Chemical potential dependence of the endpoint of the first-order phase transition in the heavy-quark region of finite-temperature lattice QCD

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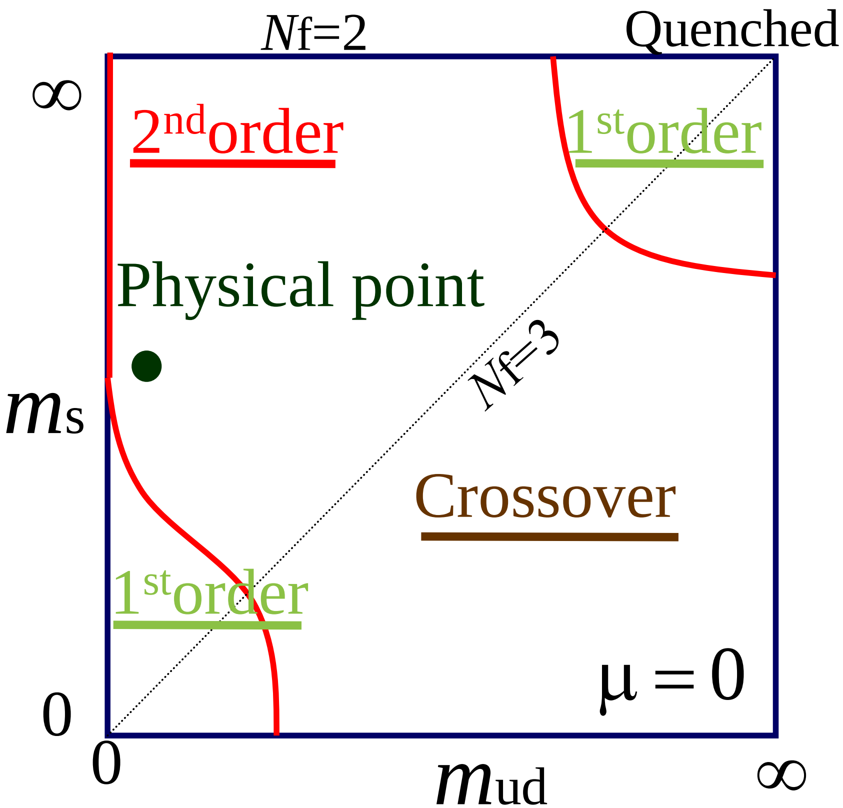
QCD phase transition in heavy quark region



WHOT-QCD Collab.
Phys.Rev.D84, 054502(2011)
Phys.Rev.D89, 034507(2014)
Phys.Rev.D101, 054505(2020)
Phys.Rev.D104, 114509(2021)
PTEP 2022, 033B05 (2022)

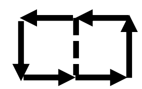
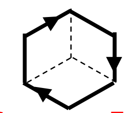
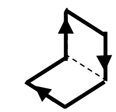
- The critical mass at which the first-order phase transition turns into a crossover
- Light quark regime
  - chiral symmetry breaking
- Heavy quark region
  - Confinement phase transition
  - Center symmetry breaking
  - Critical line at finite density
  - We study the heavy region
- It is important to calculate thermodynamic quantities as continuous functions
  - Reweighting method
  - Hopping parameter expansion

Efficient theory by hopping parameter expansion

- expectation value of physical quantity O

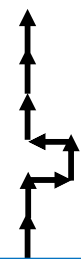
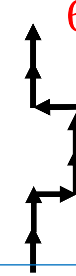
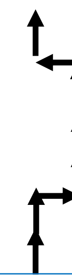
$$\langle O\rangle(\beta,\kappa) = \frac{1}{Z}\int DU\,O[U]\big(\det M(\kappa)\big)^{N_\mathrm{f}} e^{-S_g} = \frac{1}{Z}\int DU\,O[U]\,e^{-S_\mathrm{eff}}$$

- Hopping parameter expansion ($\kappa \sim 1/(\mathrm{mass})$)

$$\ln\big(\det M(\kappa)\big) = 288 N_\mathrm{site}\kappa^4 P + [768\, N_\mathrm{site}\kappa^6 (3$$  $$+$$  $$+6$$  $$)]+\cdots$$

plaquette

6-step Wilson loop

$$+12\times 2^{N_t} N_s^3 [\kappa^{N_t}\mathrm{Re}\Omega + 6N_t\kappa^{N_t+2}$$  $$+6N_t\kappa^{N_t+2}$$  $$+3N_t\kappa^{N_t+2}$$  $$]$$

Polyakov loop

Leading term

Next to leading terms (for N_t=6)

- Near the critical point of $N_t = 4$, $\det M$ can be well approximated by the lowest order terms.
- Effective action: $\boxed{S_\mathrm{eff} \approx 6N_\mathrm{site}(\beta + N_\mathrm{f} 48\kappa^4)P + 12 N_\mathrm{f}\, 2^{N_t} N_s^3 \kappa^{N_t}\mathrm{Re}\Omega}$
  - Monte Carlo simulation with the Polyakov loop term
    - $S_\mathrm{eff} \approx 6N_\mathrm{site}\beta' P + N_s^3 \lambda \mathrm{Re}\Omega$ with $\lambda = 12 N_\mathrm{f}\, 2^{N_t}\kappa^{N_t}$
- In this talk, we discuss the correct calculation method when N_t is large.

End point of the first-order phase transition

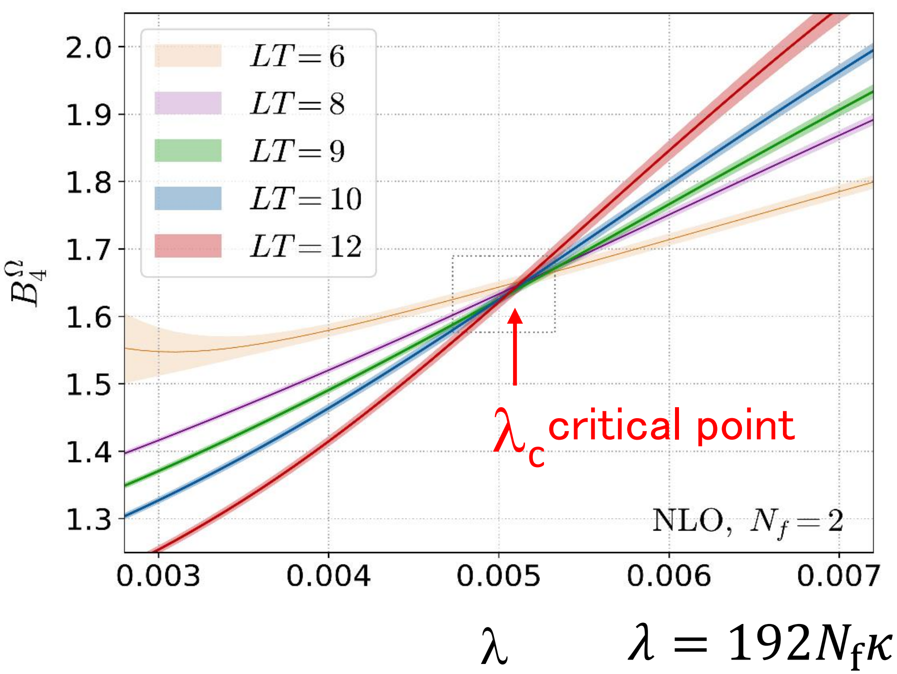
Quenched QCD with Polyakov loop term, simulation + <u>reweighting</u>

Binder cumulant $B_4 = \dfrac{\langle(\Omega - \langle\Omega\rangle)^4\rangle}{\langle(\Omega - \langle\Omega\rangle)^2\rangle^2}$

Next to leading order effect
β and λ shift

B_4 is volume independent at the critical point.

