The QCD sign problem as a total derivative

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INT University of Washington, USA, May 8, 2013

What QCD at non-zero quark chemical potential $re^{i\theta} = \det(D + \mu\gamma_0 + m)$

Ensembles with θ fixed

Why Understand the histogram method

Z and n_B build up as $\int d\theta$

How General argumets, hadron resonance gas model, strong coupling

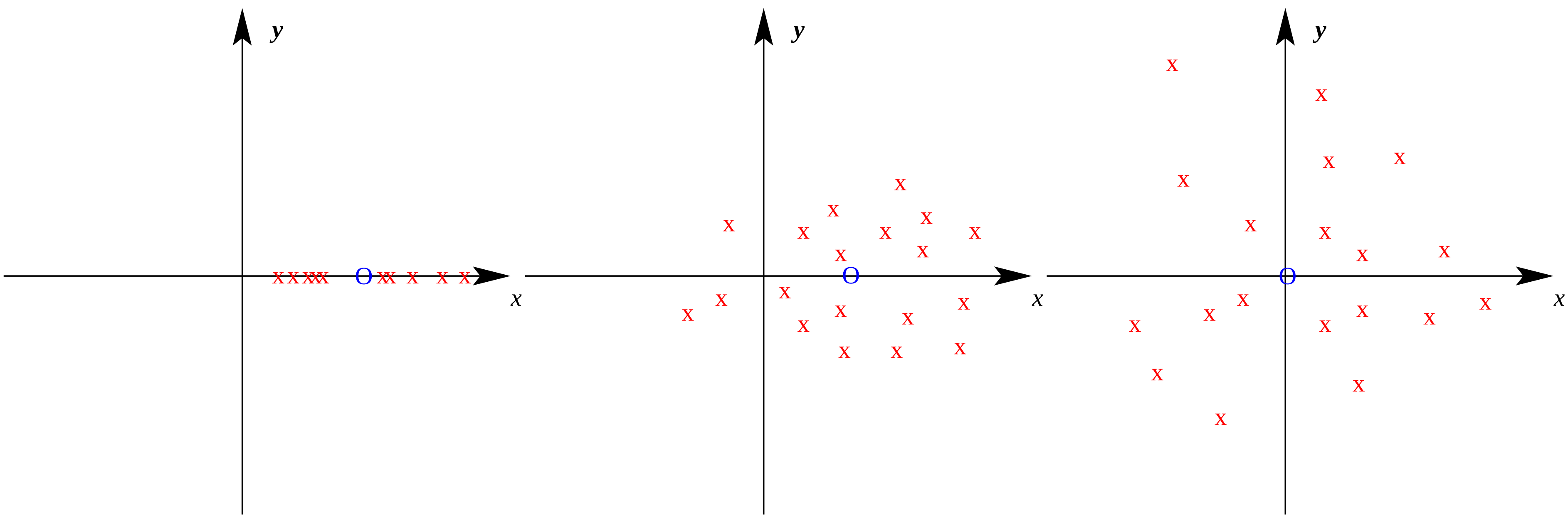
Sign problem = total derivatives wrt θ

What is a sign problem?

Severity of sign problem

$$\frac{1}{N}\sum^{N} X = O$$

No Weak Strong



The QCD sign problem

$$Z = \int dA \, \det(D + \mu\gamma_0 + m) \, e^{-S_{\mathrm{YM}}}$$

Anti Hermitian

Hermitian

$$\det(D + \mu\gamma_0 + m) = |\det(D + \mu\gamma_0 + m)| e^{i\theta}$$

The measure is not real and positive

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No QCD inequalities

hadron masses not what you think

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No QCD inequalities *hadron masses not what you think*

No Vafa-Witten theorem *symmetries not what you think*

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No Elitzur theorem — *local symmetries perhaps not what you think*

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No QCD inequalities — *hadron masses not what you think*

No Vafa-Witten theorem — *symmetries not what you think*

No Elitzur theorem — *local symmetries perhaps not what you think*

No Monte Carlo sampling of A_η — *lattice QCD not applicable*

Is the sign problem really that bad ?

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The θ-distribution: $\langle \delta(\theta - \theta') \rangle$

