First order transitions in finite temperature and density QCD with two and many flavors

Shinji Ejiri (Niigata University)

Collaboration with

Ryo Iwami (Niigata), Norikazu Yamada (KEK) & Hiroshi Yoneyama (Saga)

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Phase structure of QCD at high temperature and density

Lattice QCD Simulations

- Phase transition lines *T*
- Equation of state

 Direct simulation: Impossible at μ≠0.



QCD phase transition at finite T and μ

Expansion of the parameter space and Extrapolation

- Large chemical potential μ (at physical mass)
 - Different quark mass at low density
 - Large number of flavor
- Chiral limit of 2-flavor QCD
 (2+1)-flavor or (2+many)-flavor at finite mass
- Large volume limit
 - Complex parameter: Lee-Yang zero

Quark Mass dependence of QCD phase trantion



P. de Forcrand & O.Philipsen, 03, 07

Bielefeld-Swansea Collab., 02, 03

- On the line of physical mass, the crossover at low density $\implies 1^{st}$ order transition at high density.
- However, the 1st order region is very small, and simulations with very \bullet small quark mass are required. \implies Difficult to study.



Finite T and μ phase transition in (2+many)-flavor QCD

- Many-flavor QCD to construct Technicolor models
- Chiral phase transition of QCD
 - → Electroweak phase transition at finite temperature
- Nambu-Goldstone bosons
 - 3 bosons are absorbed into gauge bosons. (3 massless bosons)
 - The other bosons have not observed yet. (The other bosons: heavy)
 - 2 techni-felmions are massless, and the others are heavy.
- Electro-weak baryogenesis
 - Strong first order transition: required. (SM: Not strong 1st order.)
 - From the analogy of 2+1-flavor QCD, 1st order at small mass;
 2nd order or crossover at large mass.
- <u>It is important to determine the endpoint of the first order region</u> in (2+many)-flavor QCD.

Nature of phase transition of $2+N_{f}$ -flavor QCD



mud

S. E. & N. Yamada, Phys. Rev. Lett. 110, 172001 (2013)

- Assumption: $N_{\rm f}$ -flavors are heavy.
 - Hopping parameter κ expansion
- Parameter: $N_{\rm f} \kappa^{N_t} \implies 1/m_{h,ct} \sim \kappa_{ct} \propto 1/N_{\rm f}^{1/N_t}$
- As increasing $N_{\rm f}$, critical mass becomes Easy to investigate.
- Tricritical scaling: the same as (2+1)-flavor



Good test ground

Nature of 2-flavor QCD in the chiral limit 2nd order or 1st order?

Long standing problem

Light quark mass (m_1) dependence of the critical line

• Trictitical scaling behavior?





Similar study in QCD with an imaginary chemical potential: Bonati, D' Elia, de Forcrand, Philipsen, Sanfilippo, arXiv:1311.0473; 1408.5086

Singularities of QCD in the complex μ_q plane Lee-Yang zero/ Fisher zero: partition function Z=0

Prediction near the chiral limit, assuming O(4) universality

• M. Stephanov Phys. Rev. D73, 094508 (2006)



 The distribution of Z=0 → Nature of phase transition by Mote-Carlo simulations (order & universality class)

Phase transitions in many-flavor QCD

We investigate the critical surface in 2-flavor QCD and QCD with 2-light flavors + N_fmassive flavors.

- (2+Nf)-flavor QCD
 - Electro-weak baryogenesis Technicolor model
 - Good testing ground for (2+1)-flavor QCD

Plan of this talk

- Histogram method to study nature of phase transitions
- N_f-dependence of the critical heavy quark mass.
- Light quark mass-dependence of the critical curve
 - The chiral limit of 2-flavor QCD: 2nd order or 1st order?
- μ -dependence of the critical curve.
- Singularities in the complex μ plane, Lee-Yang zeros

Probability distribution function

• Distribution function (Histogram)

X: order parameters, total quark number, average plaquette etc.

$$Z(m,T,\mu) = \int dX \ W(X,m,T,\mu)$$
 histogram

• In the Matsubara formalism,

$$Z(m,T,\mu) \equiv \int DU (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$
$$W(X',m,T,\mu) \equiv \int DU \delta(X-X') (\det M(m,\mu))^{N_{\rm f}} e^{-S_g}$$

- where det*M*: quark determinant, S_g: gauge action.
- Useful to identify the nature of phase transitions
 - e.g. At a first order transition, two peaks are expected in W(X).



