Finite Density Phase Transition with Canonical Ensemble Approach

- Finite Density Algorithm with Canonical Approach
- Results on N_F = 2, and 4 with Wilson Fermion and N_F = 3 with Clover Fermion

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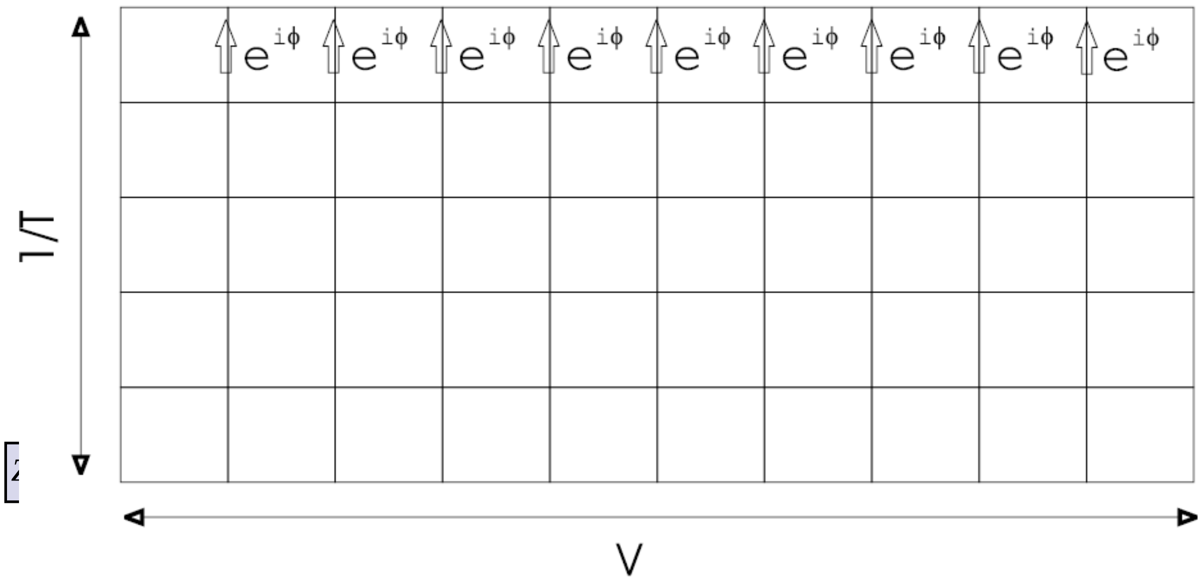
XQCD, July 23, 2008

- Finite density calculations:
  - Fugacity Expansion
  - Multi-parameter Reweighting
  - Taylor Expansion
  - Imaginary Chemical Potential
  - Canonical Ensemble with Reweighting
  - …

Canonical partition function

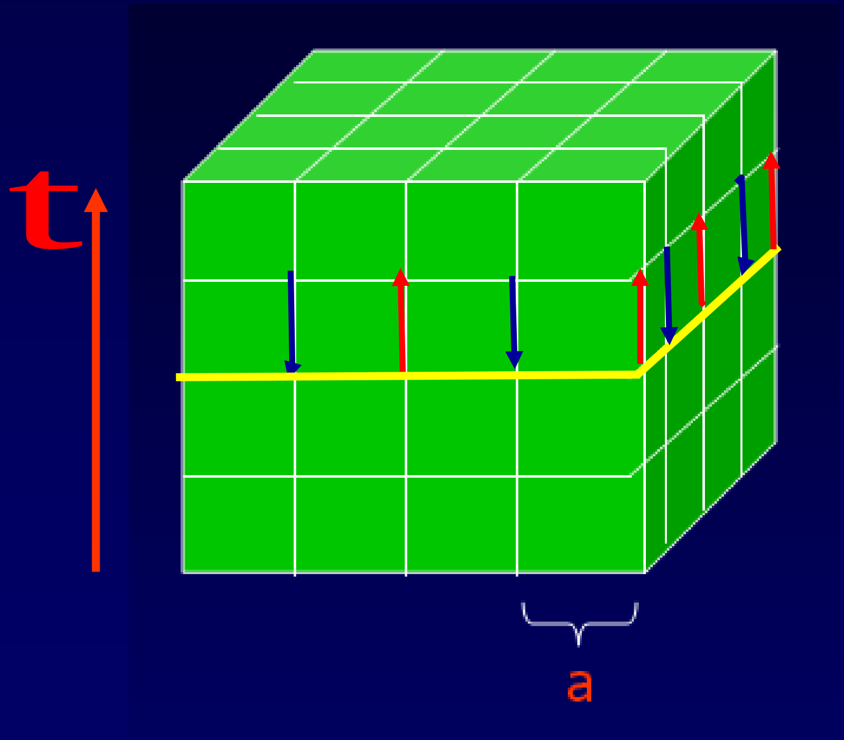


Using the fugacity expansion $Z_{GC}(V,\mu,T)=\sum_{k=-4V}^{k=4V} Z_C(V,k,T)e^{\frac{\mu}{T}k}$ we get

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

- Canonical Ensemble Approach:

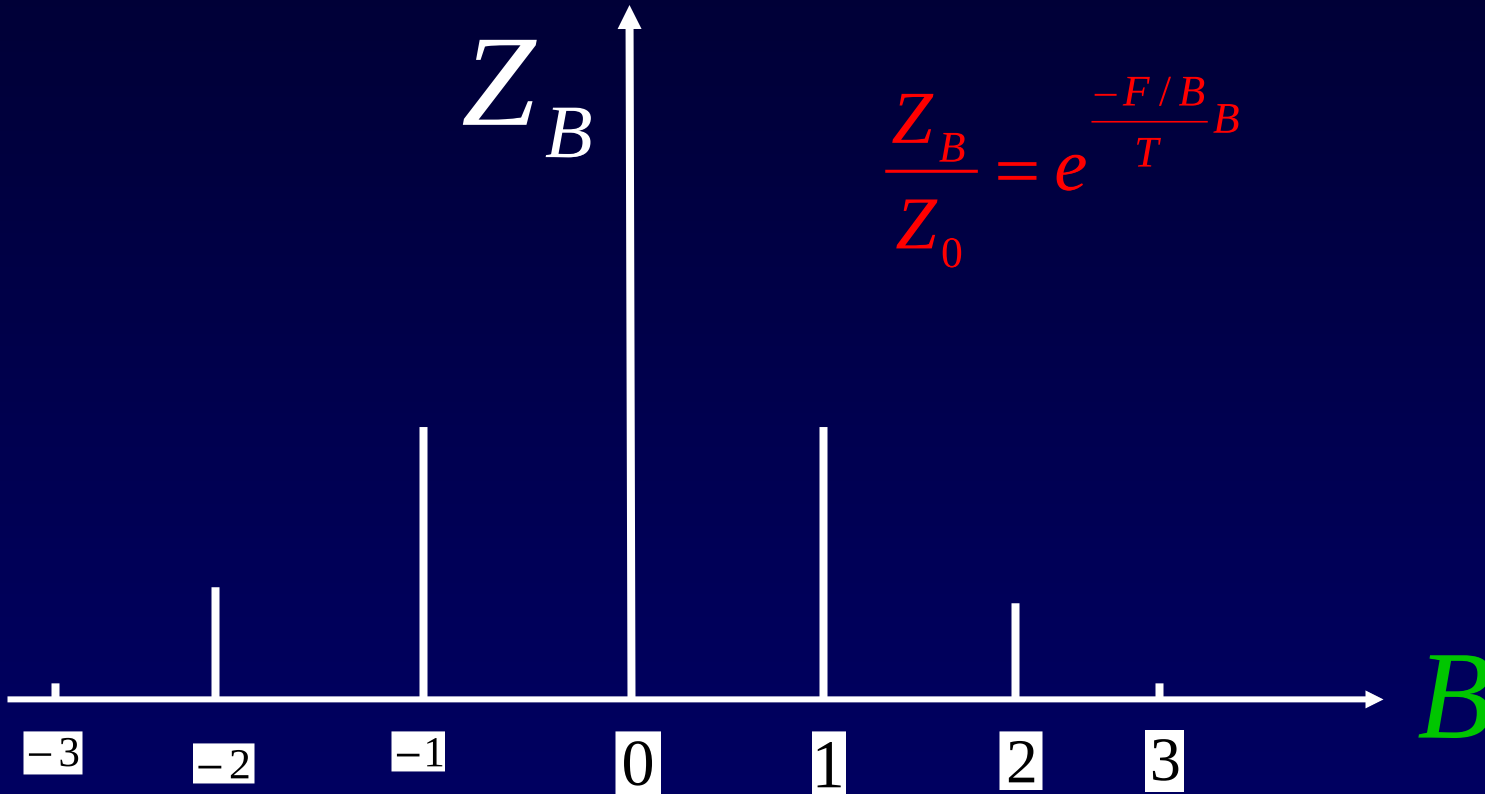
$$Z_B(T,V) = \frac{\beta}{2\pi}\int_0^{2\pi/\beta} d\mu\, Z_{GC}(i\mu) e^{-i\beta\mu B}$$
$$= \int DU\, e^{-S_g} \int_0^{2\pi} d\varphi / 2\pi\, e^{-i3B\varphi} \det M(\varphi);$$
$$M(\theta)_{m,n} = \delta_{m,n} - \kappa[(1+\gamma_4)U_4^+(n)e^{i\phi}\delta_{m,n+4} + (1-\gamma_4)U_4 e^{-i\varphi}(m)\delta_{m+4,n} + \ldots]$$



$$\det M = e^{Tr \log M(\theta)}$$

is real

Overlap Problem



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

- Avoid the Overlap Problem
  - KFL (Int. Jou. Mod. Phys. B16, 2017 (2002))

