Numerical study of the endpoint of first order phase transition lines in finite density Lattice QCD Density Fluctuations, Sign problem

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第二回クラスター階層領域研究会

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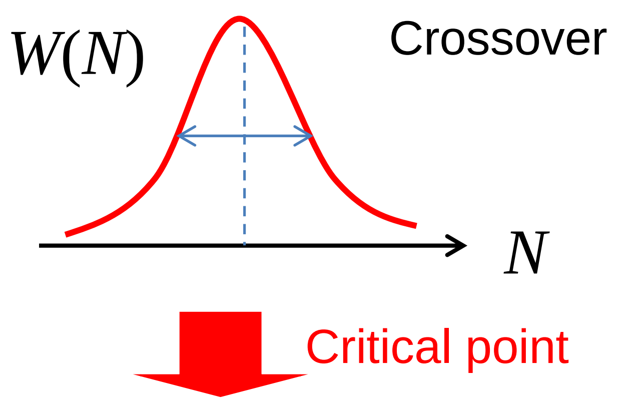
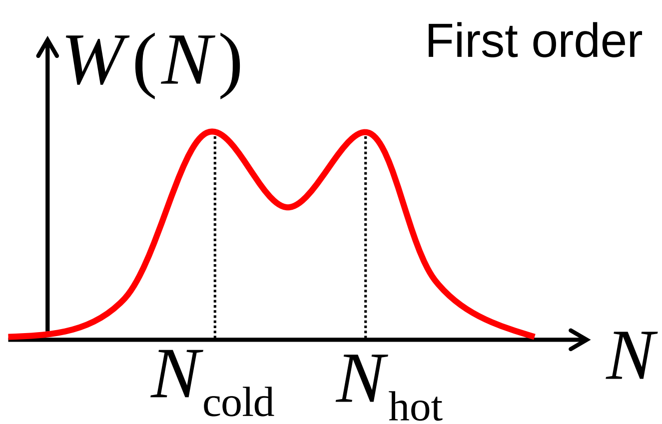
QCD phase structure at high density

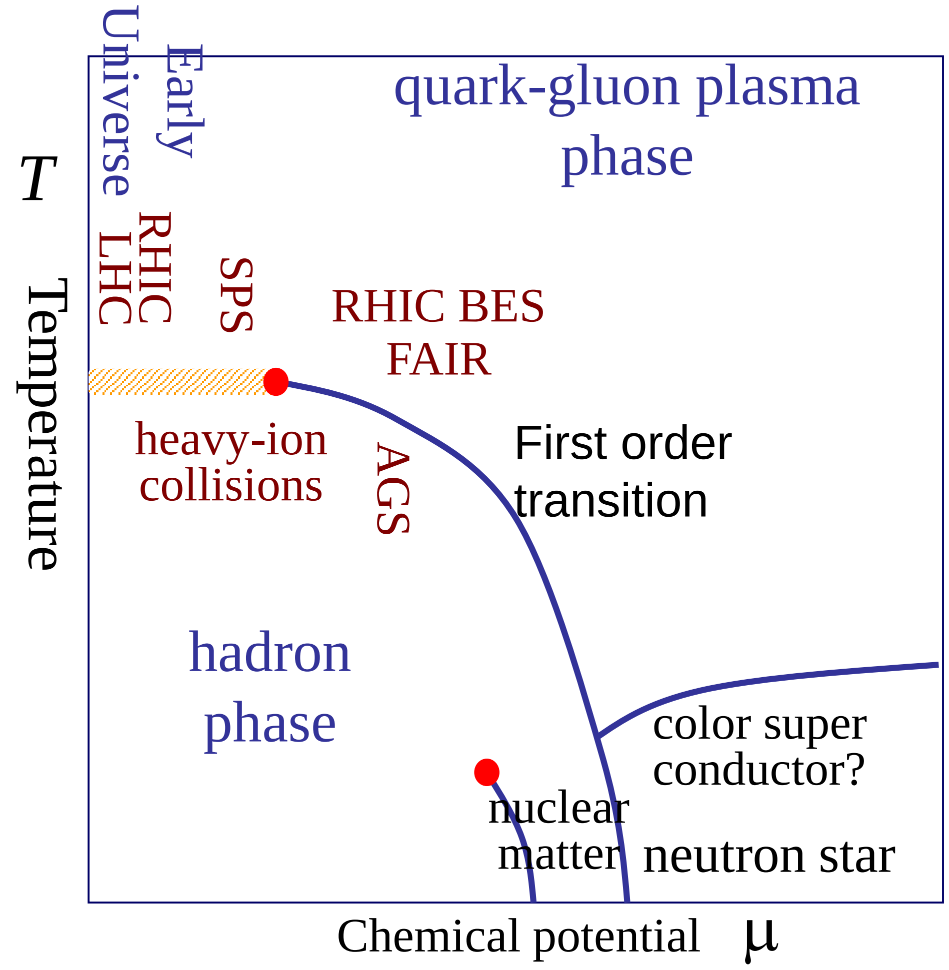
- Critical point at high density
- Baryon number fluctuation

