Reweighting and Lee-Yang Zero

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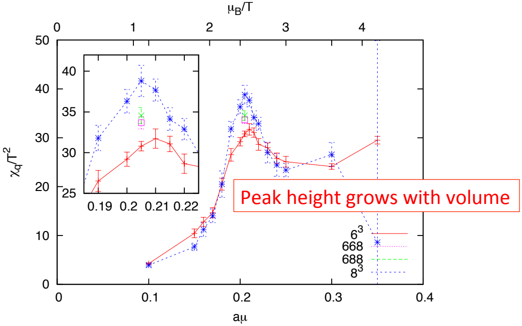
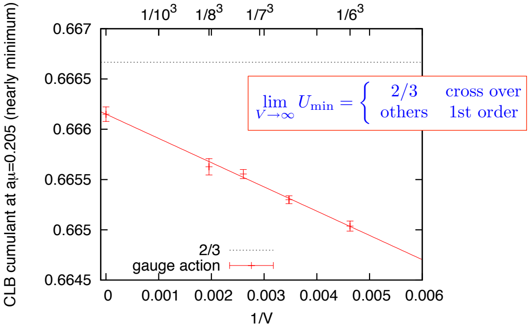
Introduction

- Following S. Takeda's talk on Monday about 4 flavors
- Phase quenched simulations of grand canonical ensembles

$$Z_{||} = \int [dU]\, e^{\beta N_p P(U)}\, |\det D(\mu; U)|^{N_f}$$

- $N_t = 4$ with Spatial Volumes of 6^3, $6^2 \cdot 8$, $6 \cdot 8^2$ and 8^3
- $4,000$ configurations for 6^3 and to $20,000 \sim 40,000$ configurations for 8^3





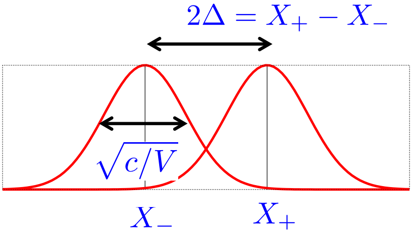
We observed weak volume scaling.

Assume a double-Gaussian distribution model

$$\chi = c\left(1 + \frac{\Delta^2}{c}V\right)$$

$$K = -\frac{2}{\left(1 + \frac{c}{\Delta^2}\frac{1}{V}\right)^2}$$

$$U = \frac{2}{3}\frac{X^4 + \Delta^4}{(X^2 + \Delta^2)^2}\left[1 - \frac{2c}{X^2 + \Delta^2}\frac{1}{V} + O(V^{-2})\right]$$



- Weak (Bad) volume scaling for χ and K when $c \sim \Delta^2 V$
- U makes the Δ contribution to the scaling smaller, while the extrapolated value depends on the existence of Δ
- We want to separate the dependence of c and Δ
- Another way is to use **Fourier transform!**

Fourier transform of two states

$$\int \mathrm{d}x \exp(ixt)\,[f(x+\Delta)+f(x-\Delta)]$$

$$\propto \left[\int \mathrm{d}x \exp(ixt) f(x)\right] \cos\Delta t$$

$$\to \exp(-\frac{t^2}{2V/c})\,\cos\Delta t \qquad \text{for } f(x) \propto \exp(-\frac{x^2}{2c/V})$$

- Completely separate the dependence of the width and the peak distance
- How to see it? $\cos\Delta t$ has zeros at $t = (2n+1)\pi/2\Delta$
- Here, the location of zeros only depend on Δ
- Not new at all. This is just Lee-Yang zero.
- Beware: Signal is suppressed exponentially with increasing t
- Beware: For this two-states model (does not need to be Gaussian), two states has to be the same to get cos function

What is Lee-Yang zero mathematically?

- Inspired by Alves, Berg & Sanielevici (1992) and Ejiri (2006)
- To find the zeros of Z with complexified $\beta = \beta^R + i\beta^I$

$$Z(\beta^R, \beta^I, \mu) = \int [\mathrm{d}U]\, e^{\beta P_{\mathrm{tot}}} \, [\det D(\mu; U)]^{N_f}$$

$$= Z(\beta^R, \beta^I = 0, \mu) \int \mathrm{d}P_{\mathrm{tot}}\, e^{i\beta^I P_{\mathrm{tot}}} \, \mathrm{Prob}(P_{\mathrm{tot}})$$

$$\mathrm{Prob}(P_{\mathrm{tot}}) = \frac{1}{Z(\beta^R, \beta^I = 0, \mu)} \int [\mathrm{d}U]\, \delta(P_{\mathrm{tot}} - P') e^{\beta^R P'} \, [\det D(\mu)]^{N_f}$$

