FEFU
FAR EASTERN FEDERAL UNIVERSITY

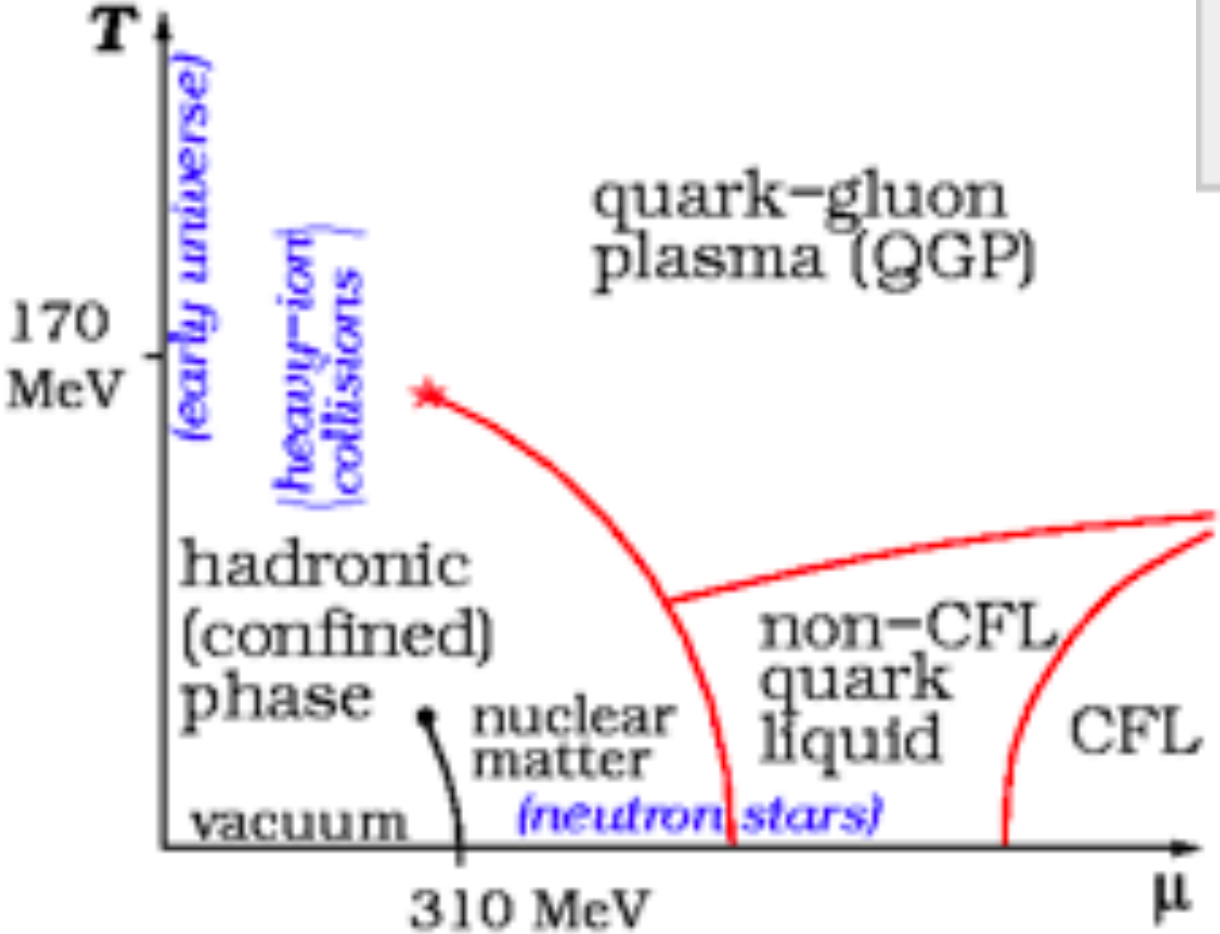
Introduction to
Finite Density Lattice QCD

Atsushi Nakamura

Oct. 3, 2019

FEFU, Vladivostok

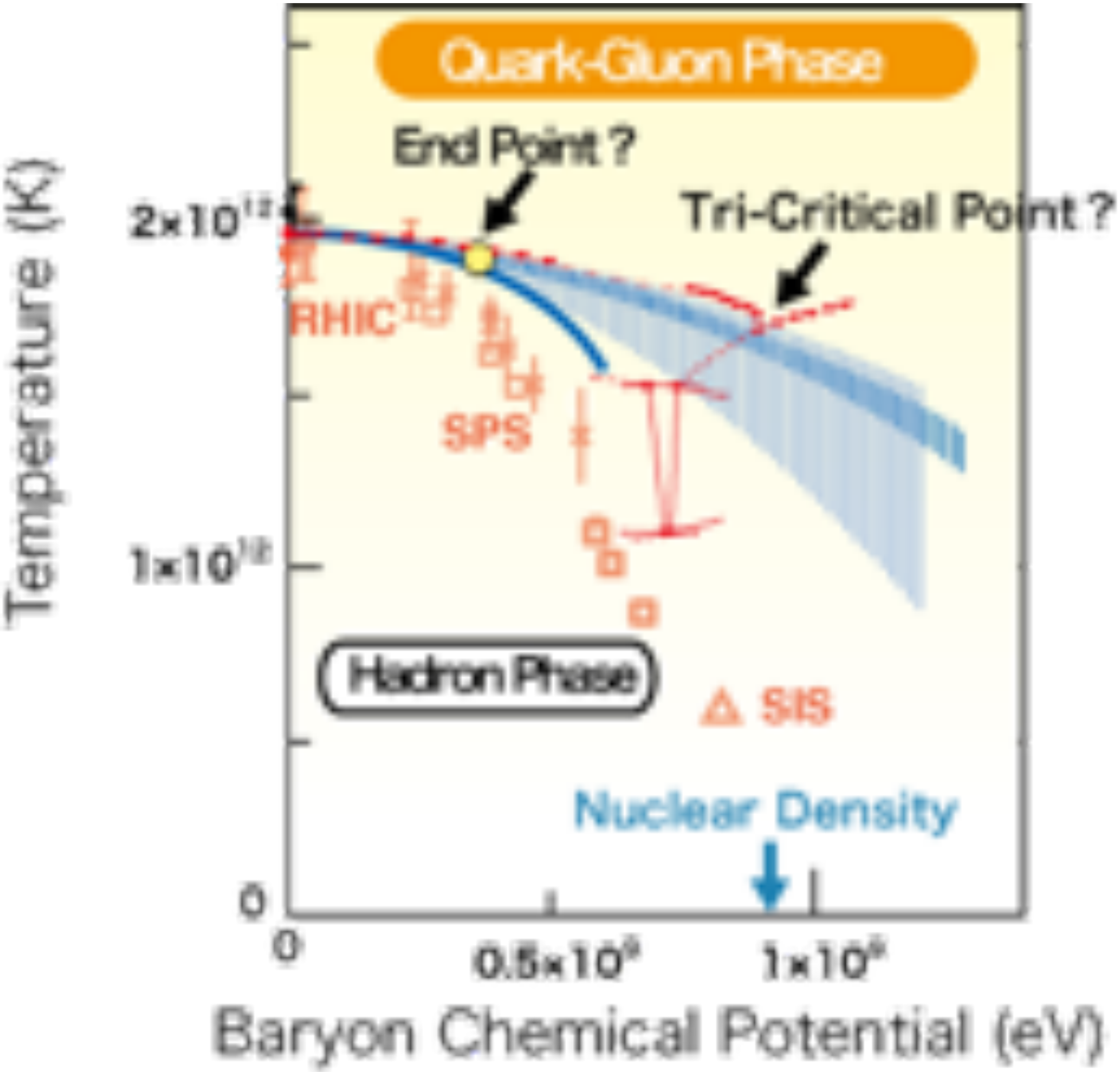
Wikipedia: QCD matter

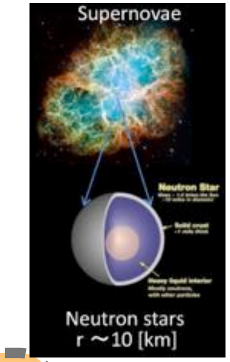


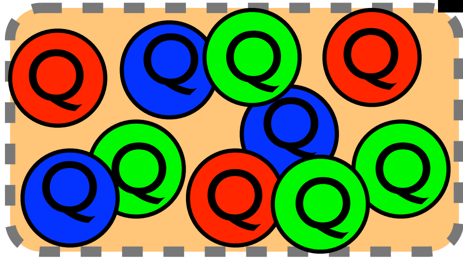
Unsolved problem in physics:

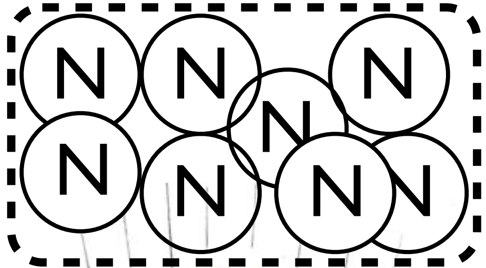
QCD in the non-perturbative regi... quark matter. The equations of ... predict that a sea of quarks and ... should be formed at high tempera... and density. What are the propert... this phase of matter?

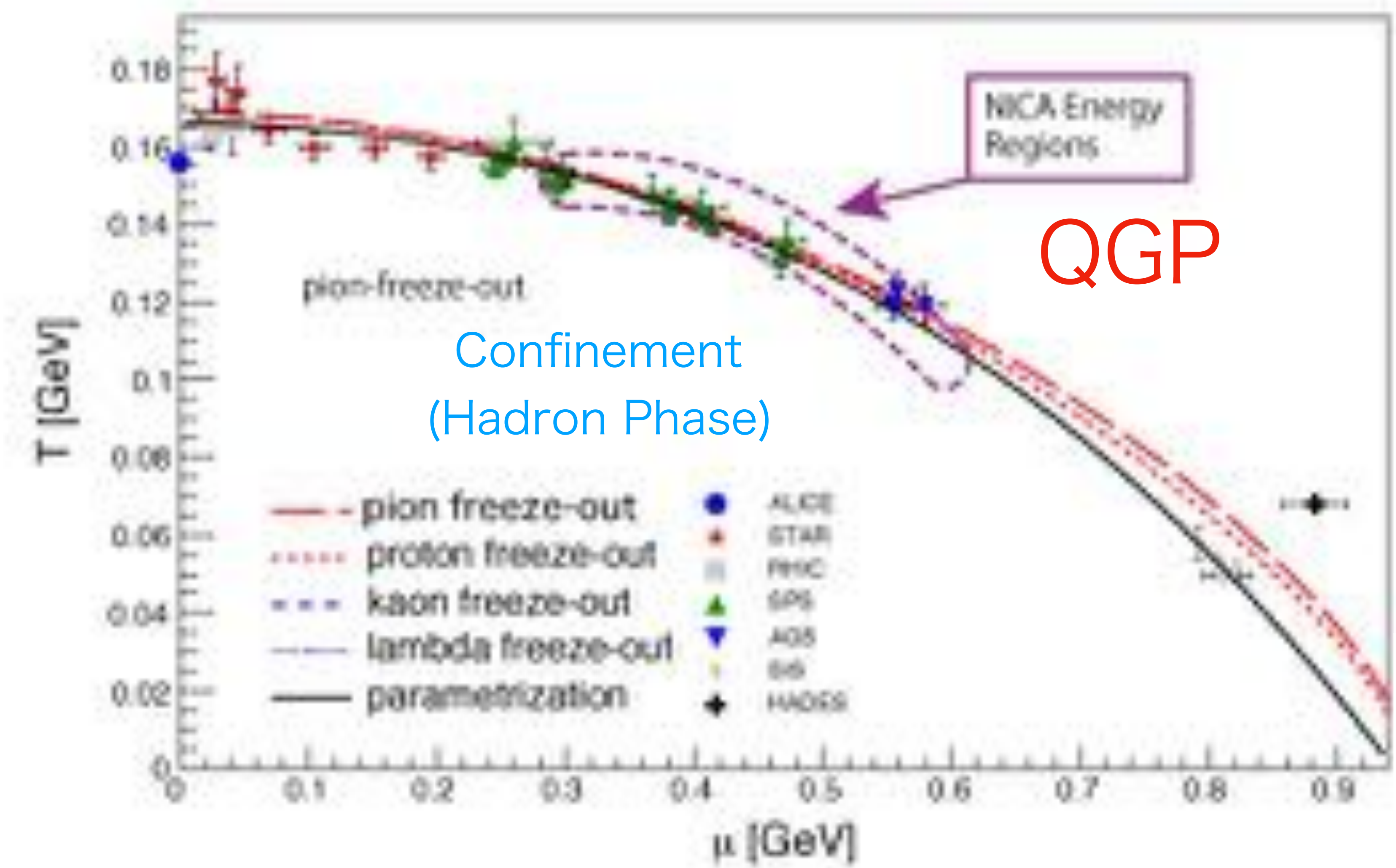
(more unsolved problems in physics)