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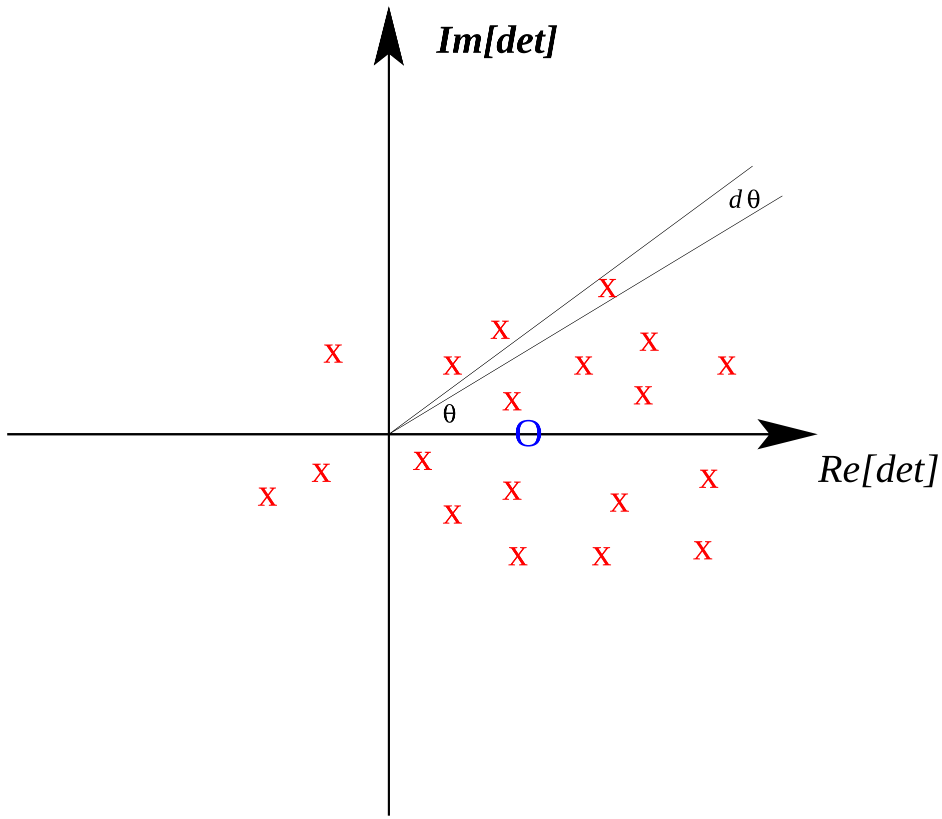

Full theory $\int d\theta \langle\delta(\theta - \theta')\rangle$

The θ-distribution is complex

$$\langle \delta(\theta - \theta') \rangle_{1+1} \quad \equiv \quad \frac{1}{Z_{1+1}} \int dA\ \delta(\theta - \theta') \det{}^2(D + \mu\gamma_0 + m) e^{-S_{YM}}$$

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$$\begin{aligned}
\langle \delta(\theta - \theta') \rangle_{1+1} &= \frac{1}{Z_{1+1}} \int dA \, \delta(\theta - \theta') |\det(D + \mu\gamma_0 + m)|^2 e^{2i\theta'} e^{-S_{YM}} \\
&= \frac{1}{Z_{1+1}} e^{2i\theta} \int dA \, \delta(\theta - \theta') |\det(D + \mu\gamma_0 + m)|^2 e^{-S_{YM}}
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$$\begin{aligned}\langle\delta(\theta-\theta')\rangle_{1+1} \quad &= \quad \frac{1}{Z_{1+1}}\int dA\, \delta(\theta-\theta')|\det(D+\mu\gamma_0+m)|^2 e^{2i\theta'} e^{-S_{YM}} \\ &= \quad \frac{1}{Z_{1+1}}e^{2i\theta}\int dA\, \delta(\theta-\theta')|\det(D+\mu\gamma_0+m)|^2 e^{-S_{YM}}\end{aligned}$$

$$\langle\delta(\theta-\theta')\rangle_{1+1} \quad = \quad \frac{Z_{1+1^*}}{Z_{1+1}}e^{2i\theta}\langle\delta(\theta-\theta')\rangle_{1+1^*}$$

The simplest thing - normalization of the θ-distribution

$$\langle \delta(\theta - \theta') \rangle_{1+1} \quad = \quad \frac{Z_{1+1^*}}{Z_{1+1}} e^{2i\theta} \langle \delta(\theta - \theta') \rangle_{1+1^*}$$

$$\int d\theta \; \langle \delta(\theta - \theta') \rangle_{1+1} \quad = \quad \int d\theta \; \langle \delta(\theta - \theta') \rangle_{1+1^*} = 1$$

