The QCD sign problem as a total derivative

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XQCD, AEC univerity of Bern, August 6, 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 $\int d\theta$

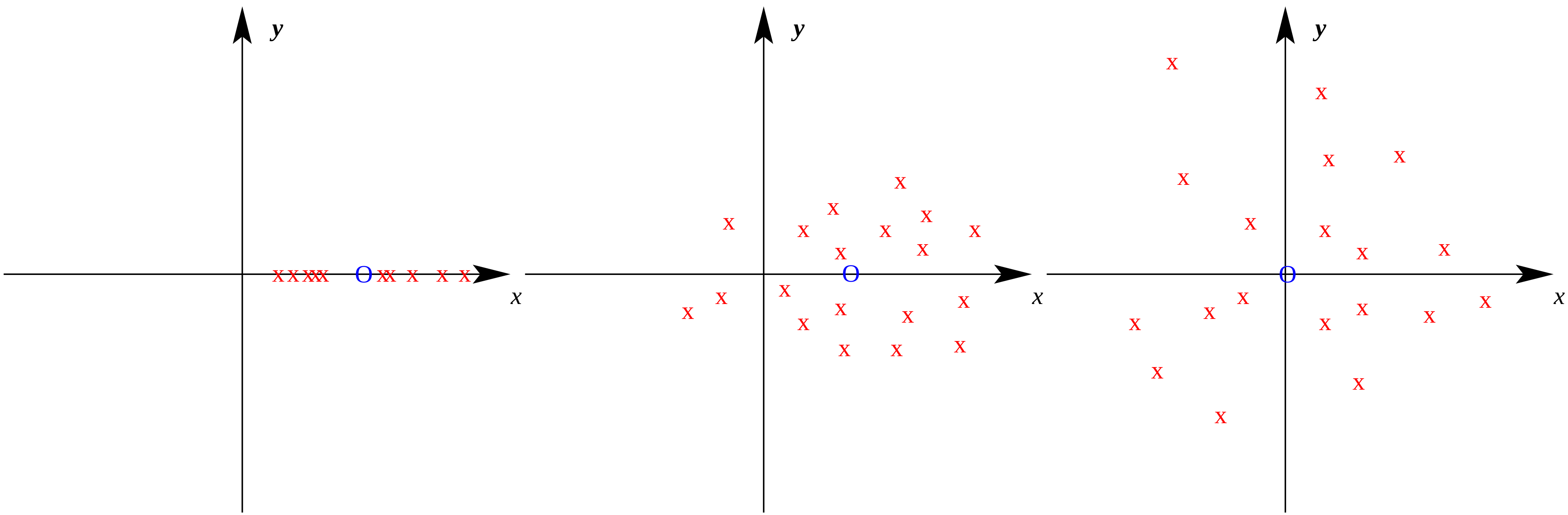
How General argumets, hadron resonance gas model, strong coupling