- The earlier procedure $$\frac{Z_{GC}(i\mu)}{Z_{GC}(i\mu_{update})} = \langle \frac{\det M(i\mu)}{\det M(i\mu_{update})} \rangle$$

  is like projection after variation (Peierls and Yoccoz)

- Need variation after projection (Zeh-Rouhaninejad-Yoccoz)

$$Z_B(T,V) = \int DU\, e^{-S_g} \left[\int_0^{2\pi} d\varphi / 2\pi\, e^{-i3B\varphi} \det M(\varphi) \right]$$

- Accept/reject based on $\det_B$.

➢ Unfortunately, this introduces fluctuation problem!

Because $$\det M = e^{Tr \log M} \sim O(e^V)$$

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

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

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

Discrete Fourier transform

$$\widetilde{\det}_k M^2(U) \equiv \frac{1}{N}\sum_{j=0}^{N-1} e^{-ik\phi_j} \det M^2(U_{\phi_j}) \qquad \phi_j = \frac{2\pi j}{N}$$

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

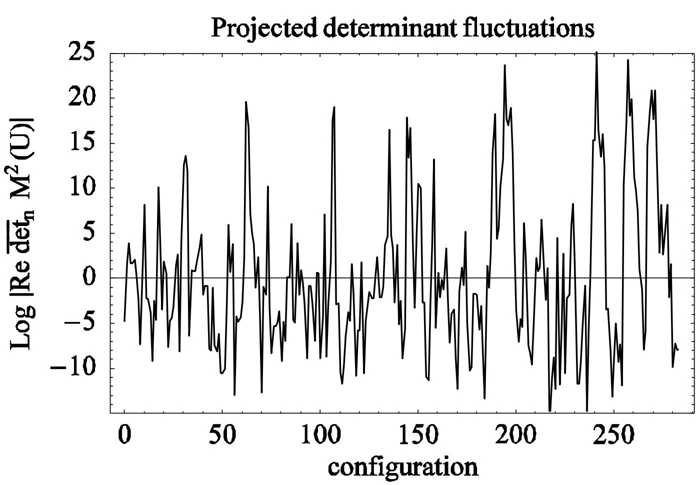
$$log \det M(U_\phi)$$ WNEM

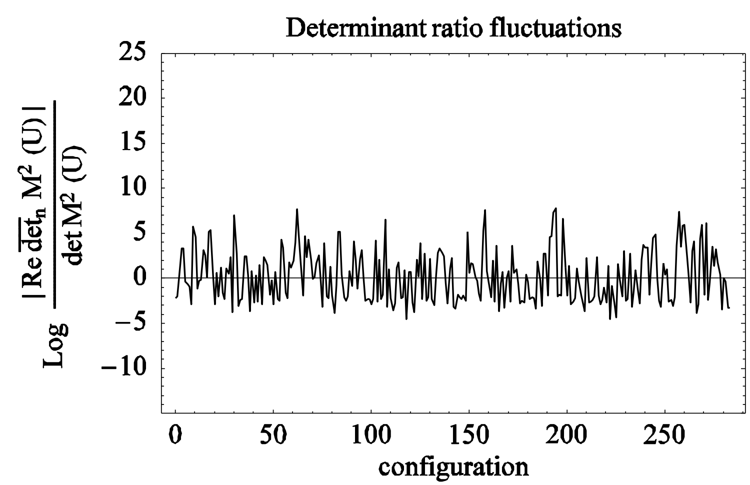
Continues Fourier transform
Useful for large k

Fluctuations

$$\underbrace{\int DU\, e^{-S_G(U)}}_{\text{Heath bath}} \underbrace{\left|\mathrm{Re}\det_n M^2(U)\right|}_{\text{Accept/Reject}}$$

$$\underbrace{\int DU\, e^{-S_G(U)} \det M^2(U,0)}_{\text{Standard HMC}} \underbrace{\frac{\left|\mathrm{Re}\det_n M^2(U)\right|}{\det M^2(U,0)}}_{\text{Accept/Reject}}$$





Instability of discrete Fourier transform

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

It's difficult to pick up the high frequency modes with discrete Fourier transform

k	3	6	9	12	15
N=51	2212.21	247.601	-22.8783	-4.53755	-0.233997
N=102	2212.21	247.601	-22.8783	-4.53755	-0.233997
N=204	2212.21	247.601	-22.8783	-4.53755	-0.233997
k	18	21	24	27	30
N=51	-0.00545724	-0.0000602919	6.70879E-7	6.70879E-7	-0.0000602919
N=102	-0.005458	-0.0000631063	-8.98294E-7	1.56917E-6	2.81435E-6
N=204	-0.005458	-0.0000634881	-1.66312E-6	-2.83726E-7	6.42123E-6

Winding number expansion (I)

In QCD

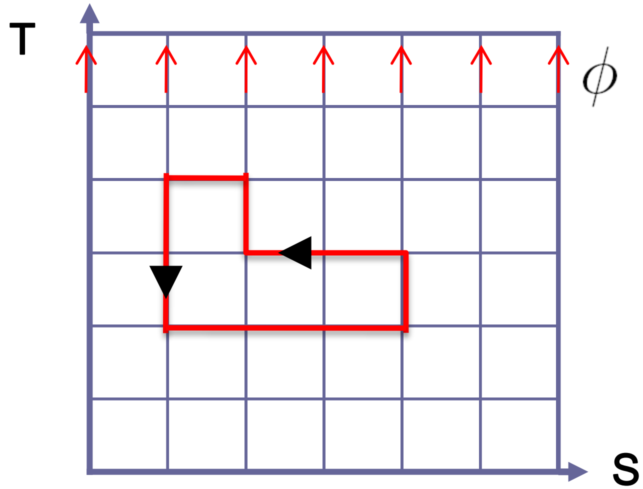
Tr log $\longrightarrow$ loop $\longrightarrow$ loop expansion

In particle number space

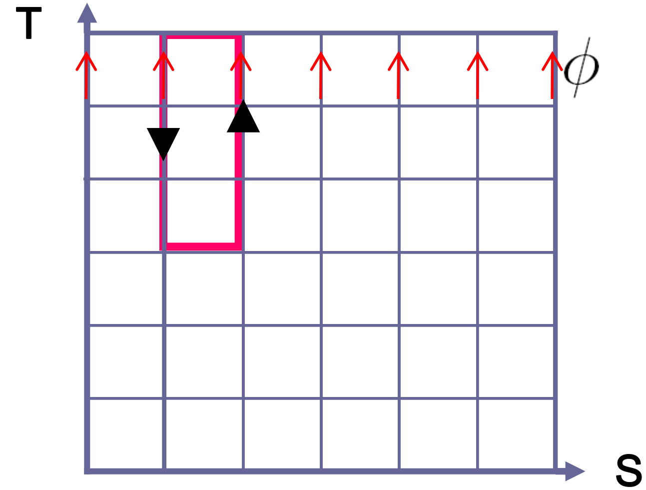
$$\begin{aligned} TrlogM(U,\phi) &= A_0(U) + \Sigma loop(U,\phi) \\ &= A_0(U) + [\sum_k e^{ik\phi} W_k(U) + e^{-ik\phi} W_k^\dagger(U)] \end{aligned}$$

