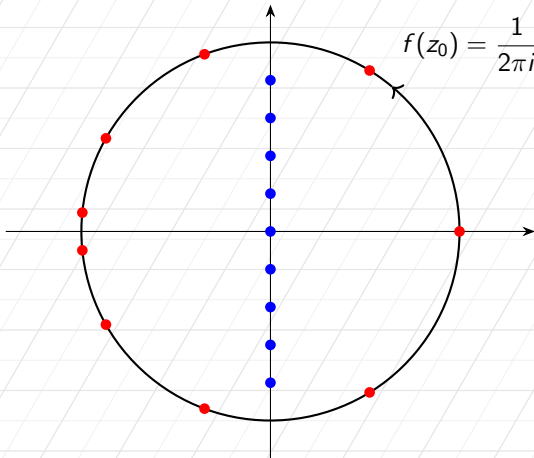
Inverse Problem



$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz$$

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

Inverse Problem



$$f(z_0) = \frac{1}{2\pi i} \oint_C \frac{f(z)}{z - z_0} dz$$

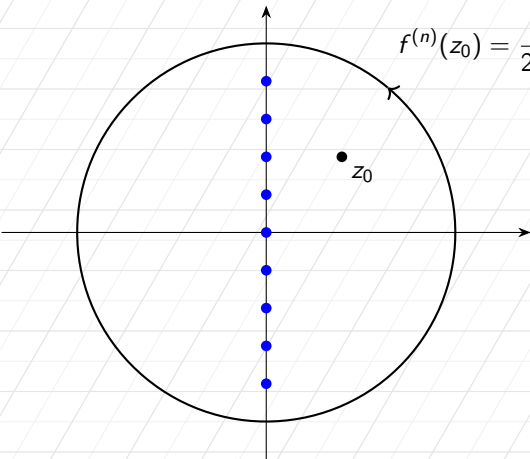
$$\chi_1(\mu_j) = \frac{1}{2\pi} \int_0^{2\pi} \frac{Re^{i\theta} \chi_1(Re^{i\theta})}{Re^{i\theta} - \mu_j} d\theta$$

Gauss-Legendre

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

$$j = 1, \dots, n$$

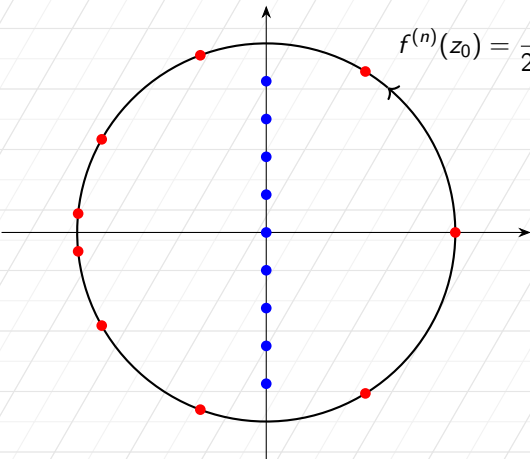
Inverse Problem With Derivatives



$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} dz$$

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

Inverse Problem With Derivatives



$$f^{(n)}(z_0) = \frac{n!}{2\pi i} \oint_C \frac{f(z)}{(z - z_0)^{n+1}} dz$$

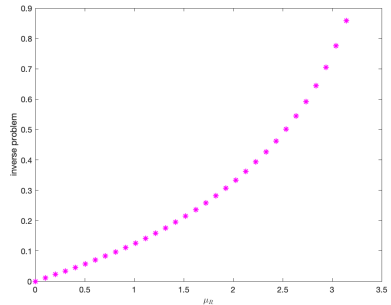
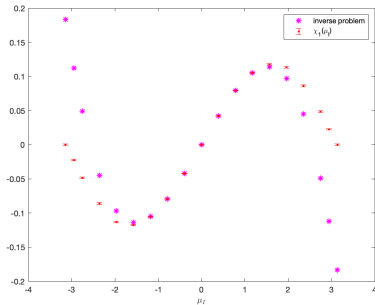
$$\chi_{n+1}(\mu_j) = \frac{n!}{2\pi} \int_0^{2\pi} \frac{Re^{i\theta} \chi_1(Re^{i\theta})}{(Re^{i\theta} - \mu_j)^{n+1}} d\theta$$

