Phase structure of QCD in the heavy quark region

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WHOT-QCD Collaboration

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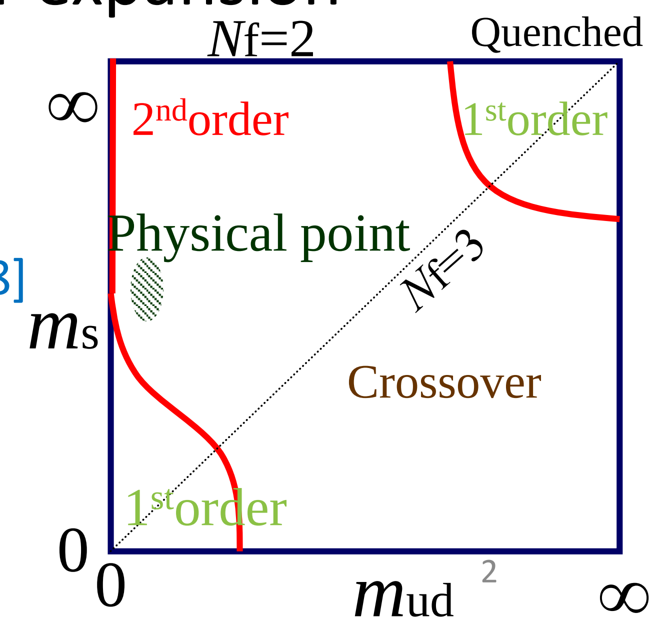
QCD phase diagram and lattice QCD, YITP Kyoto, 2021/10/28

This talk

- Important topics in the heavy quark region of Lattice QCD
- Latent heat at first order transition [PTEP,2021,013B03 (2021)]
  - Small flow time expansion method based on Gradient flow
  - Comparison to the derivative method
- End point of the first order transition region
  - Reweighting method with hopping parameter expansion
  - Determination by the shape of the histogram[PRD101,054505(2020)]
    - Truncation error of hopping parameter expansion
    - Lattice spacing dependence
    - Spatial volume dependence
  - Finite volume scaling analysis [arXiv:2108.0018]
    - Simulations with a Polyakov loop term

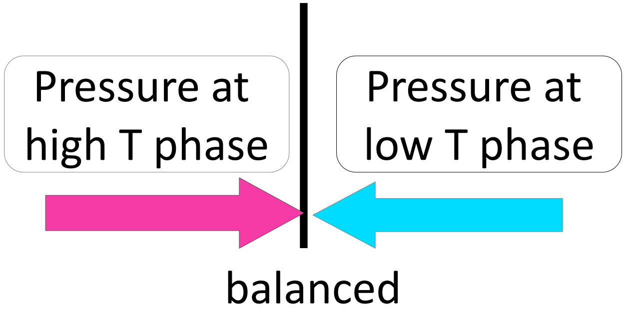


Latent heat and pressure gap in Quenched QCD

Whot-QCD, PTEP,2021,013B03 (2021)

- The latent heat (energy gap) the most basic quantity.
- The gap of pressure must vanish.

  Reliability of the calculation can be confirmed.



- Integral method cannot be used because the gap zero is assumed.
- Derivative method (F. Karsch, 1981) is required to compute the Gaps.

  (Whot-QCD, Phys. Rev. D94, 014506 (2016))
  - Non-perturbative Karsch coefficients must be calculated.
  - Large computational power is required to reduce the lattice spacing.
- We use the small flow time expansion (SFtX) method for the calculation of the energy density and pressure. [H. Suzuki, 2013]
  - Information about the Karsch coefficients are included in the formulation.

Small Flow time Expansion method [H. Suzuki (2013)]

- Compute physical quantities from flowed operators after Gradient Flow

energy-momentum tensor: $T_{\mu\nu}(x) = \lim_{t\to 0}\{c_1(t)U_{\mu\nu}(t,x) + 4c_2(t)\delta_{\mu\nu}[E(t,x) - \langle E(t,x)\rangle_0]\}$

- Gradient flow: solve "diffusion equation" → coarse graining

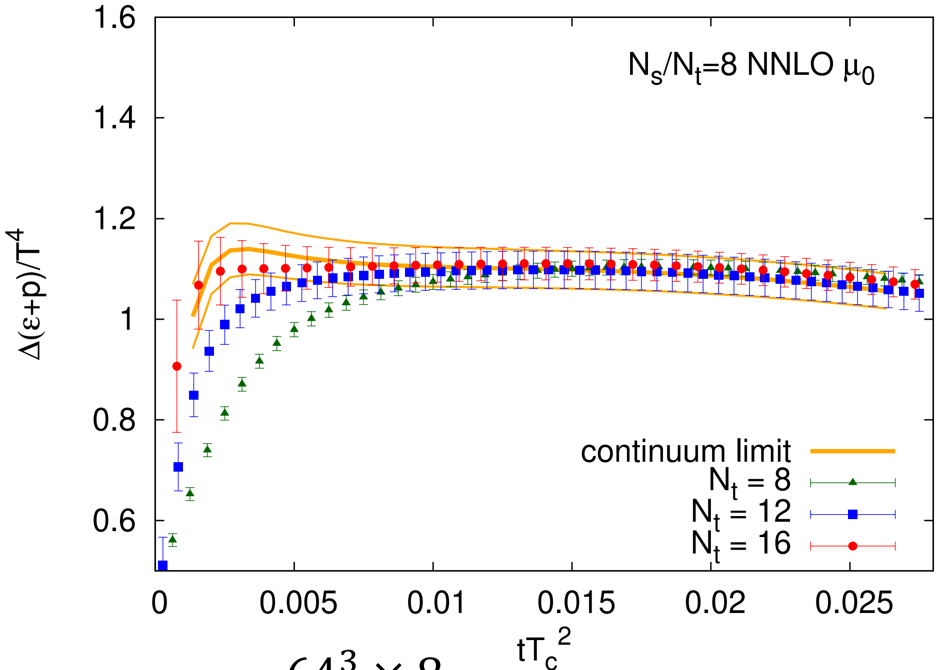
$B_\mu(t=0,x) = A_\mu(x)$ $\quad$ $G_{\mu\nu}(t,x) = \partial_\mu B_\nu(t,x) - \partial_\nu B_\mu(t,x) + [B_\mu(t,x), B_\nu(t,x)]$

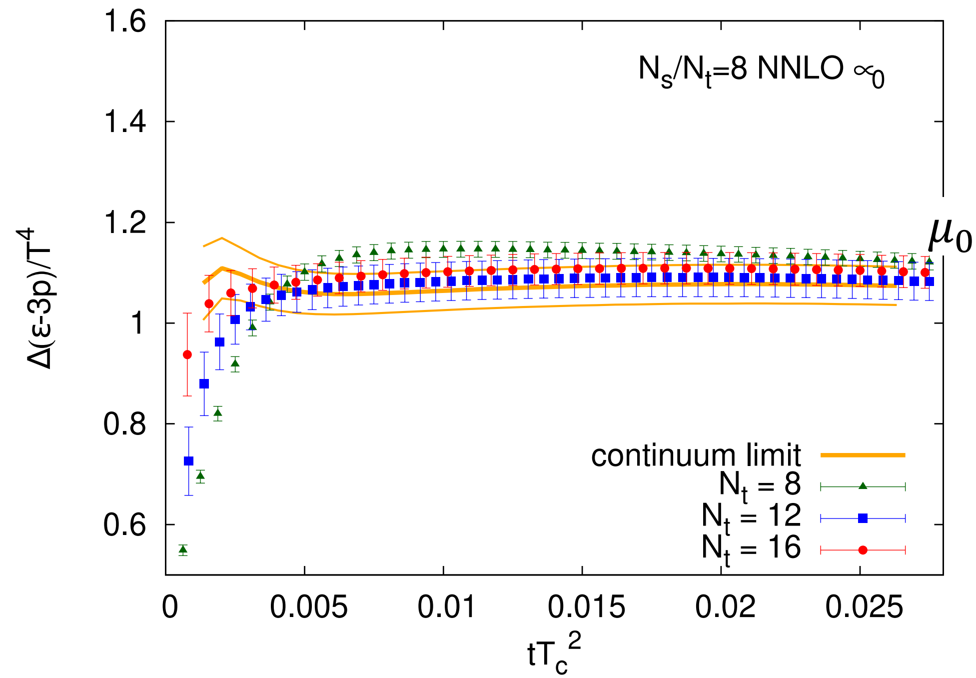
$$\partial_t B_\mu(t,x) = D_\nu G_{\mu\nu}(t,x) = -\frac{\delta S}{\delta B_\mu^a}(t,x)$$ (for Quench QCD)

- Reduce quantum fluctuations ⇒ Reduce the statistical error
- Information loss of the original lattice ⇒ continuum limit
- By the coarse graining, the theory is regularized in the continuum limit
- Physical quantities that are difficult to define on a lattice, e.g. energy-momentum tensor $T_{\mu\nu}$, can be defined in the continuum limit.
- This method is valid when flow time t is small.

⇒ We calculate with various t and extrapolate where t is small.

Latent heat and pressure gap measured at flow time t





Lattice size: $64^3 \times 8$, $96^3 \times 12$, $128^3 \times 16$

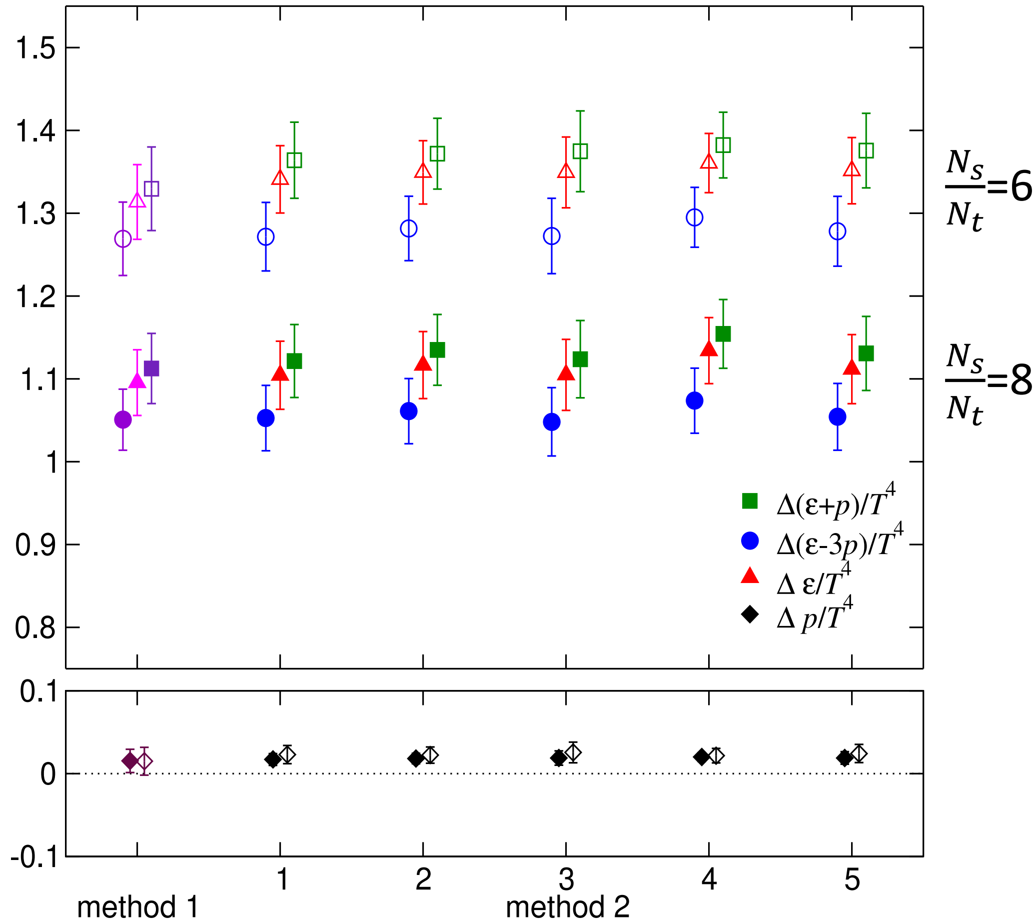
spatial volume: $V = (N_s a)^3 = \left(\frac{N_s}{N_t}\right)^3 \frac{1}{T_c^3}$ lattice spacing: $a = \frac{1}{N_t T_c}$