$N_t = 4$ $LT = N_s/N_t$



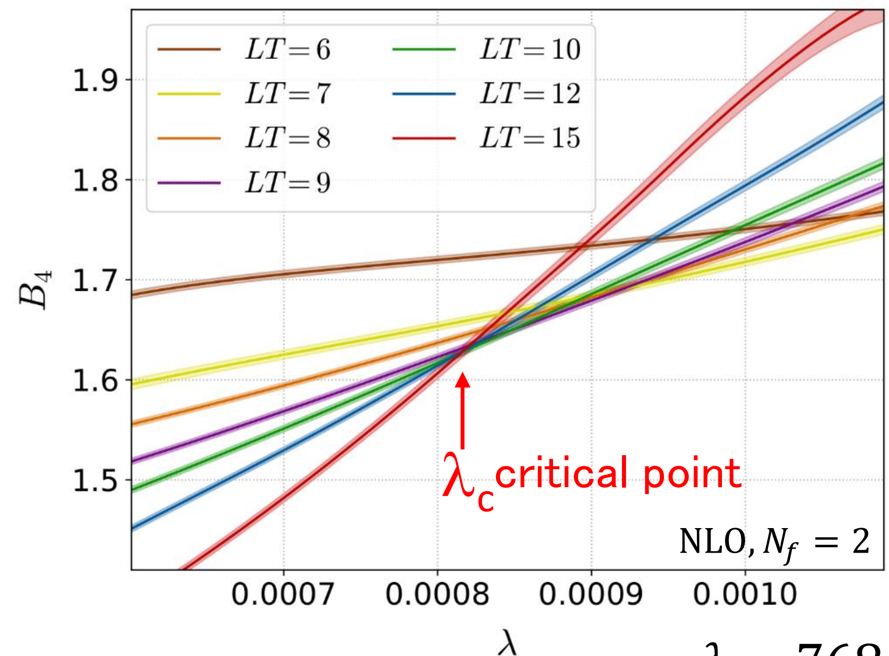
$\lambda = 192 N_f \kappa^4$

[Phys.Rev.D104, 114509(2021)]

$$\lambda_{c,\mathrm{NLO}} = 0.00503(14)$$

$$\kappa_{c,\mathrm{NLO}} = 0.0602(4)$$

$N_t = 6$



$\lambda = 768 N_f \kappa^6$

Talk by Masakiyo Kitazawa (Tue, 13:50)

$$\lambda_{c,\mathrm{NLO}} = 0.0008144(67)$$

$$\kappa_{c,\mathrm{NLO}} = 0.08997(12)$$

preliminary

- Next to leading order results

Correlation among expansion terms in HPE [PTEP 2022, 033B05 (2022)]

- Expansion terms: $\ln\det M(\kappa) = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \ln\det M}{\partial \kappa^n} \kappa^n \equiv N_{\rm site} \sum_{n=1}^{\infty} D_n \kappa^n$

$$D_n = \frac{1}{N_{\rm site}} \frac{(-1)^{n-1}}{n} \mathrm{tr}\left[\left(\frac{\partial M}{\partial \kappa}\right)^n\right] = W(n) + L(N_t, n)$$

Wilson loop type

Polyakov loop type
closed with periodic boundary

- A matrix trace is computed by the noise method at each gauge configuration.
- Separate $W(n)$ and $L(N_t, n)$ by changing the boundary conditions.
- $W^0(n)$ and $L^0(N_t, n)$ are these terms when all $U_\mu(x)$ are set to 1.

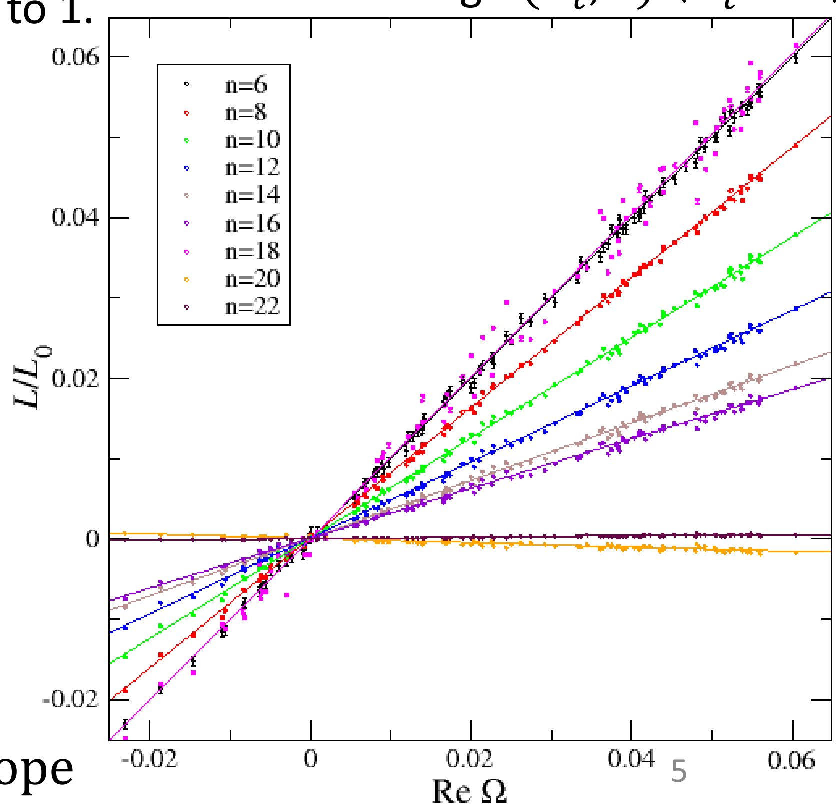
Leading order term

Polyakov loop

$$L(N_t, N_t) = L^0(N_t, N_t)\ \mathrm{Re}\ \Omega = \frac{12 \times 2^{N_t}}{N_t} \mathrm{Re}\ \Omega$$

- The correlation between $L(N_t, n)$ and ReΩ is very strong.
- Approximation: $\underline{L(N_t, n) = L^0(N_t, n) c_n\ \mathrm{Re}\ \Omega}$
- The values of c_n is found to be independent of β and κ.
- $W(n)$ terms are improvement terms for the gauge action.
  - As an improvement term, the value is very small.
  - Omitted in this talk.