Quark-Gluon Phase
End Point ?
Tri-Critical Point ?
2×10¹²
1×10¹²
RHIC
SPS
Hadron Phase
△ SIS
Nuclear Density
0
0
0.5×10⁹
1×10⁹
Temperature (K)
Baryon Chemical Potential (eV)


Supernovae
Neutron stars
r ～10 [km]

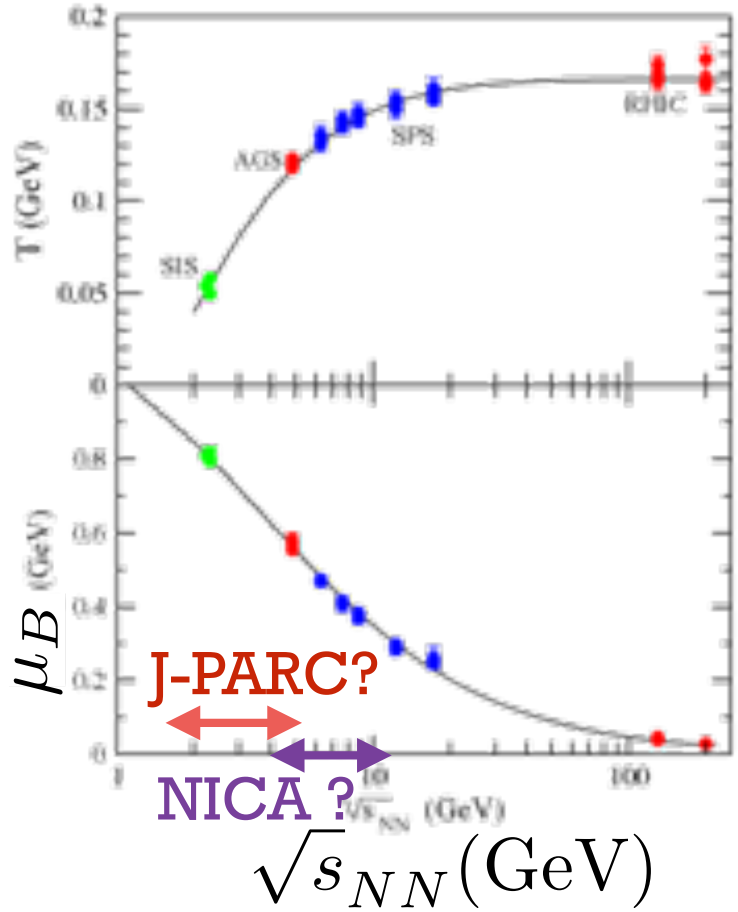






μ :Chemical Potential

D. Blaschke, J. Jankowski, and M. Naskręt
arXiv:1705.00169



J.Cleymans et al.,
Phys. Rev. C73, (2006) 034905.

Intuitive meaning of Chemical Potential μ

$$Z(\mu, T) = \mathrm{Tr}\, e^{-(H-\mu\hat{N})/T}$$
$$= e^{-F/T}$$

$$\frac{e^{-(H-\mu(\hat{N}+1))/T}}{e^{-(H-\mu\hat{N})/T}} = e^{-\Delta F/T}$$

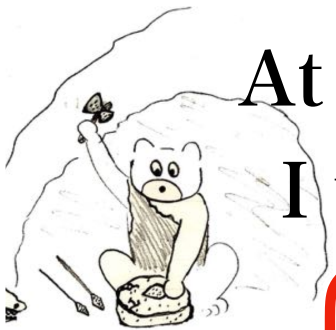
Energy for adding one more particle

Lattice QCD + μ

$\mu N = \mu \bar{\psi} \gamma_4 \psi$ **is added?**

P.Hasenfratz and F.Karsch
Physics Letters B125, (1983), 308

They found the energy density diverges.



At that time, Poland was under the martial law.
I was there, and considered it independently.

A. Nakamura
Physics Letters B149, 1984,391
Behavior of quarks and gluons at finite temperature and density in SU(2) QCD

Nakamura was thinking as follows:

In the continuum theories,

$$\mathcal{L} = \bar{\psi}[\partial_k \gamma_k + (\partial_4 + \mu)\gamma_4 + m]\psi$$

$$ip_\mu = \partial_\mu$$

On the lattice, (free case in the momentum space)

$$\Delta(p) = I - \kappa \sum_{\mu=1}^{4} \{(1-\gamma_\mu)e^{ip_\mu} + (1+\gamma_\mu)e^{-ip_\mu}\}$$

$$ip_4 \to ip_4 + \mu$$

$$I - \kappa[\sum_{\mu=1}^{3} \{(1-\gamma_\mu)e^{ip_\mu} + (1+\gamma_\mu)e^{-ip_\mu}\}]$$
$$-\kappa[(1-\gamma_4)e^{ip_4+\mu} + (1+\gamma_4)e^{-ip_4-\mu}]$$

Then we can change the hopping parameters (depending on the forward or backward)

$$\kappa e^{+\mu} \qquad \kappa e^{-\mu}$$

In the co-ordinate space with gauge field,

$$\Delta = I - \kappa \sum_{l=1}^{3} \left\{ (1-\gamma_l) U_l(x) \delta_{x', x+\hat{l}} + (1+\gamma_l) {U^\dagger}_l(x') \delta_{x', x-\hat{l}} \right\}$$
$$-\kappa e^{+\mu} (1-\gamma_4) U_\mu(x) \delta_{x', x+\hat{4}} - \kappa e^{-\mu} (1+\gamma_4) U_\mu^\dagger(x') \delta_{x', x-\hat{4}}$$

Remember $U_4 = e^{iA_4}$ **Then, we change**

$$A_4 \quad \Rightarrow \quad A_4 \to A_4 + i\mu$$

- ☑ Anyway, we had got Lattice Action with μ
- ☑ Several big groups started simulation:
  Of course SU(3).
- ☑ Nakamura could use only a small computer,
  and started a simulation with SU(2).
  (Computer room staffs at Frascatti lab. kindly
  allowed me to use their server, VAX11.)

But

Sign Problem

Lattice QCD does not work
at finite density !

Big groups failed, and only
(poor) Nakamura got results.

$$(\det \Delta(\mu))^* = \det \Delta(\mu)^\dagger = \det \Delta(-\mu^*)$$

For $\mu = 0$

$$(\det \Delta(0))^* = \det \Delta(0)$$

$\det \Delta$ ⇒ *Real*

For $\mu \neq 0$ (in general)

$\det \Delta$ ⇒ *Complex*

$$Z = \int \mathcal{D}U \prod_f \det \Delta(m_f, \mu_f) e^{-\beta S_G}$$

⇑

Complex ⇒ Sign Problem

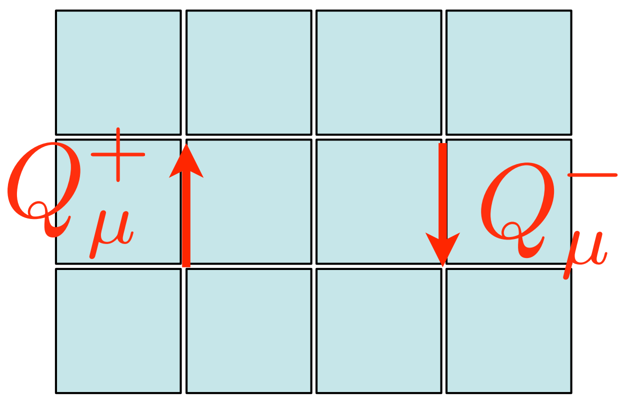
Origin of Sign Problem

Wilson Fermions $\Delta = I - \kappa Q$

KS(Staggered) Fermions $\Delta = m - Q'$

$$= m(I - \frac{1}{m}Q)$$

$$Q = \sum_{i=1}^{3}(Q_i^+ + Q_i^-) + (e^{+\mu}Q_4^+ + e^{-\mu}Q_4^-)$$



$$Q_\mu^+ = **U_\mu(x)\delta_{x',x+\hat{\mu}}$$

$$Q_\mu^- = **U_\mu^\dagger(x')\delta_{x',x-\hat{\mu}}$$

$$\det \Delta = e^{\mathrm{Tr}\log \Delta} = e^{\mathrm{Tr}\log(I-\kappa Q)}$$

$$= e^{-\sum_n \frac{1}{n}\kappa^n \mathrm{Tr} Q^n}$$

Hopping Parameter Exp.
or
Large Mass Expansion.