- Results when the same spatial volume but different lattice spacing
- Separate configurations into high T phase and low T phase

$$\frac{\Delta(\epsilon+p)}{T^4} = \langle\frac{\epsilon+p}{T^4}\rangle_{\mathrm{hot}} - \langle\frac{\epsilon+p}{T^4}\rangle_{\mathrm{cold}}, \qquad \frac{\Delta(\epsilon-3p)}{T^4} = \langle\frac{\epsilon-3p}{T^4}\rangle_{\mathrm{hot}} - \langle\frac{\epsilon-3p}{T^4}\rangle_{\mathrm{cold}}$$

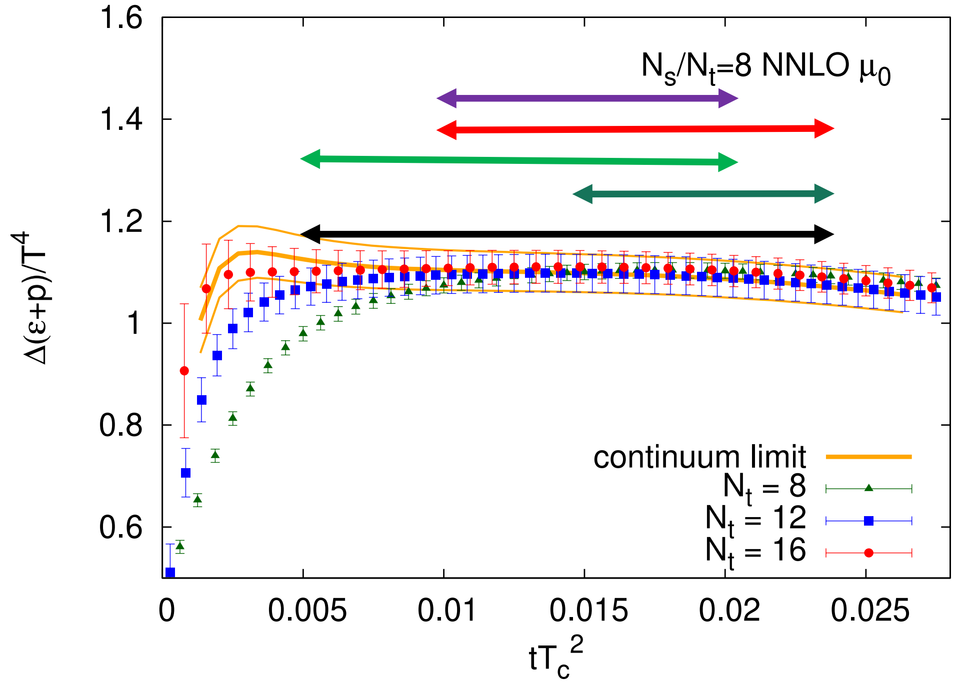
- As the flow time increased, the lattice spacing dependence disappeared.
- The orange line is the continuous limit.

Continuum limit and t → 0 limit



$t \to 0$, then $a \to 0$

$a \to 0$, then $t \to 0$

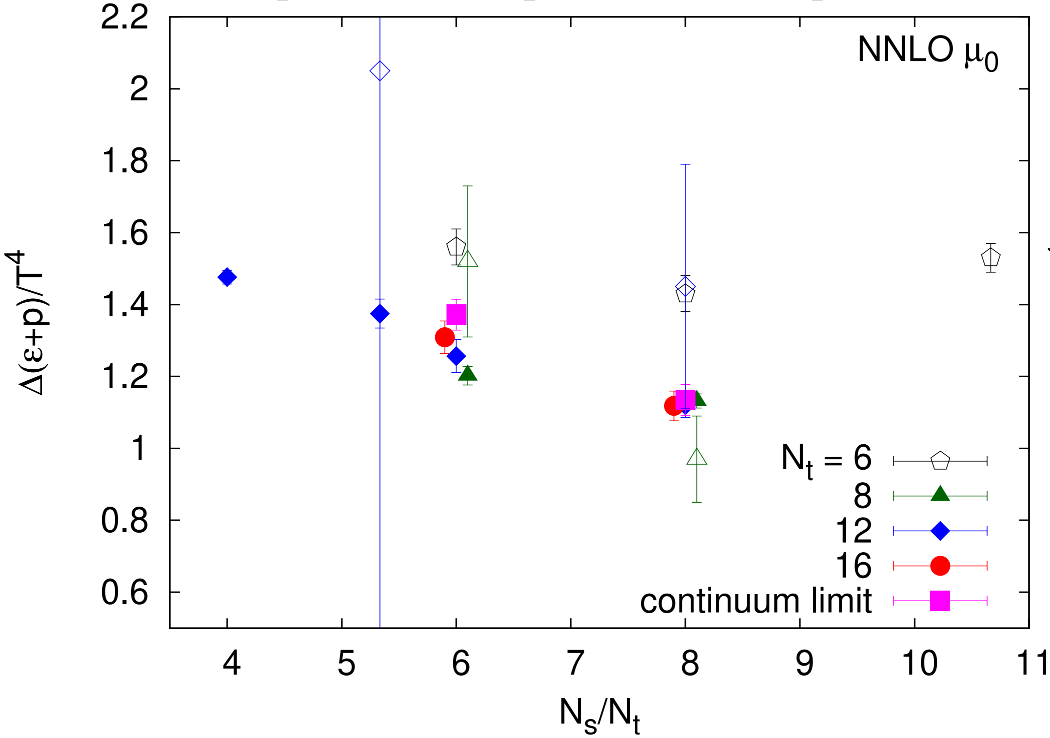


	Fit range
1 ⟷	0.010-0.020
2 ⟷	0.010-0.025
3 ⟷	0.005-0.020
4 ⟷	0.015-0.025
5 ⟷	0.005-0.025

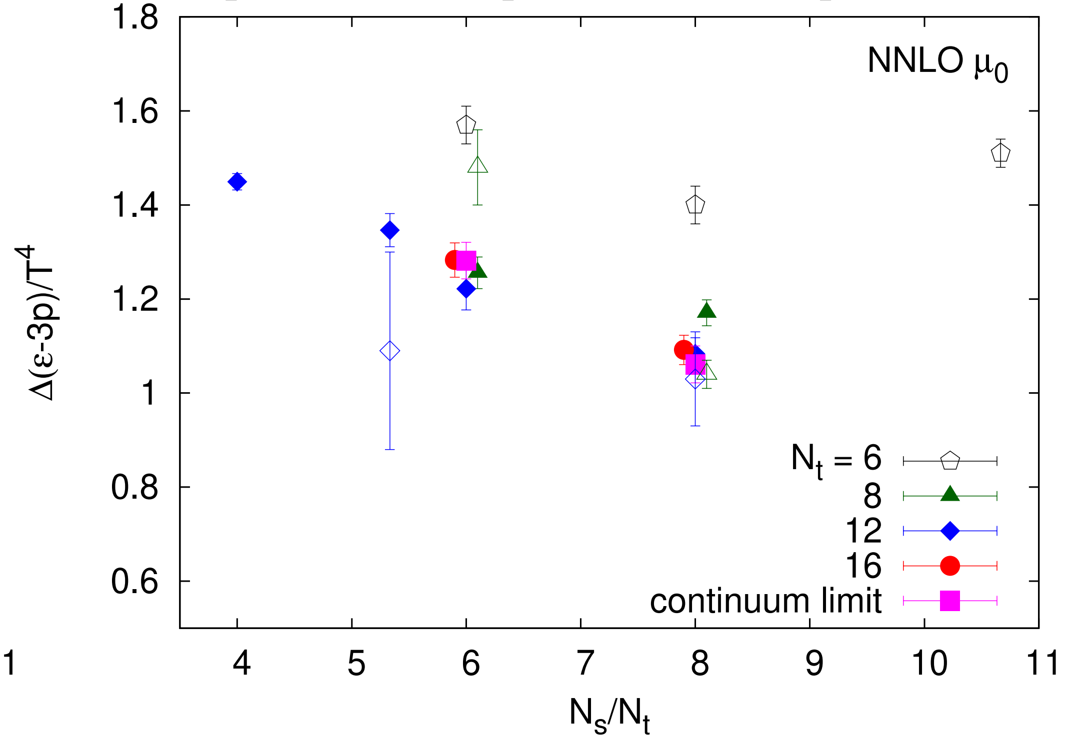
- The fit range dependence is negligible.
- One can change the order of $a \to 0$ and $t \to 0$.
- Spatial volume dependence is sizable.
- Pressure gap is zero.

