

Canonical partition functions and Lee-Yang zeros in QCD

Keitaro Nagata (KEK)

collaboration with

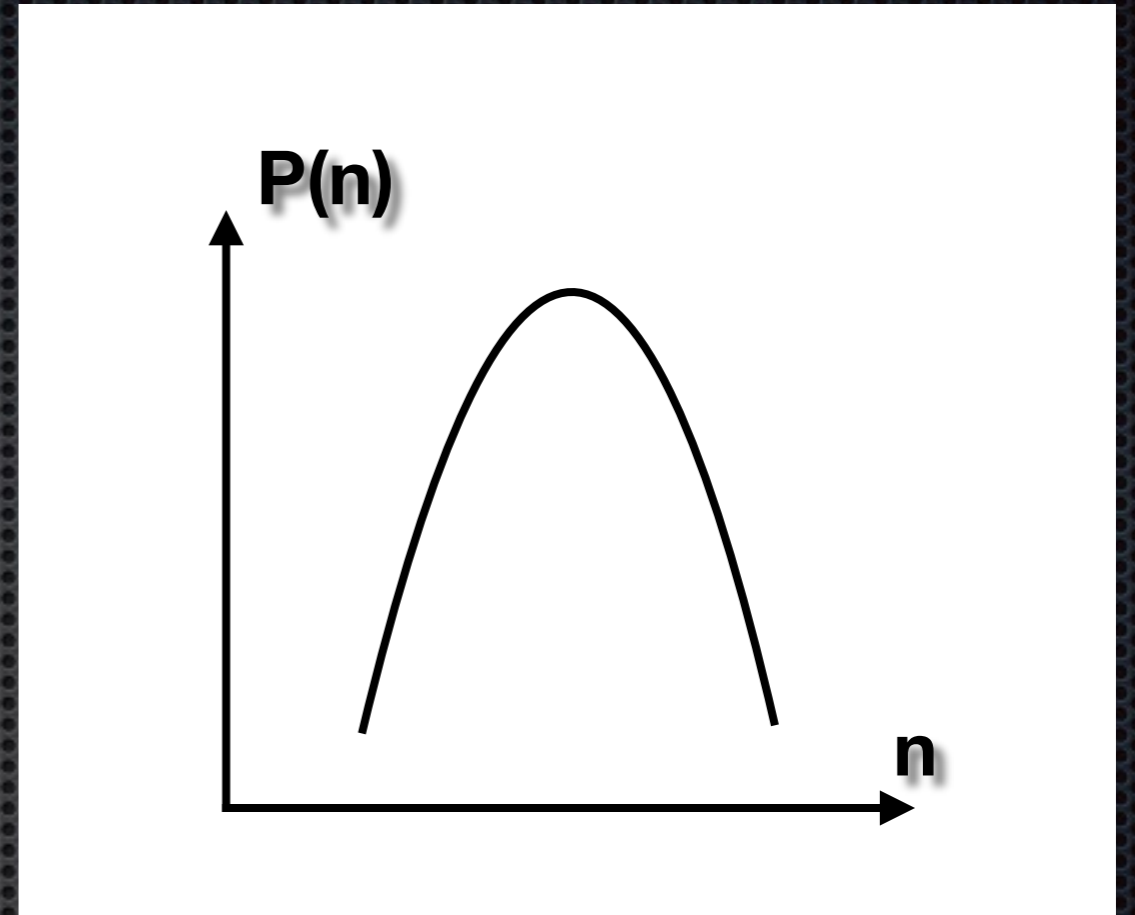
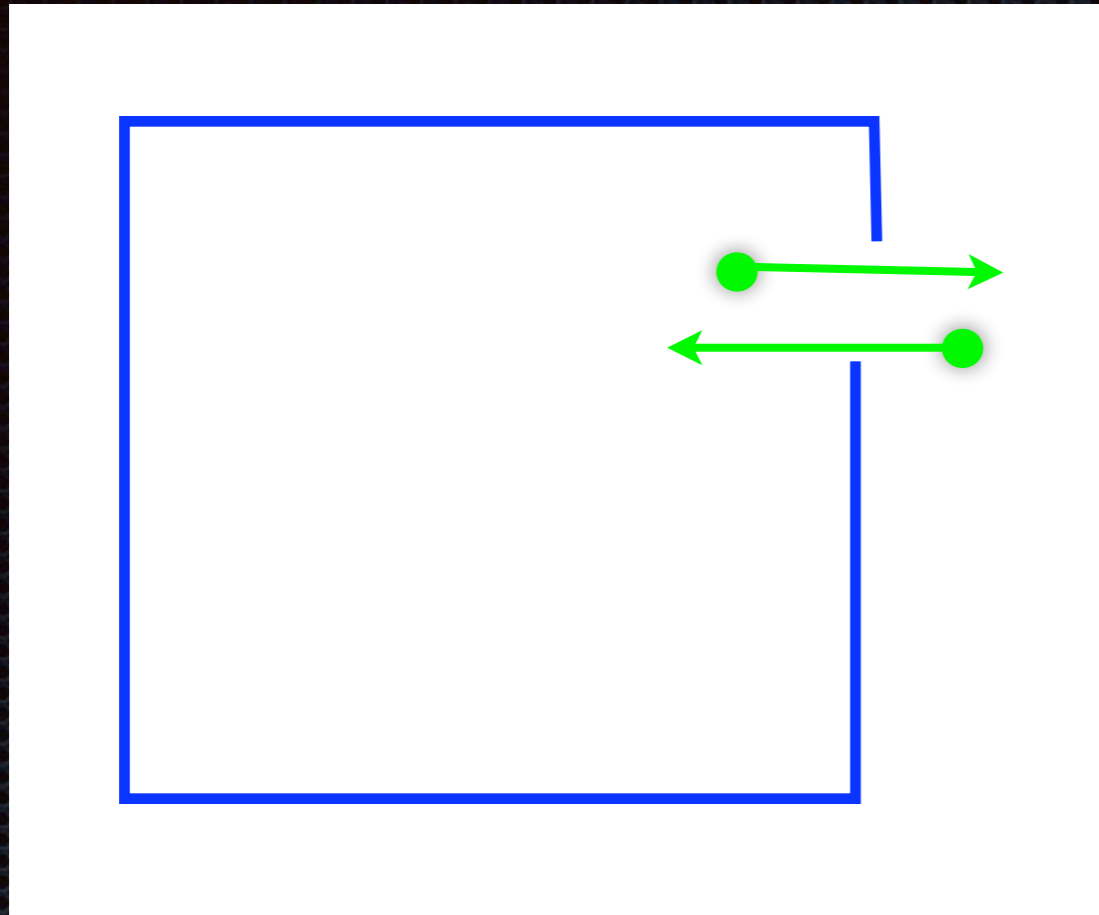
K. Kashiwa(YITP), A. Nakamura(Hiroshima),

S. M. Nishigaki(Shimane)

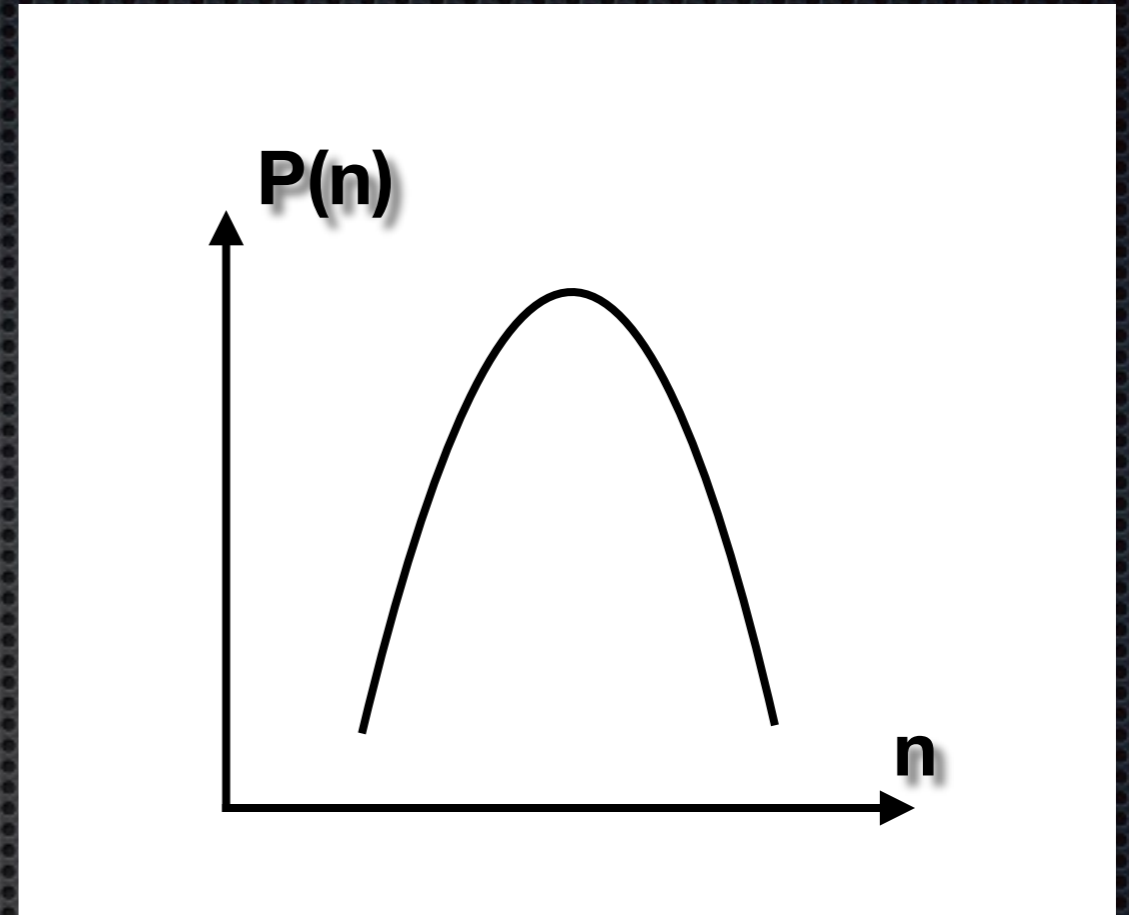
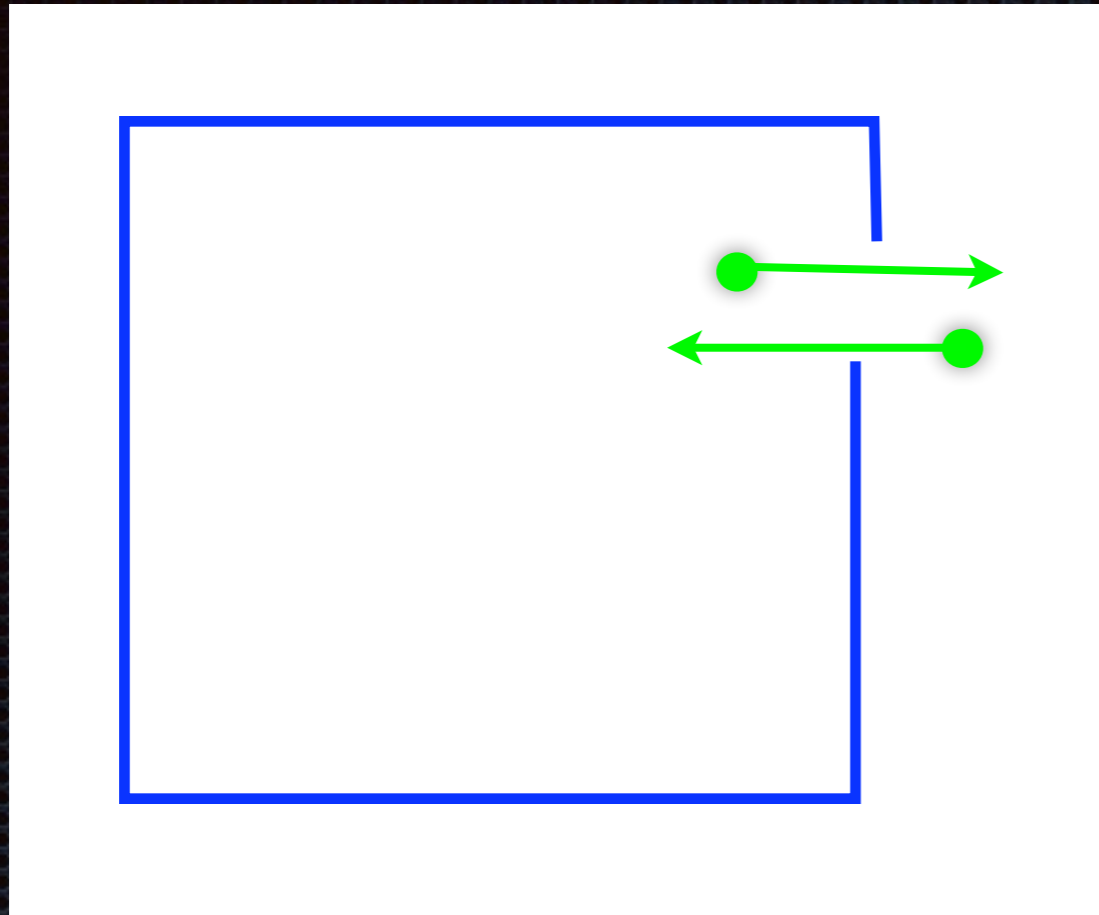
KN, S. Motoki, Y. Nakagawa, A. Nakamura, T. Saito [PTEP01A103(2012)]

A. Nakamura, KN [arXiv:1305.0760]

KN, K. Kashiwa, A. Nakamura, S. M. Nishigaki arXiv:1410.0783



A grand canonical partition function
 \Rightarrow n -particle state with a probability $P(n)$



A grand canonical partition function

=> n -particle state with a probability $P(n)$

What is the shape of this probability in QCD ?

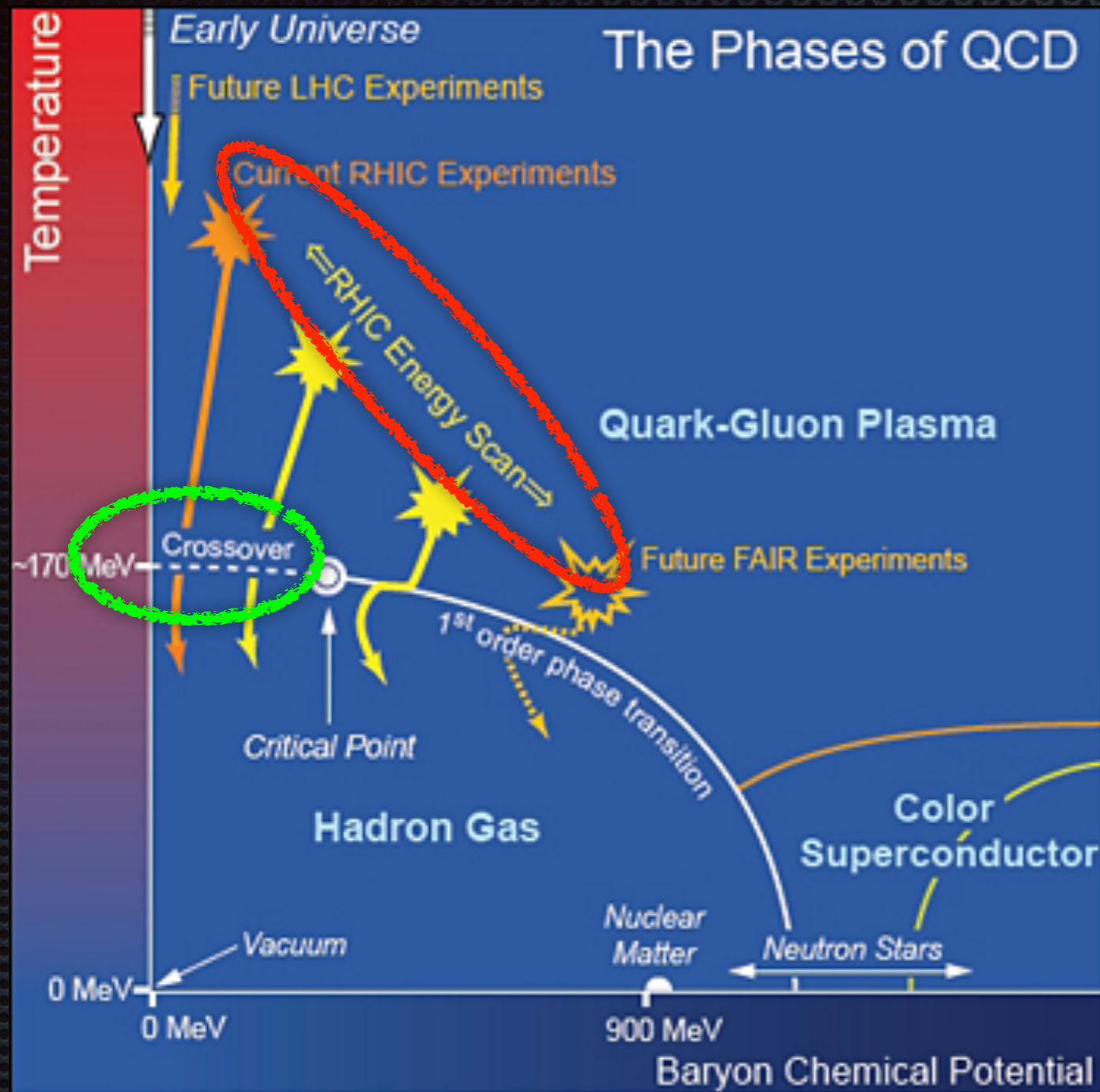
Contents

1. Introduction : motivation
2. result 1
 1. canonical partition function
 2. Lee-Yang zeros
3. result 2 - High T QCD
4. summary