- It is a Fourier transform of the probability function of $P_{\mathrm{tot}} \propto V$
- Modify our previous double-Gaussian model to be

$$\mathrm{Prob}(P_{\mathrm{tot}}) = f(x + \Delta V) + f(x - \Delta V) \quad \text{with} \quad f(x) \propto \exp(-\frac{x^2}{2cV})$$

$$Z_{\mathrm{norm}}(\beta^R, \beta^I, \mu) = \frac{Z(\beta^R, \beta^I, \mu)}{Z(\beta^R, \beta^I = 0, \mu)} \propto \exp(-\frac{(\beta^I)^2}{2/cV}) \cos \Delta V \beta^I$$

Reweighting in Lee-Yang zero

- Reweighting is a must to see the proper zero point where the Fourier transform produces a cos fonction
- Conventionally reweighting in β is used (basically using complex β)
- Need to be very carefull with β reweighting
  - Valid in a small β region suppressed exponentially by the volume
  - Unwanted scale change — we get a zero at a different lattice spacing
  - ...

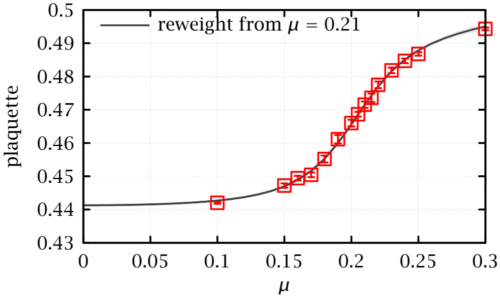
Lee-Yang zero under μ reweighting

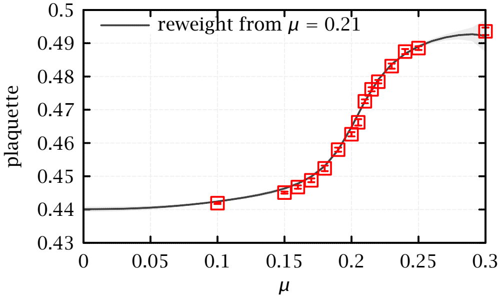
- We use the complex β, but we do not need to reweight in β
- We reweight in any parameter that can move the system to the transition
- In finite density studies, we can do μ reweighting

$$
\begin{aligned}
Z_{\text{norm}}(\beta^I, \mu') &= \frac{Z(\beta^I, \mu')}{Z(\beta^I = 0, \mu')} e^{-i\beta^I N_p \langle P \rangle_{\mu'}} \\
&= \frac{\left\langle e^{i\beta^I N_p \Delta P} \left(\frac{\det D(\mu')}{\det D(\mu_0)} \right)^{N_f} e^{iN_f \theta(\mu_0)} \right\rangle_{\mu_0}}{\left\langle \left(\frac{\det D(\mu')}{\det D(\mu_0)} \right)^{N_f} e^{iN_f \theta(\mu_0)} \right\rangle_{\mu_0}},
\end{aligned}
$$

- We calculate the ratio of determinant with Taylor expansion in μ/T
- We cut off the expansion after the 4^{th} order (the 4^{th} derivative is also used for other cumulant quantities)
- We calculate the derivatives exactly

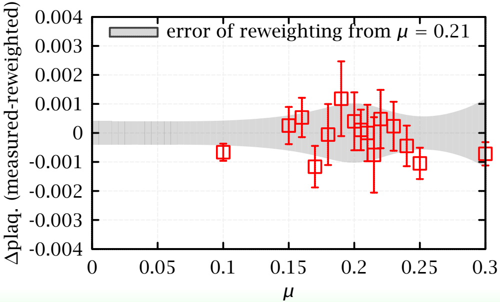
Reweighting in μ — Plaquette ($\beta = 1.6$, $\kappa = 0.1371$)

