Taylor series coefficients at $\mu = 0$ from imaginary μ computations

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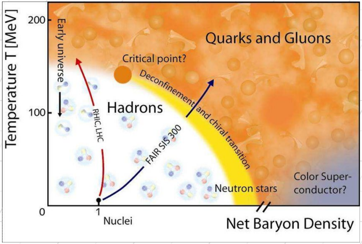
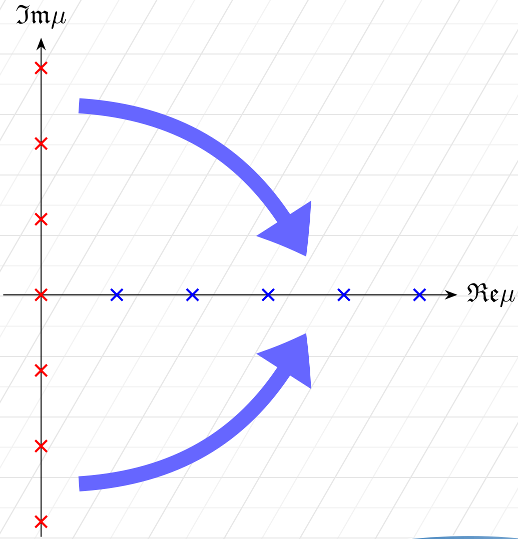
The Sign Problem

- 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

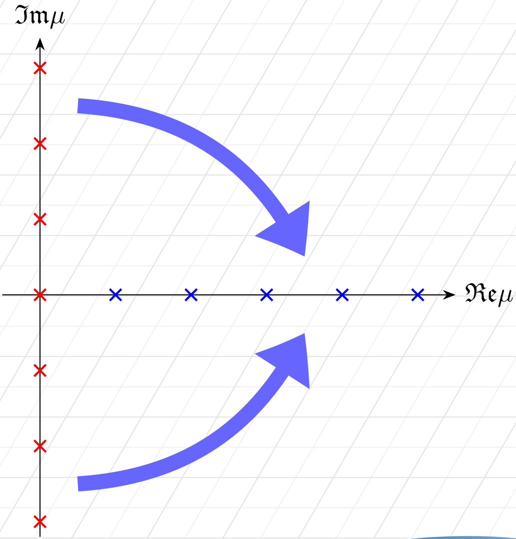


Imaginary μ



- 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
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- Propagation of the statistical uncertainty?
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Find the Taylor coefficients at $\mu = 0$

Taylor Expansion of a Generic Function

Dataset

$\{f(x_0), \ldots, f(x_{N-1})\}$

$$
\begin{cases}
f(x_0) = \sum_{k=0}^{N-1} \frac{1}{k!} f^{(k)}(0) x_0^k + O(x^N) \\
\vdots \\
f(x_{N-1}) = \sum_{k=0}^{N-1} \frac{1}{k!} f^{(k)}(0) x_{N-1}^k + O(x^N)
\end{cases}
$$

N Linear Equations!

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N Linear Equations!

N Unknown Parameters

$f^{(k)}(0)$ or $\frac{1}{k!} f^{(k)}(0), \quad k = 0, \ldots, N-1$

Generic Function and its First Derivative

Dataset

$$\{f(x_0), \ldots, f(x_{N-1})\}, \quad \{f'(x_N), \ldots, f'(x_{N+M-1})\}$$

$$\begin{cases} f(x_i) = \displaystyle\sum_{k=0}^{N+M-1} \frac{1}{k!} f^{(k)}(0) x_i^k + O(x^{N+M}) & i = 0, \ldots, N-1 \\ \quad \vdots & N+M \text{ Linear Equations!} \\ f'(x_j) = \displaystyle\sum_{k=1}^{N+M-1} \frac{k}{k!} f^{(k)}(0) x_j^{k-1} + O(x^{N+M-1}) & j = N, \ldots, N+M-1 \end{cases}$$