Correlation among $L(N_t, n)$ ($N_t = 6$)



c_n: slope

Determination of critical κ

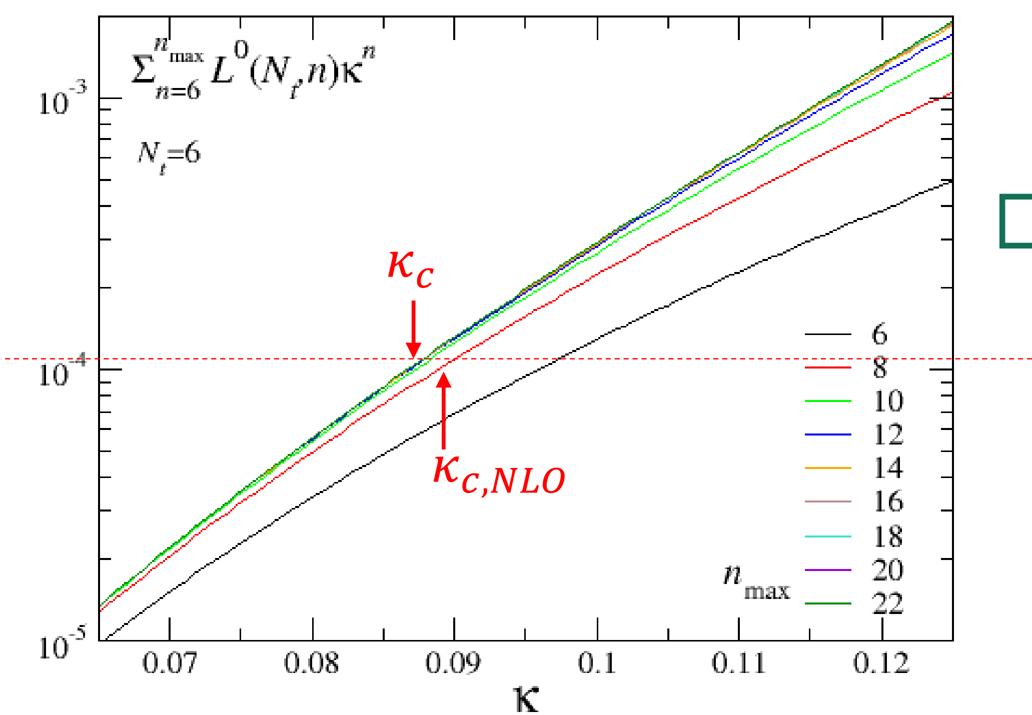
$$L(N_t, n) = L^0(N_t, n) c_n \,\mathrm{Re}\, \Omega$$

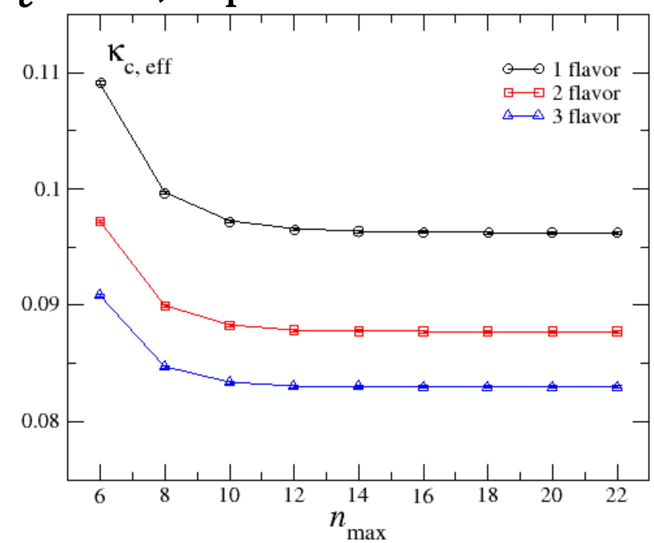
$$\frac{\ln\det M(\kappa)}{N_{\mathrm{site}}} - (\text{Wilson loops}) = \sum_{n=N_t}^{n_{\max}} L(N_t, n)\,\kappa^n \approx \mathrm{Re}\,\Omega \underbrace{\sum_{n=N_t}^{n_{\max}} L^0(N_t, n)\, c_n \kappa^n}_{\text{One parameter}}$$

- The same as determining the critical point by the first order term only.

$$\sum_{n=N_t}^{n_{\max}} L^0(N_t, n)\, c_n \kappa_{c,\mathrm{eff}}^n = L^0(N_t, N_t)\kappa_{c,\mathrm{LO}}^{N_t}$$

- Solving this equation gives us the critical κ considering the higher order terms.
- Determination of effective critical points $(N_t = 6, N_{\mathrm{f}} = 2)$





convergence value : $\kappa_c = 0.08775(11)$

κ_c = 0.0877(9) by a full QCD simulation
[Cuteri et al., Phys.Rev.D103(2021), 014513]

Critical Line of 2+1 Flavor QCD Incorporating Higher Order Effects

$$\ln\left[\prod_f \det M(\kappa_f)\right] = N_{\rm site}\,{\rm Re}\,\Omega \sum_f \sum_{n=N_t}^{n_{\max}} L^0(N_t,n)\,c_n\kappa_f^n + (\text{Wilson loops})$$