Sign problem = total derivatives wrt θ

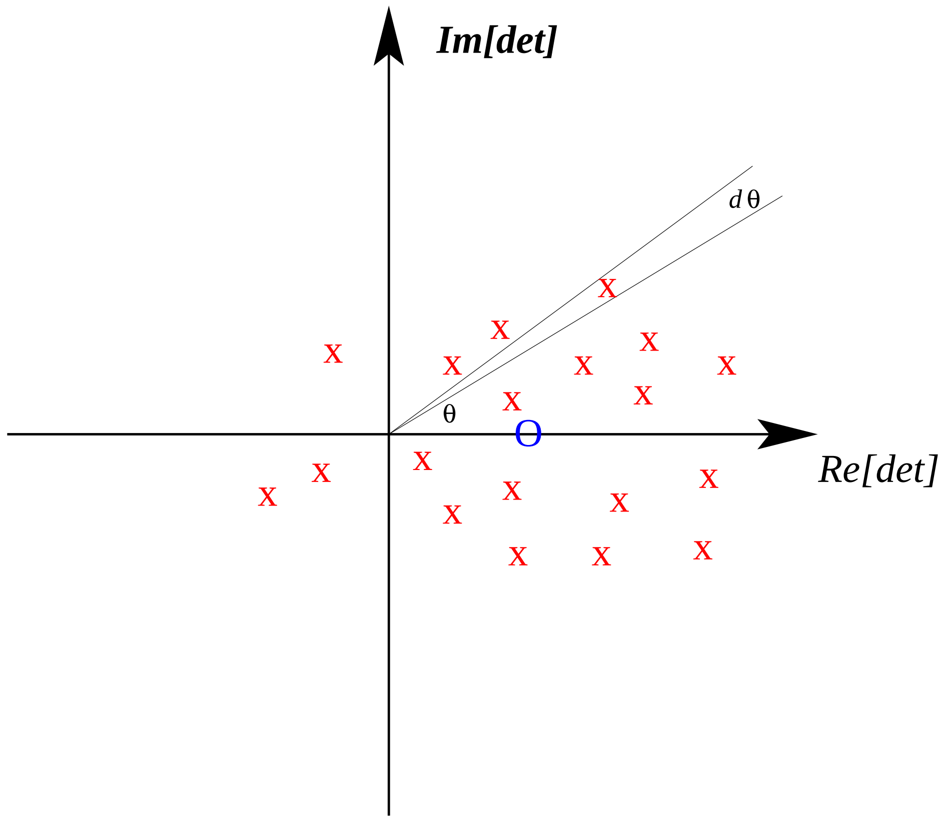
The sign problem

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

No Weak Strong



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



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

The θ-distribution is complex

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

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

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

The simplest thing - normalization of the θ-distribution

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

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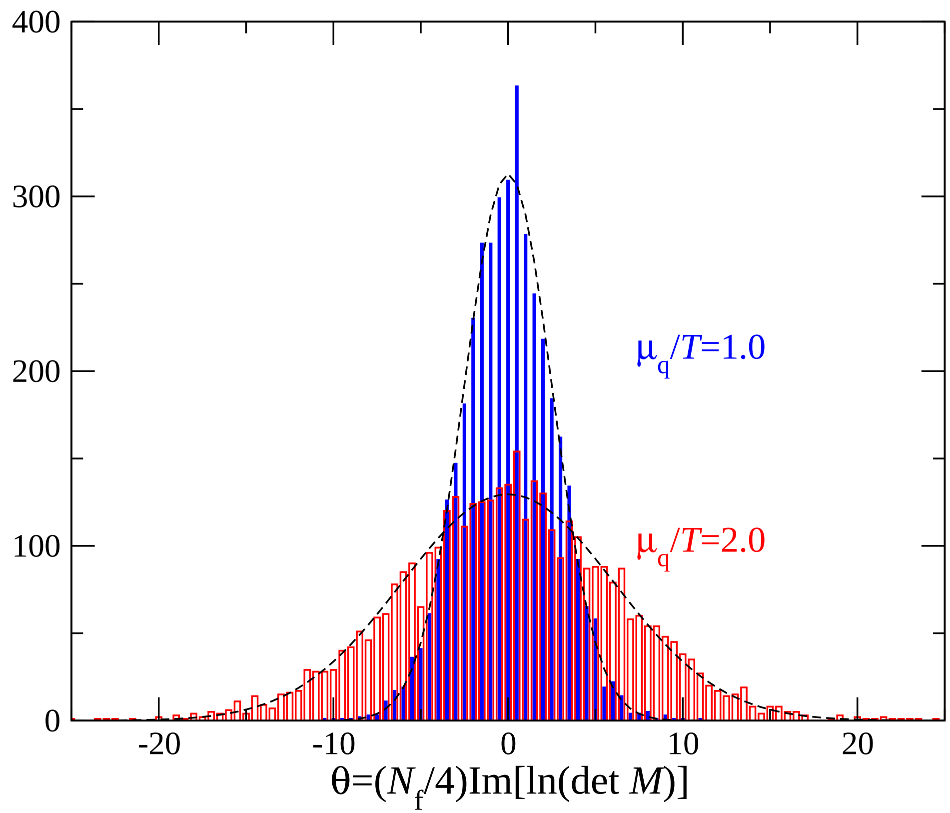
Exponential cancellations!