Closed loops do not vanish

Lowest μ depsnent terms

$$\kappa^{N_t} e^{\mu N_t} \mathrm{Tr}(Q^+ \cdots Q^+)$$

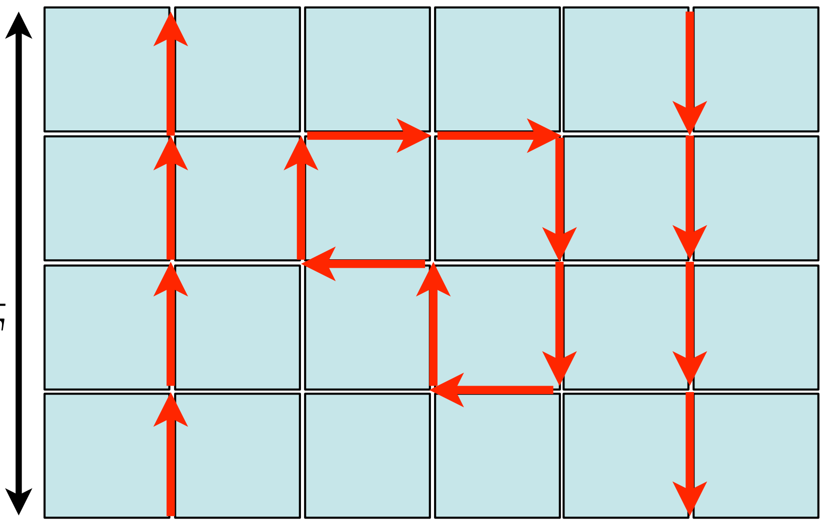
$$= ** \kappa^{N_t} e^{\mu/T} \mathrm{Tr} L$$

$$\kappa^{N_t} e^{-\mu N_t} \mathrm{Tr}(Q^- \cdots Q^-)$$

$$= ** \kappa^{N_t} e^{-\mu/T} \mathrm{Tr} L^\dagger$$

$\mathrm{Tr}L$: Polyakov Loop

$N_t = \frac{1}{T}$



Combine both

$$** \kappa^{N_t} \left(\cosh \frac{\mu}{T} \Re \mathrm{Tr} L + i \sinh \frac{\mu}{T} \Im \mathrm{Tr} L \right)$$

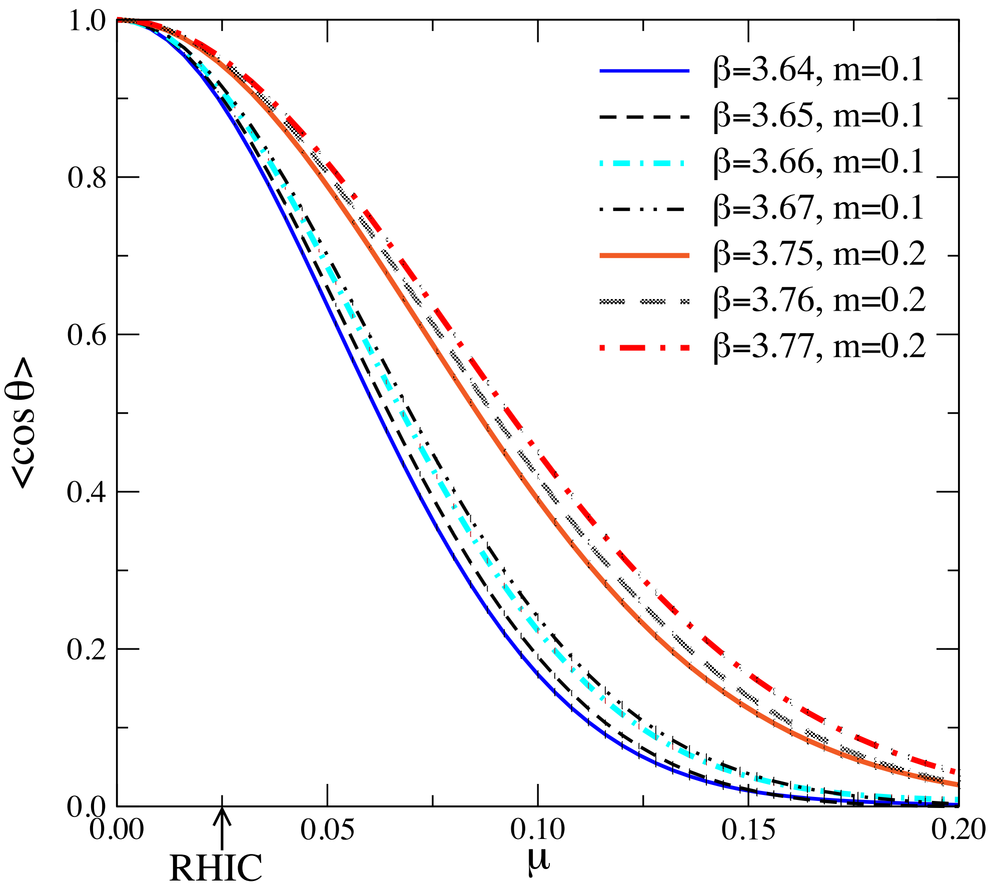
Sign Problem is sever

when μ is large

when T is low

Allton et al., Phys.Rev.D.66. 074507
(arXiv:hep-lat/0204010)

$$\det D = |\det D| e^{i\theta}$$



No Sign problem cases

1. Pure imaginary chemical potential

$$(\det \Delta(\mu))^* = \det \Delta(-\mu^*)$$

$$\mu = i\mu_I \quad \Rightarrow \quad (\det \Delta(\mu_I))^* = \det \Delta(\mu_I)$$

2. Color SU(2)

$$U_\mu^* = \sigma_2 U_\mu \sigma_2$$

$$\det \Delta(U, \gamma_\mu)^* = \det \Delta(U^*, \gamma_\mu^*) = \det \sigma_2 \Delta(U, \gamma_\mu^*) \sigma_2$$
$$= \det \Delta(U, \gamma_\mu)$$

3. Iso vector (finite iso-spin)

$$\mu_d = -\mu_u$$

$$\det \Delta(\mu_u) \det \Delta(\mu_d) = \det \Delta(\mu_u) \det \Delta(-\mu_u)$$

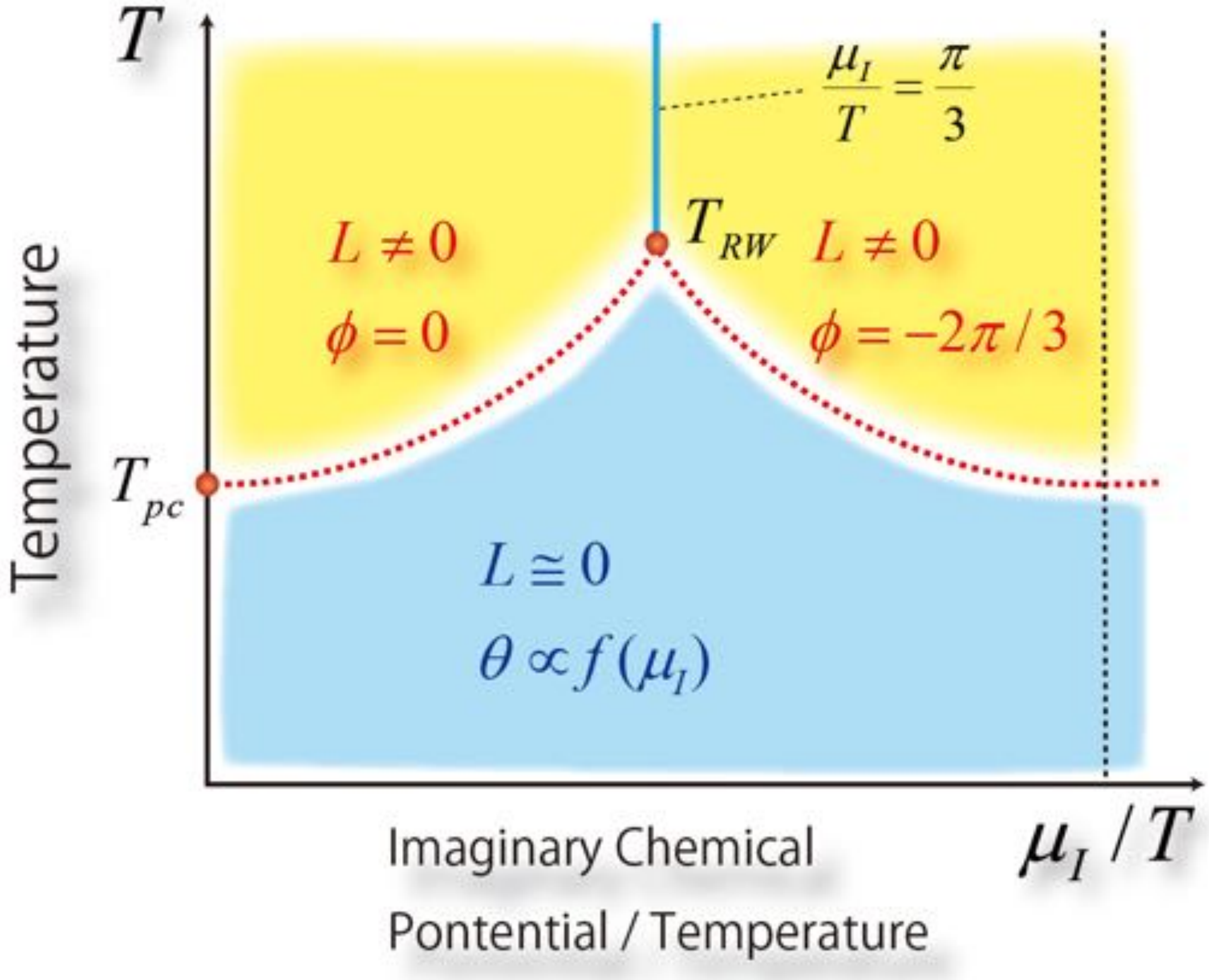
$$= \det \Delta(\mu_u) \det \Delta(\mu_u)^* = |\det \Delta(\mu_u)|^2$$ (Phase Quench)

Phase Structure in pure imaginary

$$(\det \Delta(\mu))^* = \det \Delta(\mu)^\dagger = \det \Delta(-\mu^*)$$

$$\mu = i\mu_I \Rightarrow \det \Delta\text{: Real !}$$

Phase diagram in μI region



Polyakov loop

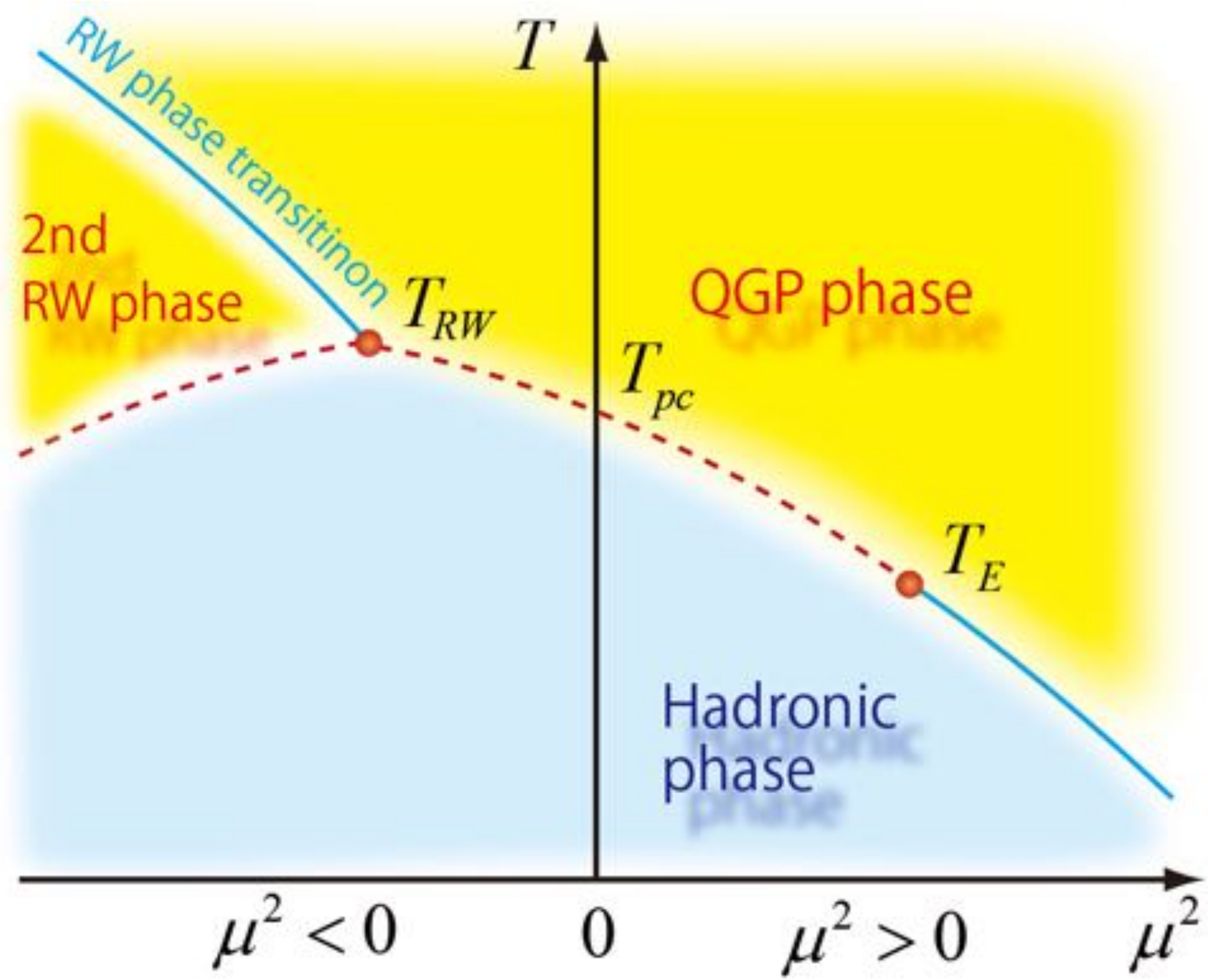
$$P = L_P \exp(i\phi_P)$$

If μ is pure imaginary

there is no sign problem.

