Study of QCD critical point using canonical ensemble method

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χQCD collaboration:
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Outline

Motivation
- QCD phase diagrams

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- QCD phase diagrams

Canonical ensemble
- Lattice formulation of QCD thermodynamics
- Canonical partition function
- Simulation details
- Projected determinant

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Results
- 2 and 4 flavors
- 3 flavors

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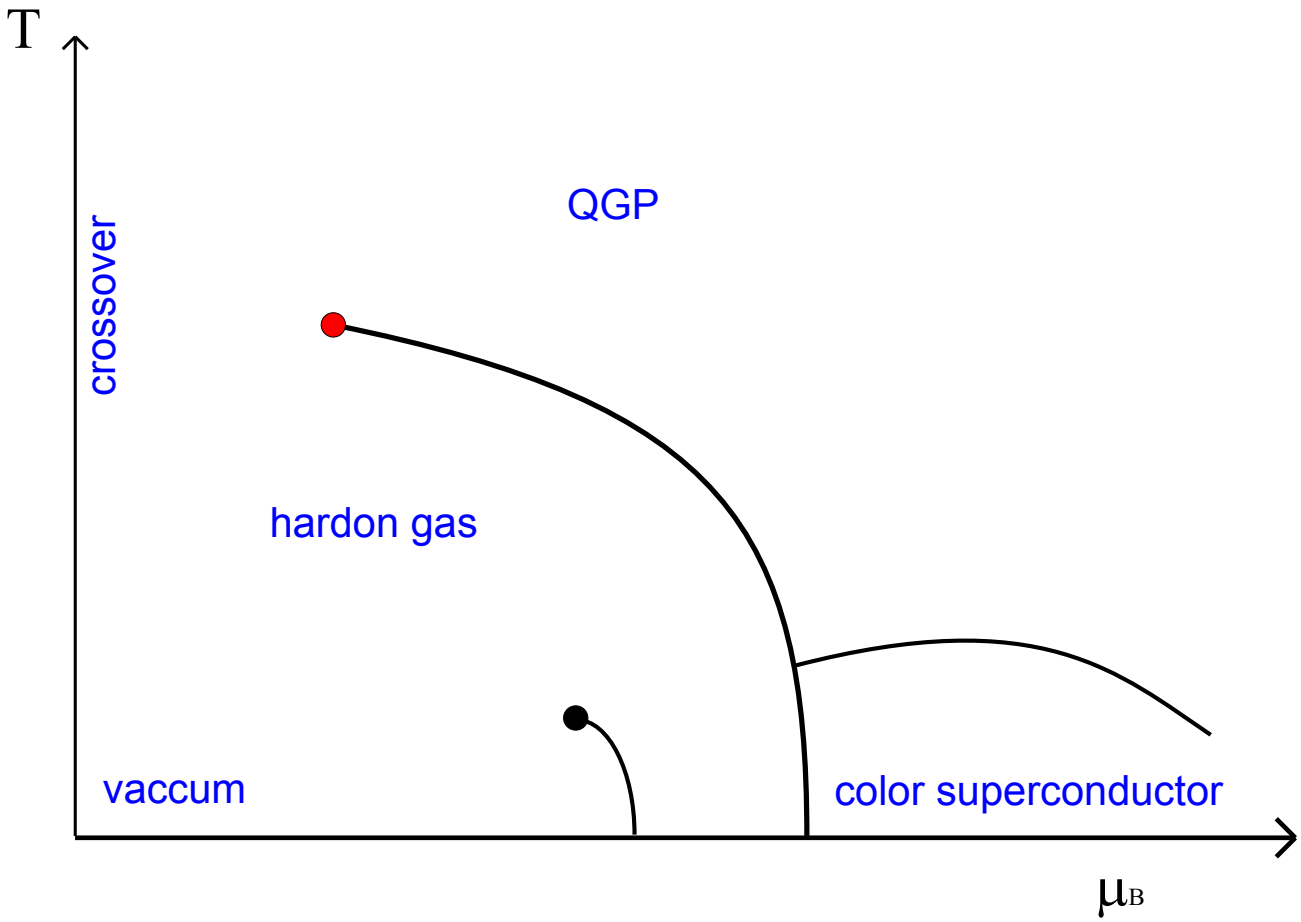
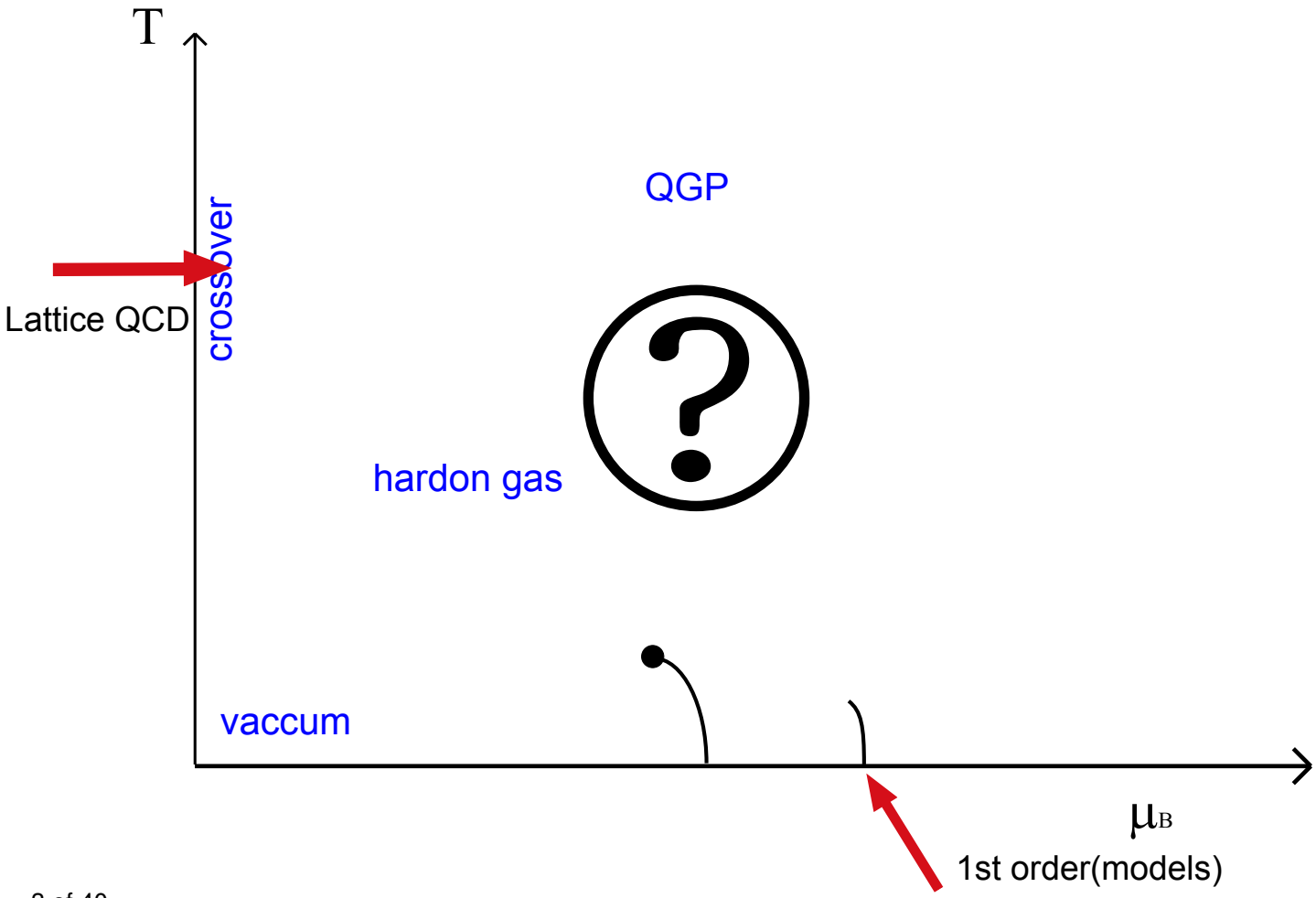
Summary

