Investigating corrections to a Gaussian distribution of the complex phase

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based on work with Jeff Greensite and Kim Splittorff

[arXiv:1306.3085 and work in preparation]

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Outline

- Motivation and introduction to the density of states method as a way to study QCD at nonzero chemical potential
- The density: distribution of the complex phase: When is it Gaussian? When are there corrections? How large are they?
 - Hadron resonance gas model
 - Strong coupling expansion
- Lattice studies (WHOT-QCD)

See also plenaries of C. Gattringer and K. Szabo

QCD phase diagram goal of current RHIC experiments [STAR Collaboration - arXiv:1007.2613]



The finite density QCD phase diagram is under investigation by both theorists and experimentalists.

One of the questions which both would like to address is the existence, and if so location, of a possible critical end point in the μ , *T*-plane.

See also talks of S. Borsanyi, C. Schmidt, and K. Szabo.

Theoretical approaches - hindered by sign problem

The sign problem is a consequence of a real, non-zero quark chemical potential μ . $\not D$ is Hermitian and has purely real eigenvalues. Since $\{\gamma_5, \not D\} = 0$ and $\{\gamma_5, \gamma_0\} = 0$,

$$(i\not\!\!D + \gamma_0\mu)\gamma_5\psi = -\gamma_5(i\not\!\!D + \gamma_0\mu)\psi.$$

so the fermion determinant resulting from integration over ψ can be written as

$$det(i\mathcal{D} + \gamma_0\mu + m) \equiv \frac{1}{2} det[(i\mathcal{D} + \gamma_0\mu + m)(-i\mathcal{D} - \gamma_0\mu + m)]$$
$$= \frac{1}{2} det[-(i\mathcal{D} + \gamma_0\mu)^2 + m^2]$$
$$\equiv re^{i\theta}.$$

Sign problem:

When $\mu \neq 0$ the fermion determinant is complex such that conventional lattice simulations using importance sampling are not possible.

Histogram method - A way to avoid the sign problem? [Ejiri et al. - Phys.Rev. D82 (2010) 014508 [arXiv: 0909.2121]] A cumulant expansion of the average phase is used by WHOT-QCD to avoid the sign problem.

$$\langle e^{i\theta} \rangle_X = \exp\left[-\frac{1}{2} \langle \theta^2 \rangle_c + \frac{1}{4!} \langle \theta^4 \rangle_c - \dots\right]$$

with

$$\begin{split} \langle \theta^2 \rangle_c &= \langle \theta^2 \rangle_X \,, \\ \langle \theta^4 \rangle_c &= \langle \theta^4 \rangle_X - 3 \langle \theta^2 \rangle_X^2 \,, \end{split}$$

Notice that $\langle e^{i\theta} \rangle_X$ is real and positive. So the sign problem is either gone, or has relocated into the higher order cumulants. One must check that the cumulant expansion converges. See also talk of S. Ejiri.

The technique of WHOT-QCD is to approximate the expansion by the first cumulant $\langle \theta^2 \rangle_c$. This corresponds to a Gaussian distribution of the complex phase (note central limit theorem). But how large are $\langle \theta^4 \rangle_c$, $\langle \theta^6 \rangle_c$, ...?

What is the density, or distribution of the complex phase? The density as a function of some fixed quantity X is defined as

$$ho(X) \equiv \int \mathcal{D}A \, \delta(X - X') \left| \det(\not D + \gamma_0 \mu + m) \right|^{N_f} e^{iN_f \theta(X')} e^{-S_{YM}}$$

The partition function is just the integral of the density

$$Z = \int \mathrm{d}X \
ho(X) \,.$$

Observables can be calculated when the density is known, using

$$\langle \mathcal{O}
angle = rac{1}{Z} \int \mathrm{d} X \;
ho(X) \mathcal{O}(X) \, .$$

Notice that $\rho(X) = Z \langle \delta(X - X') \rangle$.

It is convenient to consider the distribution $\langle \delta(X - X') \rangle$, since

$$\int \mathrm{d}X \, \left< \delta(X - X') \right> = 1$$

 \implies direct interpretation as a probability distribution.