Introduction

HHIQCD, YITP, Kyoto, March 4, 2015

Today, I would like to focus on

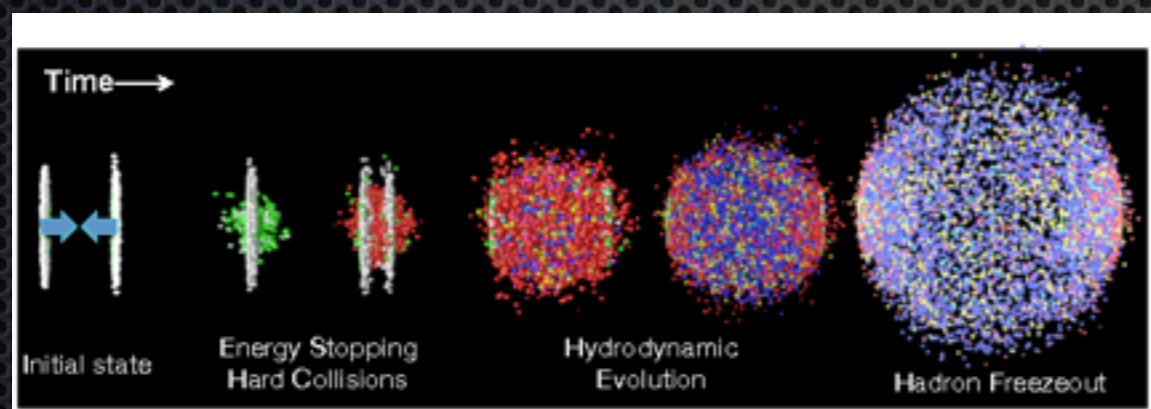


- **Beam energy scan experiment : exp. data at finite density**
- **Developments of techniques for finite density LQCD**

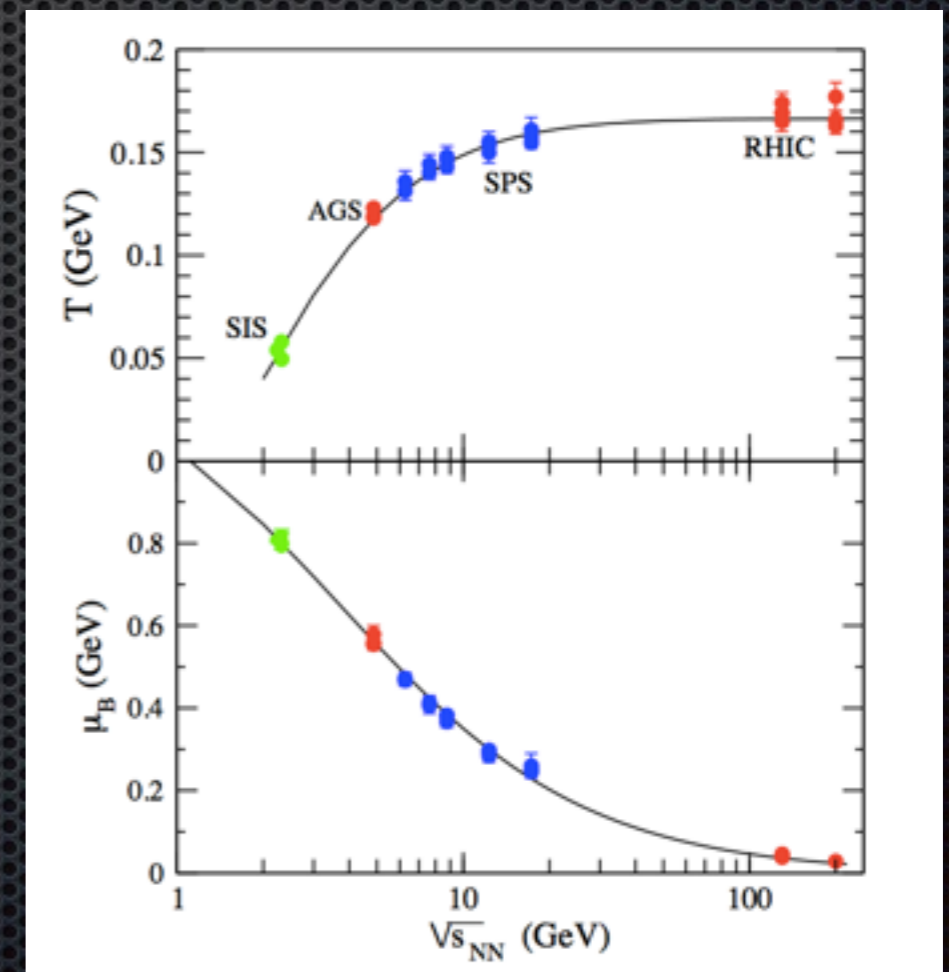
BES experiments

Investigate phase diagram using HIC with different beam energy

- Number of hadrons measured in heavy ion collision
 - success of thermal statistical models [e.g. Andronic, et., al, (2005)]
 - provide information at freeze out point (μ_B and T)



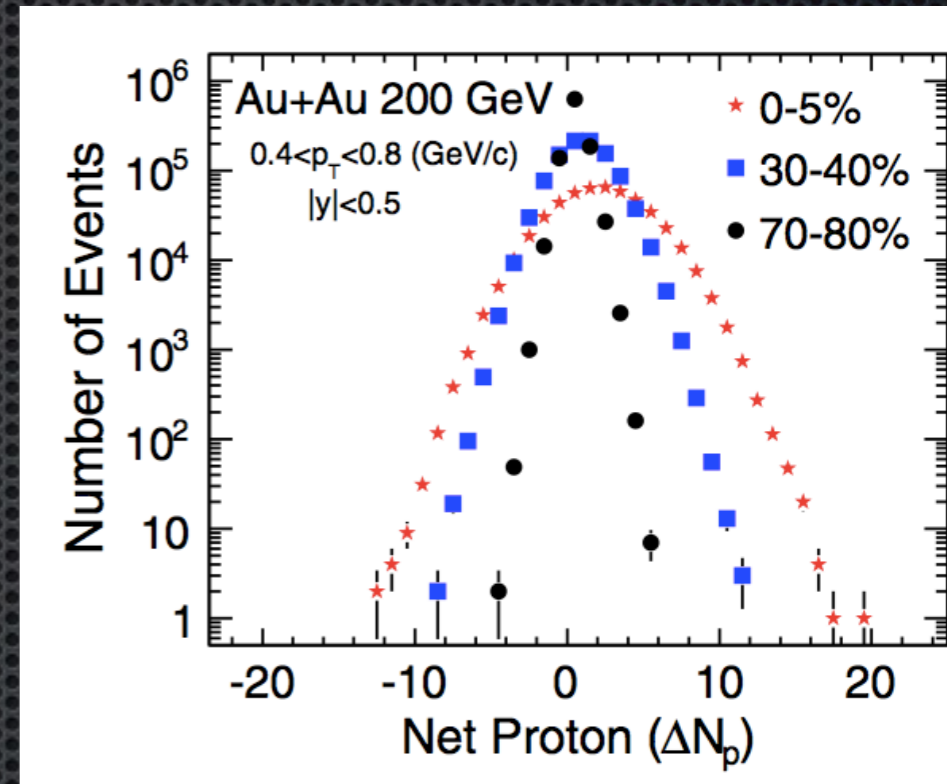
Nayak, Pramana, 79, 719('12)



Cleymans et. al. PRC73, 034905('06)

Grand canonical ?

- Due to the experimental setup, hadrons can be observed for a limited region
 - seeing a part of fireball
 - analogous to grand canonical system



Agaarwal et.al. PRL105,
022302('10), arXiv:1004.4959.

Canonical approach

a method to study the probability distribution

$$Z(\mu) = \text{tr} e^{-\beta(\hat{H} - \mu\hat{N})}$$
$$= \sum_{n=-N}^N Z_n e^{n\mu/T} = \text{probability for an n-particle state}$$

$$Z_n = \langle n | e^{-\beta\hat{H}} | n \rangle$$

(references for canonical approach)

Barbour, Davies, Sabeur, PLB215, 567(1988) 2⁴, Barbour, Bell NPB372, 385(1992)., Barbour et. al., arXiv:hep-lat/9705042

A. Hasenfratz, D. Toussaint, NPB371, 539('92) 2⁴

de Forcrand, Kratochvila NPB Proc. Suppl. 153, 62 (2006), Kratochvila, de Forcrand, 0509143, PoS Lat2005.

Ejiri, PRD78, 074507(2008) 16^{3x4}

Li, Meng, Alexandru, Liu, 0810.2349, PoS Lat(2008) , Li, 1002.4459, PoS, Lat(2009) , Li, Alexandru, Liu, Meng 1005.4158, Phys.Rev. D82 (2010) 054502 , Li, Alexandru, Liu, PRD84, 071503, arXiv: 1103.3045

Canonical approach

It can be applied to both theory and experiment.

$$Z(\mu) = \text{tr} e^{-\beta(\hat{H} - \mu\hat{N})}$$
$$= \sum_{n=-N}^N Z_n e^{n\mu/T}$$

probability to observe n-particle state

calculable in LQCD at $\mu=0$

$$Z_n = \langle n | e^{-\beta\hat{H}} | n \rangle$$

- ✦ There may be an opportunity to compare theory with exp.
- ✦ Practically, there are controversy
 - ✦ difficulty to measure neutron
 - ✦ non-equilibrium

What we can learn from distribution

Shape of the distribution ~ signal for CEP

- Higher order moments of the distribution of conserved charges are sensitive to the correlation length

$$\sigma^2 = \langle (\delta N)^2 \rangle, S = \langle (\delta N)^3 \rangle / \sigma^3, \kappa = \langle (\delta N)^4 \rangle / \sigma^4 - 3$$

- S : skewness (asymmetry)
- kappa : kurtosis : sharpness

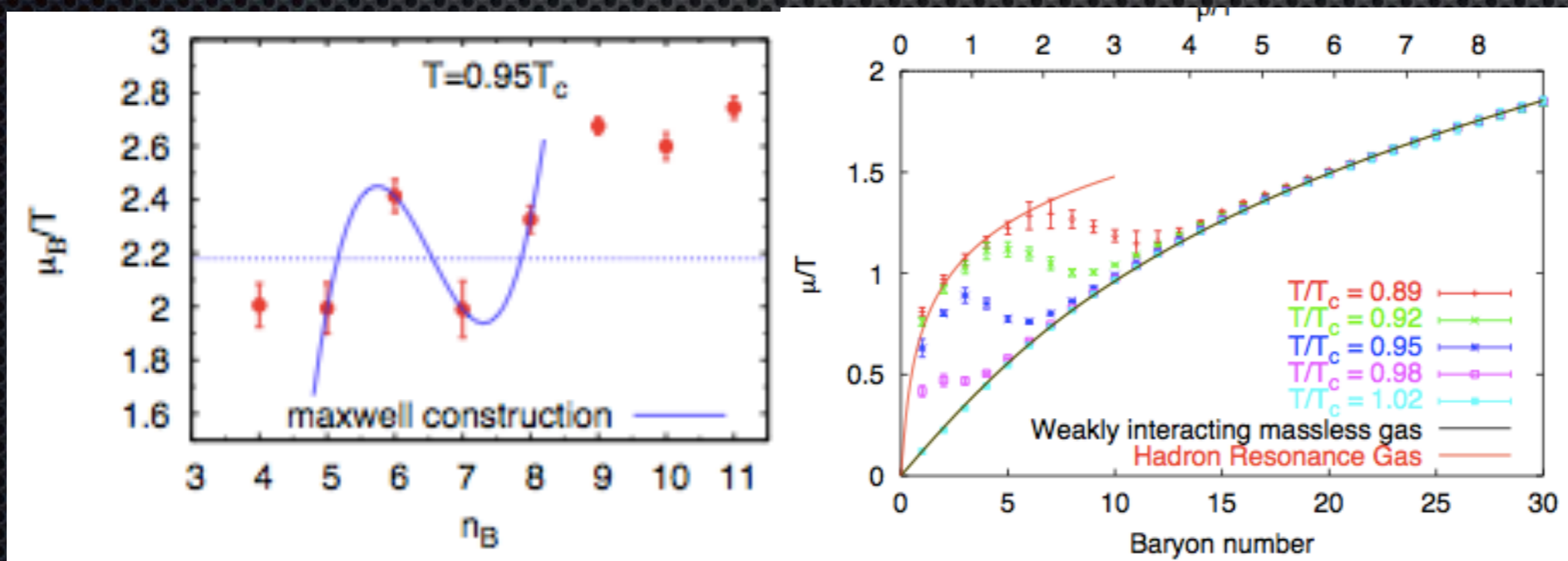
Hatta, Stephanov, PRL91, 102003(2003),
Stephanov, PRL102, 032301(2009), Asakawa,
Ejiri, Kitazawa, PRL103, 262301 (2009),
Stephanov PRL 107, 052301 (2011), etc

What we can learn from the distribution

First order phase transition from Maxwell construction

- Chemical potential \sim an energy to add one particle

$$\begin{aligned}\mu &\equiv F(n+1) - F(n), \quad (Z_n = e^{-F(n)/T}) \\ &= -T(\ln Z_{n+1} - \ln Z_n)\end{aligned}$$



(Left) A.Li, PoS Lat09,
(Right) de Forcrand &
Kratochvila, NPB Proc.
Suppl. 153, 62 (2006),

What we can learn from the distribution

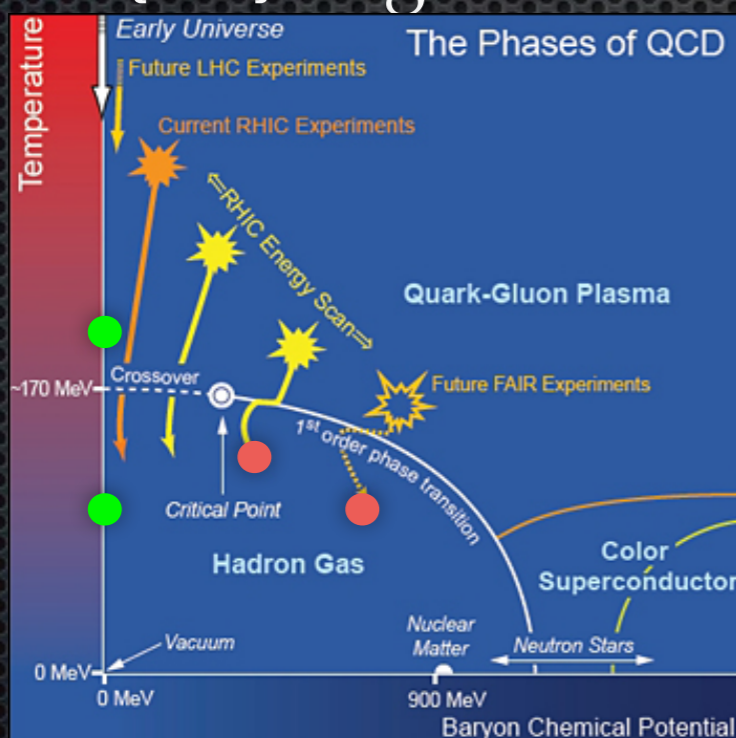
Canonical approach extends data at a given μ to wide range.

Accessible values of μ are limited both in theory and experiments

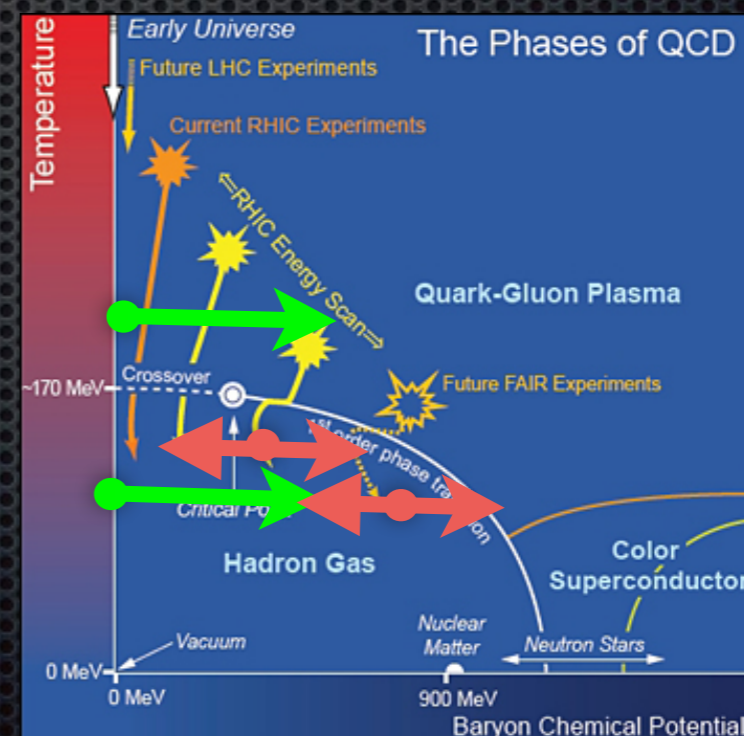
- lattice QCD(Monte Carlo) is possible at $\mu=0$
- HIC data are obtained at chem. freeze-out

