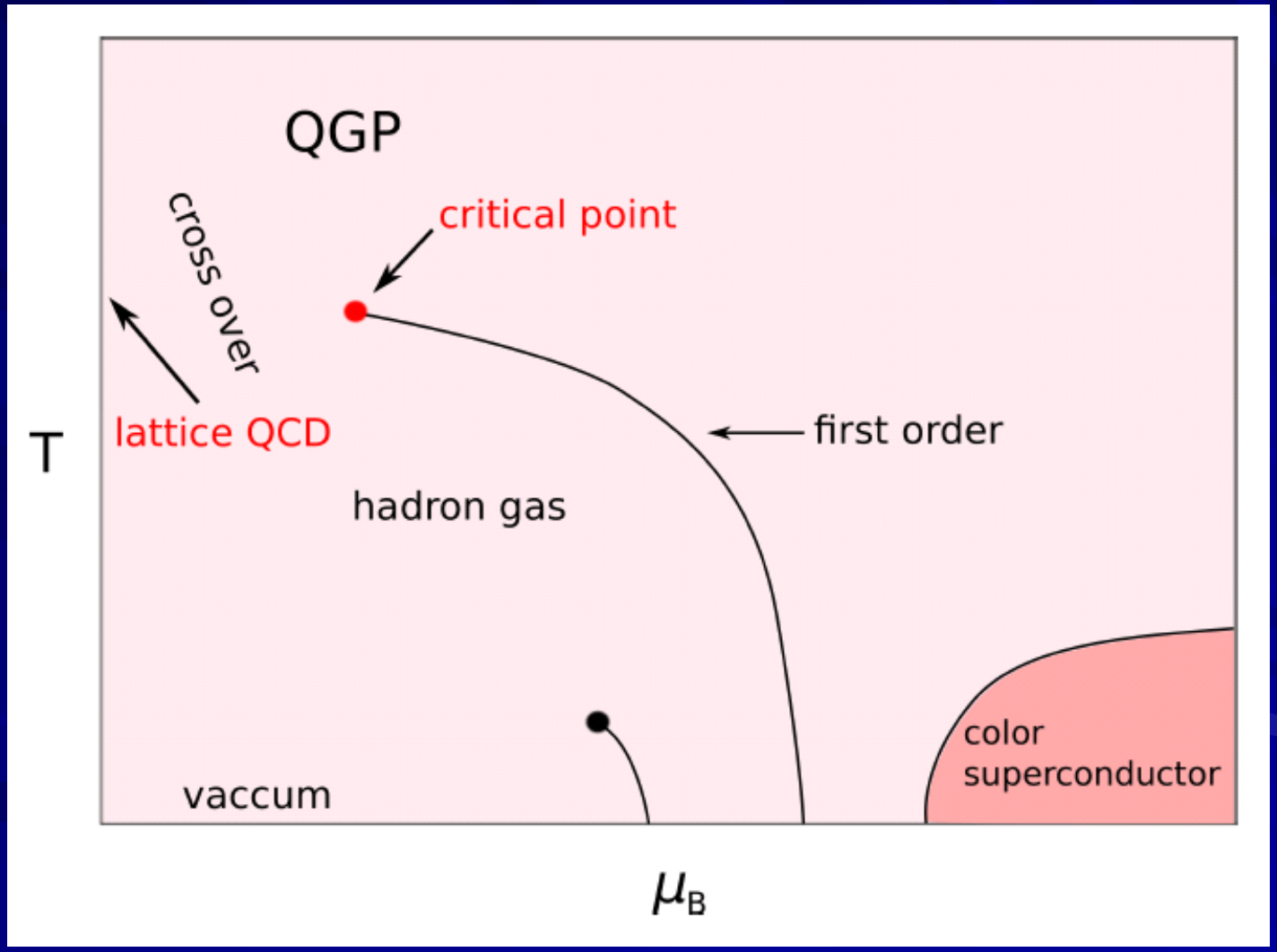
Lattice Calculation of QCD Critical Point with the Canonical Ensemble

- Finite Density Algorithm with Canonical Ensemble Approach
- Results on $N_F = 4$ with Wilson-Clover Fermion
- $N_F = 3$ with Wilson-Clover Fermion

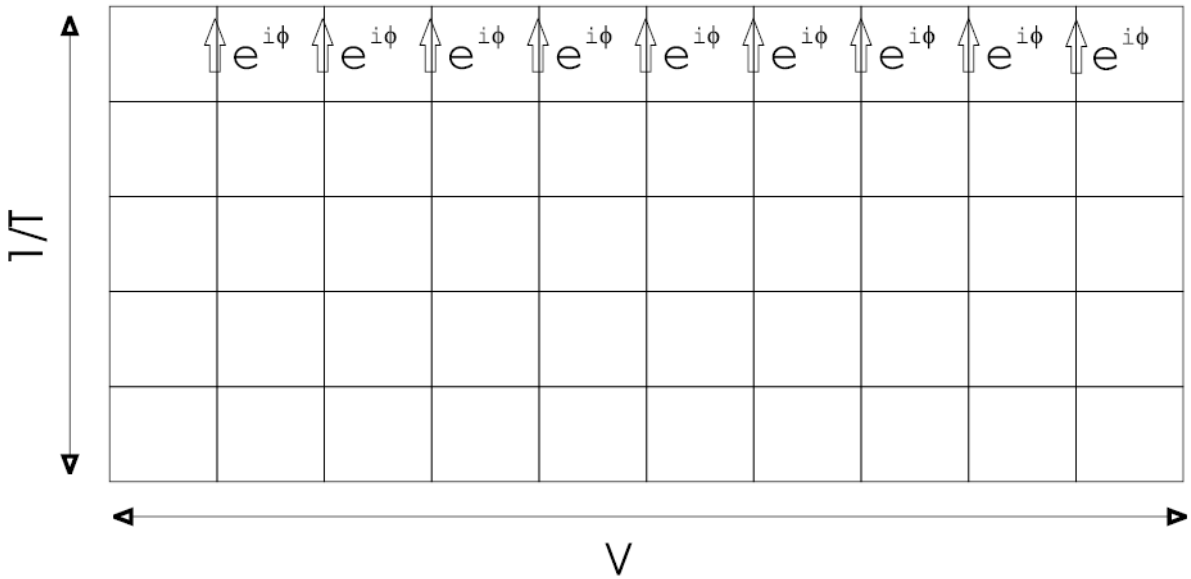
χQCD Collaboration:
Anyi Li, Andrei Alexandru, KFL, and Xiangfei Meng

BNL, Oct. 4, 2011

A Conjectured Phase Diagram



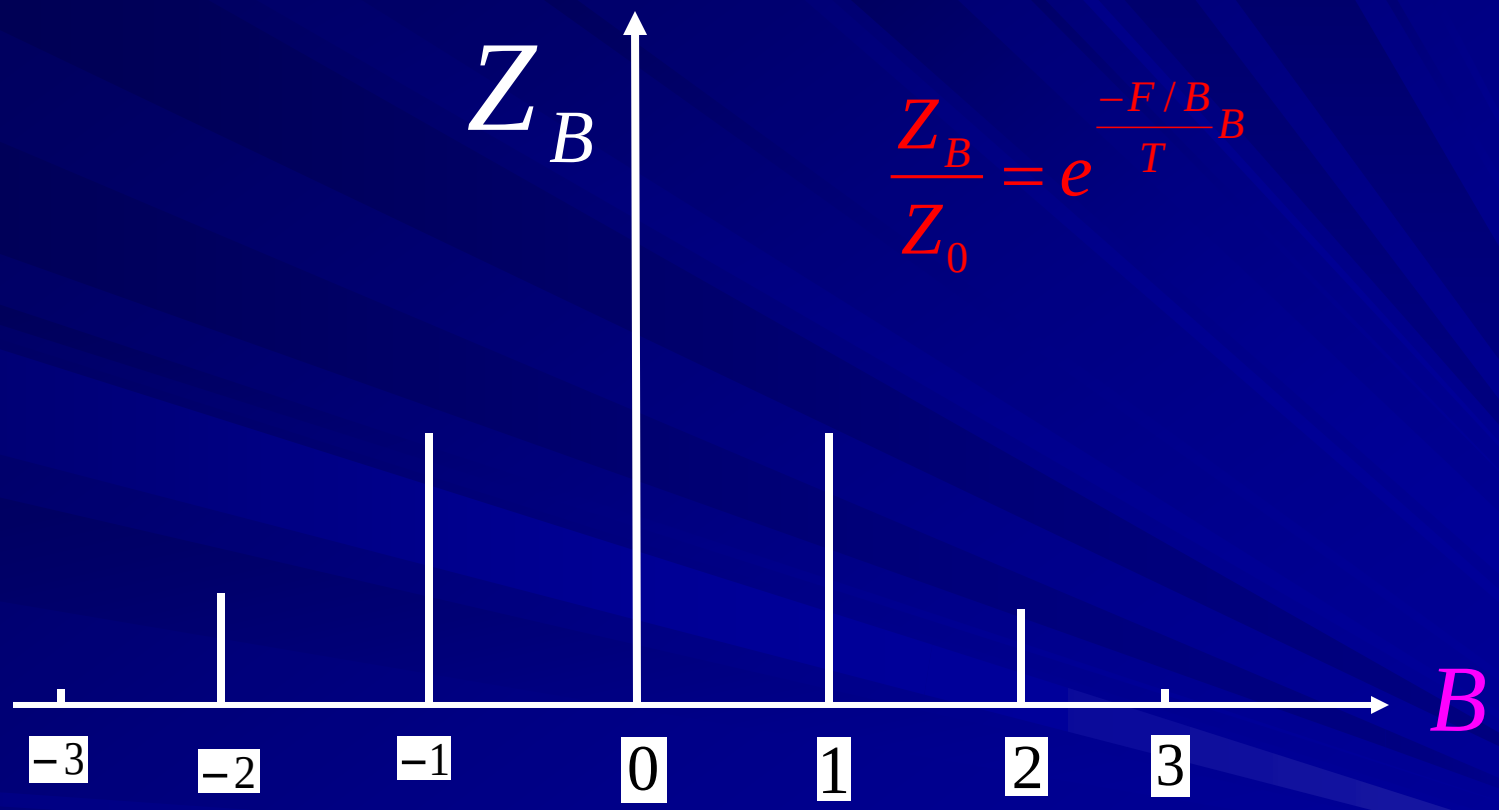
Canonical partition function



Using the fugacity expansion $Z_{GC}(V,\mu,T)=\sum_{k=-4V}^{k=4V} Z_C(V,k,T)e^{\frac{\mu}{T}k}$ we get

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

Overlap Problem



$$\frac{Z_B}{Z_0} = e^{\frac{-F/B}{T}B}$$

$$Z_{GC}(\mu/T,T,V) = \sum_{B=-V}^{V} e^{\mu B/T} Z_B(T,V)$$

Canonical approach

K. F. Liu, *QCD and Numerical Analysis* Vol. III (Springer,New York, 2005),p. 101.
Andrei Alexandru, Manfried Faber, Ivan Horva´th,Keh-Fei Liu, *PRD* 72, 114513 (2005)

Canonical ensembles

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

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

Fourier transform

$$\widetilde{\det}_k M^2(U) \equiv \frac{1}{2\pi} \int d\phi\, e^{-ik\phi} \det M^2(U_\phi)$$

Real due to
C or T, or CH

$$\det M^2(U_\phi) = e^{2 log \det M(U_\phi)}$$

$$log \det M(U_\phi)$$

WNEM

Continues Fourier transform
Useful for large k

Winding number expansion (I)

In QCD

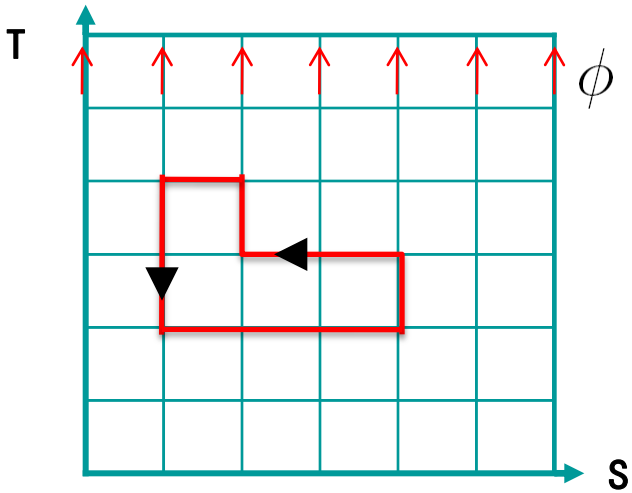
Tr log $\longrightarrow$ loop $\longrightarrow$ loop expansion