  Variance, Skewness, Kurtosis

  Provability distribution function







Quark number distribution function

- Canonical partition function: Z_c (Fugacity expansion)

$$Z_{GC}(T,\mu)=\sum_N \underline{Z_C(T,N)}\exp(N\mu/T)\equiv\sum_N W(N)$$

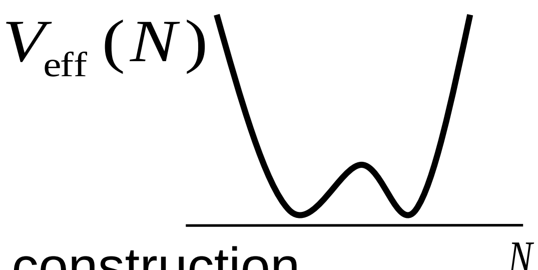
- Effective potential as a function of the quark number *N*.

$$V_{\rm eff}(N)=-\ln W(N)=-\ln Z_C(T,N)-N\frac{\mu}{T}$$

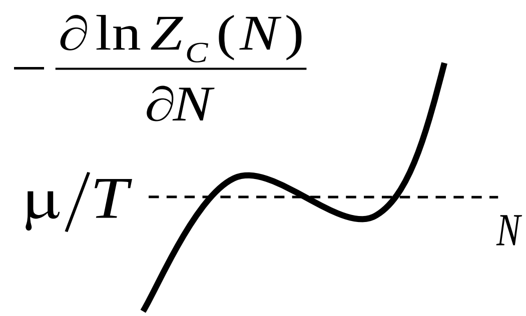
- At the minimum,

$$\frac{\partial V_{\rm eff}(N)}{\partial N}=-\frac{\partial \ln W(N)}{\partial N}=-\underline{\underline{\frac{\partial \ln Z_C(T,N)}{\partial N}}}-\frac{\mu}{T}=0$$

- First order phase transition: Two phases coexist.

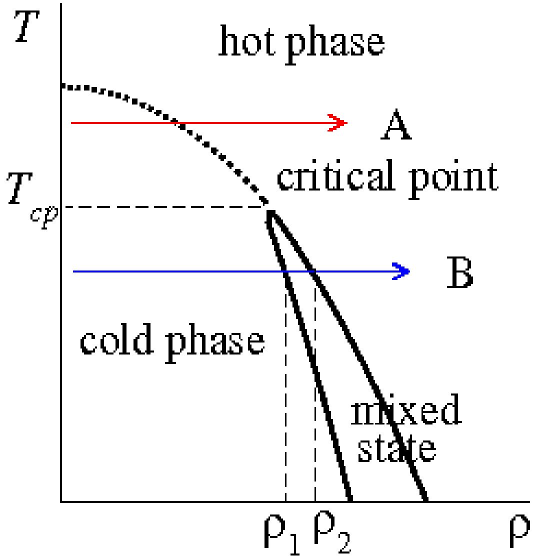


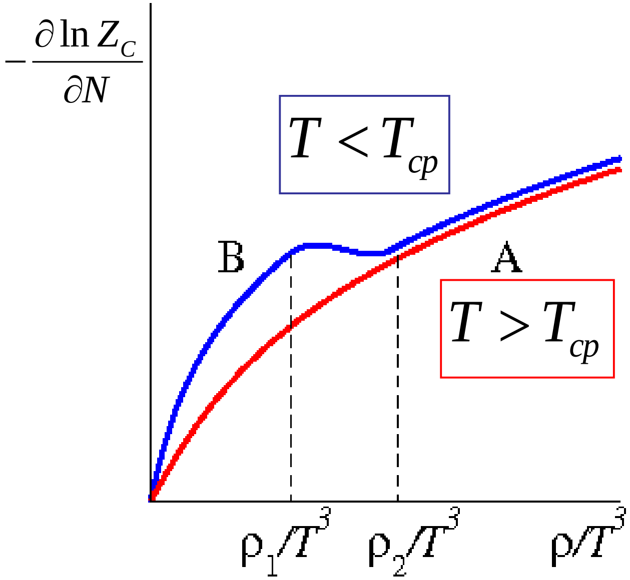
Maxwell construction



First order phase transition line

At the potential minimum, $\frac{\partial V_{\text{eff}}(N)}{\partial N} = 0,$ ⇨ $\boxed{\frac{\mu}{T} = -\frac{\partial \ln Z_C(T,N)}{\partial N}}$





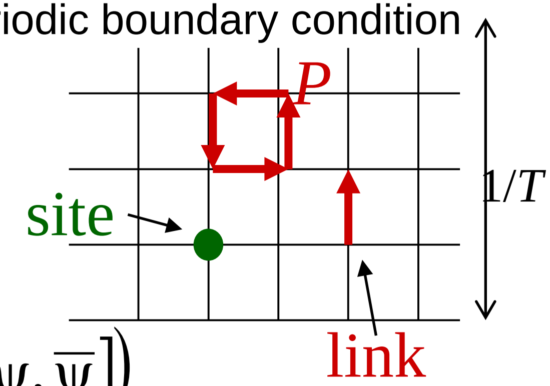
Mixed state
⬇
First order transition

Key words of this talk

- Canonical approach with a saddle point approximation
  (S.E., Phys.Rev.D78, 074507 (2008))
- Fugacity expansion = Winding number expansion
- Sign problem
- Canter symmetry

Lattice QCD simulations

- Gauge field on links $U_\mu \in SU(3)$
  Quark field on sites $\psi, \bar{\psi}$ (grassmann number)