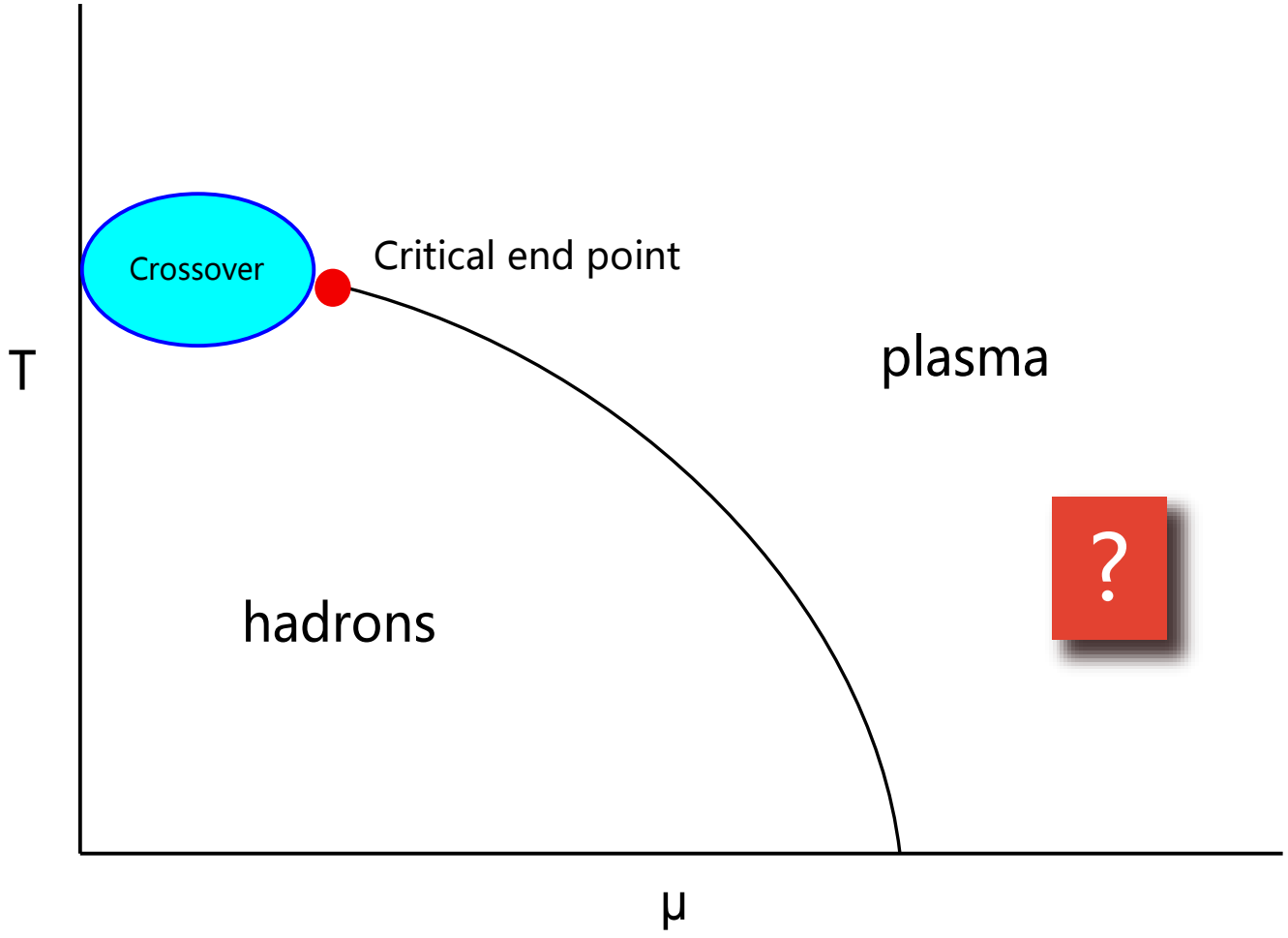
Phase diagram



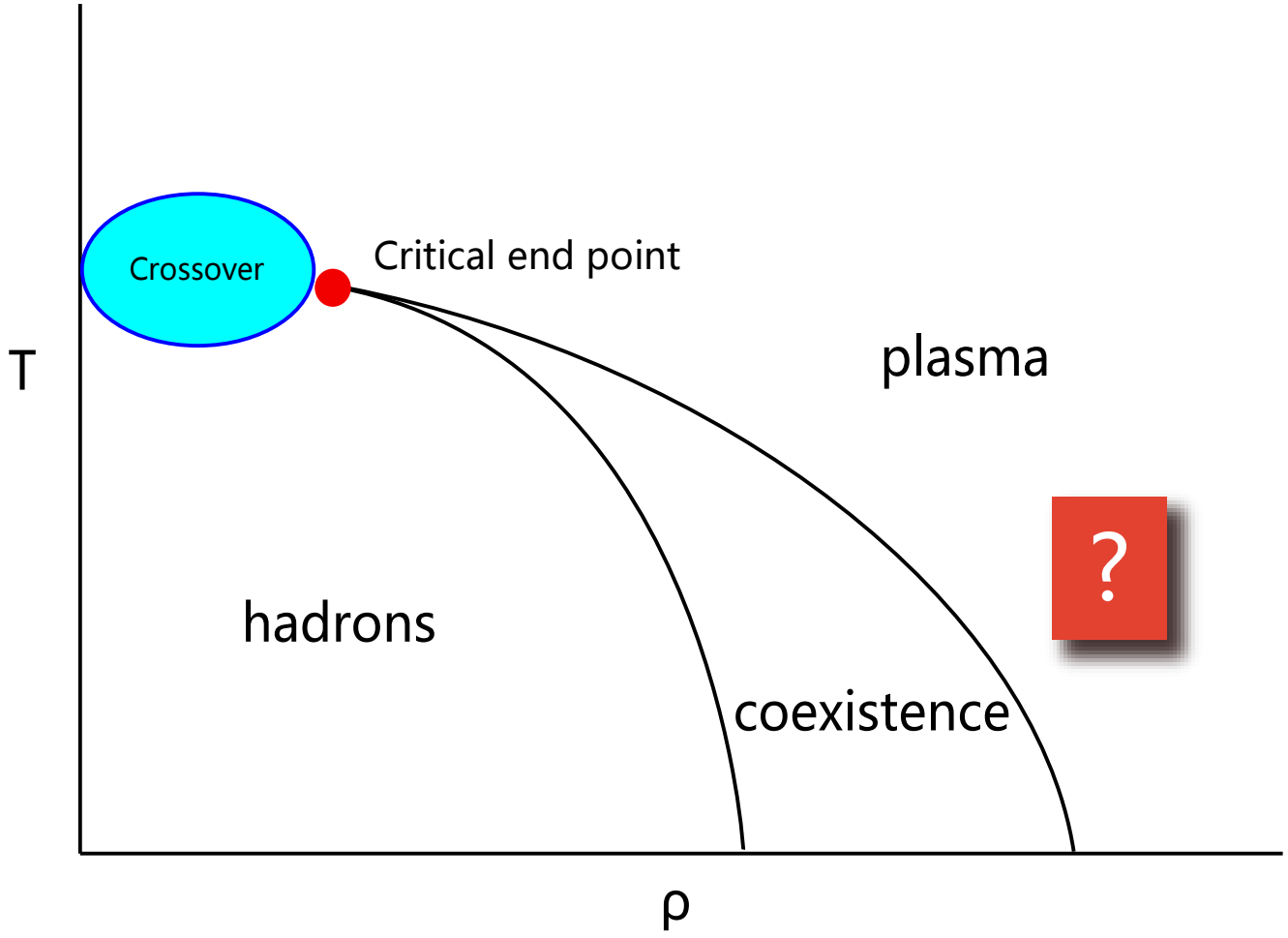
Phase diagram



Phase diagram @ GCE



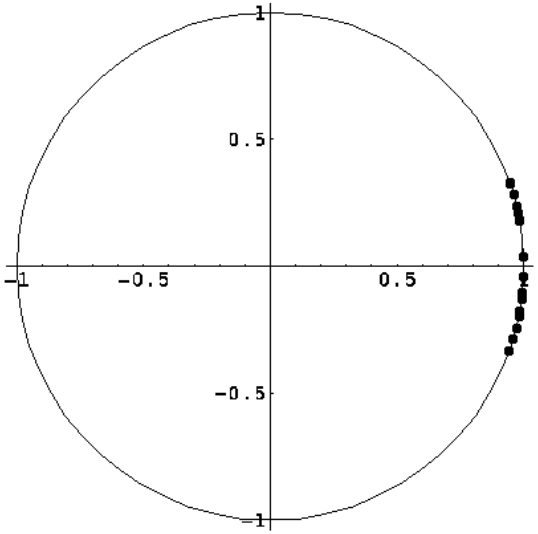
Phase diagram @ CE

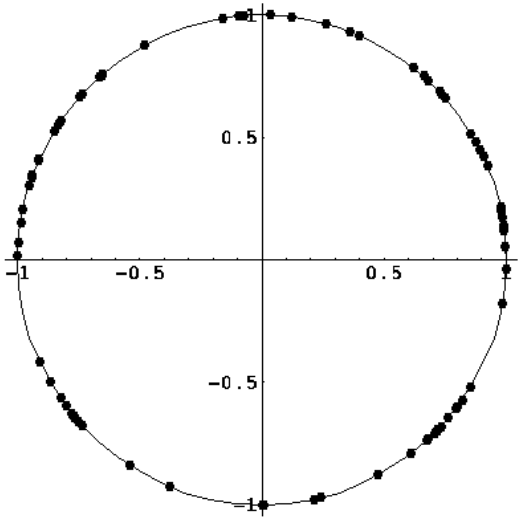


Sign problem

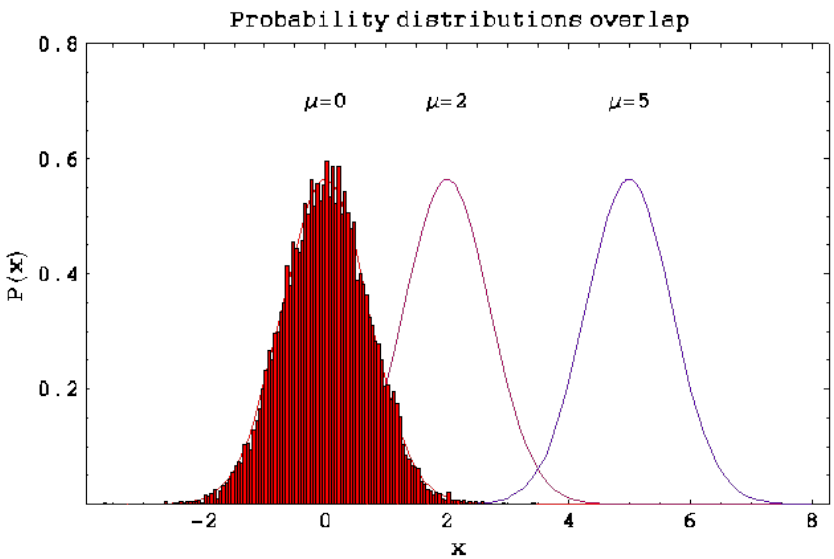
$$Z_{\mathrm{GC}}(V,T,\mu) = \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} |\mathrm{det}M^2(\mu;U)| \frac{\mathrm{det}M^2(\mu;U)}{|\mathrm{det}M^2(\mu;U)|}$$

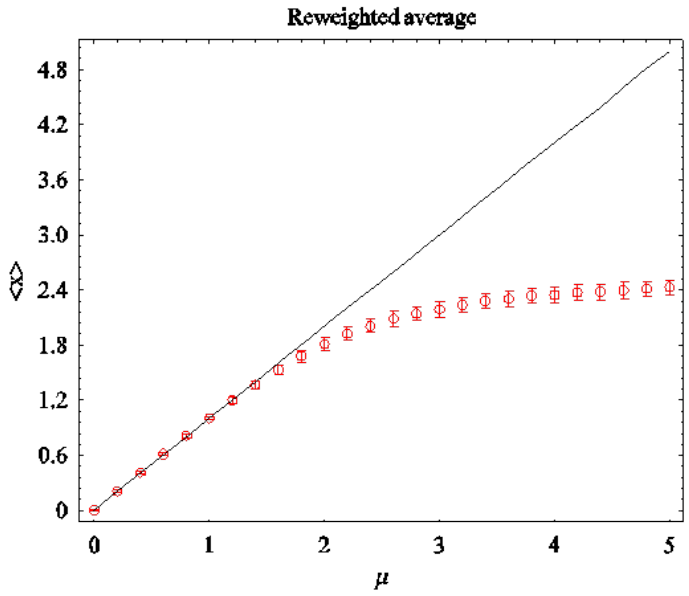
$$\langle O(U)\rangle = \frac{\langle O(U)e^{i\phi(U)}\rangle_0}{\langle e^{i\phi(U)}\rangle_0} \qquad e^{i\phi(U)} = \frac{\mathrm{det}M^2(\mu;U)}{|\mathrm{det}M^2(\mu;U)|}$$





Overlap problem





$$P(\mu;x) = \frac{1}{\sqrt{\pi}} e^{-(x-\mu)^2}$$

$$\langle x \rangle_\mu = \frac{\left\langle x \frac{P(\mu;x)}{P(0;x)} \right\rangle_0}{\left\langle \frac{P(\mu;x)}{P(0;x)} \right\rangle_0}$$

Formulation I

Use the fugacity expansion

$$Z_{\mathsf{GC}}(V,\mu,T) = \sum_{n=-4V}^{n=4V} Z_C(V,k,T)e^{\mu k/T}$$

we get

$$Z_C(V,T,k) = \frac{1}{2\pi}\int_0^{2\pi} \mathsf{d}\phi\, e^{-ik\phi} Z_{\mathsf{GC}}(V,T,\mu)|_{\mu=i\phi T}$$

Formulation II

Definition

$$\mathrm{det}_k M^2(U) \equiv \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\phi\, e^{-ik\phi}\, \det M^2(m,\mu;U)|_{\mu=i\phi T}$$

$$Z_C(V,T,k) \equiv \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \mathrm{det}_k M^2(U)$$

Formulation II

Definition

$$\det{}_k M^2(U) \equiv \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\phi\, e^{-ik\phi} \det M^2(m,\mu;U)|_{\mu=i\phi T}$$

$$Z_C(V,T,k) \equiv \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \det{}_k M^2(U)$$

Charge conjugation symmetry

$$Z_C(V,T,k) = Z_C(V,T,-k)$$

$$\langle \det{}_k M^2(U)\rangle = \langle \mathrm{Re}\det{}_k M^2(U)\rangle$$

$$Z_C(V,T,k) = \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)}\, \mathrm{Re}\det{}_k M^2(U)$$

Dynamical simulation

Canonical partition function

$$Z_C(V,T,k) = \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \mathrm{det}_k M^2(U) =$$

$$\underbrace{\int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \mathrm{det} M^2(U)}_{\text{Standard HMC}} \underbrace{\frac{|\mathrm{Re}\,\mathrm{det}_k M^2(U)|}{\mathrm{det} M^2(U)}}_{\text{Accept/Reject}} \underbrace{\frac{\mathrm{det}_k M^2(U)}{|\,\mathrm{Re}\,\mathrm{det}_k M^2(U)|}}_{\text{Phase}}$$

Dynamical simulation

Canonical partition function

$$Z_C(V,T,k) = \int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \det{}_k M^2(U) =$$

$$\underbrace{\int \mathcal{D}\mathrm{U}\, e^{-S_g(U)} \det M^2(U)}_{\text{Standard HMC}} \underbrace{\frac{|\mathrm{Re}\det{}_k M^2(U)|}{\det M^2(U)}}_{\text{Accept/Reject}} \underbrace{\frac{\det{}_k M^2(U)}{|\mathrm{Re}\det{}_k M^2(U)|}}_{\text{Phase}}$$

Accept/Reject based on $\frac{|\mathrm{Re}\det{}_k M^2(U)|}{\det M^2(U)}$ is done in the simulation. →

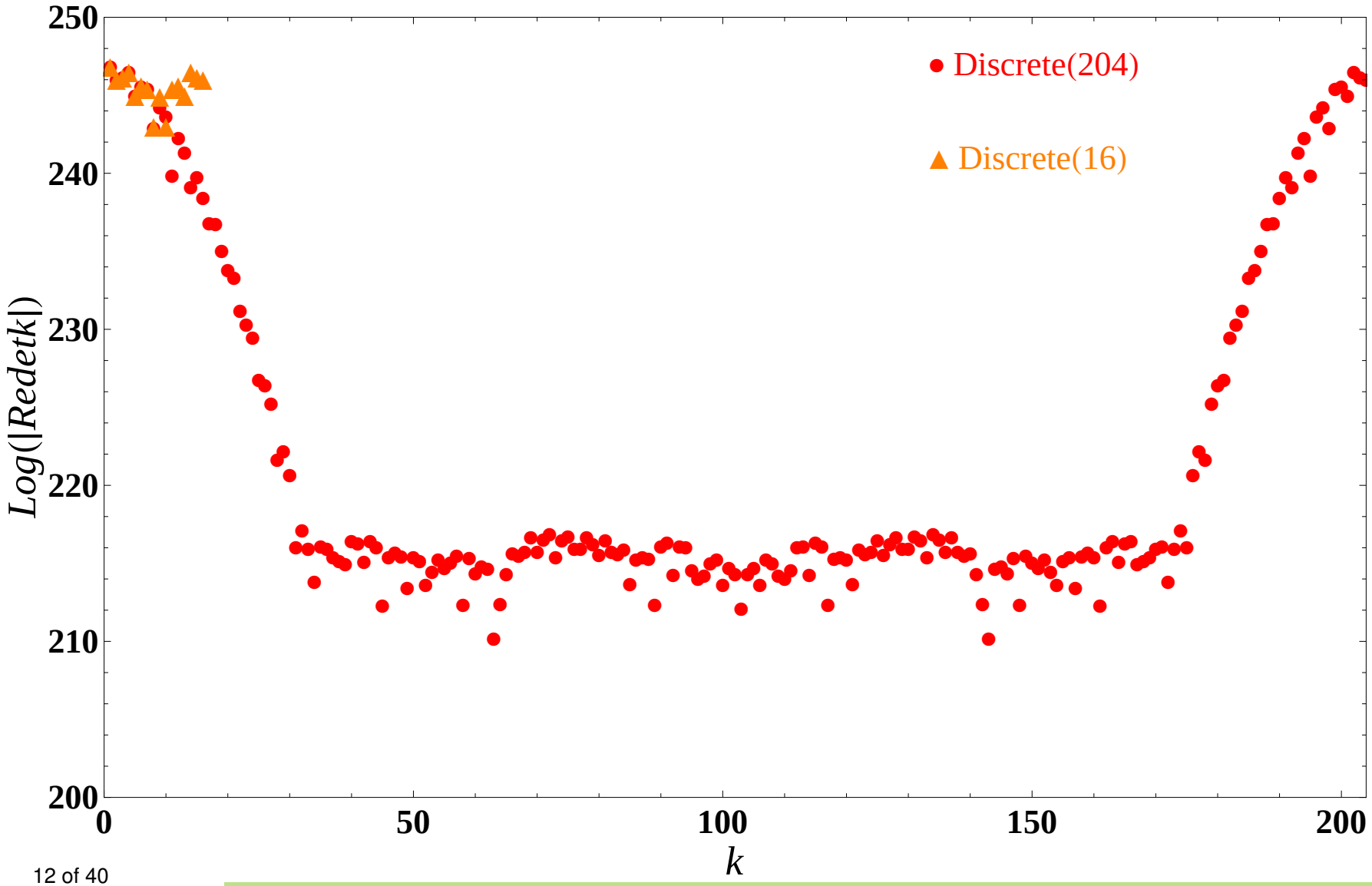
Avoid Overlap Problem ! Reduce determinant fluctuation

Discrete Fourier transform

$$\widetilde{\det}_k M^2[U] = \frac{1}{N}\sum_{j=0}^{N-1} e^{-ik\phi_j} \det M^2[U,\phi_j] \qquad \phi_j = \frac{2\pi j}{N}.$$

Numerically unstable and computationally impossible at larger k!