Comparison to the derivative method

$$\frac{\Delta(\epsilon + p)}{T^4} = \langle\frac{\epsilon + p}{T^4}\rangle_{\text{hot}} - \langle\frac{\epsilon + p}{T^4}\rangle_{\text{cold}}$$



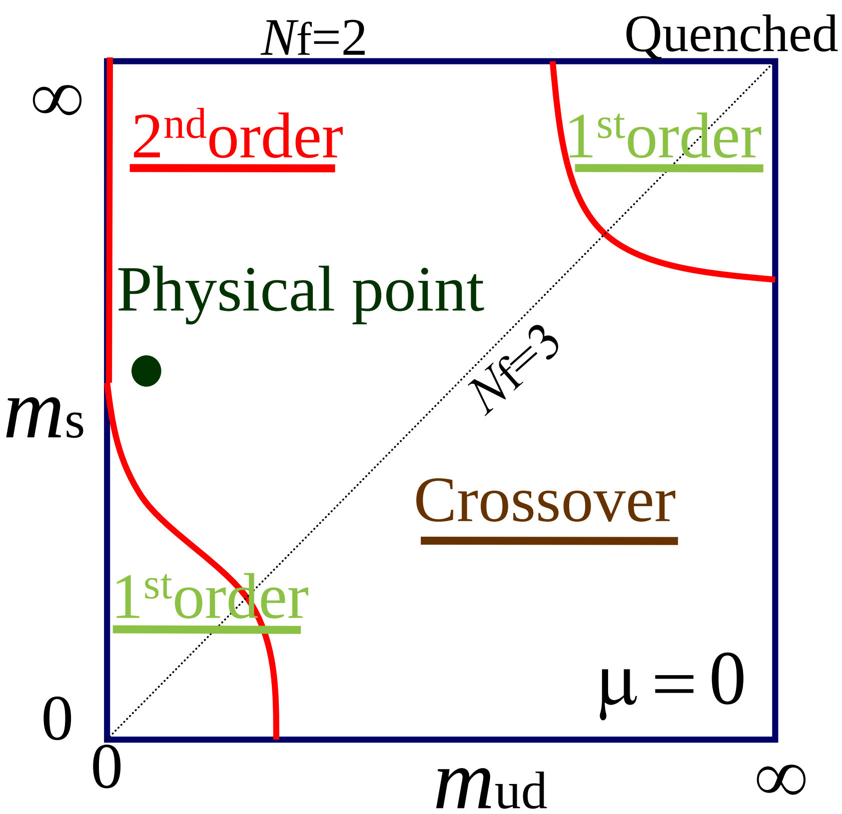
$$\frac{\Delta(\epsilon - 3p)}{T^4} = \langle\frac{\epsilon - 3p}{T^4}\rangle_{\text{hot}} - \langle\frac{\epsilon - 3p}{T^4}\rangle_{\text{cold}}$$



- Open symbols are the results by derivative method.
- The results by SFtX method and derivative method are consistent except for $N_t = 6$.
- Spatial volume dependence is observed.
- SFtX method works very well.

$$\frac{1}{T_C} = N_t a$$

Quark Mass dependence of QCD phase transition



WHOT-QCD Collab.
Phys.Rev.D84, 054502(2011)
Phys.Rev.D89, 034507(2014)
Phys.Rev.D101,054505(2020)

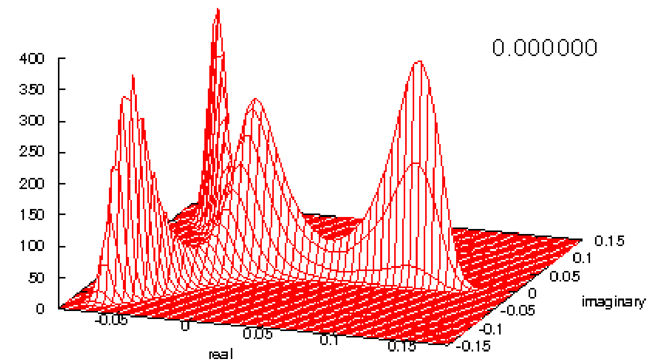
- The determination of the boundary of 1st order region: important.
- We study the boundary in the heavy quark region.
    - To understand the center symmetry breaking
    - A good practice to find the critical point in the light quark region
- In order to investigate the critical point, it is important to calculate the physical quantity as a continuous function.
- Reweighting method is useful.
    - Parameter in dynamical fermions: difficult
    - Large computational cost for quark determinant
- Hopping parameter expansion is useful to calculate the quark determinant in the heavy quark region.

Polyakov loop distribution at β_c in the complex plane

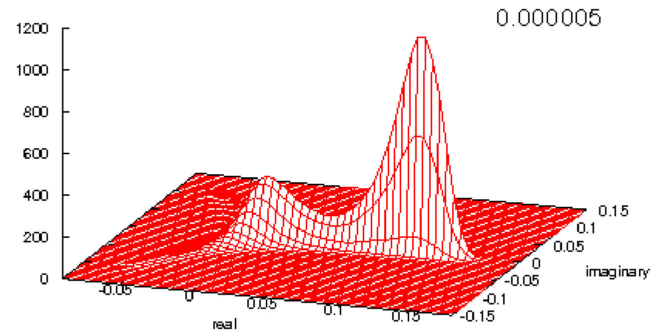
(2-flavor, $24^3 \times 4$ lattice, Phys.Rev.D89, 034507(2014))

Quenched QCD

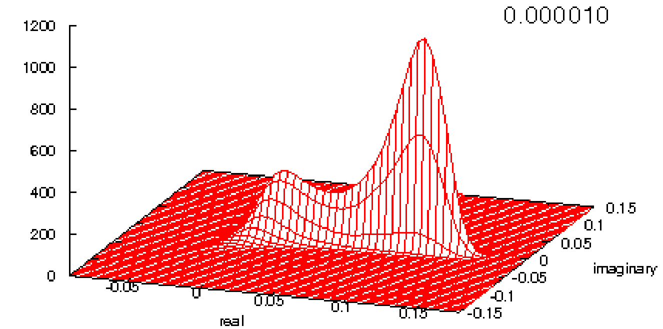
$K^4 = 0.0$ Z(3) symmetric



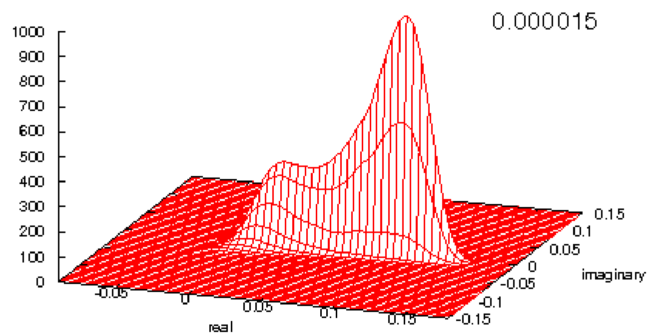
$K^4 = 5.0 \times 10^{-6}$



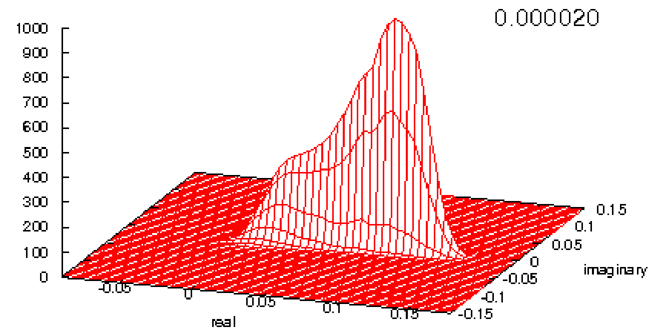
$K^4 = 1.0 \times 10^{-5}$



$K^4 = 1.5 \times 10^{-5}$

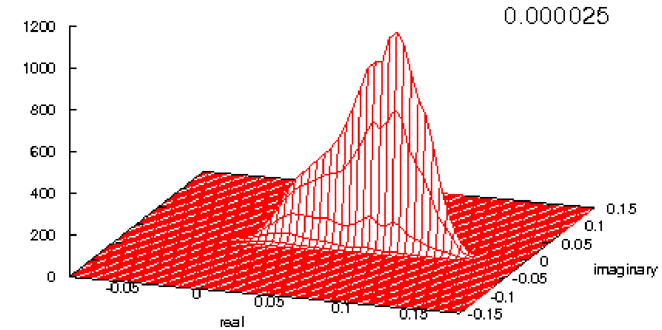


$K^4 = 2.0 \times 10^{-5}$



critical point

$K^4 = 2.5 \times 10^{-5}$



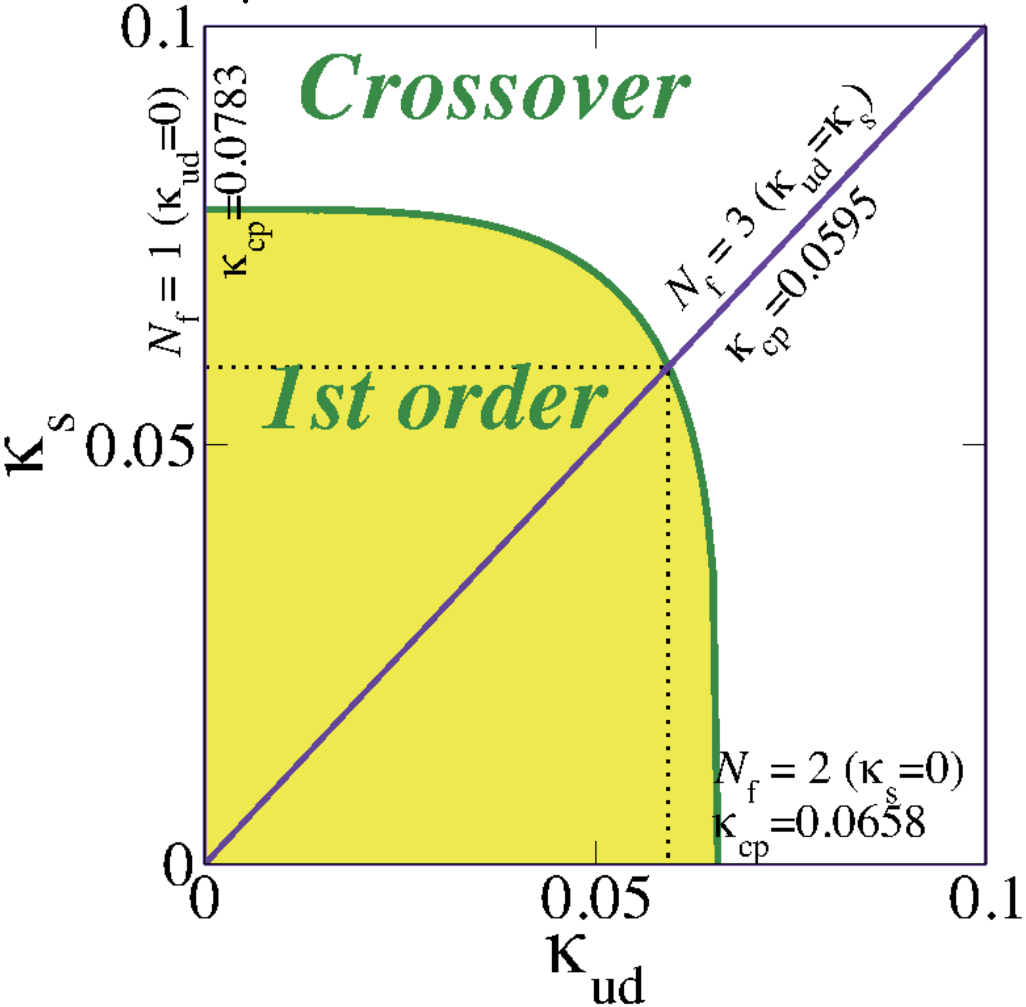
K: hopping parameter ~ 1/(mass)