$$(\det \Delta(\mu))^* = \det \Delta(-\mu^*)$$

Imaginary to real chemical potential



Many Approaches to Sign Problem

- Taylor Expansion
- Canonical Approach
- Density of State
- Complex Langevin

Canonical Approach

proposed by
A.Hasenfratz and Toussaint in 1992
to solve the sign problem.
But it did not work.
We traced the cause and solve it with
multiple precision numerical calculations

Canonical Approach

$$Z(\mu, T) \Longleftrightarrow Z_n(T)$$

Grand Canonical — Canonical

$$Z(\mu, T) = \mathrm{Tr}\, e^{-(H-\mu\hat{N})/T}$$

$$= \sum_n \langle n| e^{-(H-\mu\hat{N})/T} |n\rangle$$

If $[H, \hat{N}] = 0$

$$= \sum_n \langle n| e^{-H/T} |n\rangle\, e^{\mu n/T}$$

$$= \sum_n Z_n(T) \xi^n \qquad \left(\xi \equiv e^{\mu/T}\right)$$

Fugacity

Personal History about Sign Problem

We were looking for

A Reduction Formula for Wilson Fermions

$$\det \Delta = \det Q$$

Matrix Δ is smaller than Q

- ☆Keitaro Nagata and Atsushi Nakamura
  Phys. Rev. D82,094027 (arXiv:1009.2149)
- ☆A. Alexandru and U. Wenger
  Phys.Rev.D83:034502,2011 (arXiv:1009.2197)
- ☆ One more group

For KS Fermions, the reduction formula was known.

- Gibbs Formula(*)
  - P.E.Gibbs, Phys.Lett. B172 (1986) 53-61

$$
\begin{aligned}
\det \Delta &= z^{-N} \begin{vmatrix} -B(-V) - z & 1 \\ -V^2 & -z \end{vmatrix} \\
&= \left| \begin{pmatrix} BV & 1 \\ -V^2 & 0 \end{pmatrix} - zI \right| \\
&= \det (P - zI) \\
&= \prod (\lambda_i - z)
\end{aligned}
$$

P

$z \equiv e^{-\mu}$

- P is $(2 \times N_c \times N_x \times N_y \times N_z)^2$ (Matrix Reduction)
- Determinant for any value of μ

*) A similar formula was developped by Neuberger (1997) for a chiral fermion and applied by Kikukawa(1998).

The same matrix transformation like KS case cannot be employed, due to the fact that

$r \pm \gamma_4$ have no inverse, if the Wilson term $r = 1$.

Gibbs started to multiply V to the fermion matrix Δ.

Instead, we multiply $P = (c_a r_- + c_b r_+ V z^{-1})$

Here,

$$
V = \left(\begin{array}{c|c|ccc|c}
0 & U_4(t=1) & 0 & \cdots & & 0 \\ \hline
0 & 0 & U_4(t=2) & \cdots & & 0 \\ \hline
0 & 0 & 0 & \cdots & & \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
 & & & \cdots & U_4(t=N_t-2) & 0 \\ \hline
0 & 0 & & \cdots & 0 & U_4(t=N_t-1) \\ \hline
-U_4(t=N_t) & 0 & & \cdots & 0 & 0
\end{array}\right)
$$

c_a and c_b are arbitary non-zero numbers.

$$\det P = (c_a c_b z^{-1})^{N/2}$$

if we take the following trick, Borici (2004)

$$r_+ r_- = \frac{r^2 - 1}{4} = \epsilon \to 0$$

where $r_\pm \equiv \dfrac{r \pm \gamma_4}{2}$

After very long calculation (See Nagata-Nakamura arXiv:1009.2149), we get

$$\det \Delta(\mu) = (c_a c_b)^{-N/2} z^{-N/2}$$

$$\times \left(\prod_{i=1}^{N_t} \det(\alpha_i) \right) \det \left(z^{N_t} + Q \right)$$

$$\frac{\det \Delta(\mu)}{\det \Delta(0)} = \frac{\det(\xi + Q)}{\det(1+Q)}$$

$$\xi \equiv e^{-\mu/T}$$

(fugacity)

Q is $(4N_cN_xN_yN_z) \times (4N_cN_xN_yN_z)$ matrix.

No N_t !

In case of KS matrix, the corresponding matrix is $(2N_cN_xN_yN_z) \times (2N_cN_xN_yN_z)$

Diagonalize Q,

$$Q \to \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \cdots & \\ & & & \lambda_{N_{red}} \end{pmatrix}$$

$$\det(\xi + Q) = \prod (\xi + \lambda_n)$$

λ_n does not depend on μ.

⇨ Once we calculate λ_n, we can evaluate $\det \Delta(\mu)$ for any μ.

$$\det(\xi + Q) = \prod(\xi + \lambda_k) = \sum C_n \xi^n$$

$$Z = \int \mathcal{D}U \det \Delta e^{-\beta S_G}$$

$$Z = \sum_n \left(\int \mathcal{D}U C_n e^{-\beta S_G} \right) \xi^n$$
$$= \sum_n z_n \, \xi^n$$

$$\xi \equiv e^{\mu/T}$$

Fugacity Expansion

$$Z(\mu, T) = \sum_n z_n(T)(e^{\mu/T})^n$$

$Z(\mu, T)$: Grand Canonical Partition Function

$z_n(T)$: Canonical Partition Function

Inverse transformation:

$$z_n = \int \frac{d\theta}{2\pi} e^{i\theta n} Z_{GC}(\theta \equiv \frac{\mathrm{Im}\mu}{T}, T)$$

A.Hasenfratz and Toussaint (1992)

z_n can be determined in imaginary μ regions.

This is Canonical approach by

A.Hasenfratz and Toussaint (1992)

$$Z_n = \int \frac{d\theta}{2\pi} e^{in\theta} Z(\theta = \frac{\mu_I}{T})$$

In pure Imaginary μ , there is no sign problem.

It was known that this method does not work.

Why ???

Check by an analytic method (Winding Number Expansion)

$$Z_n = \int \frac{d\theta}{2\pi} e^{in\theta} Z(\theta = \frac{\mu_I}{T})$$

A. Hasenfratz and D. Toussaint

$$Z(\mu) = \int DU \det \Delta(\mu) e^{-S_G}$$

Kentucky: Winding Number Expansion

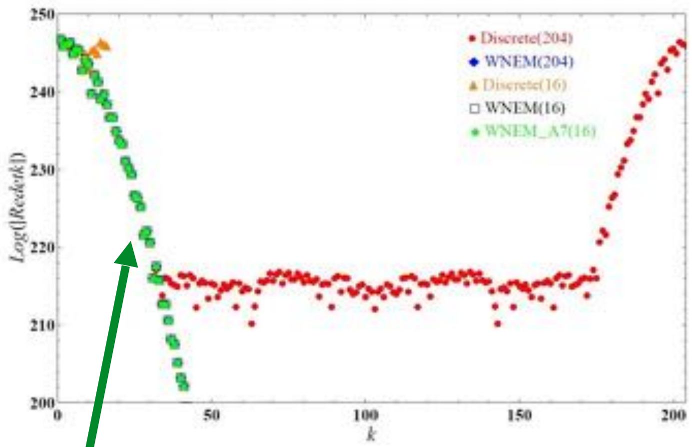
Meng et al., 2008

The original method does not work due to numerical errors.

$$\det \Delta = \exp(Tr \log \Delta)$$

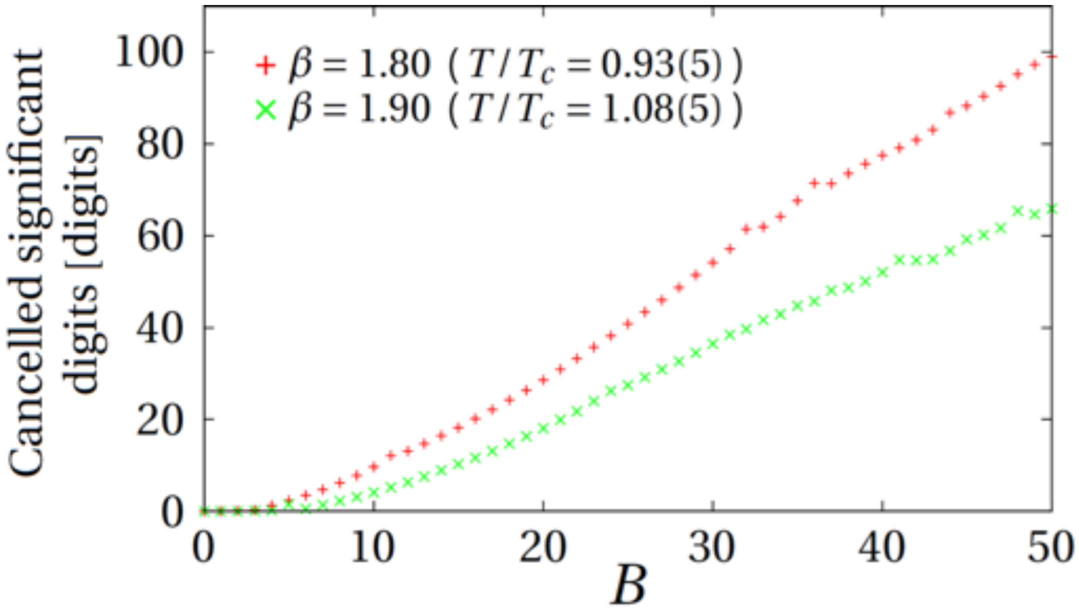
$$\log(I - \kappa Q) = -\sum_n \frac{\kappa^n Q^n}{n}$$