In particle number space

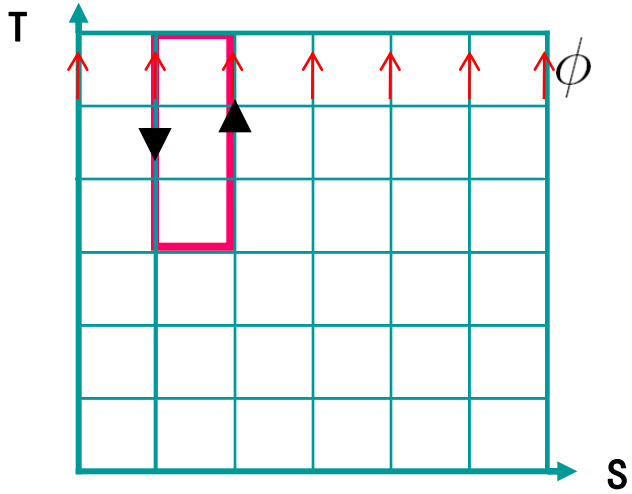
$$
\begin{aligned}
TrlogM(U,\phi) &= A_0(U) + \Sigma loop(U,\phi) \\
&= A_0(U) + [\sum_k e^{ik\phi} W_k(U) + e^{-ik\phi} W_k^\dagger(U)]
\end{aligned}
$$

Where $W_n = \frac{1}{2\pi}\int_0^{2\pi} e^{-ik\phi} trlogM(U,\phi)$

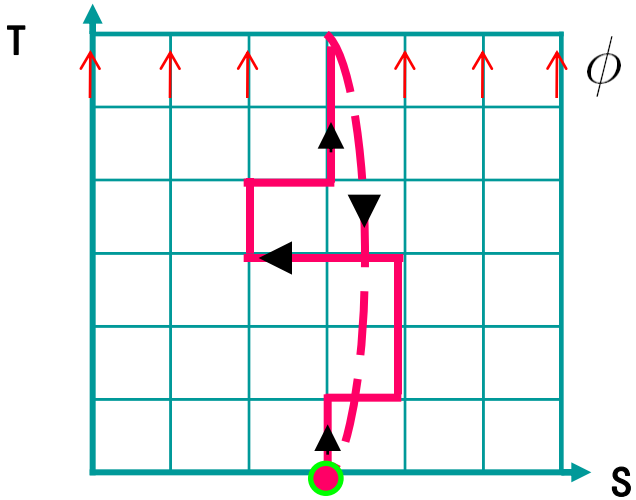
$$
\begin{aligned}
TrlogM(U,\phi) &= A_0(U) + [\sum_k e^{ik\phi} W_k(U) + e^{-ik\phi} W_k^\dagger(U)] \\
&= A_0(U) + \sum_k A_k \cos(k\phi + \delta_k)|_{A_k = 2|W_k|, \delta_k = \delta_{W_k}}
\end{aligned}
$$



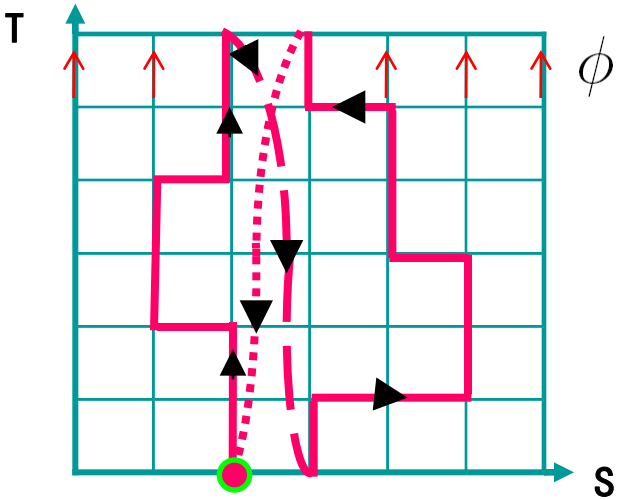
A_0



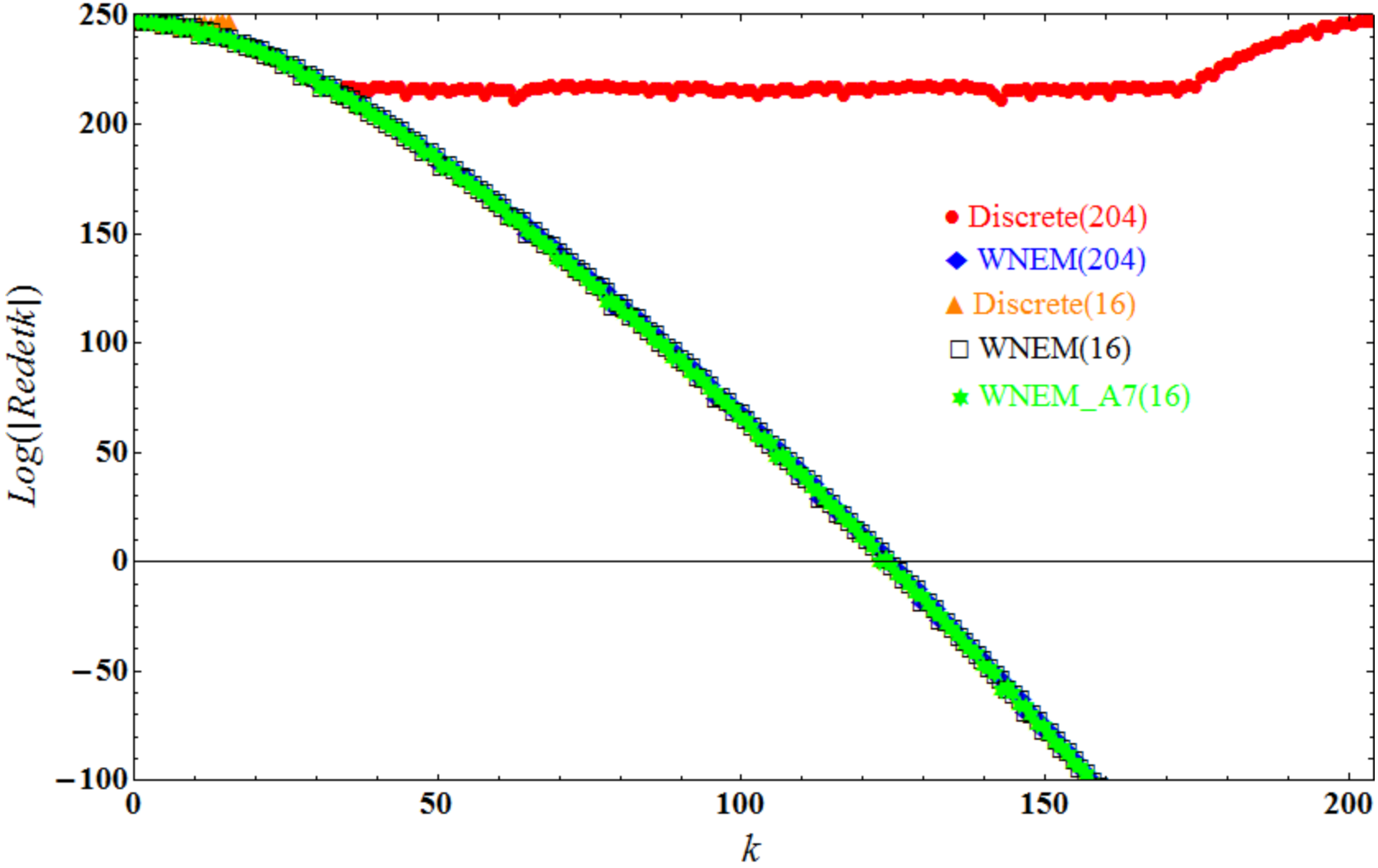
A_0



A_1



A_2


250
200
150
100
50
0
−50
−100
0
50
100
150
200
k
Log(|Redetk|)
Discrete(204)
WNEM(204)
Discrete(16)
WNEM(16)
WNEM_A7(16)

Observables

Polyakov loop

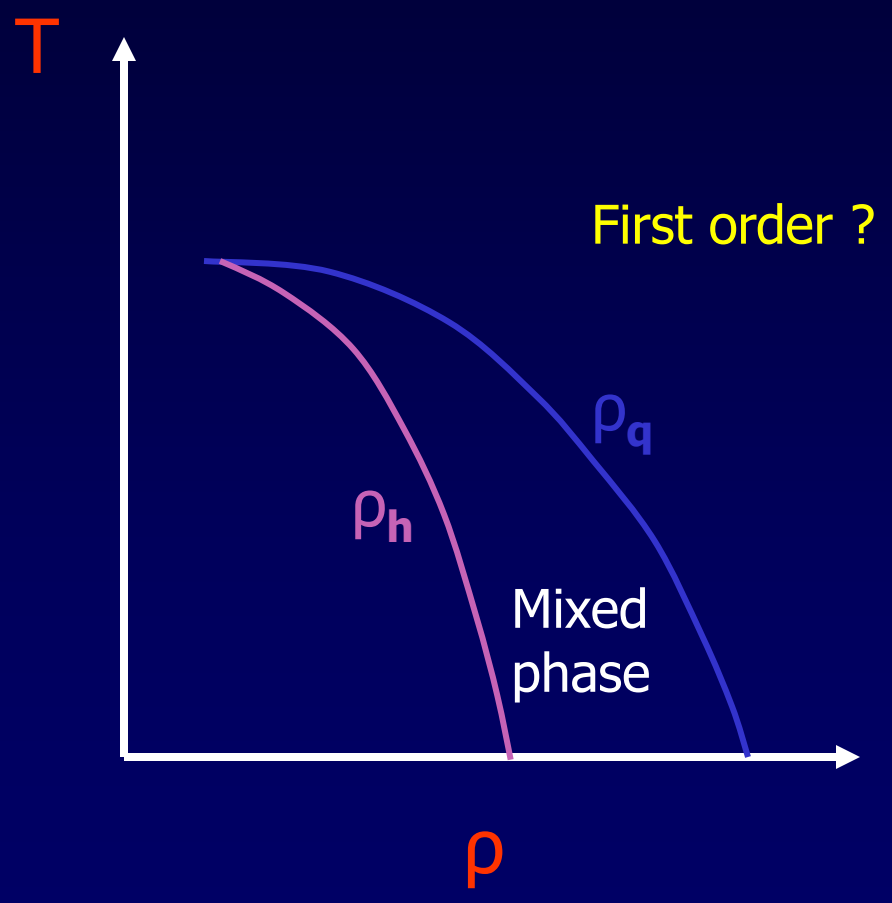
$$\langle |P| \rangle_{k'} = \frac{\langle R(U,k')|P(U)|\rangle_0}{\langle R(U,k')\rangle_0} \qquad R(U,k') = \frac{\widetilde{\det}_k M^2(U)}{|\operatorname{Re}\widetilde{\det}_k M^2(U)|}$$

