Center symmetry and the sign problem of finite density lattice gauge theory

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Abstract

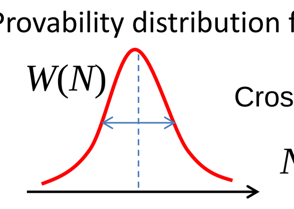
We study the phase transition of QCD at finite temperature and density by focusing on the probability distribution function of quark density. The phase transition of QCD is expected to change its properties as the density changes, and the probability distribution function gives important information for understanding the nature of the phase transition. The numerical simulation of QCD at high density has the serious problem of "sign problem".

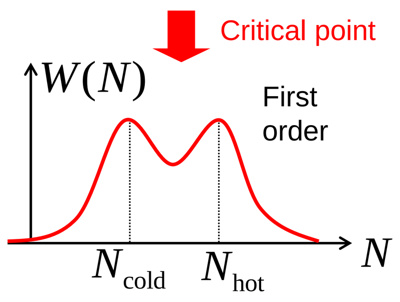
In this study, we consider the center symmetry, which is important for understanding the phase transition of lattice gauge theory, and propose a method to avoid the sign problem using the symmetry. We aim to establish a method to calculate probability distribution functions of physical quantities such as quark density by numerical simulation.

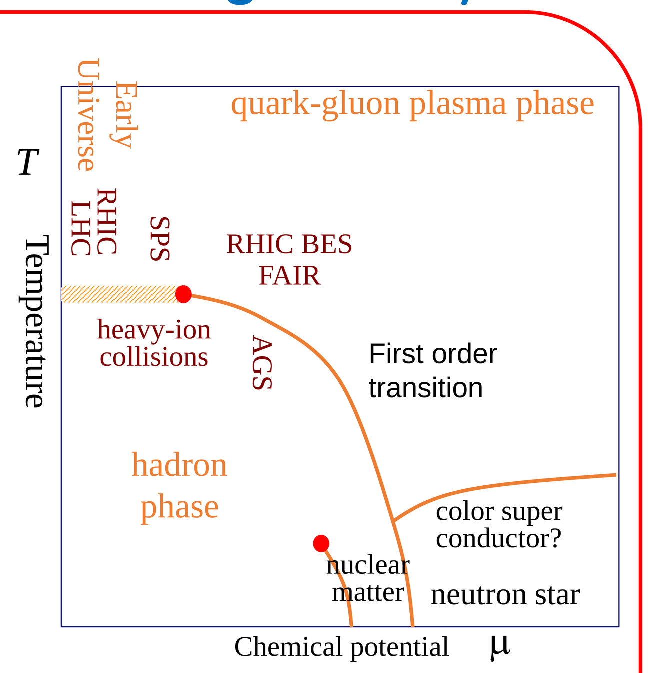
QCD phase structure at high density

- 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)

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

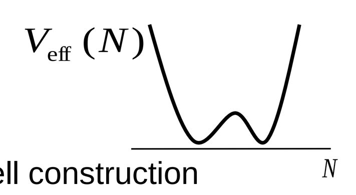
- Effective potential as a function of the quark number N.

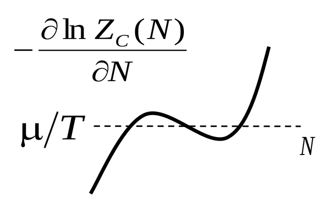
$$V_{\rm eff}(N)=-\ln W(N)=-\ln Z_C(T,N)-N\frac{\mu}{T}$$

- At the minimum,

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

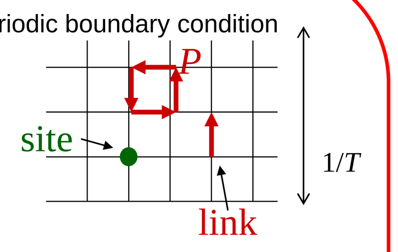
- First order phase transition: Two phases coexist.