Different ways to measure the complex phase WHOT-QCD calculates

$$\langle e^{i\theta} \rangle_{P,F} = rac{\langle \delta(P'-P)\delta(F'-F)e^{i\theta(F',P')} \rangle_{pq}}{\langle \delta(P'-P)\delta(F'-F) \rangle_{pq}} \,,$$

and

$$\langle \delta(P-P')\delta(F-F')\rangle = \langle e^{i\theta} \rangle_{P,F} \langle \delta(P-P')\delta(F-F') \rangle_{Pq},$$

where *P* is the average plaquette, and $F \equiv N_f \ln \left| \frac{\det(\vec{p} + \gamma_0 \mu + m)}{\det(\vec{p} + m)} \right|$, and *pq* refers to the phase-quenched theory.

We calculate

$$\langle e^{i \mathcal{N}_f heta'}
angle_{\mathcal{P} q} = rac{1}{Z_{\mathcal{P} q}} \int \mathcal{D} A \; e^{i \mathcal{N}_f heta'} \left| \det(D \!\!\!\!/ + \gamma_0 \mu + m)
ight| e^{-\mathcal{S}_{YM}} \, ,$$

and

$$\langle \delta(\theta - \theta') \rangle = rac{Z_{pq}}{Z} e^{iN_f \theta} \langle \delta(\theta - \theta')
angle_{pq} \, .$$

Warning:

We hope to draw some analogies between our work and that of WHOT-QCD but they will be qualitative.

Moments of the complex phase

[Lombardo, Splittorff, Verbaarschot - Phys.Rev. D80 (2009) 054509 [arXiv:0904.2122]]

The distribution can be calculated analytically from the Fourier transform

$$\langle \delta(\theta - \theta')
angle = 2 \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} e^{-2ip\theta} \langle e^{2ip\theta'}
angle \,.$$

We just need to calculate the moments

$$\langle e^{2i
ho heta'}
angle = rac{Z_{YM}}{Z} igg\langle rac{\det^{
ho}({D\!\!\!/} + \gamma_0 \mu + m)}{\det^{
ho}({D\!\!\!/} - \gamma_0 \mu + m)} \det^{N_f}({D\!\!\!/} + \gamma_0 \mu + m) igg
angle_{YM} \, ,$$

which we get using the

- hadron resonance gas model
- lattice strong coupling + hopping expansion

Gaussian or not?

1. Hadron resonance gas

$$\langle e^{2ip\theta'} \rangle_{pq} = \exp[-p^2 x_1],$$

 \implies the distribution is gaussian!

$$\langle \delta(\theta-\theta') \rangle_{pq} = 2 \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} e^{-2ip\theta} e^{-p^2 x_1} = \frac{1}{\sqrt{\pi x_1}} e^{-\theta^2/x_1}.$$

2. Strong coupling expansion

$$\langle e^{2ip\theta'} \rangle_{pq} = \exp[-p^2 x_1 - p^4 x_2 - p^6 x_3 - \dots],$$

 \implies the distribution has corrections!

$$\langle \delta(\theta - \theta') \rangle_{pq} = 2 \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} e^{-2ip\theta} e^{-p^2 x_1} e^{-p^4 x_2 - p^6 x_3 - \dots}$$

Cumulants: x_n

The cumulant expansion of the moments takes the form

$$\ln \langle e^{2ip\theta'} \rangle_{pq} = \sum_{n=1}^{\infty} \frac{(2ip)^n}{n!} \langle \theta^n \rangle_c \,.$$

Plugging in our expression from the strong coupling expansion $\langle e^{2ip\theta'} \rangle_{pq} = e^{-p^2 x_1 - p^4 x_2 - \dots}$ shows that each cumulant corresponds to one of the x_n ,

$$x_n = -rac{(2i)^{2n}}{(2n)!} \langle heta^{2n}
angle_c \,.$$

These are simply added to obtain $-\ln \langle e^{2i\theta'} \rangle_{pq}$.

 \implies

It is necessary that $x_1 \gg x_2$, x_3 , x_4 , ... for the gaussian approximation to succeed.