Critical surface in the heavy quark region of (2+1)-flavor QCD [Phys.Rev.D84, 054502(2011); Phys.Rev.D89, 034507(2014)]

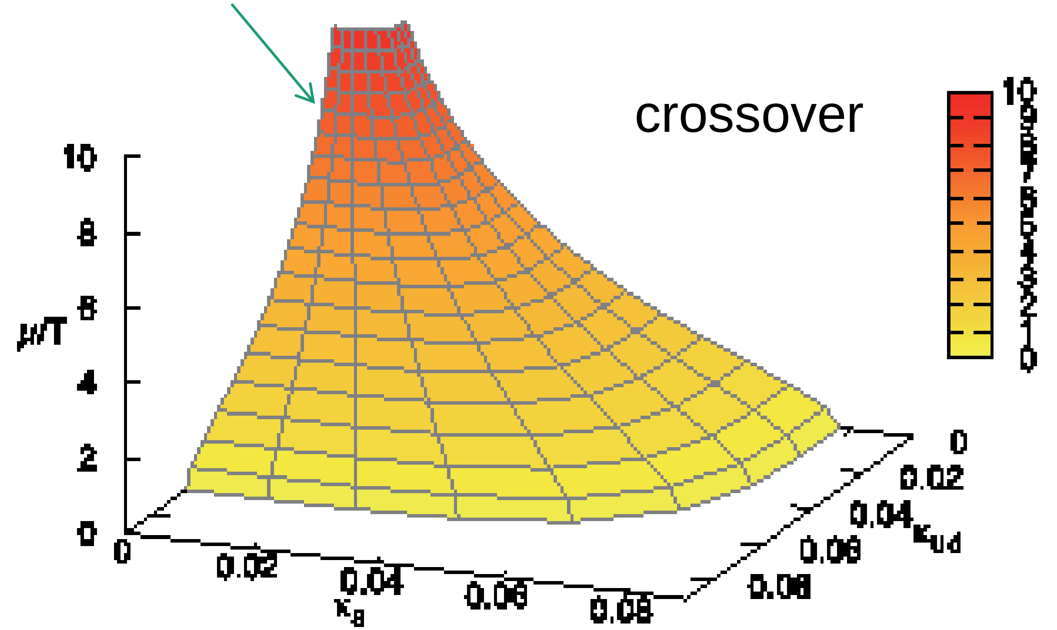
Quenched QCD simulations + reweighting

$\left(24^3 \times 4\,\text{lattice}\right)$

$\mu = 0$



Critical surface at finite density



$\frac{m_{PS}}{T_c} \approx 16.$ at κ_{cp} for 2-flavor

Histogram method

- Probability distribution function (Histogram)

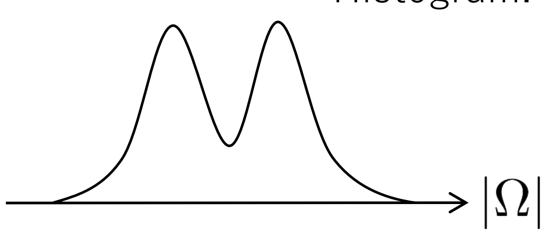
  Ω: Polyakov loop (order parameter)

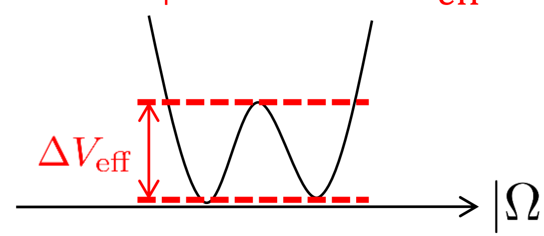
$$W(\Omega;\beta,K) \equiv \frac{1}{Z}\int DU\ \delta\left(\Omega-\widehat{\Omega}\right)\left(\det M(K)\right)^{N_{\mathrm{f}}} e^{-S_g}$$

(S_g: gauge action, M: quark matrix)

- Effective potential $\quad V_{\mathrm{eff}} = -\ln W$

First order transition





- Critical point of K: $\Delta V_{\mathrm{eff}} = 0$

Reweighting method in the heavy quark region

- Quenched QCD simulations + reweighting

$$W(\Omega;\beta,K) = \frac{1}{Z}\int DU\ \delta(\Omega-\hat{\Omega})\left(\det M(K)\right)^{N_f} e^{-S_g}$$

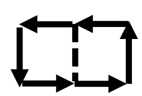
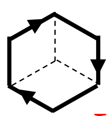
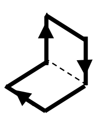
Histogram

$$= \frac{\left\langle \delta(\Omega-\hat{\Omega})\left(\det M(K)\right)^{N_f}\right\rangle_{\text{quench}}}{\left\langle \left(\det M(K)\right)^{N_f}\right\rangle_{\text{quench}}}$$

  - Multi-point (β) reweighting method is used.

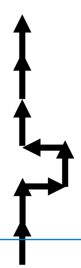
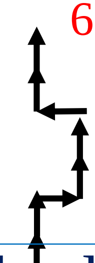
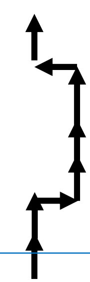
- Hopping parameter expansion $(K \sim 1/(ma))$

for N_t=6

$$\ln\left(\det M(K)\right) = 288 N_{\text{site}} K^4 P + [768\, N_{\text{site}} K^6 (3$$  $$+$$  $$+6$$  $$)] + \cdots$$

plaquette

6-step Wilson loop

$$+12 \times 2^{N_t} \times N_s^3 \left[\underline{K^{N_t} \mathrm{Re}\Omega} + 6N_t K^{N_t+2}\right.$$  $$+\, 6N_t K^{N_t+2}$$  $$+\, 3N_t K^{N_t+2}$$  $$\left.\right]$$

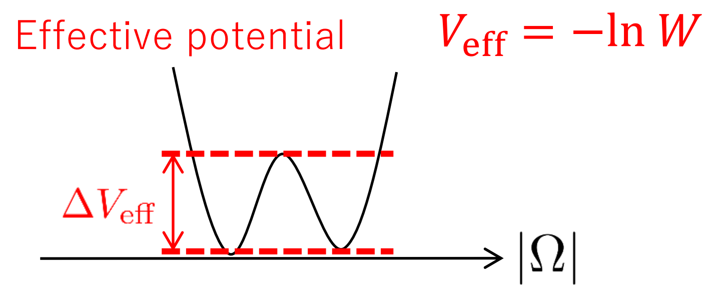
Polyakov loop

Leading term

Next to leading terms

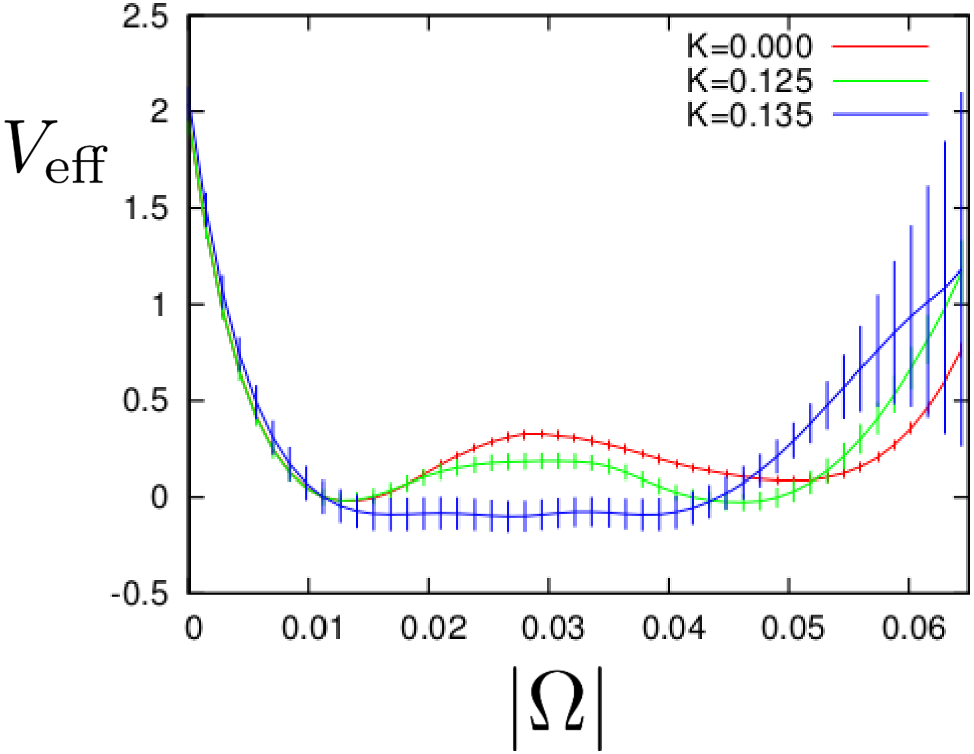
* plaquette and 6-step Wilson loop can be absolved into the gauge action.

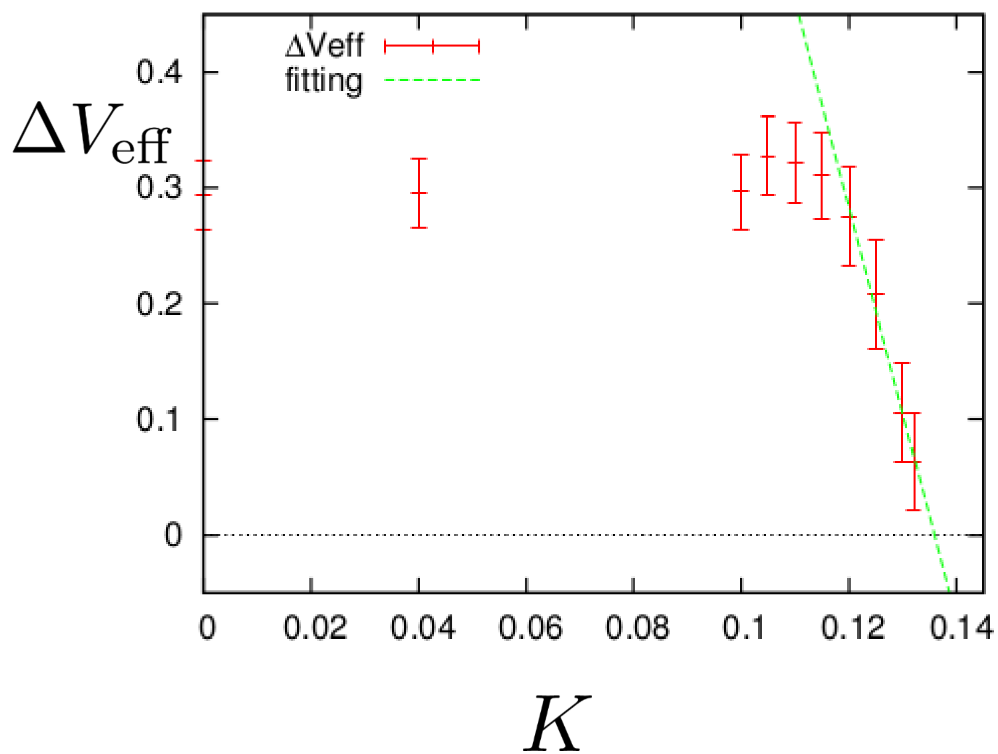
Determination of K_{ct} (leading order calculation)