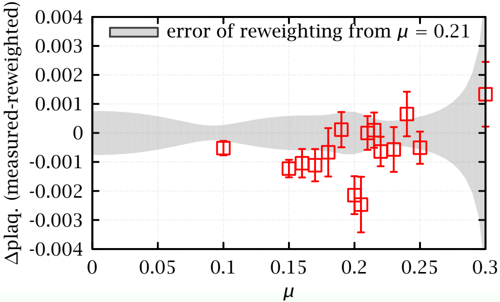




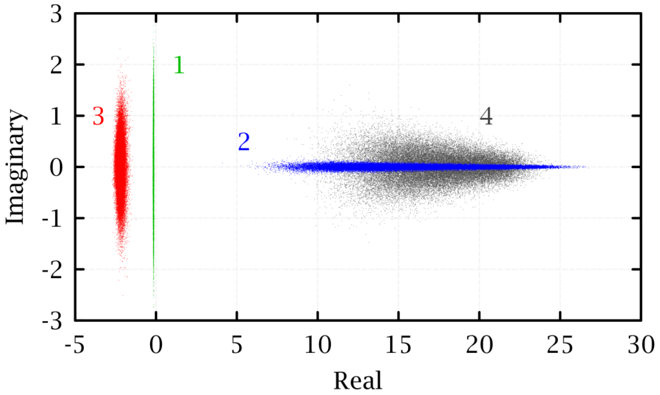
$6^3 \times 4$

$8^3 \times 4$





Reweighting in μ — $\ln \det D$ derivatives at $\mu = 0$

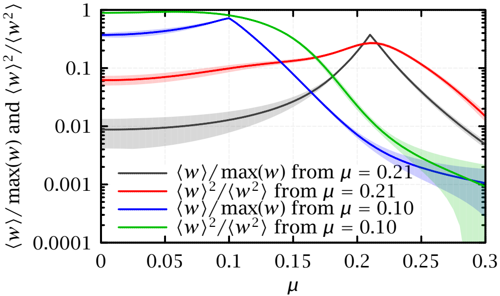


$$\frac{\partial^n}{\partial \mu^n} \ln \det D \bigg|_{\mu=0} = \mathrm{Tr}\, \frac{\partial^n}{\partial \mu^n} \ln D \bigg|_{\mu=0}$$

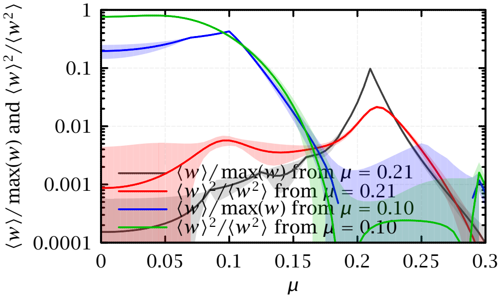
for $n = 1, 2, 3, 4$

- Data taken from 4 flavors, $\beta = 1.60$, $\kappa = 0.1371$, $\mu = 0.21$, $8^3 \times 4$.
- μ derivatives of the Dirac operator at $\mu = 0$ from Taylor expansion upto the 4^{th} derivative
- At $\mu = 0$, odd derivatives are purely imaginary, while even ones are real
- For these derivatives from Taylor expansion, 4 terms for $n = 1$, 3 terms for $n = 2$, 2 terms for $n = 3$, and only 1 term for $n = 4$

Reweighting in μ — change of reweighting factor



$6^3 \times 4$



$8^3 \times 4$

- Change of weight with μ reweighting with 4 flavors at $\beta = 1.6$, $\kappa = 0.1371$
- Two different definitions of the effective number of configurations

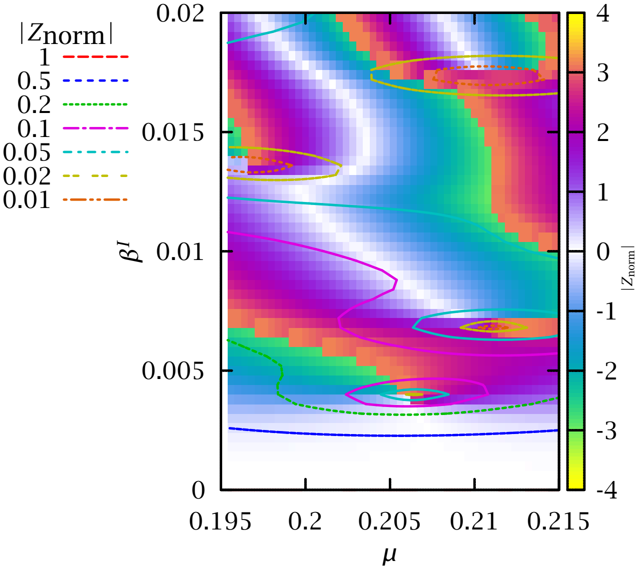
$$N_{\text{Optimism}} = \frac{\langle w\rangle^2}{\langle w^2\rangle} N_{\text{conf}}$$