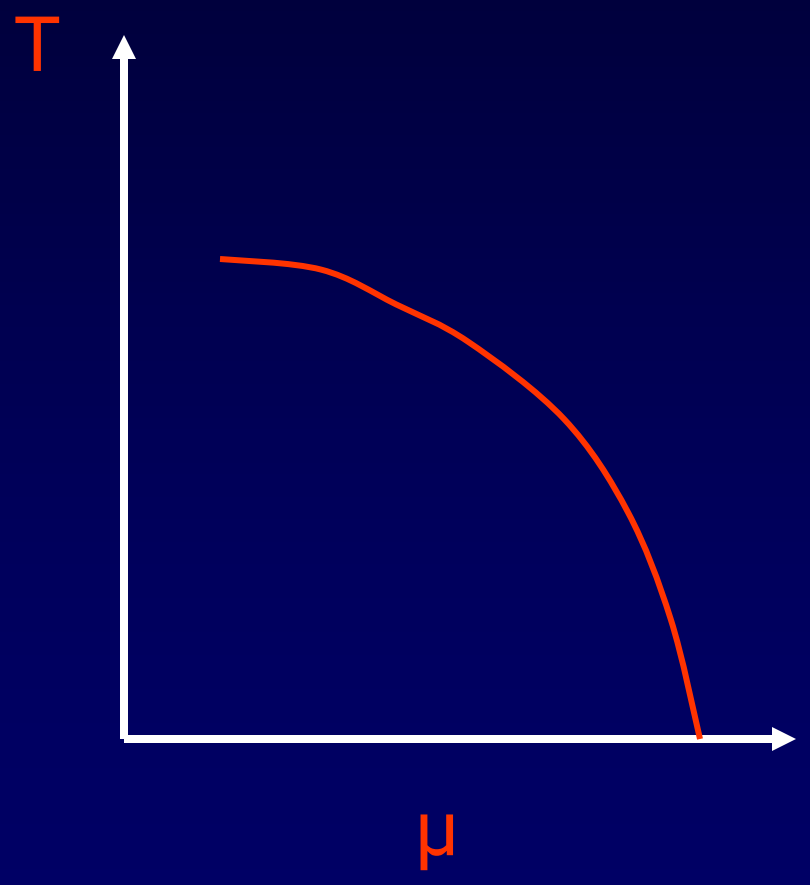
Phase

Baryon chemical potential

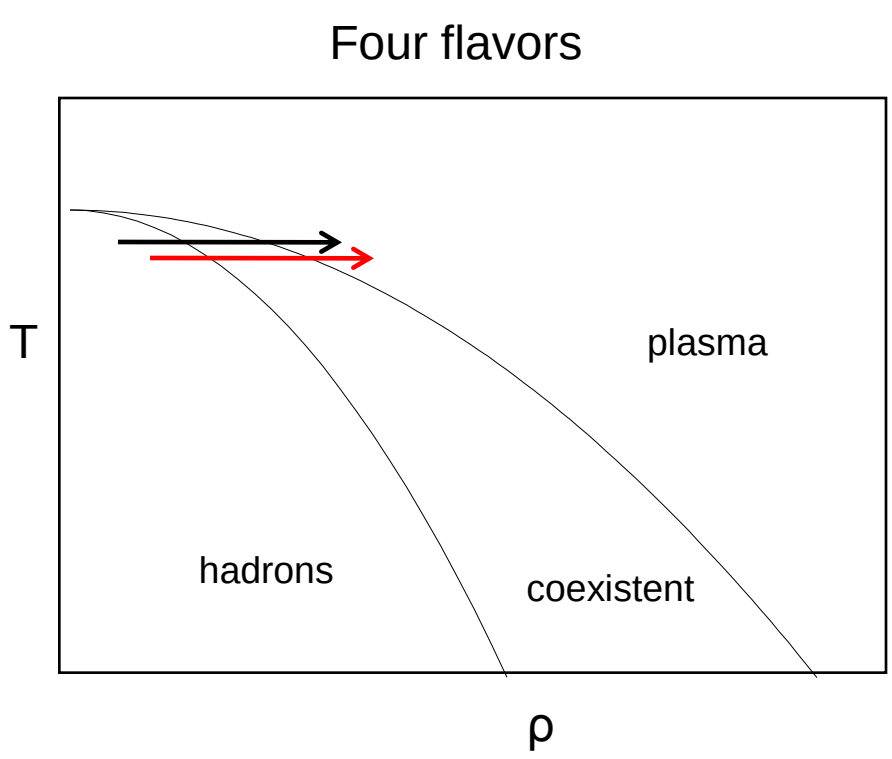
$$\begin{aligned}
\langle \mu \rangle_{n_B} &\equiv \frac{F(n_B+1)-F(n_B)}{(n_B+1)-n_B} \\
&= -\frac{1}{\beta}\ln\frac{\widetilde{Z}_C(3n_B+3)}{\widetilde{Z}_C(3n_B)} \\
&= -\frac{1}{\beta}\ln\frac{1}{\widetilde{Z}}\int \mathcal{D}U e^{-S_g(U)}|\operatorname{Re}\widetilde{\det}_{3n_B} M^2(U)|\frac{\operatorname{Re}\widetilde{\det}_{3n_B+3} M^2(U)}{|\operatorname{Re}\widetilde{\det}_{3n_B} M^2(U)|}
\end{aligned}$$