Plaquette and Polyakov loop

site_

periodic bounda

Dynamical variables

- Gauge field: $U_{\mu} \in SU(3)$, on a link
- Quark field: $\psi, \overline{\psi}$, Grassmann, on a site

Standard gauge action $(\beta = 6/g^2)$

$$S_{g} = -\beta \sum_{n,\mu\neq\nu} \frac{1}{3} \operatorname{tr} \left[U_{\mu}(n) U_{\nu}(n+\hat{\mu}) U_{\mu}^{\dagger}(n+\hat{\nu}) U_{\nu}^{\dagger}(n) \right]$$

= *P*: plaquette

Polyakov loop

$$\Omega = \frac{1}{N_s^3} \sum_{n=1}^{\infty} \frac{1}{3} \operatorname{tr} \left[U_4(\vec{n}, 1) U_4(\vec{n}, 2) \cdots U_4(\vec{n}, N_t) \right]$$

Complex: $\Omega = \Omega_R + i\Omega_I$

Reweighting method for plaquette distribution function

$$W(P,\beta,m,\mu) \equiv \int DU\delta(\hat{P}-P) \prod_{f=1}^{N_{\rm f}} \det M(m_f,\mu_f) e^{6N_{\rm site}\beta\hat{P}} \qquad \frac{S_g = -6N_{\rm site}\beta\hat{P}}{(\beta = 6/g^2)}$$

plaquette P (1x1 Wilson loop for the standard action)

^

 $R(P,\beta,\beta_0m,m_0,\mu) \equiv W(P,\beta,m,\mu)/W(P,\beta_0,m_0,0) \qquad \text{(Reweight factor)}$

$$R(P) = \frac{\left\langle \delta(\hat{P} - P) e^{6N_{\text{site}}(\beta - \beta_0)\hat{P}} \prod_{f} \frac{\det M(m_f, \mu_f)}{\det M(m_0, 0)} \right\rangle_{(\beta_0, \mu = 0)}}{\left\langle \delta(\hat{P} - P) \right\rangle_{(\beta_0, \mu = 0)}} = \left\langle e^{6N_{\text{site}}(\beta - \beta_0)\hat{P}} \prod_{f} \frac{\det M(m_f, \mu_f)}{\det M(m_0, 0)} \right\rangle_{P:\text{fixed}}$$

Effective potential:

$$V_{\text{eff}}(P,\beta,m,\mu) = -\ln[W(P,\beta,m,\mu)] = V_{\text{eff}}(P,\beta_0,m_0,0) - \ln R(P,\beta,\beta_0m,m_0,\mu)$$
$$\ln R(P) = \frac{6N_{\text{site}}(\beta-\beta_0)P}{6} + \ln\left\langle \prod_f \frac{\det M(m_f,\mu_f)}{\det M(m_0,0)} \right\rangle_{P:\text{fixed}}$$

First order transition point: two phases coexist Plaquette distribution function

- Performing simulations of 2-flavor QCD,
- Dynamical effect of N_f-flavors are included by the reweighting.
- We assume *N*_f-flavors are heavy.
- Hopping parameter (κ) expansion (Wilson quark)

$$N_{\rm f} \ln \left(\frac{\det M(\kappa,\mu)}{\det M(0,0)} \right) = N_{\rm f} \left(288N_{\rm site} \kappa^4 P + 12 \cdot 2^{N_t} N_s^3 \kappa^{N_t} \left(\cosh(\mu/T) \Omega_R + i \sinh(\mu/T) \Omega_I \right) + \cdots \right)$$

plaquette: P Polyakov loop: $\Omega_R + i \Omega_I$

• Effective potential

$$2-\text{flavor} crossover + 2+\text{Nf-flavor} 1 \text{st order transition}$$

$$V_{\text{eff}}(P,\beta,\kappa) = -\ln[R(P,\kappa)W(P,\beta,0)] = V_{P,\beta,0} + \frac{2+\text{Nf-flavor}}{1-\ln[R(P,K)]} = V_{P,\beta,0} + \frac{2+\text{Nf-fla$$