$$\det \Delta = \exp(\sum_n (W_n \xi^n + W_{-n} \xi^{-n}))$$



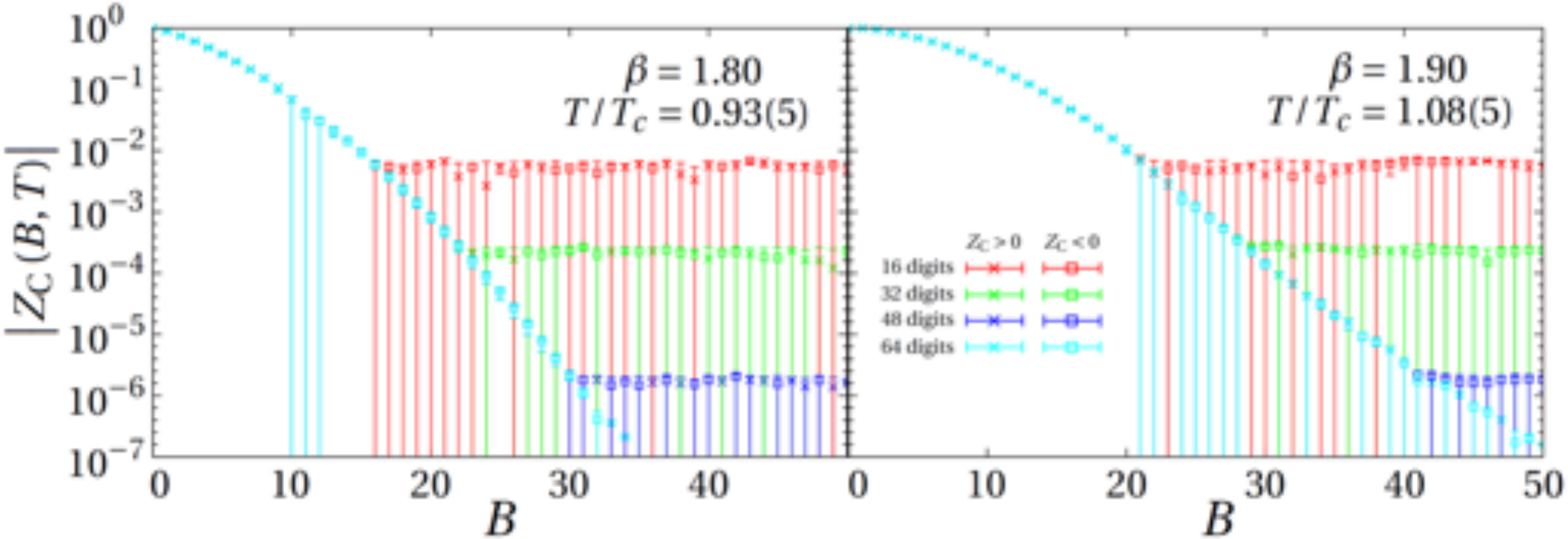
Take W_n for $|n| \leq 6$ and do the Fourier Trans. analytically.

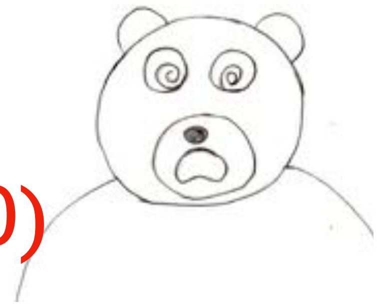
Big Cancellation in FFT !



S.Oka, arXiv:1511.04711
Talk at LATTICE 2015

Fukuda, Nakamura, Oka,
arXiv:1511.04711
Phys.RevD93, 094508 (2016)





θintegration → Multi-Precision (50 - 100)

$$z_n = \int \frac{d\theta}{2\pi} e^{i\theta n} Z_{GC}(\theta \equiv \frac{\mathrm{Im}\mu}{T}, T)$$

Using Multiple-precision, we have beaten Sign Problem.

But to make Canonical Approach workable,

we had to solve 2 problems:

1. Z_{GC} is not a direct observable in lattice QCD

2. We should perform simulations at many imaginary μ points.

Integration Method

Not Z_G but n_B in imaginary μ → z_n

$$n_B = \frac{1}{3V} T \frac{\partial}{\partial \mu} \log Z_G$$

$$= \frac{N_f}{3 N_s^3 N_t} \int \mathcal{D}U e^{-S_G} \mathrm{Tr} \Delta^{-1} \frac{\partial \Delta}{\partial \mu} \det \Delta$$

(For pure imaginary μ, n_B is also imaginary)

Then, for fixed T

$$Z(\theta \equiv \frac{\mu}{T}) = \exp(V \int_0^{\theta} n_B d\theta')$$

$$z_k = \frac{3}{2\pi} \int_{-\pi/3}^{+\pi/3} d\theta \exp\left(i\, k\theta + \int_0^{\theta} n_B d\theta' \right)$$

- Multi-precision calculation
- Integration Method

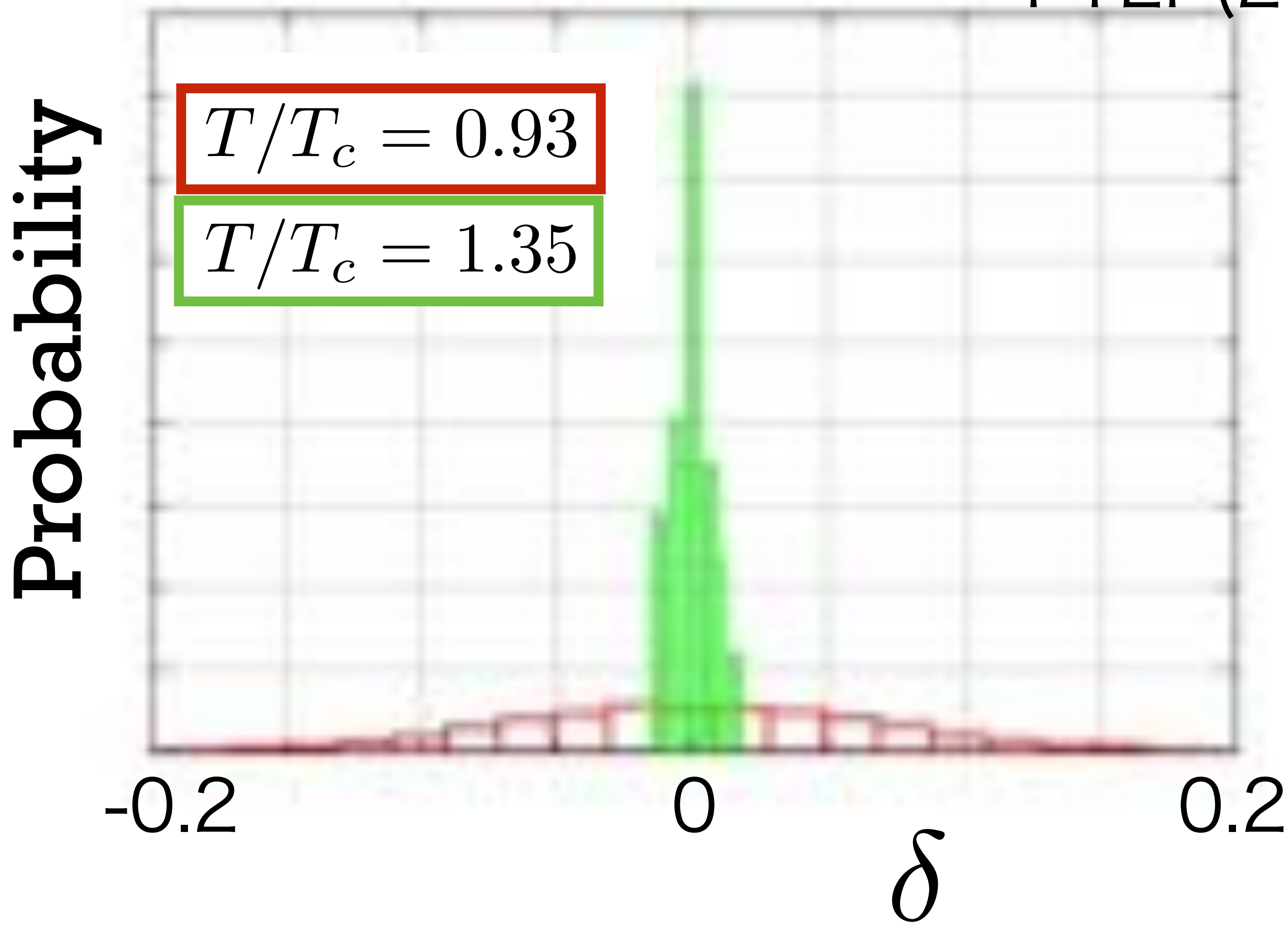
I thought we have beaten
Sign Problem.

But !

Hidden Sign Problem ?

Z_n have phase on each configuration !

V.Goy et al.,
PTEP(2017) 031D01



$z_n \simeq |z_n| e^{in\delta}$

$Z_n = \langle z_n \rangle$ are real positive.

References

A.Li et al.(Kentucky), Phys.Rev.D82:054502,2010, arXiv:1005.4158

A.Suzuki et al.(Zn Collaboration), Lattice 2016 Proceedings,

V.Goy et al.(Vladivostok), Prog Theor Exp Phys (2017) (3): 031D01,arXiv:1611.08093

Where comes the phase of z_n ?

A.Li et al.(Kentucky), Phys.Rev.D82:054502,2010, arXiv:1005.4158

$$Z = \int \mathcal{D}U \left(\det \Delta(\mu)\right)^{N_f} e^{-S_G} \quad = e^{\log(1-\kappa Q)}$$

$$\begin{aligned}\det \Delta(\mu) &= \det(1-\kappa Q(\mu)) \\ &= \exp\left(A_0 + \sum_{n>0}[e^{in\phi}W_n + e^{-in\phi}W_n^{\dagger}]\right) \\ &= \exp\left(A_0 + \sum_n A_n \cos(n\phi + \delta_n)\right)\end{aligned}$$

$$\begin{aligned} A_n &\equiv 2|W_n| \\ \delta_n &\equiv arg(W_n) \end{aligned}$$

We use $W_{-n} = W_n$

Then,

$$z_n \propto \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1\cos(\phi+\delta_1) + A_1\cos(2\phi+\delta_2)\cdots}$$

In the lowest order,

$$\int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1 \cos(\phi+\delta_1)} = e^{A_0} \int_{\delta_1}^{2\pi+\delta_1} \frac{d\phi'}{2\pi} e^{-ik(\phi'-\delta_1)} e^{A_1 \cos\phi'}$$

$$= e^{A_0+ik\delta_1} \int_{\delta_1}^{2\pi+\delta_1} \frac{d\phi'}{2\pi} e^{-ik\phi'} e^{A_1 \cos\phi'}$$

$$= e^{A_0+ik\delta_1} \int_0^{2\pi} \frac{d\phi'}{2\pi} e^{-ik\phi'} e^{A_1 \cos\phi'}$$