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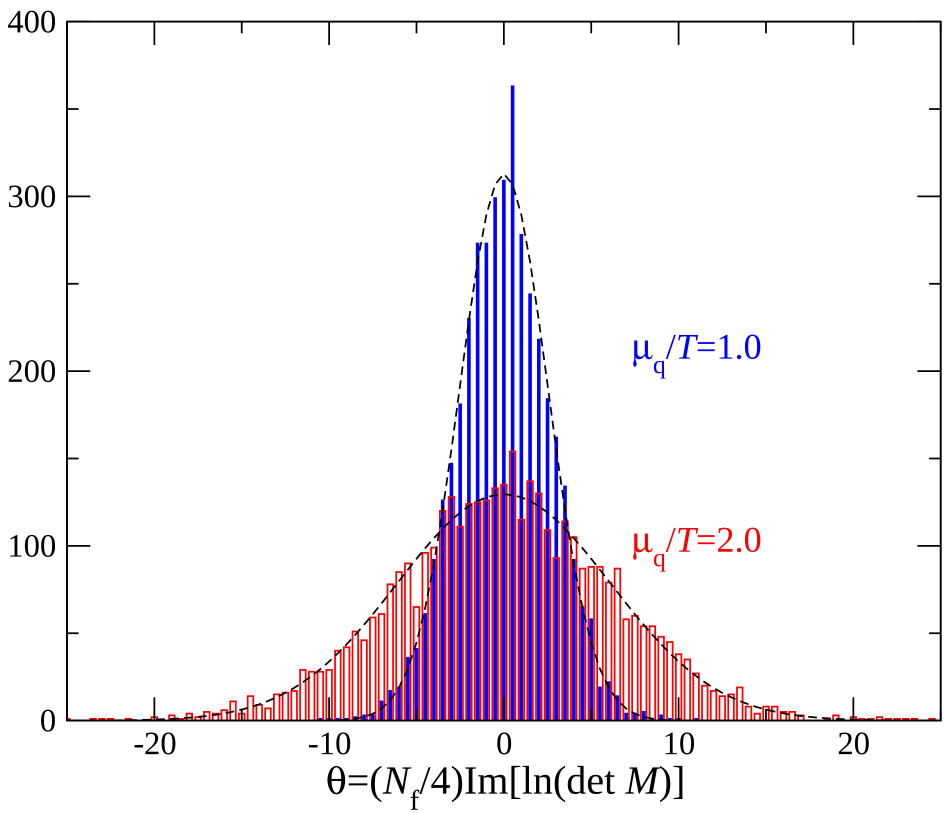
Exponential cancellations!

$\mu < m_\pi/2$ VS $\mu > m_\pi/2$

Alford Kapustin Wilczek PRD 59 (1999) 054502
Splittorff, Verbaarschot PRL 98 (2007) 031601

Dorota Grabowska, David Kaplan, Amy Nicholson PRD 87, 014504 (2013)

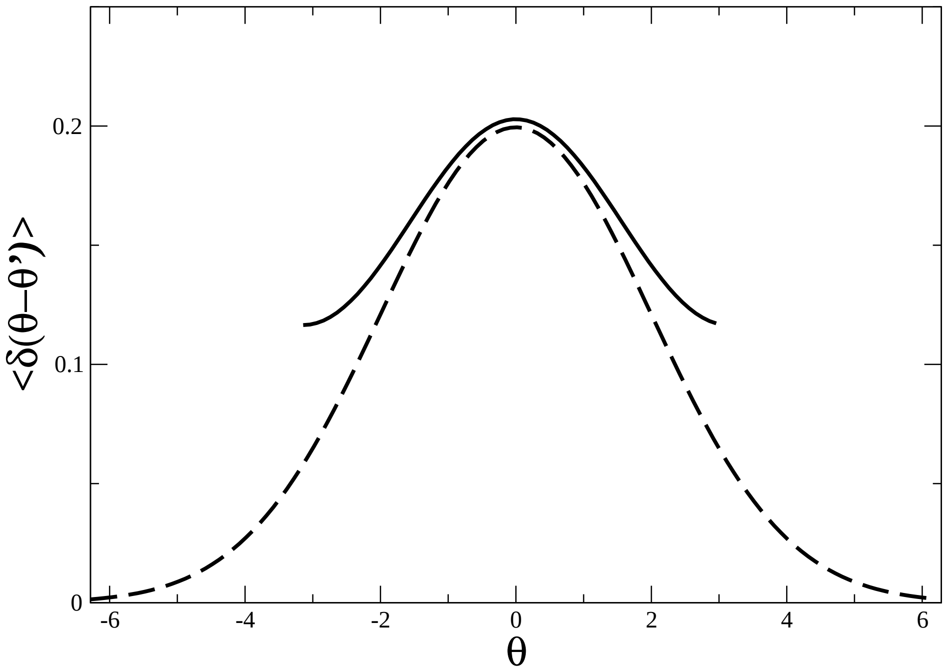
The θ-distribution from the lattice $\mu < m_\pi/2$