Lattice QCD simulations at finite density

- Gauge field on links $U_\mu \in SU(3)$
- Grand partition function (Matsubara formulation)



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

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

$$S_q=\sum_{i=1}^{N_f}\bar\psi_i M\psi_i$$ Quark action

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

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

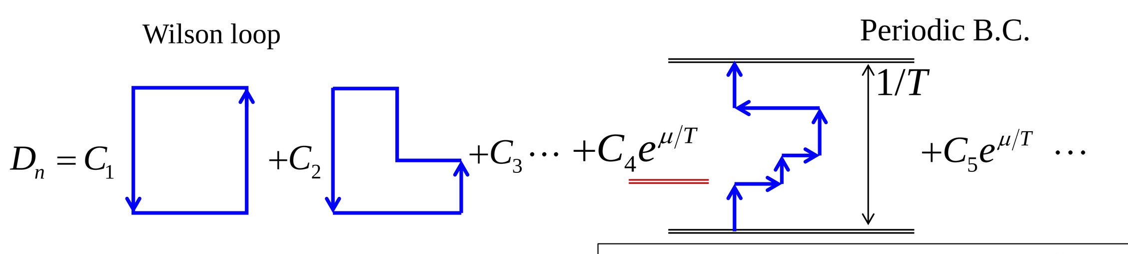
Gauge fields are generated with this weight.

Loop expansion and quark number

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

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

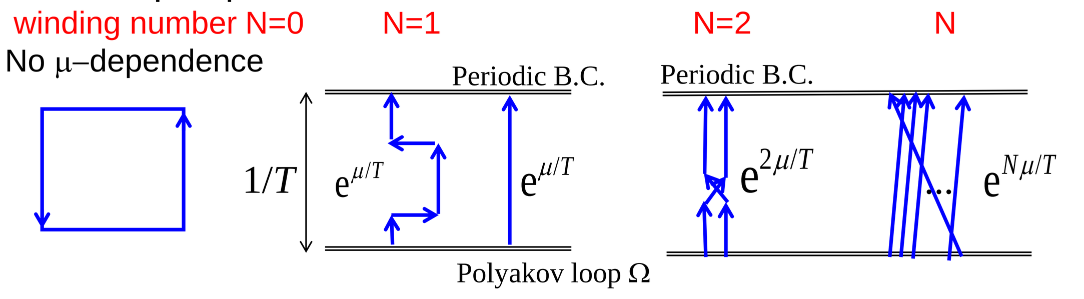
- D_n : Sum of all connected n-step Wilson loops



$$D_n=(-1)^{n+1}(n-1)!\,tr\left[\left(\frac{\partial M}{\partial K}\right)^n\right]_{K_0=0}$$

Chemical potential, Fugacity expansion

Wilson loop expansion of ln det M



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

$$\Omega=\frac{1}{3}{\rm tr}[U_4U_4U_4\cdots U_4]\qquad \langle\Omega\rangle=e^{-F/T}=0 \qquad \langle\Omega\rangle\neq 0$$

Confinement phase — Deconfinement phase

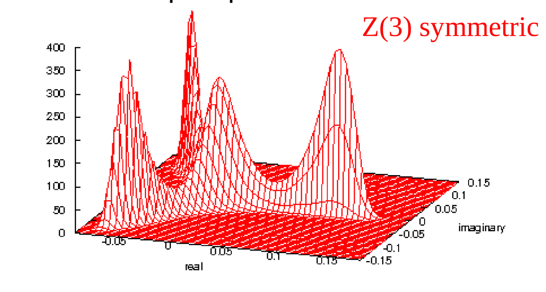
- Chemical potential enhances winding current loops (static currents).
- Classify the Wilson loops by the winding number.
- Fugacity expansion: expansion with the winding number N.