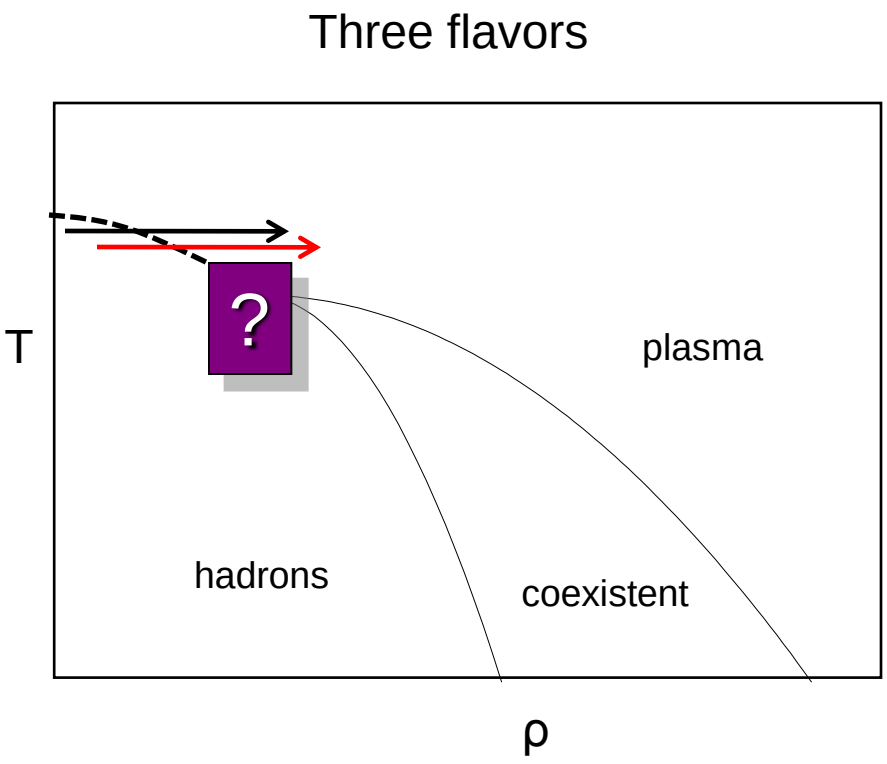
Phase Diagrams

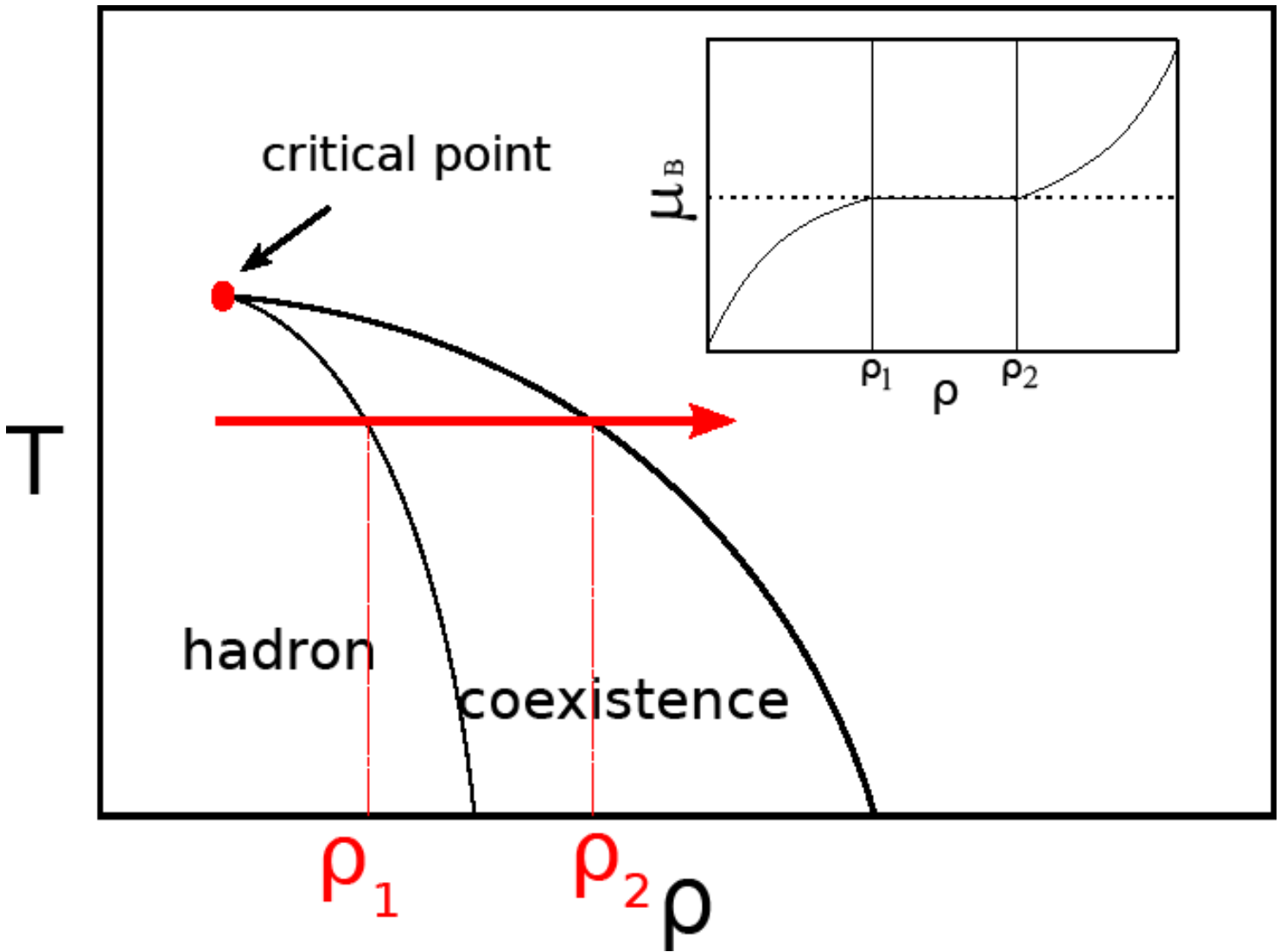




Phase diagram

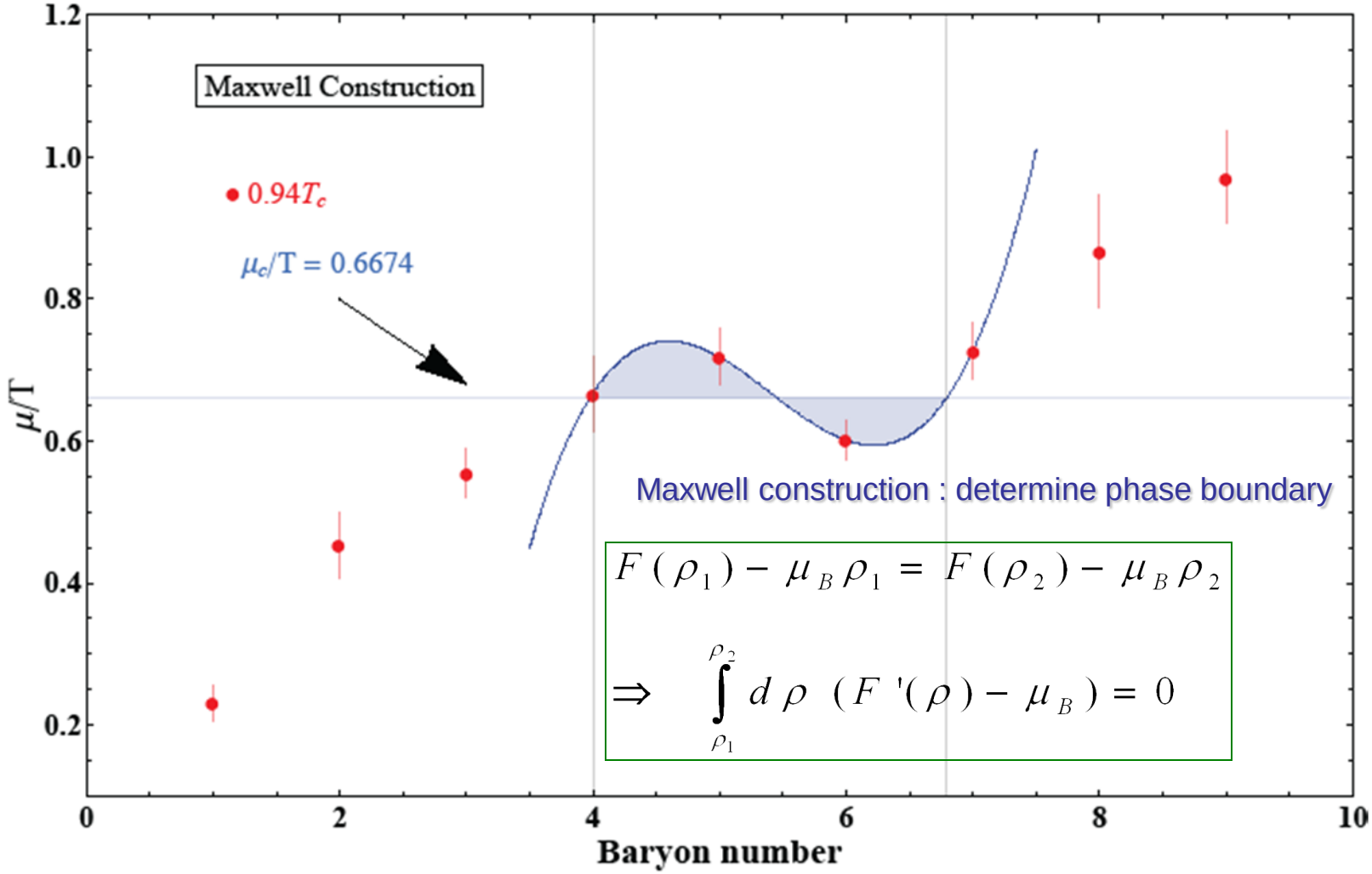





critical point
μ_B
ρ_1
ρ
ρ_2
T
hadron
coexistence
ρ_1
ρ_2
ρ

Phase Boundaries from Maxwell Construction

N_f = 4 Wilson gauge + fermion action

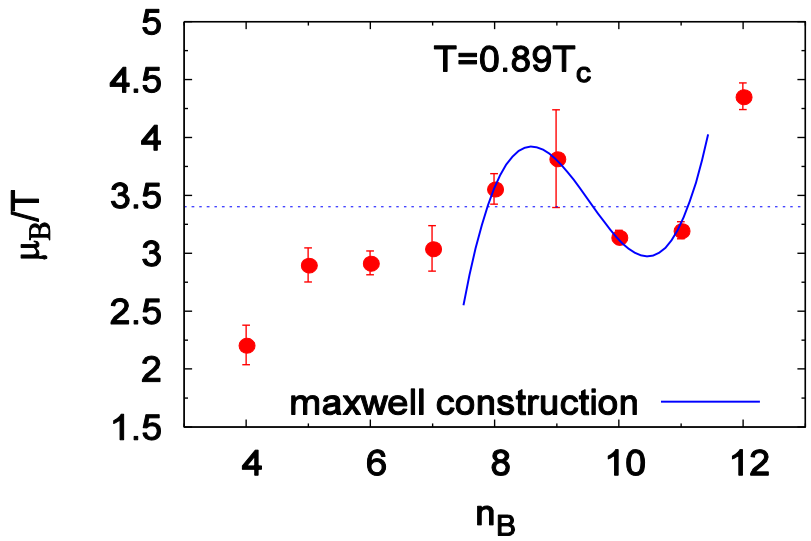


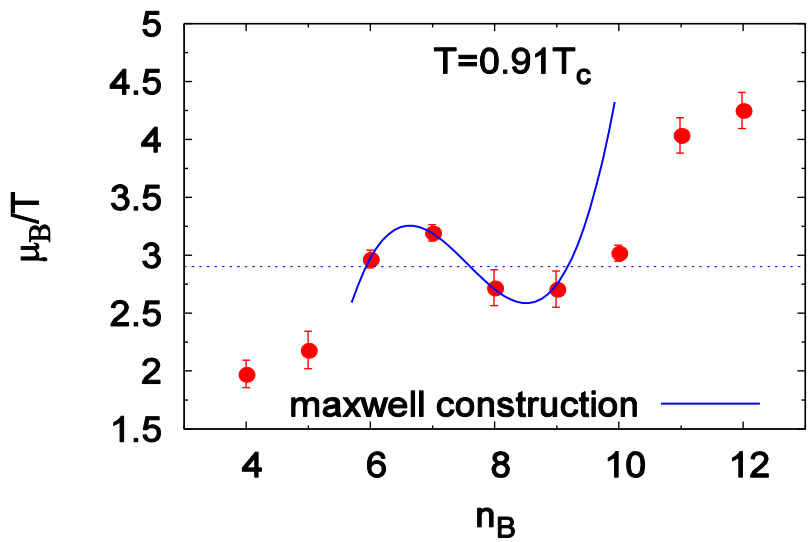
Maxwell construction : determine phase boundary

$$F(\rho_1) - \mu_B \rho_1 = F(\rho_2) - \mu_B \rho_2$$

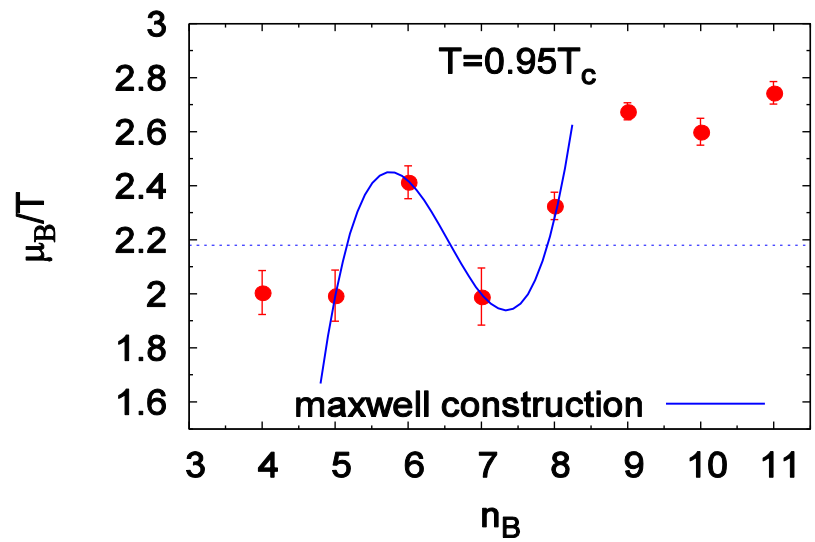
$$\Rightarrow \int_{\rho_1}^{\rho_2} d\rho \, (F'(\rho) - \mu_B) = 0$$

Baryon Chemical Potential for $N_f = 4$ ($m_\pi \sim 0.8$ GeV)