$N_t = 6$ lattice (24^3x6)

Effective potential





K_{ct}=0.1359(30)

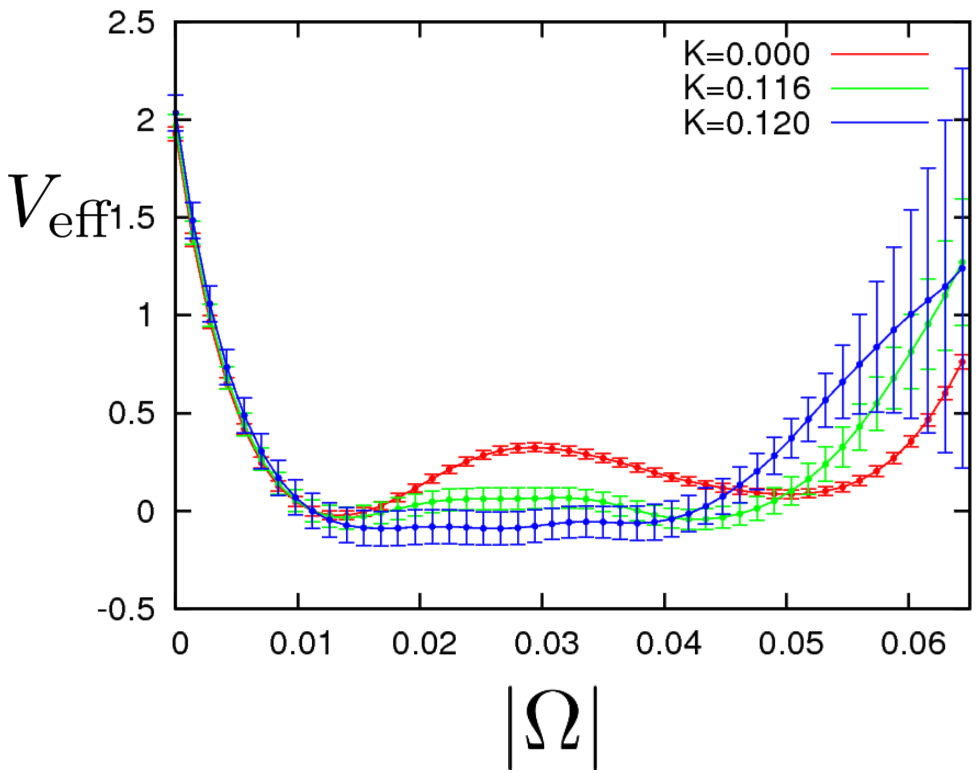
Lattice	Configurations
24^3x6	676,190
32^3x6	1,172,000
24^3x8	342,821

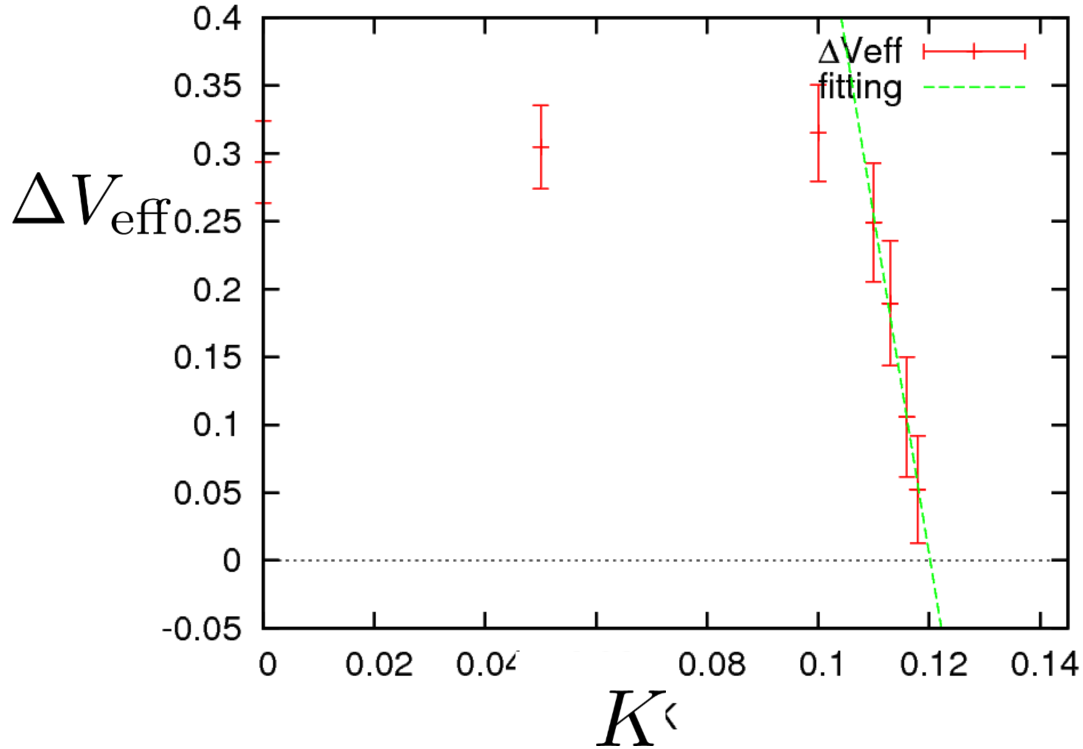
Determination of K_c (Next to leading order calculation)

To estimate the truncation error of the hopping parameter, the next to leading contribution is computed.

$N_t = 6$ lattice (24^3x6)

Effective potential





K_{ct}=0.1202(19)

Lattice	Configurations
24^3x6	676,190
32^3x6	1,172,000
24^3x8	342,821

Determination of Critical K for 2-flavor QCD

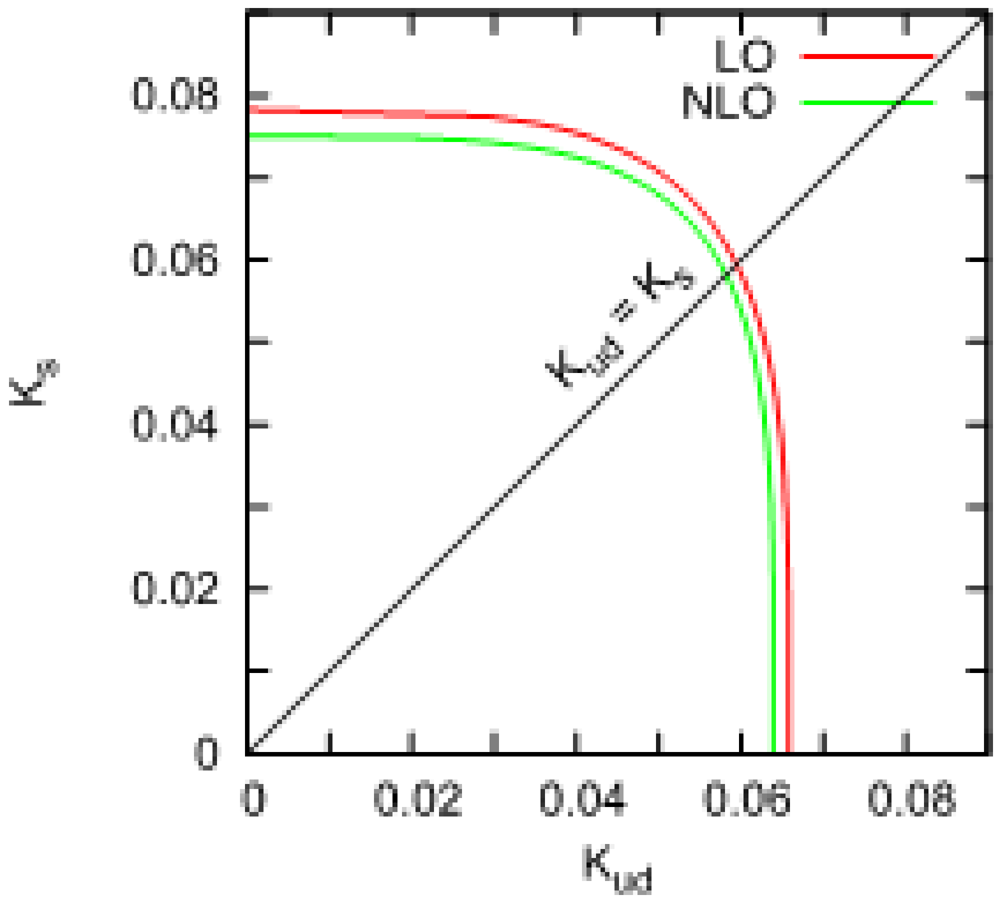
[WHOT-QCD, Phys.Rev.D101,054505(2020)]

	Leading order		Next to leading order	
Lattice	K_{ct}	m_{PS}/T_c	K_{ct}	m_{PS}/T_c
24^3x4	0.0658(10)	15.47(14)	0.0640(10)	15.73(14)
24^3x6	0.1359(30)	7.43(78)	0.1202(19)	11.15(42)
24^3x8	> 0.18			