- Grand partition function (Matsubara formulation)

$$Z = \int \prod_{x,\mu} dU_\mu(x) \prod_x d\psi(x) d\bar{\psi}(x) \exp\left(-S_g[U] - S_q\left[U, \psi, \bar{\psi}\right]\right)$$

$$S_g = -6N_{\rm site}\beta P, \qquad P = \frac{1}{6N_{\rm site}} \sum_{n,\mu\neq\nu} \frac{1}{3} {\rm tr}\left[U_\mu(n) U_\nu(n+\hat{\mu}) U_\mu^\dagger(n+\hat{\nu}) U_\nu^\dagger(n)\right] \quad \text{(plaquette)}$$

- Grassmann integral

$$Z = \int \prod_{x,\mu} dU_\mu(x) \left(\det M\right)^{N_{\rm f}} e^{-S_g}, \qquad S_q = \sum_{i=1}^{N_{\rm f}} \bar{\psi}_i M \psi_i$$

- Monte-Carlo method: Path integral, generating configurations
- Physical quantity O

$$\langle O \rangle_{(\beta,m)} = \frac{1}{Z} \int \underline{DU_\mu}\, O\left[U_\mu\right] \underline{\left(\det M\right)^{N_{\rm f}} e^{-S_g(\beta)}}$$

Gauge fields are generated with this weight.

Loop expansion and quark number

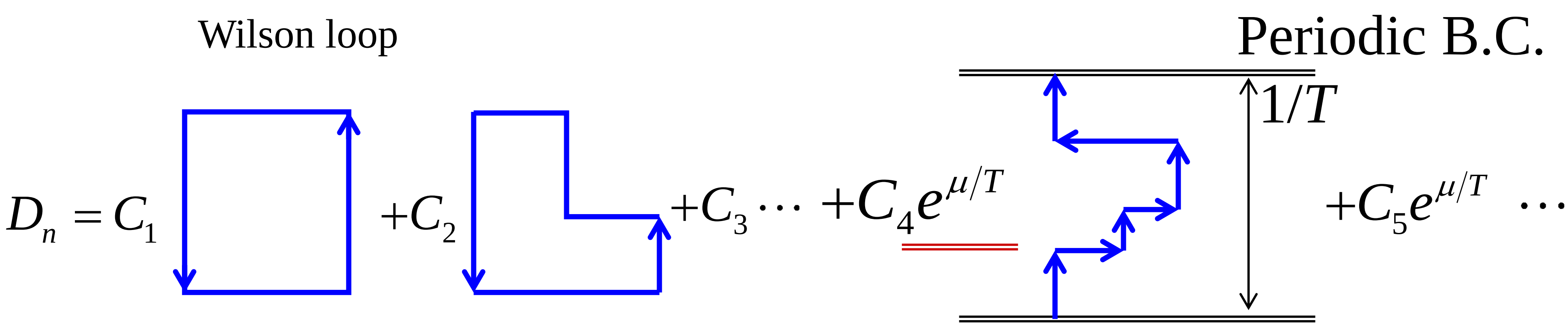
- Grand partition function

$$Z = \int \prod_{x,\mu} dU_\mu(x) \left(\det M\right)^{N_f} e^{-S_g}$$

- Hopping parameter expansion [K~1/(quark mass)]

$$\ln\left(\det M(K)\right) = \sum_{n=0}^{\infty} \frac{1}{n!}\left[\frac{\partial^n\left(\ln \det M\right)}{\partial K^n}\right]_{K=0} K^n = \sum_{n=1}^{\infty} \frac{1}{n!} D_n K^n$$

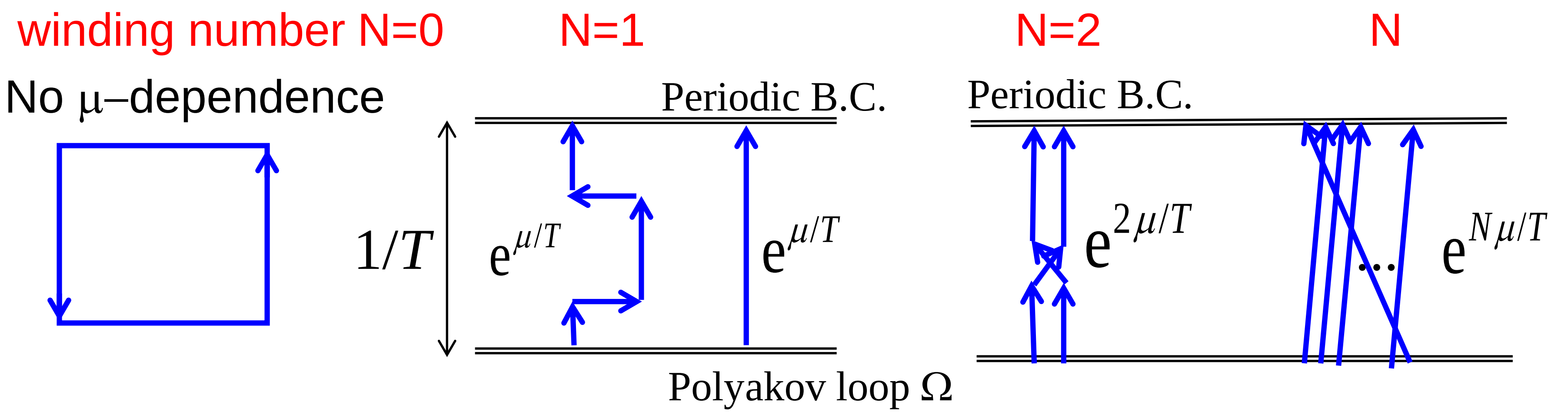
- D_n : Sum of all n-step Wilson loops (connected)