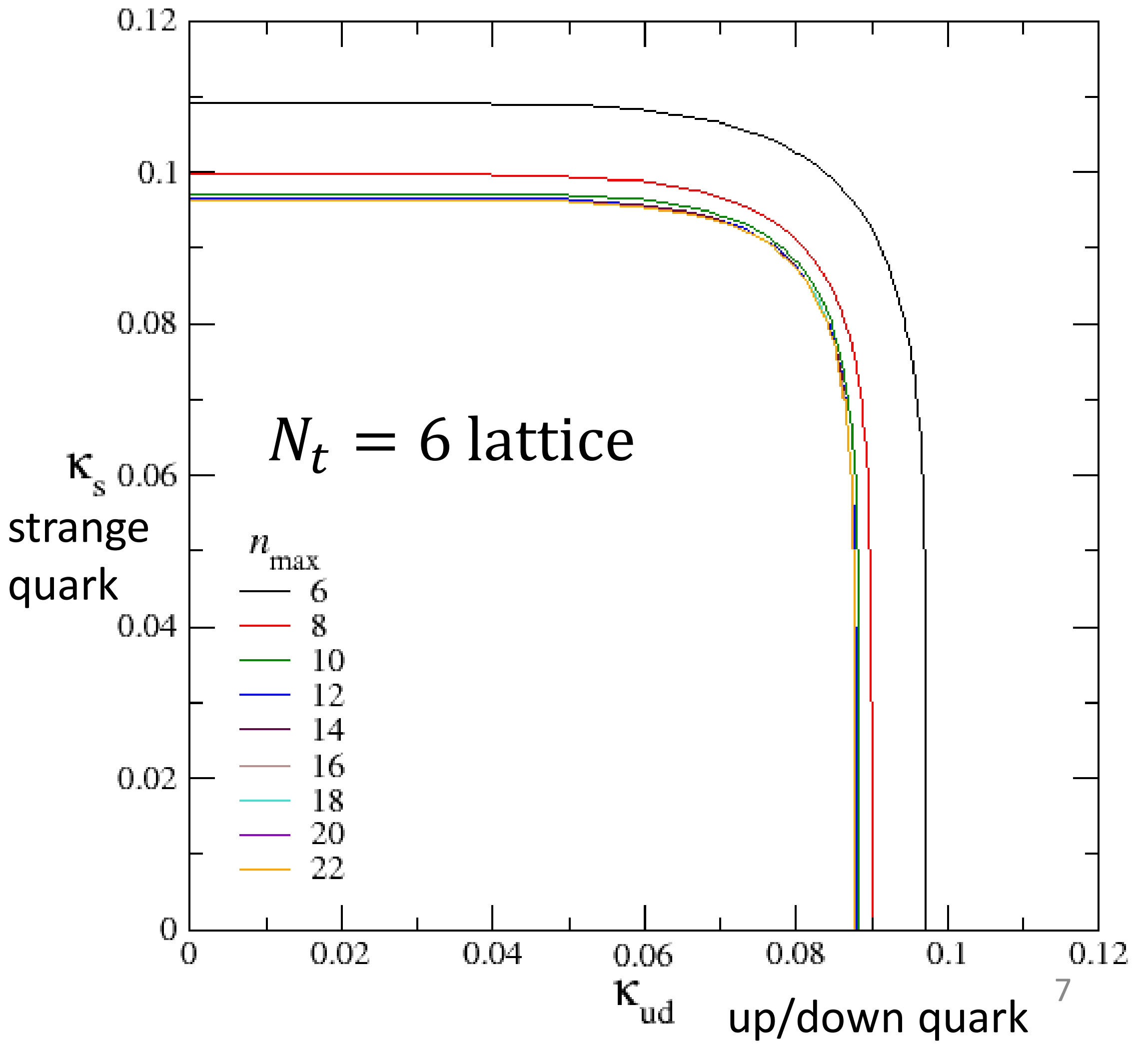
$$\boxed{2\sum_{n=N_t}^{n_{\max}} L^0(N_t,n)\,c_n\kappa_{c,ud}^n + \sum_{n=N_t}^{n_{\max}} L^0(N_t,n)\,c_n\kappa_{c,s}^n = 2L^0(N_t,N_t)\kappa_{c,\text{2f, LO}}^{N_t}}$$

Solve this equation.

Once one κ_c is determined, the critical line can be obtained for any number of flavors by using c_n.

The critical line converges at $n_{\max} \geq 12$.

$N_t = 8$ simulations are in progress. Kitazawa's talk



Critical point in finite density QCD

[Phys.Rev.D89, 034507(2014)]

$$\boxed{U_4(x) \Rightarrow e^{\mu a} U_4(x), \quad U_4^\dagger(x) \Rightarrow e^{-\mu a} U_4^\dagger(x)}$$ in $\det M$

$$\boxed{\Omega \Rightarrow e^{\mu/T}\Omega, \quad \Omega^* \Rightarrow e^{-\mu/T}\Omega^*}$$ Polyakov loop

$$\ln\det M(\kappa,\mu) = 288 N_{site}\kappa^4 P + 6\cdot 2^{N_t} N_s^3 \kappa^{N_t}\left(e^{\frac{\mu}{T}}\Omega + e^{-\frac{\mu}{T}}\Omega^*\right) + \cdots$$

$$= 288 N_{\mathrm{site}}\kappa^4 P + 12\cdot 2^{N_t} N_s^3 \underline{\kappa^{N_t}(\cosh(\mu/T)}\,\mathrm{Re}\Omega + i\,\underline{\underline{\sinh(\mu/T)\,\mathrm{Im}\Omega}}) + \cdots$$

phase

$$\boxed{\kappa^{N_t} \Longrightarrow \kappa^{N_t}\cosh(\mu/T)}$$

Determination with $N_t = 4$

Phys.Rev.D89, 034507(2014)

- First order term is dominant in HPE.
- Critical point : Solve $\underline{\kappa_c^{N_t}(\mu)\cosh(\mu/T) = \kappa_c^{N_t}(0)}$
- The contribution from the complex phase is small.

Complex phase of $(\det M)^{N_f}$ The sign problem is not serious (because $\tanh(\mu/T) < 1$)

$$\theta = 12\cdot 2^{N_t} N_s^3 N_f \kappa_c^{N_t}(0)\,\underline{\tanh(\mu/T)}\,\mathrm{Im}\Omega$$

When incorporating higher-order terms for $N_t = 6$

$$\boxed{\cosh\left(\frac{\mu}{T}\right)\sum_{n=N_t}^{n_{\max}} L^0(N_t,n)\, c_n \kappa_c^n(\mu) = L^0(N_t,N_t)\kappa_{c,\mathrm{LO}}^{N_t}(0)}$$

Finite density hopping parameter expansion

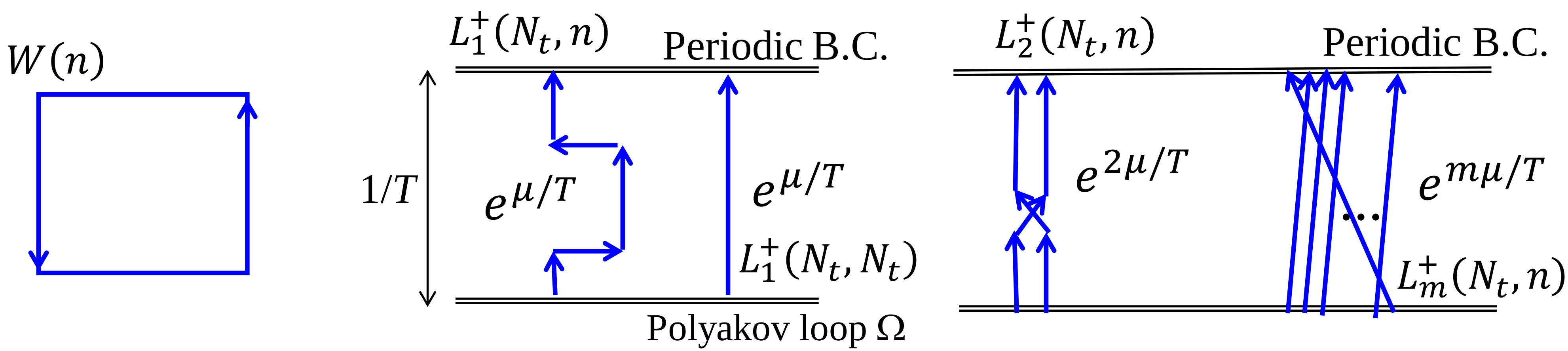
$$\boxed{L_m(N_t,n) = L_m^+(N_t,n) + L_m^-(N_t,n)}$$

$$\ln\det M(\kappa) = N_{\mathrm{site}} \sum_{n=1}^{\infty} D_n \kappa^n$$

$$= N_{\mathrm{site}} \sum_{n=1}^{\infty} \left(W(n) + \sum_{m=1}^{\infty} e^{m\mu/T} L_m^+(N_t,n) + \sum_{m=1}^{\infty} e^{-m\mu/T} L_m^-(N_t,n) \right) \kappa^n$$

$$= N_{\mathrm{site}} \sum_{n=1}^{\infty} \left(W(n) + \sum_{m=1}^{\infty} \cosh\left(\frac{m\mu}{T}\right) L_m(N_t,n) + \underbrace{\sum_{m=1}^{\infty} i \sinh\left(\frac{m\mu}{T}\right) 2\,\mathrm{Im}L_m^+(N_t,n)}_{\text{Complex Phase}} \right) \kappa^n$$

$$L_m^+(N_t,n) = \left(L_m^-(N_t,n)\right)^*, \quad 2i\,\mathrm{Im}L_m^+(N_t,n) = L_m^+(N_t,n) - L_m^-(N_t,n)$$



We ignore the phase and $m \geq 2$ terms, since $m \geq 2$ terms are very small for $N_t = 6$.