Gauss-Legendre

$$\chi_{n+1}(\mu_j) \simeq \frac{n!}{2\pi} \sum_{k=1}^n w_k \frac{Re^{i\theta_k} \hat{\chi}_{1k}}{(Re^{i\theta_k} - \mu_j)^{n+1}}$$

$$j = 1, \dots, n$$

Inverse Problem Plots



Analytic continuation from $\mu^2 < 0$

$$\mu = \{+0.3928i, +0.7853i, +1.178i, +1.571i, \dots\}$$

$$\chi_1(\mu) = \sum_{k=0}^{\infty} \frac{\chi_{2k+1}(0)}{(2k+1)!} \mu^{2k+1}$$

Analytic continuation from $\mu^2 < 0$

$$\mu = \{+0.3928i, +0.7853i, +1.178i, +1.571i, \dots\}$$

$$\Downarrow$$

$$\mu^2 = \{-0.1543, -0.6167, -1.388, -2.468, \dots\}$$

$$\chi_1(\mu) = \sum_{k=0}^{\infty} \frac{\chi_{2k+1}(0)}{(2k+1)!} \mu^{2k+1}$$

$$\tilde{\chi}_1(\mu^2) = \chi_1(\mu) / \mu$$

Analytic continuation from $\mu^2 < 0$

$$\mu = \{+0.3928i, +0.7853i, +1.178i, +1.571i, \dots\}$$

$$\Downarrow$$

$$\mu^2 = \{-0.1543, -0.6167, -1.388, -2.468, \dots\}$$

$$\chi_1(\mu) = \sum_{k=0}^{\infty} \frac{\chi_{2k+1}(0)}{(2k+1)!} \mu^{2k+1}$$

$$\tilde{\chi}_1(\mu^2) = \chi_1(\mu) / \mu$$

► Polynomial fit in μ^2

Analytic continuation from $\mu^2 < 0$

$$\mu = \{+0.3928i, +0.7853i, +1.178i, +1.571i, \dots\}$$

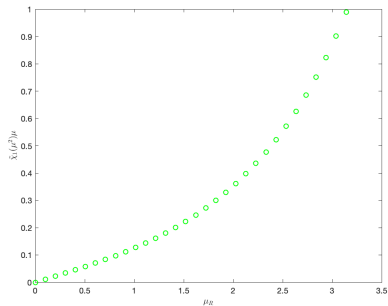
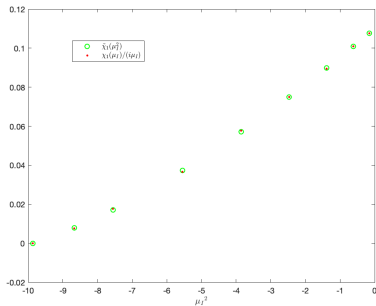
$$\downarrow$$

$$\mu^2 = \{-0.1543, -0.6167, -1.388, -2.468, \dots\}$$

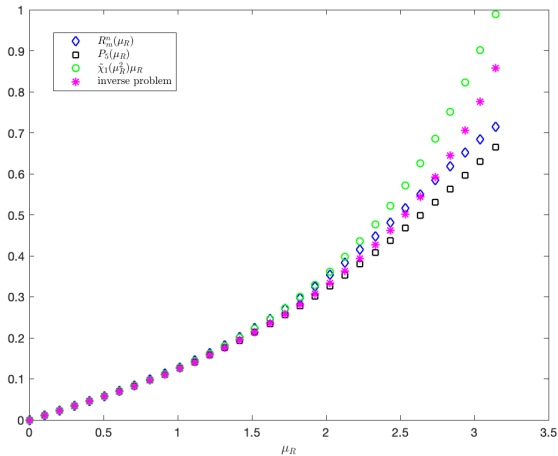
$$\chi_1(\mu) = \sum_{k=0}^{\infty} \frac{\chi_{2k+1}(0)}{(2k+1)!} \mu^{2k+1}$$