Rewighting of the effective potential

$$\ln R(P) = \ln \left\langle e^{6N_{\text{site}}(\beta-\beta_0)\hat{P}} \prod_f \frac{\det M(\kappa_f, \mu_f)}{\det M(\kappa_0, 0)} \right\rangle_{P:\text{fixed}} \approx \ln \left\langle \exp(6hN_s^3\hat{\Omega}_R) \right\rangle_{P:\text{fixed}} + (\text{linear term of } P)$$

$$\left\langle \text{degenerate mass case at } \mu=0 \right\rangle$$

 $V_{\text{eff}}(P,\beta,h,\mu) = V_{\text{eff}}(P,\beta_0,0,0) - \ln \overline{R}(P,h,\mu) + \text{ (linear term of } P)$

$$\overline{R}(P) = \left\langle \exp\left(6N_s^3 h \Omega_R\right) \right\rangle_{P:\text{fixed}} \quad \text{(for the case of } \mu=0\text{)}$$

Wilson quark

$$h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_t}$$

Staggered quark

$$h = N_{\rm f} / \left(4 \left(2m_{\rm h} \right)^{N_t} \right)$$

• β -dependence is only in the linear term.

Phase structure of (2+many)-flavor QCD

P4-imprived staggered Simulations

*N*f=2 p4-staggered, $m_π/m_ρ$ ≈0.7 data: Beilefeld-Swansea Collab., PRD71,054508(2005) 16³x4 lattice.

Improved-Wilson Simulations

Iwasaki gauge action + N_f =2 clover -Wilson fermion action, κ =0.145, 0.475, 0.150, 0.1505,

 $m_{\pi}/m_{\rho} = 0.6647, 0.5761, 0.4677, 0.4575, 16^3 \text{x4}$ lattice.

Dynamical heavy quark effect is added by the reweighting method.

det*M*: Hopping parameter expansion

Curvature of the effective potential $V_{\text{eff}}(P,\beta,h,\mu) = V_{\text{eff}}(P,\beta_0,0,0) - \ln \overline{R}(P,h,\mu) + \text{ (linear term of }P)$ $\overline{R}(P) = \left\langle \exp(6N_s^3h\Omega_R) \right\rangle_{P:\text{fixed}} \text{ (for the case of }\mu=0)$

Wilson quark

$$h = 2N_{\rm f} \left(2\kappa_{\rm h} \right)^{N}$$

Staggered quark

$$h = N_{\rm f} / \left(4 \left(2m_{\rm h} \right)^{N_t} \right)$$

- Linear term of *P* is irrelevant to the curvature
- β -dependence is only in the linear term.
- The curvature is independent of β .

$$\chi_P$$
: plaquette susceptibility
 $\frac{d^2 V_{\text{eff}}(0)}{dP^2} \approx \frac{6N_{\text{site}}}{\chi_P}$

$$\frac{d^2 V_{\text{eff}}}{dP^2}(P,h,\mu) = \frac{d^2 V_{\text{eff}}}{dP^2}(P,0,0) - \frac{d^2 \ln \overline{R}}{dP^2}(P,h,\mu)$$

2-flavor

• If there exists the negative curvature region,

First order transition (double-well potential)



Curvature of the effective potential



Slope of the effective potential

$$V_{\text{eff}}(P,\beta,h,\mu) = V_{\text{eff}}(P,\beta_0,0,0) - \ln \overline{R}(P,h,\mu) + \quad \text{(linear term of } P)$$

$$\implies \frac{dV_{\text{eff}}}{dP}(P,h,\mu) = \frac{dV_{\text{eff}}}{dP}(P,0,0) - \frac{d\ln \overline{R}}{dP}(P,h,\mu) + \quad \text{(constant term)}$$

- The shape of dV_{eff}/dP is independent of β .
- If dV_{eff}/dP is an S-shaped function,

First order phase transition (double-well potential).