$L(N_t,n) \approx L^0(N_t,n) c_n \,\mathrm{Re}\,\Omega$ at $\mu = 0$ ➡ $\cosh\left(\frac{\mu}{T}\right) L(N_t,n) \approx \cosh\left(\frac{\mu}{T}\right) L^0(N_t,n) c_n \,\mathrm{Re}\,\Omega$

Critical point at finite density (ignoring complex phase)

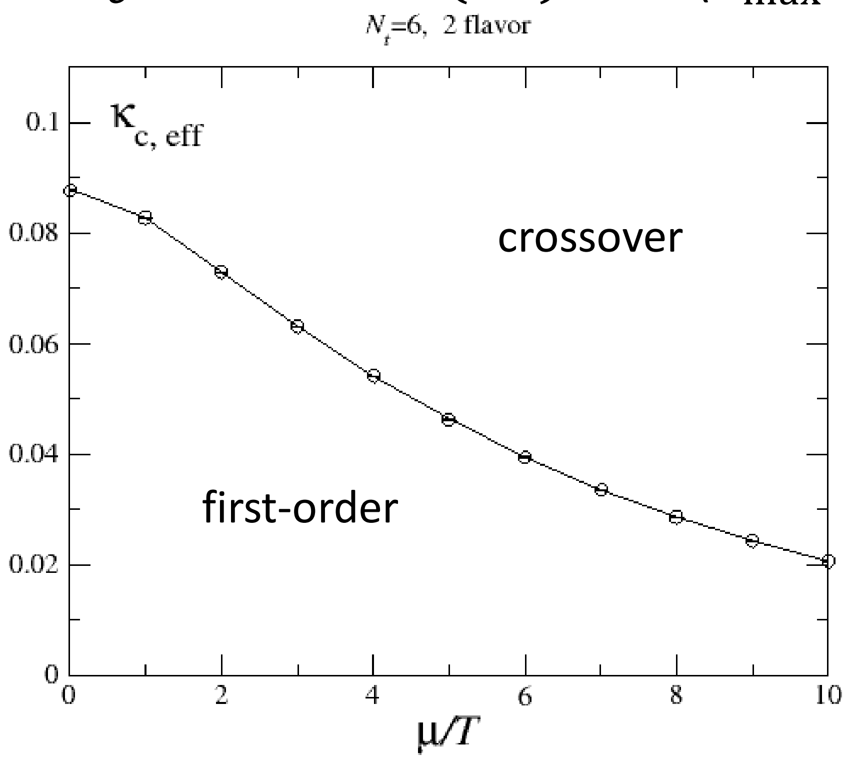
$$\cosh\left(\frac{\mu}{T}\right)\sum_{n=N_t}^{n_{\max}} L^0(N_t,n)\, c_n \kappa_{c,\mathrm{eff}}^n(\mu) = L^0(N_t,N_t)\kappa_{c,\mathrm{LO}}^{N_t}(0)$$

- Solve this equation

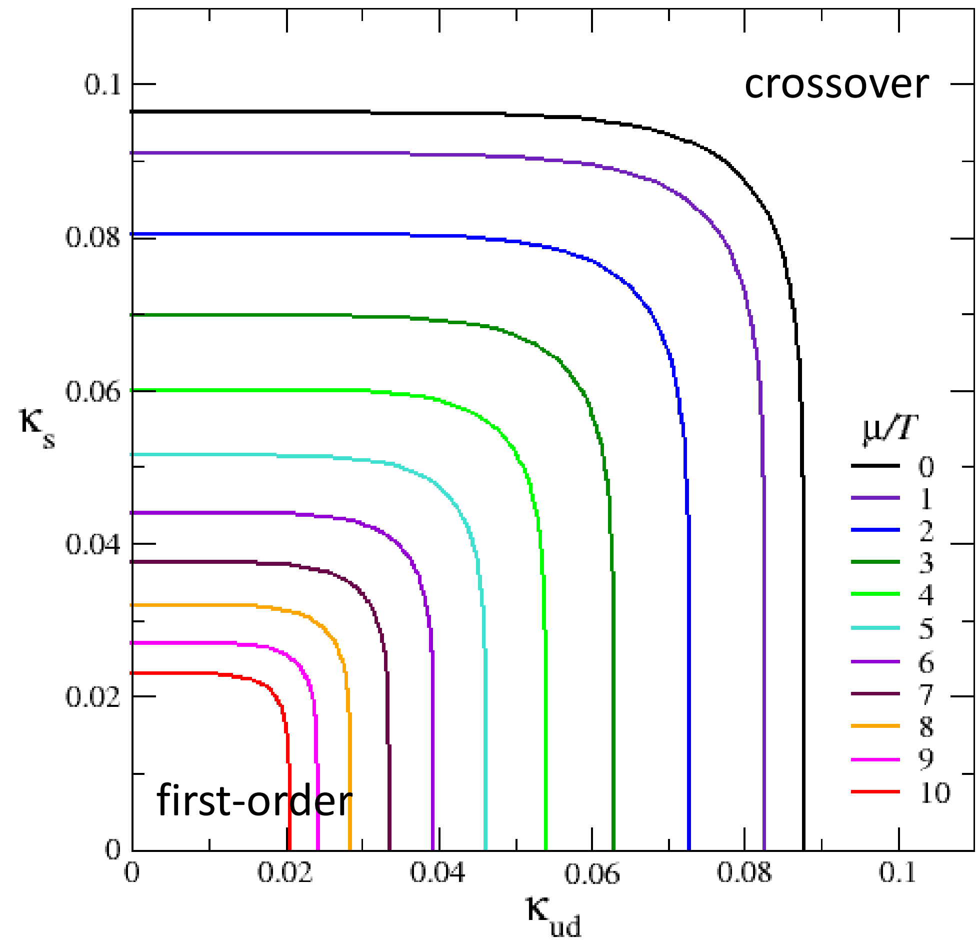
$N_t = 6,\ N_{\mathrm{f}} = 2$ case

$\kappa_{c,\mathrm{NLO}} = 0.08997(12)$ preliminary

$\kappa_c = 0.08775(11)$ $(n_{\max} = 22)$



$N_t = 6,\ N_{\mathrm{f}} = 2+1$ case



The higher the density, the smaller the first-order phase transition region.