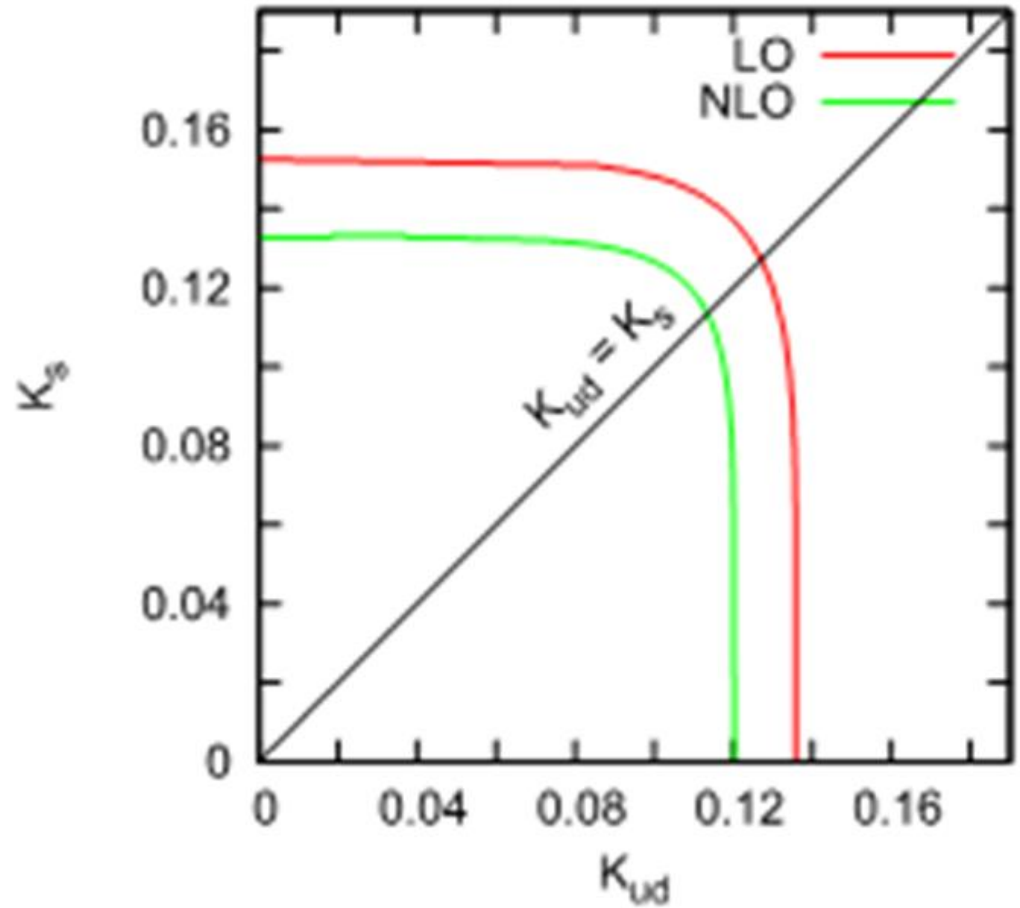
- In the study on a 24^3x4 lattice, the truncation error of the hopping parameter expansion is negligible.
- The truncation error is visible for the 24^3x6 lattice.
- Pseudo-scalar meson mass m_{PS} measured by T=0 full QCD simulations at K_c for N_t=6 is smaller than that for N_t=4.

Determination of Kc in 2+1 flavor QCD

24^{3}x4 lattice



24^{3}x6 lattice



LO: leading order NLO: next to leading order

- Difference between the leading order and next to leading calculations are sizeable for the 24^{3}x6 lattice.

Truncation error of hopping parameter expansion

$$\ln \det M\,(K) = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \ln \det M}{\partial K^n} K^n \equiv N_{\rm site} \sum_{n=1}^{\infty} D_n\, K^n$$

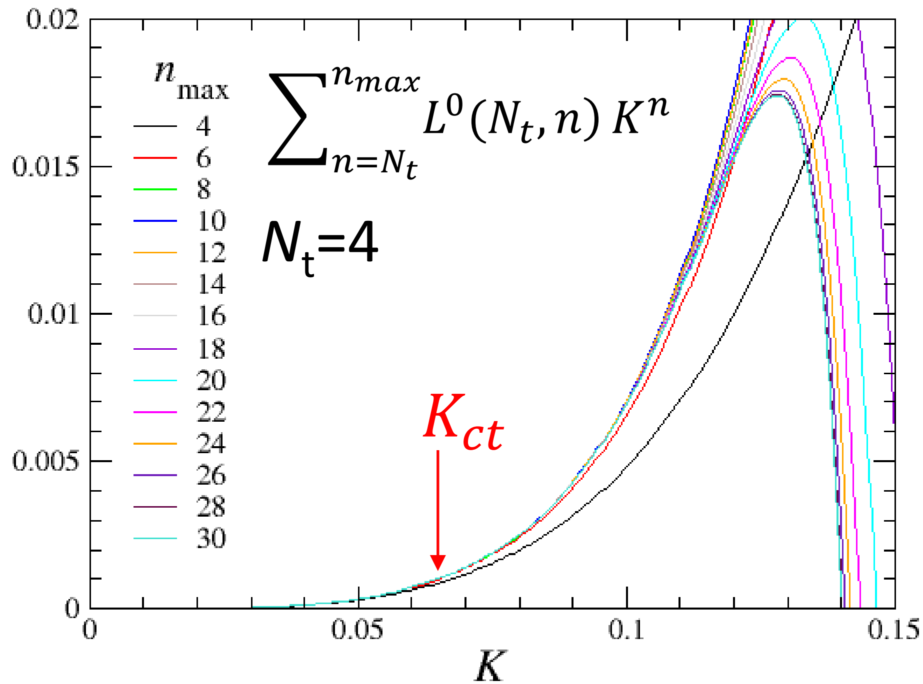
$$D_n = \frac{1}{N_{\rm site}} \frac{(-1)^{n-1}}{n} \operatorname{tr}\left[\left(\frac{\partial M}{\partial K}\right)^n\right] = W(n) + L(N_t, n)$$

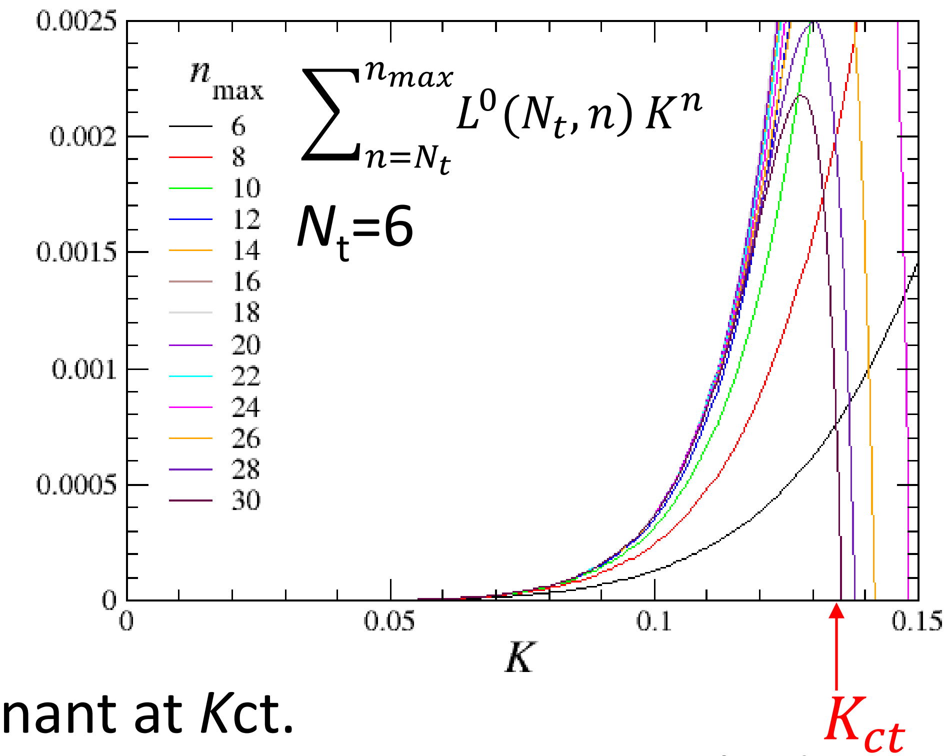
Wilson loop type

Polyakov loop type
Closed by the boundary condition

The case of all $U_\mu(x) = 1$. Then, all Polyakov loops are 1.

Because it is uniform in space-time, it is enough to calculate one diagonal element.





leading order

- *Nt*=4: The leading order term is dominant at *K*ct.
- *Nt*=6: Higher order terms are large at *K*ct.

Effective critical K

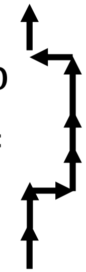
Leading order term

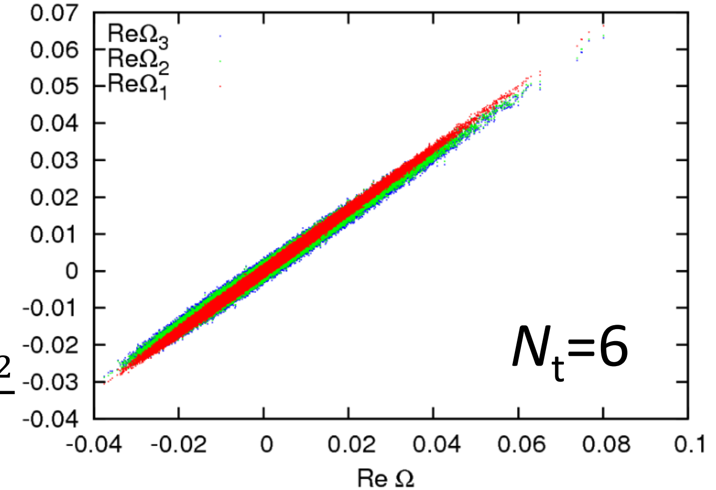
$$L(N_t,N_t)=L^0(N_t,N_t)\,\mathrm{Re}\,\Omega=\frac{12\times 2^{N_t}}{N_t}\mathrm{Re}\,\Omega$$

Next to leading order term

$$L(N_t,N_t+2)=L^0(N_t,N_t+2)\,\frac{2\mathrm{Re}\,\Omega_1+\cdots+2\mathrm{Re}\,\Omega_{N_t/2-1}+\mathrm{Re}\Omega_{N_t/2}}{N_t-1}$$

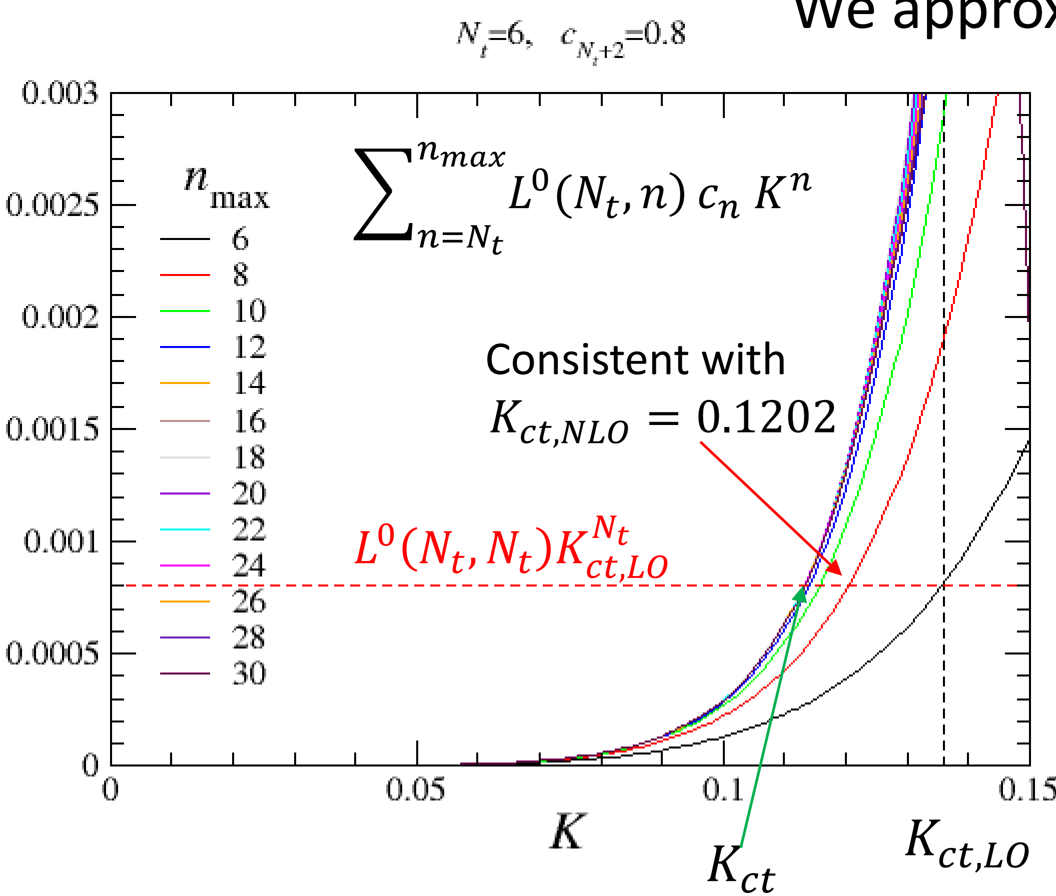
Bent Polyakov loop

$\Omega_3=$ 



Polyakov loop

- Polyakov loop and bent Polyakov loops are strongly correlated.