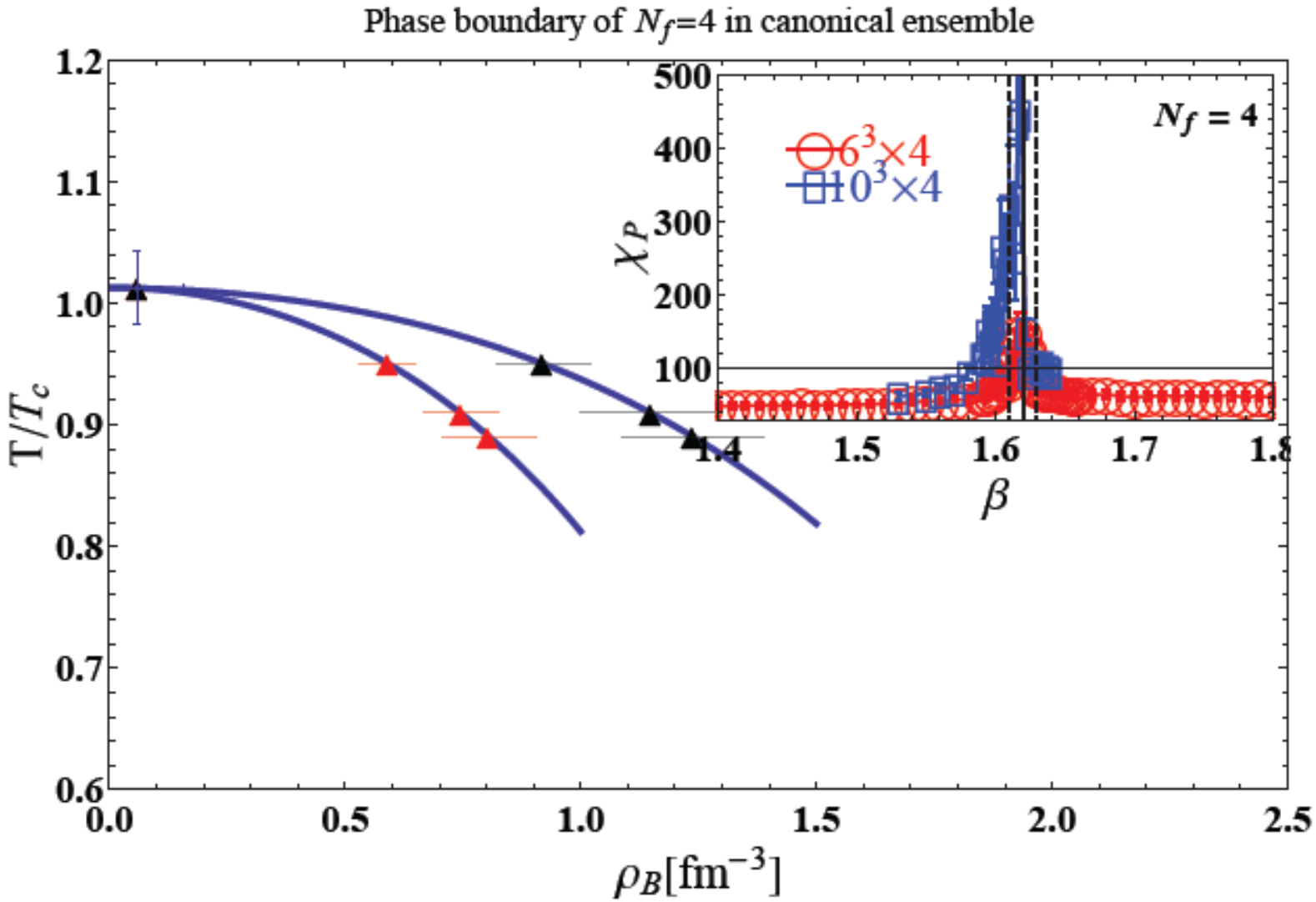




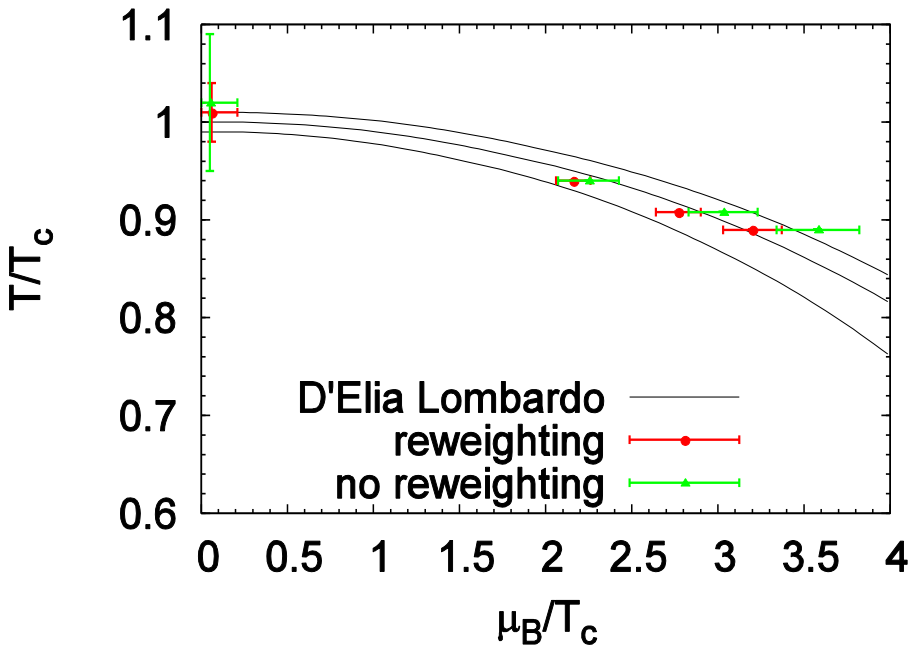
$6^3 \times 4$ lattice,
Clover fermion

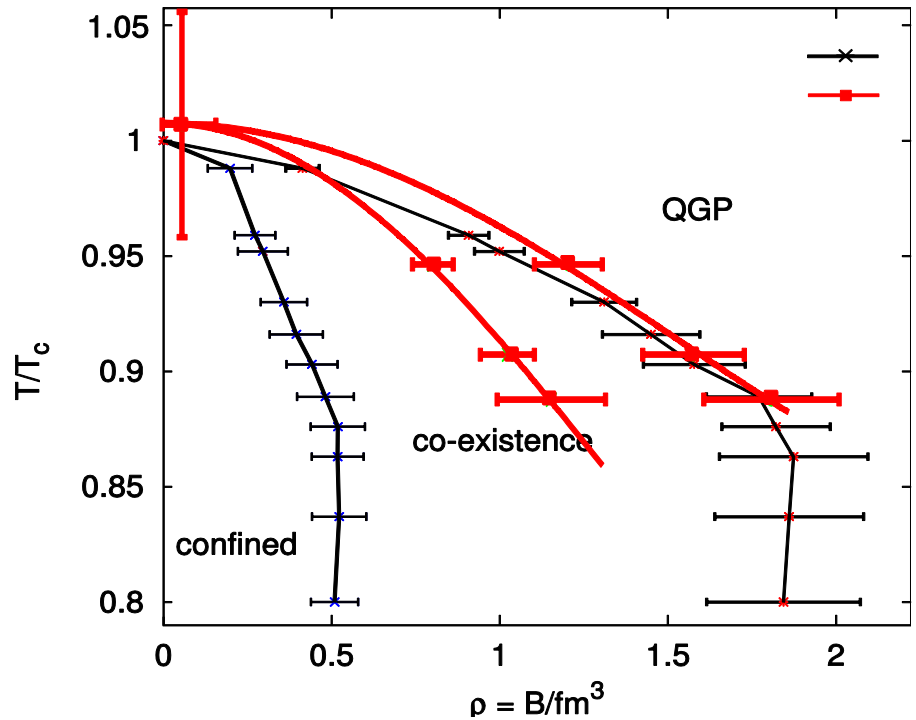


Phase boundary



Phase Boundaries





Ph. Forcrand,S.Kratochvila, Nucl. Phys. B (Proc. Suppl.) 153 (2006) 62

4 flavor (taste) staggered fermion

$N_F = 3$

A. Alexandru and U. Wenger, Phys. Rev. D83:034502 (2011)

- Dimension reduction in determinant calculation

$$\det M = \det Q \times \det[e^{-i\phi/2} + T \cdot U e^{i\phi/2}]$$

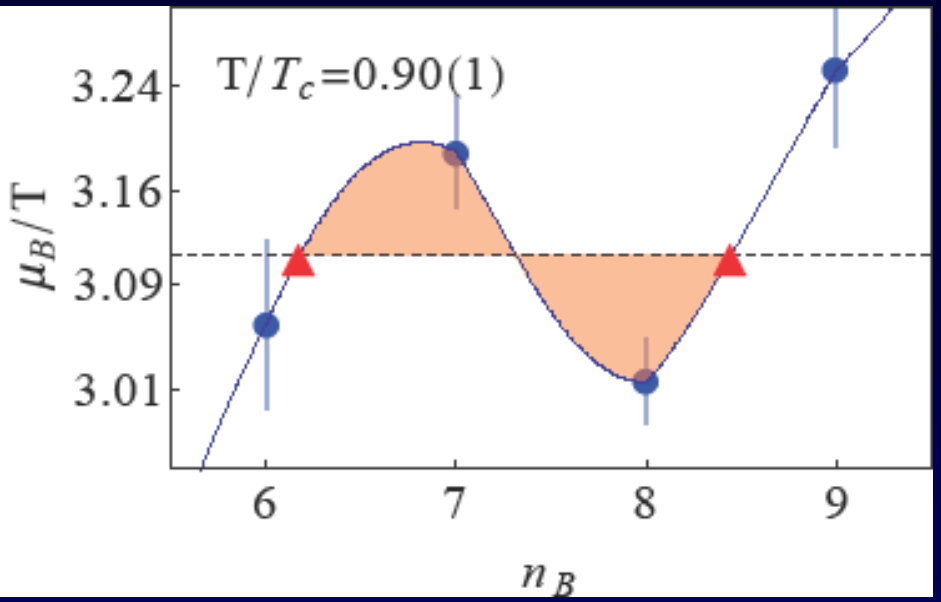
where the dimensions of Q and T·U are $4N_C L_S^3$.

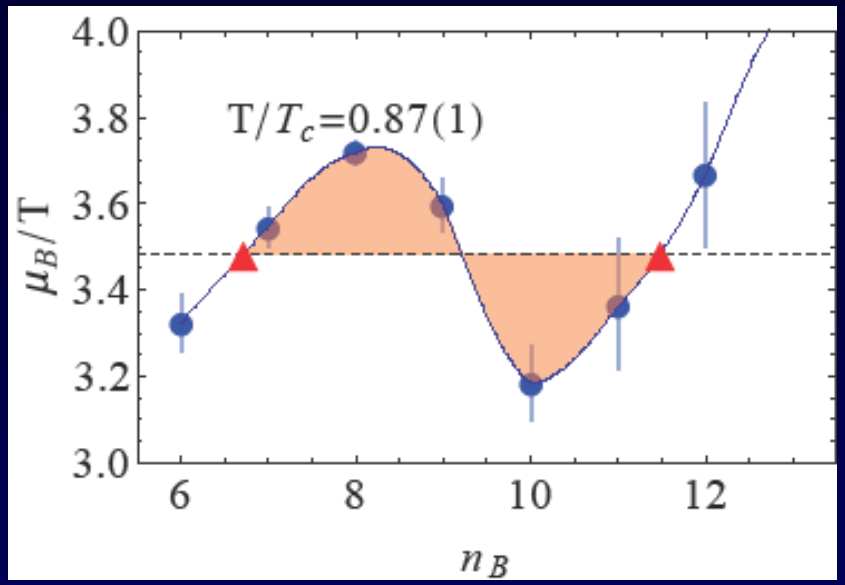
- Eigenvalues of the time-reduced matrix admits exact F.T.

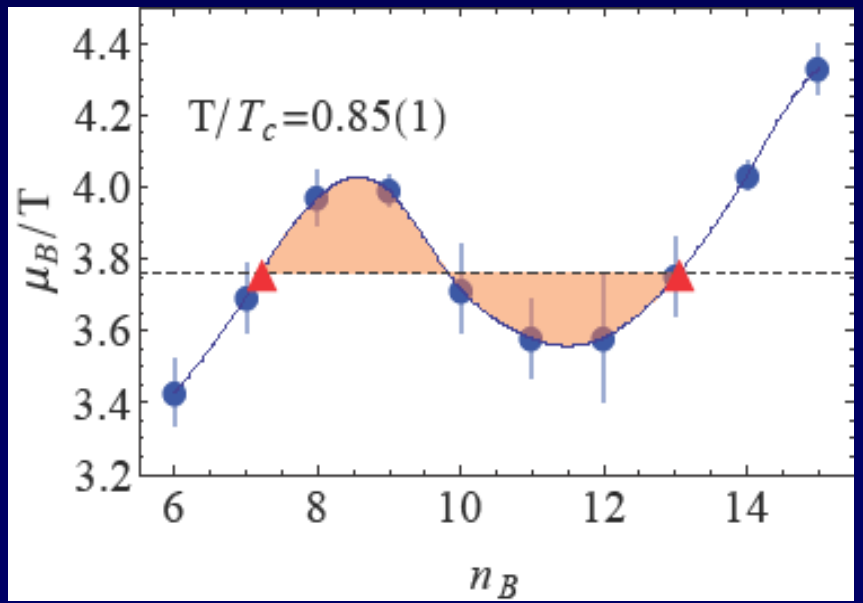
$$\det M = \det Q \times e^{i\phi 2 N_C L_S^3} \prod_{i=1}^{4 N_C L_S^3} (e^{-i\phi} + \lambda_i)$$

Three flavor case
(m_π ~ 0.7 GeV, a~ 0.3 fm)

6^3 x 4 lattice,
Clover fermion

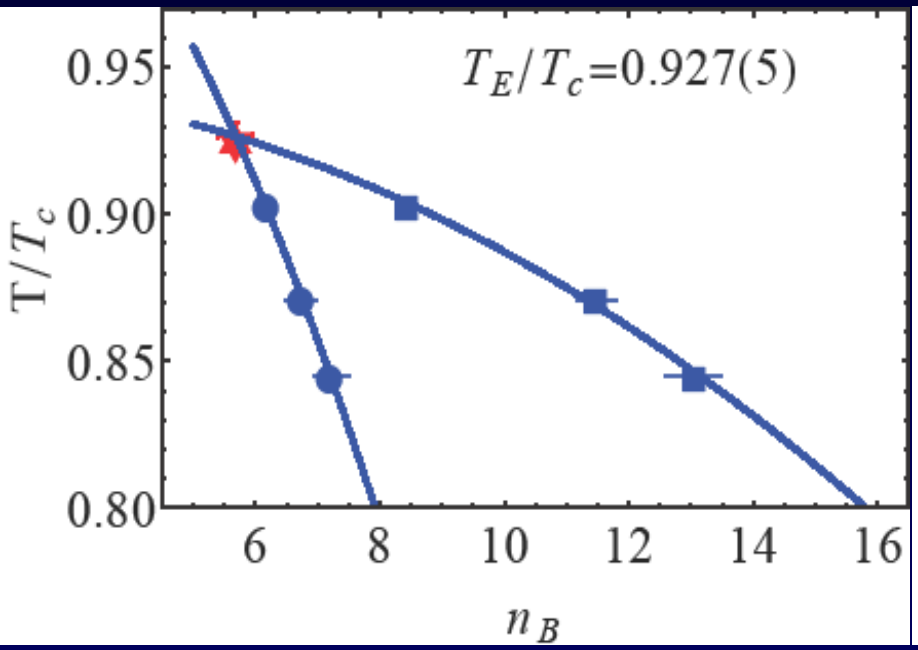


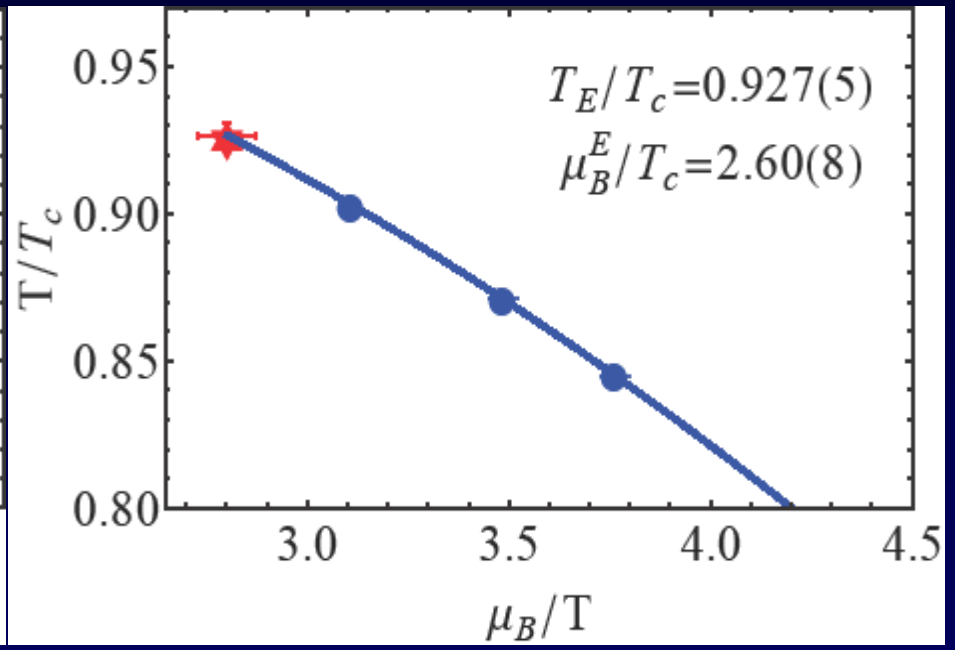




Critial Point of N_f = 3 Case

m_π ~ 0.7 GeV, 6^3 x 4 lattice, a ~ 0.3 fm





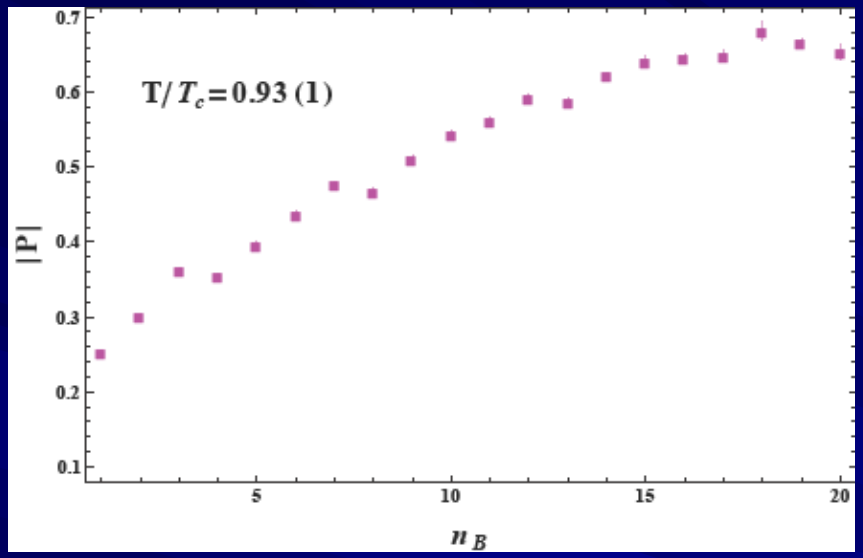
T_{CP} = 0.927(5) T_C (~ 157 MeV)