Complex phase in the hopping parameter expansion

$$\ln \det M(\kappa)$$

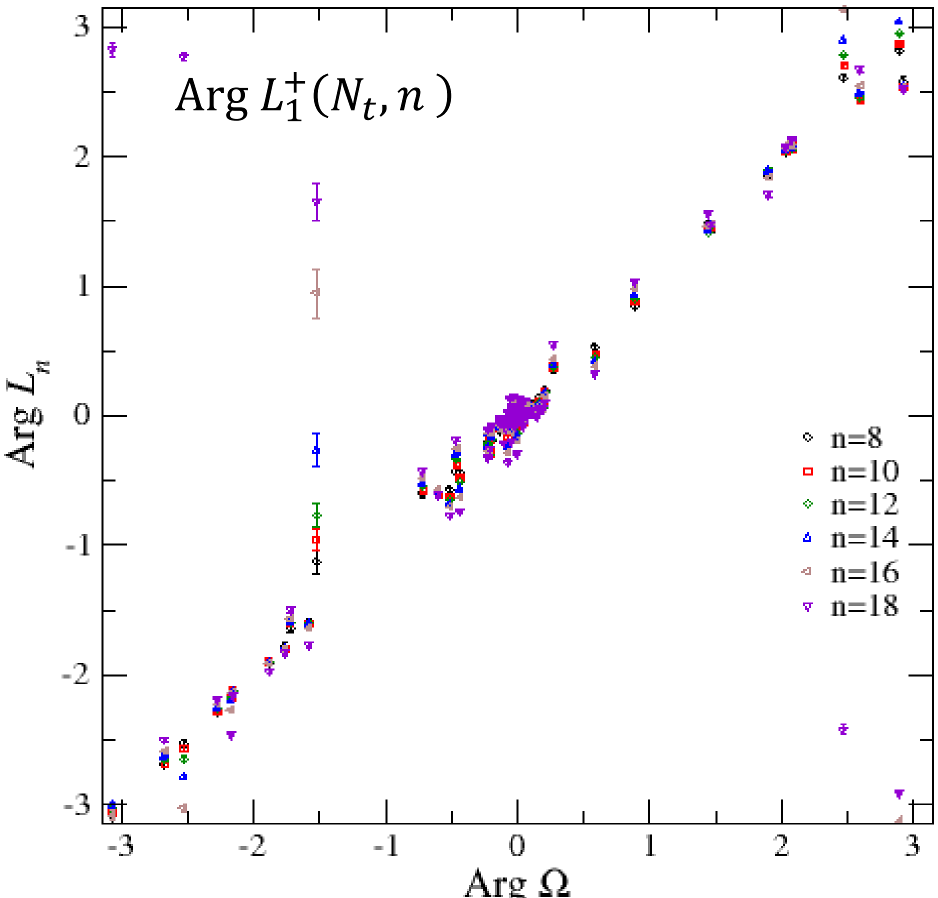
$$= N_{\text{site}} \sum_{n=1}^{\infty} \left(W(n) + \sum_{m=1}^{\infty} \cosh\left(\frac{m\mu}{T}\right) L_m(N_t, n) + \underline{\sum_{m=1}^{\infty} i \sinh\left(\frac{m\mu}{T}\right) 2\, \mathrm{Im} L_m^{+}(N_t, n)} \right) \kappa^n$$

Complex Phase

In the lowest order

$$2i\, \mathrm{Im} L_1^{+}(N_t, N_t) = L_1^{+}(N_t, N_t) - L_1^{-}(N_t, N_t) = L^0(N_t, N_t)\, i \mathrm{Im}\Omega$$

argument of complex



- Strong correlation between Arg $L_1^{+}(N_t, n)$ and Arg Ω

$$\mathrm{Arg}\, L_1^{+}(N_t, n) \approx \mathrm{Arg}\, \Omega$$

$$\frac{\mathrm{Im} L_1^{+}(N_t, n)}{\mathrm{Re}\, L_1^{+}(N_t, n)} \approx \frac{\mathrm{Im}\, \Omega}{\mathrm{Re}\, \Omega}$$

We can approximate as

$$\underline{2L^{+}(N_t, n) \approx L^0(N_t, n) c_n\, \Omega}$$

$$(2\, \mathrm{Im} L^{+}(N_t, n) = L^0(N_t, n) c_n \mathrm{Im}\Omega)$$

For $m \geq 2$, there was no appreciable correlation within error.

Reweighting method at finite density

- Quark determinant: $\left(\det M\,(\kappa,\mu)\right)^{N_\mathrm{f}} = |\det M(\kappa,\mu)|^{N_\mathrm{f}} e^{i\theta}$
- If $2\ \mathrm{Im} L_m^+(N_t,n) = L^0(N_t,n) c_n \mathrm{Im}\,\Omega$, then the complex phase is

$$\theta = N_\mathrm{f} N_\mathrm{site} \sum_{n,m} \sinh\left(\frac{m\mu}{T}\right) 2\ \mathrm{Im} L_m^+(N_t,n)\ \kappa^n \approx N_\mathrm{f} N_\mathrm{site} \sum_n \sinh\left(\frac{\mu}{T}\right) L^0(N_t,n) c_n \kappa^n\ \mathrm{Im}\,\Omega$$

- Expectation value of $F(x)$ with $x = \mathrm{Re}\Omega$ by the reweighting method

$$\langle F(x)\rangle_{(\beta,\kappa,\mu)} = \frac{1}{Z}\int DU\, F\left(\det M(\kappa,\mu)\right)^{N_\mathrm{f}} e^{-S_g} = \frac{\int DU\, F \cos\theta |\det M(\kappa,\mu)|^{N_\mathrm{f}} e^{-S_g}}{\int DU \cos\theta |\det M(\kappa,\mu)|^{N_\mathrm{f}} e^{-S_g}}$$

$$= \frac{\int F(x) \langle\cos\theta\rangle_{x=\mathrm{Re}\Omega} W(x) dx}{\int \langle\cos\theta\rangle_{x=\mathrm{Re}\Omega} W(x) dx}$$

- $\langle\cos\theta\rangle_{x=\mathrm{Re}\Omega}$ is the expectation value calculated by classifying the value of $\mathrm{Re}\Omega$,
- $W(x)$ with $x = \mathrm{Re}\Omega$ is the probability distribution of $\mathrm{Re}\Omega$ when configurations are generated by $|\det M(\kappa,\mu)|^{N_\mathrm{f}}$ (phase quench simulation).
- We estimate the shift from the Phase-ignoring critical line by the effect of $\langle\cos\theta\rangle_x$.
- We calculate $\langle\cos\theta\rangle_x$ on the critical line and discuss the shift by $\langle\cos\theta\rangle_x$.