Winding number expansion



Winding number expansion

$$\det M(U,\phi) = \exp(\mathrm{Tr}\log M(U,\phi))$$

Winding number expansion

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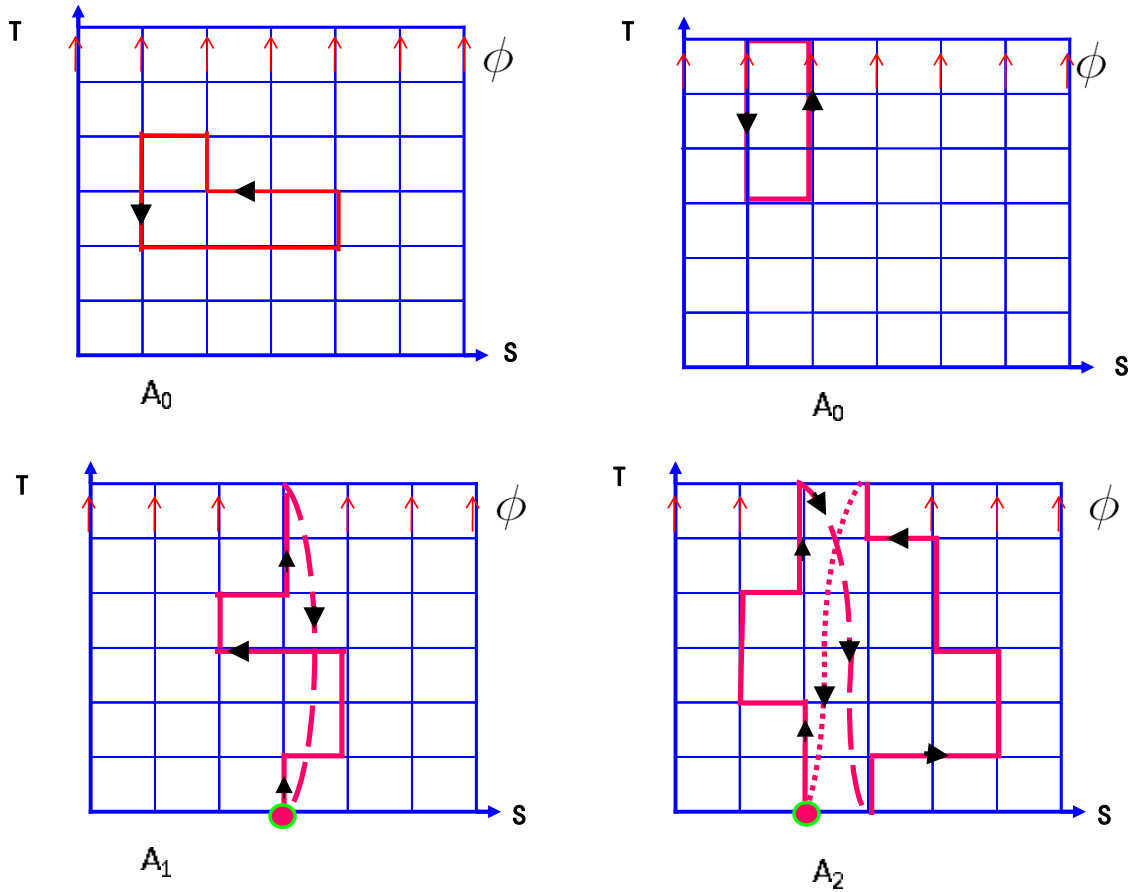
$Tr\log$ → loop → loop expansion



Winding number expansion I

Loop expansion

$$\begin{aligned}\mathrm{Tr}\log M(U,\phi) &= A_0(U) + [\sum_n e^{in\phi} W_n(U) + e^{-in\phi} W_n^\dagger(U)] \\ &= A_0(U) + \sum_n A_n \cos(n\phi + \delta_n),\end{aligned}$$

Winding number expansion I

Loop expansion

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Analytical solution

$$\int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1 \cos(\phi+\delta_1)} = e^{A_0 + ik\delta_1} \mathrm{I}_k(A_1)$$

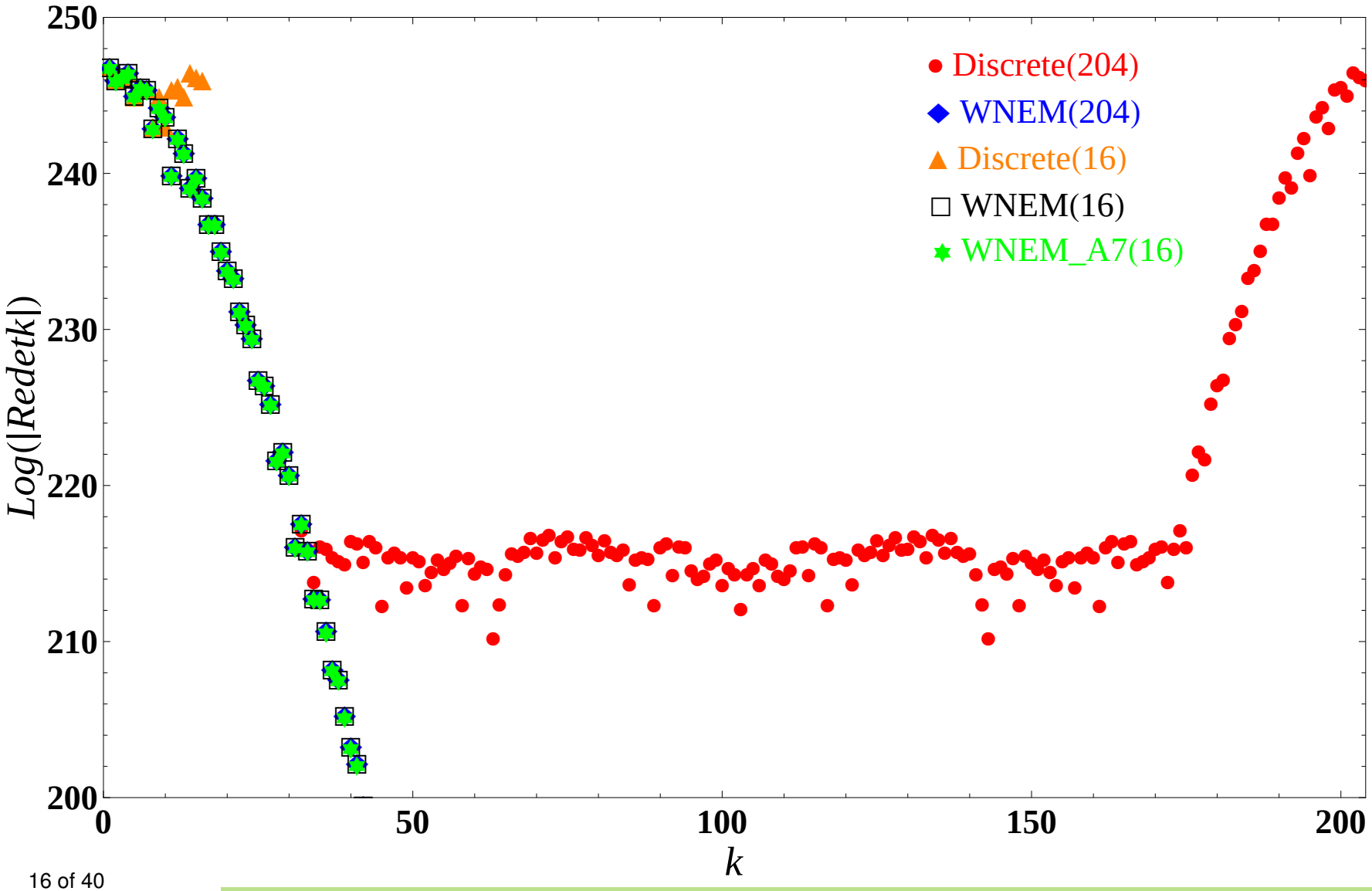
Winding number expansion II

Analytical solution

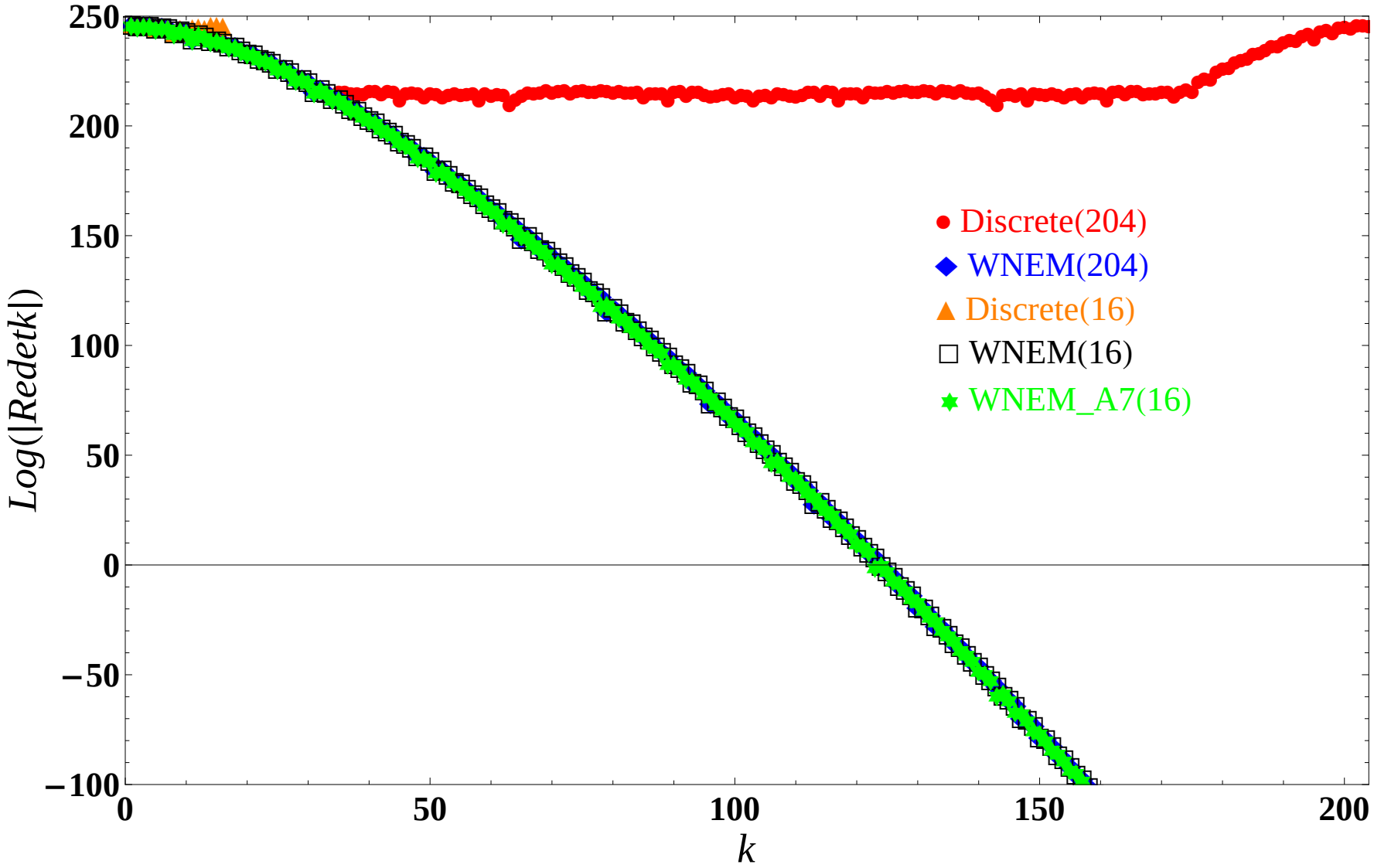
$$
\begin{aligned}
& \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1 \cos(\phi+\delta_1)} e^{A_2 \cos(2\phi+\delta_2) + A_3 \cos(3\phi+\delta_3) + \ldots} \\
= & \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1 \cos(\phi+\delta_1)} (1 + A_2 \cos(2\phi+\delta_2) + \frac{1}{2!} A_2^2 \cos(2\phi+\delta_2)^2 + \ldots) \times \\
& (1 + A_3 \cos(3\phi+\delta_3) + \frac{1}{2!} A_3^2 \cos(3\phi+\delta_3)^2 + \ldots) \times \ldots \\
= & c_{00} \mathrm{I}_k(A_1) + c_{+01} \mathrm{I}_{k+1}(A_1) + c_{-01} \mathrm{I}_{k-1}(A_1) + c_{+02} \mathrm{I}_{k+2}(A_1) + c_{-02} \mathrm{I}_{k-2}(A_1) + \ldots
\end{aligned}
$$

More discussion:
X. Meng, A. Li, A. Alexandru, KF Liu arXiv:0811.2112v2 [hep-lat]
Christof Gattringer, Ludovit Liptak arXiv:0906.1088v1 [hep-lat]

Winding number expansion



Winding number expansion



Measurements

Baryon chemical potential

$$\langle\mu\rangle_{n_B} = \frac{F(n_B+1)-F(n_B)}{(n_B+1)-n_B} = -\frac{1}{\beta}\ln\frac{Z_C(3n_B+3)}{Z_C(3n_B)} = -\frac{1}{\beta}\ln\frac{\langle\gamma(U)\rangle_o}{\langle\alpha(U)\rangle_o}$$

$$\begin{aligned}\alpha(U) &= \frac{\mathrm{Re}\,\det_{3n_B}M^2(U)}{|\mathrm{Re}\,\det_{3n_B}M^2(U)|} \quad \text{and}\\ \gamma(U) &= \frac{\mathrm{Re}\,\det_{3n_B+3}M^2(U)}{|\mathrm{Re}\,\det_{3n_B}M^2(U)|}.\end{aligned}$$

Polyakov loop

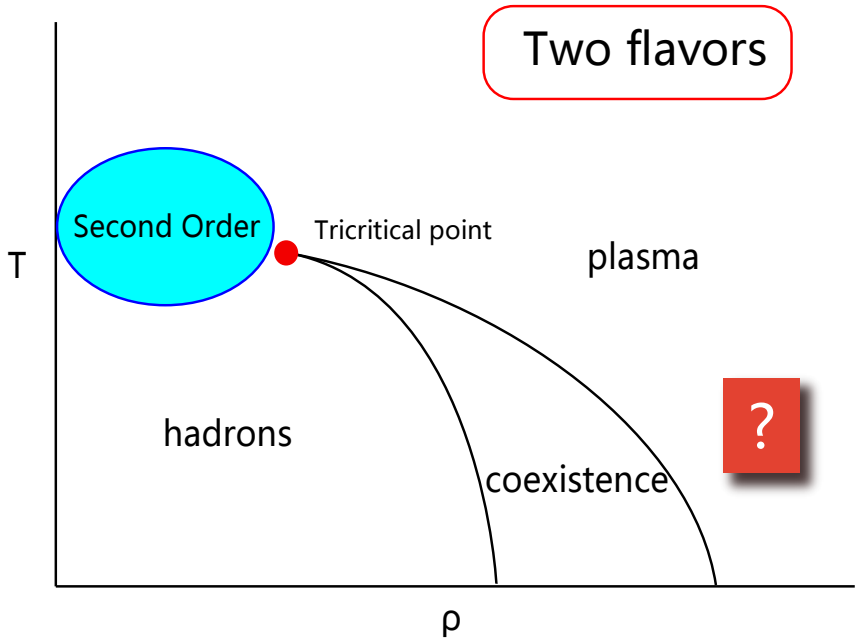
$$\langle|P|\rangle = \frac{\langle|P|\alpha\rangle_0}{\langle\alpha\rangle_0}$$