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

$$c_{N_t}=1,\quad c_{N_t+2}=0.813(3)$$

Well approximated by $c_{N_t+2n}\approx(0.8)^n$

$$\ln\det M(K)/N_{\rm site}-(\text{Wilson loops})=$$

$$\sum_{n=N_t}^{n_{max}} L(N_t,n)\,K^n=\mathrm{Re}\,\Omega\sum_{n=N_t}^{n_{max}} L^0(N_t,n)\,c_nK^n$$

Only one parameter

Solving the equation,

$$\boxed{\sum_{n=N_t}^{n_{max}} L^0(N_t,n)\,c_nK_{ct}^n=L^0(N_t,N_t)K_{ct,LO}^{N_t}}$$

Truncation error can be removed.

Finite-size scaling analysis for K_{ct} determination

- Binder cumulant is computed at Tc to determine the critical point.
- Universality class is discussed.

Volume dependence of Critical K determined by histogram method

[WHOT-QCD, Phys.Rev.D101,054505(2020)]

Lattice	K_{ct}
24^3x6	0.1359(30)
32^3x6	0.1286(40)
36^3x6	[overlap problem]

- K_c becomes smaller as the volume increases.
- 36^3x6 lattice: overlap problem arises before K_{ct}.
- Reweighting form quenched simulation dose not work for large volume.

  → Simulations with a Polyakov loop term.

Simulations with the Polyakov loop term Ω

[Kiyohara et al., arXiv:2108.0018]

- Simulations with an effective action

$$S_{\mathrm{eff}} = -6N_s^3\beta P + N_s^3\lambda \mathrm{Re}\Omega$$

  - The Polyakov loop term corresponds to the leading order contribution of the hopping parameter expansion of ln det M.

$$\lambda = 384\ K^4 \quad \text{(for 2-flavor, } N\text{t=4)}$$

- Heat bath algorithm is applicable. → small computational cost.
- Overlap problem can be avoided.
- We include the next to leading contribution of the hopping parameter expansion by the reweighting.
- Nt=4: Large volume is more important than small lattice spacing.
  - Truncation error of hopping parameter expansion: small
- Lattice size: Nt=4, Ns=24, 32, 36, 40, 48 $\quad V = (N_s a)^3 = \left(\frac{N_s}{N_t}\right)^3 \frac{1}{T_c^3}$
- High statistics: 6×10^5 measurements for each parameter

Binder cumulant

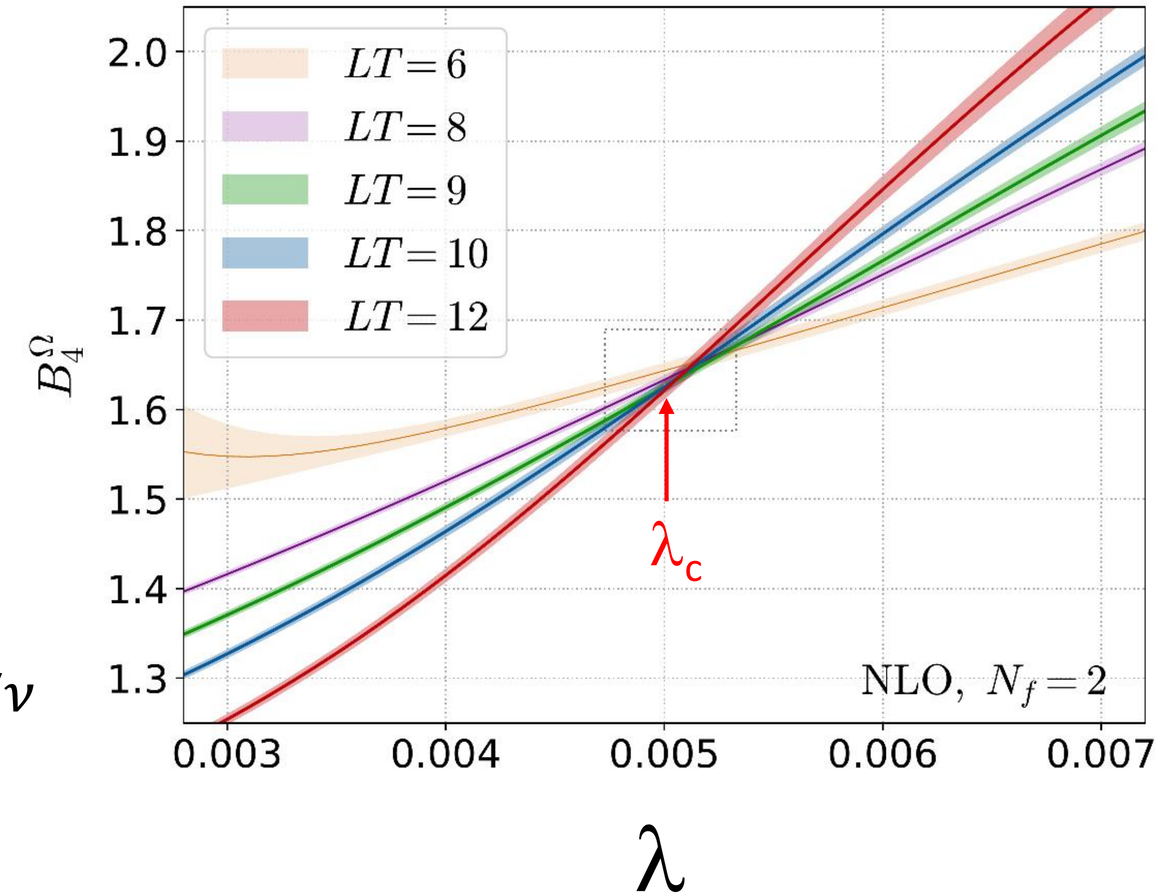
$$B_4 = \frac{\langle(\Omega - \langle\Omega\rangle)^4\rangle}{\langle(\Omega - \langle\Omega\rangle)^2\rangle^2}$$

- No volume dependence at the critical point λ_c
- 3D Ising universality class: B_4=1.604 at λ_c and ν=0.63.
- Results of $N_t = 4, N_f = 2$
- Intersect around $B_4 \approx 1.6$
- Fit the data by

  $$B_4 = B_c + c(\lambda - \lambda_c)(LT)^{1/\nu}$$

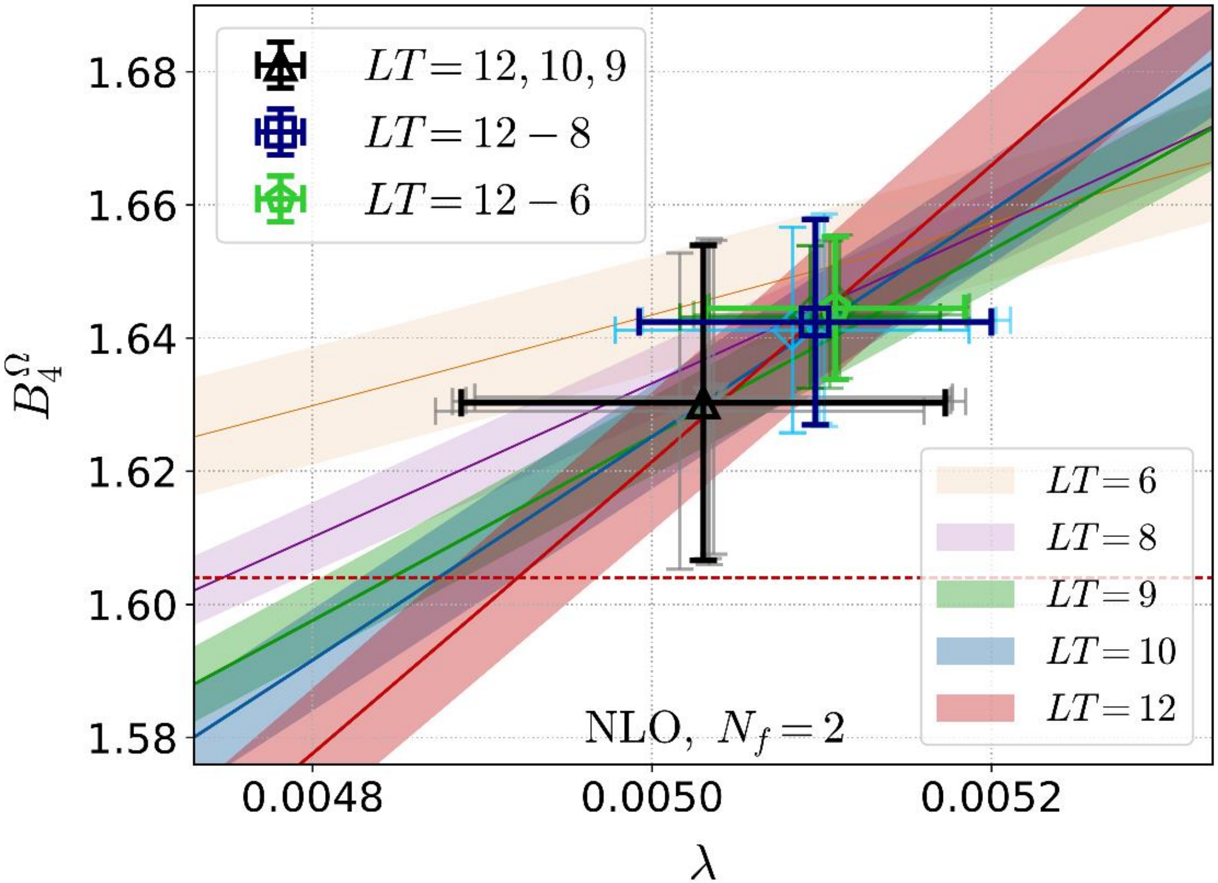
  - 4 fit parameters

$$LT = N_s/N_t$$



[Kiyohara et al., arXiv:2108.0018]