$$\tilde{\chi}_1(\mu^2) = \chi_1(\mu) / \mu$$

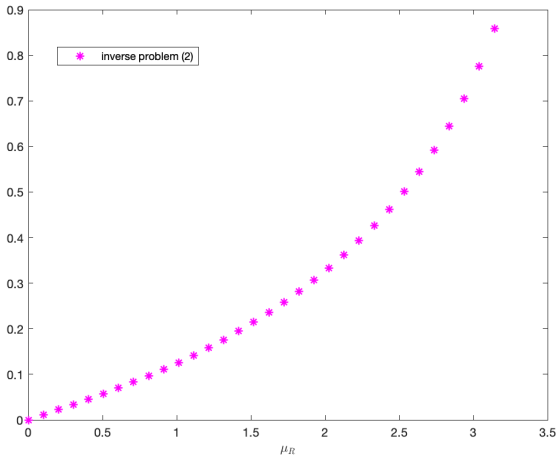
- ▶ Polynomial fit in μ^2
- ▶ Recover the original function by multiplying by μ

μ^2 Fit Plots

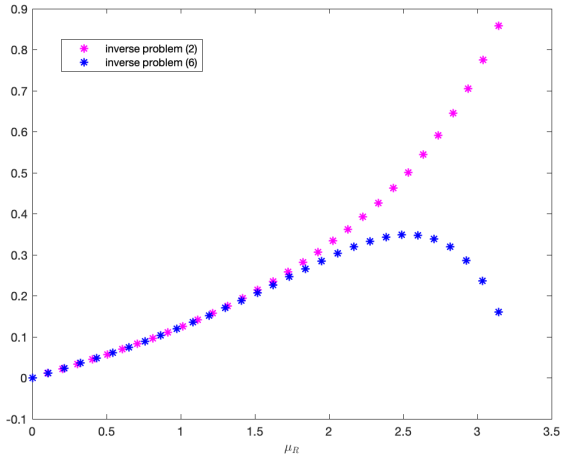
Results Comparison



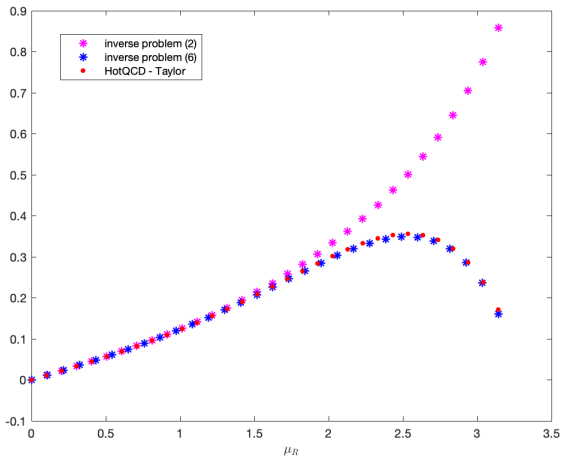
What About the Errors?



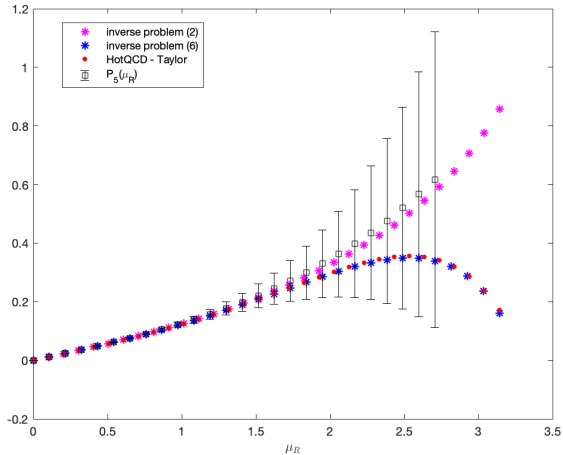
What About the Errors?



What About the Errors?



What About the Errors?



In Conclusion...

- ▶ Various methods, with very different ways of operation, have been used for analytical continuation from imaginary μ_B/T to real μ_B/T
- ▶ There is a common region ($\mu_B/T \lesssim 1.5$) where every method agree with each other, with *small* error bars
- ▶ Outside this region ($\mu_B/T \gtrsim 1.5$), they significantly deviate from each other, but stay within the *much larger* error bars
- ▶ Beyond a given treshold, each method has a high systematic sensitivity with respect to the choice of the input data
- ▶ A thorough error analysis (both statistical and systematic) is being performed