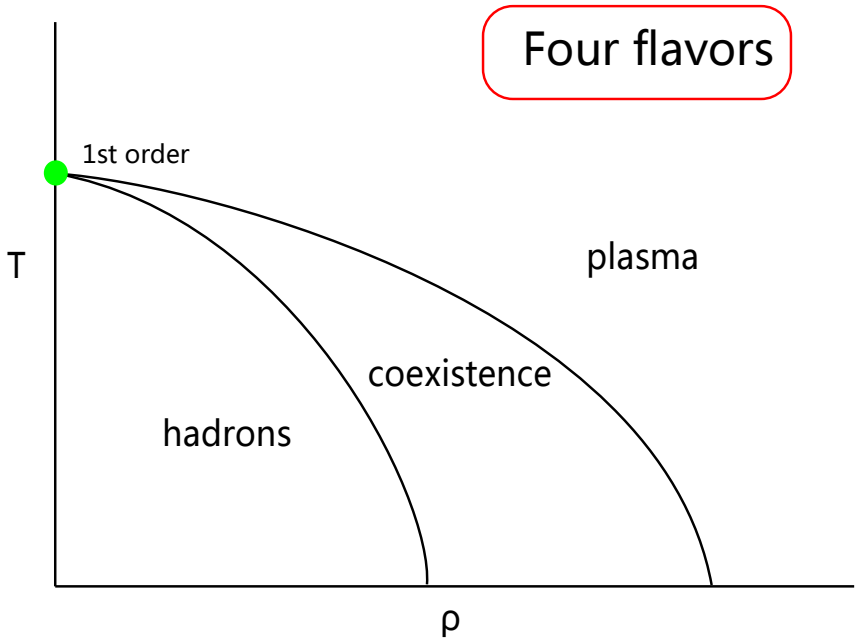
Simulation parameters

Simulation parameters

N_f	lattice size	gauge action	fermion action	m_π
2	$6^3 \times 4$	Iwasaki	Clover	$720(10)$ MeV
4	$6^3 \times 4$	Iwasaki	Clover	$810(20)$ MeV
3	$6^3 \times 4$	Iwasaki	Clover	$730(15)$ MeV

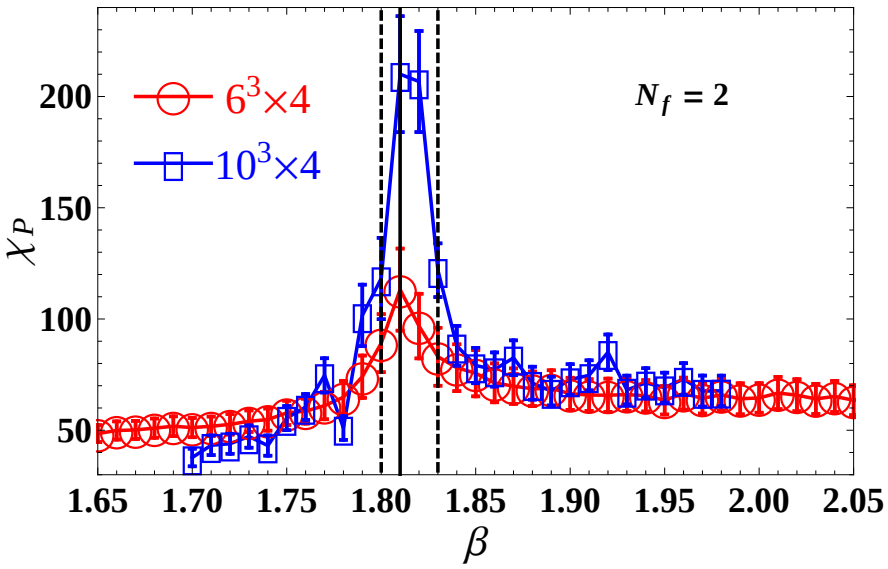
Sketch of phase diagram

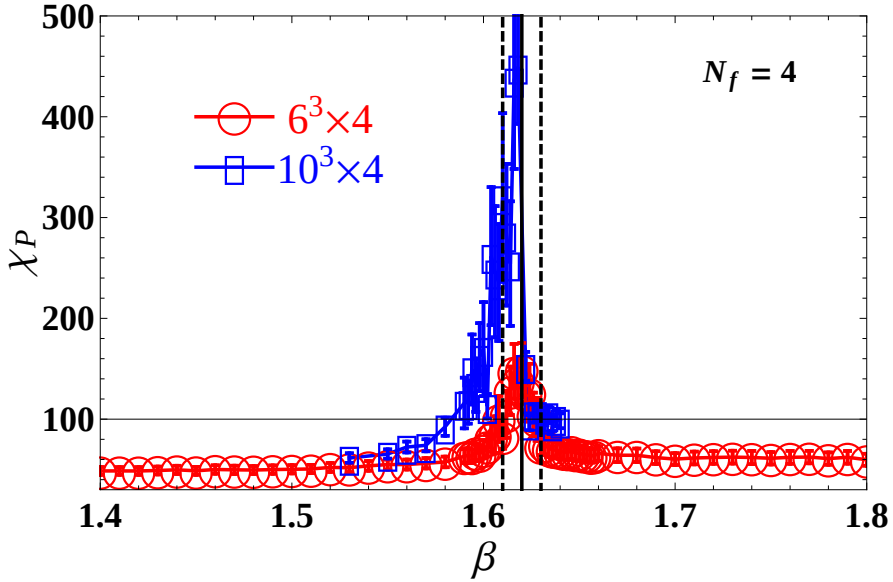




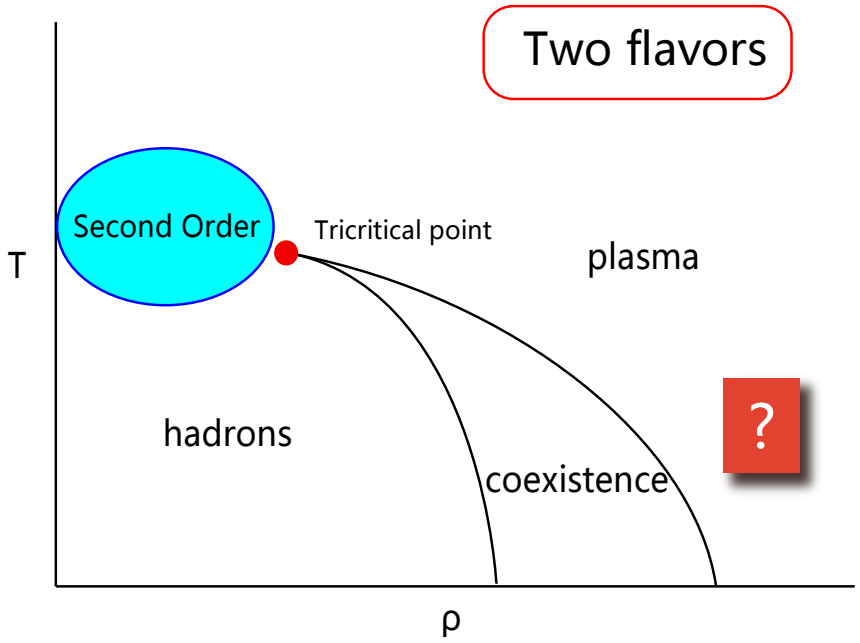
Zero chemical potential phase transition