Central limit theorem $\longrightarrow$ Gaussian

Ejiri PRD 77 (2008) 014508

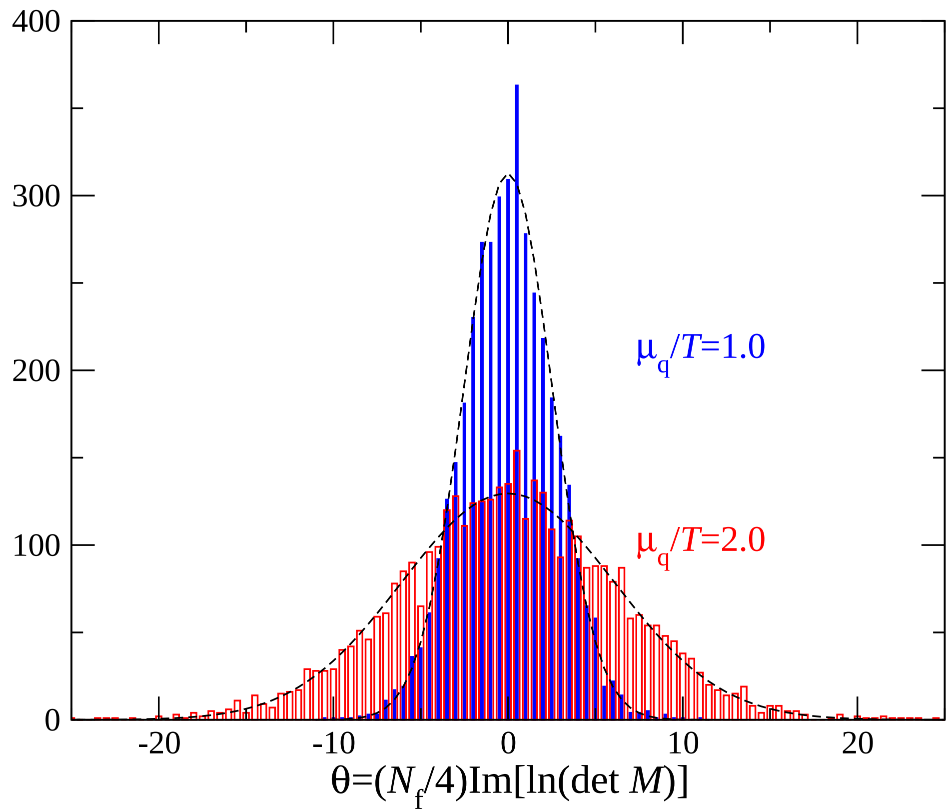
Gaussian folded onto $[-\pi : \pi]$



Multiply by $e^{2i\theta}$ to get $\langle\delta(\theta - \theta')\rangle_{1+1}$

Histogram method

(*a.k.a. Density of states method or Factorization method*)



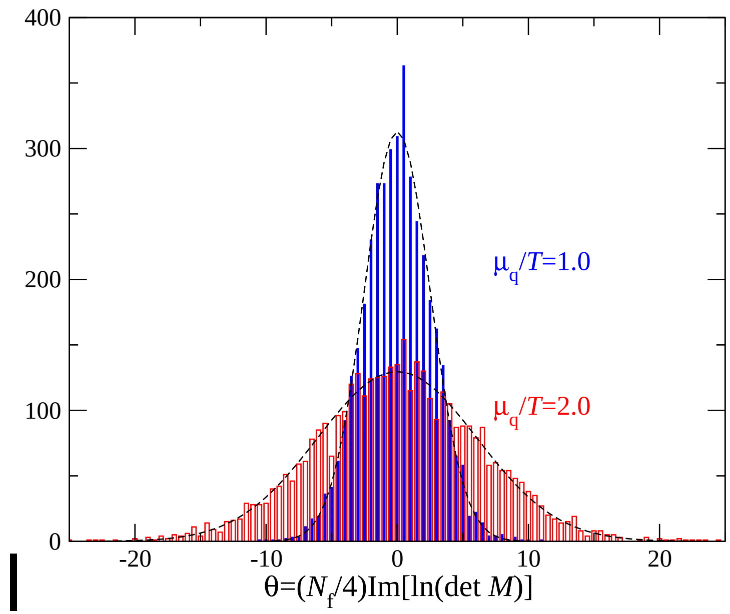
Measure the width of the Gaussian and do the θ integral analytically.

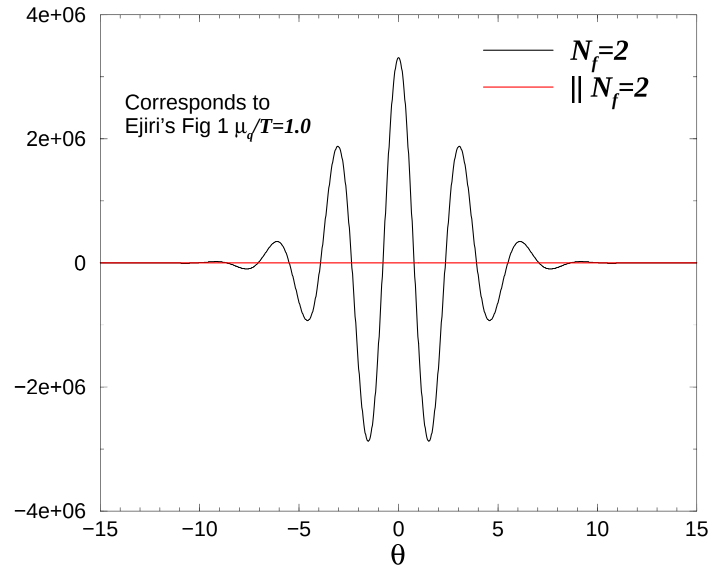
Anagnostopoulos Nishimura PRD 66 (2002) 106008