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

{Zn} is given



Z(μ) for any μ

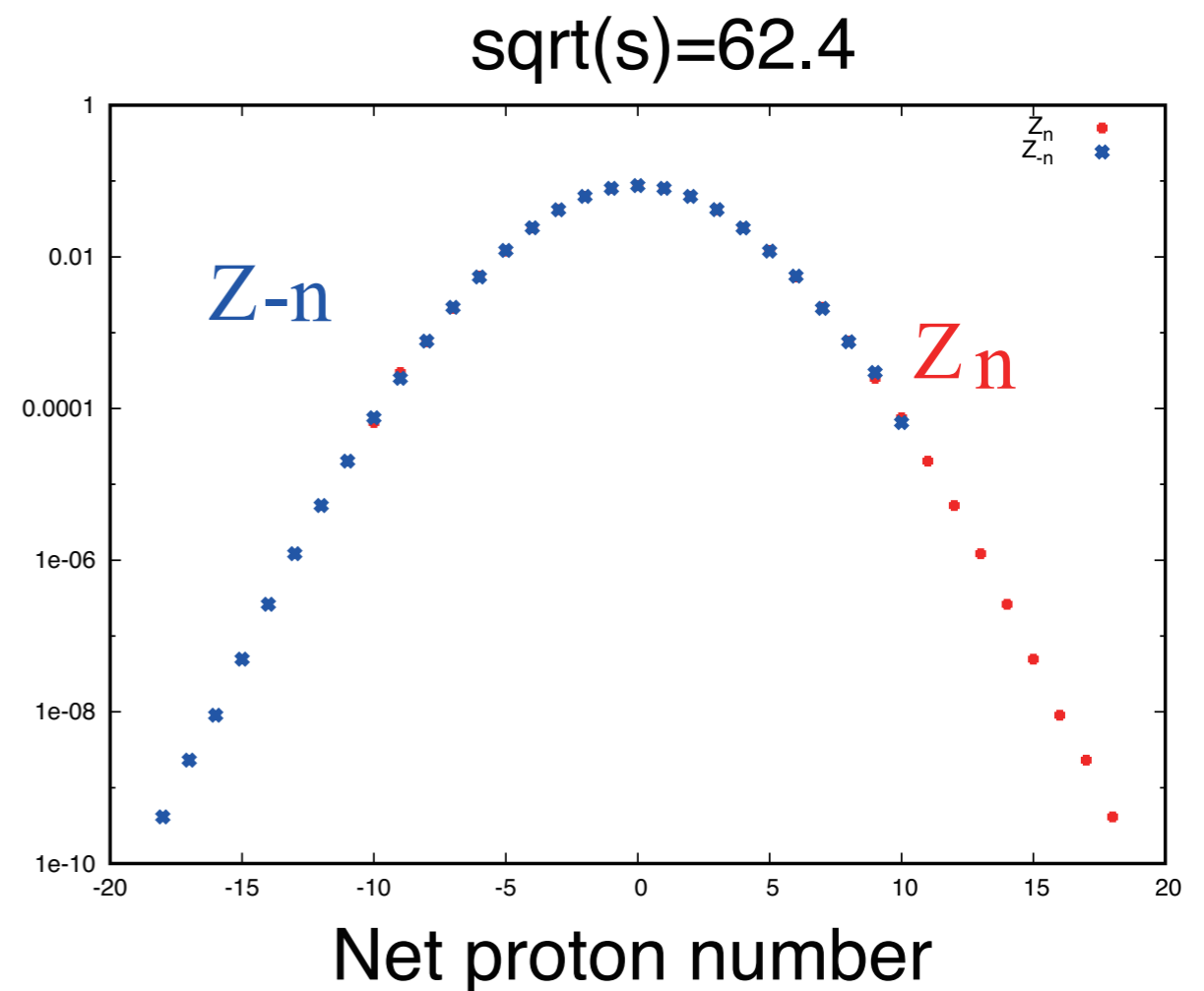
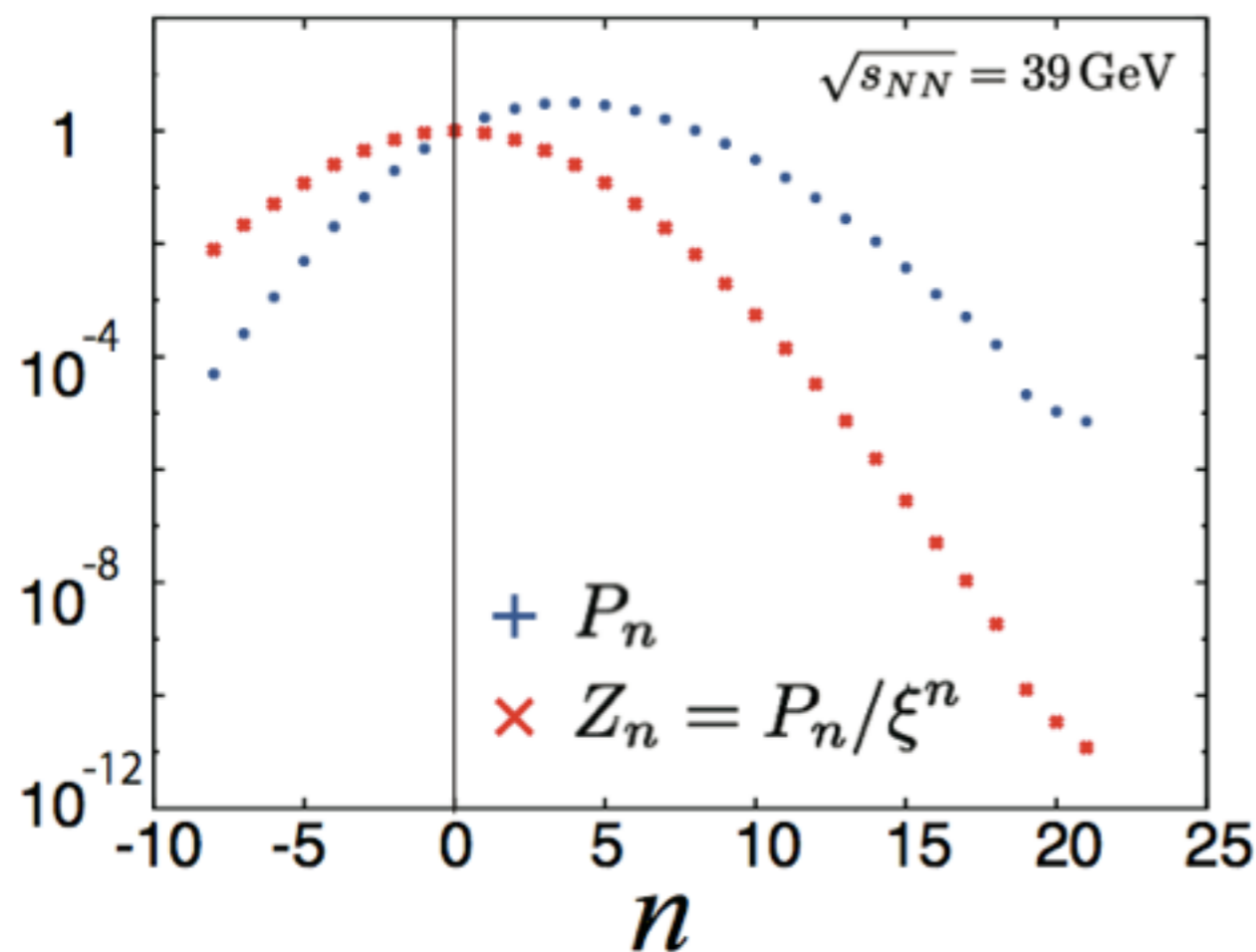


What can we learn from the distribution

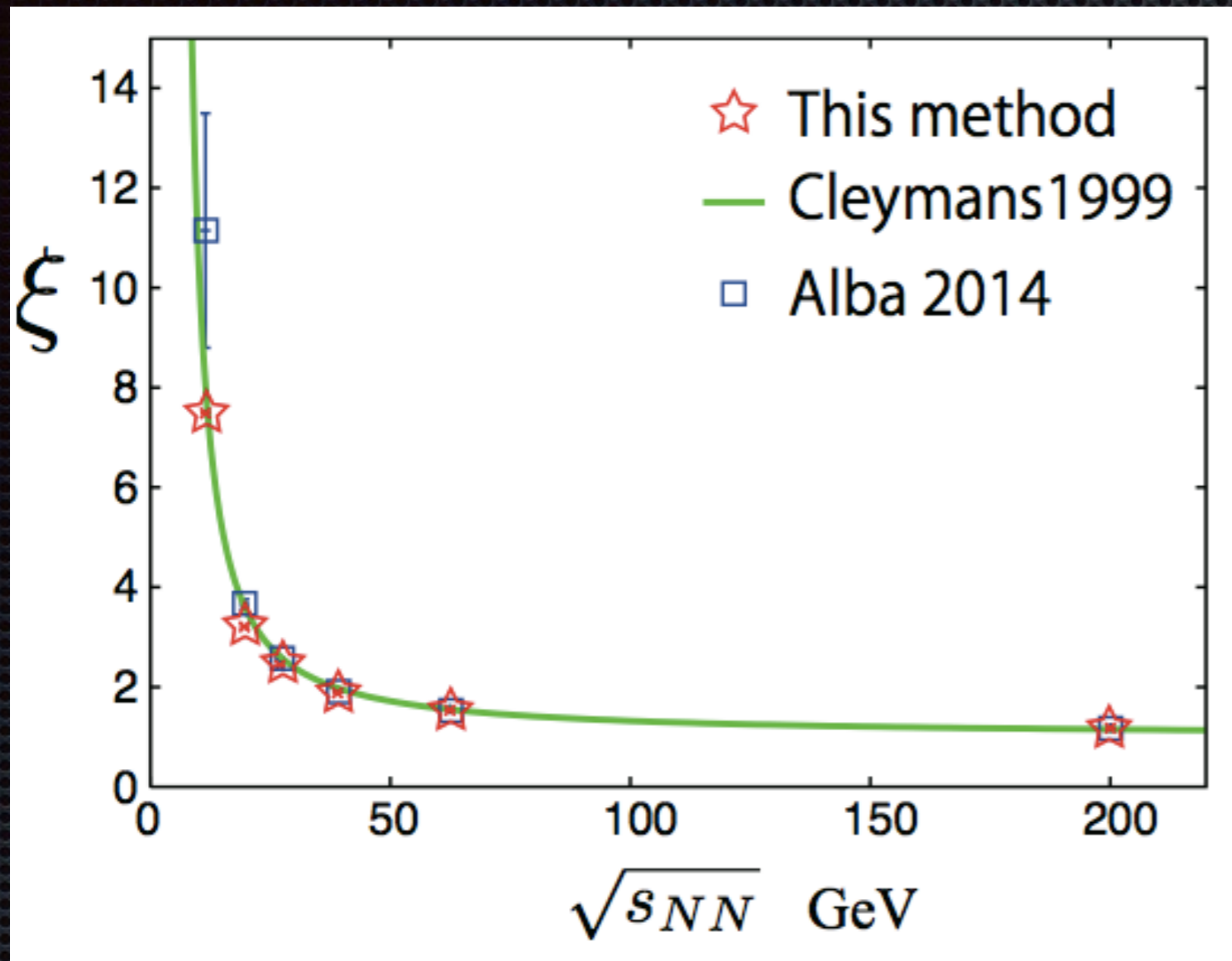
Canonical approach extends data at a given μ to wide range.

$$P_n \propto Z_n e^{n\mu/T}$$

Application to experimental data of proton number distribution [Nakamura, Nagata(2013)]



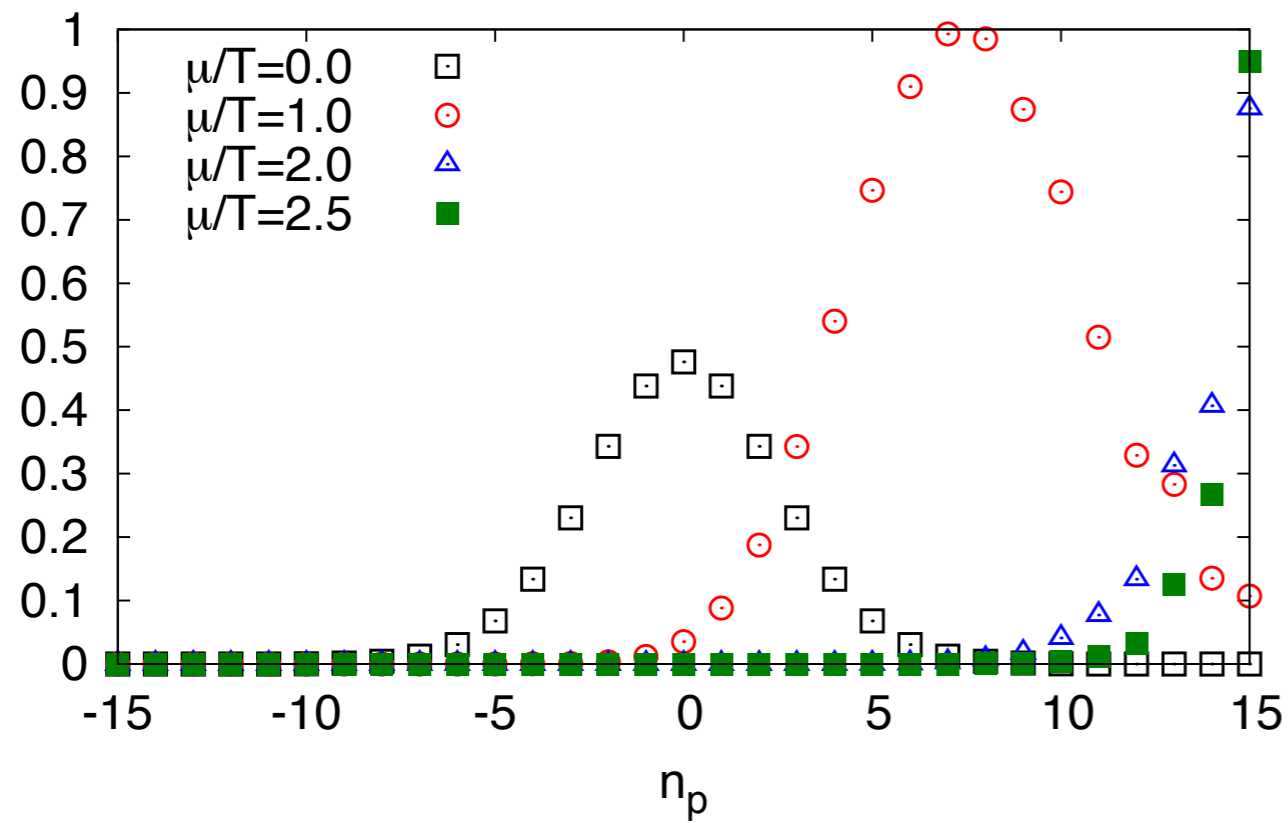
Extraction of Zn and μ/T



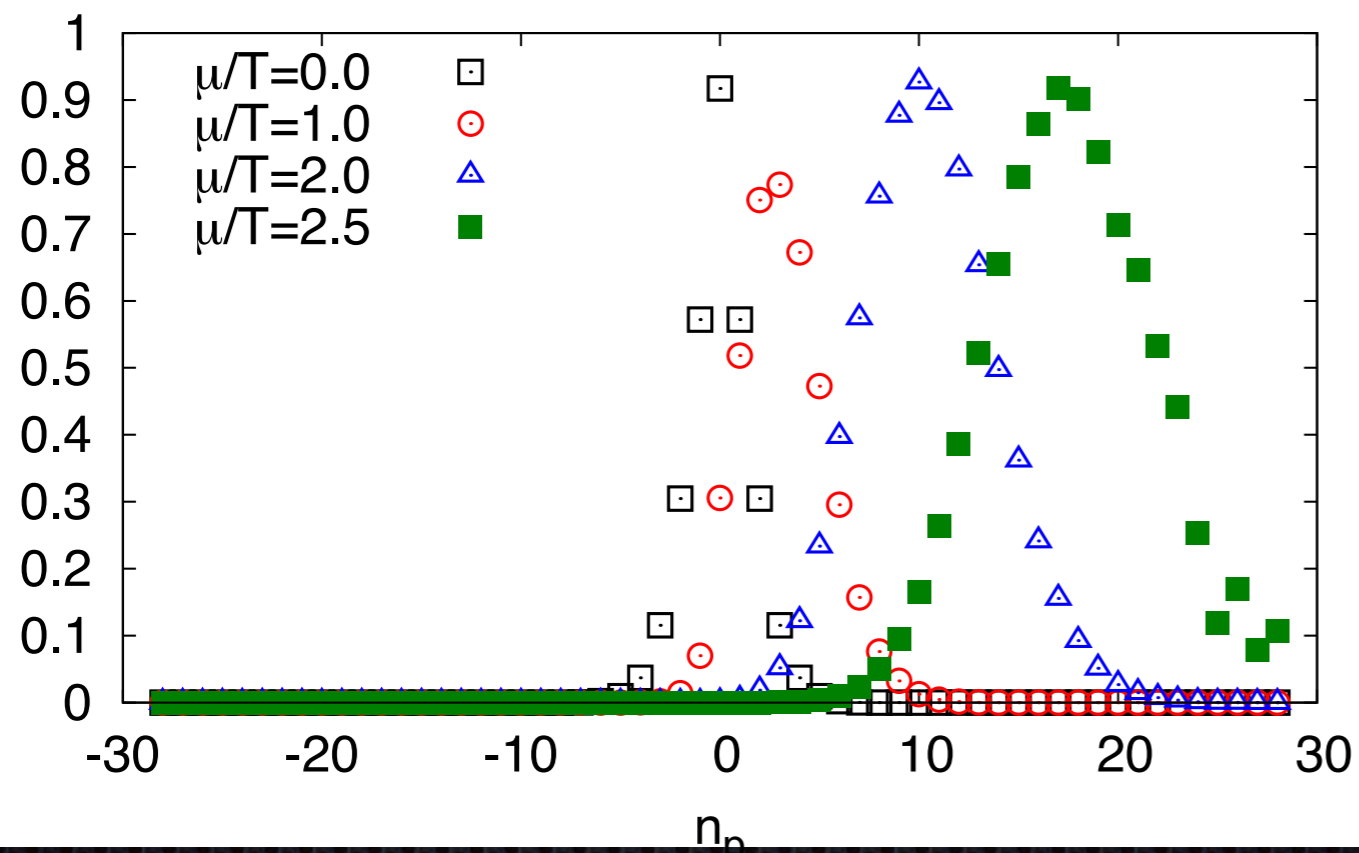
$$\xi = \exp(\mu/T)$$

- ✦ μ/T from the CP invariance vs thermal statistical

$Z(n_p) e^{n_p \mu/T}$, $\text{sqrts}_{NN}=200$



$Z(n_p) e^{n_p \mu/T}$, $\text{sqrts}_{NN}=11.5$



Studies of Z_n

- ✦ Higher order moments can be a signal
- ✦ However, it is unclear if freeze out points in experiments hit CEP
- ✦ The data would contain information of finite density QCD even if the CEP is achieved.