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

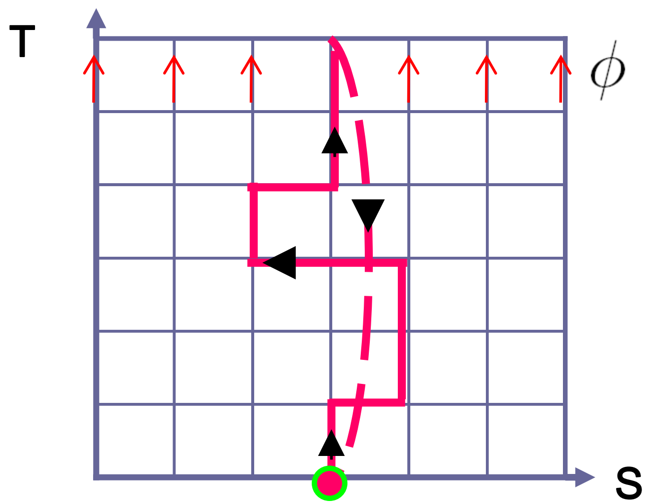
$$\begin{aligned} TrlogM(U,\phi) &= A_0(U) + [\sum_k e^{ik\phi} W_k(U) + e^{-ik\phi} W_k^\dagger(U)] \\ &= A_0(U) + \sum_k A_k \cos(k\phi + \delta_k)|_{A_k = 2|W_k|, \delta_k = \delta_{W_k}} \end{aligned}$$



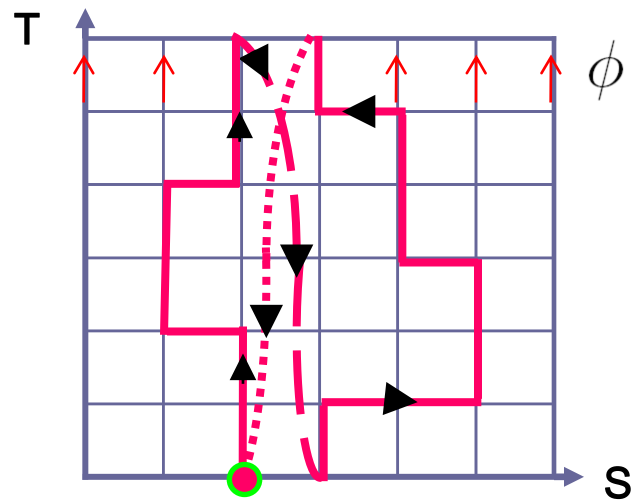
A_0



A_0



A_1



A_2

Winding number expansion (II)

For

$$detM(U,\phi) = \exp(TrlogM(U,\phi))$$

So

$$\log detM(U,\phi) = A_0 + A_1\cos(\phi+\delta_1) + A_2\cos(2\phi+\delta_2) + ...$$

$$detM(U,\phi) = \exp[A_0 + A_1\cos(\phi+\delta_1) + A_2\cos(2\phi+\delta_2) + ...]$$

The first order of winding number expansion

$$detM(U,\phi)_{k=1} = \exp(A_1\cos(\phi+\delta_1))$$

Here the important is that the FT integration of the first order term has analytic solution

$$\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ik\phi}e^{[A_1\cos(\phi+\delta_1)]} = e^{ik\delta_1}I_k(A_1)$$

$I_k(x)$ *is Bessel function of the first kind .*

Winding number expansion (III)

For higher order, Taylor expansion is used

$$
\begin{aligned}
&\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ik\phi}e^{A_1\cos(\phi+\delta_1)}e^{A_2\cos(\phi+\delta_2)+A_3\cos(\phi+\delta_3)+\ldots+A_6\cos(\phi+\delta_6)\ldots} \\
= \; &\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ik\phi}e^{A_1\cos(\phi+\delta_1)}(1+A_2\cos(2\phi+\delta_2)+\frac{1}{2!}A_2^2\cos(2\phi+\delta_2)^2+\ldots) \\
&(1+A_3\cos(3\phi+\delta_3)+\frac{1}{2!}A_3^2\cos(3\phi+\delta_3)^2+\ldots)*\ldots) \\
= \; &c_{00}I_k(A_1)+c_{+01}I_{k+1}(A_1)+c_{-01}I_{k-1}(A_1)+c_{+02}I_{k+2}(A_1)+c_{-02}I_{k-2}(A_1)+\ldots \\
&+c_{+26}I_{k+26}(A_1)+c_{-26}I_{k-26}(A_1)+\ldots
\end{aligned}
$$

Here, we use the Euler's formula to get the final expression

$$
\cos(k\phi+\delta_k) \;=\frac{1}{2}(\exp[i(k\phi+\delta_k)]+\exp[-i(k\phi+\delta_k)])
$$

Winding number expansion (IV)

The parameters of Winding number expansion---Fourier series

$$f(\phi) = \frac{1}{2}a_0 + \sum_{k=1}^{\infty} a_k cos(k\phi) + \sum_{k=1}^{\infty} b_k sin(k\phi)$$