Wilson loop : quark current loop, indicator of the confinement

Chemical potential, Fugacity expansion

- Wilson loop expansion of $\ln \det M$



Polyakov loop Ω : static current loop, order parameter of the confinement

$$\Omega = \frac{1}{3}\mathrm{tr}\left[U_4 U_4 U_4 \cdots U_4\right]$$

$\langle \Omega \rangle = e^{-F/T} = 0$ Confinement phase

$\langle \Omega \rangle \neq 0$ Deconfinement phase

- Chemical potential enhances winding current loops (static currents).
- Classify the Wilson loops by the winding number.
- Fugacity expansion: expansion with the winding number *N*.

$$Z_{GC}(T,\mu) = \sum_{N=-3V}^{3V} Z_C(N,T)\exp(N\mu/T)$$

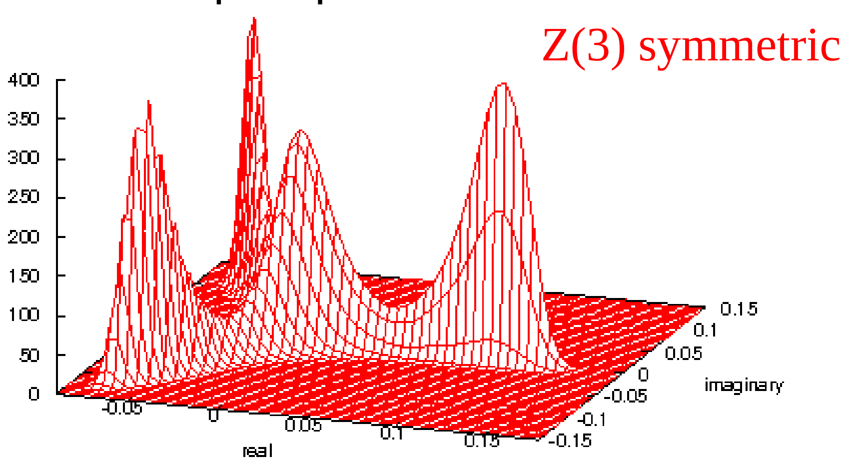
Z(3) center symmetry

- Quenched QCD (no dynamical quarks, det$M$=1)
- Center of SU(3) group $U_{\text{center}} = \omega I,\ \omega = \{1,\ e^{\frac{2\pi i}{3}},\ e^{\frac{4\pi i}{3}}\}$
- On one time slice, $U_4 \Rightarrow \omega U_4$
- Action of gauge fields and integral measure are invariant.

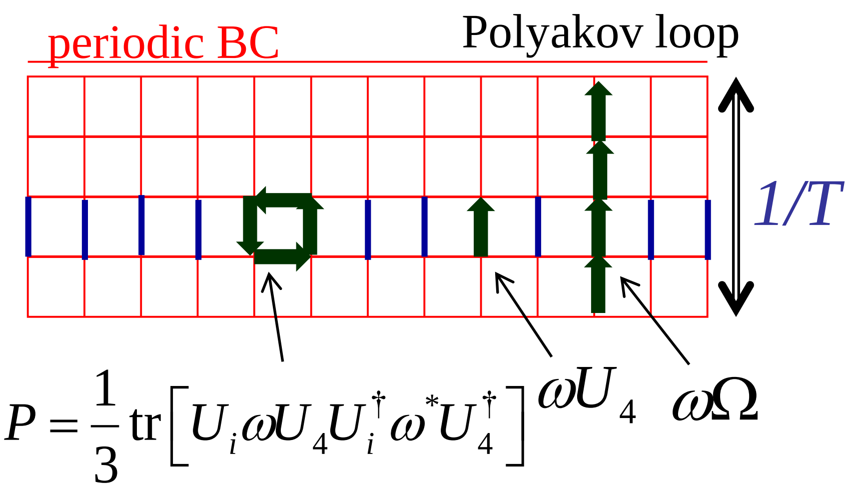
$$DU = D(UV),\ \ UV \in SU(3) \qquad P \Rightarrow \frac{1}{3}\mathrm{tr}\left[U_i \omega U_4 U_i^\dagger \omega^* U_4^\dagger\right] = P$$

- Polyakov loop Ω changes as $\langle\Omega\rangle \Rightarrow \omega\langle\Omega\rangle$
- $\langle\Omega\rangle = 0$ when the symmetry is unbroken.

Ω in the complex plane



Probability distribution at T_c



Roberge-Weiss symmetry

$$U_4 \Rightarrow \omega U_4$$

- Fugacity expansion (with dynamical quarks)