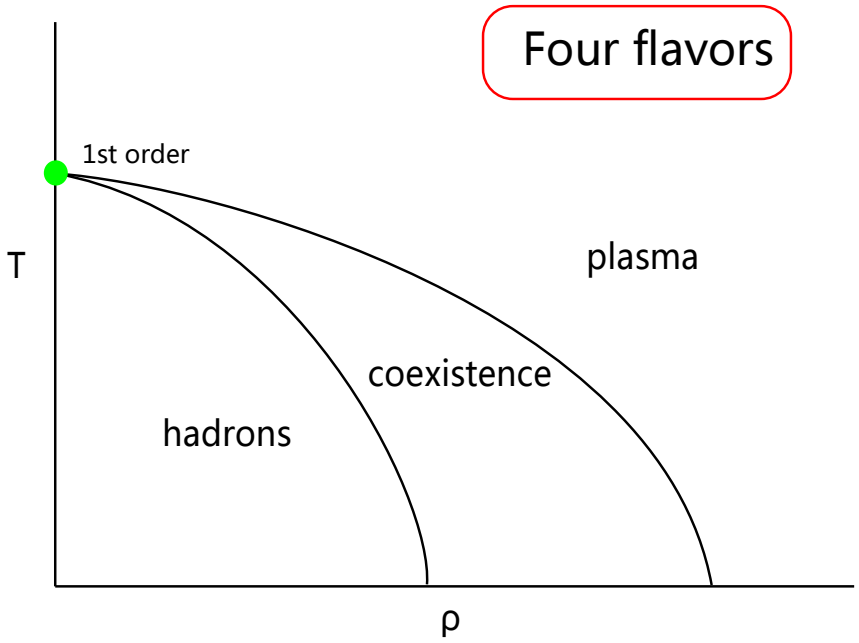
Susceptibility of Polyakov loop



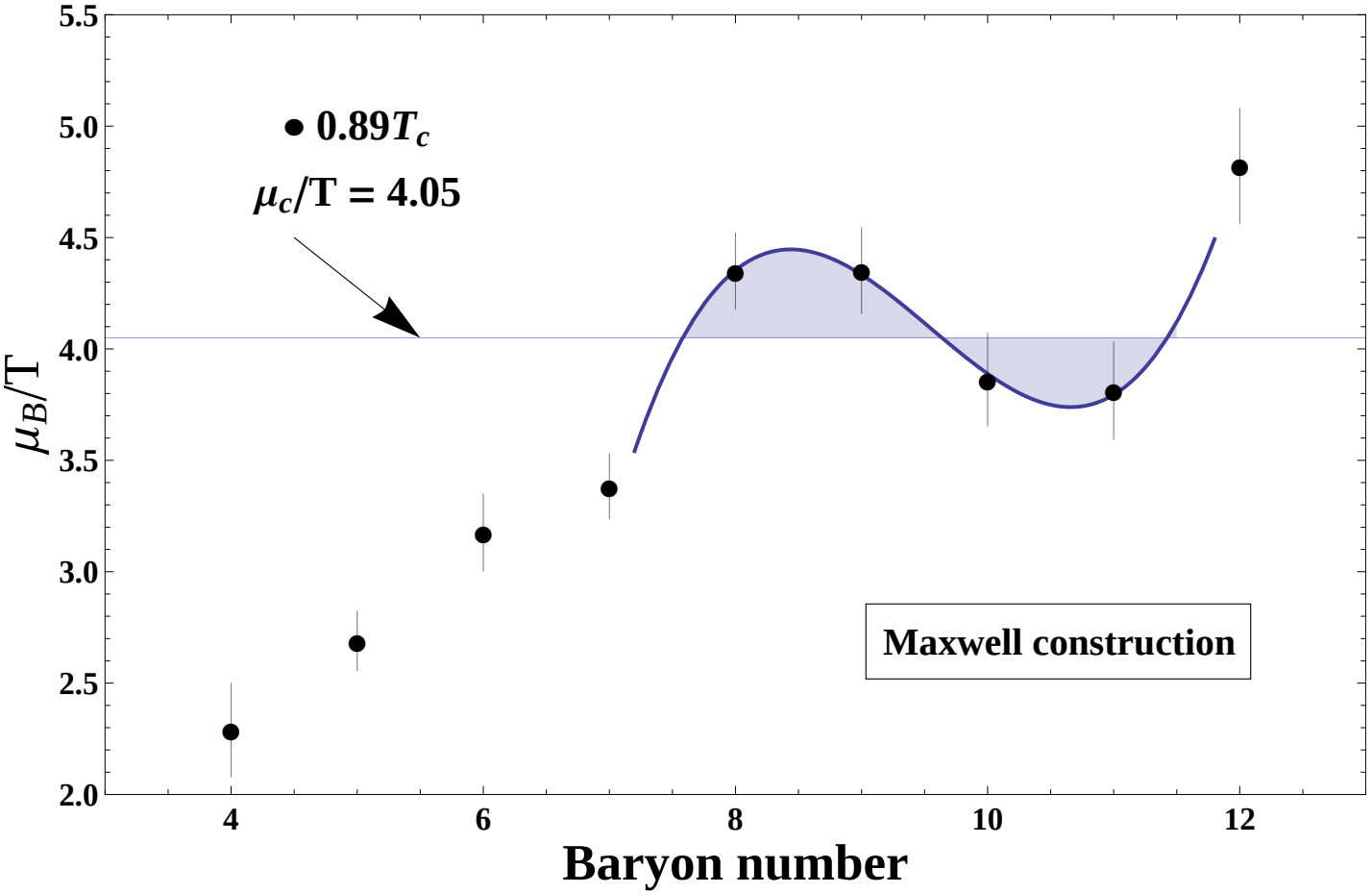


Sketch of phase diagram





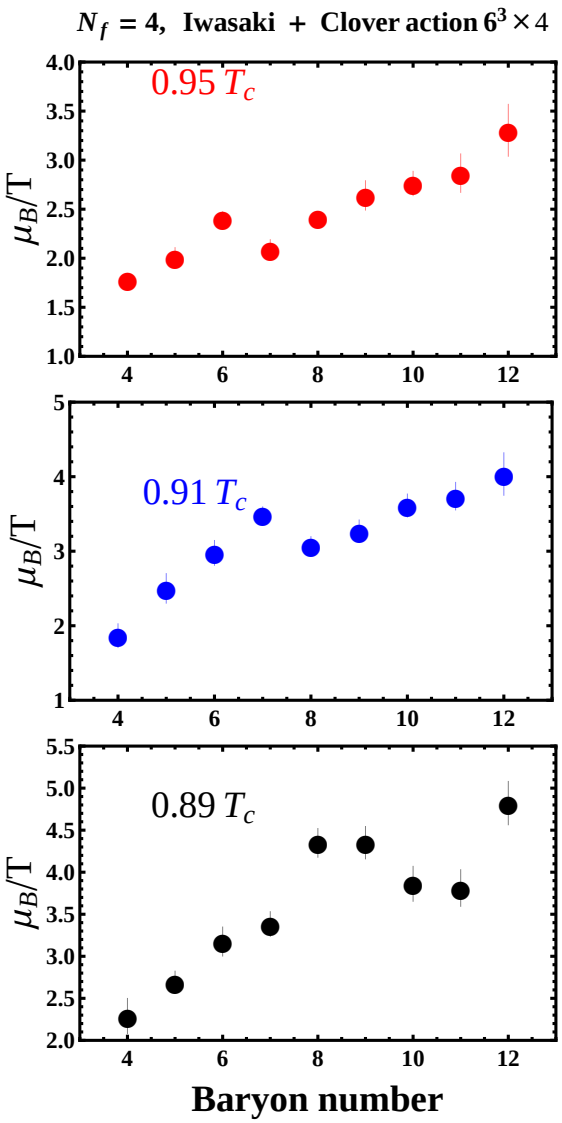
Maxwell construction

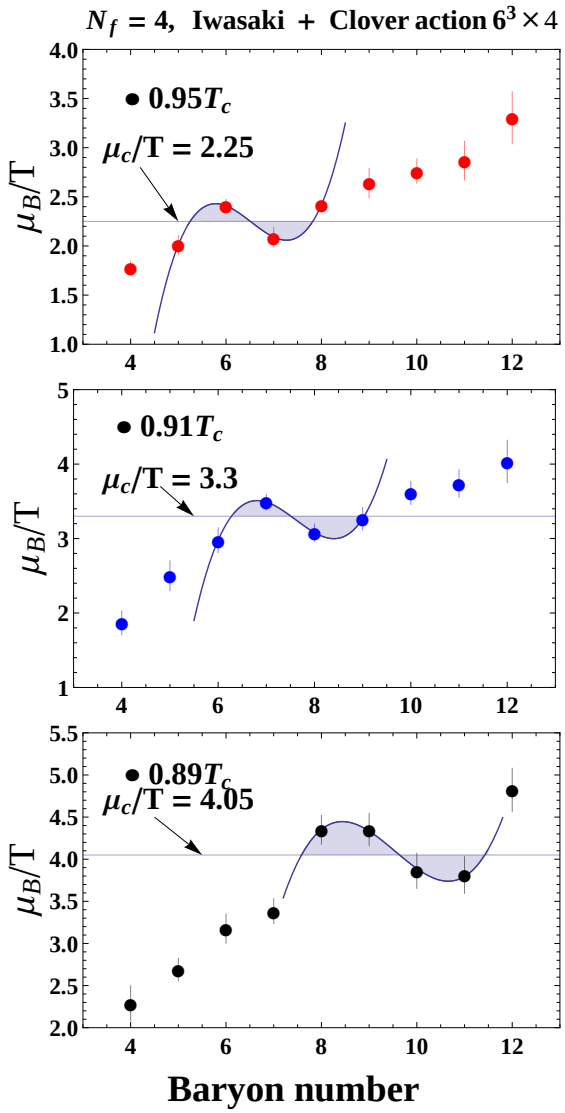


"S-shape"

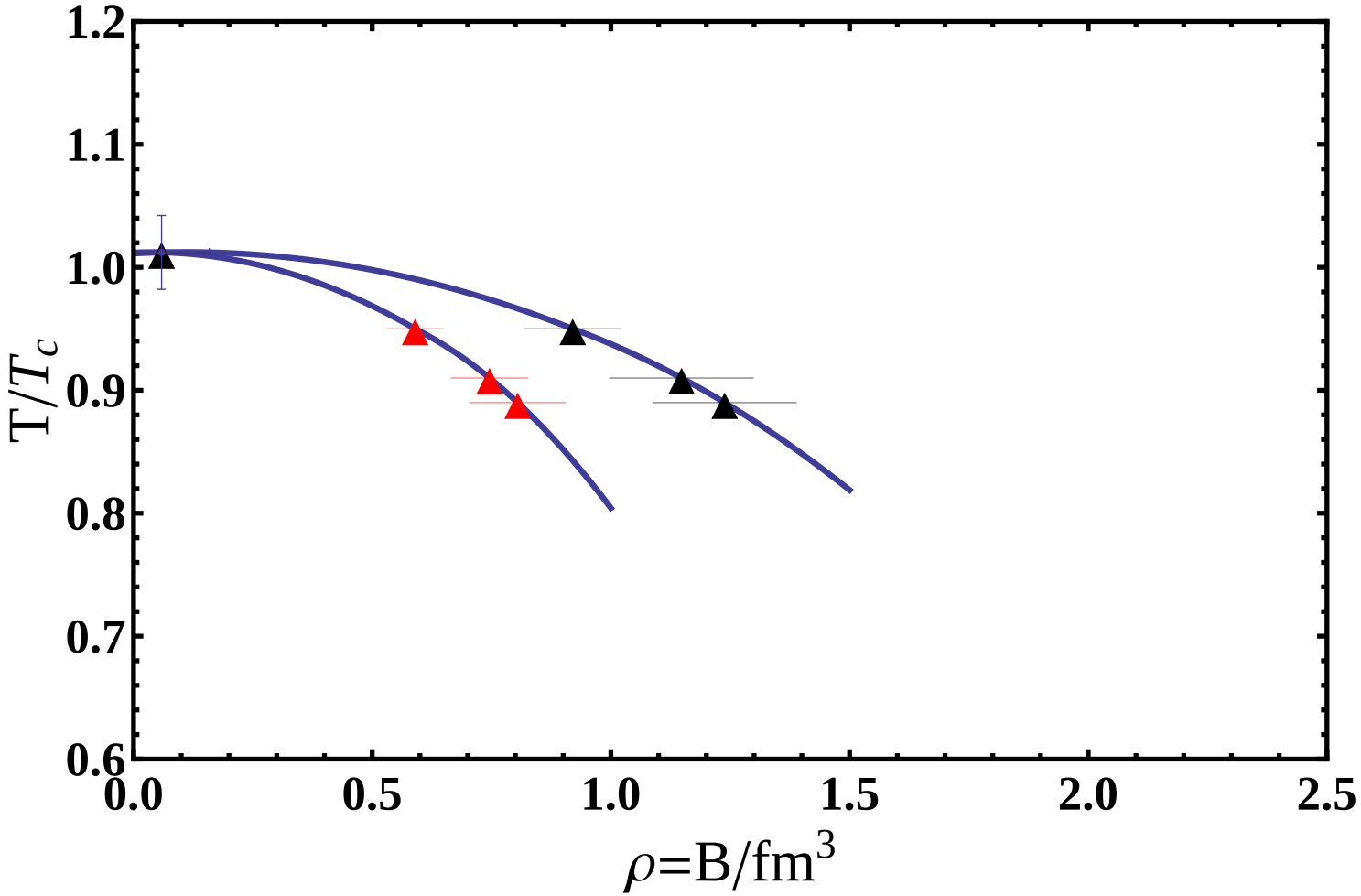
First order (Finite volume effect)

4 flavors

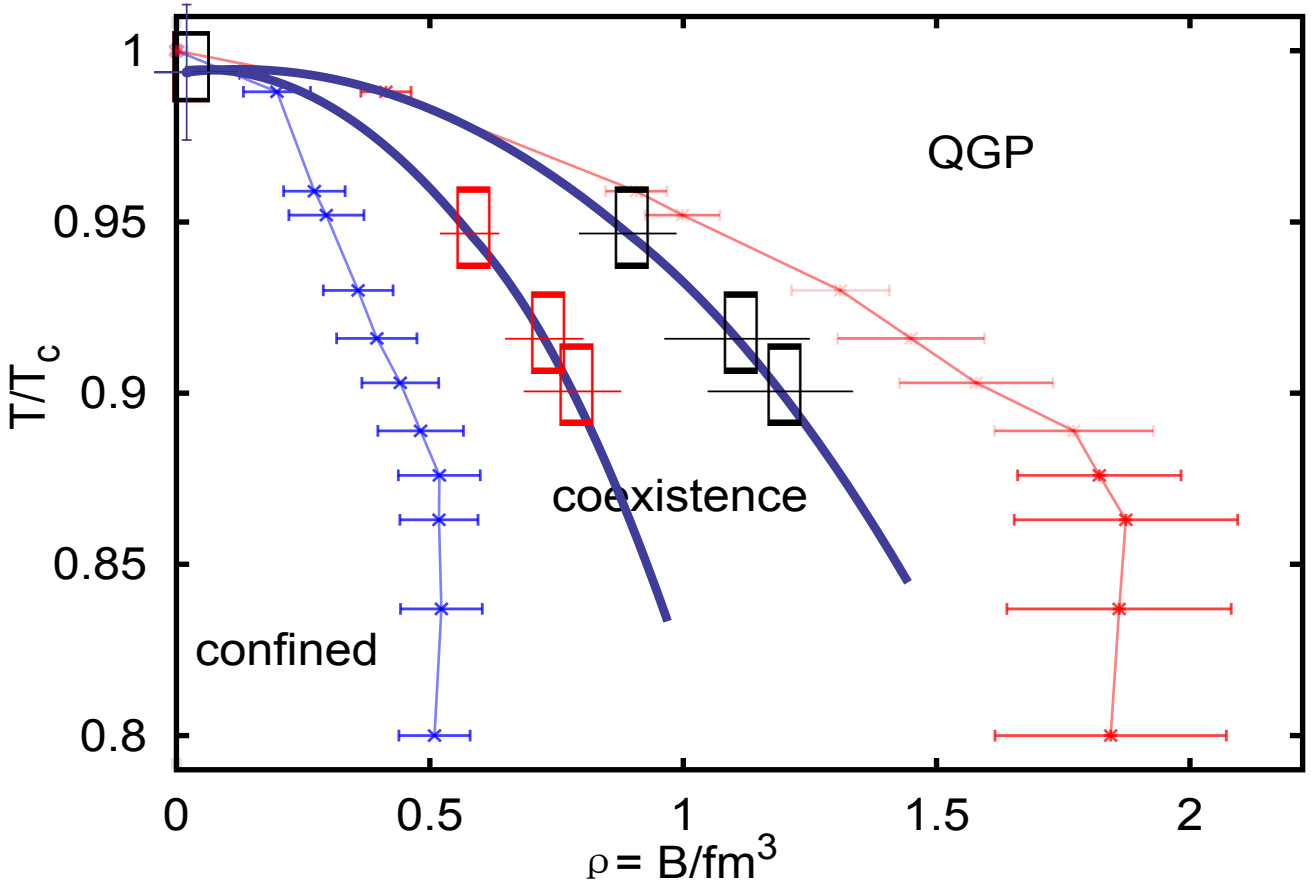

N_f = 4, Iwasaki + Clover action $6^3 \times 4$
0.95 T_c
0.91 T_c
0.89 T_c
μ_B/T
Baryon number


N_f = 4, Iwasaki + Clover action $6^3 \times 4$
● 0.95T_c
μ_c/T = 2.25
● 0.91T_c
μ_c/T = 3.3
● 0.89T_c
μ_c/T = 4.05
μ_B/T
Baryon number