$$= e^{A_0+ik\delta_1} I_k(A_1)$$

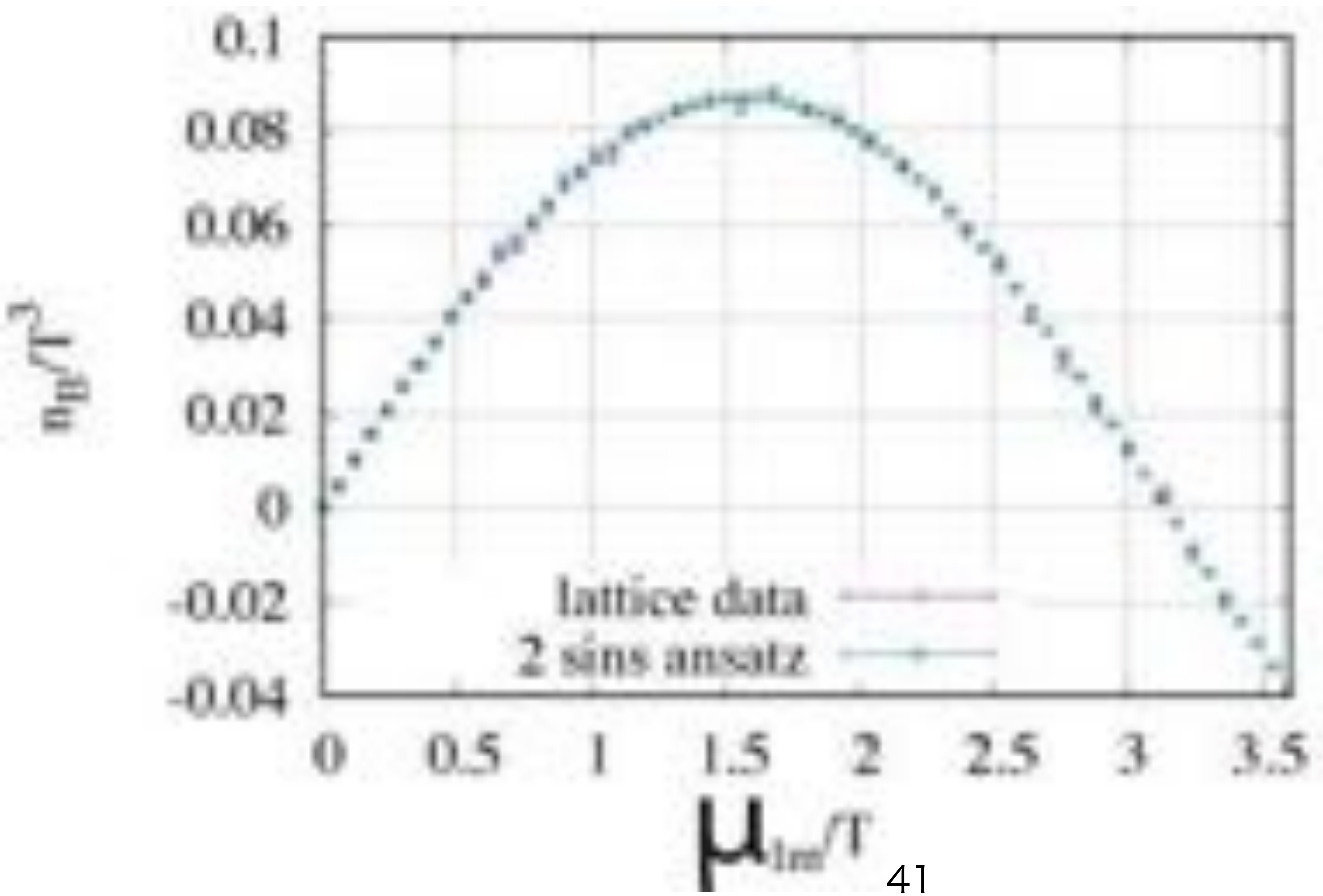
$$\propto z_k$$

where we use

$$I_n(z) = \frac{(-1)^n}{2\pi} \int_0^{2\pi} e^{z\cos t} e^{-int} dt$$

A Remark of Function Form of $n_B(\mu_I)$

Preliminary



$n_B(\mu_I)$ is well approx-imated by sine function at *T*<*Tc*.

Takahashi et al. Phy. Rev. D 91 (1) (2015) 014501.
Bornyakov et al., Phys.Rev. D95, 094506 (2017)

Number density in Imaginary μ

We expand the number density as

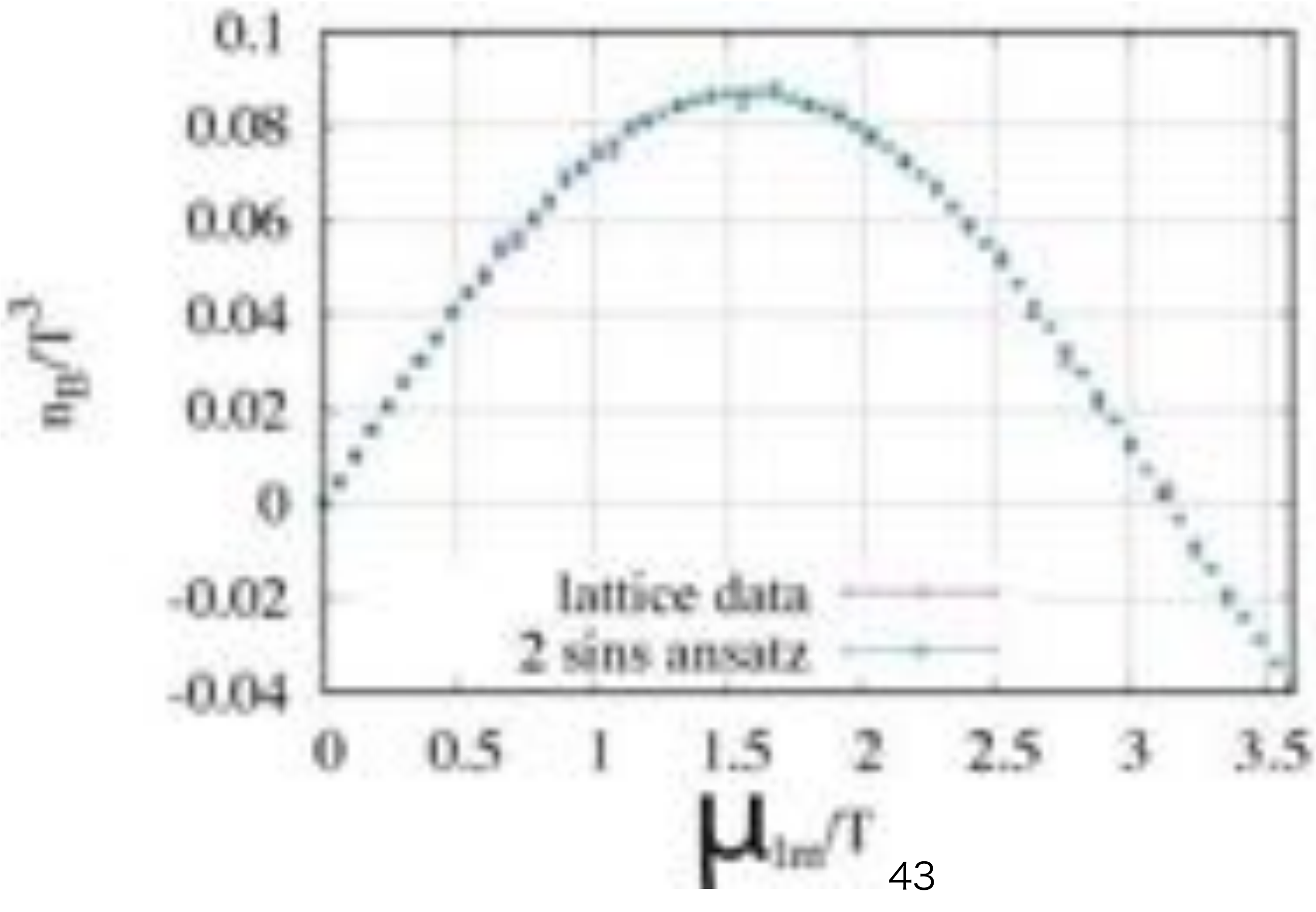
$$n_B/T^3 = \sum_{k=1}^{k_{max}} f_{3k} \sin(k\theta)$$ **Confinement phase** $T < T_c$

$$n_B/T^3 = \sum_{k=1}^{k_{max}} a_{2k-1} \theta^{2k-1}$$ **DeConfinement phase** $T > T_c$

Fittine functions are much more robust
against the hidden sign problem,
because a fitting curve include many points.

$$\theta \equiv \frac{\mu}{T}$$

A Remark of Function Form of $n_B(\mu_I)$



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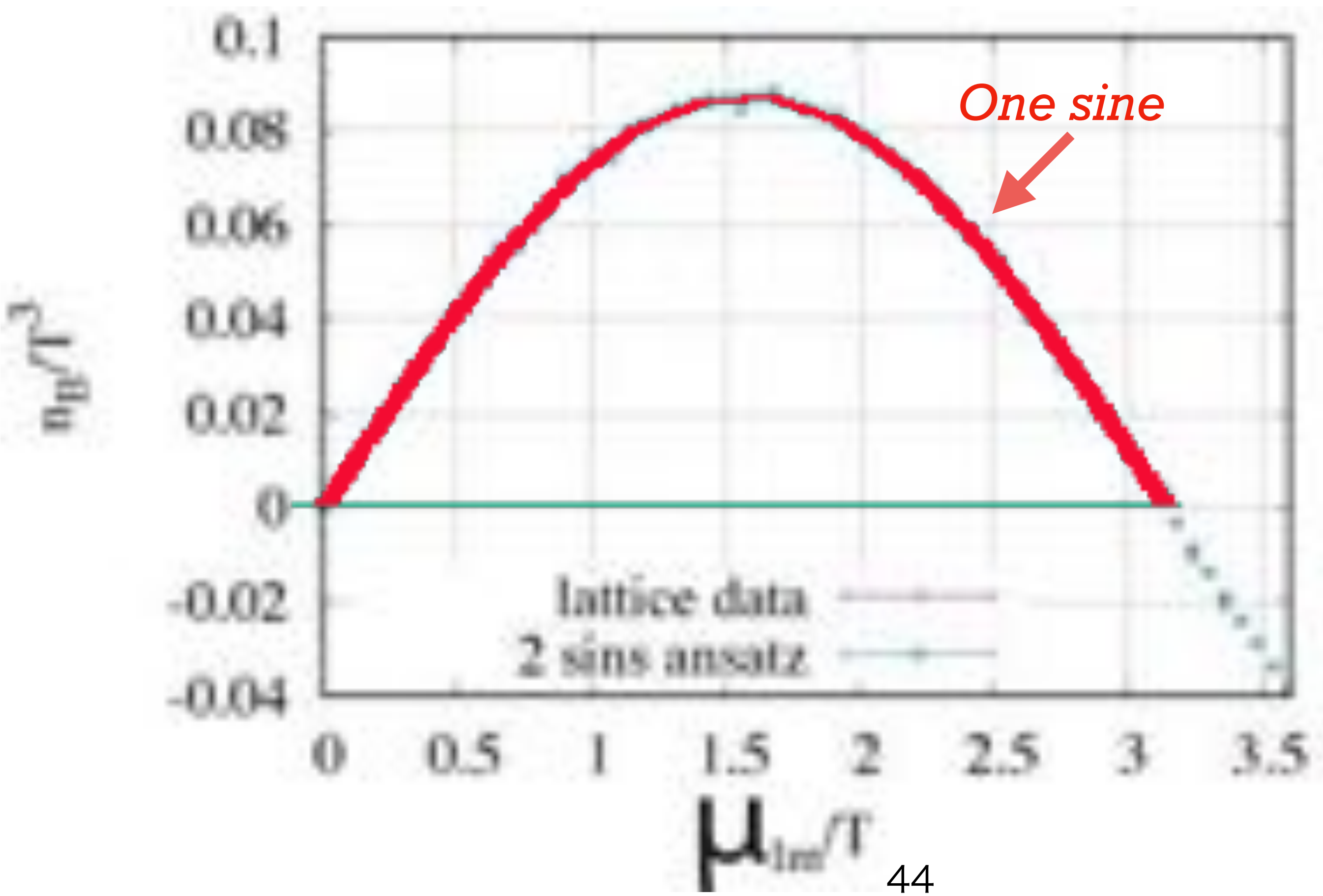

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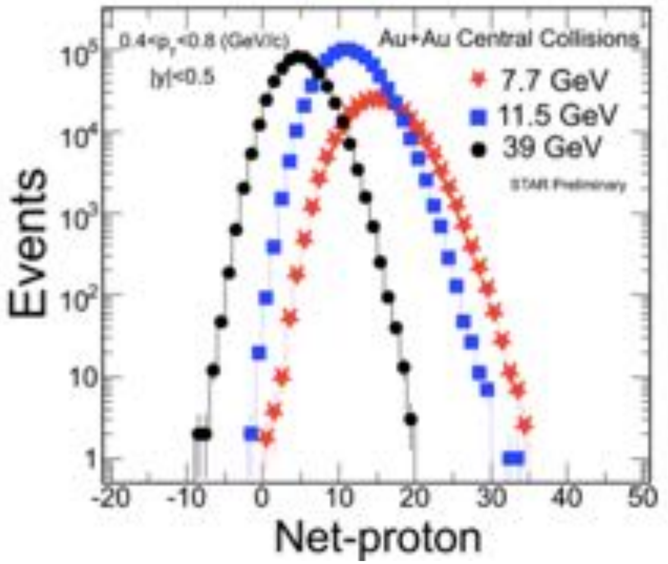
Takahashi et al. Phy. Rev. D 91 (1) (2015) 014501.
Bornyakov et al., Phys.Rev. D95, 094506 (2017)

- Now we can say we have beaten Sign Problem for T>0 by Canonical Approach.