S-shaped function at large h

 $h = 2N_{\rm f} (2\kappa_{\rm h})^{N_t}$ for Wilson quark

$N_{\rm f}$ -dependence of the critical mass $h_c = 0.0614(69)$ (p4-staggared, $m_{\pi}/m_{ ho} \approx 0.7$)

• Critical mass increases as $N_{\rm f}$ increases.

$$h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_t} \quad \Longrightarrow \quad \kappa_{\rm h}^c = \frac{1}{2} \left(\frac{h_c}{2N_{\rm f}}\right)^{1/N_t}$$

- When $N_{\rm f}$ is large, κ is small. Then, the hopping parameter (κ) expansion is good.
- On the hand, when $N_{\rm f}$ is small, the κ -expansion is bad.
- In a quenched simulation with N_t=4, the first and second terms becomes comparable around κ=0.18.
- For $N_{\rm f}$ =10, $N_{\rm t}$ =4, $h_c = 0.0614(69)$ $\implies \kappa_h^c \approx 0.118$
 - It may be applicable for $N_{\rm f}$ ~10.

Phase structure of (2+many)-flavor
QCD using Wilson quark action
2-flavor QCD simulations + reweighting
Light quark mass dependence of the critical line

• Is there a first order transition region in 2-flavor QCD?



Light quark mass dependence



• The derivative of V_{eff} becomes an S-shaped function at large h.

• Critical point: light quark mass dependence is small in this region.



- Critical point: light quark mass dependence is small in the region we investigated.
- The red & green lines are the critical point at $m_l = \infty$ (N_f=0+16).
- The first order transition in the massless 2-flavor QCD is not suggested.

The effective potential at finite $\boldsymbol{\mu}$

Reweighting factor

$$\ln R(P) = \ln \left\langle \left(\frac{\det M(m,\mu)}{\det M(m,0)} \right)^2 \left(\frac{\det M(h,\mu_h)}{\det M(0,0)} \right)^{N_f} \right\rangle_{P:\text{fixed}}$$

light quarks heavy quarks

Light quark determinant: Taylor expansion up to $O(\mu^6)$ for staggered $O(\mu^2)$ for Wilson

$$N_{\rm f} \ln \det M(\mu) = N_{\rm f} \sum_{n=0}^{N} \left[\frac{1}{n!} \left(\frac{\mu}{T} \right)^n \frac{{\rm d}^n \ln \det M}{{\rm d}(\mu/T)^n} \right] \qquad \qquad \theta: \text{ complex phase} \\ \theta \equiv \operatorname{Im} \ln \det M$$

Heavy quark determinant: Hopping parameter expansion

$$N_{\rm f} \ln\left(\frac{\det M(\kappa,\mu_h)}{\det M(0,0)}\right) = N_{\rm f} 288N_{\rm site}\kappa^4 P + 6N_s^3 h \cosh\left(\frac{\mu_h}{T}\right) \left(\Omega_R + i \tanh\left(\frac{\mu_h}{T}\right)\Omega_I\right) + \cdots + h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_t}$$

$$2 \text{ control parameters}$$
²⁶

Avoiding the sign problem at finite $\boldsymbol{\mu}$

• Cumulant expansion method (SE,PRD77,014508(2008), WHOT-QCD,PRD82,014508(2010))

$$\langle e^{i\theta} \rangle = \exp\left[i\langle \theta \rangle_{c} - \frac{1}{2}\langle \theta^{2} \rangle_{c} - \frac{i}{3!}\langle \theta^{3} \rangle_{c} + \frac{1}{4!}\langle \theta^{4} \rangle_{c} + \cdots\right]$$

cumulants

$$\langle \theta \rangle_{C} = \langle \theta \rangle, \ \langle \theta^{2} \rangle_{C} = \langle \theta^{2} \rangle - \langle \theta \rangle^{2}, \ \langle \theta^{3} \rangle_{C} = \langle \theta^{3} \rangle - 3 \langle \theta^{2} \rangle \langle \theta \rangle + 2 \langle \theta \rangle^{3}, \ \langle \theta^{4} \rangle_{C} = \cdots$$