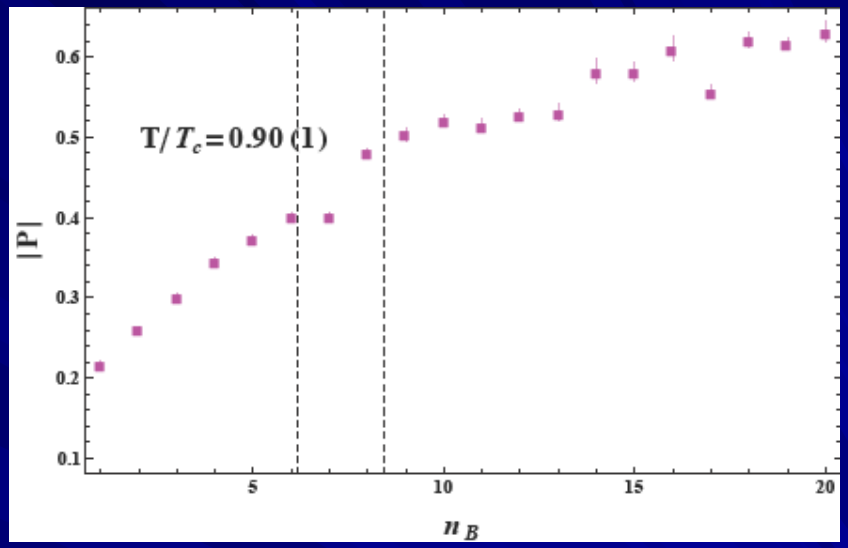
μ_{CP} = 2.60(8) T_C (~ 441 MeV)