Extrapolation



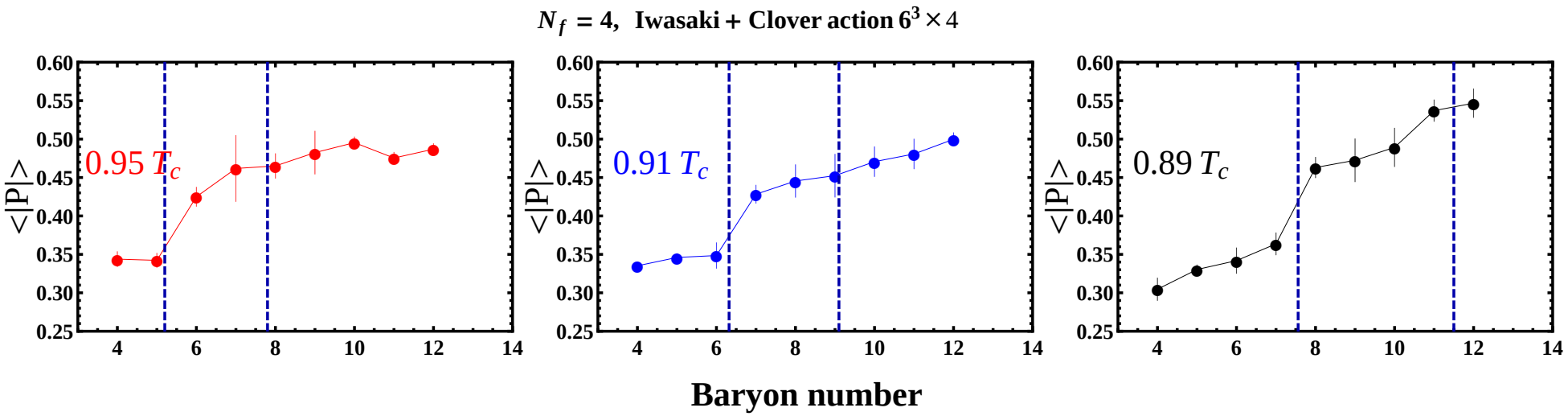
Extrapolation



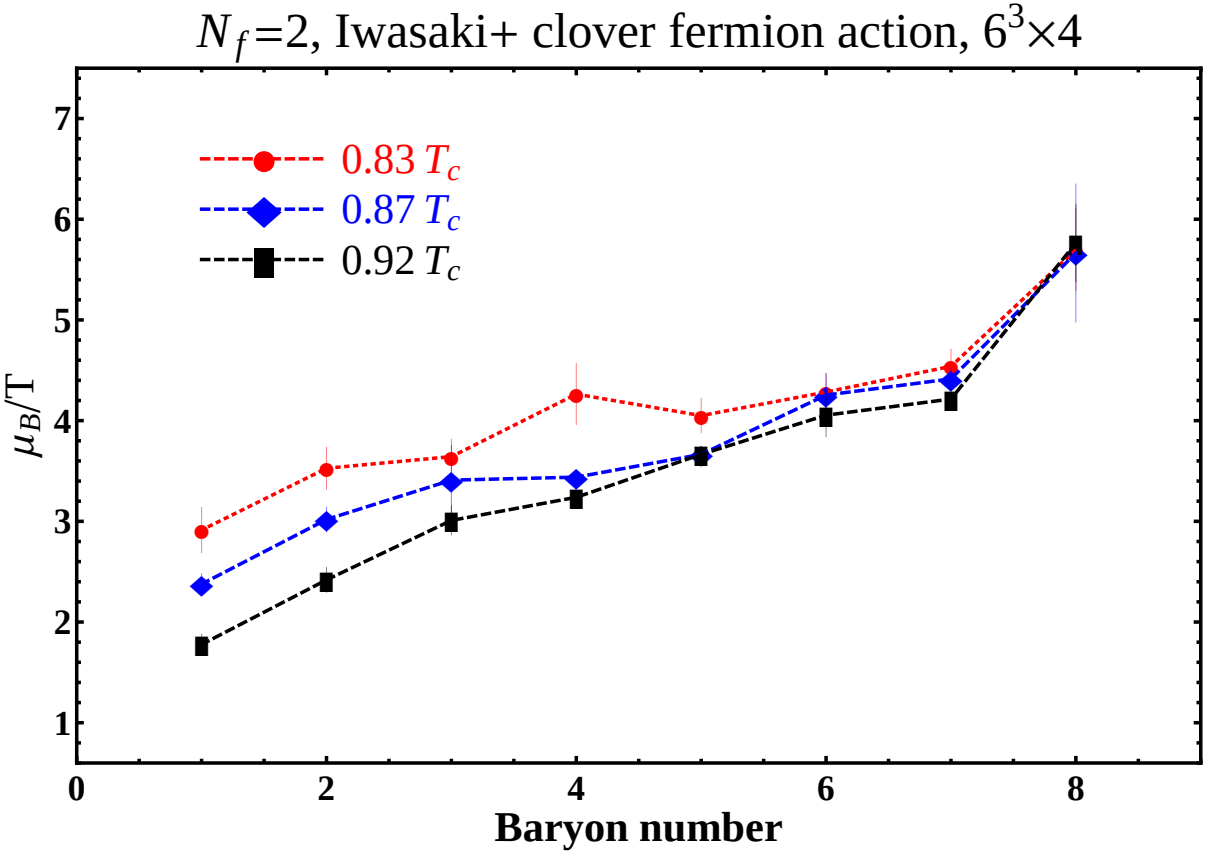
$m_\pi \approx 300\,\text{MeV} \quad 6^3 \times 4$

Philippe de Forcrand, Slavo Kratochvila Nucl. Phys. B (Proc. Suppl.) 153 (2006) 62

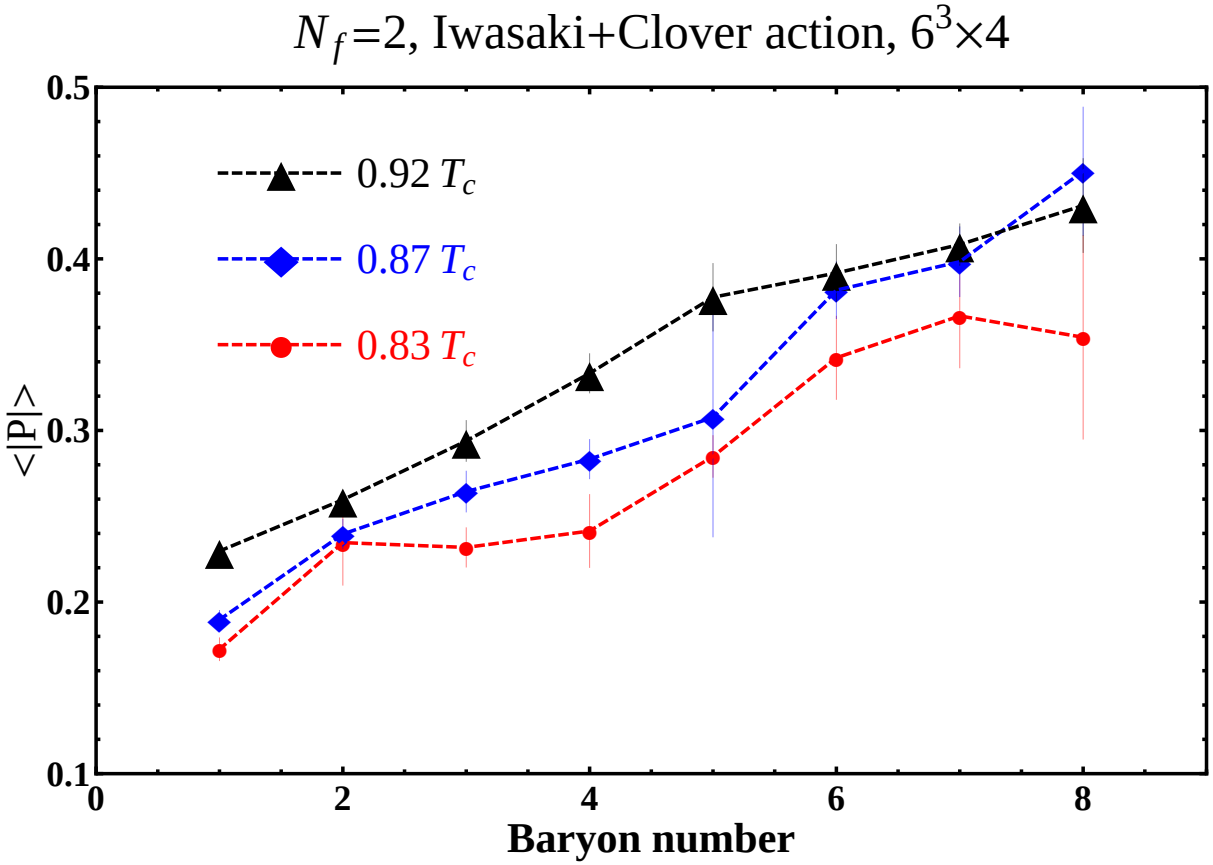
4 flavors


N_f = 4, Iwasaki + Clover action $6^3 \times 4$
0.95 T_c
0.91 T_c
0.89 T_c
<|P|>
Baryon number

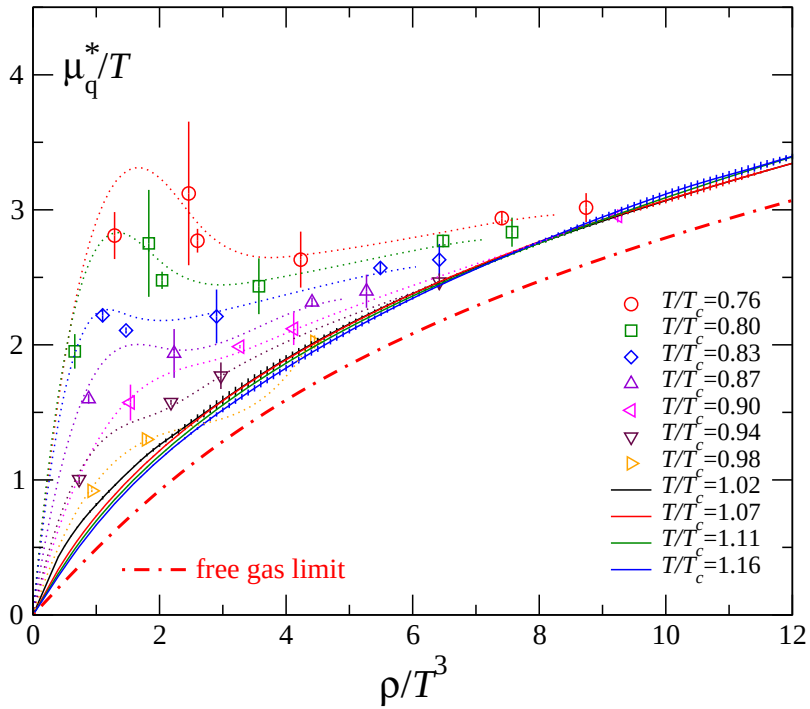
2 flavors

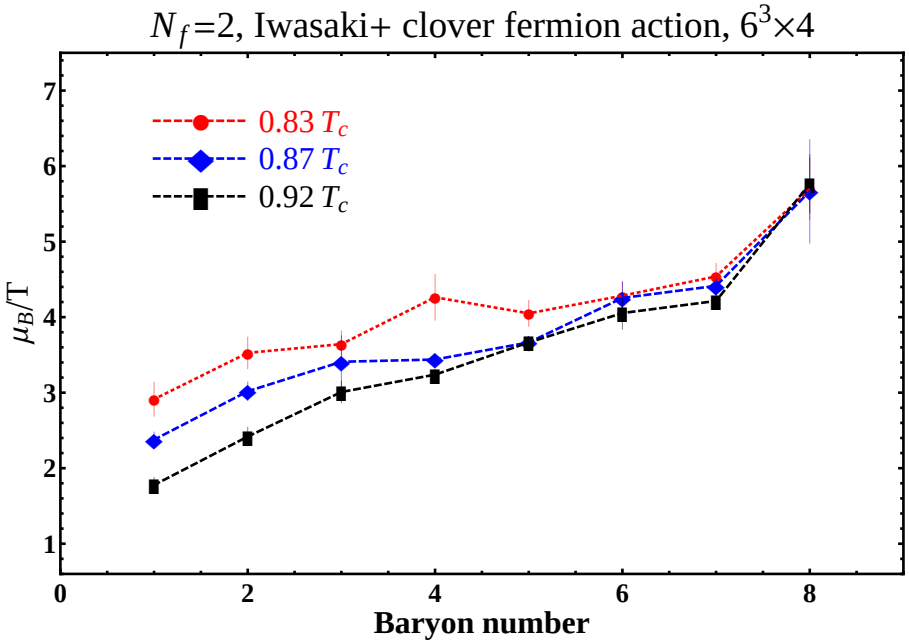

N_f=2, Iwasaki+ clover fermion action, $6^3\times4$
0.83 T_c
0.87 T_c
0.92 T_c
μ_B/T
Baryon number
0
2
4
6
8
1
2
3
4
5
6
7

2 flavors


N_f=2, Iwasaki+Clover action, $6^3\times4$
0.92 T_c
0.87 T_c
0.83 T_c
<|P|>
0.5
0.4
0.3
0.2
0.1
0
2
4
6
8
Baryon number