  Under Z(3) center transformation $\left(\omega = e^{2\pi i/3}\right)$, Zc(N) changes as $(\omega^N = e^{2\pi i N/3})$

$$Z_{GC}(T,\mu) = \sum_N Z_C(N,T) e^{N 2\pi i/3} e^{N\mu/T}$$

  This is the same as the transformation: $\mu/T \rightarrow \mu/T + 2\pi i/3$

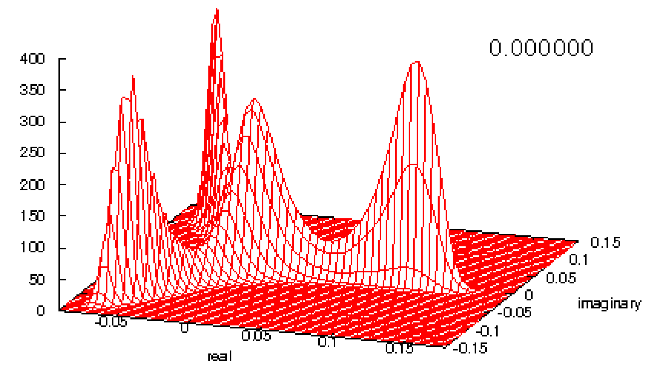
  Roberge-Weiss symmetry:

$$Z_{GC}(T,\mu) = Z_{GC}(T,\mu + 2\pi i T/3)$$

- $Z_C(N,T)=0$ when $N \neq 3 \times$ (integer) $(\omega^3=1,\ 1+\omega+\omega^2=0)$

$$Z_{GC}(T,\mu) = \frac{1}{3}\left(Z_{GC}(T,\mu) + Z_{GC}(T,\mu + 2\pi i T/3) + Z_{GC}(T,\mu + 4\pi i T/3)\right)$$

$$= \sum_{n=0}^{\infty} Z_C(3n,T)\ e^{3n\mu/T}$$



Center symmetry in U(1) gauge theory

- Centers of group are all members $U_\mu = e^{i\theta}$.
- Under the center transformation,

$$Z_{GC}(T,\mu) = \sum_N Z_C(N,T)\underline{e^{iN\theta}}e^{N\mu/T}, \qquad Z_{GC}(T,\mu) = Z_{GC}(T,\mu + i\theta T)$$

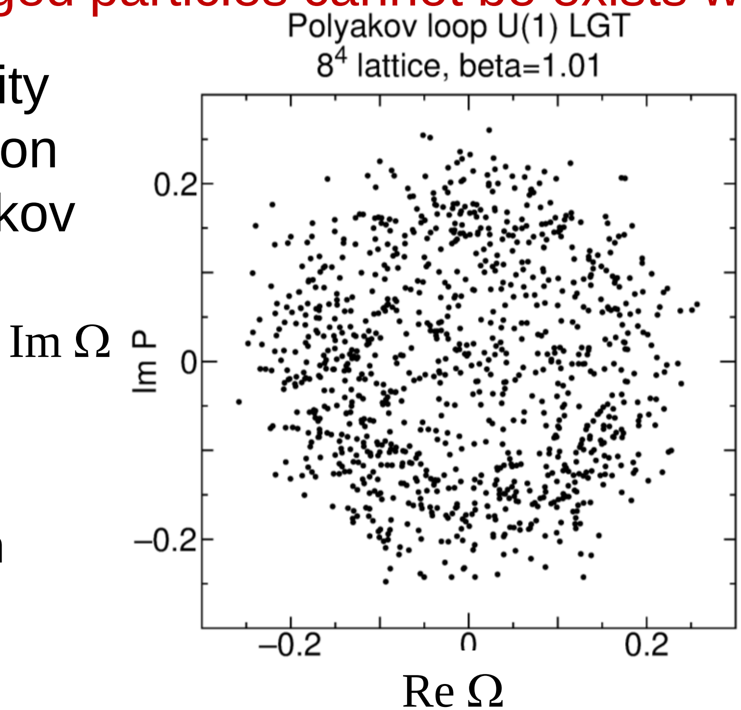
- Except for N=0, the canonical partition function is zero.

$$Z_{GC}(T,\mu) = \frac{1}{2\pi}\int\left[\sum_N Z_C(N,T)e^{iN\theta}e^{N\mu/T}\right]d\theta = Z_C(0,T)$$

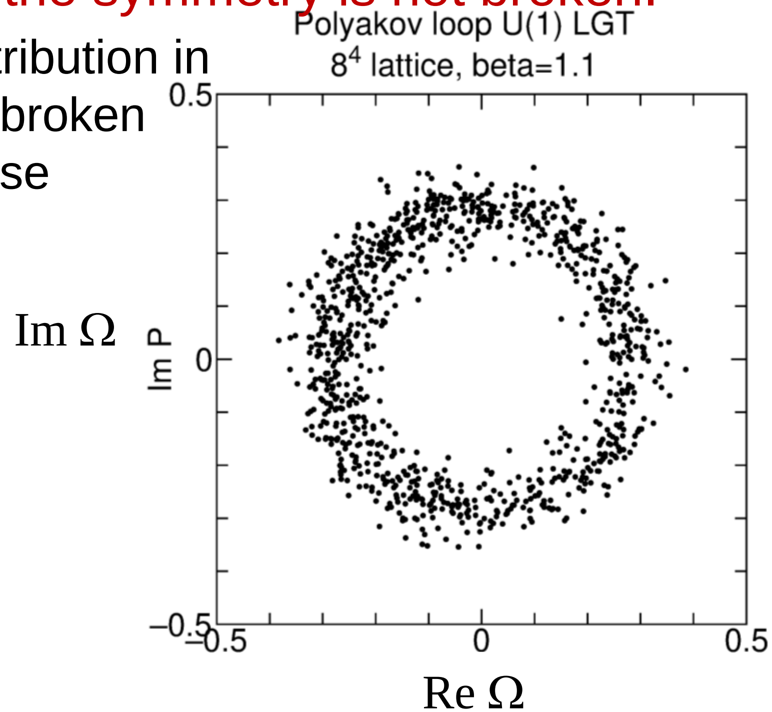
Charged particles cannot be exists when the symmetry is not broken.