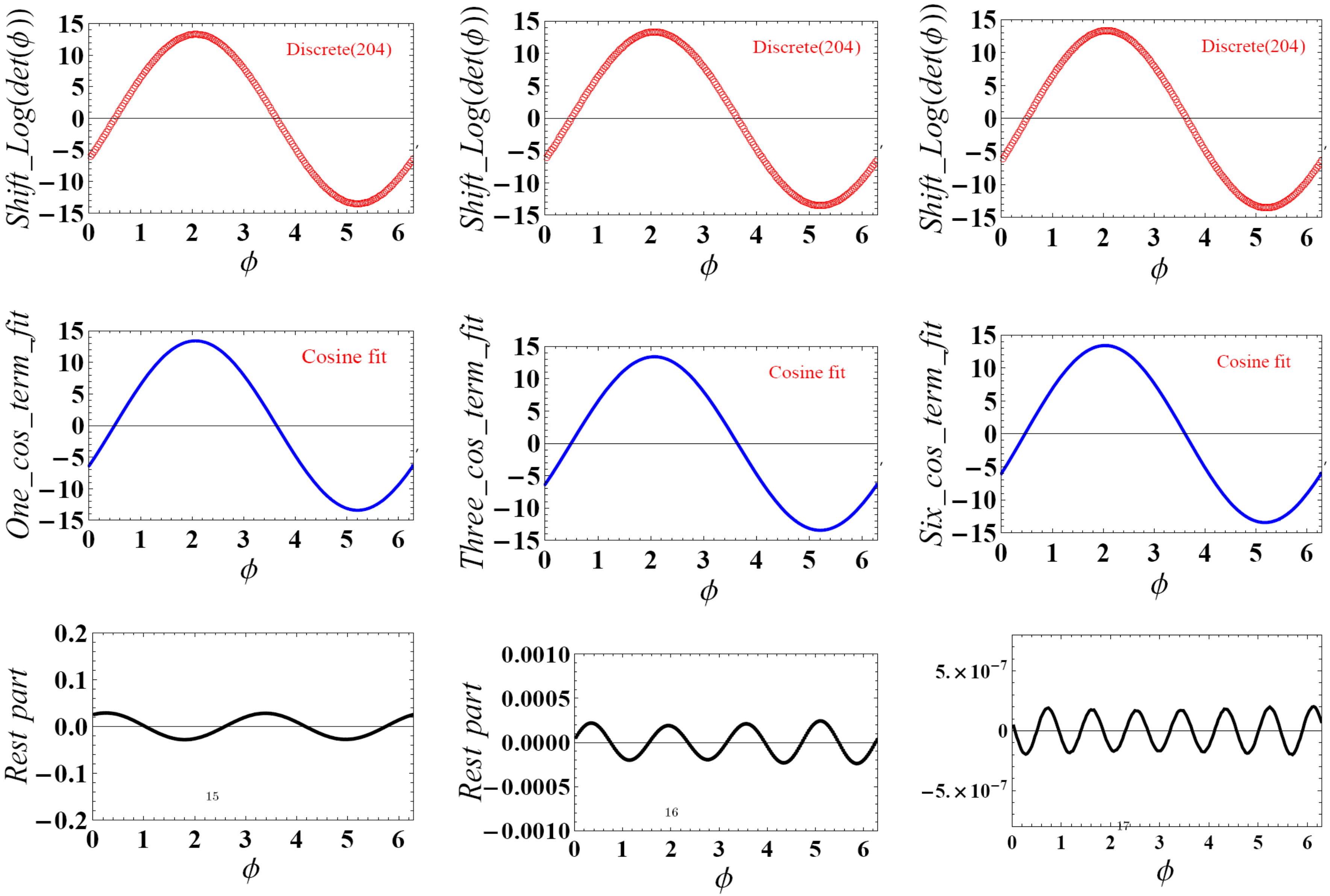
$$\delta_k = arctan(\frac{-b_k}{a_k})$$

$$A_k = \frac{a_k}{cos(\delta_k)}$$

The recursion of Bessel function

$$I_{k-1}(A) = \frac{2k}{A} I_k(A) + I_{k+1}(A)$$

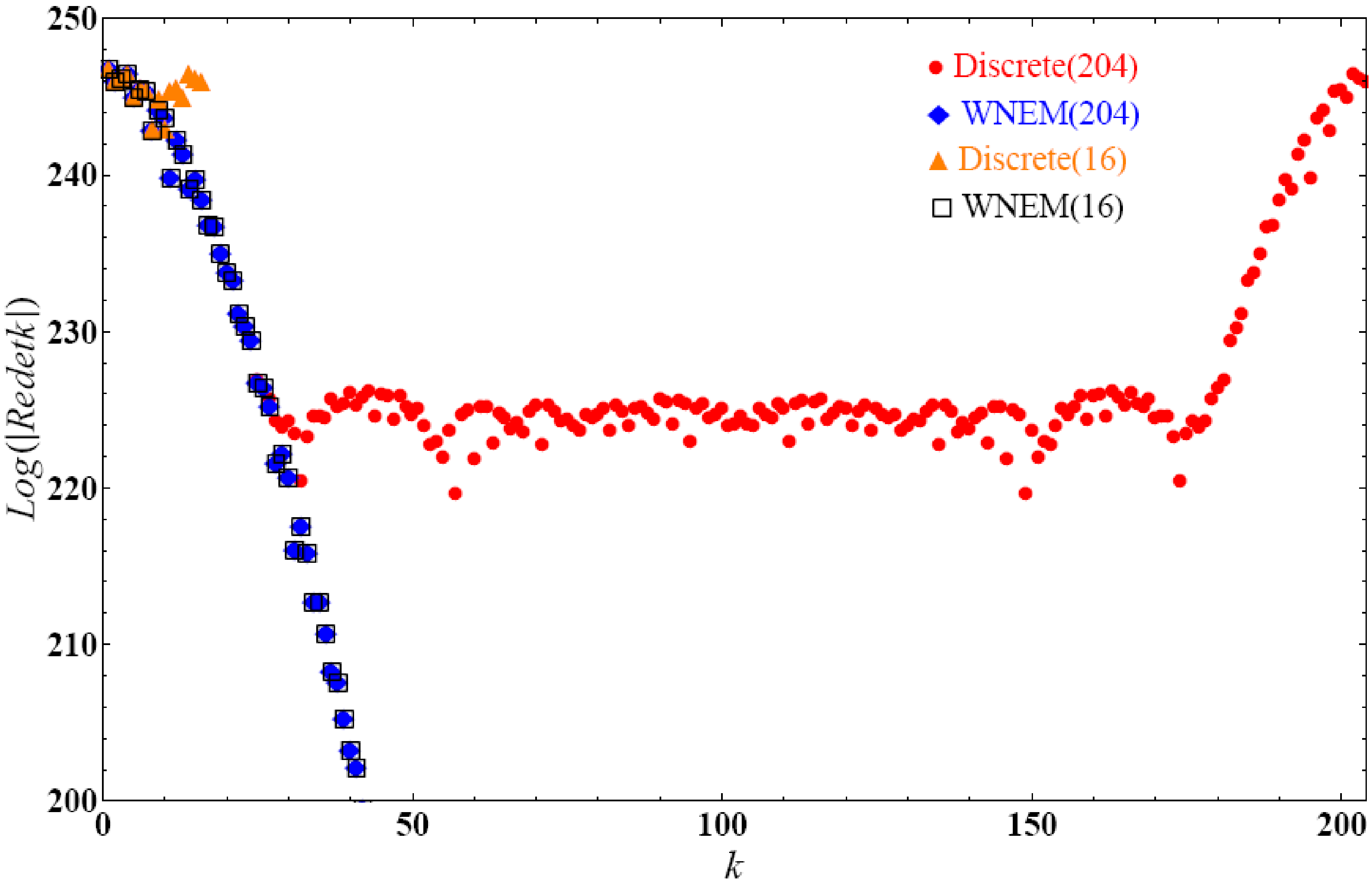
Winding number expansion test (I)



Winding number expansion test (II)

	Nd=16	Nd=24	Nd=36	Nd=200
A0	2.357308e+02	2.357308e+02	2.357308e+02	2.357308e+02
A1	-1.341400e+01	-1.341400e+01	-1.341400e+01	-1.341400e+01
A2	2.820535e-02	2.820535e-02	2.820534e-02	2.820534e-02
A3	4.135219e-04	4.135043e-04	4.134942e-04	4.134755e-04
A4	2.148188e-04	2.147950e-04	2.147792e-04	2.147547e-04
A5	2.641758e-05	2.639153e-05	2.637794e-05	2.636227e-05
A6	2.289491e-06	2.286772e-06	2.291285e-06	2.305249e-06

Winding number expansion test (III)



Observables

Polyakov loop

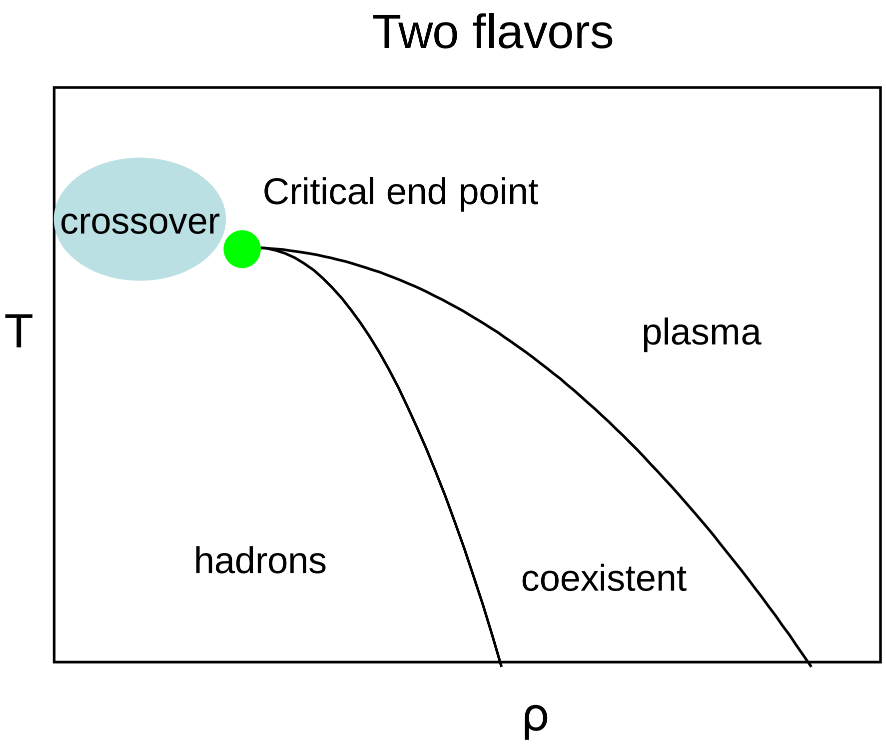
$$\langle |P| \rangle_{k'} = \frac{\langle R(U,k') |P(U)| \rangle_0}{\langle R(U,k') \rangle_0} \qquad R(U,k') = \frac{\widetilde{\det}_k M^2(U)}{|\,\mathrm{Re}\,\widetilde{\det}_k M^2(U)|}$$