2 flavors

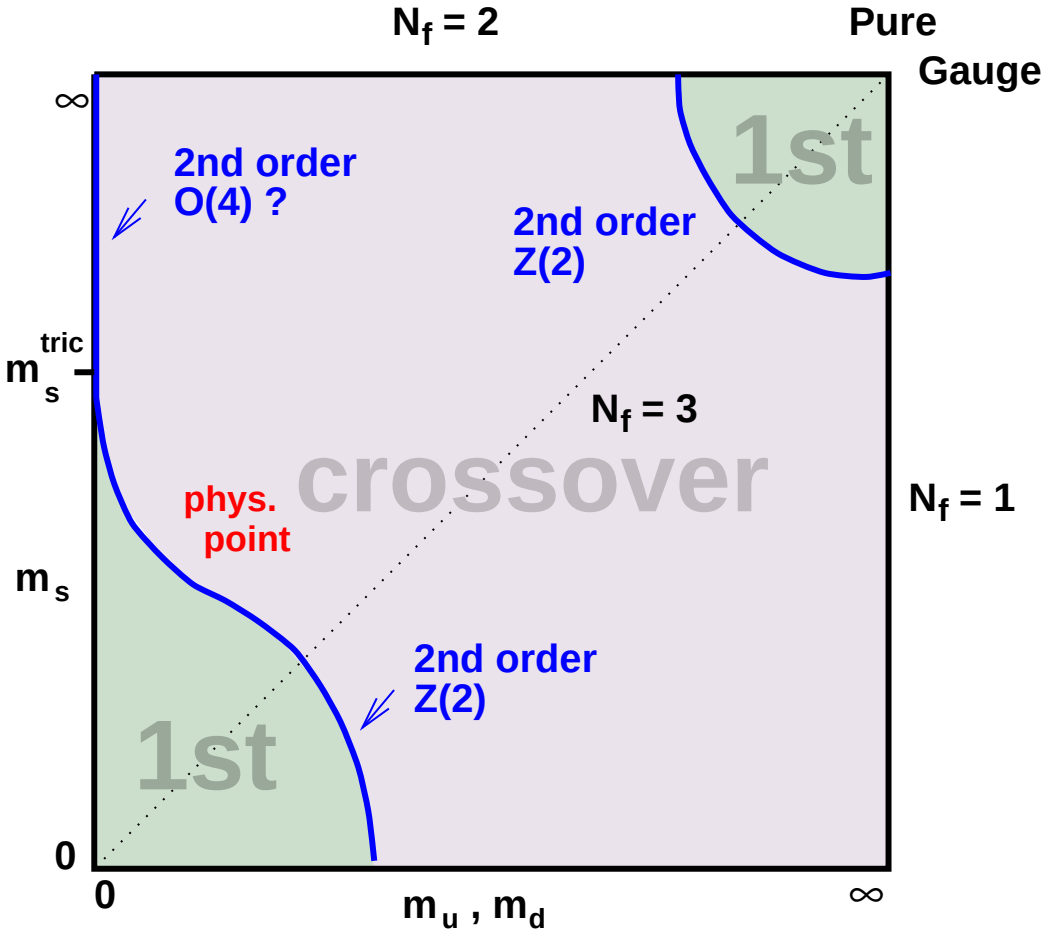




$m_\pi \approx 770\,\text{MeV} \quad 16^3 \times 4$

Shinji Ejiri Phys.Rev.D78:074507,2008 62

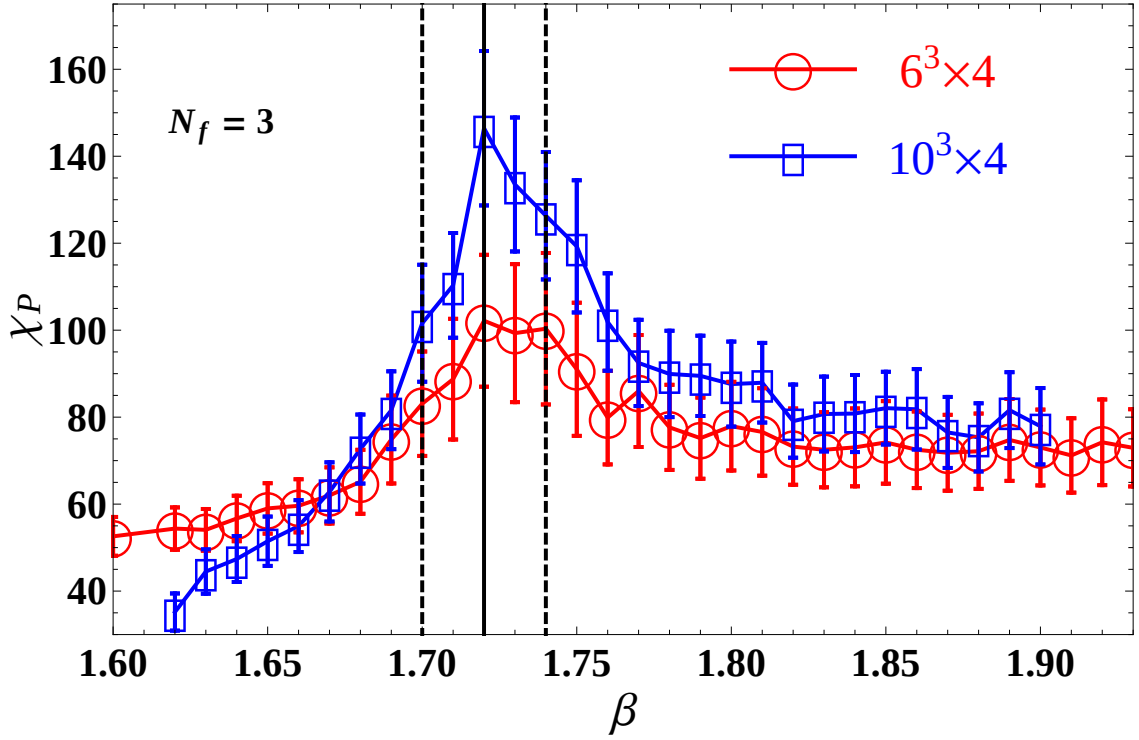
Zero chemical potential



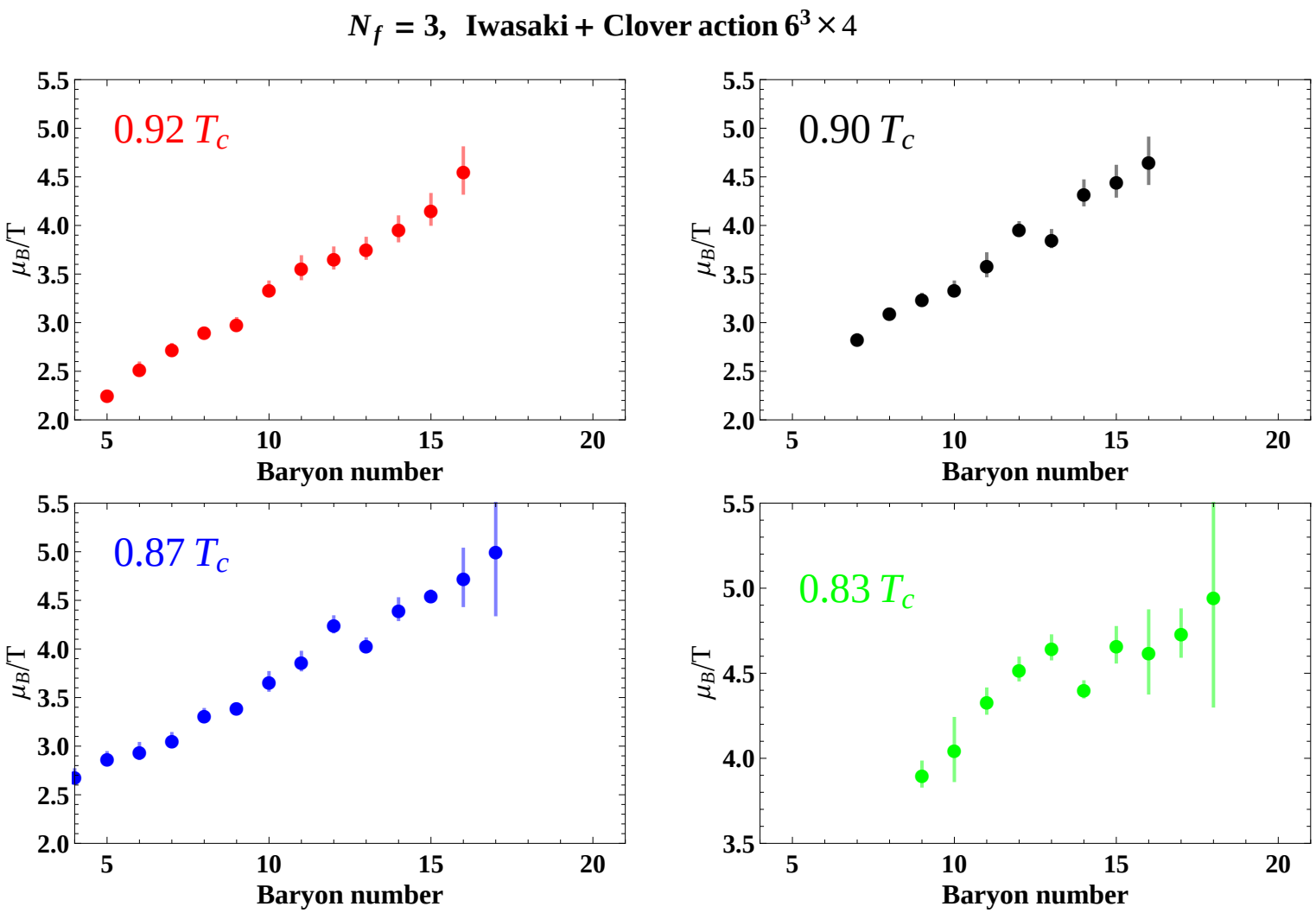
Philippe de Forcrand, Owe Philipsen arXiv:0811.3858v1 [hep-lat]

Zero chemical potential phase transition

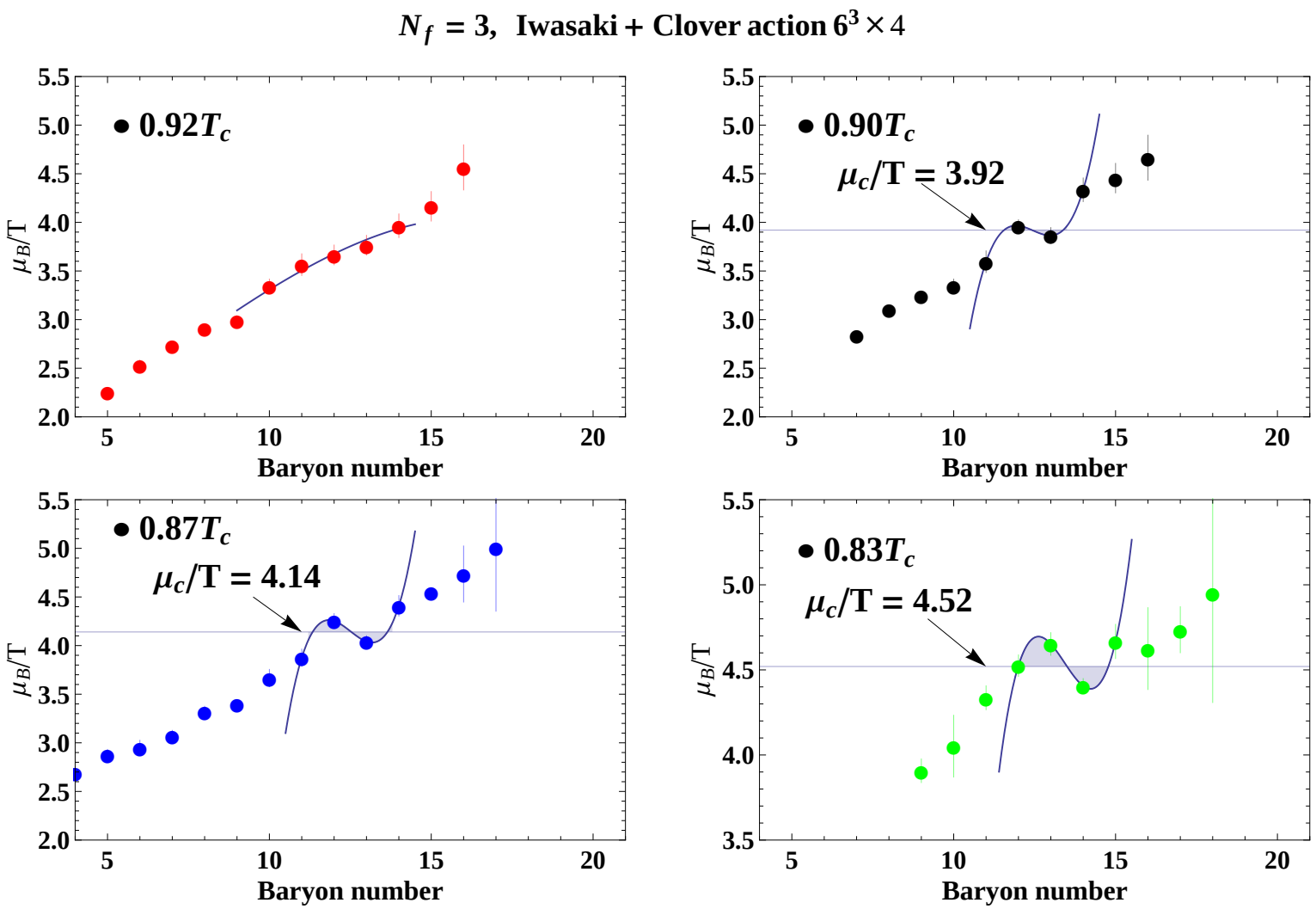
Susceptibility of Polyakov loop



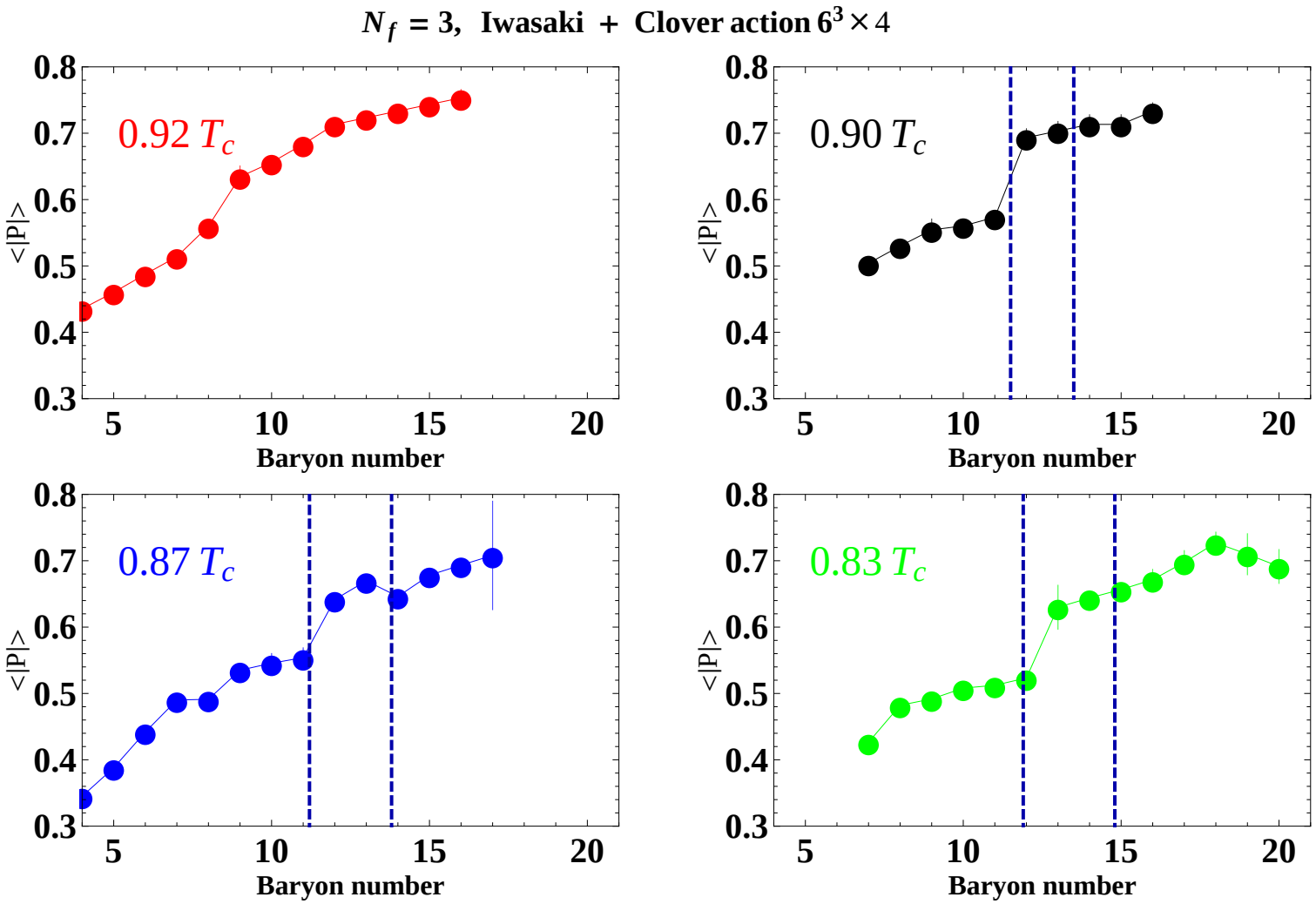
3 flavors


$N_f = 3$, Iwasaki + Clover action $6^3 \times 4$
0.92 T_c
0.90 T_c
0.87 T_c
0.83 T_c
μ_B/T
Baryon number