 $\rightarrow 0$

- <u>Odd terms</u> vanish from a symmetry under $\mu \leftrightarrow -\mu \ (\theta \leftrightarrow -\theta)$ Source of the complex phase
- If the distribution of θ is Gaussian, $\langle \theta^2 \rangle_c$ term dominates.
- Assuming the Gaussian distribution, we approximate

$$\left\langle e^{i\theta} \right\rangle \approx \exp\left[-\frac{1}{2}\left\langle \theta^2 \right\rangle_C\right]$$

 $\rightarrow 0$

Critical line at finite density (staggered)

$$h = 2N_{\rm f} \left(2\kappa_{\rm h}\right)^{N_{\rm f}}$$

for Wilson quarks

$$h = N_{\rm f} \left/ \left(4 \left(2 m_{\rm h} \right)^{N_t} \right) \right.$$

for staggered quarks

- Calculations of detM: Taylor expansion up to O(μ⁶)
- Distribution function of the complex phase of detM: approximated by a Gaussian function



S. E. & N. Yamada, Phys. Rev. Lett. 110, 172001 (2013)



The first order region becomes wider as increasing μ . 28

μ -dependence of critical h



The effect from the phase of heavy-flavor is small (< 30%). The Critical κ_h decreases exponentially as μ_h . Hopping parameter expansion is good for large μ_h .

Singularities of QCD in the complex μ_q **plane** M. Stephanov Phys. Rev. D73, 094508 (2006)

- Lee-Yang zero/ Fisher zero: partition function Z=0
 - Prediction near the chiral limit, assuming O(4) universality



- Singularities exist at large Im(μq) even for crossover.
 - Application range of Taylor expansion of $\frac{p}{T^4} = \frac{1}{VT^3} \ln Z$
- The distribution of Z=0 → Nature of phase transition by Mote-Carlo simulations (order & universality class)

Singularities of pure SU(3) gauge theory in the complex β plane (SE, Phys.Rev.D73,054502(2006))

Relation between distribution of Z=0 and plaquette distribution function



Lee-Yang zeros in the complex β for pure SU(3)

• Normalized partition function (reweighting for Imaginary β)

$$Z(\beta) = \int DU \exp[6(\beta_{\text{Re}} + i\beta_{\text{Im}})N_{\text{site}}P] \qquad \left(N_{\text{site}} = N_s^3 N_t = VN_t\right)$$
$$Z_{\text{norm}} = \left|\frac{Z(\beta_{\text{Re}}, \beta_{\text{Im}})}{Z(\beta_{\text{Re}}, 0)}\right| = \left|\left\langle\exp(i6\beta_{\text{Im}}N_{\text{site}}P)\right\rangle_{(\beta_{\text{Re}}, 0)}\right| = \left|\left\langle\exp(i6\beta_{\text{Im}}N_{\text{site}}\Delta P)\right\rangle_{(\beta_{\text{Re}}, 0)}\right|$$
$$\therefore \left|\exp(i6\beta_{\text{Im}}N_{\text{site}}\langle P\rangle\right) = 1, \ \left(\Delta P = P - \langle P\rangle\right)$$

• Plaquette distribution function (histogram)

$$w(\Delta P') = \frac{1}{Z} \int DU\delta(P' - P) e^{6\beta_{\text{Re}}N_{\text{site}}P}$$
$$Z_{\text{norm}}(\beta) = \left| \int \exp(i6\beta_{\text{Im}}N_{\text{site}}\Delta P) w(\Delta P) dP \right|$$



 $\implies \text{Fourier transformation} \quad (\Delta P \rightarrow \beta_{\text{Im}} N_{\text{site}})$



$$\theta = 6\beta_{\rm Im}N_{\rm site}\Delta P \implies Z_{\rm norm} = \left|\int e^{i\theta}w(\Delta P(\theta))d\theta\right| / (6\beta_{\rm Im}N_{\rm site})$$