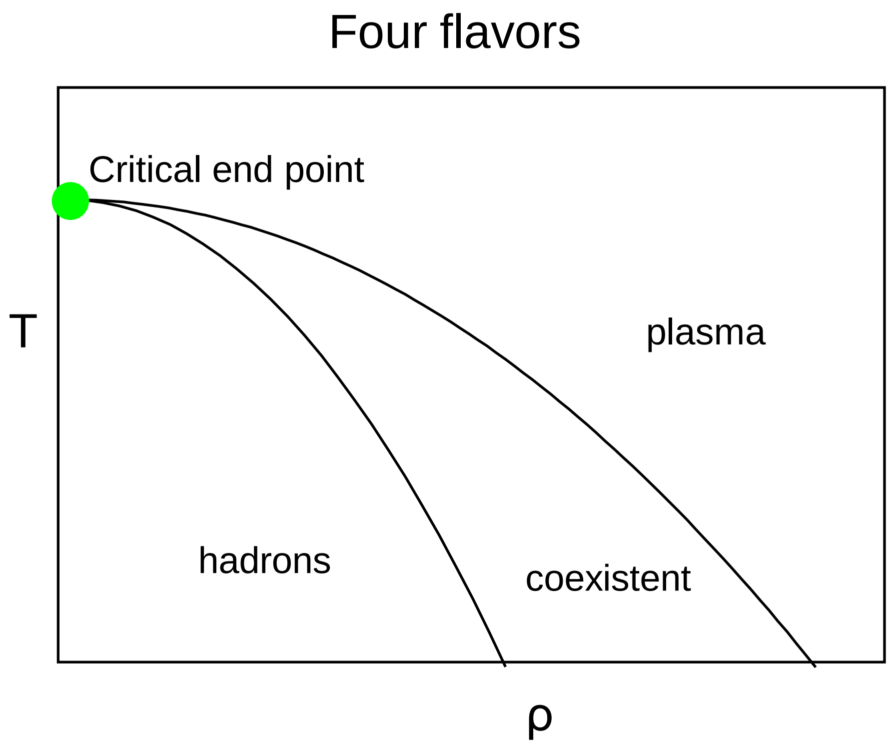
Phase

Baryon chemical potential

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

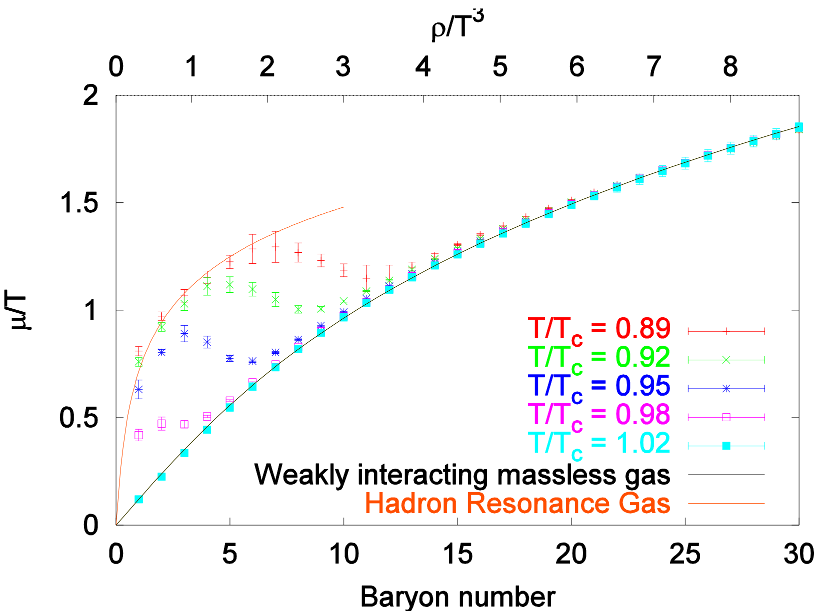
Phase diagram

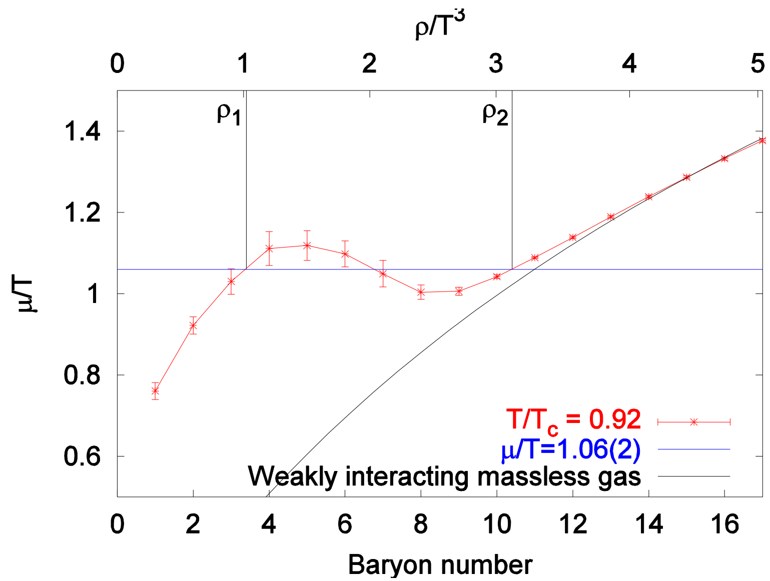




Phase boundary

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