Complex phase along the critical line κ_c

- Because $\cosh\left(\frac{\mu}{T}\right)\sum_n L^0(N_t,n)\, c_n \kappa_c^n(\mu) = L^0(N_t,N_t)\kappa_{c,\mathrm{LO}}^{N_t}$ on the line of κ_c.
- $\theta \approx N_\mathrm{f} N_\mathrm{site} \sum_n \sinh\left(\frac{\mu}{T}\right) L^0(N_t,n) c_n \kappa_c^n(\mu)\ \mathrm{Im}\,\Omega \approx N_\mathrm{f} N_\mathrm{site} L^0(N_t,N_t)\kappa_{c,\mathrm{LO}}^{N_t}(0)\tanh\left(\frac{\mu}{T}\right)\mathrm{Im}\,\Omega$
- $\theta = N_\mathrm{s}^3 \lambda_{c,\mathrm{LO}} \tanh\left(\frac{\mu}{T}\right)\mathrm{Im}\,\Omega$ $\quad(\lambda = N_t N_\mathrm{f} L^0(N_t,N_t)\kappa^{N_t} = 12 N_\mathrm{f}\, 2^{N_t}\kappa^{N_t})$
- Because $\lambda_{c,\mathrm{LO}}$ is small and $\tanh\left(\frac{\mu}{T}\right) < 1$, $\ln\langle\cos\theta\rangle$ is computable without sign problem.

- If the volume is very large, $\ln\langle\cos\theta\rangle$ cannot be calculated, so in that case we use the cumulant expansion

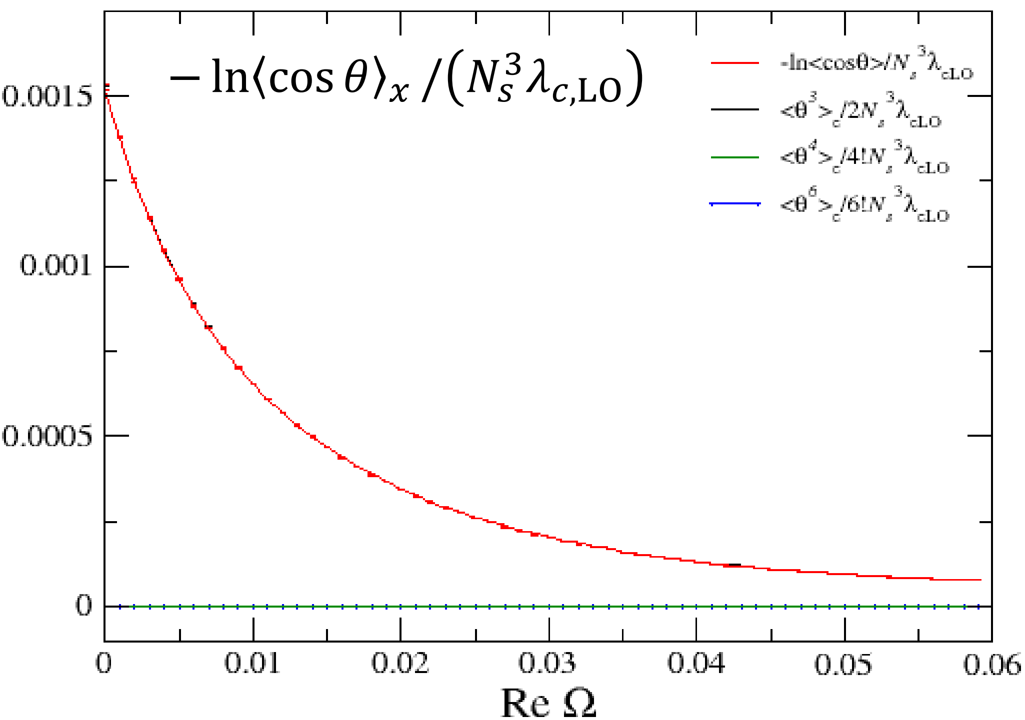
$$\ln\langle\cos\theta\rangle \approx -\frac{1}{2!}\langle\theta^2\rangle_c + \frac{1}{4!}\langle\theta^4\rangle_c - \frac{1}{6!}\langle\theta^6\rangle_c + \cdots$$

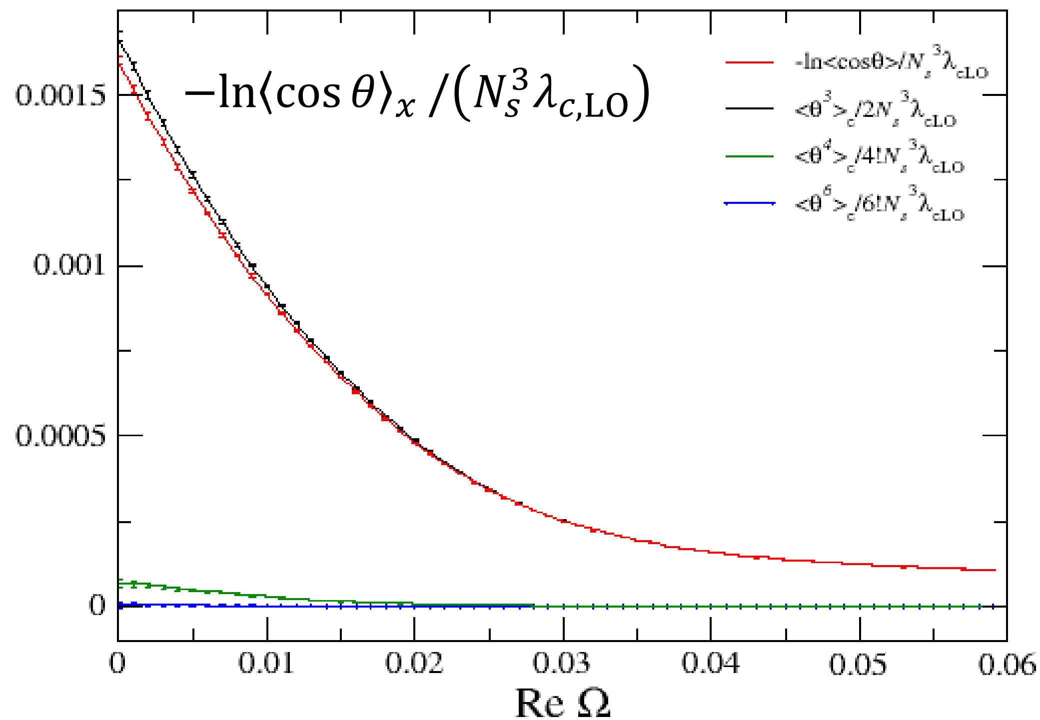
$$\langle\theta^2\rangle_c = \langle\theta^2\rangle, \qquad \langle\theta^4\rangle_c = \langle\theta^4\rangle - 3\langle\theta^2\rangle^2, \qquad \langle\theta^6\rangle_c = \langle\theta^6\rangle - 15\langle\theta^4\rangle\langle\theta^2\rangle + 30\langle\theta^2\rangle^3, \cdots$$