Generic Function and its First Derivative

Dataset

$$\{f(x_0), \dots, f(x_{N-1})\}, \quad \{f'(x_N), \dots, f'(x_{N+M-1})\}$$

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$N + M$ Unknown Parameters

$f^{(k)}(0)$ or $\frac{1}{k!} f^{(k)}(0)$, $\quad k = 0, \dots, N+M-1$

Odd Function and its First Derivative

Dataset

$$\{f(x_0),\dots,f(x_{N-1})\},\quad \{f'(x_N),\dots,f'(x_{N+M-1})\},\quad f(-x)=-f(x)$$

$$\begin{cases} f(x_i) \approx \displaystyle\sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} f^{(2k+1)}(0) x_i^{2k+1} & i=0,\dots,N-1 \\ \quad\vdots & N+M \text{ Linear Equations!} \\ f'(x_j) \approx \displaystyle\sum_{k=0}^{N+M-1} \frac{2k+1}{(2k+1)!} f^{(2k+1)}(0) x_j^{2k} & j=N,\dots,N+M-1 \end{cases}$$

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Odd Function and its First Derivative

Dataset

$$\{f(x_0), \dots, f(x_{N-1})\}, \quad \{f'(x_N), \dots, f'(x_{N+M-1})\}, \quad f(-x) = -f(x)$$

$$\begin{cases} f(x_i) \approx \sum_{k=0}^{N+M-1} \frac{1}{(2k+1)!} f^{(2k+1)}(0) x_i^{2k+1} & i = 0, \dots, N-1 \\ \vdots & N+M \text{ Linear Equations!} \\ f'(x_j) \approx \sum_{k=0}^{N+M-1} \frac{2k+1}{(2k+1)!} f^{(2k+1)}(0) x_j^{2k} & j = N, \dots, N+M-1 \end{cases}$$

$N + M$ Unknown Parameters

$$f^{(2k+1)}(0) \text{ or } \frac{1}{(2k+1)!} f^{(2k+1)}(0), \qquad f^{(2k)}(0) = 0, \qquad k = 0, \dots, N+M-1$$

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The Linear System (1)

$$\begin{pmatrix} 1 & x_0 & \frac{x_0^2}{2!} & \cdots & \frac{x_0^{(N-3)}}{(N-3)!} & \frac{x_0^{(N-2)}}{(N-2)!} & \frac{x_0^{(N-1)}}{(N-1)!} \\ 1 & x_1 & \frac{x_1^2}{2!} & \cdots & \frac{x_1^{(N-3)}}{(N-3)!} & \frac{x_1^{(N-2)}}{(N-2)!} & \frac{x_1^{(N-1)}}{(N-1)!} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & x_{N-2} & \frac{x_{N-2}^2}{2!} & \cdots & \frac{x_{N-2}^{(N-3)}}{(N-3)!} & \frac{x_{N-2}^{(N-2)}}{(N-2)!} & \frac{x_{N-2}^{(N-1)}}{(N-1)!} \\ 1 & x_{N-1} & \frac{x_{N-1}^2}{2!} & \cdots & \frac{x_{N-1}^{(N-3)}}{(N-3)!} & \frac{x_{N-1}^{(N-2)}}{(N-2)!} & \frac{x_{N-1}^{(N-1)}}{(N-1)!} \end{pmatrix} \begin{pmatrix} f(0) \\ f^{(1)}(0) \\ f^{(2)}(0) \\ \vdots \\ f^{(N-3)}(0) \\ f^{(N-2)}(0) \\ f^{(N-1)}(0) \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{pmatrix}$$

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The Linear System (1)

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- Pro: More accurate results
- Con: Worse condition number

Condition Number

$$\text{Cond}(A) = \frac{|\lambda_{\max}(A)|}{|\lambda_{\min}(A)|},$$

$\lambda_{\min/\max}(A) =$ min/max eigenvalue of A

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The Linear System (2)

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^{(N-3)} & x_0^{(N-2)} & x_0^{(N-1)} \\ 1 & x_1 & x_1^2 & \dots & x_1^{(N-3)} & x_1^{(N-2)} & x_1^{(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 1 & x_{N-2} & x_{N-2}^2 & \dots & x_{N-2}^{(N-3)} & x_{N-2}^{(N-2)} & x_{N-2}^{(N-1)} \\ 1 & x_{N-1} & x_{N-1}^2 & \dots & x_{N-1}^{(N-3)} & x_{N-1}^{(N-2)} & x_{N-1}^{(N-1)} \end{pmatrix} \begin{pmatrix} f(0) \\ f^{(1)}(0) \\ \frac{f^{(2)}(0)}{2!} \\ \vdots \\ \frac{f^{(N-3)}(0)}{(N-3)!} \\ \frac{f^{(N-2)}(0)}{(N-2)!} \\ \frac{f^{(N-1)}(0)}{(N-1)!} \end{pmatrix} = \begin{pmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_{N-2}) \\ f(x_{N-1}) \end{pmatrix}$$