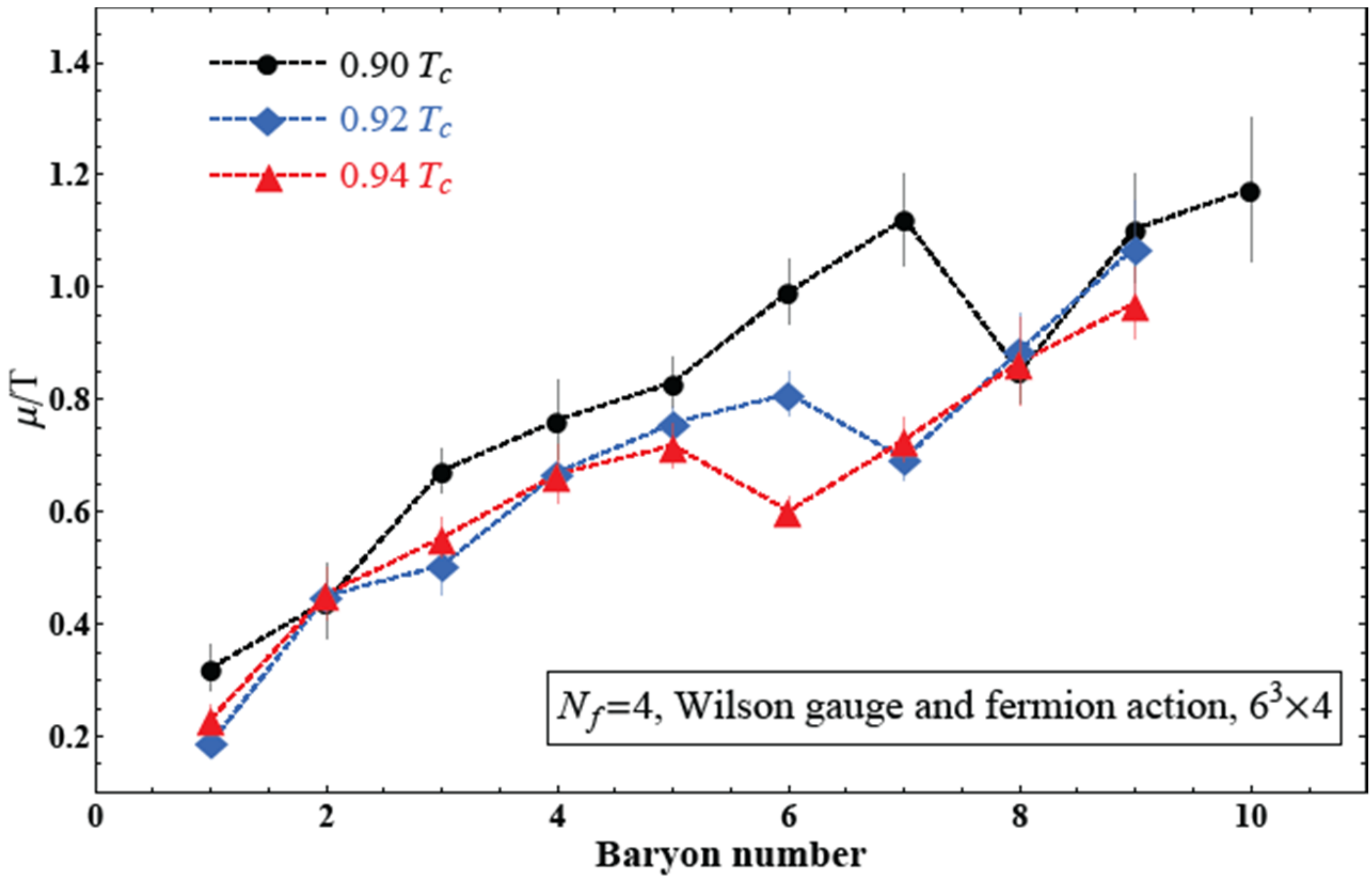




Maxwell construction : determine phase boundary

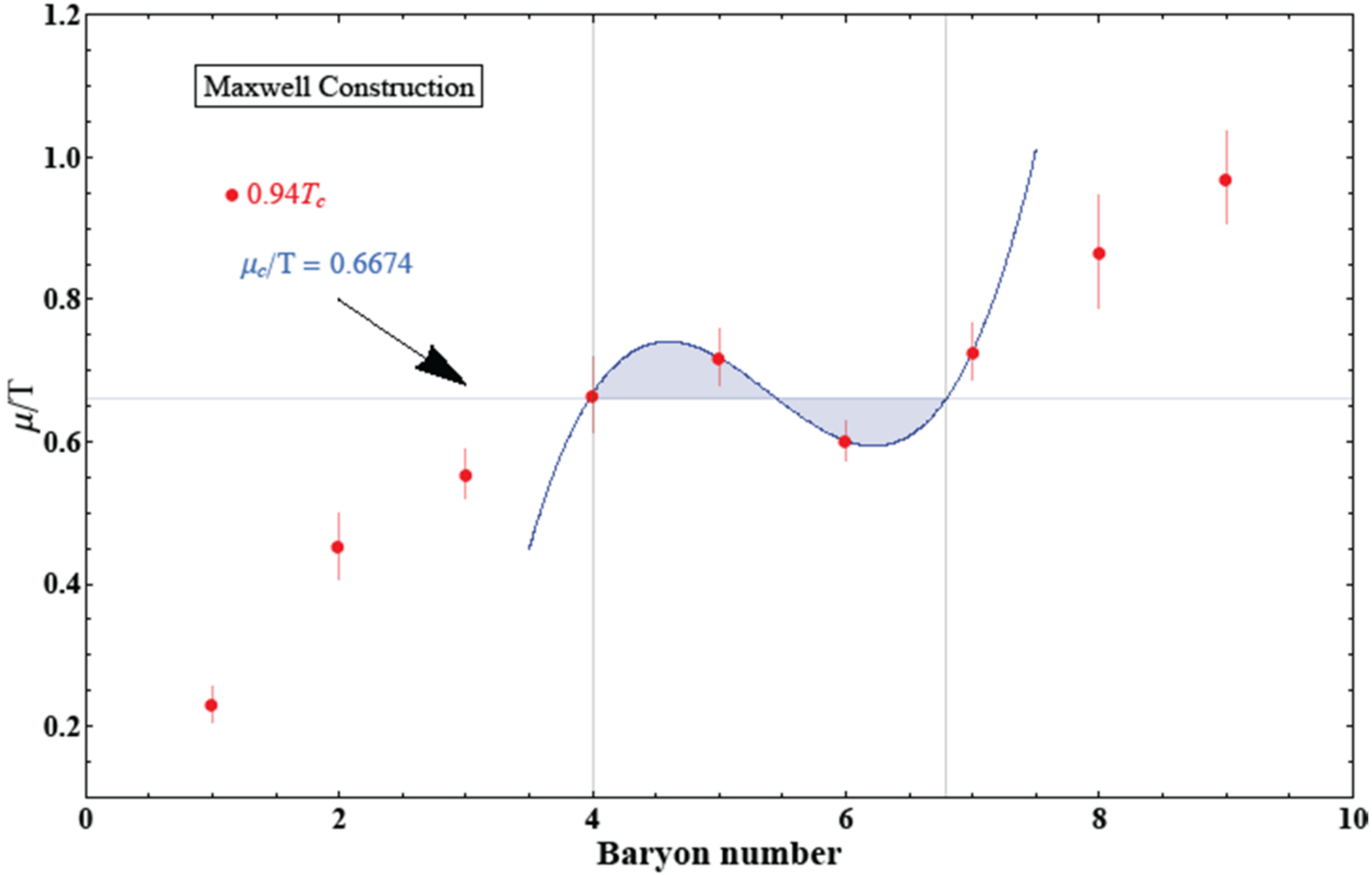
Baryon Chemical Potential

N_f = 4 Wilson gauge + fermion action



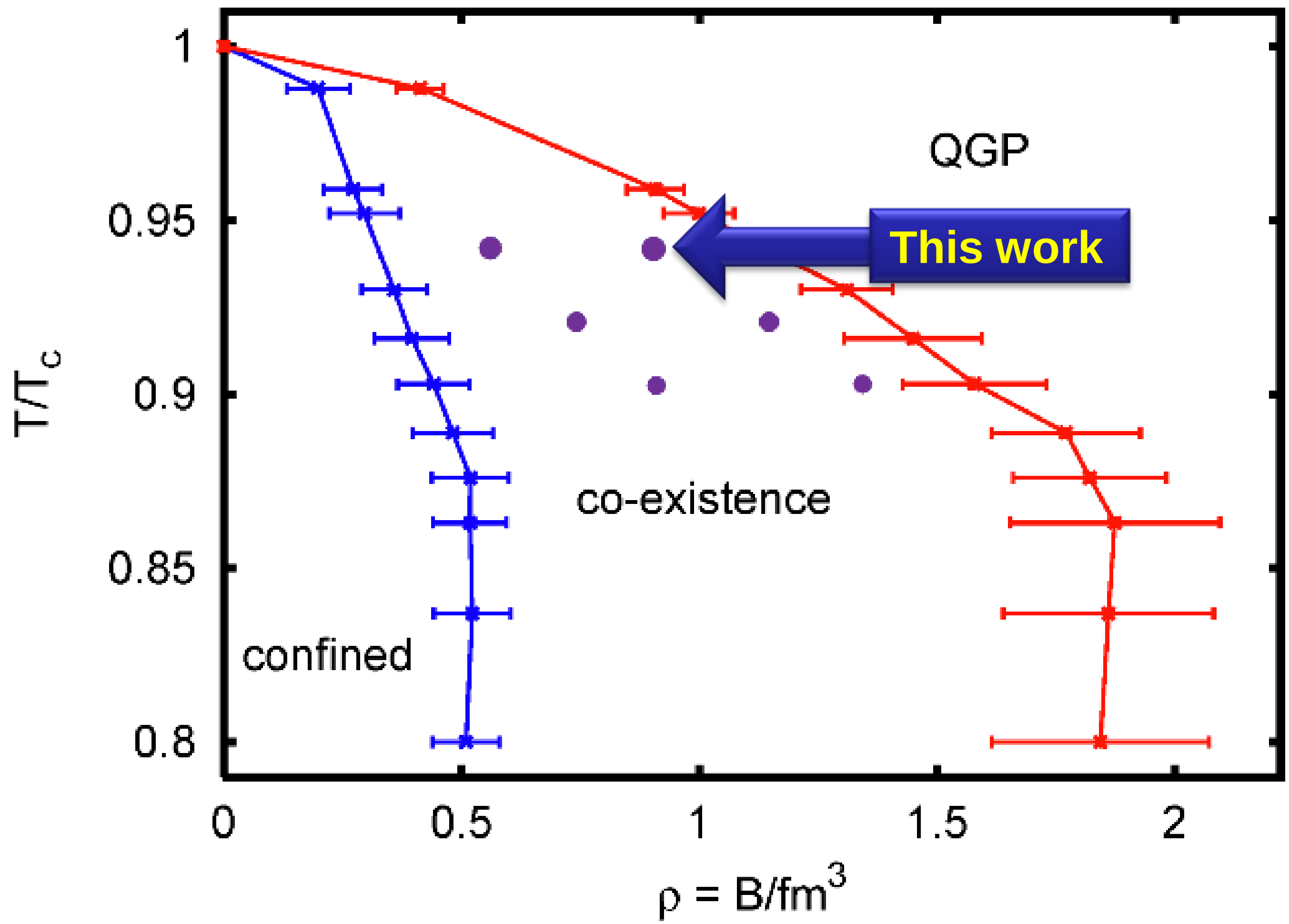
Maxwell Construction

N_f = 4 Wilson gauge + fermion action



Phase Boundary (Preliminary)