Hadron resonance gas

To obtain the moments from the HRG we must calculate

$$\langle e^{2ip heta'}
angle = rac{Z_{YM}}{Z} \left\langle rac{\det^p(D + \gamma_0 \mu + m)}{\det^p(D - \gamma_0 \mu + m)} \det^{N_f}(D + \gamma_0 \mu + m) \right\rangle_{YM}$$

Notice that this vev corresponds to a partition function of a theory with $p + N_f$ quarks, and p "ghost quarks" from the det in the denominator.

To obtain the expectation value it is necessary to compute the spectrum of the quarks and ghost quarks, which proceeds in precisely the same way as calculating the hadron spectrum of the standard model.

See also talk of C. Schmidt.

Hadron resonance gas - spectra

[Amsler, DeGrand, Krusche - Quark Model review for the Particle Data Group] Our calculation of the moments $\langle e^{2ip\theta'} \rangle$ includes all possible spectral combinations of mesons with spin 0 and 1, and baryons with spin $\frac{1}{2}$ and $\frac{3}{2}$ for $2p + N_f$ flavors.



The contributions are obtained by decomposing

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\mathbf{n}\otimes\mathbf{n}\otimes\mathbf{n}\,,
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and

 ${\bf n}\otimes {\bf \bar n}\,,$

where **n** is the fundamental representation, from $SU(2(2p + N_f))$ to $SU(2p + N_f) \times SU(2)_{spin}$.

Hadron resonance gas - results

To obtain $\langle e^{2ip\theta'} \rangle$, add up the free energies from all possible hadronic states. Assuming they are free, these are, for mesons and baryons

$$F_{g}^{M}(\mu_{I}) = -g \frac{m_{M}^{2} T^{2}}{\pi^{2}} \sum_{n=1}^{\infty} \frac{1}{n^{2}} \mathrm{K}_{2}(nm_{M}/T) \cosh\left[2nI_{3}\mu_{I}\beta\right],$$

$$F_g^B(\mu_B - 2I_3\mu_I) = g \frac{m_B^2 T^2}{\pi^2} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} K_2(nm_B/T) \cosh\left[(\mu_B - 2I_3\mu_I)n\beta\right],$$

with spin degeneracy g = 2s + 1.

Noting that each ghost quark contributes a factor of -1 to the free energy, and $-\mu$ to the chemical potential, the result is

$$\langle e^{2ip\theta'} \rangle_{pq} = e^{-p^2 x_1}$$
 with $x_1 = F^M(2\mu) - F^M(0) + F^B(3\mu) - F^B(0)$.

where $F^{M}(\mu) = k_{M} [F_{1}^{M}(\mu) + F_{3}^{M}(\mu)]$, and $F^{B}(\mu) = k_{B} [2F_{2}^{B} + F_{4}^{B}(\mu)]$.

The higher order cumulants are zero.

Taylor expansion - simulations needed

It is in principle possible to have higher order cumulants. This can be seen by performing a Taylor expansion of $\log \langle e^{2i\rho\theta'} \rangle$ around $\mu/T = 0$. Defining $M(\mu) \equiv \det(\Bar{P} + \gamma_0\mu + m)$ and $D^{(n)}(\mu) \equiv \frac{\partial^n}{\partial(\mu/T)^n} \frac{M(\mu)^{p+N_f}}{M(-\mu)^p}$,

$$\begin{split} \log\left[\frac{Z_{YM}}{Z}\left\langle\frac{M(\mu)^{p+N_{f}}}{M(-\mu)^{p}}\right\rangle_{YM}\right] &= \frac{1}{2!}\left(\frac{\mu}{T}\right)^{2}\left[\frac{\langle D^{(2)}(0)\rangle_{YM}}{\langle M(0)^{N_{f}}\rangle_{YM}}\right] \\ &+ \frac{1}{4!}\left(\frac{\mu}{T}\right)^{4}\left[\frac{\langle D^{(4)}(0)\rangle_{YM}}{\langle M(0)^{N_{f}}\rangle_{YM}} - 3\frac{\langle D^{(2)}(0)\rangle_{YM}}{\langle M(0)^{N_{f}}\rangle_{YM}^{2}}\right] \\ &+ \frac{1}{6!}\left(\frac{\mu}{T}\right)^{6}\left[\frac{\langle D^{(6)}(0)\rangle_{YM}}{\langle M(0)^{N_{f}}\rangle_{YM}} - 15\frac{\langle D^{(2)}(0)\rangle_{YM}\langle D^{(4)}(0)\rangle_{YM}}{\langle M(0)^{N_{f}}\rangle_{YM}^{2}} + 30\frac{\langle D^{(2)}(0)\rangle_{YM}^{3}}{\langle M(0)^{N_{f}}\rangle_{YM}^{3}}\right] \\ &+ \mathcal{O}\left(\frac{\mu}{T}\right)^{8} - \log\left[\frac{Z}{Z_{YM}}\right]. \end{split}$$