Complex phase fluctuation at the critical point

- $\langle \theta^n \rangle_c = \left[N_s^3 \lambda_{c,\mathrm{LO}} \tanh(\mu/T) \right]^n \langle (\mathrm{Im}\Omega)^n \rangle_c$ on the critical line for $\tanh(\mu/T) = 1$
- Even with $N_s = 90$, the phase fluctuation is small. $\langle \cos\theta \rangle$ can be easily calculated.
- $\ln\langle \cos\theta \rangle_x \approx -\frac{1}{2}\langle \theta^2 \rangle_c$ This indicates an approximately Gaussian distribution.
- Then, the volume dependence is $\langle \theta^2 \rangle_c \sim N_s^3$.
- The volume dependence of $\ln\langle \cos\theta \rangle_x / \left(N_s^3 \lambda_{c,\mathrm{LO}} \right)$ is small. $(x = \mathrm{Re}\Omega)$

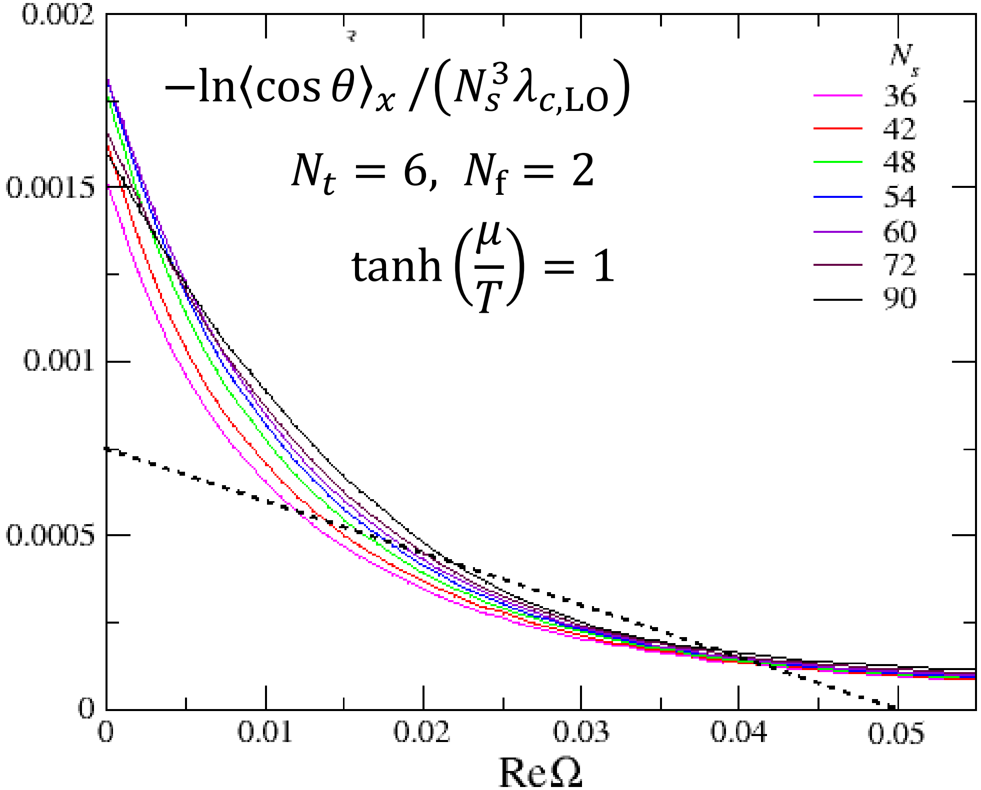
$36^3 \times 6$ lattice $\tanh(\mu/T) = 1$ $90^3 \times 6$ lattice





Effect from the phase fluctuation to κ_c

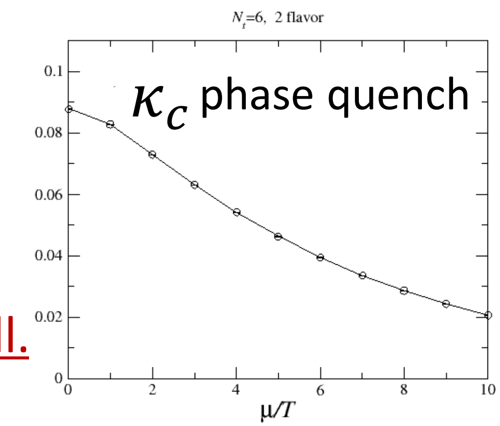
volume dependence



$$\langle F(x)\rangle = \frac{\int F(x)\,\langle\cos\theta\rangle_{x=\mathrm{Re}\Omega} W(x)dx}{\int \langle\cos\theta\rangle_{x=\mathrm{Re}\Omega} W(x)dx}$$

Approximation: black dashed line

$$-\ln\langle\cos\theta\rangle_x / (N_s^3\lambda_{c,\mathrm{LO}}) = d_0 + d_1\mathrm{Re}\Omega$$
$$\approx 0.00075 - 0.015\ \mathrm{Re}\Omega$$



Effect from the phase fluctuation is very small.

- On the Phase-ignoring critical line,

$$N_\mathrm{f}\ln|\det M| - (\mathrm{WL}) \approx N_\mathrm{site}N_\mathrm{f}\cosh\left(\frac{\mu}{T}\right)\sum_n L^0(N_t,n)c_n\kappa^n\mathrm{Re}\Omega = N_s^3\lambda_{c,\mathrm{LO}}\mathrm{Re}\Omega$$

$$\theta = N_s^3\lambda_{c,\mathrm{LO}}\tanh\left(\frac{\mu}{T}\right)\mathrm{Im}\Omega$$

$$\langle\cos\theta\rangle_{\mathrm{Re}\Omega}|\det M|^{N_\mathrm{f}} \approx \exp\left[\ln\langle\cos\theta\rangle_{\mathrm{Re}\Omega} + N_s^3\lambda_{c,\mathrm{LO}}\mathrm{Re}\Omega\right] \approx C\exp\left[N_s^3\lambda_{c,\mathrm{LO}}(1-d_1)\mathrm{Re}\Omega\right]$$

- Multiplying $\langle\cos\theta\rangle$ is the same as $\lambda \to \lambda(1-d_1)$. For $\tanh\left(\frac{\mu}{T}\right) = 1, d_1 \approx -0.015$.
- The phase effect reduces λ_c by 1.5%, i.e. κ_c is 0.25% smaller. $(\lambda = 12N_\mathrm{f}\,2^{N_t}\kappa^{N_t})$

Conclusion and outlook

- We discussed how to efficiently determine the critical point of QCD in the heavy quark region, including the finite density region.
- There is a strong correlation between the expansion terms of the hopping parameter expansion.
  - Approximation: $L(N_t, n) = L^0(N_t, n) c_n \operatorname{Re} \Omega$
- We performed numerical simulations with the effective theory.

$$S_{\text{eff}} = 6N_{\text{site}}\beta' P + N_s^3 \lambda \text{Re}\Omega \,.$$

- Based on this effective theory with the reweighting method, the critical point of the heavy quark region can be determined relatively easily, even if the lattice spacing is small.
  - $N_t = 6$ (Kitazawa's talk) → $N_t = 8$ (in progress) → Continuum limit
- The study at finite density is possible. The critical point decreases exponentially as the chemical potential increases.