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

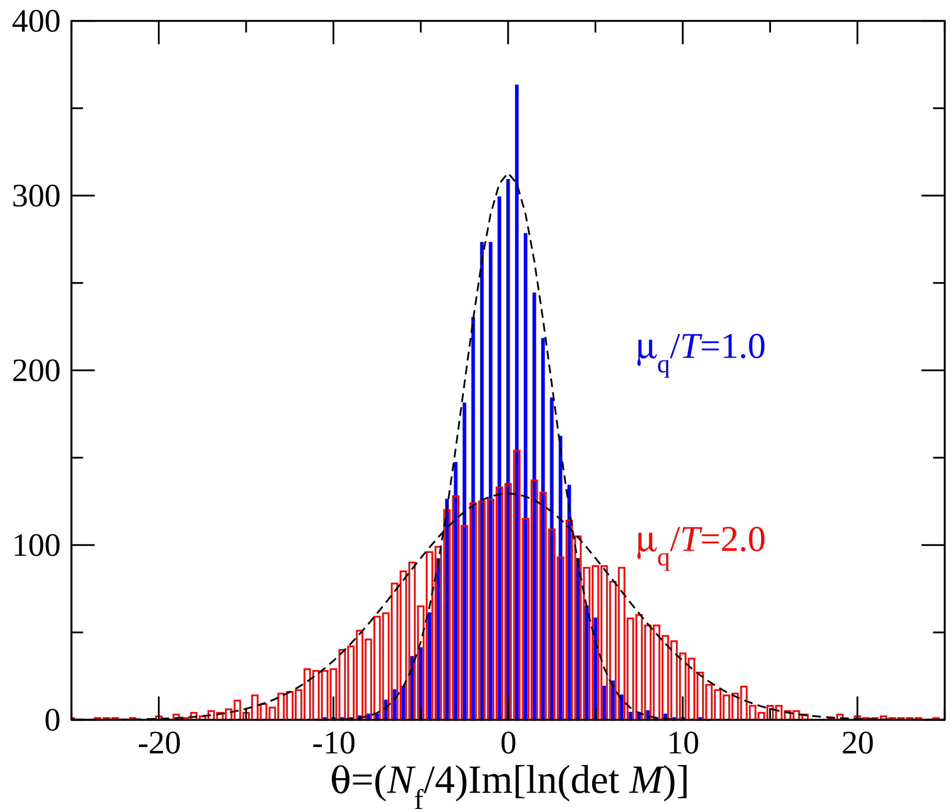


Central limit theorem $\longrightarrow$ Gaussian

Ejiri PRD 77 (2008) 014508

Histogram method

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



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

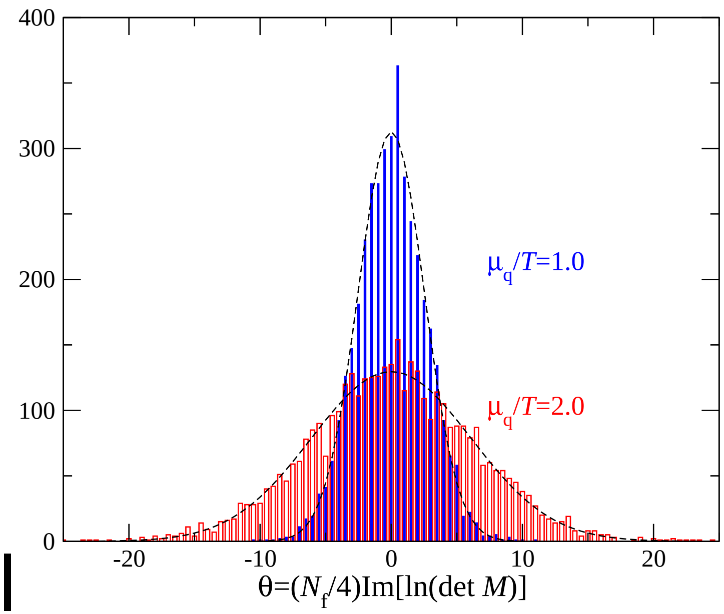
Anagnostopoulos Nishimura PRD 66 (2002) 106008