It is important to study the shape of the distribution theoretically.

- ✦ find properties sensitive to the shape
- ✦ clarify its physical meaning

Lattice QCD simulations

Lattice simulations

Canonical approach: extends data at a given μ to wide range
How do we obtain Zn ? : reduction formula + reweighing

$$Z(\mu) = \int \mathcal{D}U (\det \Delta(\mu))^{N_f} e^{-S_g}$$

• Reduction formula

$$\det \Delta = \xi^{-N_{\text{red}}/2} C_0(\{U\}) \prod (\xi + \lambda_n(\{U\})), \quad \xi = e^{-\mu/T},$$

$$= C_0 \sum_{n=-N_{\text{red}}/2}^{N_{\text{red}}/2} c_n \xi^n$$

[Gibbs ('86). Hasenfratz, Toussaint('92).
Adams('03, '04), Borici('04). KN&AN('10),
Alexandru & Wenger('10)]

• We use a reweighing in μ

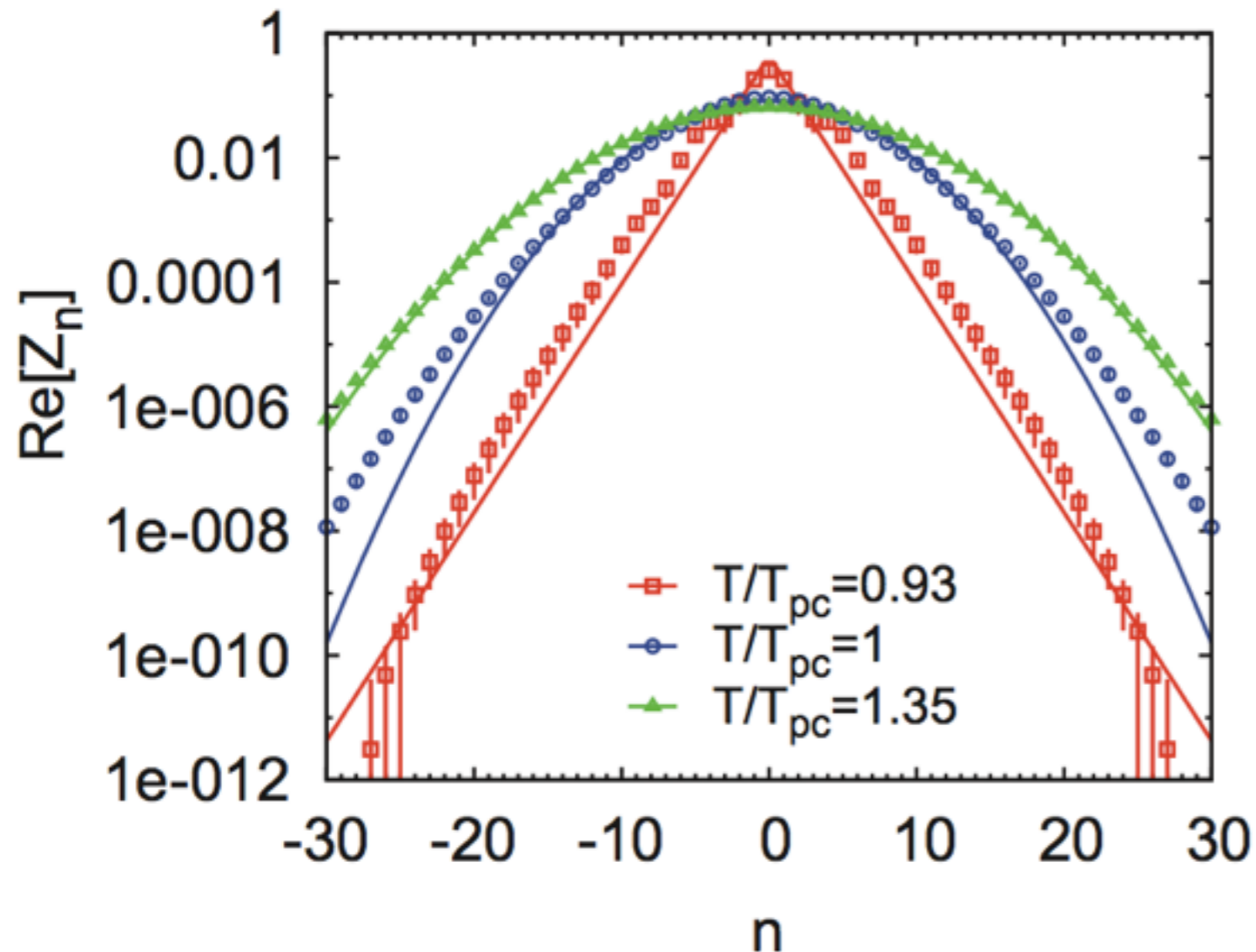
[Barbour, et. al. ('91).]

$$Z(\mu) = \sum Z_n e^{n\mu/T}, \quad Z_n \propto \left\langle \frac{C_0^{N_f} d_n}{(\det \Delta(0))^{N_f}} \right\rangle$$

Lattice simulations

- gauge configurations are generated at $\mu = 0$ and use reweighting
- volume : $8^3 \times 4$, $10^3 \times 4$
- mass : $m_{ps}/m_v \sim 0.8$
- action : clover-improved Wilson fermion + renormalization improved gauge
- # of statistics : 400 (20 trajectory-intervals, 3000 therm.)

Result - Zn



Lines :

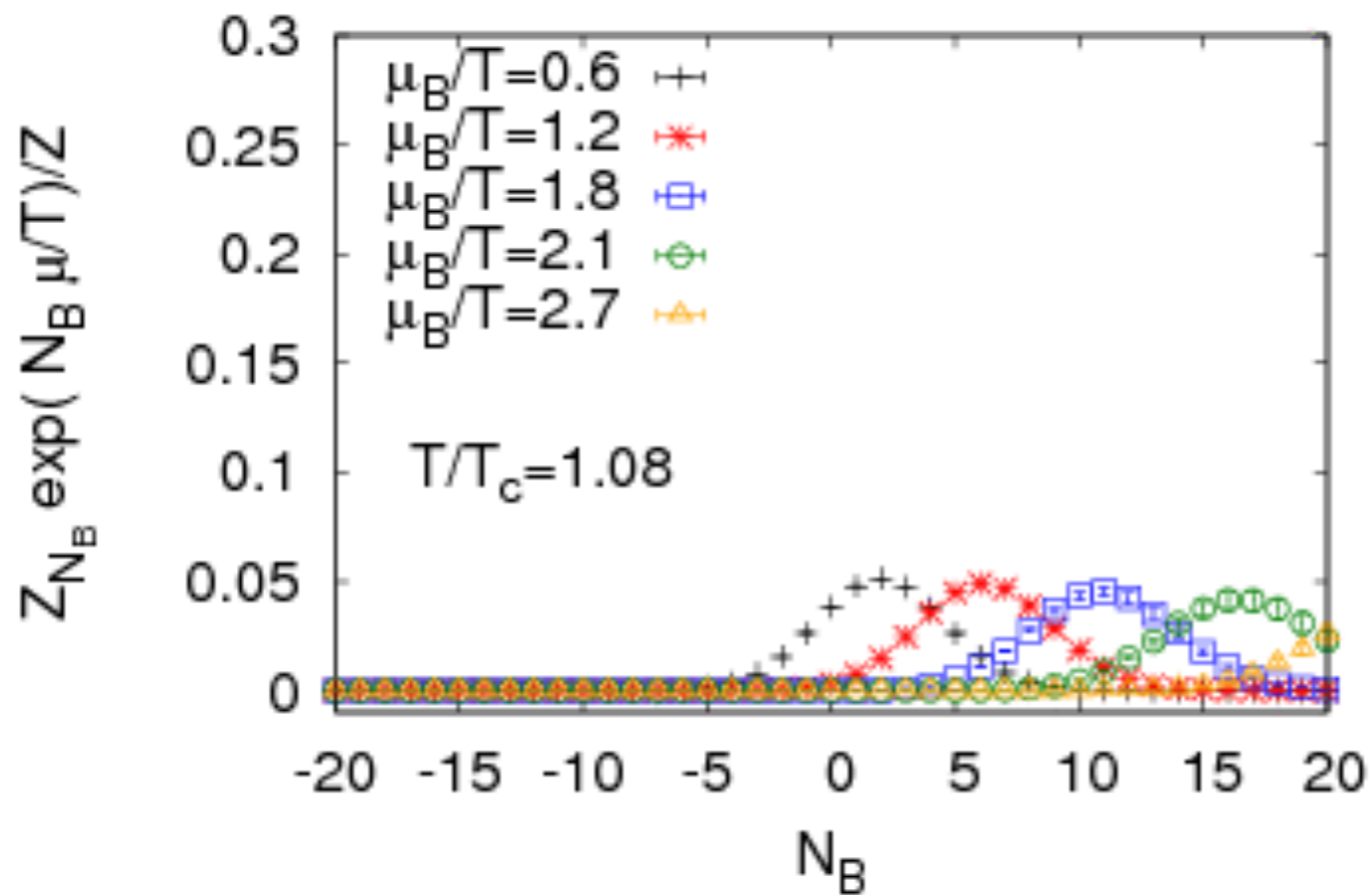
Gaussian for $T/T_{pc} = 1.35$ and 1 ,
 $\exp(-a|n|)$ for $T/T_{pc} = 0.93$.

[KN, S. Motoki, Y. Nakagawa, A. Nakamura, T. Saito, PTEP(2012). 1

- ✦ volume : $8^3 \times 4$, $10^3 \times 4$, mass : $m_{ps}/m_v \sim 0.8$
- ✦ gauge configurations are generated at $\mu = 0$ and use reweighting
- ✦ action : clover-improved Wilson fermion + renormalization improved gauge
- ✦ # of statistics : 400 (20 trajectory-intervals, 3000 therm.)

Result - $Z_n \exp(\mu/T)$ at high T

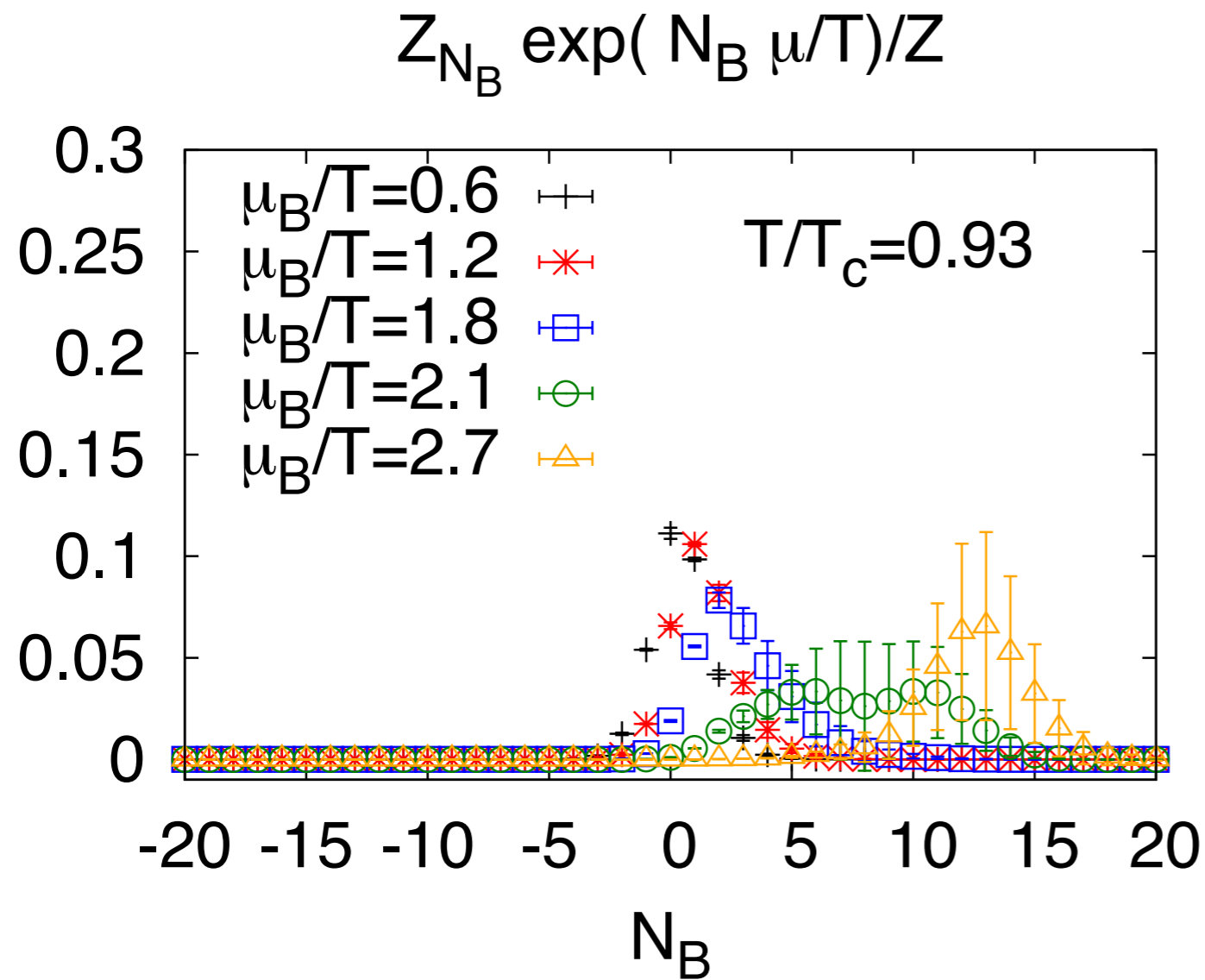
If Z_n is the Gaussian, then the baryon number distribution is also Gaussian.