Probability distribution of Polyakov loop

near the phase transition



Distribution in the broken phase

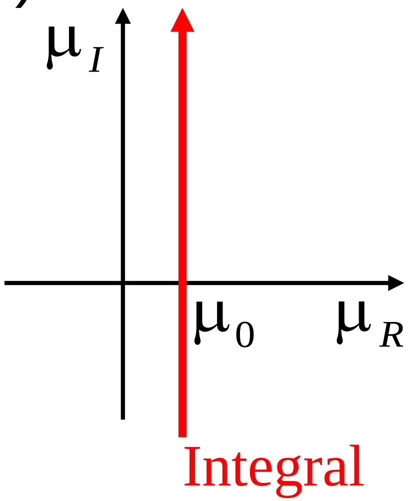


Canonical partition function

- Fugacity expansion (Laplace transformation)

$$Z_{GC}(T,\mu)=\sum_N \underline{\underline{Z_C(T,N)}}\exp(N\mu/T) \qquad \rho = N/V$$

canonical partition function



- Inverse Laplace transformation

$$Z_C(T,N)=\frac{1}{2\pi}\int_{-\pi}^{\pi} d(\mu_I/T)\, e^{-N(\mu_0/T+i\mu_I/T)} Z_{GC}(T,\mu_0+i\mu_I)$$

Arbitrary μ_0

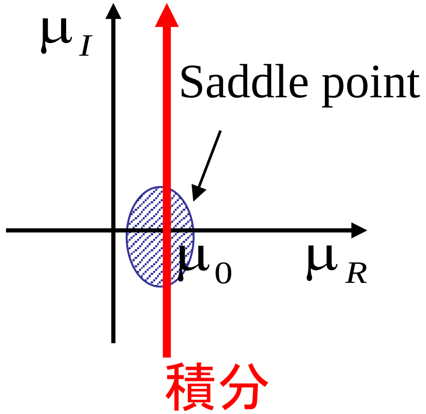
$$\frac{Z_{GC}(\mu)}{Z_{GC}(0)}=\frac{1}{Z_{GC}(0)}\int DU(\det M(\mu))^{N_f} e^{-S_g} = \left\langle \left(\frac{\det M(\mu)}{\det M(0)}\right)^{N_f} \right\rangle_{\mu=0}$$

Integral path though a saddle point

- – Note: periodicity $Z_{GC}(T,\mu+2\pi iT/3)=Z_{GC}(T,\mu)$
- – det$M(\mu)$: Quark determinant

Saddle point approximation

(S.E., Phys. Rev. D78, 074507 (2008))



- Inverse Laplace transformation

$$Z_C(T,N)=\frac{3}{2\pi}\int_{-\pi/3}^{\pi/3} d(\mu_I/T)\, e^{-N(\mu_0/T+i\mu_I/T)} Z_{GC}(T,\mu_0+i\mu_I)$$

$$=\frac{3Z_{GC}(0)}{2\pi}\left\langle \int_{-\pi/3}^{\pi/3} d(\mu_I/T)\, e^{-N(\mu_0/T+i\mu_I/T)} \left(\frac{\det M(\mu_0+i\mu_I)}{\det M(0)}\right)^{N_f} \right\rangle$$

- Saddle point approximation (valid for large *V, 1/V*-expansion)
  - Taylor expansion at the saddle point. Gauss integral.

$$\mu_0/T = z_0$$

Saddle point: z_0 $$\left[\frac{N_{\rm f}}{V}\frac{\partial(\ln\det M)}{\partial(\mu/T)}-\rho\right]_{\frac{\mu}{T}=z_0}=0$$

$$\rho = N/V$$

$$V \equiv N_s^3$$

Saddle point approximation

- Canonical partition function in a saddle point approximation

$$\frac{Z_C(T,\rho)}{Z_{GC}(T,0)} = \frac{3}{\sqrt{2\pi}} \left\langle \exp\left[N_{\rm f} \ln\left(\frac{\det M(z_0)}{\det M(0)} \right) - V\rho z_0 \right] e^{-i\alpha/2} \sqrt{\frac{1}{V\left|D''(z_0)\right|}} \right\rangle_{(T,\mu=0)}$$

$$\equiv \frac{3}{\sqrt{2\pi}} \left\langle \exp(F + i\theta) \right\rangle_{(T,\mu=0)}$$

Saddle point: z_0

$$D''\left(\frac{\mu}{T}\right) = \frac{N_{\rm f}}{V} \frac{\partial^2 (\ln \det M)}{\partial (\mu/T)^2} \equiv \left|D''\right| e^{i\alpha}$$

- Chemical potential

$$\frac{\mu^*(\rho)}{T} \equiv \frac{-1}{V} \frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\left\langle z_0 \exp(F + i\theta) \right\rangle_{(T,\mu=0)}}{\left\langle \exp(F + i\theta) \right\rangle_{(T,\mu=0)}}$$

saddle point reweighting factor

⇨ Similar to the reweighting method (sign problem & overlap problem)

In the case of heavy quark (small K)

$\mu/T = z$

$$D\left(K, \frac{\mu}{T}\right) \equiv \frac{N_f}{N_s^3} \ln(\det M(K,\mu)) = N_f N_t 288 K^4 P + 6 \times 2^{N_t} N_f K^{N_t} \left(e^{\mu/T} \underline{\Omega} + e^{-\mu/T} \underline{\Omega^\dagger}\right) + \cdots$$