Fodor Katz Schmidt JHEP 0703:121,2007

Ejiri PRD 77 (2008) 014508

The exponential cancellations





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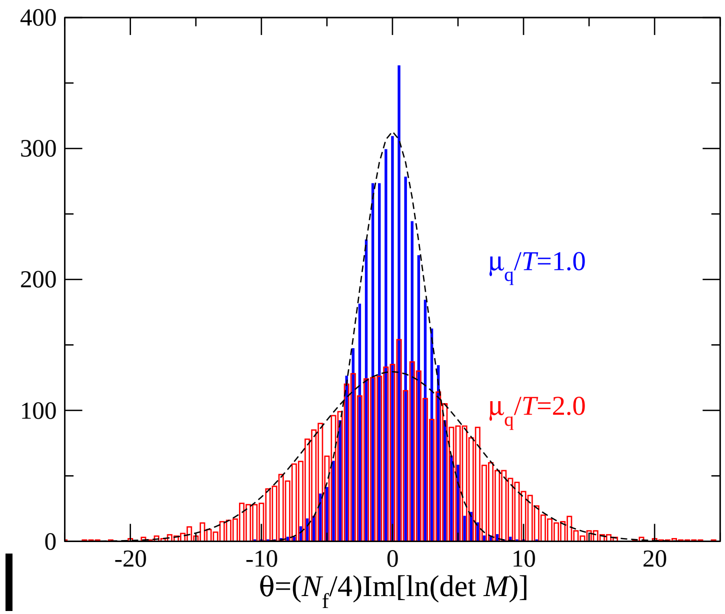

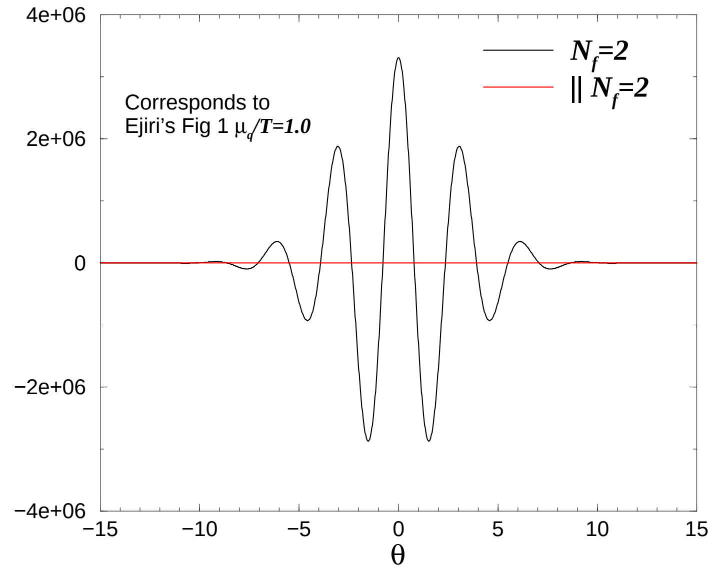

The Gaussian fit needs to be good

Is $\langle \delta(\theta - \theta') \rangle_{1+1^*}$ Gaussian?

Is $\langle \delta(\theta - \theta') \rangle_{1+1^*}$ Gaussian?

Check analytically!

Michael G. Endres, David B. Kaplan, Jong-Wan Lee, Amy N. Nicholson, PoS (Lattice 2011) Plenary
Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, *to appear*

The delta function

$$\langle \delta(\theta - \theta') \rangle_{1+1} \equiv \frac{1}{Z_{1+1}} \int dA\ \delta(\theta - \theta') \det{}^2(D + \mu\gamma_0 + m) e^{-S_{YM}}$$

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$$\delta(\theta - \theta') = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp \; e^{ip(-\theta+\theta')}$$

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$$\langle \delta(\theta - \theta') \rangle_{1+1} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp \; e^{-ip\theta} \langle e^{ip\theta'} \rangle_{1+1}$$

The moments of the phase factor

$$\langle e^{ip\theta'} \rangle_{N_f} \equiv \frac{1}{Z_{N_f}} \left\langle \frac{\det^{N_f+p/2}(D+\mu\gamma_0+m)}{\det^{p/2}(D-\mu\gamma_0+m)} \right\rangle$$

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Compute these moments for all p and pluck them back into

$$\langle \delta(\theta - \theta') \rangle_{1+1} = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp\, e^{-ip\theta} \langle e^{ip\theta'} \rangle_{1+1}$$

General form of the moments $(\mu < m_\pi/2)$

$$\langle e^{ip\theta'} \rangle_{N_f} = e^{-p/2(N_f+p/2)X_1 - (p/2(N_f+p/2))^2 X_2 + \ldots}$$

where the X_j's are extensive

General form of the moments $(\mu < m_\pi/2)$

$$\langle e^{ip\theta'}\rangle_{N_f} = e^{-p/2(N_f+p/2)X_1-(p/2(N_f+p/2))^2X_2+\ldots}$$

where the X_j's are extensive

Gaussian dist of $\theta \Leftrightarrow X_j = 0$ for all $j > 1$

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, *to appear*

Gaussian distribution found in

- 1-loop chiral perturbation theory
- Hadron resonance gas model
- Strong coupling QCD at large N_c *confined and deconfined*

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, *to appear*

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But ... strong coupling QCD for $N_c = 3$ has corrections to Gaussian

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Greensite Myers Splittorff, *to appear*