- Pro: Better condition number
- Con: Less accurate results

Condition Number

$$\mathrm{Cond}(A) = \frac{|\lambda_{\max}(A)|}{|\lambda_{\min}(A)|},$$
$$\lambda_{\min/\max}(A) = \min/\max \text{ eigenvalue of } A$$

Toy Model: $\sin(x)$

4 equally spaced input points in range $(0, 0.5i]$

	Points Only	Points and Parity
$f^{(k)}(0)$	0) $-9.519e^{-21} - 6.183e^{-05}i$	1) $+1.000e^{+00} + 1.205e^{-15}i$
	1) $+1.001e^{+00} + 0.000e^{+00}i$	3) $-1.000e^{+00} + 1.972e^{-13}i$
	2) $+9.660e^{-17} + 9.878e^{-03}i$	5) $+1.000e^{+00} + 2.959e^{-11}i$
	3) $-1.051e^{+00} + 3.075e^{-16}i$	7) $-1.007e^{+00} + 2.716e^{-09}i$
	Condition n.: $5.044e^{+03}$	Condition n.: $2.975e^{+07}$
$\frac{f^{(k)}(0)}{k!}k!$	0) $-1.294e^{-16} - 6.183e^{-05}i$	1) $+1.000e^{+00} + 1.150e^{-15}i$
	1) $+1.001e^{+00} - 1.554e^{-15}i$	3) $-1.000e^{+00} + 1.886e^{-13}i$
	2) $+1.130e^{-14} + 9.878e^{-03}i$	5) $+1.000e^{+00} + 2.830e^{-11}i$
	3) $-1.051e^{+00} + 4.002e^{-14}i$	7) $-1.007e^{+00} + 2.597e^{-09}i$
	Condition n.: $1.127e^{+03}$	Condition n.: $6.522e^{+03}$

Toy Model: $\sin(x)$

4 equally spaced input points in range $(0, 0.5i]$

	Points, Parity and 1st derivative	
$f^{(k)}(0)$	$1) +1.000e^{+00} + 1.858e^{-15}i$	$3) -1.000e^{+00} + 3.546e^{-13}i$
	$5) +1.000e^{+00} + 9.966e^{-11}i$	$7) -1.000e^{+00} + 2.614e^{-08}i$
	$9) +1.000e^{+00} + 5.224e^{-06}i$	$11) -1.005e^{+00} + 5.798e^{-04}i$
	$13) +5.220e^{-03} - 3.019e^{-06}i$	$15) -1.262e^{-05} + 7.304e^{-09}i$
	Condition n.: $5.658e^{+20}$	
$\frac{f^{(k)}(0)}{k!}k!$	$1) +1.000e^{+00} + 3.281e^{-15}i$	$3) -1.000e^{+00} - 4.122e^{-13}i$
	$5) +1.000e^{+00} - 1.145e^{-09}i$	$7) -1.000e^{+00} - 1.217e^{-06}i$
	$9) +1.000e^{+00} - 9.956e^{-04}i$	$11) -9.729e^{-01} - 6.334e^{-01}i$
	$13) +1.294e^{+01} - 2.826e^{+02}i$	$15) +2.789e^{+03} - 6.651e^{+04}i$
	Condition n.: $6.385e^{+08}$	

With LatticeQCD data[1]

Objective: The first two nontrivial derivatives of the barion number density $\chi_1(\mu)$ at $\mu = 0$

Input data: Baryon number density for $\mu \in \{+0.3928i, +0.7853i, +1.178i, +1.5709i\}$

	$\chi_2(0)$	$\chi_4(0)$	Cond. n.
$\chi_k(0)$	0.12278	0.466	352
$\frac{\chi_k(0)}{(k-1)!}$	0.12278	0.466	291
$\chi_k^{odd}(0)$	0.10973 ± 0.00140	0.081 ± 0.028	$3.25e^{+5}$
$\frac{\chi_k^{odd}(0)}{(k-1)!}$	0.10973	0.081	489
HotQCD	0.10870 ± 0.00004	0.084 ± 0.004	

[1] From the Bielefeld-Parma collaboration

In Conclusion...

- Discrepancy between HotQCD data and Bielefeld-Parma data is less than the error obtained through statistical bootstrap
- Lower order derivatives more stable than higher order derivatives

In the future:

- Thorough study of statistical errrors
- Comparison with another method of analytic continuation[2]

[2] See talk by F. Di Renzo