$$P_n \propto Z_n e^{n\mu/T}$$

Result - Zn $\exp(\mu/T)$ at low T

Increasing μ at low T, a non-trivial shape change has been observed



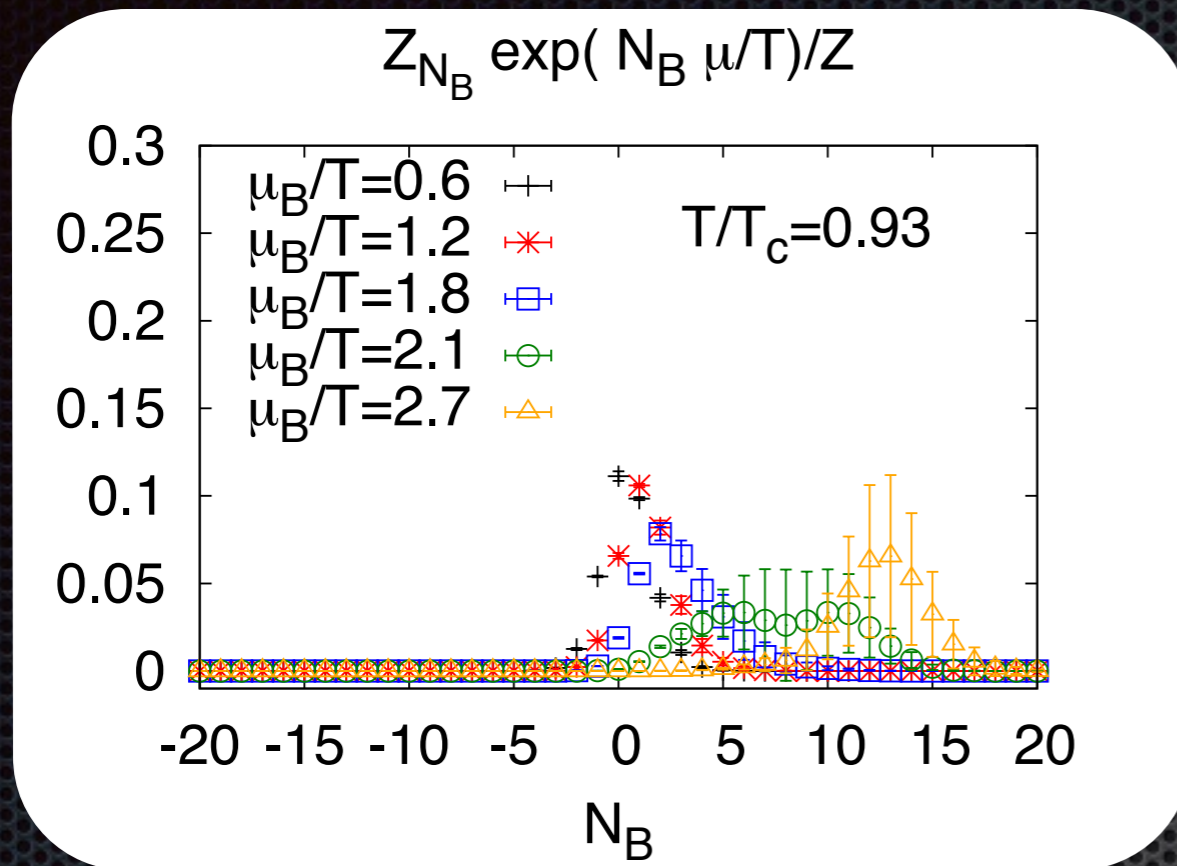
$T/T_c = 0.93$

$\mu_B/T = 1.8$: right tail

$\mu_B/T = 2.1$: flat

$\mu_B/T = 2.7$: left tail

Baryon number distribution & fluctuations

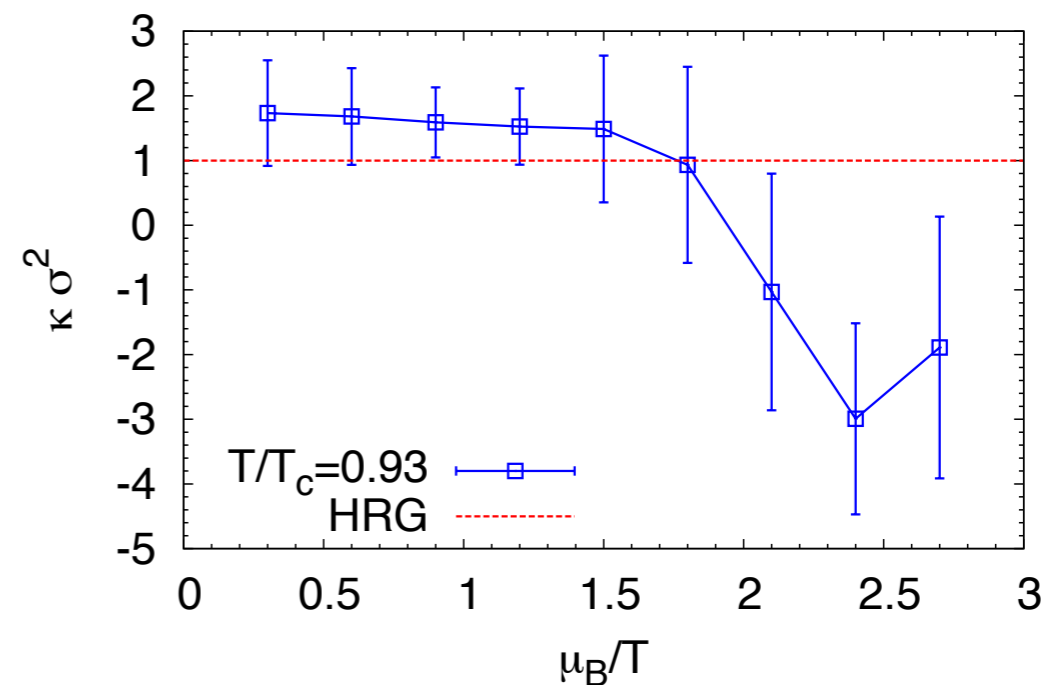
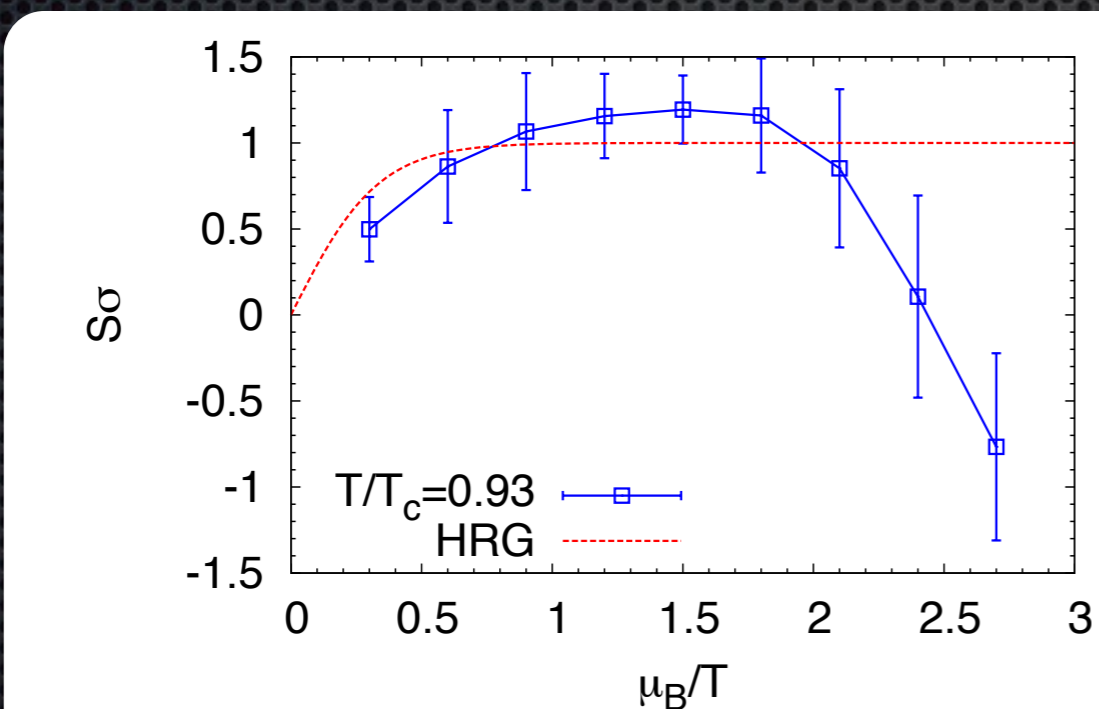


$$\langle (\delta N)^m \rangle = \sum_{n_B} (\delta N)^m Z_{n_B} e^{n_B \mu_B / T} / Z_{GC}$$

$$\sigma^2 = \langle (\delta N)^2 \rangle$$

$$S = \frac{\langle (\delta N)^3 \rangle}{\sigma^3}$$

$$\kappa = \frac{\langle (\delta N)^4 \rangle}{\sigma^4} - 3$$



Lee-Yang zeros : from CPF to Phase transition

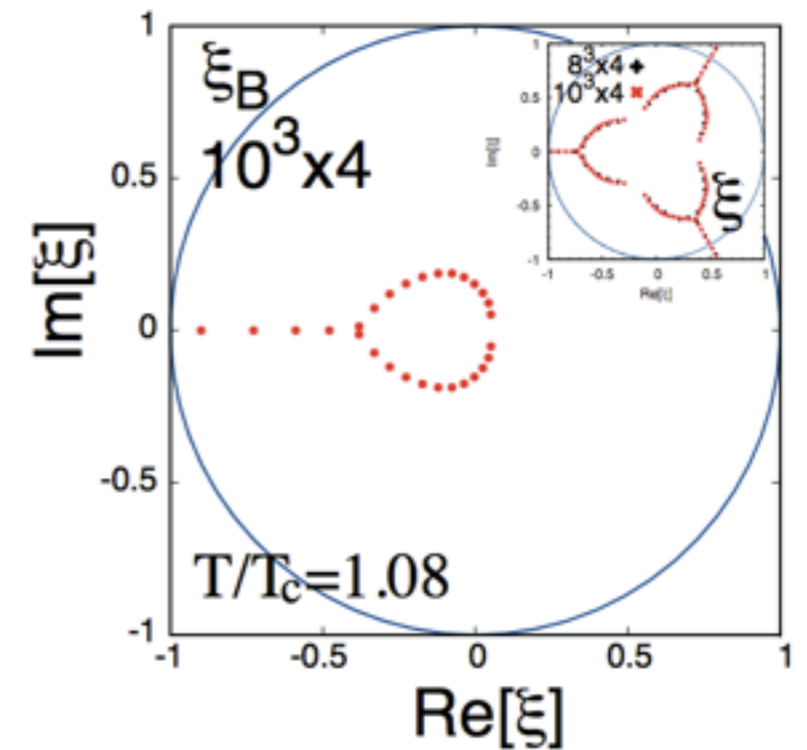
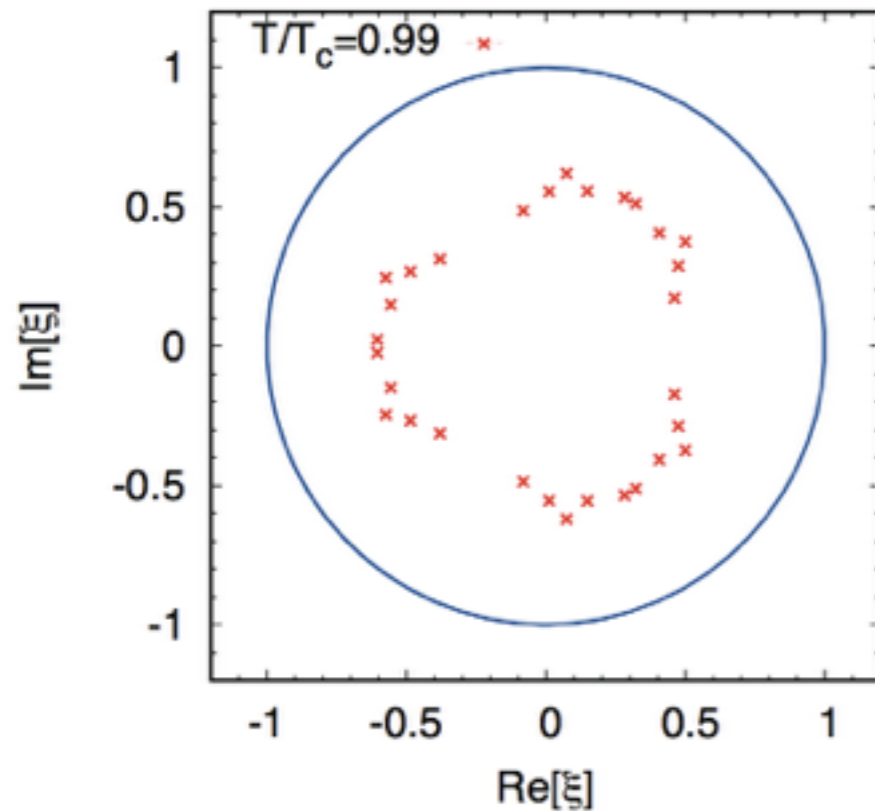
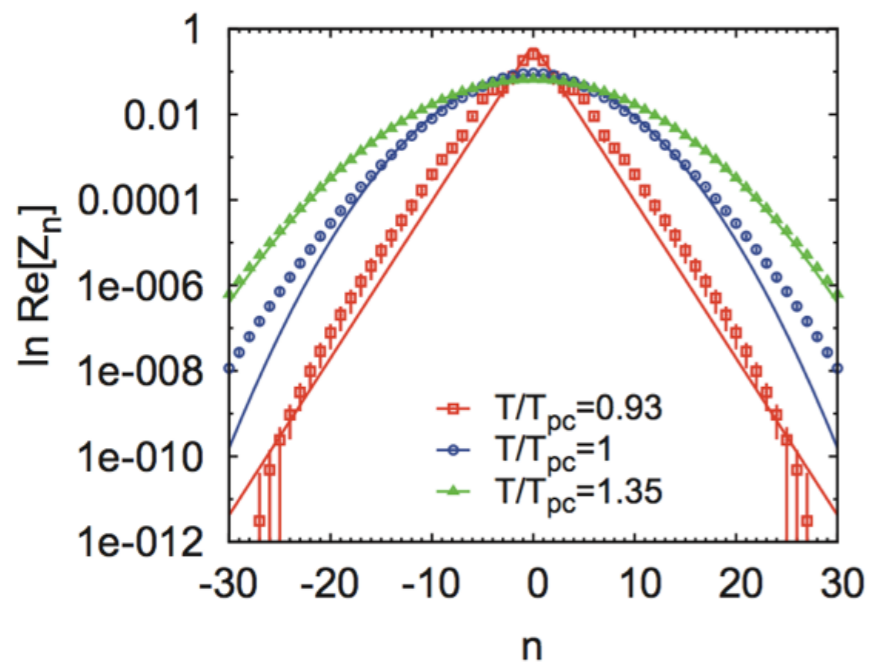
Lee-Yang zero Theorem :

zeros of the partition function control the analyticity of the free energy [Lee & Yang 1952]

$$Z(\mu) = \sum Z_n e^{n\mu/T}$$
$$\propto \prod (1 - \xi/\xi_i)$$

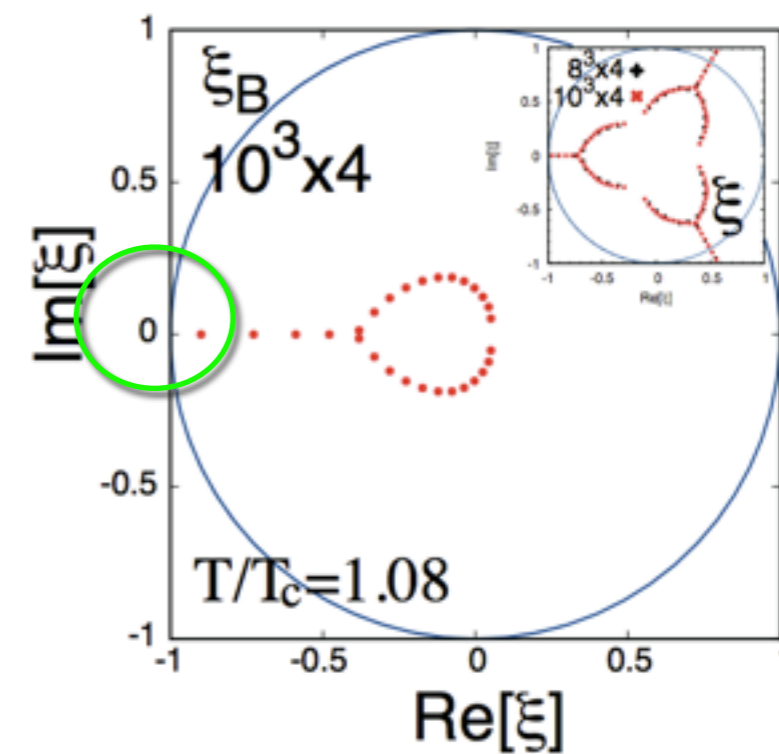
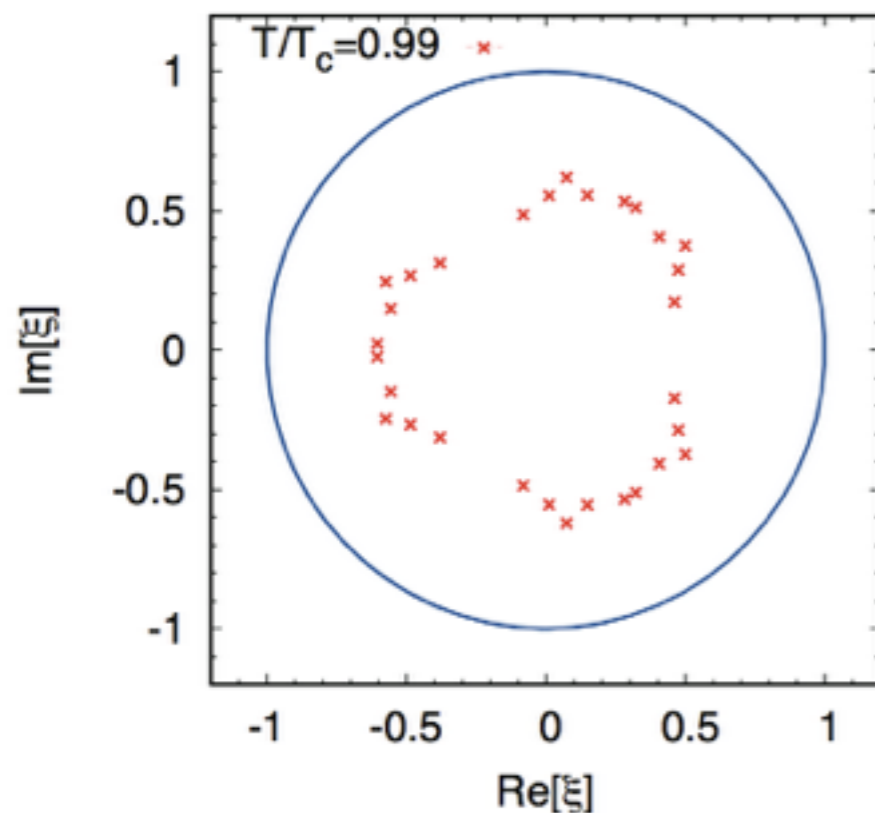
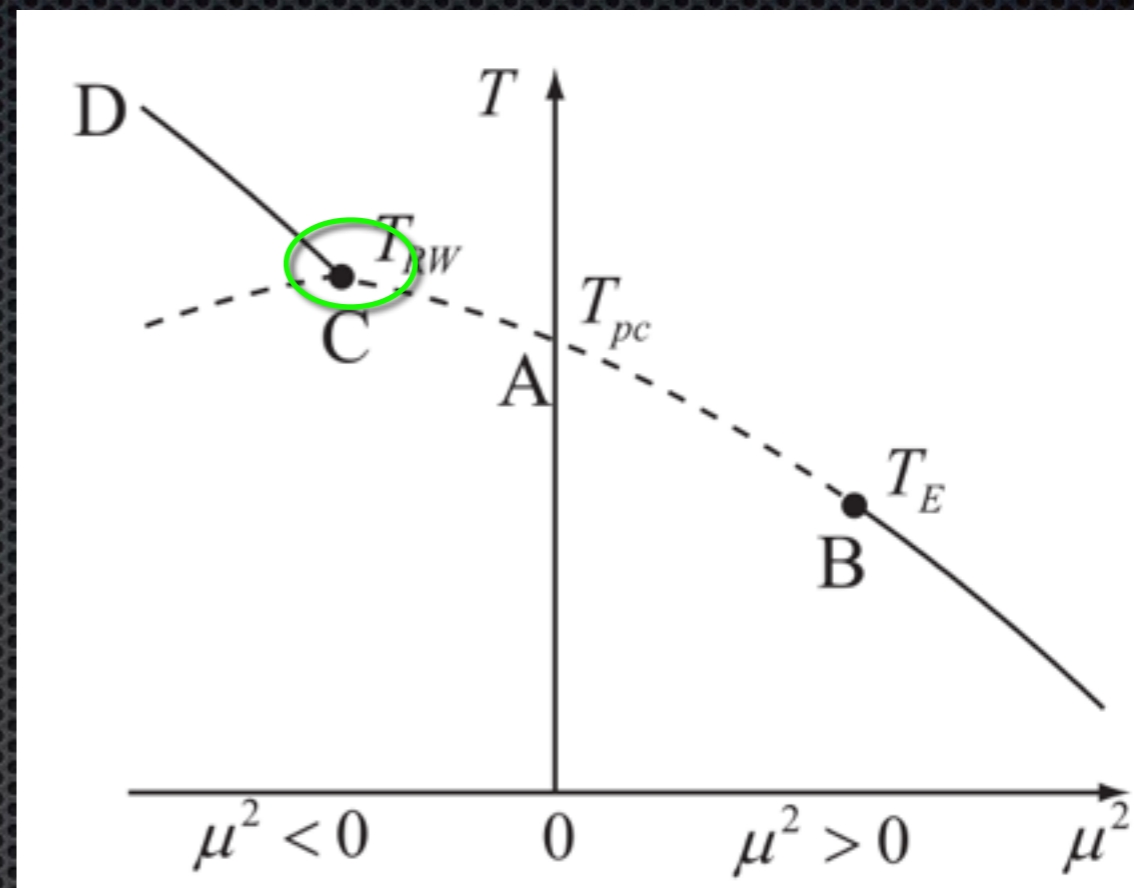
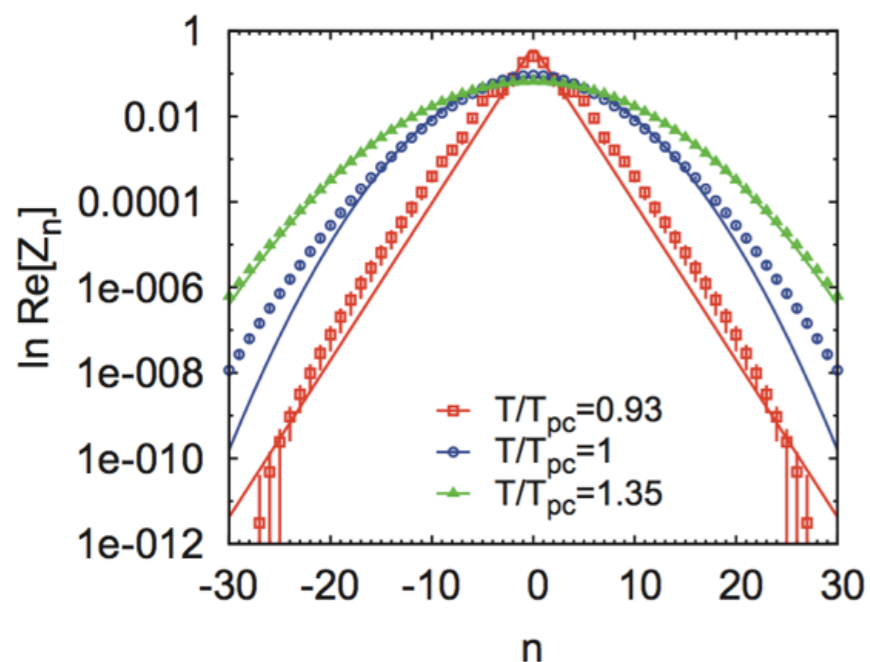
Result-Lee-Yang zeros