In CPT at 1-loop

Number of charged pions

$$\langle e^{ip\theta'} \rangle_{N_f} = e^{-p/2(N_f+p/2)V\Delta G_0}$$

ΔG_0 is the difference between charged and neutral pions

In CPT at 1-loop

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ΔG_0 is the difference between charged and neutral pions

$$\Delta G_0 = \frac{m_\pi^2 T^2}{\pi^2} \sum_{n=1}^{\infty} \frac{K_2(\frac{m_\pi n}{T})}{n^2} \left[\cosh(\frac{2\mu n}{T}) - 1 \right]$$

Challenge

Compute the moments of the phase factor

$$\langle e^{ip\theta'} \rangle_{N_f} \equiv \frac{1}{Z_{N_f}} \left\langle \frac{\det^{N_f+p/2}(D+\mu\gamma_0+m)}{\det^{p/2}(D-\mu\gamma_0+m)} \right\rangle$$

in your favorite approach to QCD.

Masanori Hanada, Carlos Hoyos, Andreas Karch, Laurence G. Yaffe arXiv:1201.3718

The sign problem as a total derivative

The distribution of n_B with θ

$$\langle n_B \delta(\theta - \theta') \rangle_{1+1}$$

$$\equiv \qquad \frac{1}{Z_{1+1}} \lim_{\tilde{\mu}\to\mu} \frac{d}{d\tilde{\mu}} \int dA \; \delta(\theta - \theta'(\mu)) \det{}^2(D + \tilde{\mu}\gamma_0 + m) e^{-S_{YM}}$$

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Recall

$$\delta(\theta - \theta'(\mu)) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dp \; e^{-ip\theta} \frac{\mathrm{det}^{p/2}(D + \mu\gamma_0 + m)}{\mathrm{det}^{p/2}(D - \mu\gamma_0 + m)}$$

The general form of

$$\frac{1}{Z_{N_f}}\left\langle \frac{\det^{p/2}(D+\mu\gamma_0+m)}{\det^{p/2}(D-\mu\gamma_0+m)}\det{}^{N_f}(D+\tilde{\mu}\gamma_0+m)\right\rangle = \exp[\text{polynomial in } p]$$

where

$$\lim_{\tilde{\mu}\to\mu} e^{\text{polynomial in } p} = e^{-p/2(N_f+p/2)X_1-(p/2(N_f+p/2))^2X_2+\ldots}$$

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$$\langle n_B\delta(\theta-\theta')\rangle_{N_f} = \int\frac{dp}{2\pi}e^{-ip\theta}(c_0+c_1p+c_2p^2+\dots)e^{-p/2(N_f+p/2)X_1-\dots}$$

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... looks pretty complicated ... but in fact ...

Total derivatives

We found

$$\langle n_B \delta(\theta - \theta') \rangle_{N_f} = \int \frac{dp}{2\pi} e^{-ip\theta} (c_0 + c_1 p + c_2 p^2 + \ldots) e^{-p/2(N_f + p/2)X_1 - \ldots}$$

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But this is simply

$$\begin{aligned}
& \langle n_B \delta(\theta - \theta')\rangle_{N_f} \\
= \quad & \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \left(c_0 + \frac{c_1}{-i}\frac{\partial}{\partial\theta} + \frac{c_2}{(-i)^2}\frac{\partial^2}{\partial\theta^2} + \ldots \right) e^{-ip\theta} e^{-p/2(N_f + p/2)X_1 + \ldots} \\
= \quad & \left(c_0 + \frac{c_1}{-i}\frac{\partial}{\partial\theta} + \frac{c_2}{(-i)^2}\frac{\partial^2}{\partial\theta^2} + \ldots \right) \langle \delta(\theta - \theta')\rangle_{N_f}
\end{aligned}$$

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Signal

Noise

Example

$$\langle n_B \delta(\theta - \theta') \rangle_{N_f} = \int \frac{dp}{2\pi} e^{-ip\theta} (c_0 + c_1 p + c_2 p^2 + \ldots) e^{-p/2(N_f + p/2) X_1 - \ldots}$$

In 1-loop chiral perturbation theory only $c_1 \neq 0$

Example

$$\langle n_B \delta(\theta - \theta') \rangle_{N_f} = \int \frac{dp}{2\pi} e^{-ip\theta} (c_0 + c_1 p + c_2 p^2 + \ldots) e^{-p/2(N_f + p/2)X_1 - \ldots}$$