Singularities of full QCD with complex μ μ_{q} : complex $Z(\beta, \mu_{q}) = \int R(P, \mu_{q}) W(P, \beta) dP$ $S_{g} = -6N_{site}\beta P$ (Reweight factor) (Weight factor at $\mu_{q}=0$) $(\det M(\mu_{q}))^{*} = \det M(-\mu_{q}^{*})$ \square $R^{*}(P, \mu_{q}) = R(P, \mu_{q}^{*}) \neq R(P, \mu_{q})$

 $R(P,\mu_q) = e^{i\phi(P,\mu_q)} |R(P,\mu_q)|$

Reweight factor: complex

Z≠0

 P_+

$$Z(\beta, \mu_q) = \int e^{i\phi(P)} \left| \frac{R(P, \mu_q) W(P, \beta) dP}{= \exp(-V_{\text{eff}}(P, \beta, \mu_q))} \right|$$

When V_{eff} is a double-well potential And $\phi(P_+) - \phi(P_-) \approx \pi + 2\pi n$, Lee-Yang zeros appear. $Z(\beta, \mu_q) \sim C(e^{i\phi(P_+)} + e^{i\phi(P_-)})$

Numerical calculation of the reweighting factor 2 approximations (SE, Phys.Rev.D77,014508(2008))

• Estimation of det*M* by a Taylor expansion up to $O(\mu_q^6)$

$$N_{\rm f} \ln \det M(\mu) = N_{\rm f} \sum_{n=0}^{N} \left[\frac{1}{n!} \left(\frac{\mu}{T} \right)^n \frac{{\rm d}^n \ln \det M}{{\rm d}(\mu/T)^n} \right]$$

• Sign problem: If $e^{i\theta}$ changes its sign,

$$\left\langle \left(\frac{\det M(\mu)}{\det M(0)} \right)^{N_f} \right\rangle_{P \text{ fixed}} \equiv \left\langle e^{i\theta} F \right\rangle_P << \text{(statistical error)}$$

- Gaussian approximation
 - Distribution function of θ : Gaussian.

$$\langle e^{i\theta}F\rangle_{P} \approx \langle F\exp\left[i\langle\theta\rangle_{C}-\frac{1}{2}\langle\theta^{2}\rangle_{C}-\frac{i}{3!}\langle\theta^{3}\rangle_{C}+\frac{1}{4!}\langle\theta^{4$$



cumulant expansion

 $\left\langle \Theta \right\rangle_{C} = \left\langle \Theta \right\rangle_{F,P}, \ \left\langle \Theta^{2} \right\rangle_{C} = \left\langle \Theta^{2} \right\rangle_{F,P} - \left\langle \Theta \right\rangle_{F,P}^{2}, \ \left\langle \Theta^{3} \right\rangle_{C} = \left\langle \Theta^{3} \right\rangle_{F,P} - 3\left\langle \Theta^{2} \right\rangle_{F,P} \left\langle \Theta \right\rangle_{F,P} + 2\left\langle \Theta \right\rangle_{F,P}^{3}, \ \left\langle \Theta^{4} \right\rangle_{C} = \cdots$

<..>*F*,*P*: expectation values fixed *F* and *P*.



Singularities in the complex μ_q plane

(SE & Yoneyama, in progress)



• Probability distribution function becomes a double-peaked function at large $\mu{\rm Im}$ as well as large $\mu{\rm Re}.$

Summary

- We studied the phase structure of (2+Nf)-flavor QCD.
 - This model is interesting for the feasibility study of the electroweak baryogenesis in the technicolor scenario.
- Applying the reweighting method, we determine the critical mass of heavy flavors terminating the first order region.
 - The critical mass becomes larger with $N_{\rm f}$.
 - The first order region becomes wider as increasing μ .
 - The light quark mass dependence of the critical heavy quark mass is small in the region we investigated.
 - The first order transition in 2-flavor QCD is not suggested.
- This may be a good approach for the determination of boundary of the first order region in (2+1)-flavor QCD at finite density.
- In the complex μ plane, the probability distribution function becomes a double-peaked function at large $\mu{\rm Im}$