▪ [Nakamura, Nagata(2013)]



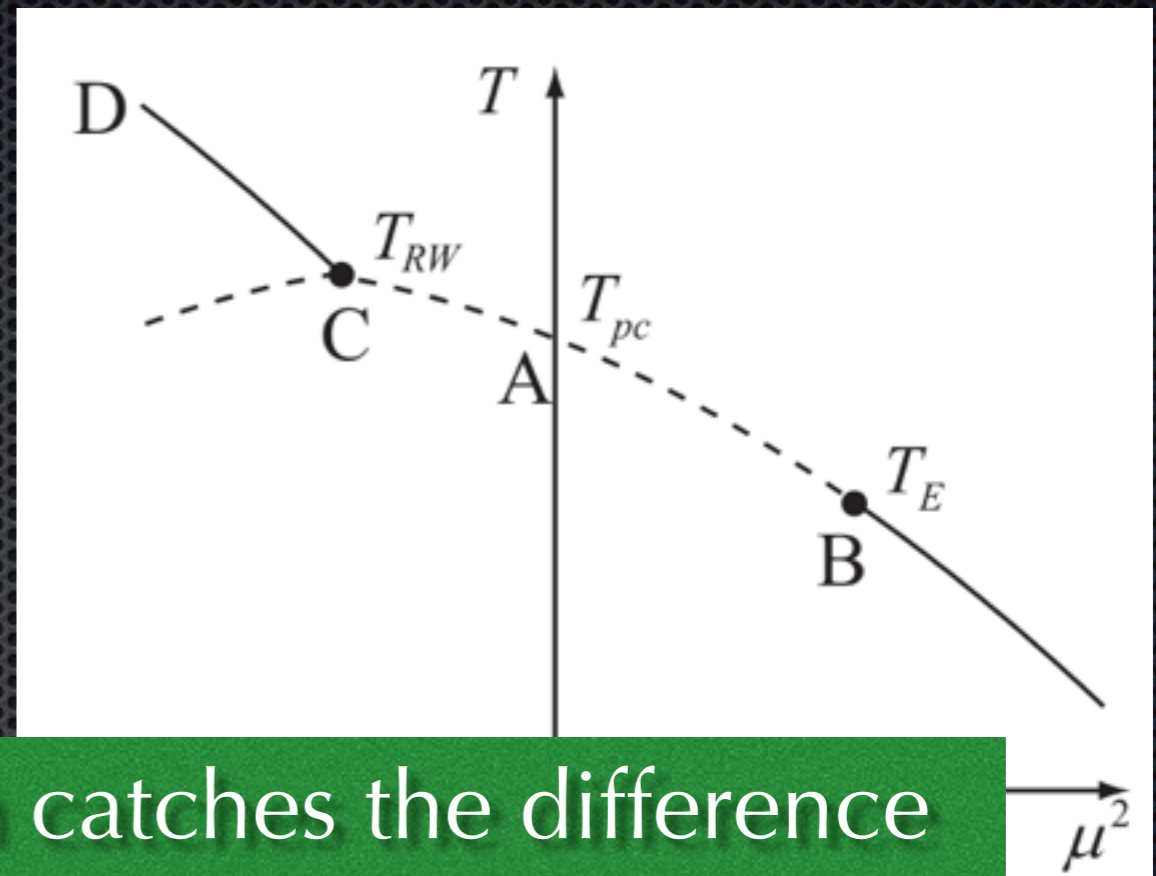
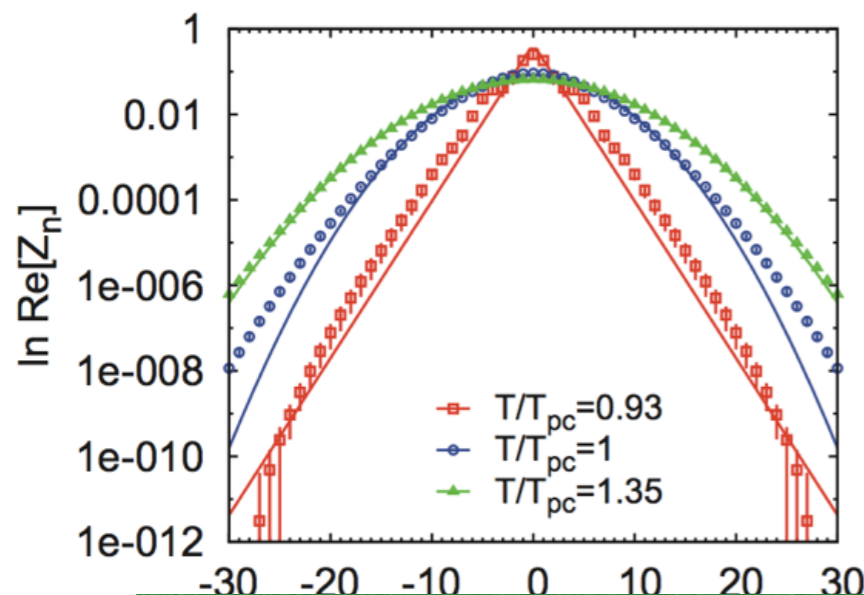
Result-Lee-Yang zeros

▪ [Nakamura, Nagata(2013)]

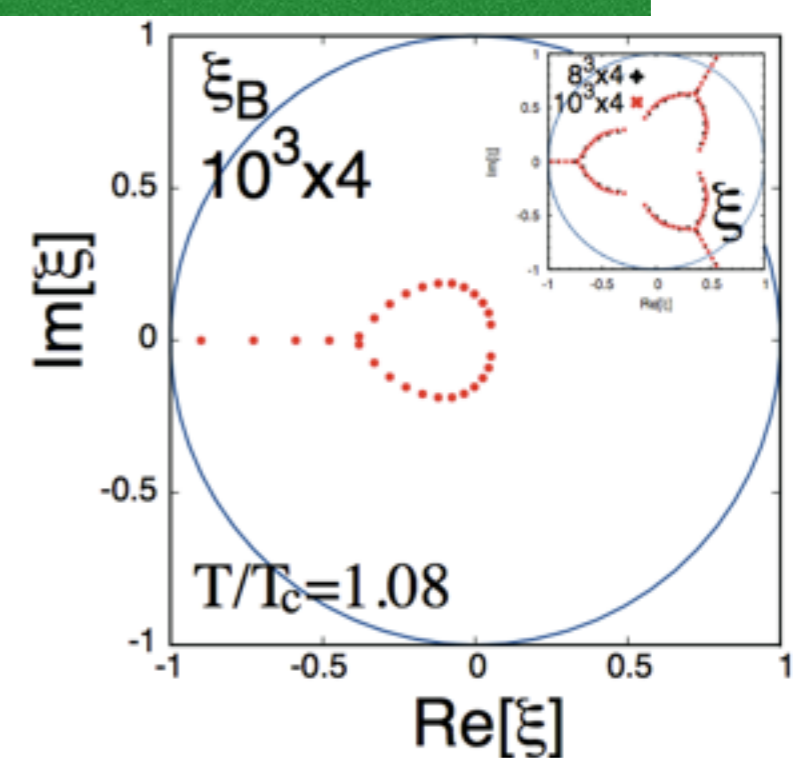
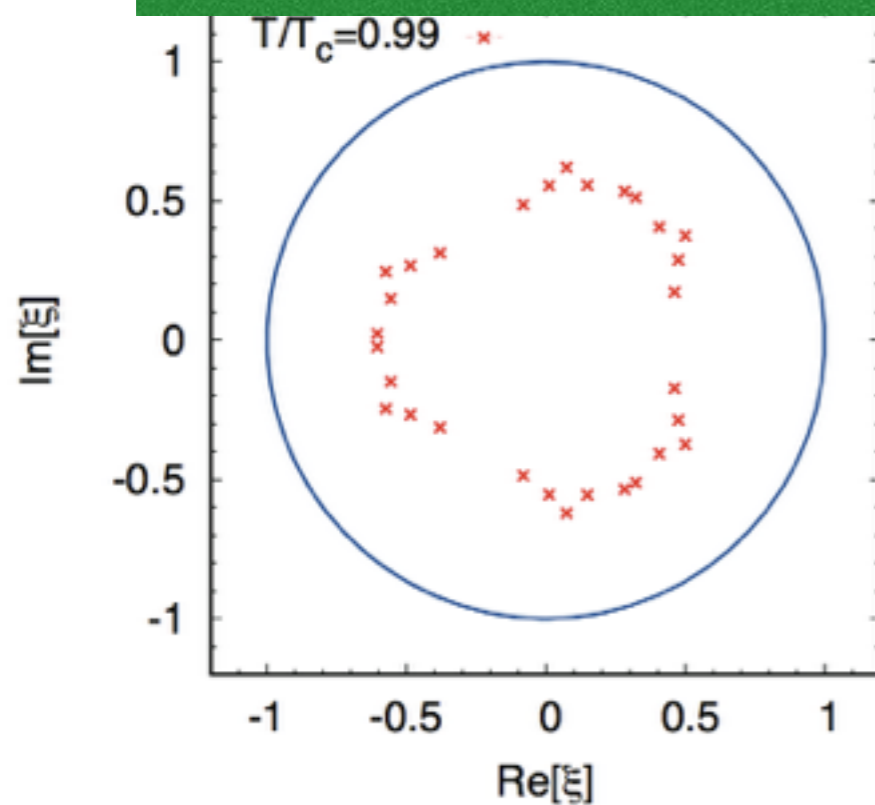


Result-Lee-Yang zeros

▪ [Nakamura, Nagata(2013)]



Lee-Yang zero distribution catches the difference between T_c and T_{RW}



Result - 2

Questions and Subtleties in the calculation

- Lee-Yang zeros are sensitive to Z_n ; We need careful analysis
- There remains some questions
 - error bars in Z_n : statistical stability
 - truncation of the polynomial : convergence

$$Z(\mu) = \sum_{n=-\infty}^{\infty} Z_n e^{n\mu/T} \rightarrow \sum_{n=-n_0}^{n_0} Z_n e^{n\mu/T} + (|n| > n_0)$$

We focus on high T region, and perform

- analytic calculation
- reanalysis of lattice data

Analytic calculation of Zn of high T QCD

Properties of high T QCD leads to Gaussian Zn

- Zn can be obtained from the F.T.

$$Z_n = \int Z(\theta) e^{in\theta} d\theta, \quad \mu/T = i\theta, (\theta \in \mathbb{R})$$

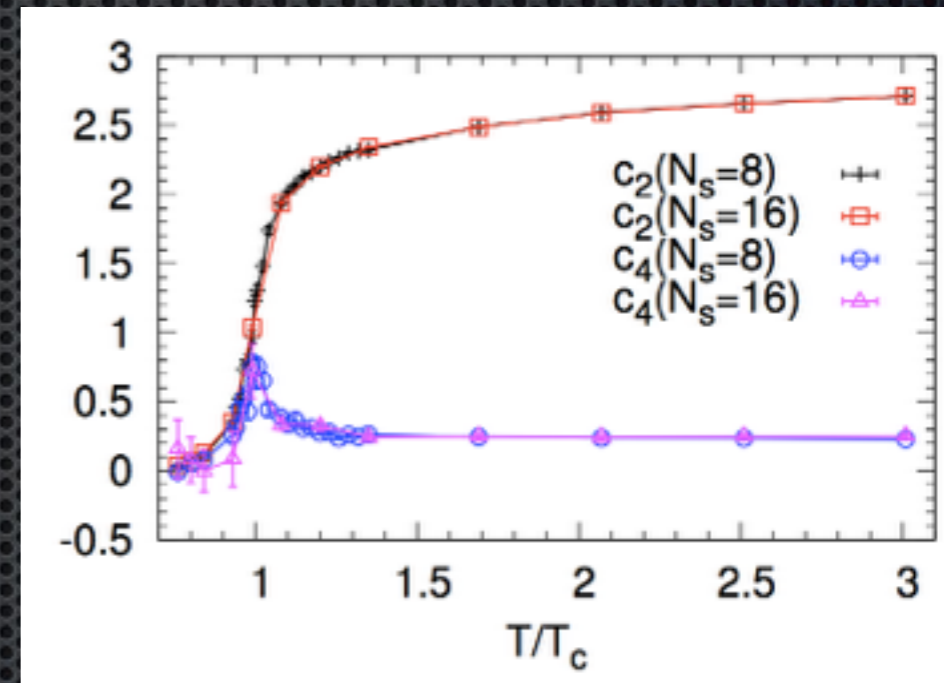
- Use properties of high T QCD

$$-\frac{f}{T^4} = c_0 + c_2(\mu/T)^2 + c_4(\mu/T)^4$$

$$Z\left(\frac{\mu_I}{T}\right) = Z\left(\frac{\mu_I}{T} + \frac{2\pi}{N_c}\right).$$

- also use the saddle point approximation

$$Z_n = C e^{-n^2/(4T^3 V c_2)}, \quad (n \equiv 0 \pmod{3})$$



Nagata, Nakamura, JHEP(2012)

Analytical calculation of LY zeros of high T QCD

Gaussian Zn + RW periodicity leads to Lee-Yang zeros as

$$\frac{\mu}{T} = \frac{(2l+1)\pi i}{3} - \frac{3(2k+1)}{4VT^3 c_2}$$

Analytical calculation of LY zeros of high T QCD

Gaussian Zn + RW periodicity leads to Lee-Yang zeros as

$$\frac{\mu}{T} = \frac{(2l+1)\pi i}{3} - \frac{3(2k+1)}{4VT^3c_2}$$

High T QCD

$$Z_n = C e^{-n^2/(4T^3Vc_2)}, \quad (n \equiv 0 \pmod{3})$$

$$Z(\mu) = C \sum_{n_B=-\infty}^{\infty} e^{-9n_B^2/(4T^3Vc_2) + 3n_B\mu/T}$$

Theta function

$$\vartheta(z, \tau) = \sum_{n=-\infty}^{\infty} e^{-\pi i n^2 \tau + 2\pi i n z}$$

$$i\pi\tau = 9/(4T^3Vc_2),$$
$$2\pi i z = 3\mu/T$$

$$\vartheta(z, \tau) = 0 \Leftrightarrow z = l + k\tau + \frac{1}{2} + \frac{\tau}{2}, \quad (k, l \in \mathbb{Z})$$

Alternative calculation

Cancellation of two types of free energy allows $Z=0$

- Cancellation of free energies [Biskup et al('01)]

$$Z = e^{-V f_I/T} + e^{-V f_{II}/T}$$

$$\begin{cases} \operatorname{Re}[f_I - f_{II}] = 0 \\ \frac{V}{T} \operatorname{Im}[f_I - f_{II}] = (2k - 1)\pi, (k \in \mathbb{Z}) \end{cases}$$

- Approximate solution for $c_2 \gg c_4$

$$(\mu_R, \mu_I) = \left(\frac{3(2k - 1)}{4VT^3 c_2}, -\pi/3 \right)$$

- It is also possible to solve it in the presence of c_4
- f_I and f_{III} , and f_{II} and f_{III} .