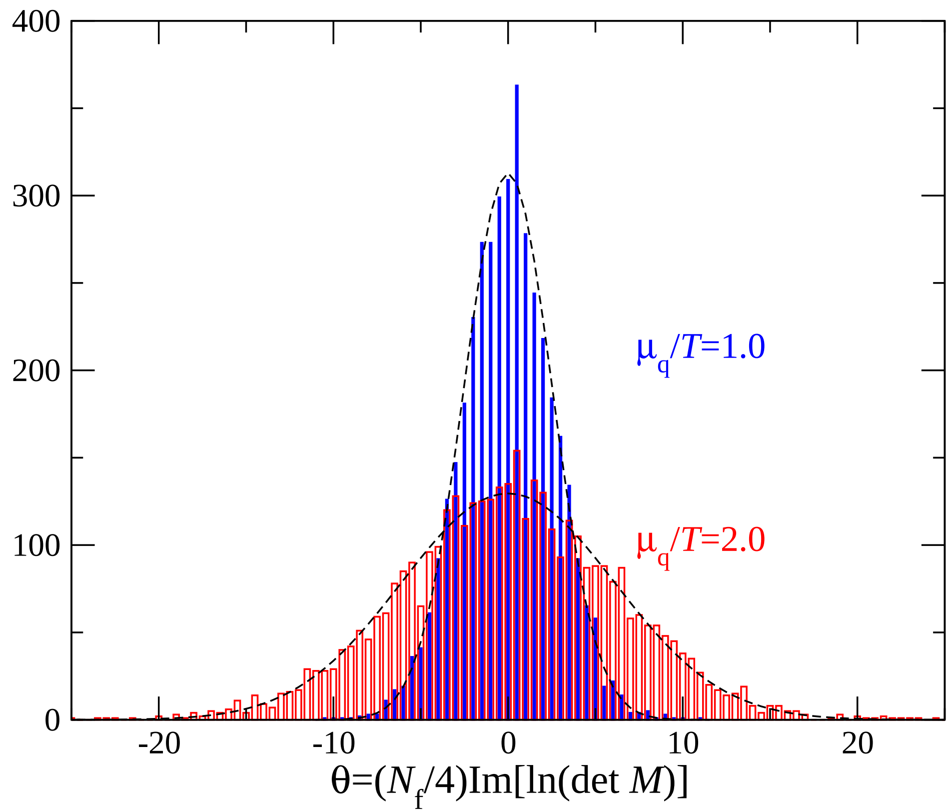
In 1-loop chiral perturbation theory only $c_1 \neq 0$

$$\langle n_B \rangle_{N_f} \quad = \quad \int d\theta \left(\frac{c_1}{-i} \frac{\partial}{\partial \theta} \right) \langle \delta(\theta - \theta') \rangle_{N_f} = 0$$

Only Noise

Histogram method

(*a.k.a. Density of states method or Factorization method*)



Check the Gaussian carefully and check for total derivatives.

Anagnostopoulos Nishimura PRD 66 (2002) 106008

Fodor Katz Schmidt JHEP 0703:121,2007

Ejiri PRD 77 (2008) 014508

⋮

Total derivatives and volume

In 1-loop chiral perturbation theory

$$\begin{aligned}
&\langle n_B \delta(\theta - \theta')\rangle_{1+1} \\
&= \quad [\lim_{\tilde{\mu}\to\mu} \frac{d}{d\tilde{\mu}} V\Delta G_0(-\mu,\tilde{\mu})] \frac{e^{V\Delta G_0}}{\sqrt{\pi V\Delta G_0}} (1 + i\frac{\theta}{V\Delta G_0}) e^{2i\theta} e^{-\theta^2/V\Delta G_0}
\end{aligned}$$