$$N_{\text{Pessimism}} = \frac{\langle w\rangle}{\max(w)} N_{\text{conf}}$$

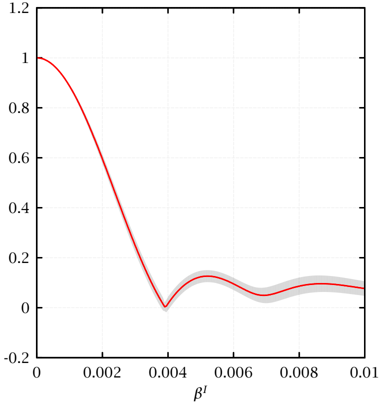
$$w = \mathrm{Re}\left[\frac{\det D(\mu')}{|\det D(\mu_0)|}\right]^{N_f}$$

Reweight from μ_0 to μ'

The normalized partition function (from $\mu = 0.205, 8^3$)

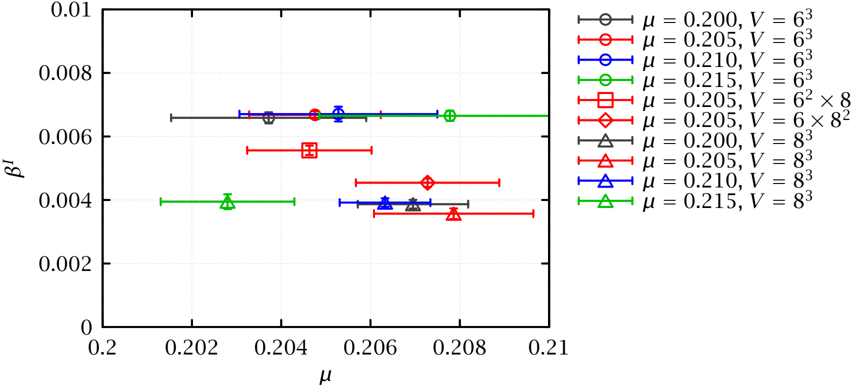


contour and phase



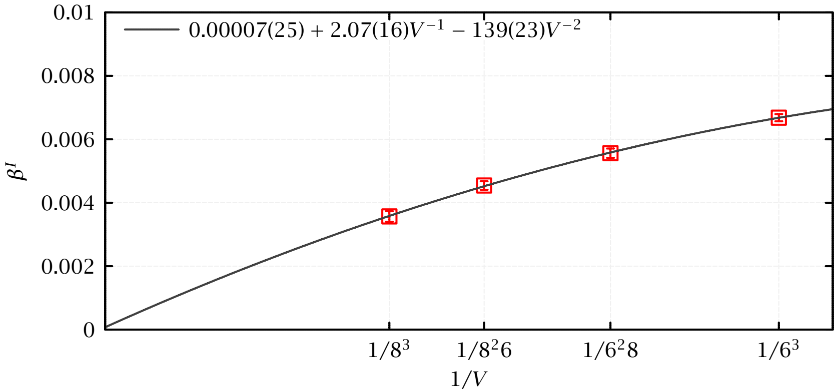
at μ of the first zero

The position of the first zero in β^I - μ plane



- Positions of zeros in β^I - μ plane with 4 flavors, $\beta = 1.60$, $\kappa = 0.1371$
- Errors are estimated by finding zero of each Jackknife
- Consistent except result from $\mu = 0.215$

Volume scaling of the location of the first zero



- Data from 4 flavors, $\beta = 1.60$, $\kappa = 0.1371$, $\mu = 0.205$
- There are higher order (V^{-2}) dependence of the first zero
- Double-Gaussian model $\Rightarrow \cos \Delta V \beta^I \Rightarrow \beta^I_{\text{zero}} \propto 1/\Delta V$
- When the volume is small ($V \lesssim 8^3$), the volume averaged peak distance (difference between the two states) is likely to have volume dependence

Conclusions and outlook

- What we have learnt
  - We have investigated the location of parition function zeros by reweighting in μ direction
  - Avoided the complication of β reweighting with conventional methods
  - Locations of the first zero are consistent across different ensembles simulated at different μ
  - Our data shows possible volume dependence of the peak distance between two states at the transition with small volumes ($V \lesssim 8^3$)

- What we are planning to do
  - Do the actual Fourier transformation for other quantities
  - Improving μ reweighting by using the properties of dirac operator derivatives at $\mu = 0$
  - Apply this method to 3 flavors