Evaluating the derivatives and collecting terms with like powers of p results in a series of special relationships which must hold to make $x_2, x_3, ... = 0$. For example, to make $x_2 = 0$ at $\mathcal{O}(\frac{\mu}{T})^4$ it is required that

$$\langle M(0)^{N_f} \rangle_{YM} \langle M(0)^{N_f-4} M'(0)^4 \rangle_{YM} = 3 \langle M(0)^{N_f-2} M'(0)^2 \rangle_{YM}^2$$
 (check?) 14

Lattice strong coupling expansion [Langelage, Lottini, Philipsen - JHEP 1102 (2011) 057[arXiv:1010.0951]]

After integrating out the spatial link variables the lattice Yang-Mills partition function can be simplified by using the character expansion

$$Z_{YM} = \int_{SU(N_c)} \prod_{z} \mathrm{d}W_{z} \prod_{\langle xy \rangle} \left[1 + \sum_{R} \lambda_{R} \left[\chi_{R}(W_{x}) \chi_{R}(W_{y}^{\dagger}) + \chi_{R}(W_{x}^{\dagger}) \chi_{R}(W_{y}) \right] \right]$$

 $\chi_R(W_x) = \operatorname{Tr}_R(W_x)$ are characters of Polyakov lines $W_x = \prod_{\tau=1}^{N_\tau} U_0(\mathbf{x}, \tau)$. The $\sum_{\langle xy \rangle}$ is over nearest neighbor sites.

The λ_R are expansion parameters in powers of $\frac{1}{g^2 N_c}$. We work at leading order, which includes only the fundamental representation, no higher dimensional representations or decorations, such that

$$e^{-S_{YM}} o 1 + \lambda_1 \sum_{\langle xy
angle} \left[\operatorname{tr}(W_x) \operatorname{tr}(W_y^{\dagger}) + \operatorname{tr}(W_x^{\dagger}) \operatorname{tr}(W_y) \right],$$

with $\lambda_1 = \left(\frac{1}{g^2 N_c}\right)^{N_\tau}$.

See also talks of J. Langelage, M. Neuman, and W. Unger.

Hopping expansion - static quark limit [Langelage, Lottini, Philipsen - JHEP 1102 (2011) 057[arXiv:1111.4953]]

The fermion determinant can be approximated in the static, heavy quark limit by the hopping expansion

$$\log \det(\not D + \gamma_0 \mu + m) = a_1 h[e^{\mu/T} \operatorname{Tr} W_x + e^{-\mu/T} \operatorname{Tr} W_x^{\dagger}] + a_2 h^2 [e^{2\mu/T} \operatorname{Tr} (W_x^2) + e^{-2\mu/T} \operatorname{Tr} (W_x^{\dagger 2})] + \dots$$

For Wilson fermions

$$a_n = 2 \frac{(-1)^n}{n}$$
, $h = (2\kappa_f)^{N_t}$, $\kappa_f = \frac{1}{ma+d+1}$.

By calculating the moments $\langle e^{2ip\theta'} \rangle$, we obtain the leading order contribution to the x_n , which is at least $\mathcal{O}(h^{2n})$.

At $\mathcal{O}(\lambda_1^0)$, we calculate the leading order to $x_1, ..., x_6$. At $\mathcal{O}(\lambda_1)$, we compute the leading order to $x_1, ..., x_3$.

In both cases the calculations are performed in the confined phase. See also talks of J. Langelage and M. Neuman.