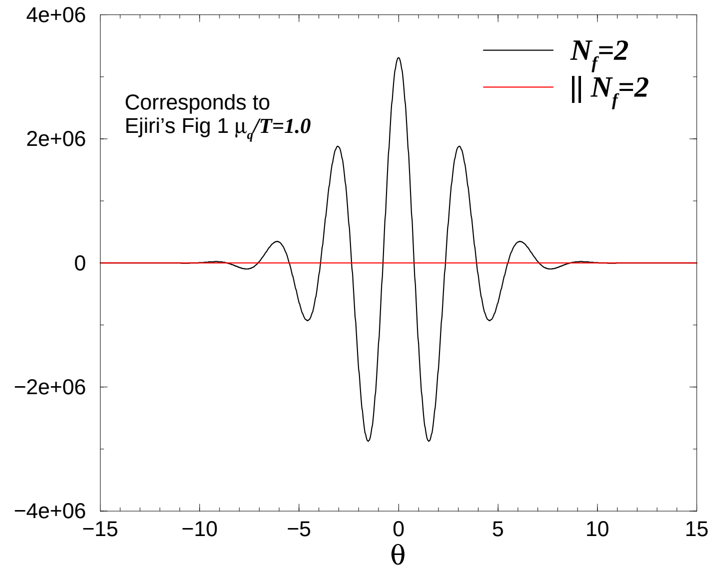
Fodor Katz Schmidt JHEP 0703:121,2007

Ejiri PRD 77 (2008) 014508

:

The exponential cancellations





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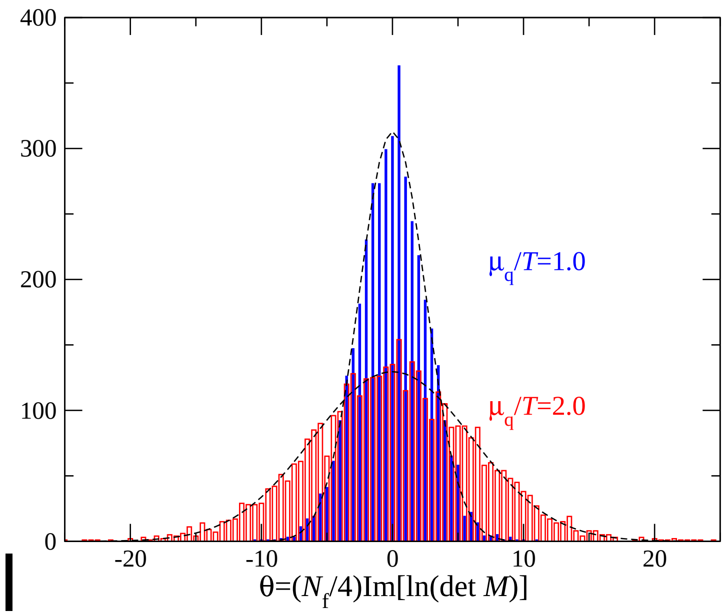

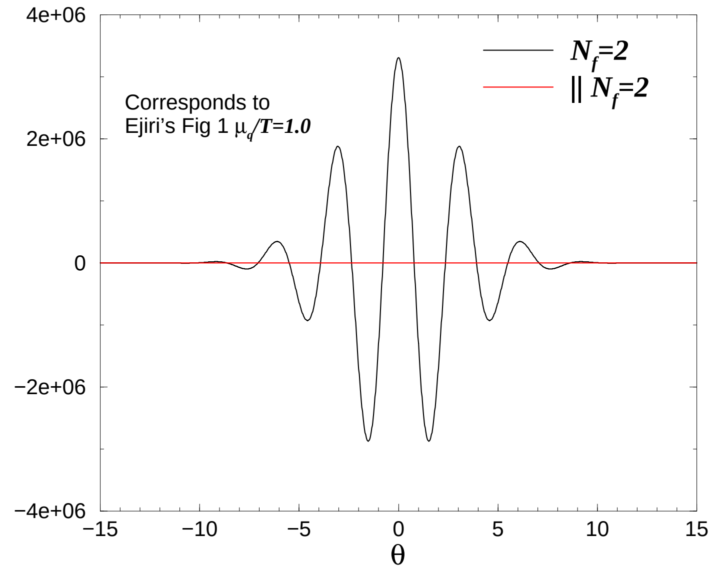

The Gaussian fit needs to be good

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

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

Check analytically!