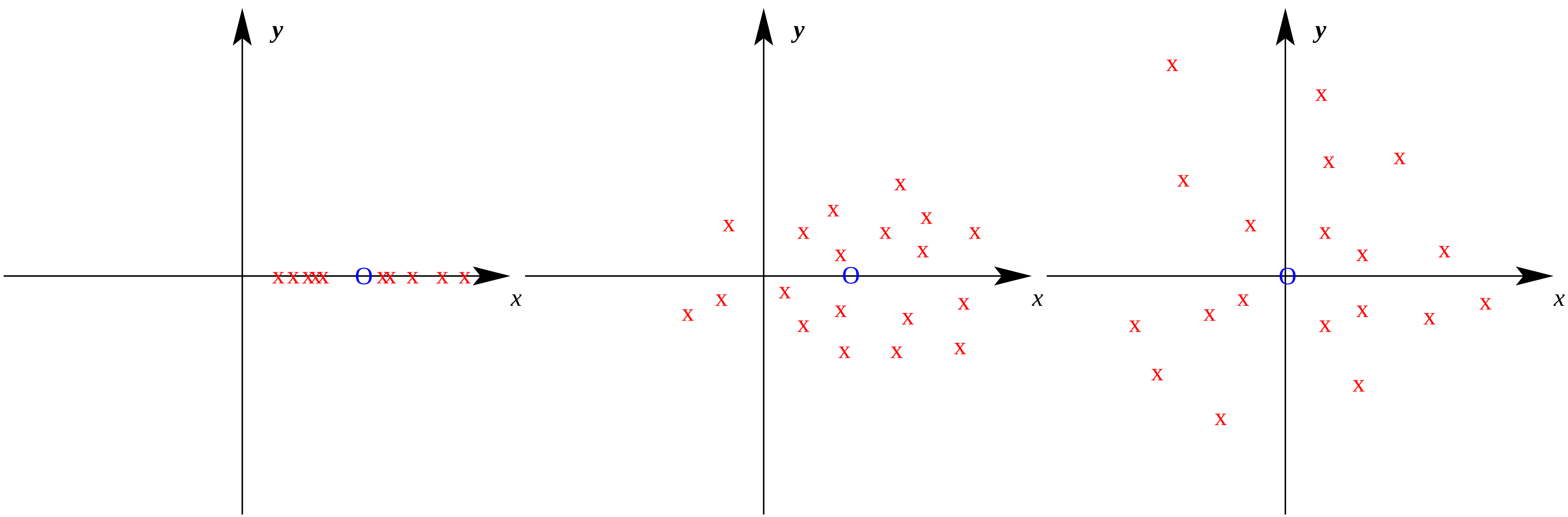
Severity of sign problem

$$\frac{1}{N}\sum^{N} X = O$$

No

Weak

Strong



Conclusions

Interplay between lattice QCD and analytic QCD is essential to understand QCD at $\mu \neq 0$

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Here:

Fixed θ

Studied how $\langle n_B \rangle$ builds up

Non-Gaussian terms even for $\mu < m_\pi/2$

Sign problem as total derivative

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Interplay between lattice QCD and analytic QCD is essential to understand QCD at $\mu \neq 0$

Here:

Fixed θ

Studied how $\langle n_B \rangle$ builds up

Non-Gaussian terms even for $\mu < m_\pi/2$

Sign problem as total derivative

Next: Implement in lattice QCD and Extend to $\mu > m_\pi/2$

In CPT at mean field level

Bosonic mean field rules

$$\langle e^{2ip\theta'}\rangle_{N_f} = e^{-(|p+N_f/2|-N_f/2)V\Delta\Omega}$$

$\Delta\Omega$ is the difference between the mean field terms

In CPT at mean field level

Bosonic mean field rules

$$\langle e^{2ip\theta'} \rangle_{N_f} = e^{-(|p+N_f/2|-N_f/2)V\Delta\Omega}$$

$\Delta\Omega$ is the difference between the mean field terms

$$\Delta\Omega = 2\mu^2 F^2 + \frac{\Sigma^2 m^2}{2\mu^2 F^2} - 4m\Sigma$$

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

The θ-distribution ($\mu > m_\pi/2$)

$$\langle \delta(2\theta - 2\theta') \rangle = \frac{1}{\pi} \sum_{p=-\infty}^{\infty} e^{-2ip\theta} \langle e^{2ip\theta'} \rangle_{N_f}$$

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Lorentzian (on $[-\pi/2 : \pi/2]$)

$$\langle\delta(2\theta - 2\theta')\rangle_{1+1} = e^{2i\theta}\frac{e^{V\Delta\Omega}}{2\pi}\frac{\sinh(V\Delta\Omega)}{\cosh(V\Delta\Omega) - \cos(2\theta)}$$

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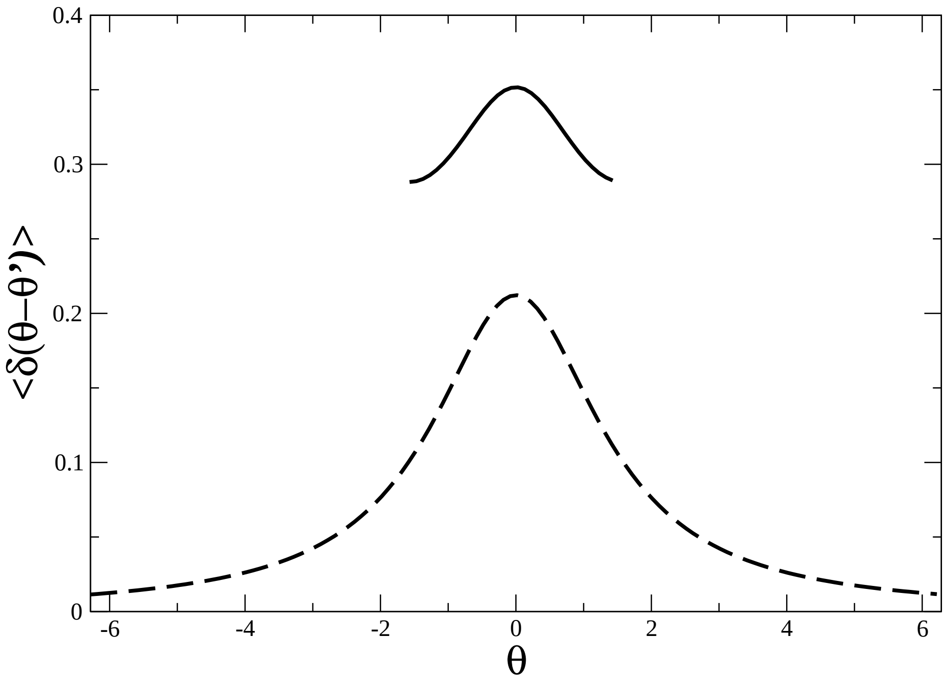
Central limit theorem fails!

Lorentzian folded onto $[-\pi/2 : \pi/2]$



Multiply by $e^{2i\theta}$ to get $\langle\delta(2\theta - 2\theta')\rangle_{1+1}$