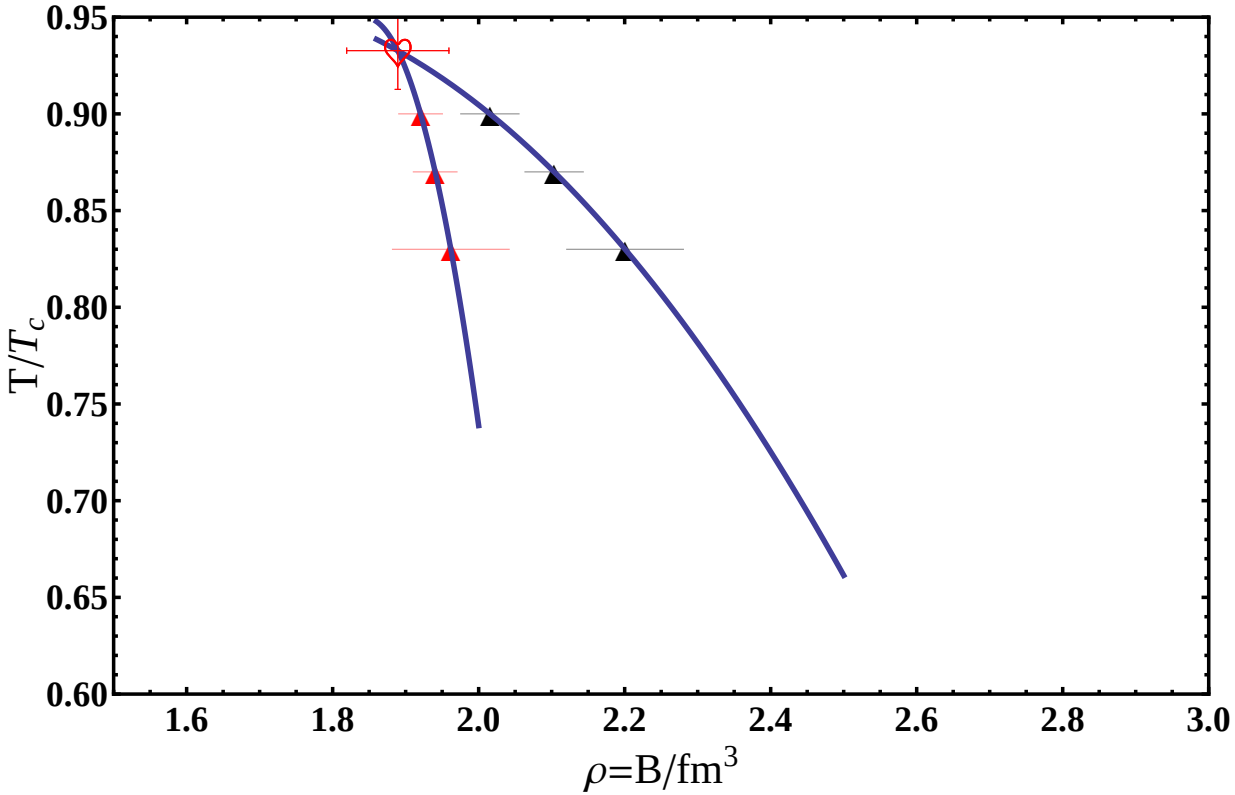
3 flavors


N_f = 3, Iwasaki + Clover action $6^3 \times 4$
● $0.92T_c$
● $0.90T_c$
μ_c/T = 3.92
● $0.87T_c$
μ_c/T = 4.14
● $0.83T_c$
μ_c/T = 4.52
μ_B/T
Baryon number

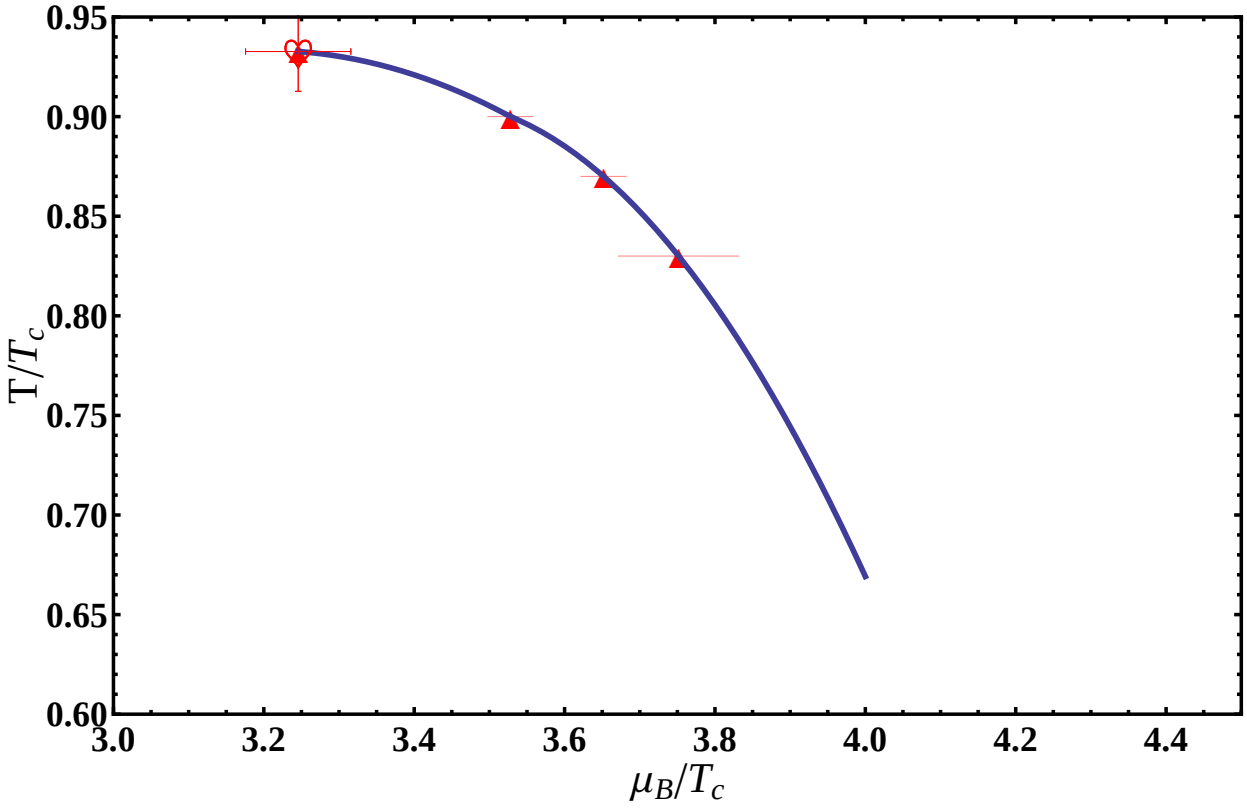
3 flavors


N_f = 3, Iwasaki + Clover action $6^3 \times 4$
0.92 T_c
0.90 T_c
0.87 T_c
0.83 T_c
<|P|>
Baryon number
0.3
0.4
0.5
0.6
0.7
0.8
5
10
15
20

3 flavors


0.95
0.90
0.85
0.80
0.75
0.70
0.65
0.60
T/T_c
1.6
1.8
2.0
2.2
2.4
2.6
2.8
3.0
ρ=B/fm^3

3 flavors



At CEP $T_E/T_c(\mu_B = 0) = 0.93(2) \quad \mu_c^B/T_E = 3.25(7)$

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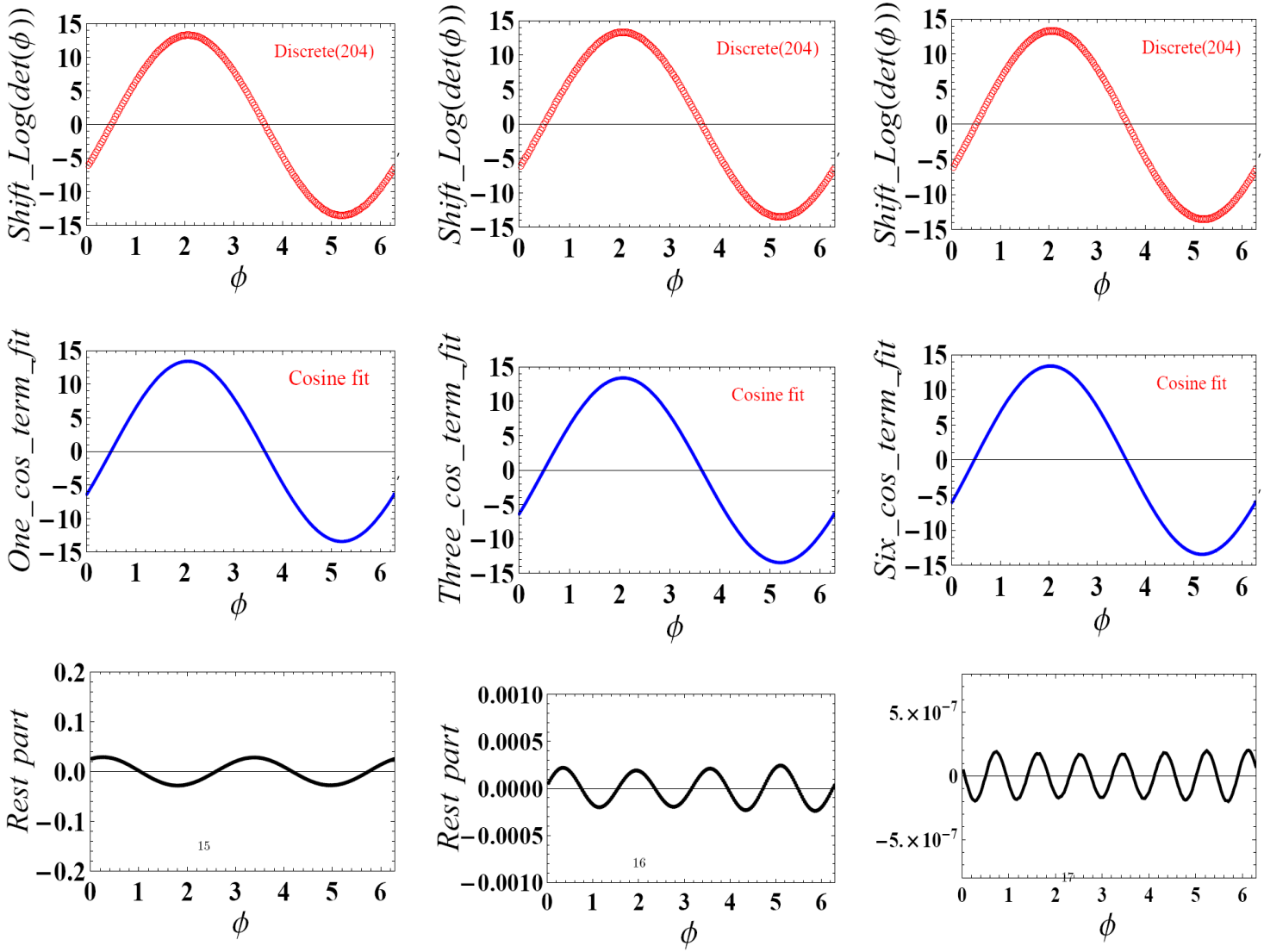
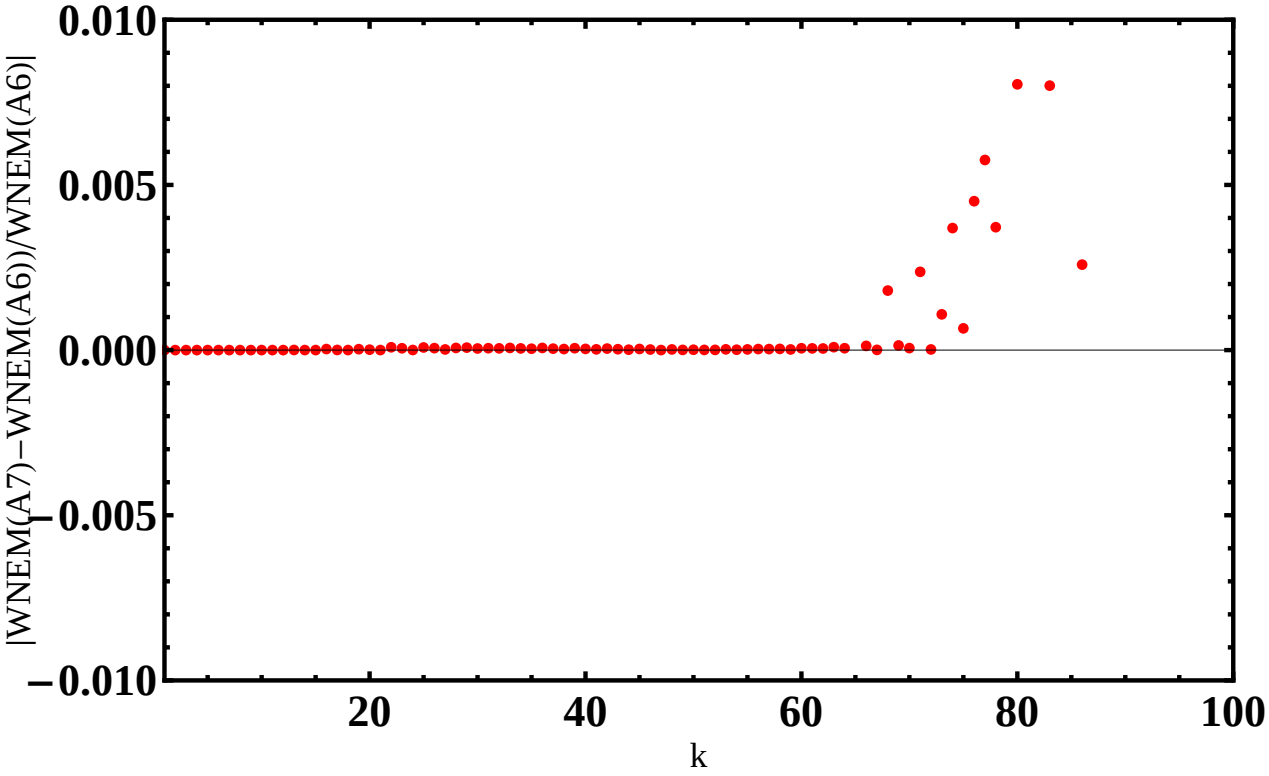
- Wilson fermion on $6^3 \times 4$ lattice with $m_\pi \approx 700$ MeV shows $N_f = 2$ is 2nd order (?) down to $0.83T_c$, $N_f = 4$ is first order.
- Iwasaki + Clover fermion on $6^3 \times 4$ lattice with $m_\pi \approx 700$ MeV results for $N_f = 3$ are first order. Critical end point is determined by extrapolation.

Future plan

- Lighter quark masses
- Chiral fermions (Overlap fermion)
- Larger volume, Fold projected determinant into molecule dynamics
- Measurements of other physical quantities (Hardon mass, chiral condensation)

Winding number expansion



Winding number expansion