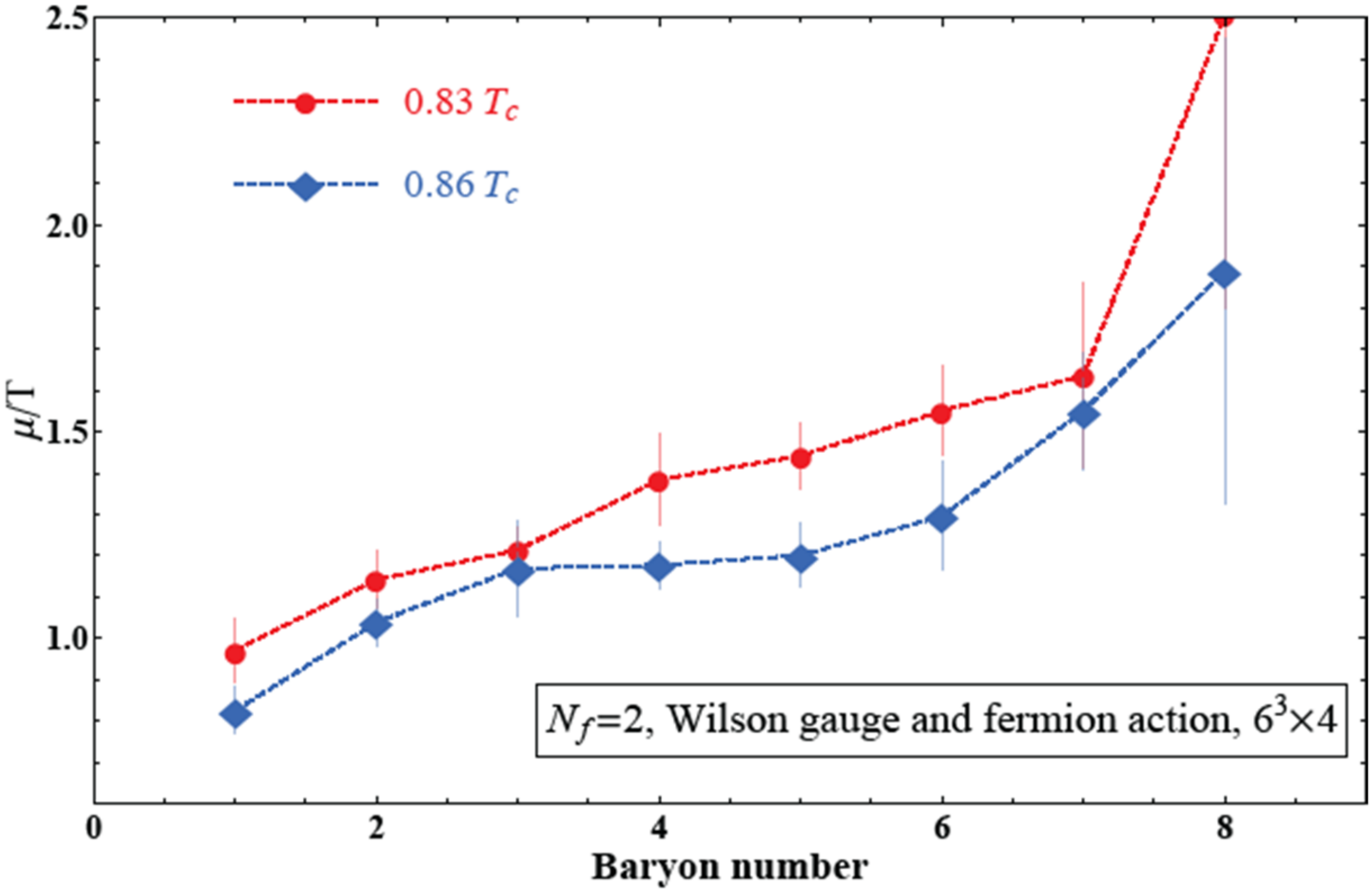
$N_f = 4$



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

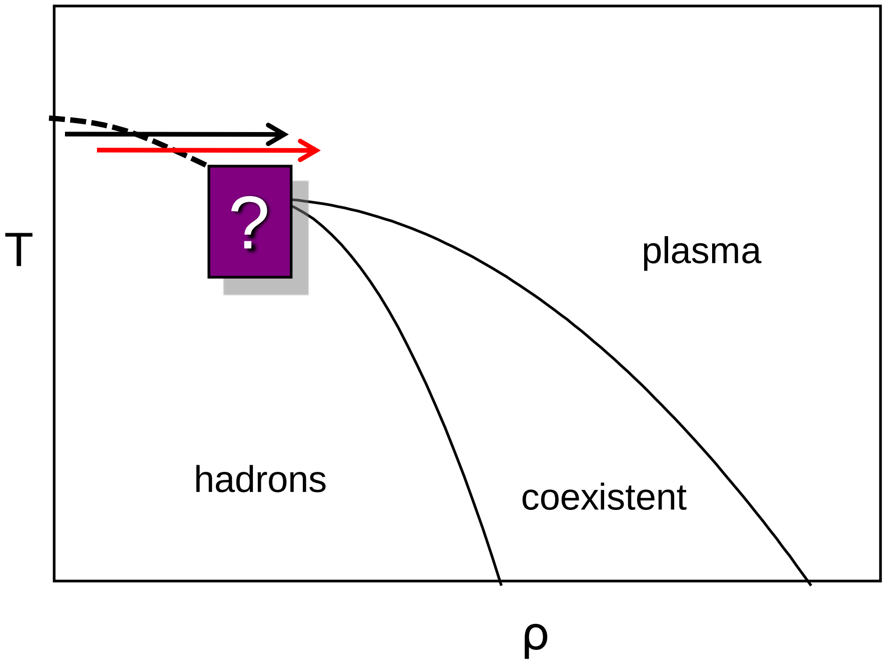
Baryon Chemical Potential

N_f = 2 Wilson gauge + fermion action

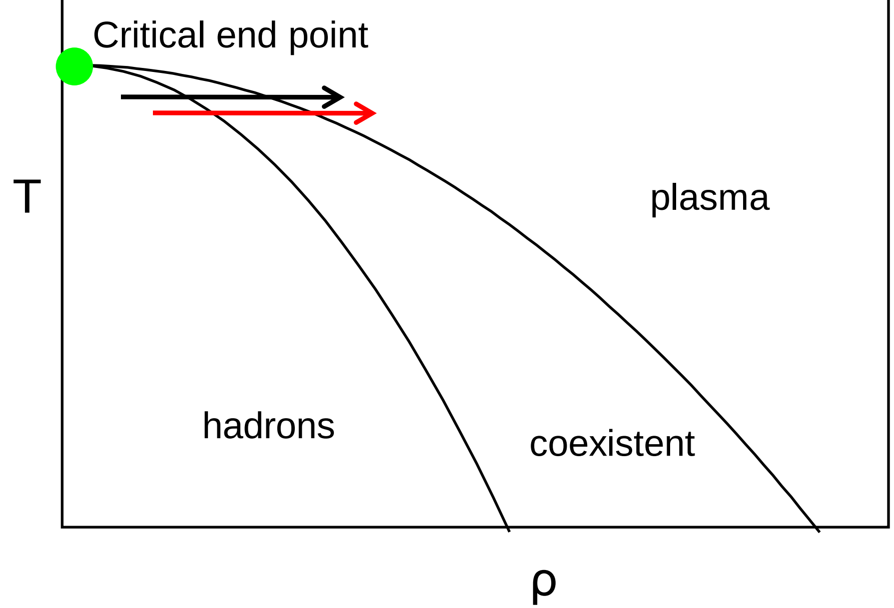


Phase diagram

Two flavors

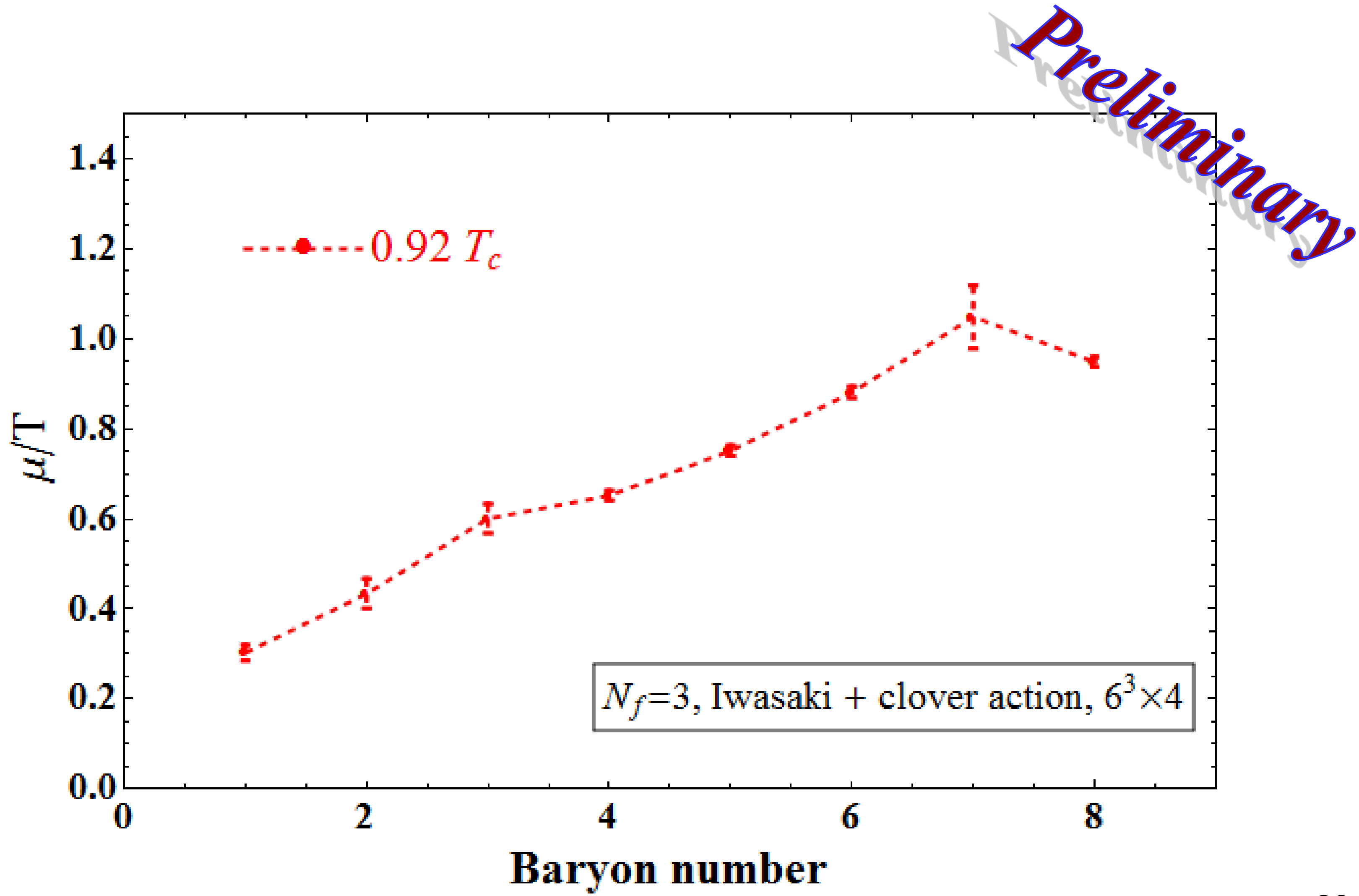


Four flavors



Three Flavors (Preliminary)