Homework: Calculating vevs of Polyakov lines in the confined phase

At each order, all contributions which result in color singlets must be obtained. We define $P_n = \text{Tr}(W_x^n)$, $P_n^* = \text{Tr}(W_x^{\dagger n})$. Here are some example vevs which appear in the calculations.

$$\begin{array}{l} \langle P_1 P_1^* \rangle_{YM} = \text{singlets in } \mathbf{3} \otimes \mathbf{\bar{3}} = 1 \,, \\ \langle P_1^2 P_1^{*2} \rangle_{YM} = \text{singlets in } \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{\bar{3}} \otimes \mathbf{\bar{3}} = 2 \,, \\ \langle P_1^3 \rangle_{YM} = \text{singlets in } \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} = 1 \,, \\ \langle P_1^4 P_1^* \rangle_{YM} = \text{singlets in } \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{3} \otimes \mathbf{\bar{3}} = 3 \,, \\ \langle P_2 P_1 \rangle_{YM} = \langle (P_1^2 - 2P_1^*) P_1 \rangle_{YM} = -1 \,, \end{array}$$

Note that the third and fourth vevs only contribute for SU(3), and that the last is -2 when $N_c = \infty$.

. . .

Strong coupling results in the confined phase $\mathcal{O}(\lambda_1^0)$

	$N_c = 3$	$N_c = \infty$
<i>x</i> ₁	$4a_1^2h^2\sinh^2(\mu/T)+\mathcal{O}(h^3)$	"
x ₂	$4h^{5}\sinh^{4}(\mu/T)\cosh(\mu/T)\left[8a_{1}^{3}a_{2}-a_{1}^{5}N_{f} ight]N_{s}+\mathcal{O}(h^{6})$	$0+\mathcal{O}(h^6)$
<i>x</i> ₃	$-rac{8}{9}N_sa_1^6h^6\sinh^6(\mu/T)+\mathcal{O}(h^7)$	$0+\mathcal{O}(h^7)$
<i>x</i> 4	$-rac{44}{45}N_sa_1^8h^8\sinh^8(\mu/T)+{\cal O}(h^9)$	$0+\mathcal{O}(h^9)$
<i>x</i> 5	$-rac{112}{225} N_{s} a_{1}^{10} h^{10} \sinh^{10}(\mu/T) + \mathcal{O}(h^{11})$	$0+\mathcal{O}(h^{11})$
<i>x</i> ₆	$rac{3488}{14175} N_{s} a_{1}^{12} h^{12} \sinh^{12}(\mu/T) + \mathcal{O}(h^{13})$	$0+\mathcal{O}(h^{13})$

		$N_c = 3$	$N_c = \infty$
$O(\lambda_1)$	<i>x</i> ₁	$0+\mathcal{O}(h^3)$	$0 + \mathcal{O}(h^3)$
0(/1)	<i>x</i> ₂	$-24\lambda_1 N_s a_1^4 h^4 \sinh^4(\mu/T) + \mathcal{O}(h^5)$	$0 + \mathcal{O}(h^5)$
	<i>x</i> 3	$-80\lambda_1 N_s a_1^6 h^6 \sinh^6(\mu/T) + \mathcal{O}(h^7)$	$0 + \mathcal{O}(h^7)$

The presence of $x_n \neq 0$ for n > 1 implies that there are non-zero higher order cumulants, unless $N_c = \infty$. Also, they should become more significant with increasing μ/T or β , or decreasing m.

Strong coupling Results - Cumulants



Even though the higher order cumulants, x_n , are non-zero at strong coupling they are small compared to x_1 in the regime of validity of the hopping expansion $h e^{\mu/T} \ll 1$, in the limit $\lambda_1 \rightarrow 0$ ($\beta \rightarrow 0$).

The plots include all contributions of x_1 , x_2 , up to $\mathcal{O}(h^6)$ at $\mathcal{O}(\lambda_1^0)$, and the leading order contributions to $x_3, ..., x_6$.

Are the higher order cumulants ever significant compared to x_1 ? This is a question that should be addressed in simulations.

Strong coupling Results - Distribution



Calculating $\langle \delta(\theta - \theta') \rangle_{pq}$ from the cumulants gives a distribution which is indistinguishable from a gaussian by eye.