Saddle point $z_0 = x_0 + iy_0$, where $\frac{\partial}{\partial z}[D(z) - \rho z] = \left[\frac{\partial D}{\partial z}(z) - \rho\right] = 0$

$y_0 = -Arg(\hat{\Omega})$

Absorb the complex phase into z_0

$$\sinh(x_0) = \frac{\rho}{12 \times 2^{N_t} N_f K^{N_t} |\Omega|}$$

$$x_0 = \ln\left[\frac{\bar{\rho}}{3 \times 2^{N_t+2} N_f \kappa^{N_t}} \frac{1}{|\hat{\Omega}|} + \sqrt{\left(\frac{\bar{\rho}}{3 \times 2^{N_t+2} N_f \kappa^{N_t}} \frac{1}{|\hat{\Omega}|}\right)}\right]$$

$D(z_0), D''(z_0)$ at the saddle point

$$D(z_0) = 288 N_t N_f \kappa^4 \hat{P} + 3 \times 2^{N_t+2} N_f \kappa^{N_t} |\hat{\Omega}| \cosh x_0 + \cdots$$

$$D''(z_0) = 3 \times 2^{N_t+2} N_f \kappa^{N_t} |\hat{\Omega}| \cosh x_0 + \cdots$$

x_0, $D(z_0)$, $D''(z_0)$ are real functions of $|\Omega|$

Canonical partition function by a saddle point ap.

$$Z_C(T,N) = \frac{3}{\sqrt{2\pi}} Z_{GC}(T,0,0) \left\langle \exp\left[V D(z_0) - N(x_0 + i y_0) - \frac{1}{2} \ln V |D''(z_0)| \right] \right\rangle_{T,\kappa=0,\mu_q=0}$$

$$= \frac{3}{\sqrt{2\pi}} Z_{GC}(T,0,0) \left\langle \exp\left[F + i\theta \right] \right\rangle_{T,\kappa=0,\mu_q=0}$$

Quenched QCD simulations

$$\begin{cases} F \equiv V D(z_0) - N x_0 - \frac{1}{2} \ln[V |D''(z_0)|] \\ \theta \equiv -N y_0 \quad (y_0 = -Arg(\hat{\Omega})) \end{cases}$$

real part F and imaginary part θ

θ makes the sign problem

F is a function of $|\Omega|$

θ is $N\,\mathrm{Arg}(\Omega)$

$$(N = V\rho)$$

$\langle \ldots \rangle_{|\Omega|}$:

Average fixing $|\Omega|$

In the Monte-Carlo method, we take an average fixing $|\Omega|$.

$$\frac{-1}{V} \frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\langle z_0 \exp(F + i\theta) \rangle_{(T,\kappa=\mu=0)}}{\langle \exp(F + i\theta) \rangle_{(T,\kappa=\mu=0)}} \approx \frac{\int x_0 e^F \langle \cos\theta \rangle_{|\Omega|} w(|\Omega|) d|\Omega|}{\int e^F \langle \cos\theta \rangle_{|\Omega|} w(|\Omega|) d|\Omega|}$$

Sign problem

$$\frac{-1}{V}\frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\int x_0 e^F \langle \cos\theta \rangle_{|\Omega|} w(|\Omega|)}{\int e^F \langle \cos\theta \rangle_{|\Omega|} w(|\Omega|)}$$

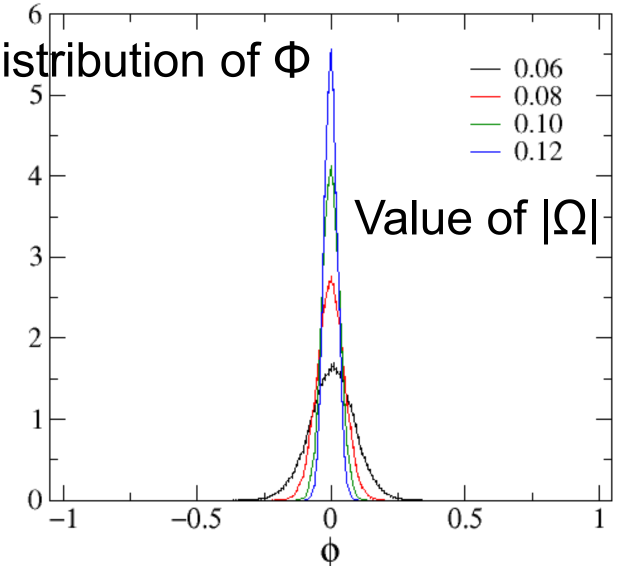
$$\langle \cos\theta \rangle_{|\Omega|} = \int_{-\pi}^{\pi} \cos(N\phi)\; w(|\Omega|,\phi)\, d\phi$$

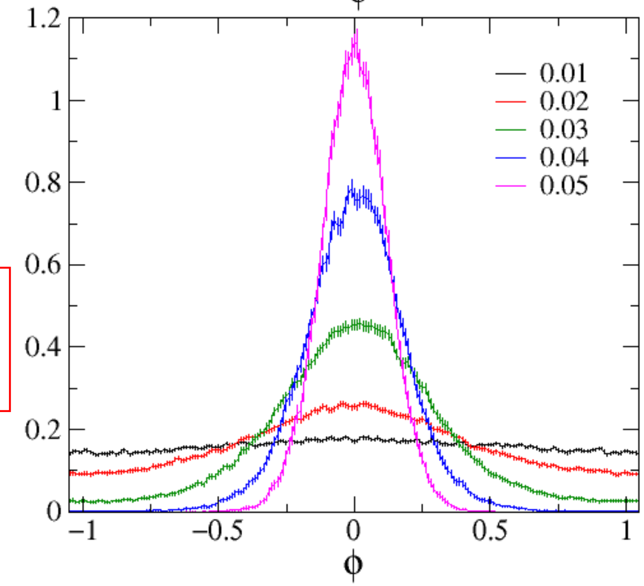
$$\theta = N\phi = V\rho\phi \qquad \text{(Quenched QCD)}$$