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, arXiv:1306.3085 and *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 ($\mu < m_\pi/2$)

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

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, arXiv:1306.3085 and *to appear*

Gaussian distribution found in

- 1-loop chiral perturbation theory
- Hadron resonance gas model

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, *to appear*

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But ... strong coupling QCD for $N_c = 3$ beyond 3rd order in the hopping parameter has corrections to Gaussian

Lombardo Splittorff Verbaarschot PRD 80 (2009) 054509

Greensite Myers Splittorff, *to appear*

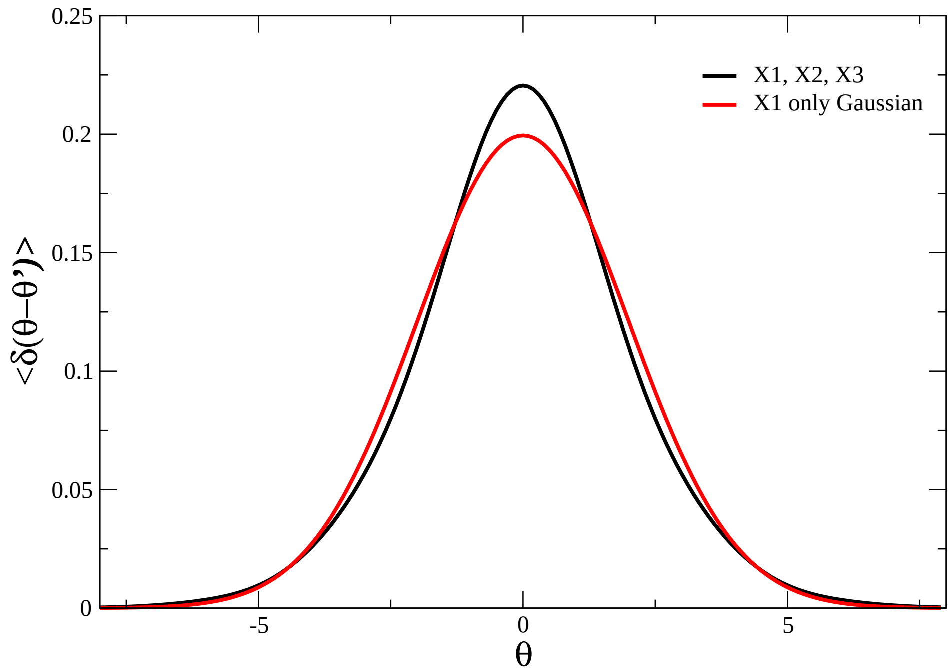
Warning: $\langle \delta(\theta - \theta') \rangle$ looks Gaussian at large volumes!

Example with 20% correction to the free energy

$$\langle\delta(\theta-\theta')\rangle = \frac{1}{2\pi}\int dp\; e^{-i\theta p} e^{-p^2 X_1 - p^4 X_2 - p^6 X_3}$$

$X_1 = V$; $X_2 = -.2V$; $X_3 = 0.02V$ (Black)