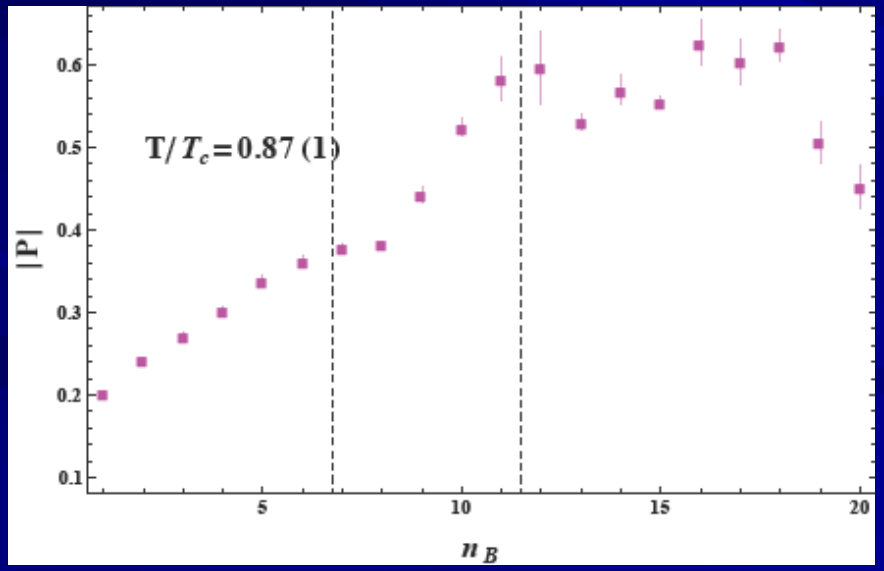
Transition density ~ 5-8 ρ_{NM}

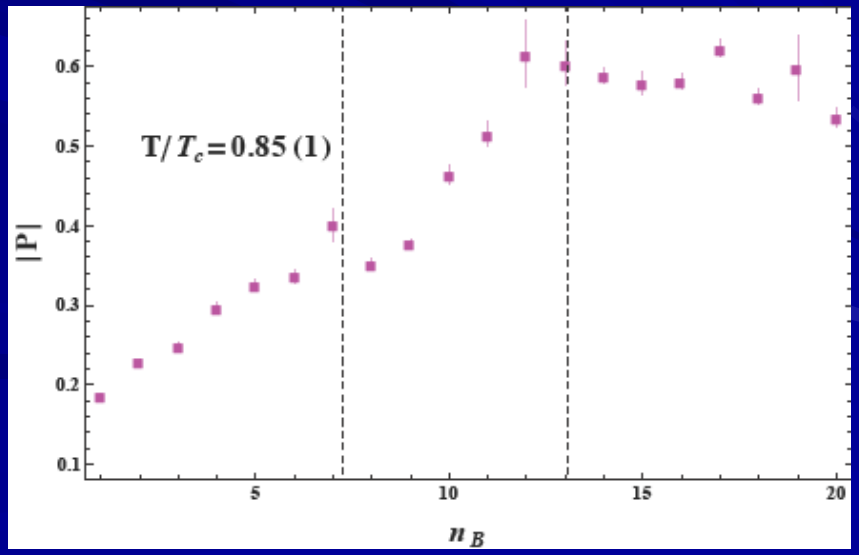
Nature of phase transition

Polyakov Loops

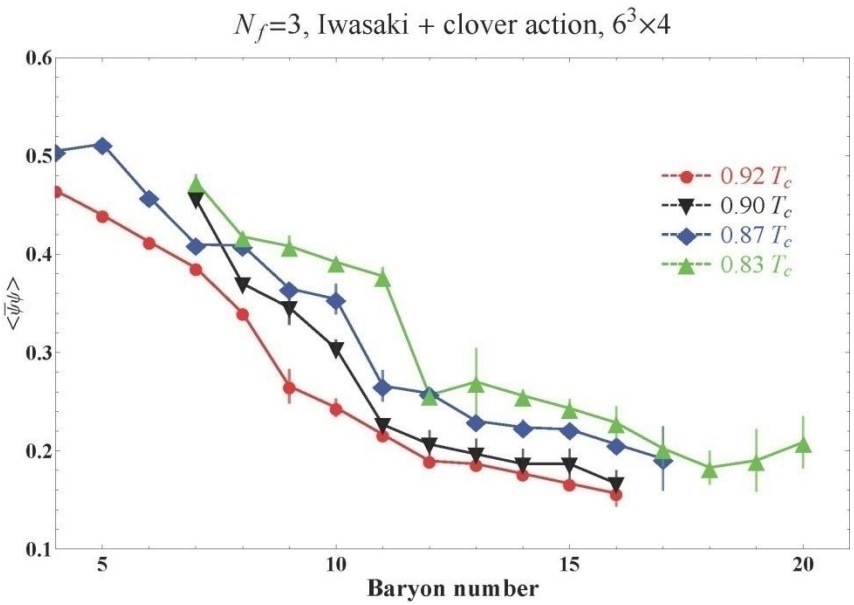


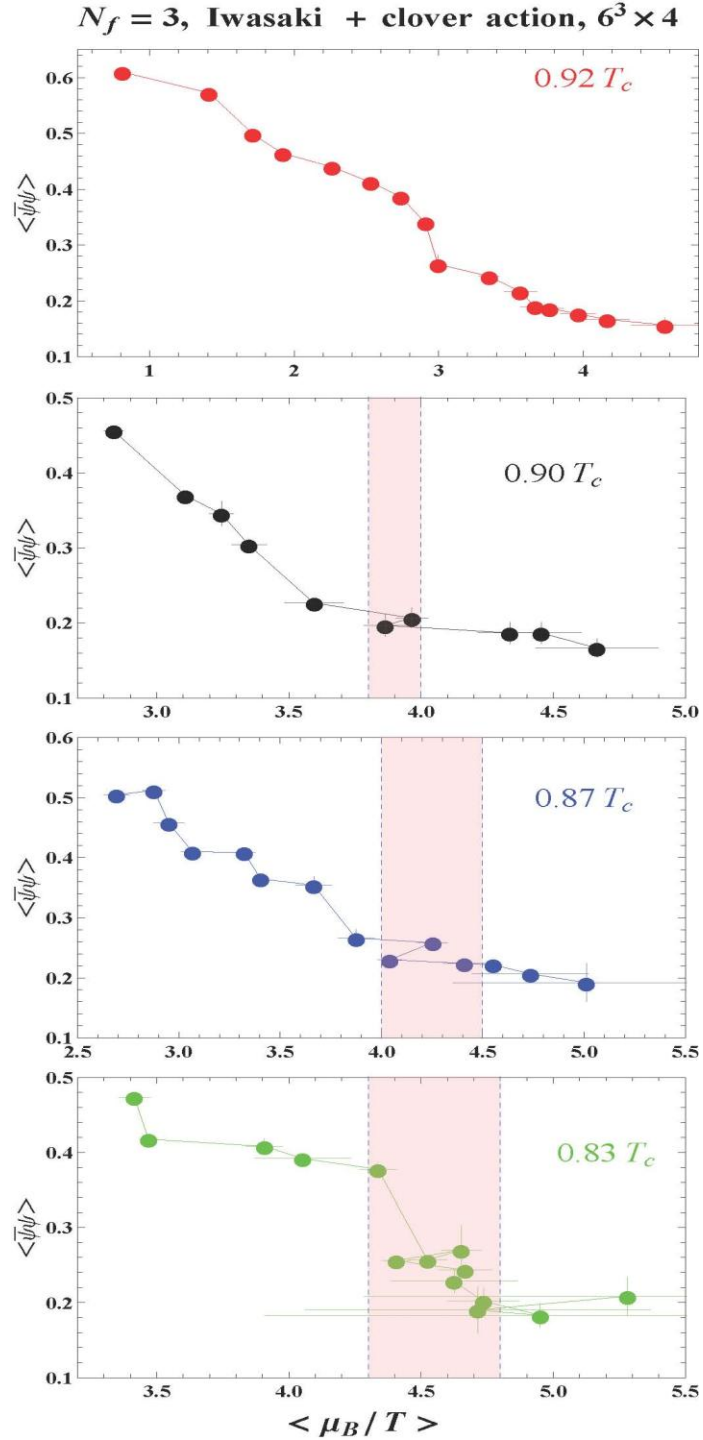




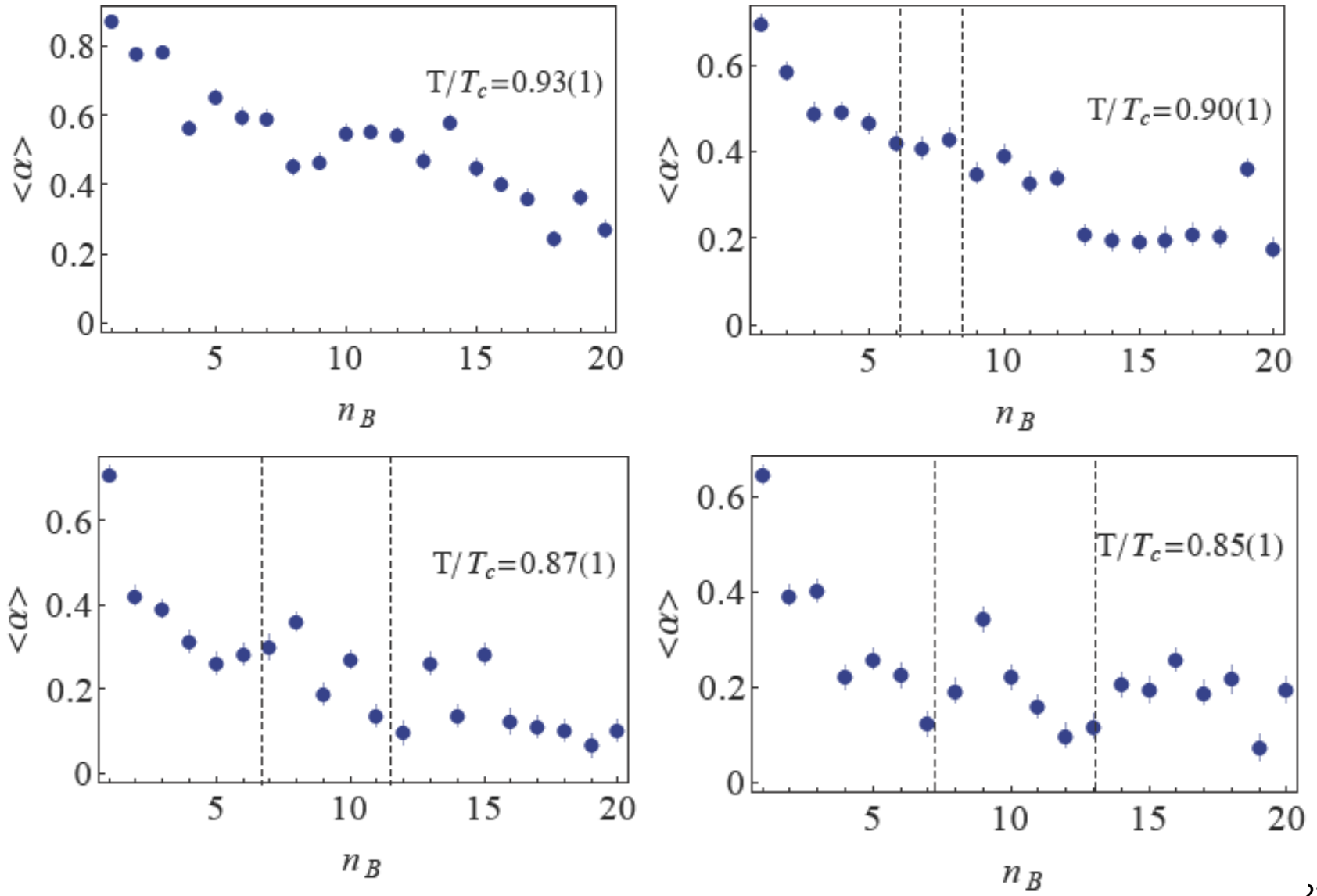


Quark Condensate





Sign Problem?



Fluctuations

- Fluctuations of the baryon number in grand canonical ensemble

$$\left\langle N^k \right\rangle_{GC} = T^{k-1} V \left(\frac{\partial^k p}{\partial \mu^k} \right)$$

- In canonical ensemble at the thermodynamic limit

$$F(V,T,N) \equiv -T \log Z_C(T,V,N)$$

$$\left\langle N^k \right\rangle_C = T \left(\frac{\partial \mu}{\partial N} \right)^{-1} \frac{\partial \left\langle N^{k-1} \right\rangle_C}{\partial N} = T \left(\frac{\partial^2 F}{\partial N^2} \right)^{-1} \frac{\partial \left\langle N^{k-1} \right\rangle_C}{\partial N};$$

$$\left\langle N^2 \right\rangle_C = \left\langle N^2 \right\rangle - \left\langle N \right\rangle^2 = T \left(\frac{\partial \mu}{\partial N} \right)^{-1};$$

$$\left\langle N^3 \right\rangle_C = \left\langle N^3 \right\rangle - \left\langle N \right\rangle^3 = T^{-3} \left(\frac{\partial \mu}{\partial N} \right)^{-3} \frac{\partial^3 F}{\partial N^3}.$$

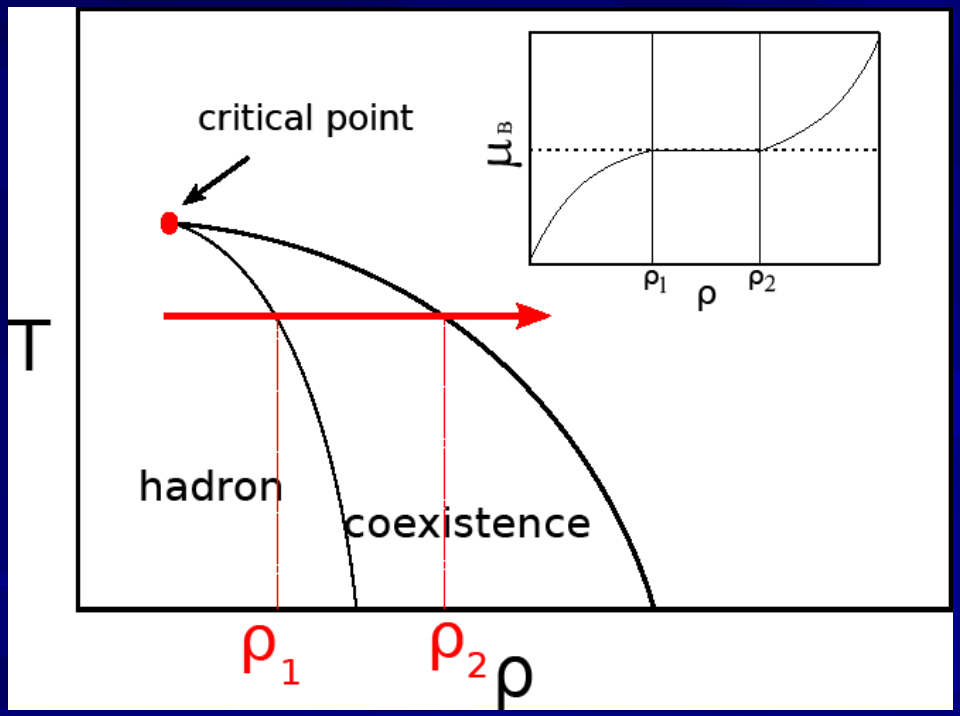
- The second moment is evaluated by

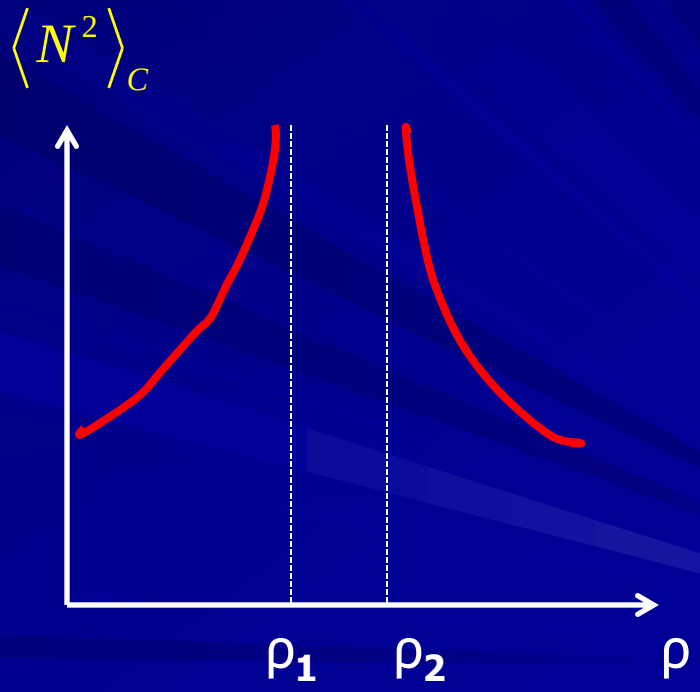
$$\left\langle N^2 \right\rangle_C^{-1} = \log Z_C(N+1) + \log Z_C(N-1) - 2 \log Z_C(N)$$

$$= \log \left\langle \frac{\det_{3(N+1)} M}{\det_{3N} M} \right\rangle + \log \left\langle \frac{\det_{3(N-1)} M}{\det_{3N} M} \right\rangle$$

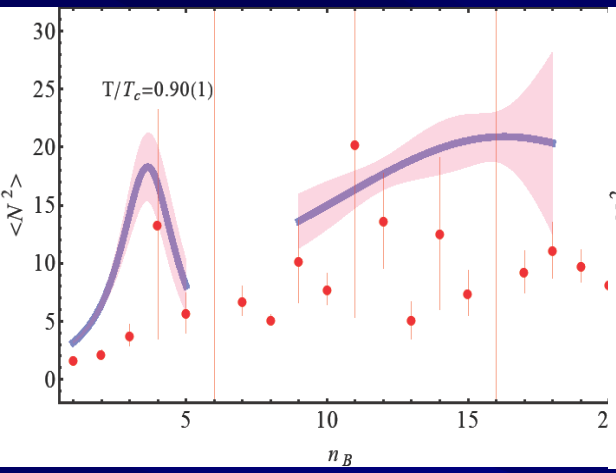
Variance

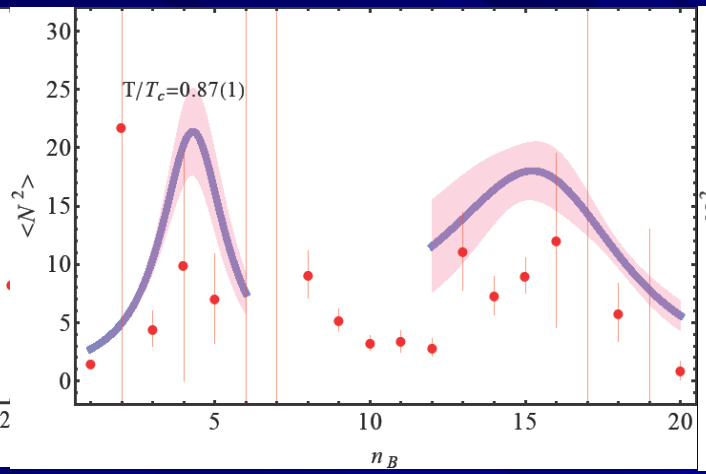
$$\langle N^2 \rangle_C = T \left(\frac{\partial \mu}{\partial N} \right)^{-1}$$