Analytical calculation of LY zeros of high T QCD

$$\frac{\mu}{T} = \underbrace{\frac{(2l+1)\pi i}{3}}_{\text{angular}} - \underbrace{\frac{3(2k+1)}{4VT^3 c_2}}_{\text{radial}}$$

$$\xi = \exp(-\mu/T)$$

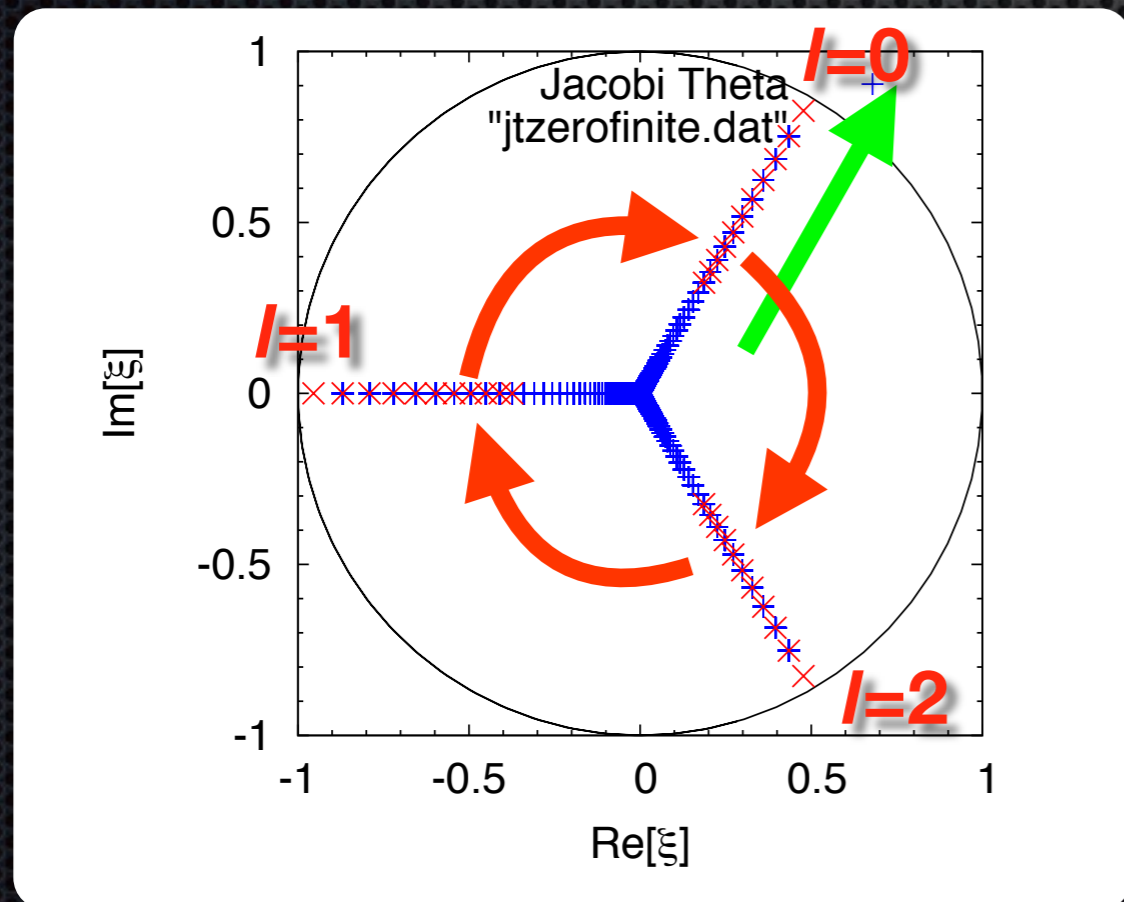
Analytical calculation of LY zeros of high T QCD

$$\frac{\mu}{T} = \frac{(2l+1)\pi i}{3} - \frac{3(2k+1)}{4VT^3 c_2}$$

angular

radial

$$\xi = \exp(-\mu/T)$$



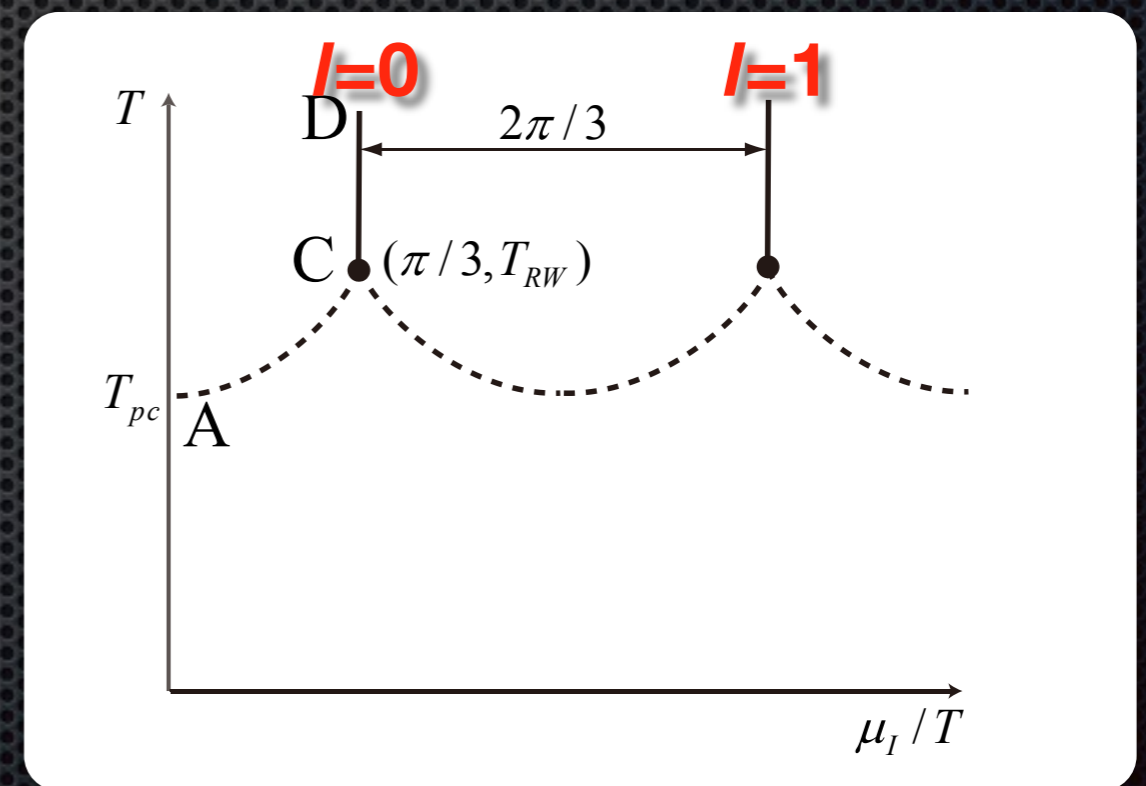
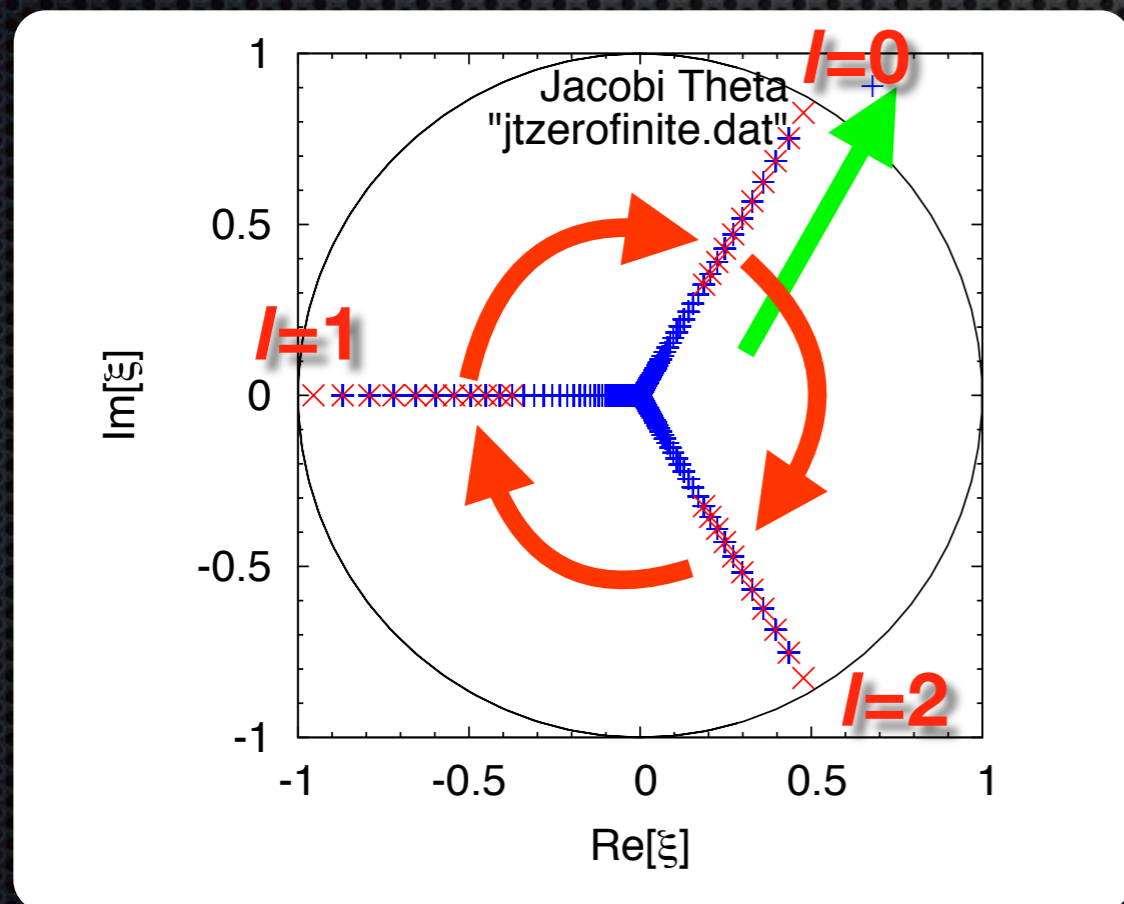
Analytical calculation of LY zeros of high T QCD

$$\frac{\mu}{T} = \frac{(2l+1)\pi i}{3} - \frac{3(2k+1)}{4VT^3c_2}$$

angular

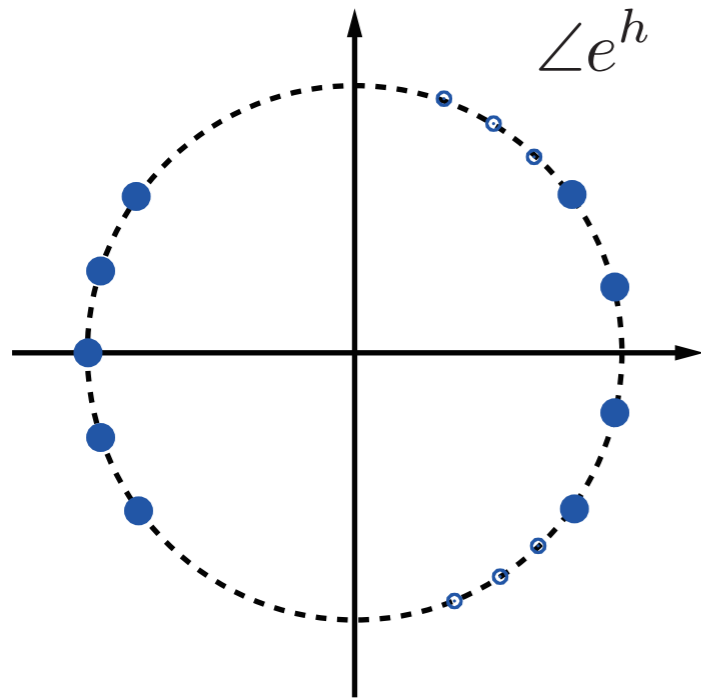
radial

$$\xi = \exp(-\mu/T)$$

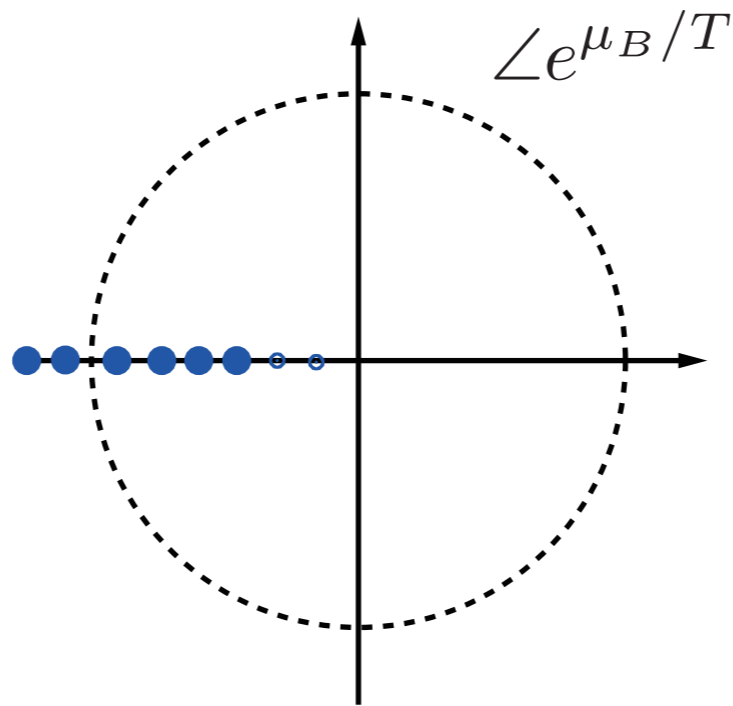


Lee-Yang zeros : Ising vs free fermion gas

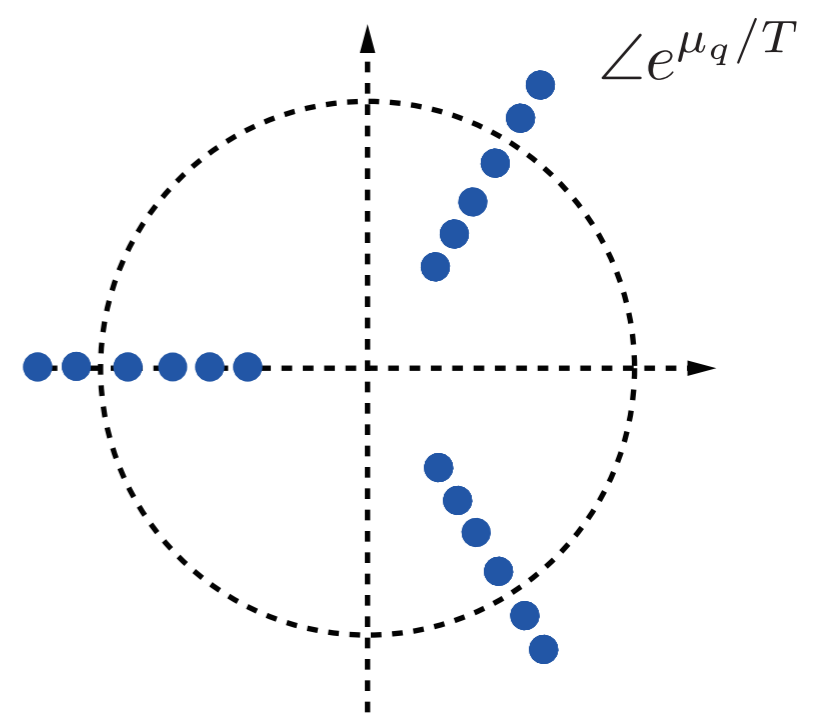
a) Ising



b) high T QCD



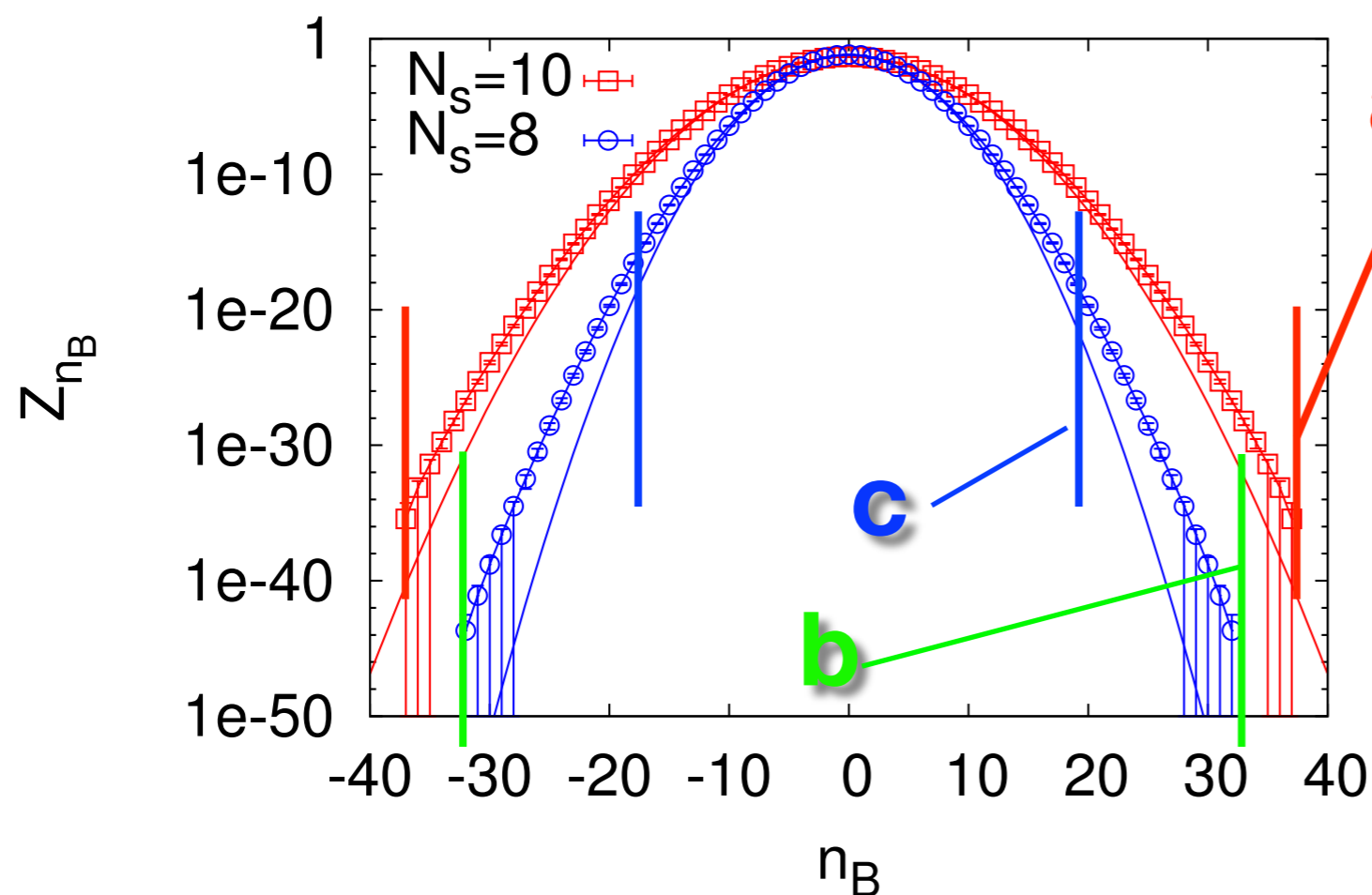
c) high T QCD



Reanalysis of Lattice data & analytic result

- We reanalyze previous lattice data.
 - errors of Z_n : bootstrap analysis (1000 BS samples.)
 - estimate the convergence
 - finite size scaling