N_f = 3 Iwasaki gauge + Clover fermion action, m_π ~0.8 GeV



Summary

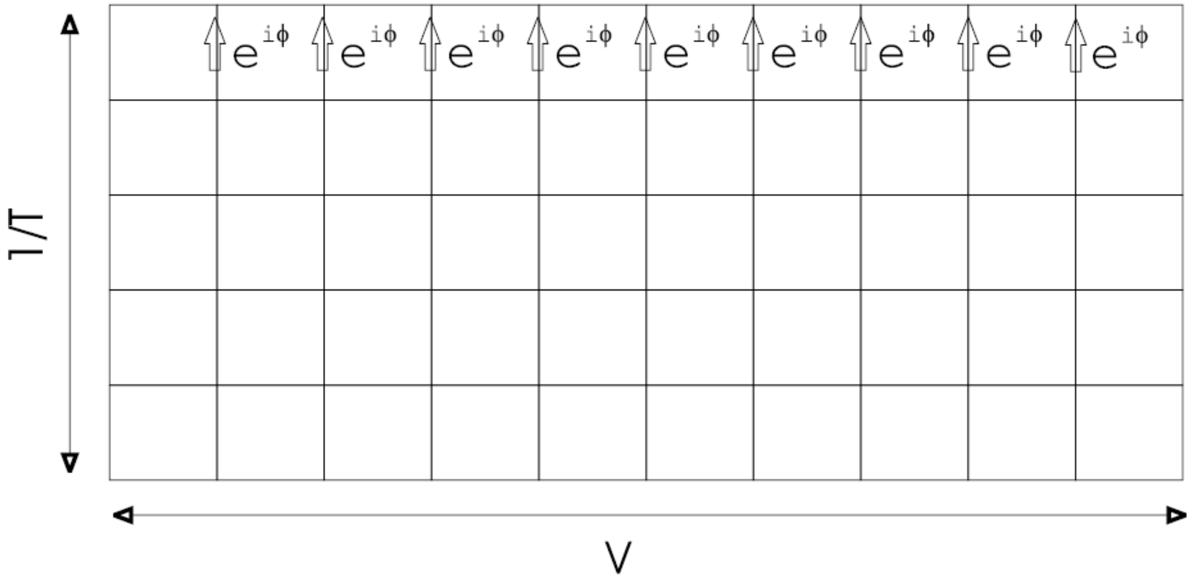
- Canonical Ensemble Approach overcomes the overlap problem and alleviates the fluctuation problem. No sign problem for $T > 0.8\ T_c$.
- Wilson fermion on $6^3 \times 4$ lattice with $m_\pi \sim$ 1 GeV shows $N_F = 2$ is crossover (?) down to $0.83\ T_c$, $N_F = 4$ is first order.
- Iwasaki + Clover fermion on $6^3 \times 4$ lattice with $m_\pi \sim 0.8$ GeV results for $N_F = 3$ are forthcoming.

Future (wish list)

- Larger volume → HNMC (A. Alexandru, et al. arXiv:0711.2678)
- Smaller masses
- Chiral fermion action
- Lower temperature (sign problem)

Triality

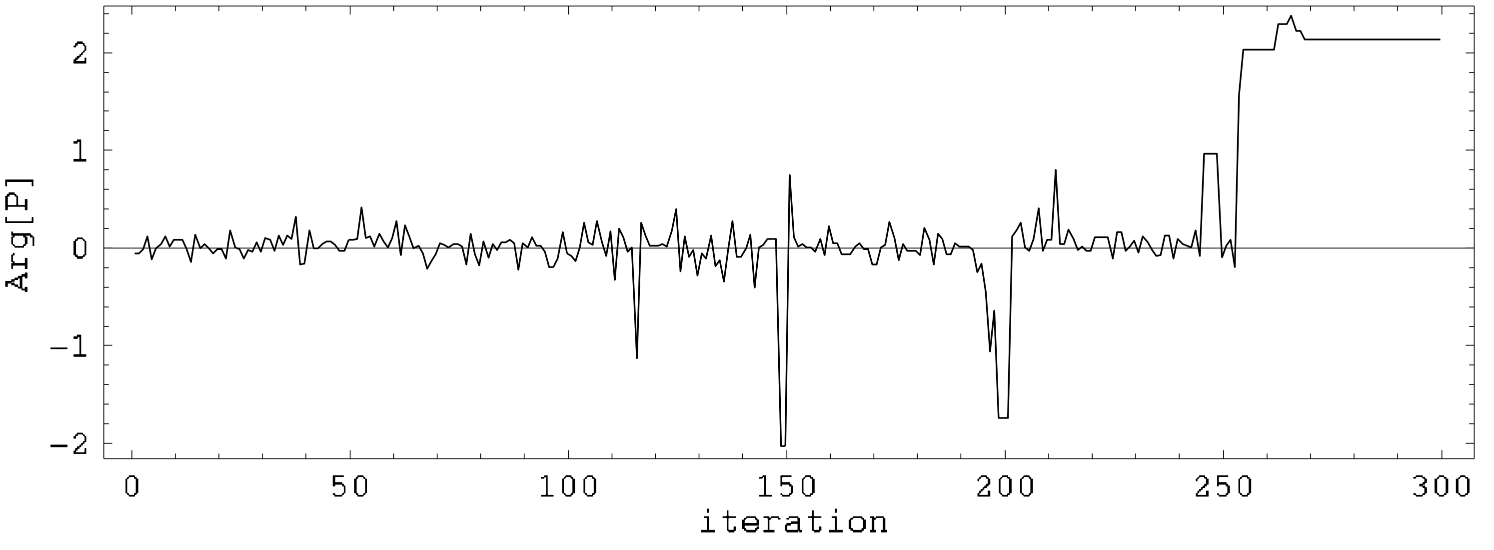
$$Z_{GC}(\mu = \mu_R + i(\mu_I + \frac{2\pi T}{3})) = Z_{GC}(\mu = \mu_R + i\mu_I)$$



$$\phi \to \phi \pm \frac{2\pi}{3}$$

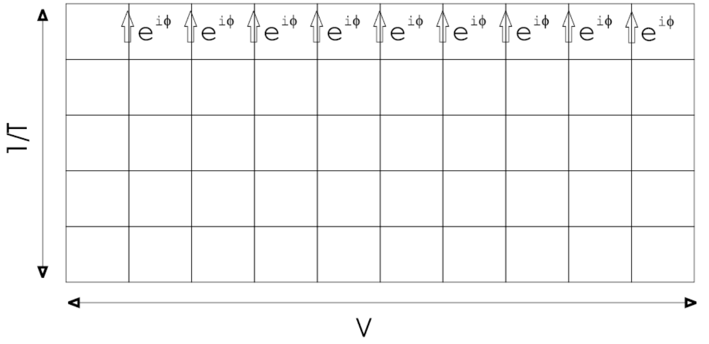
$$\boxed{Z_C(V,n,T) = 0 \; if \;\; n \neq 3B}$$

Z(3) hopping



$$\frac{\left(\dfrac{\left|\operatorname{Re}\det_n M^2(U)\right|}{\det M^2(U,0)}\right)_0}{\left(\dfrac{\left|\operatorname{Re}\det_n M^2(U)\right|}{\det M^2(U,0)}\right)_1} \approx \frac{\det M^2(U_1,0)}{\det M^2(U_0,0)} \approx 0$$

Z(3) hopping



$$U \to U(\pm 2\pi/3)$$