$X_1 = V$; $X_2 = 0$; $X_3 = 0$ (Red) $\qquad V = 2$



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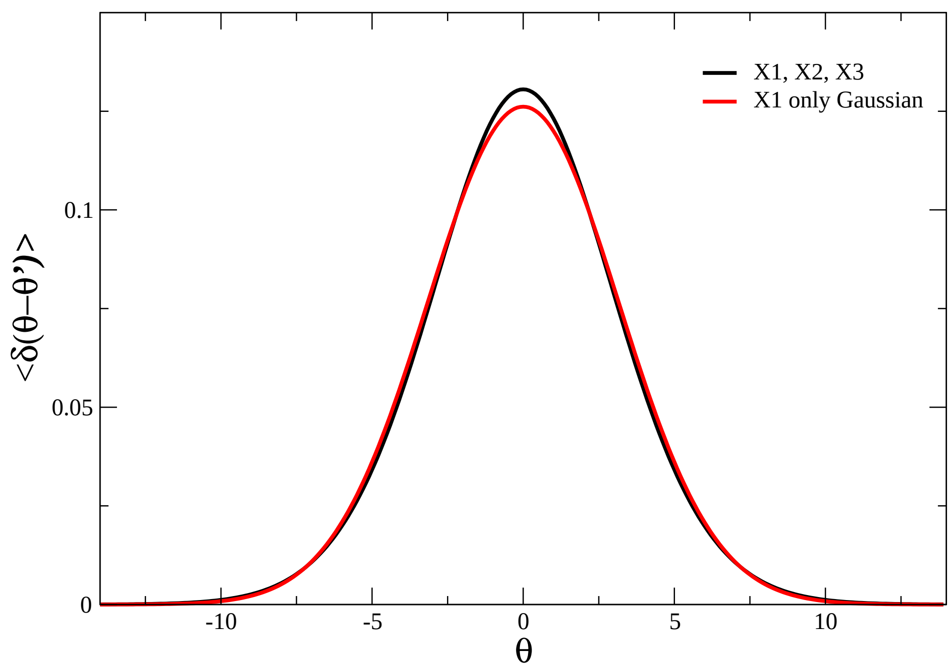
$X_1 = V$; $X_2 = -.2V$; $X_3 = 0.02V$ (Black)

$X_1 = V$; $X_2 = 0$; $X_3 = 0$ (Red) $V = 5$



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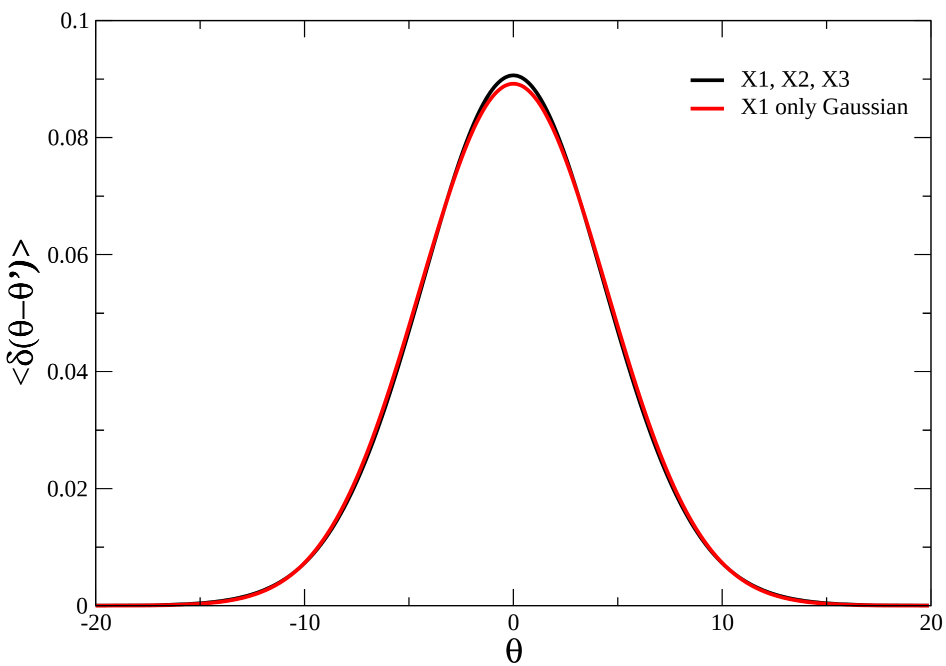
$X_1 = V$; $X_2 = -.2V$; $X_3 = 0.02V$ (Black)