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

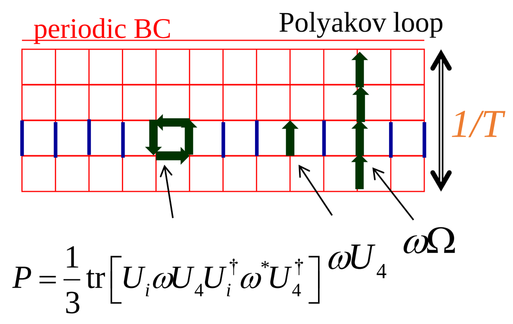
Z(3) center symmetry

- Quenched QCD (no dynamical quarks, $\det M$=1)
- Center of SU(3) group $\qquad U_{\rm center}=\omega I,\ \omega=\{1,\ e^{\frac{2\pi i}{3}},\ e^{\frac{4\pi i}{3}}\}$
- On one time slice, $\quad U_4\Rightarrow\omega U_4$
- Action of gauge fields and integral measure are invariant.
  $DU=D(UV),\ UV\in SU(3) \qquad P\Rightarrow\frac{1}{3}{\rm tr}\left[U_i\,\omega U_4 U_i^\dagger\,\omega^* U_4^\dagger\right]=P$
- Polyakov loop Ω changes as $\quad \langle\Omega\rangle\Rightarrow\omega\langle\Omega\rangle$
- $\langle\Omega\rangle=0$ when the symmetry is unbroken.

Ω in the complex plane



Probability distribution at T_c



$$P=\frac{1}{3}{\rm tr}\left[U_i\omega U_4U_i^\dagger\omega^*U_4^\dagger\right]\qquad \omega U_4 \quad \omega\Omega$$

- Fugacity expansion (including dynamical quarks) $\qquad U_4\Rightarrow\omega U_4$

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

$$Z_{GC}(T,\mu)=\sum_N Z_C(N,T)e^{N2\pi i/3}e^{N\mu/T}$$

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

Roberge-Weiss symmetry: $\quad Z_{GC}(T,\mu)=Z_{GC}(T,\mu+2\pi iT/3)$

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

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

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

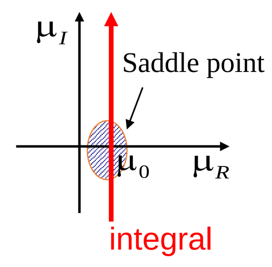
Canonical partition function

- Fugacity expansion (Laplace transformation)

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

canonical partition function

- Inverse Laplace transformation



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

Arbitrary μ_0

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

- Note: periodicity $\quad Z_{GC}(T,\mu+2\pi iT/3)=Z_{GC}(T,\mu)$

Integral path though a saddle point

- det$M(\mu)$: Quark determinant

Saddle point approximation (S.E., Phys. Rev. D78, 074507 (2008))

- Inverse Laplace transformation

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

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

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

Saddle point: z_0 $\qquad \left[\frac{N_f}{V}\frac{\partial(\ln\det M)}{\partial(\mu/T)}-\rho\right]_{\frac{\mu}{T}=z_0}=0 \qquad \mu_0/T=z_0,\quad V\equiv N_s^3,\quad \rho=N/V$

- Canonical partition function in a saddle point approximation

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

$$\equiv\frac{1}{\sqrt{2\pi}}\langle\exp(F+i\theta)\rangle_{(T,\mu=0)}$$

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

- Derivative of Zc

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

saddle point — reweighting factor

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

In the case of heavy quark (small K)

$$D\left(K,\frac{\mu}{T}\right)\equiv\frac{N_f}{N_s^3}\ln(\det M(K,\mu))=N_fN_t288K^4P+6\times2^{N_t}N_fK^{N_t}(e^{\mu/T}\hat\Omega+e^{-\mu/T}\hat\Omega^\dagger)+\cdots$$

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

$y_0=-Arg(\hat\Omega)$ $\quad$ Absorb the complex phase into z_0

$$\sinh(x_0)=\frac{\rho}{12\times2^{N_t}N_fK^{N_t}|\hat\Omega|}\qquad x_0=\ln\left[\frac{\bar\rho}{3\times2^{N_t+2}N_fK^{N_t}}\frac{1}{|\hat\Omega|}+\sqrt{\left(\frac{\bar\rho}{3\times2^{N_t+2}N_fK^{N_t}}\frac{1}{|\hat\Omega|}\right)^2+1}\right]$$