Experimental Data

In 2012, at Wuhan

STAR@RHIC



Prof.Nu Xu

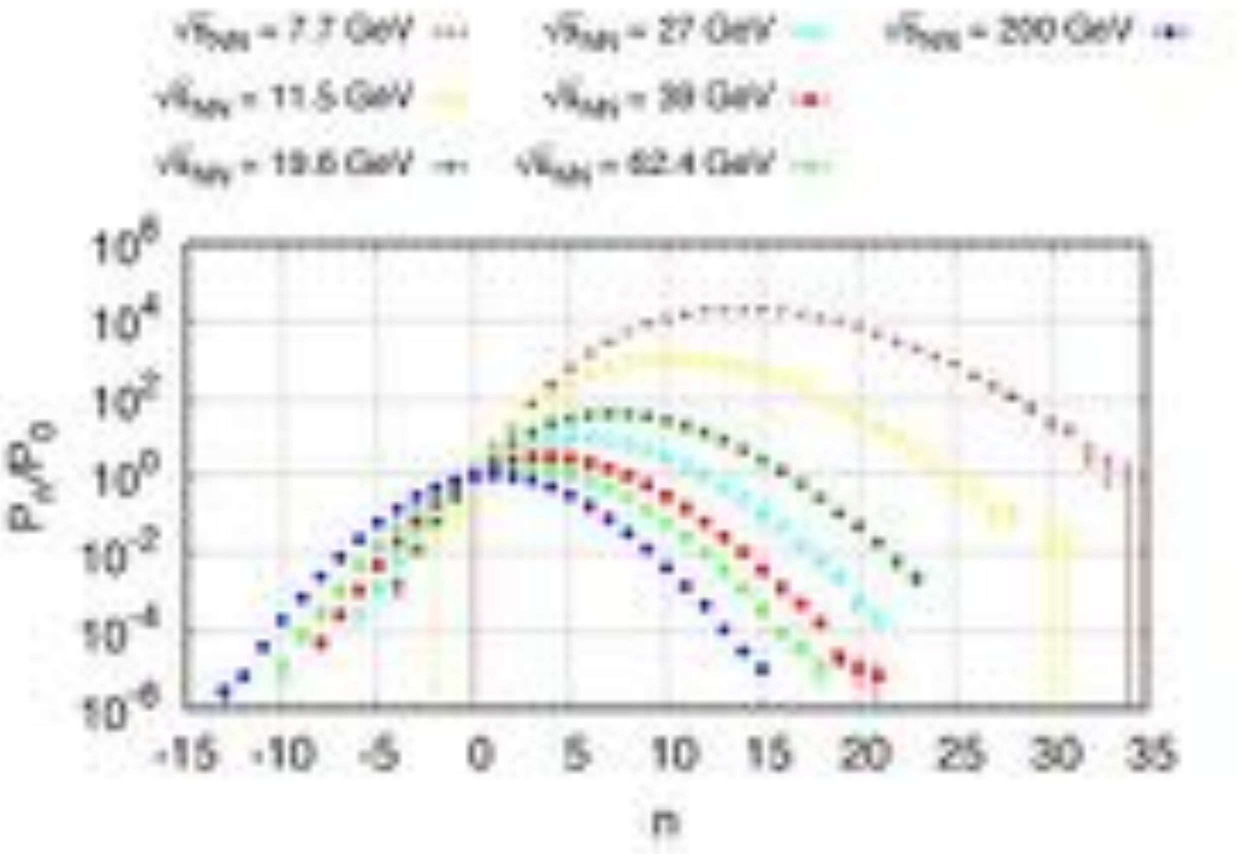
This is Canonical !

We thank Prof.Nu Xu
and Prof.Luo!

$$Z(\mu, T) = \sum_n Z_n(T)(e^{\mu/T})^n$$

Experimental data and Fugacity Expansion

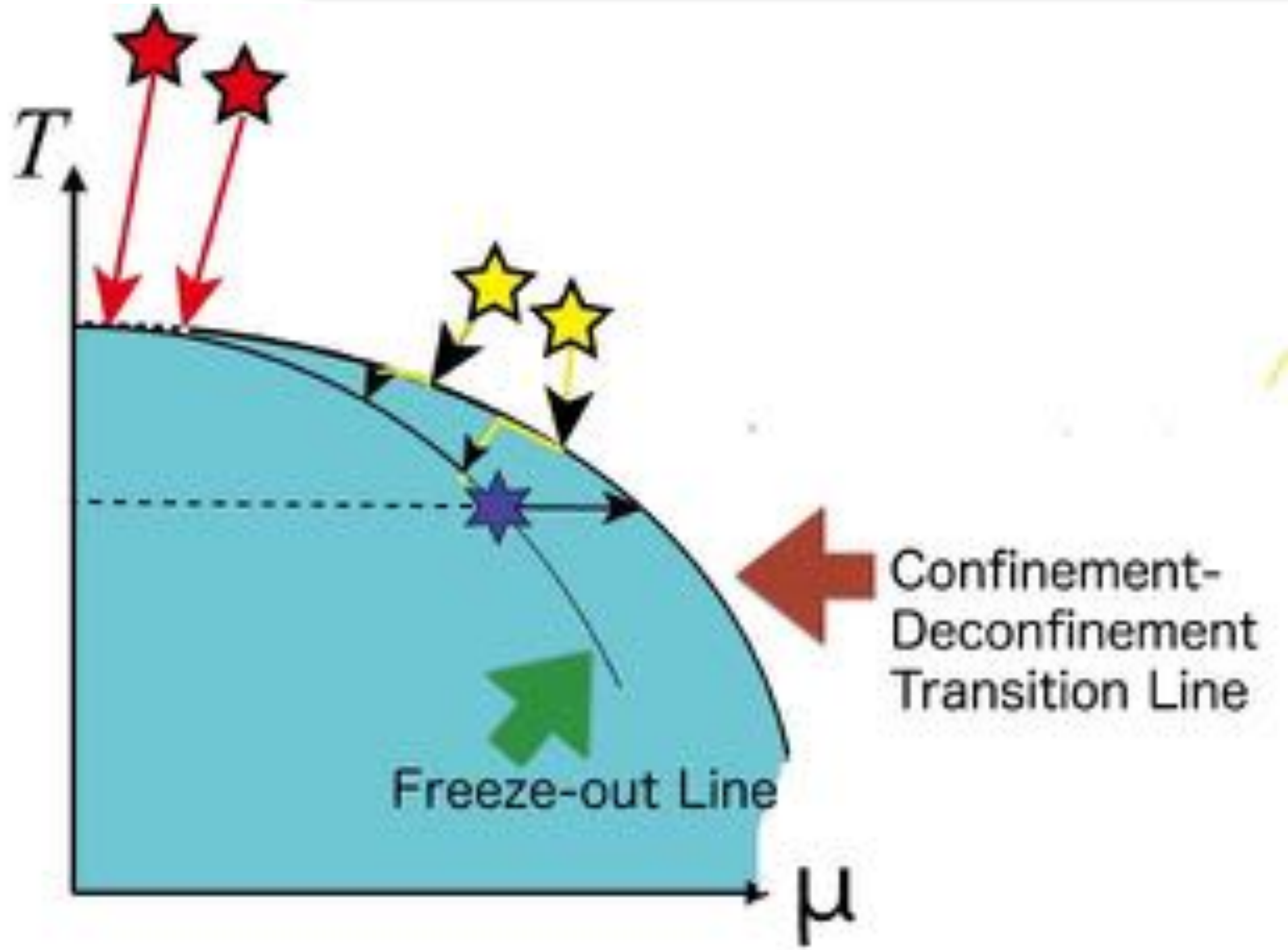
$$Z(\mu, T) = \sum_n Z_n(T) z_n(T)^n$$



You combine Experimental data.
It means you are in the confinement phase.
So no chance to see the Phase transition.

How to find QCD phase transition line ?

$$Z(\mu, T) = \sum_n z_n(T)(e^{\mu/T})^n$$

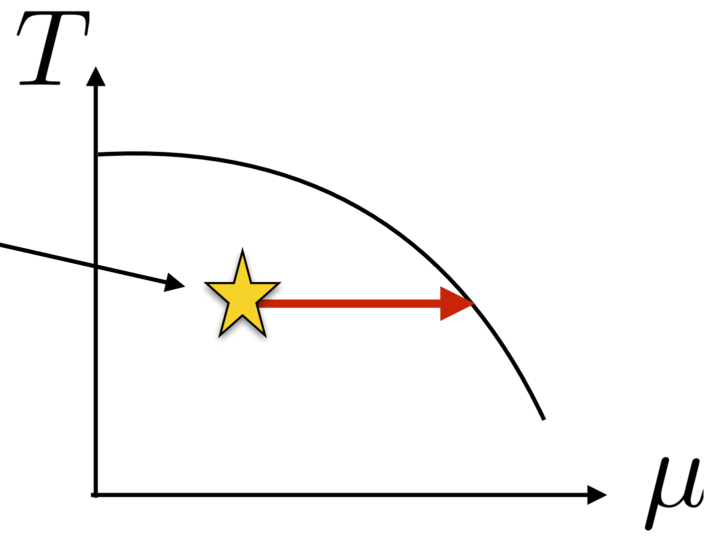


Information hidden in Fugacity Expansion ?

$$Z(\mu, T) = \sum_n z_n(T)(e^{\mu/T})^n$$

★ Experimentally

Determine $Z_n(T)$ here.
Then see QCD Phase
at higher density !