$X_1 = V$; $X_2 = 0$; $X_3 = 0$ (Red) $V = 10$



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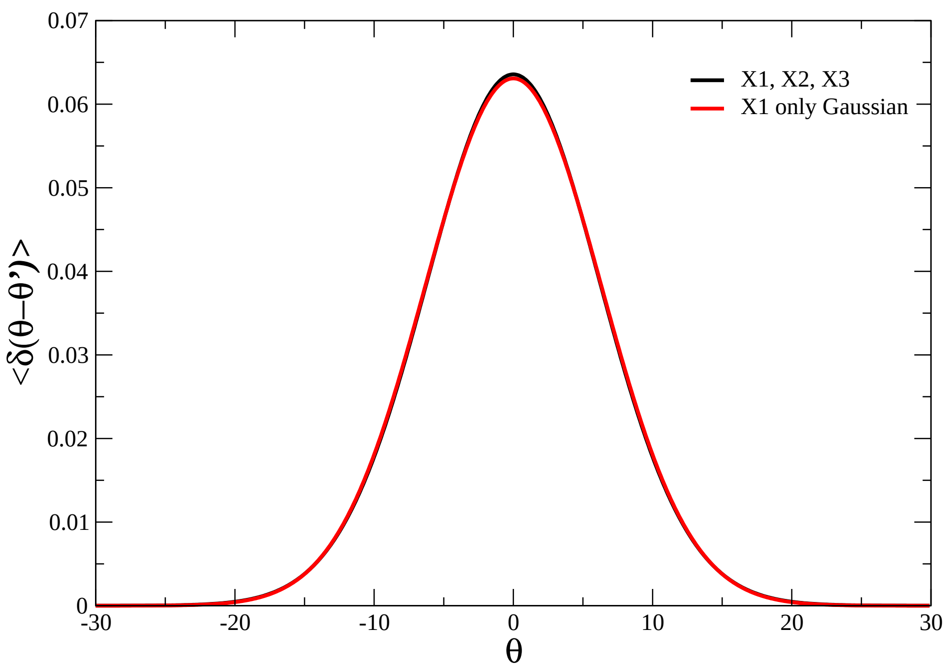
$X_1 = V$; $X_2 = 0$; $X_3 = 0$ (Red) $\qquad V = 20$



Reason: The effect of X_2 is $1/V$ suppressed in $\langle \delta(\theta - \theta') \rangle$ (for $\theta \ll V$)

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Consistent with the central limit theorem

However:

We want to obtain $\langle e^{i\theta} \rangle$ from the distribution

$$\langle \delta(\theta - \theta') \rangle = \frac{1}{2\pi} \int dp\, e^{-i\theta p} e^{-p^2 X_1 - p^4 X_2 - p^6 X_3}$$

Analytically this is trivial

$$\int d\theta\, e^{i\theta} \langle \delta(\theta - \theta') \rangle = e^{-X_1 - X_2 - X_3}$$

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But if we only capture the Gaussian (ie. X_1) we make a 20$\%$ error

Conclusion: The effect of X_2 is $1/V$ suppressed in $\langle\delta(\theta-\theta')\rangle$. But is nevertheless needed to get the correct free energy.

The sign problem as a total derivative

The distribution of n_B with θ

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

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

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We are after

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

The sign problem as total derivatives

$$\langle n_B \delta(\theta - \theta') \rangle_{N_f} = \left(c_0 + \frac{c_1}{-i} \frac{\partial}{\partial \theta} + \frac{c_2}{(-i)^2} \frac{\partial^2}{\partial \theta^2} + \ldots \right) \langle \delta(\theta - \theta') \rangle_{N_f}$$

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Signal

Noise

$$\langle n_B \rangle_{1+1} = \int d\theta \; \langle n_B \delta(\theta - \theta') \rangle_{1+1} = c_0$$

Example

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

Conclusions

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

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

Here:

- Fixed θ
- Non-Gaussian terms even for $\mu < m_\pi/2$
- Sign problem as total derivative

Additional slides

The distribution of n_B with θ

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Recall

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

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

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

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

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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