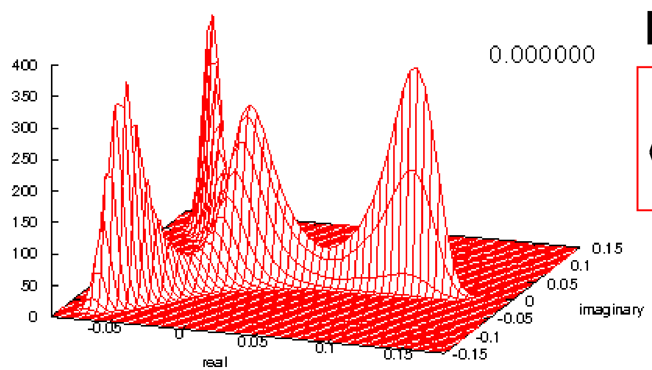
- Fourier transformation of the distribution function W(Φ).
- Ω : large distribute near Φ~0

$$w(\phi) \sim e^{-a\phi^2 - b\phi^4 - c\phi^6 - \cdots}$$ Gaussian distribution

- Ω:small distribution becomes wide.







If Gaussian distribution

$$\langle \cos(N\phi) \rangle \approx e^{-N^2 \langle \theta^2 \rangle / 2}$$

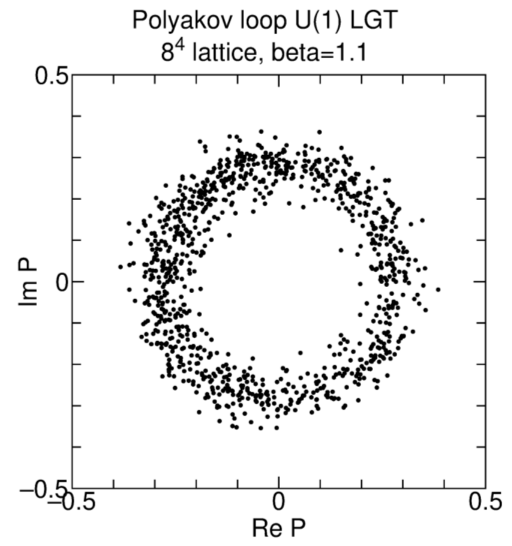
No sign problem

Sign problem in U(1) gauge theory

$$\frac{-1}{V}\frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\left\langle z_0 e^{F+i\theta}\right\rangle_{(T,\kappa=\mu=0)}}{\left\langle e^{F+i\theta}\right\rangle_{(T,\kappa=\mu=0)}} \approx \frac{\int x_0 e^F \left\langle \cos\theta\right\rangle_{|\Omega|} w(|\Omega|)\, d|\Omega|}{\int e^F \left\langle \cos\theta\right\rangle_{|\Omega|} w(|\Omega|)\, d|\Omega|}$$

- Fourier transformation of $w(\phi)$ $\qquad \theta = N\phi = V\rho\phi$

$$\left\langle \cos\theta\right\rangle_{|\Omega|} = \int_{-\pi}^{\pi} \cos(N\phi)\; w(\phi)\, d\phi$$



- From the U(1) center symmetry,
  The distribution function is constant.

$$w(\phi) = \frac{1}{2\pi} \quad \Rightarrow \quad \left\langle \cos\theta\right\rangle_{|\Omega|} = 0$$

- Adding det$M$ with infinitesimal 1/(mass)

$$\frac{-1}{V}\frac{\partial \ln Z_C(T,\rho)}{\partial \rho} \approx \frac{\int x_0 e^F \underline{|\Omega|^N}\; w(|\Omega|)\; d|\Omega|}{\int e^F \underline{|\Omega|^N}\; w(|\Omega|)\; d|\Omega|}$$

Sign problem is removed.

Application to SU(3) and light quark

- The quark determinant: $\ln \det M = \sum_N F_N \; e^{N\mu/T}$
- This analysis is applicable when $\ln \det M \approx F_1 \; e^{\mu/T}$ is a good approximation.
- For the case of $\ln \det M \approx F_1 \; e^{\mu/T} + F_2 e^{2\mu/T} + \cdots$, complex phase remains. But, it is O(K^{2Nt}) at most.
- SU(3) gauge theory: the Polyakov loop is U(1) symmetric (not Z(3)) in the large volume limit, if the Z(3) center symmetry is unbroken (low T phase).
- In the high temperature phase of SU(3) gauge theory, the probability distribution of complex phase is well-approximated by a gaussian function.

Summary and outlook

- We discussed the computational method of the probability distribution function of baryon number, which is important to understand QCD phase transition.
- The numerical simulation of QCD at high density has the serious problem of "sign problem". In this study, we considered the center symmetry, and proposed a method to avoid the sign problem using the symmetry.
- We aim to establish a method to calculate the probability distribution function by numerical simulation.