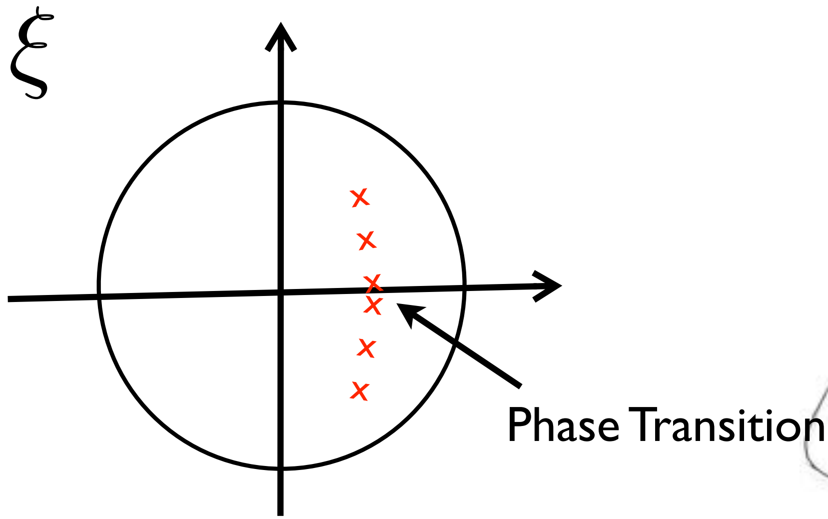
$$Z(\xi, T) = \sum_{n=-N_{max}}^{+N_{max}} Z_n(T)\,\xi^n$$

Lee-Yang Zeros (1952)

Zeros of $Z(\xi)$ in Complex Fugacity Plane.

$$Z(\alpha_k) = 0$$

Great Idea to investigate a Statistical System

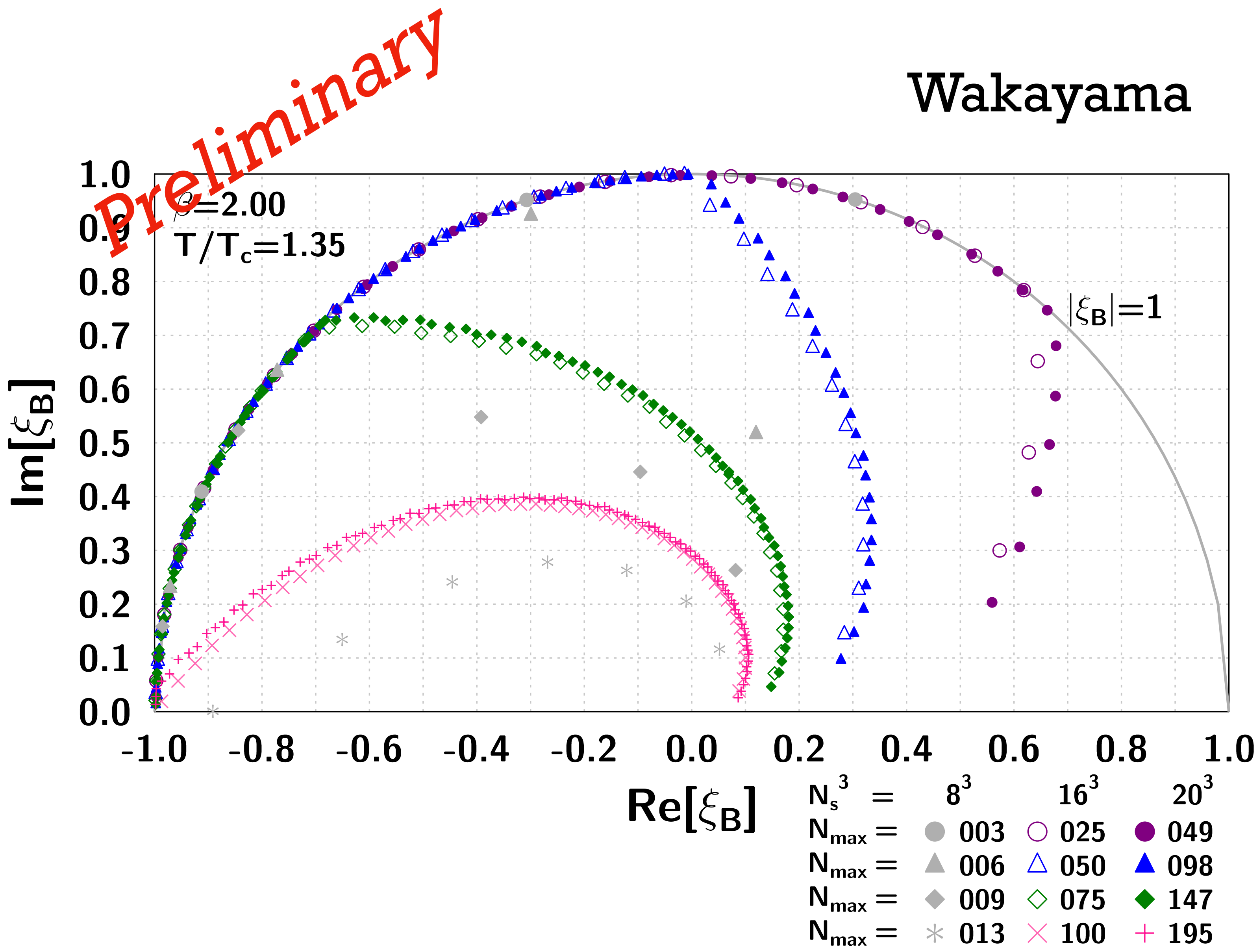


☆Time consuming part is to solve

$$f(\xi) = \prod_k (\xi - \alpha_k)$$

☆Nikolai found a very fast algorithm.

➡ Then, we can obtain results easily.


Preliminary
Wakayama
β=2.00
T/T_c=1.35
|ξ_B|=1
Im[ξ_B]
Re[ξ_B]
1.0 0.9 0.8 0.7 0.6 0.5 0.4 0.3 0.2 0.1 0.0
-1.0 -0.8 -0.6 -0.4 -0.2 0.0 0.2 0.4 0.6 0.8 1.0
N_s^3 = 8^3 16^3 20^3
N_max = 003 025 049
N_max = 006 050 098
N_max = 009 075 147
N_max = 013 100 195

What should we do next？

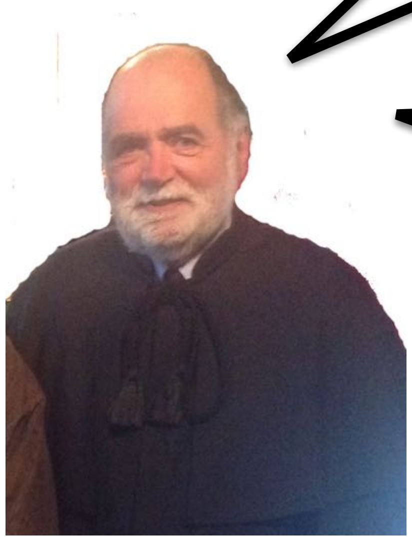
Sign Problem is now solved for T>0, and
it is time to analyze the finite density QCD.

But people do not know it. Why ?

It takes very
long time until
your idea is understood.

Because your
Approach is
different.

But I use
only Statistical
Mechanics !?



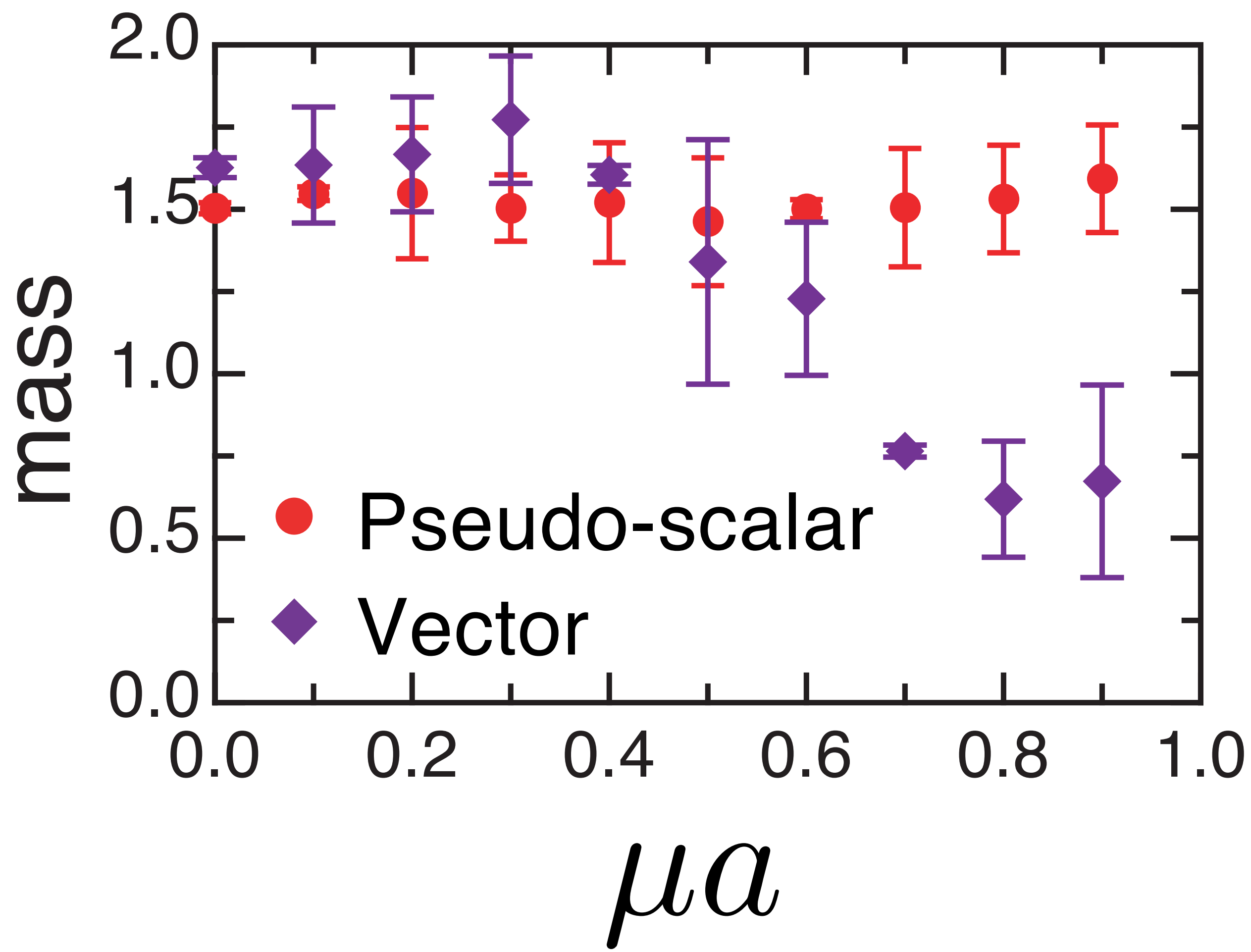
What should we do next ?

- Let the world to know that the Sign Problem was solved by Vladivostok group
  - Canonical approach + Multiple precision beat the sign problem
- SU(2) can access large finite real μ
  - Long time ago, I observed a strange behavior of rho meson at finite μ

Muroya, Nakamura and Nonaka

arXiv 0211010 Phys. Lett. B551,(2003) pp305-310

$\kappa = 0.160$ 4^3x8 SU(2)



Vector meson
mass drops !

2+1 (u/d+s) Simulation because the s-quark effects cannot be neglected at finite temperature,

$m_s \sim 100\mathrm{MeV}$

$(T_c \sim 200\mathrm{MeV})$

This simulation is very important for NICA and J-PARC.

2+1 (u/d+s) Simulation because the s-quark effects cannot be neglected at finite temperature,

$m_s \sim 100\mathrm{MeV}$

$(T_c \sim 200\mathrm{MeV})$

Odd-flaver simulation

E.I.Zolotarev, “Application of elliptic functions to the questions of functions deviating least and most from zero”, Zap. Imp. Akad. N St. Petersburg, 30 (1877), no.5; reprinted in his Collected works, Izdat, Akad. Nauk SSSR, Moscow, 1932, p.1-59

$$\frac{1}{\sqrt{x^2}} \sim C \prod_n \frac{x^2 + a_n}{x^2 + b_n} = \sum \frac{c_n}{x^2 + d_n}$$

OK, we explore the new world, Hadronic matter at Finite Density, with our Tool !