Critical point and Z(2) Universality class



- No volume dependence at the critical point λ_c
- 3D Z(2) universality class: B_4=1.604 at λ_c and ν=0.63.
- Consistent with 3D Ising universality.
- λ_c=0.00503 → K_c=0.0602(4) is smaller than the result by the histogram method: 0.0640(10)

(NLO, 24^3x4 lattice)

Fit result $N_t = 4$

$$B_4 = B_c + c(\lambda - \lambda_c)(LT)^{1/\nu}$$

N_s/N_t =6, 8, 9, 10, 12

- λ_c=0.00511(8)(2)
- B_{cp}=1.645(11)(2)
- ν=0.593(18)(3)

N_s/N_t =8, 9, 10, 12

- λ_{cp}=0.00510(10)(2)
- B_{cp}=1.643(15)(2)
- ν=0.614(29)(3)

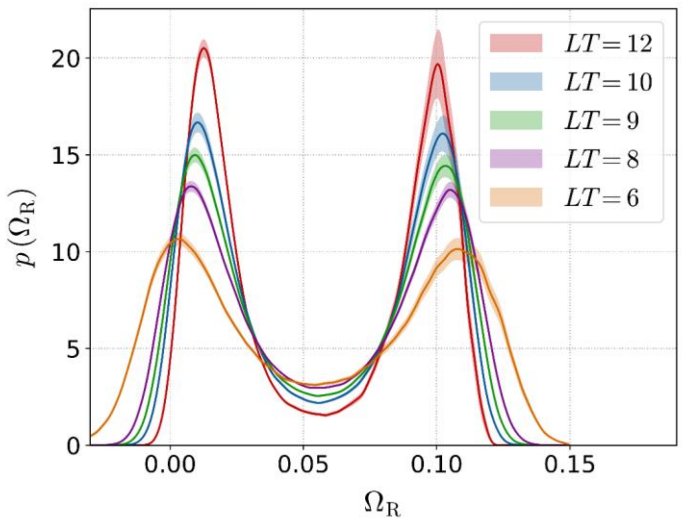
Final result

N_s/N_t=9, 10, 12

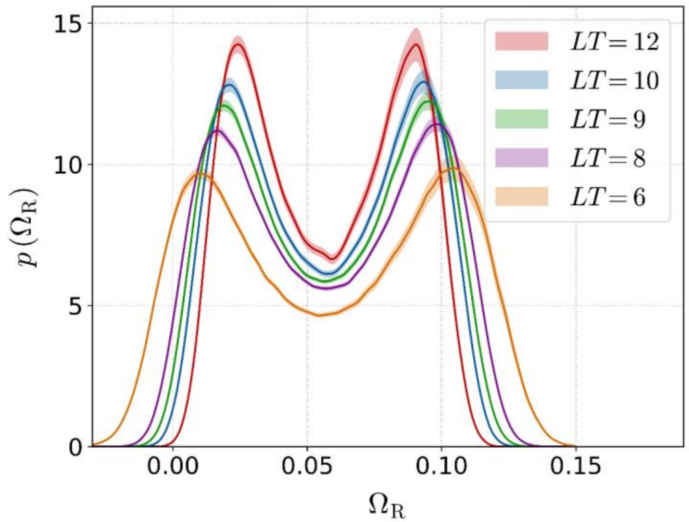
- λ_{cp}=0.00503(14)(2)
- B_{cp}=1.630(24)(2)
- ν=0.614(48)(3)

Volume dependence of the histogram

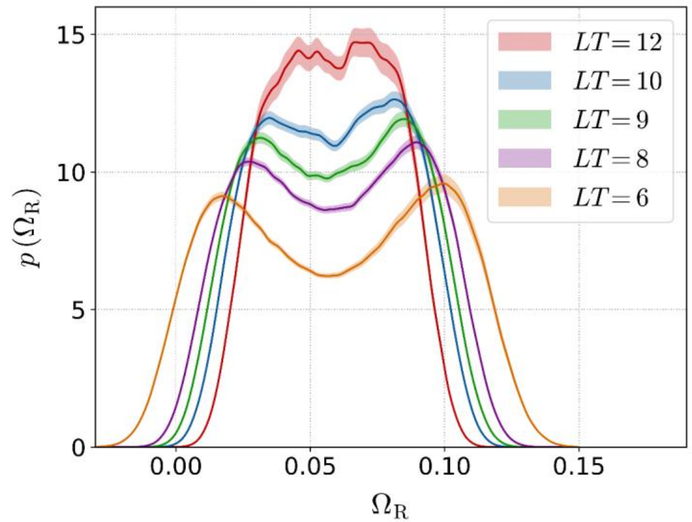
λ=0.003



λ=0.005



λ=0.007



λ_c=0.00503(14)(2)

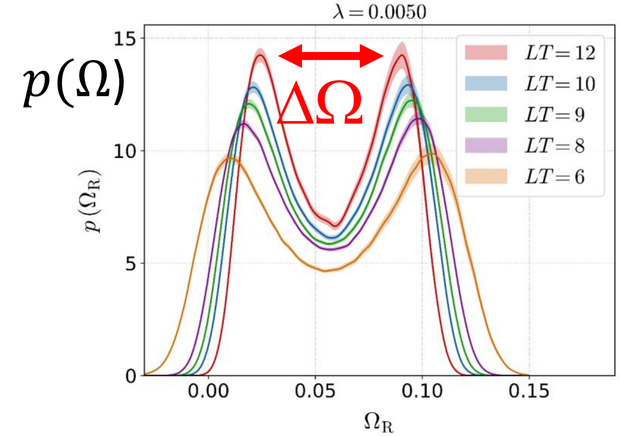
- $\lambda<\lambda_c$, The middle dent in the histogram gets deeper as the volume increases. (first order)
- $\lambda>\lambda_c$, the middle dent becomes shallower and disappears. (crossover)
- λ_c is the boundary that divides one peak or two peaks in the volume infinity limit.

Finite volume Scaling of the gap

- Assuming the gap $\Delta\Omega$ corresponds to (magnetization)/(volume) of 3D ising,

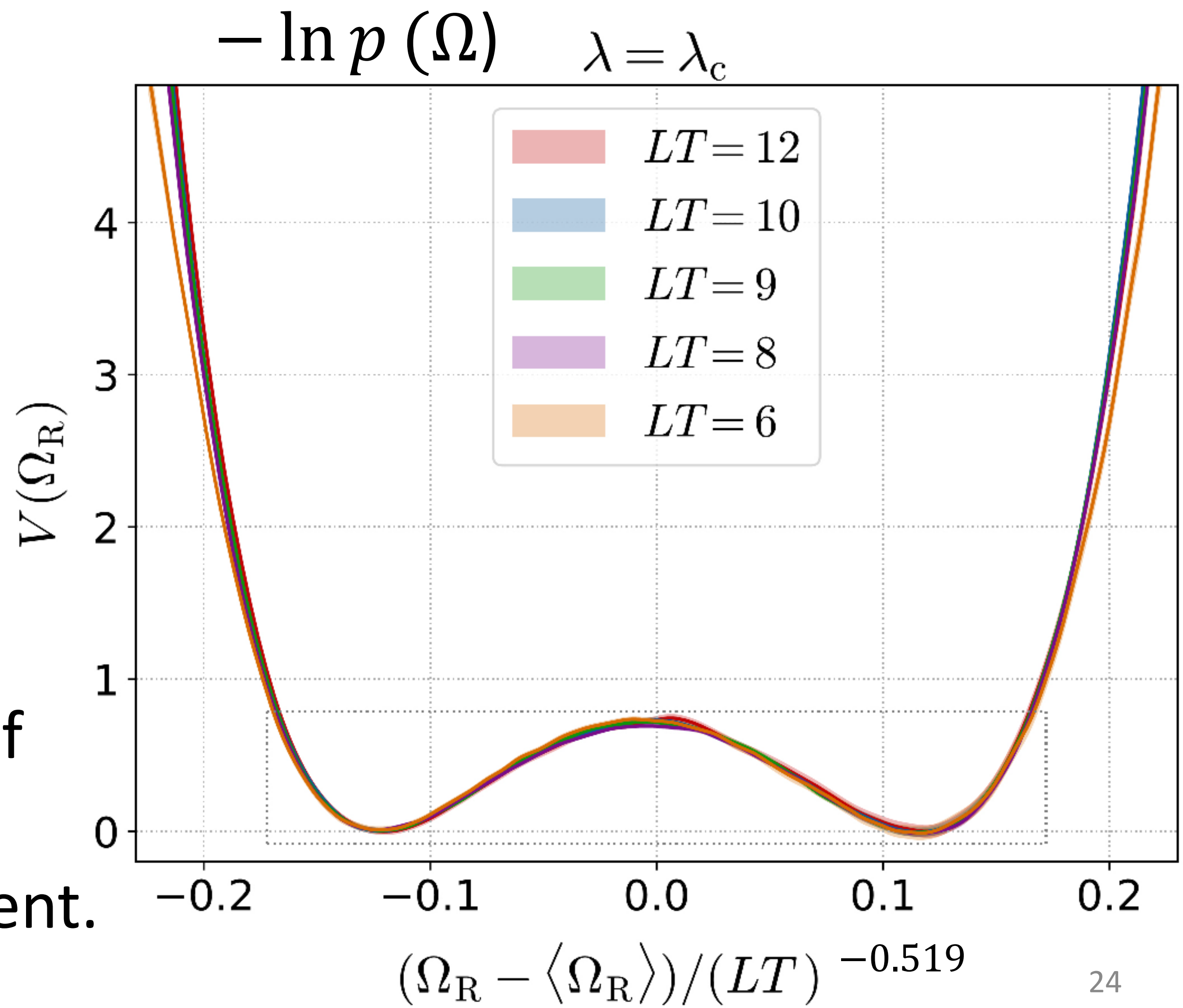
$$\Delta\Omega \ \propto LT^{-0.519}$$

is expected at λ_c.



In the limit $LT \to \infty$,
$\Delta\Omega$ vanises.
Single well in the volume infinity limit.

If we find the critical point from the shape of the histogram, Kc is highly volume-dependent.



Summary and out look

- Latent heat at first order transition were computed using small flow time expansion method based on Gradient flow.
  - We compared the results with those by the derivative method.
- We studied the location of critical point at which the first order phase transition changes to crossover in the heavy quark region by investigating the histogram of the Polyakov loop and applying the finite-size scaling analysis.
  - simulations of quenched QCD or quench + Polyakov loop term
  - reweighting method
  - quark determinant: hopping parameter expansion
  - Scaling behavior at λ_c is consistent with 3D ising model.
- Truncation error of the hopping parameter expansion: Method to remove the truncation error: proposed.
- If we try to find the critical point from the shape of the histogram, error due to finite volume effect is large.
- Study of the critical point on fine lattices is important.