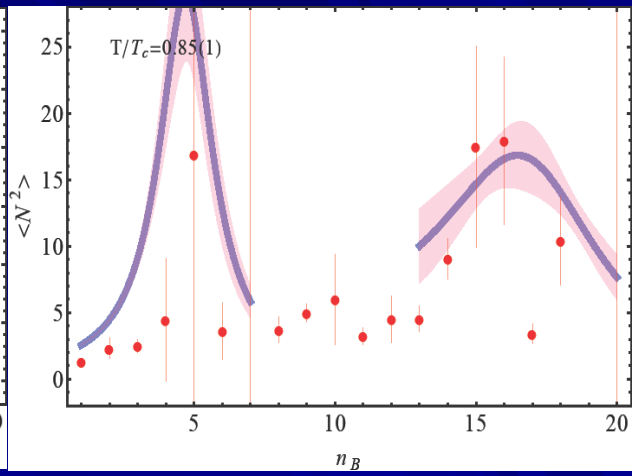


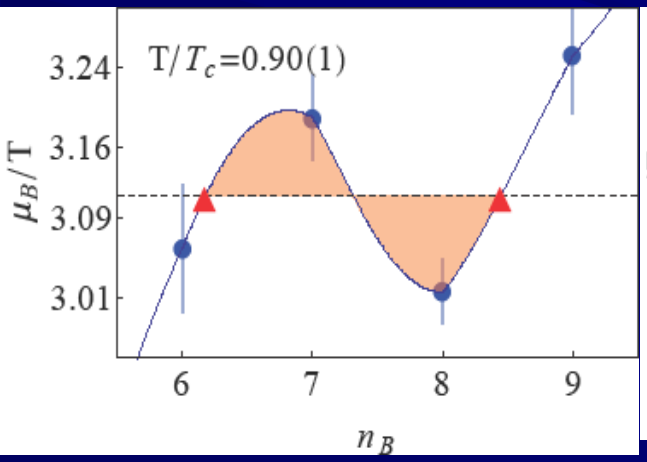


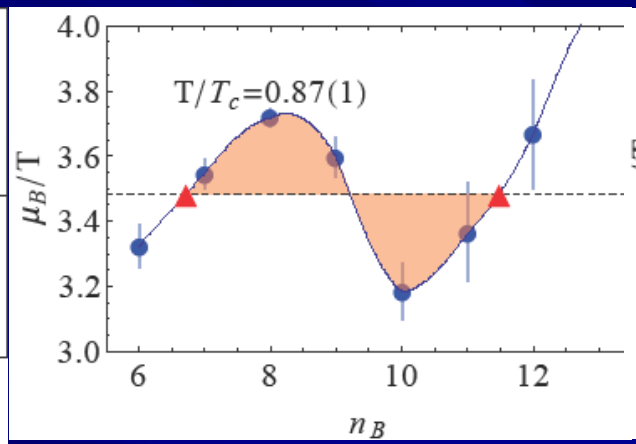
Second moment <N²>

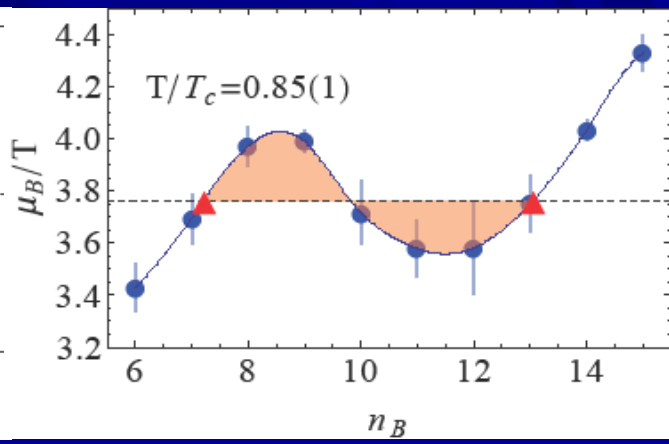


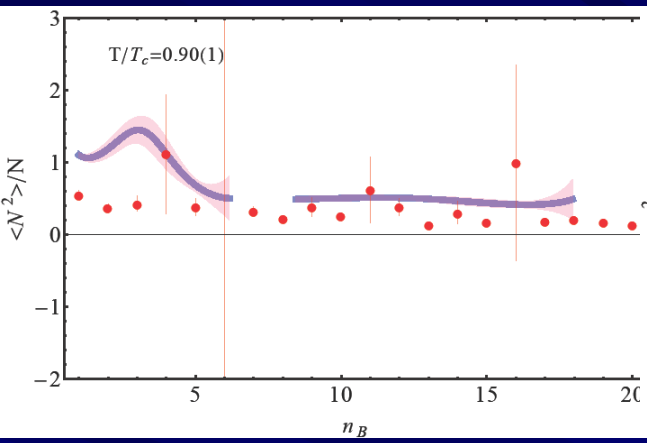


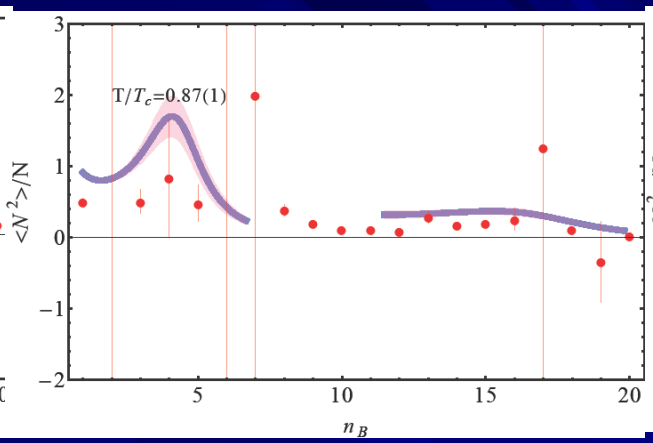


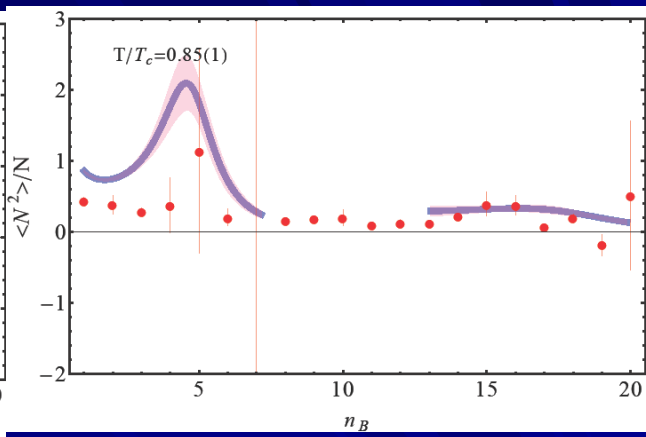


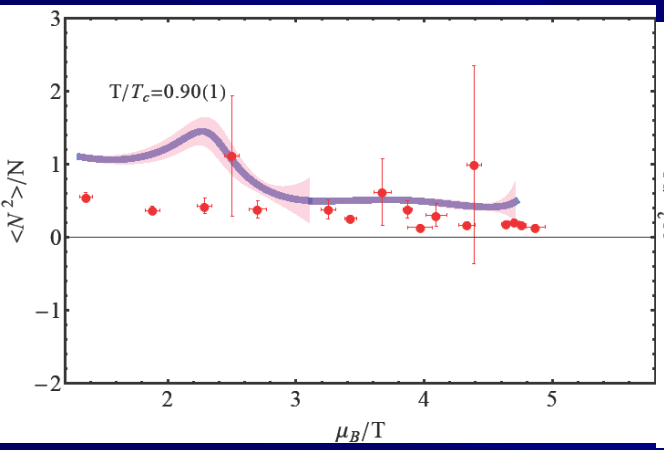


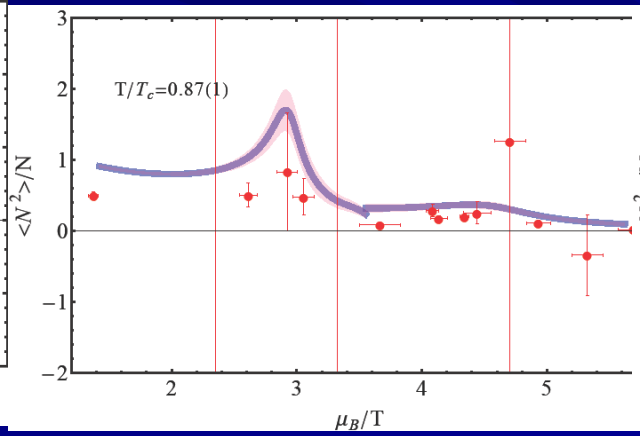


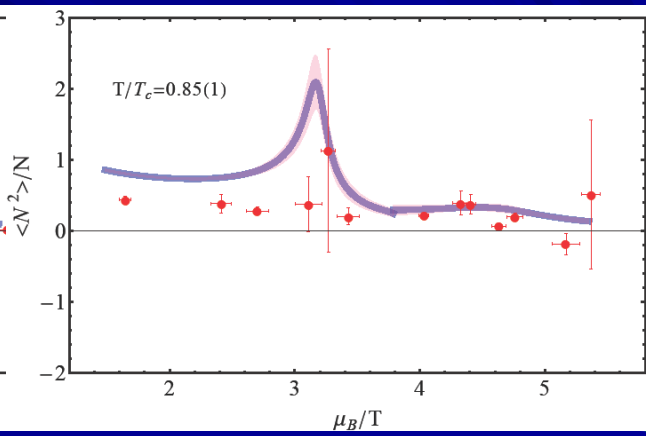

T/T_c=0.90(1)
$<N^2>/N$
n_B


T/T_c=0.87(1)
$<N^2>/N$
n_B

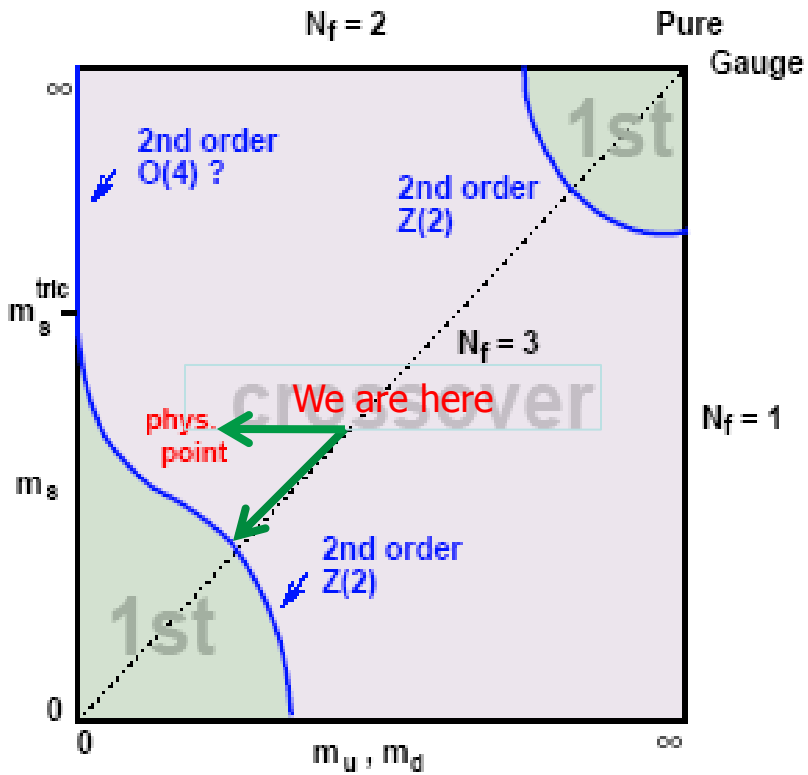

T/T_c=0.85(1)
$<N^2>/N$
n_B


T/T_c=0.90(1)
$<N^2>/N$
μ_B/T


T/T_c=0.87(1)
$<N^2>/N$
μ_B/T

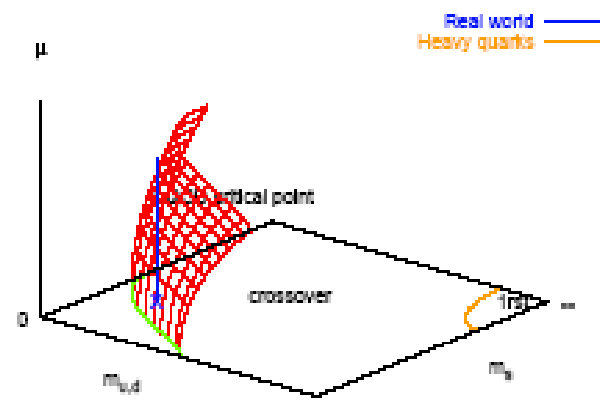

T/T_c=0.85(1)
$<N^2>/N$
μ_B/T

Two different scenarios

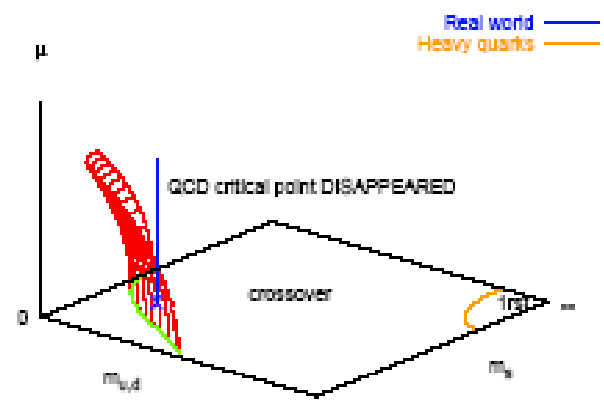


Philippe de Forcrand, Owe Philipsen arXiv:0811.3858v1 [hep-lat]

$$\partial m_c^2/\partial \mu^2 > 0$$



$$\partial m_c^2/\partial \mu^2 < 0$$



Challenges for more realistic calculations

- Smaller quark masses: HYP smearing, larger volume.
- Larger volume:
  - larger quark number k to maintain the same baryon density → numerically more intensive to calculate the projected determinant (L_s^9).
  - Unbiased estimator of determinant.
  - Acceptance rate and sign problem → isospin chemical potential in HMC and A/R with $\det_k$.

Summary

- Calculation with small volume and large quark mass notwithstanding, direct observation of the first order phase transition and the critical point is afforded in the canonical ensemble approach.
- Problem with precise numerical evaluation of $\det_k$ for large k is overcome.
- Simulations at smaller quark masses and larger volumes free from acceptance rate and sign problems are essential to the full understanding of the realistic situation.