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

$$D(z_0)=288N_tN_f\kappa^4\hat P+3\times2^{N_t+2}N_f\kappa^{N_t}|\hat\Omega|\cosh x_0+\cdots$$

$$D''(z_0)=3\times2^{N_t+2}N_f\kappa^{N_t}|\hat\Omega|\cosh x_0+\cdots$$

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

Canonical partition function by a saddle point ap.

$$\frac{Z_C(T,\rho)}{Z_{GC}(T,0)}=\frac{1}{\sqrt{2\pi}}\left\langle\exp\left[VD(z_0)-N(x_0+iy_0)-\frac{1}{2}\ln V|D''(z_0)|\right]\right\rangle_{(T,\mu=0,K=0)}$$

$$\equiv\frac{1}{\sqrt{2\pi}}\langle\exp(F+i\theta)\rangle_{(T,\mu=0,K=0)}$$

Quenched QCD simulations

$$F\equiv VD(z_0)-Nx_0-\frac{1}{2}\ln[V|D''(z_0)|]$$
$$\theta\equiv-Ny_0\quad(y_0=-Arg(\hat\Omega))$$

real part F and imaginary part θ makes the sign problem

F is a function of $|\Omega|$
θ is $N\,{\rm Arg}(\Omega)$ $\qquad (N=V\rho)$

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

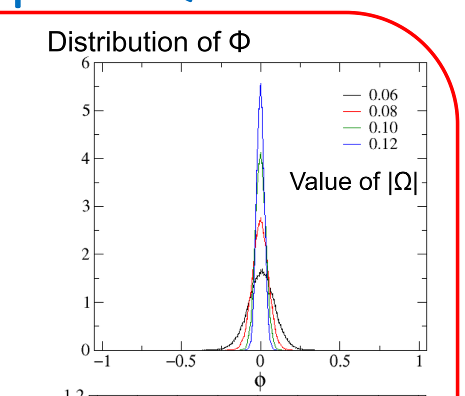
In the Monte-Carlo method, we take an average fixing $|\Omega|$.

$$\frac{-1}{V}\frac{\partial\ln Z_C(T,\rho)}{\partial\rho}\approx\frac{\langle z_0\exp(F+i\theta)\rangle_{(T,\kappa=\mu=0)}}{\langle\exp(F+i\theta)\rangle_{(T,\kappa=\mu=0)}}\approx\frac{\int x_0e^F\langle\cos\theta\rangle_{|\Omega|}w(|\Omega|)d|\Omega|}{\int e^F\langle\cos\theta\rangle_{|\Omega|}w(|\Omega|)d|\Omega|}$$

Sign problem in heavy quark QCD

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

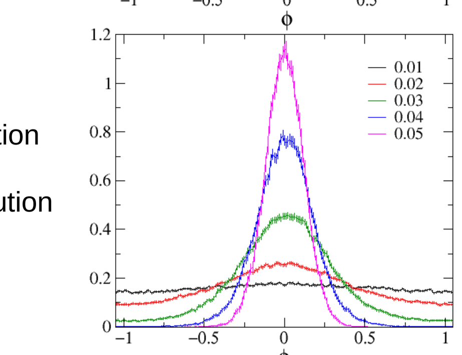
$\theta=N\phi=V\rho\phi \qquad$ (Quenched QCD)



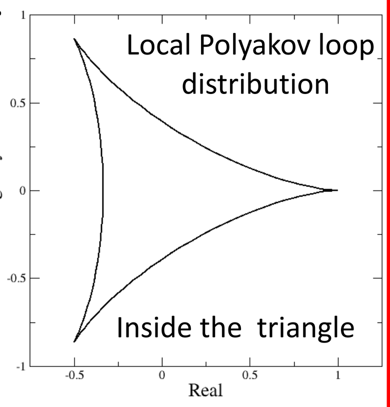
- Fourier transformation of the distribution function $W(\phi)$.
- Ω : large distribute near ϕ =0
  - Center symmetry is broken (high T).