Total derivatives and volume

In 1-loop chiral perturbation theory

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

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

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

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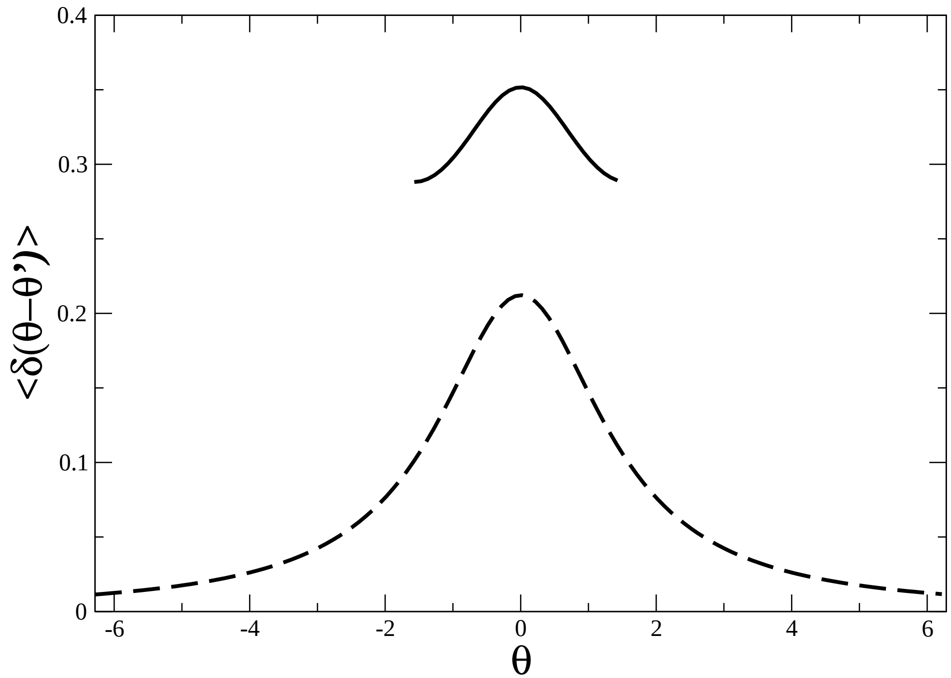
$$\langle\delta(2\theta - 2\theta')\rangle_{1+1} = e^{2i\theta}\frac{e^{V\Delta\Omega}}{2\pi}\frac{\sinh(V\Delta\Omega)}{\cosh(V\Delta\Omega) - \cos(2\theta)}$$

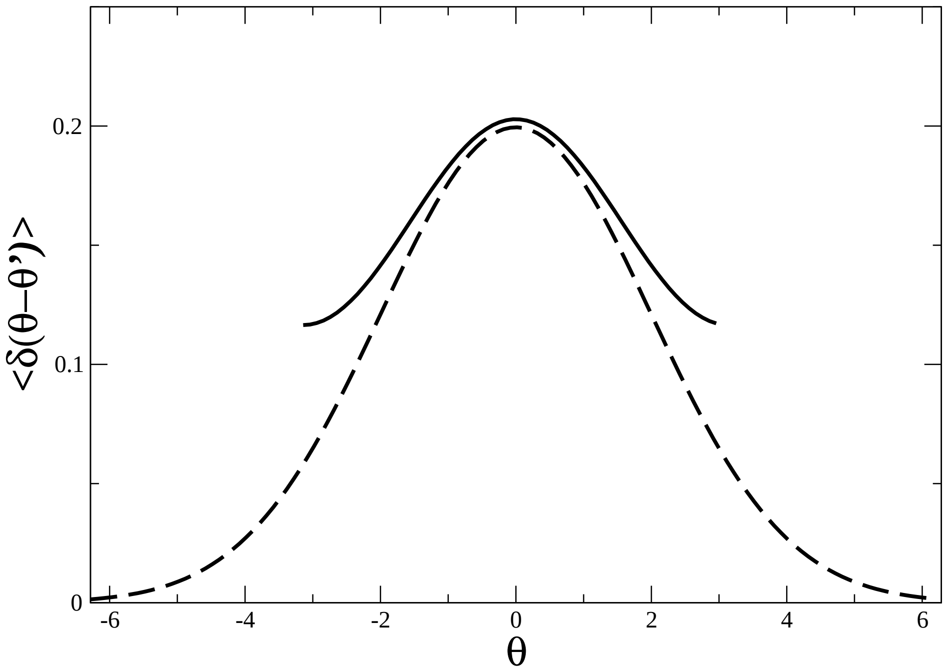
Central limit theorem fails!

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



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

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



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