However, there are $\mathcal{O}(\frac{1}{V})$ corrections which are made visible by calculating the difference

$$rac{\langle \delta(heta- heta')
angle_{pq}-g(heta)}{g(heta)}\,,$$

where $g(\theta) = \frac{1}{\sqrt{\pi x_1}} e^{-x_1 \theta^2}$ is the gaussian distribution.

What if higher order cumulants were significant?



If we choose hypothetical values of the cumulants x_1 , x_2 , ..., such that $\frac{x_2}{x_1}$ is more significant we find that the distribution still appears indistinguishable from a gaussian.

Considering the difference

$$\langle \delta(heta - heta')
angle - g(heta),$$

it is clear that the distribution contains corrections which are $\mathcal{O}(\frac{1}{V})$.

WHOT-QCD Results - Cumulants (Heavy quarks) [Fig. 5 in PoS LATTICE2011 (2011) 214 [arXiv:1202.6113] - Saito et al.]



Cumulants $Green = \langle \theta^2 \rangle_c$,

$$\mathsf{Red} = \langle \theta^4 \rangle_c \, .$$

- unimproved Wilson quark action
- heavy quark limit
- $24^3 \times 4$ lattice

WHOT-QCD Results - Histograms (Light quarks)

[Fig. 3 in PoS LATTICE2011 (2011) 208 [arXiv:1111.2116] - Nakagawa et al.]



Phase quenched distribution of the complex phase.

- improved Wilson quark action
- light quarks: $\frac{m_{\pi}}{m_{
 ho}} = 0.8$
- $8^3 \times 4$ lattice

WHOT-QCD Results - Binder cumulant (Light quarks) [Fig. 2 in Phys.Rev. D77 (2008) 014508 [arXiv:0706.3549] - Ejiri]



• improved staggered quark action

• light quark limit:
$$\frac{m_{\pi}}{m_{
ho}} \approx 0.7$$

Notice, B_4^{θ} will always go to 3 in the large volume limit. $\langle \theta^4 \rangle_c = (B_4^{\theta} - 3) \langle \theta^2 \rangle^2 = \mathcal{O}(V)$, and $\langle \theta^2 \rangle^2 = \mathcal{O}(V^2)$. Therefore $B_4^{\theta} - 3 = \mathcal{O}\left(\frac{1}{V}\right) \implies$ Calculate $\langle \theta^4 \rangle_c$ directly.

The the 4th cumulant in expansion of $\langle e^{iN_{\rm f}\theta}\rangle$ is defined by

$$\langle \theta^4 \rangle_c = \langle \theta^4 \rangle - 3 \langle \theta^2 \rangle^2$$
.

The 4th Binder cumulant is the ratio

$$B_4^{ heta} \equiv rac{\langle heta^4
angle}{\langle heta^2
angle^2} \, .$$

$$\implies B_4^{\theta} = 3 \text{ if } \langle \theta^4 \rangle_c = 0.$$

• $16^3 \times 4$ lattice

WHOT-QCD Results - Cumulants (Light quarks)

[Fig. 4 in PoS LATTICE2011 (2011) 208 [arXiv:1111.2116] - Nakagawa et al.]



Cumulants $\begin{aligned} \textit{Blue} &= \frac{1}{2} \langle \theta^2 \rangle_c \,. \\ \textit{Red} &= \frac{1}{4!} \langle \theta^4 \rangle_c \,. \end{aligned}$

- improved Wilson quark action
- light quarks: $\frac{m_{\pi}}{m_{
 ho}} = 0.8$
- $8^3 \times 4$ lattice

Conclusions

- Corrections to a Gaussian approximation of the distribution of the complex phase are present at large quark mass and coupling strength. These appear to grow as the quark mass and the coupling strength decrease.
- The higher order cumulants are O(V) in log⟨e^{iN_fθ}⟩_{pq} but they are suppressed by O(¹/_V) in the distribution ⟨δ(θ − θ')⟩_{pq}, so it appears very gaussian in the confined phase. Also, the Binder cumulant B^θ₄ will only have O(¹/_V) corrections.
- Therefore, in simulations where the gaussian approximation is used it is important to calculate the higher order cumulants directly to determine if they small enough to neglect.

Thanks for your attention!

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