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

$\langle\cos(N\phi)\rangle\ \approx\ e^{-N^2\langle\phi^2\rangle/2}$ $\quad$ If Gaussian distribution No sign problem



- Ω : large distribute near $|\Omega|$=0
  - Local Polyakov loop has Z(3) center symmetry.
  - The distribution of the spatial average Ω has U(1) (not Z(3)) in the large volume limit, if the Z(3) center symmetry is unbroken (low T).
  - Central limit theorem: Gaussian distribution
  - The variances for the real and imaginary directions, $\overline{x^2}$ and $\overline{y^2}$, are the same.



→ U(1) symmetric Gaussian distribution:

$$W(|\Omega|,\phi)\sim e^{-a(x^2+y^2)}=e^{-a|\Omega|^2}$$

$$\overline{x^2}=\int_{-\pi}^{\pi}(r\cos\theta)^2\ w(r,\theta)\ dr\ d\theta=\int_{-\pi/N}^{\pi/N}\frac{r^2}{2}w(r,\theta)\ dr\ d\theta$$

$$\overline{y^2}=\int_{-\pi}^{\pi}(r\sin\theta)^2\ w(r,\theta)\ dr\ d\theta=\overline{x^2}$$

Local Polyakov loop dist. $w(r,\phi)$: Z(3) symmetric

$$\overline{x^2}=\int_{-\pi/N}^{\pi/N}r^2\sum_{n=1}^{N}\frac{1+\cos2(\theta+2\pi n/N)}{2}w(r,\theta)\ dr\ d\theta$$

$$=\int_{-\pi/N}^{\pi/N}r^2\frac{1+{\rm Re}(e^{2i\theta}\sum_{n=1}^{N}e^{4\pi n/N})}{2}w(r,\theta)\ dr\ d\theta=\int_{-\pi/N}^{\pi/N}\frac{r^2}{2}w(r,\theta)\ dr\ d\theta$$

Expectation values at infinitesimal 1/(mass)

$$\langle\cos(N\phi)\rangle_{|\Omega|}^{(\varepsilon)}=\frac{\langle\cos(N\phi)\ e^{\varepsilon{\rm Re}\Omega}\rangle_{|\Omega|}}{\langle e^{\varepsilon{\rm Re}\Omega}\rangle_{|\Omega|}}=\int_{-\pi}^{\pi}\cos(N\phi)\ e^{\varepsilon|\Omega|\cos\phi}d\phi\Big/\int_{-\pi}^{\pi}e^{\varepsilon|\Omega|\cos\phi}d\phi$$

$$\langle\cos(N\phi)\ e^{\varepsilon\cos\phi}\rangle_{|\Omega|}=\int_{-\pi}^{\pi}\cos(N\phi)\ e^{\varepsilon\cos\phi}d\phi\ =\frac{1}{N!\,2^{N-1}}\varepsilon^N|\Omega|^N+O(\varepsilon^{N+1})$$

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

Sign problem is solved.

- The quark determinant: $\quad \ln\det M=\sum_N F_N\ e^{N\mu/T}$
- This analysis is applicable when $\ \ln\det M\approx F_1\ e^{\mu/T}+F_1^*\ e^{-\mu/T}$ is a good approximation.
- For the case of $\ \ln\det M\approx F_1e^{\mu/T}+F_2e^{2\mu/T}+\cdots$, complex phase remains. But, it is O(K^{2Nt}) at most.
- Because F_n is $O(\Omega^n)$, F_n ($n\geq2$) is small when Ω is small.

Center symmetry in U(1) gauge theory

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

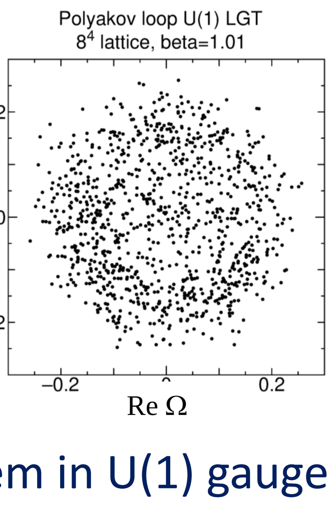
$$Z_{GC}(T,\mu)=\sum_N Z_C(N,T)e^{iN\theta}e^{N\mu/T},\qquad Z_{GC}(T,\mu)=Z_{GC}(T,\mu+i\theta T)$$

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

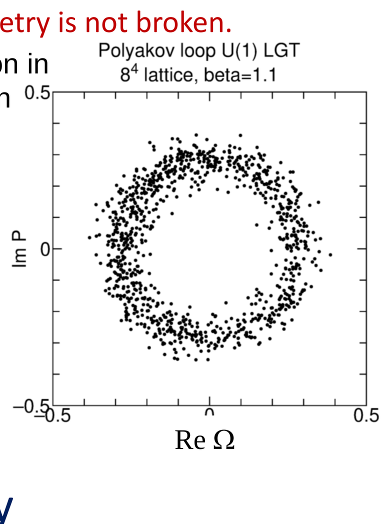
$$Z_{GC}(T,\mu)=\frac{1}{2\pi}\int\left[\sum_N Z_C(N,T)e^{iN\theta}e^{N\mu/T}\right]d\theta=Z_C(0,T)$$

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



Sign problem in U(1) gauge theory

$$\frac{-1}{V}\frac{\partial\ln Z_C(T,\rho)}{\partial\rho}\approx\frac{\langle z_0e^{F+i\theta}\rangle_{(T,\kappa=\mu=0)}}{\langle e^{F+i\theta}\rangle_{(T,\kappa=\mu=0)}}\approx\frac{\int x_0e^F\langle\cos\theta\rangle_{|\Omega|}w(|\Omega|)d|\Omega|}{\int e^F\langle\cos\theta\rangle_{|\Omega|}w(|\Omega|)d|\Omega|}$$

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

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

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

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

- Using the center symmetry: $\quad Z_{GC}(T,\mu)=\frac{1}{2\pi}\int Z_{GC}(T,\mu+i\xi)\ d\xi$
- For for $Z_{GC}(T,\mu+i\xi)$,
  The saddle point changes as $z_0\rightarrow z_0+i\xi$,
  $D(z_0)$, $D''(z_0)$ do not change.
- We write the quark determinant:

$$\ln\det M=\sum_N F_N\ e^{N\mu/T}\equiv\sum_N|F_N|e^{i\phi_N}\ e^{N\mu/T}$$

- If $\ \ln\det M\approx F_1\ e^{\mu/T}+F_1^*\ e^{-\mu/T}\ $ is a good approximation.
- Saddle point is denoted as $\quad z_0+i\xi=x_0+i(\phi_1+\delta+\xi)$
  - Integral of ξ $\qquad (y_0\equiv\phi_1+\delta)$
- Under the infinitesimal source $\qquad \langle\cos(\theta)\rangle^{(\varepsilon)}=\frac{\langle\cos(\theta)\ e^{\varepsilon{\rm Re}F_1}\rangle}{\langle e^{\varepsilon{\rm Re}F_1}\rangle}$

$$\frac{-1}{V}\frac{\partial\ln Z_C(T,\rho)}{\partial\rho}\approx\frac{\int DU_\mu\ x_0\exp F\ \cos\eta|F_1|^N}{\int DU_\mu\exp F\ \cos\eta\ |F_1|^N}$$

Sign problem is almost avoided. $\qquad \eta=V\rho\delta+V{\rm Im}D-\frac{\alpha}{2}$