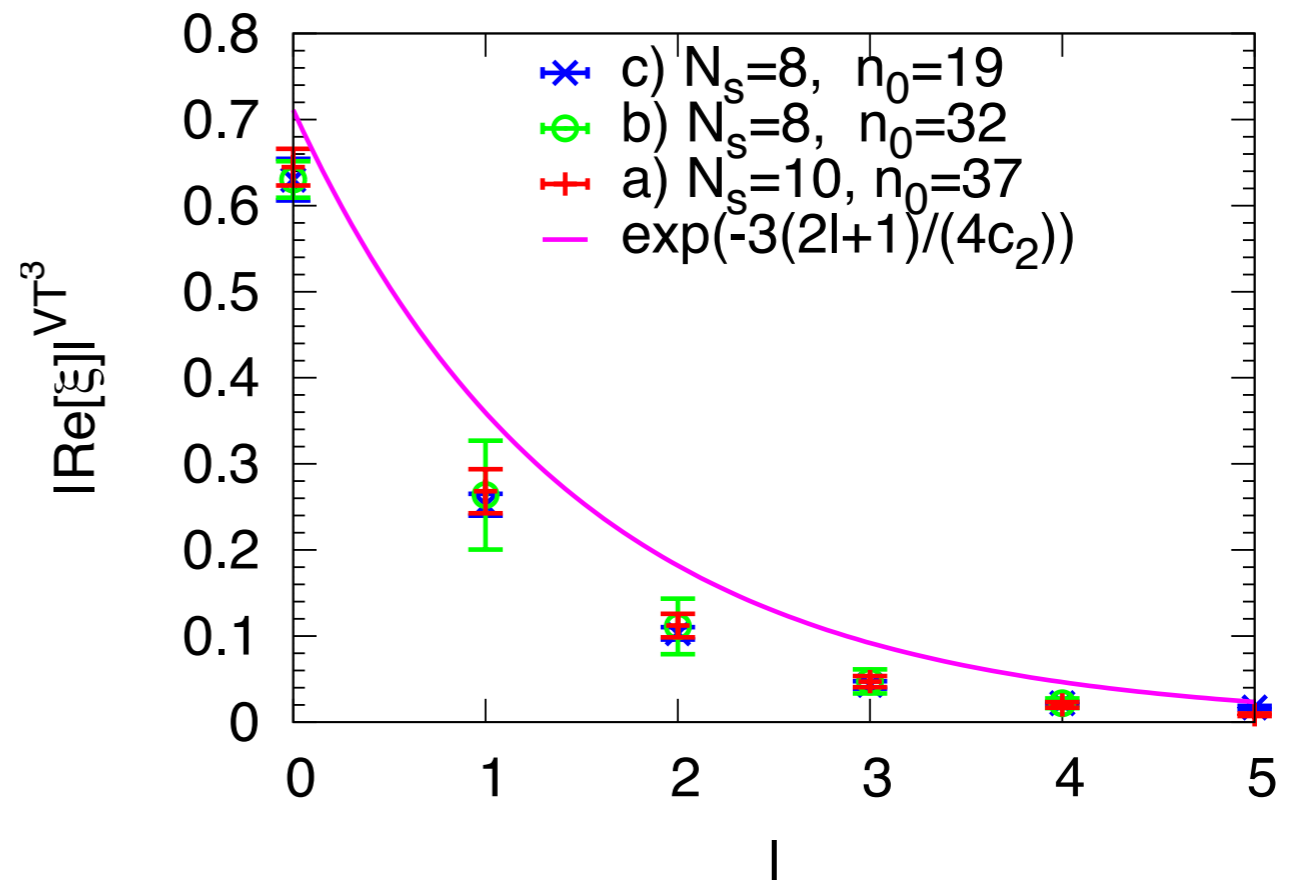
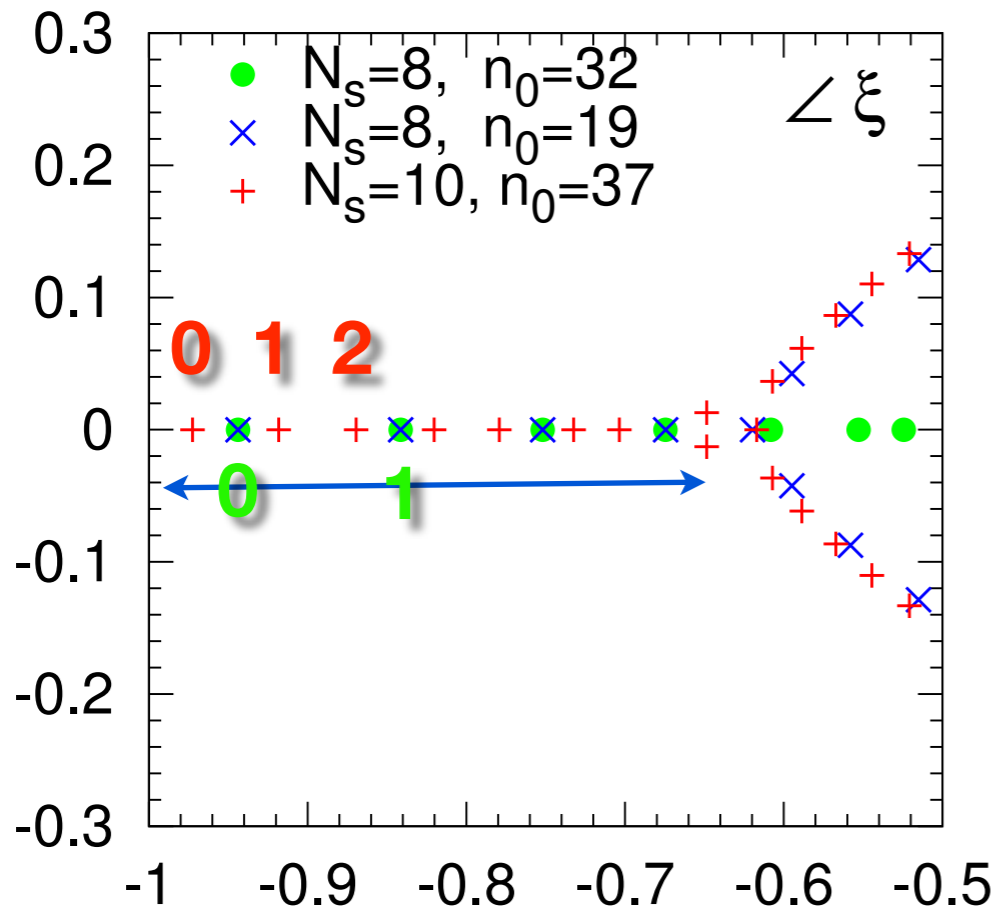
$$|\operatorname{Re}[\xi]|^{VT^3} = \exp(-(3k + 1)/(4c_2))$$



- a) $N_s=10$ $n_0=37$**
- b) $N_s=8$ $n_0=32$**
- c) $N_s=8$ $n_0=19$**

Reanalysis of Lee-Yang zeros for high T QCD

Analytic and lattice calculation are consistent !

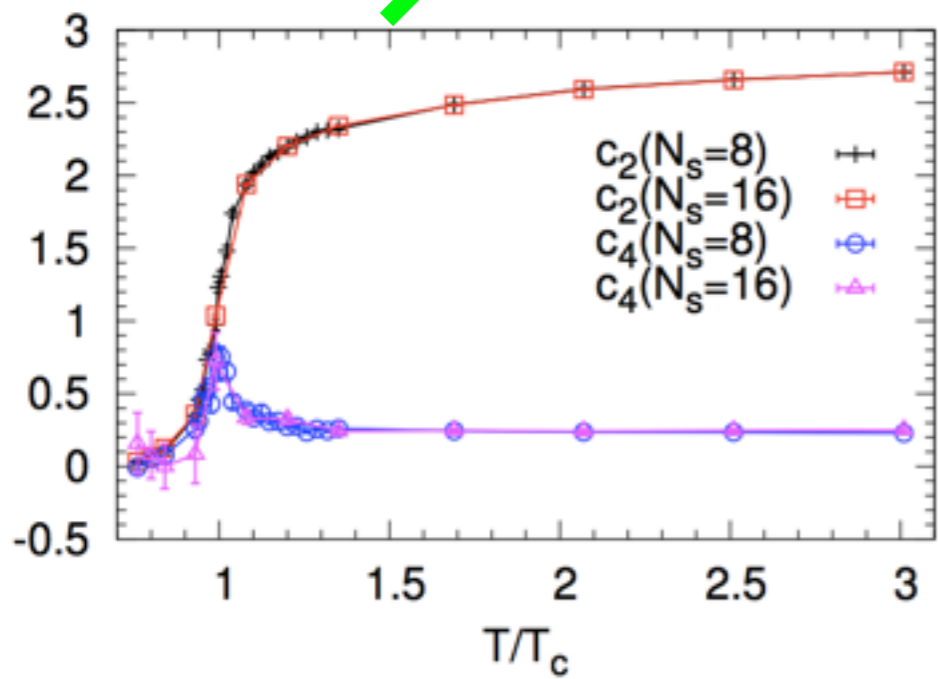


Solid Line : $|\text{Re}[\xi]|^{VT^3} = \exp(-3(2l+1)/(4c_2))$

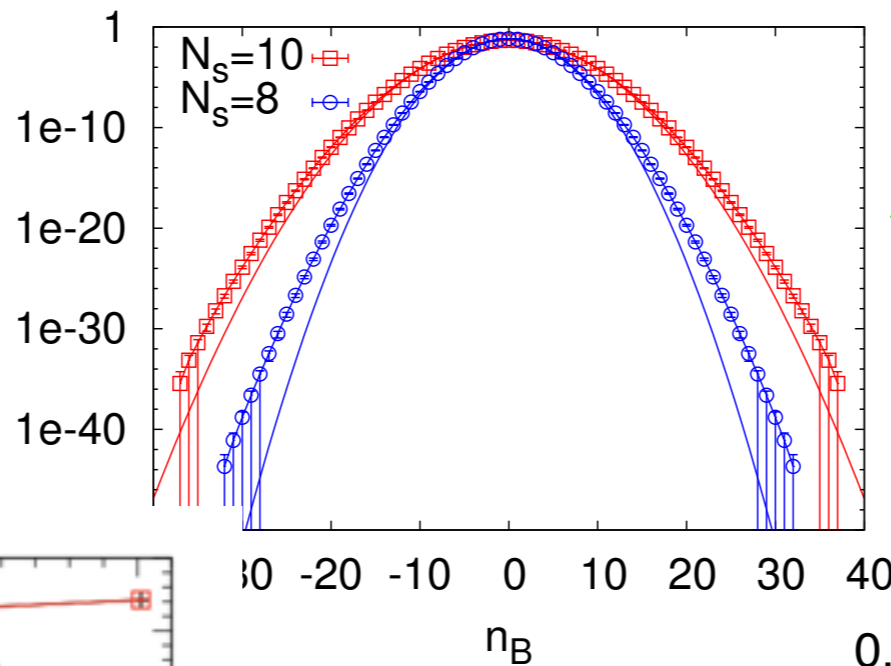
- ✦ Lee-Yang zeros near the unit circle are statistically stable
- ✦ b)-c) : convergence ok
- ✦ a)-c) : volume scaling consistent with the analytic one.
- ✦ underestimation : saddle point approximation

implication

c2-dominance
RW periodicity

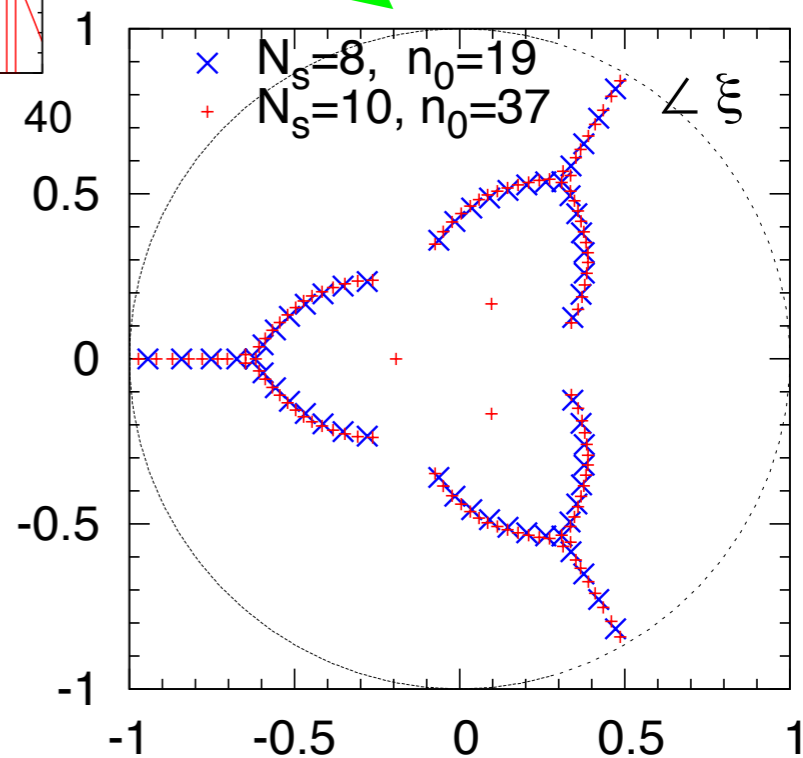


**Completion of
deconfinement**



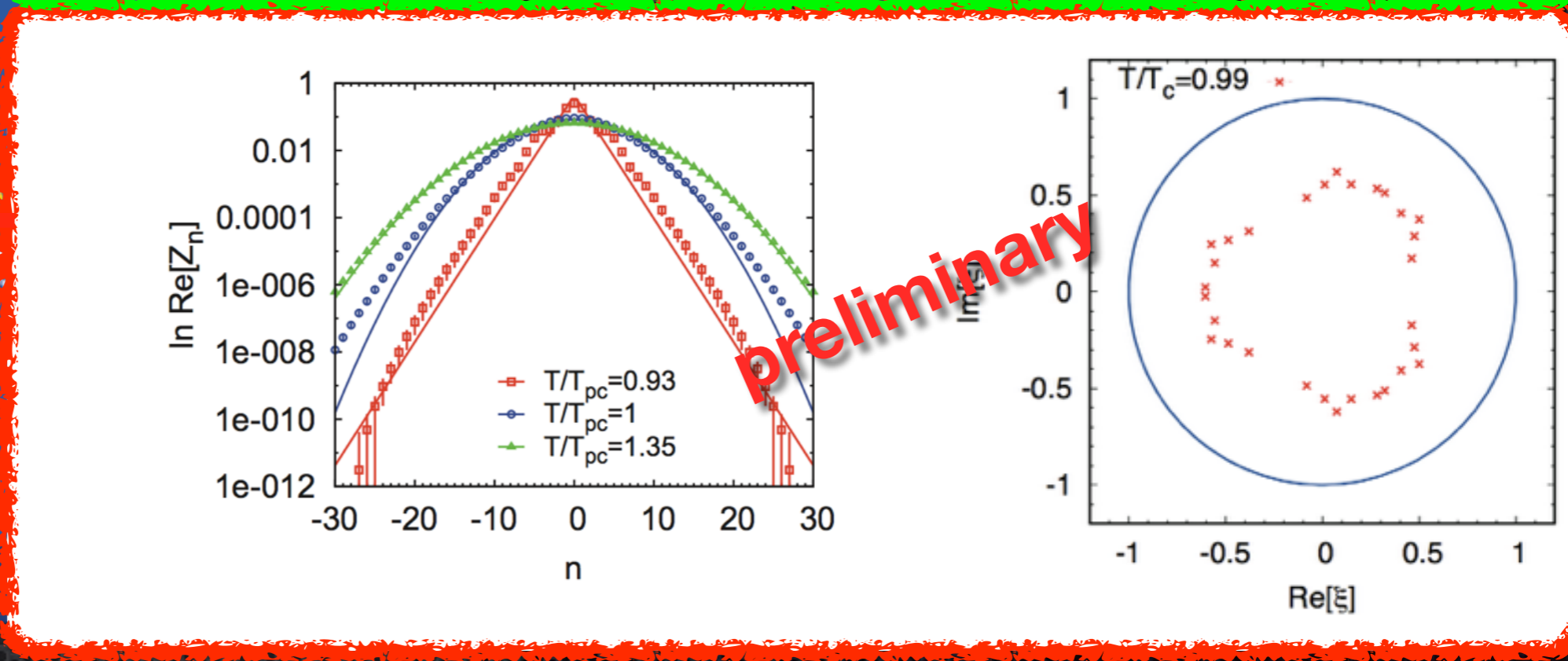
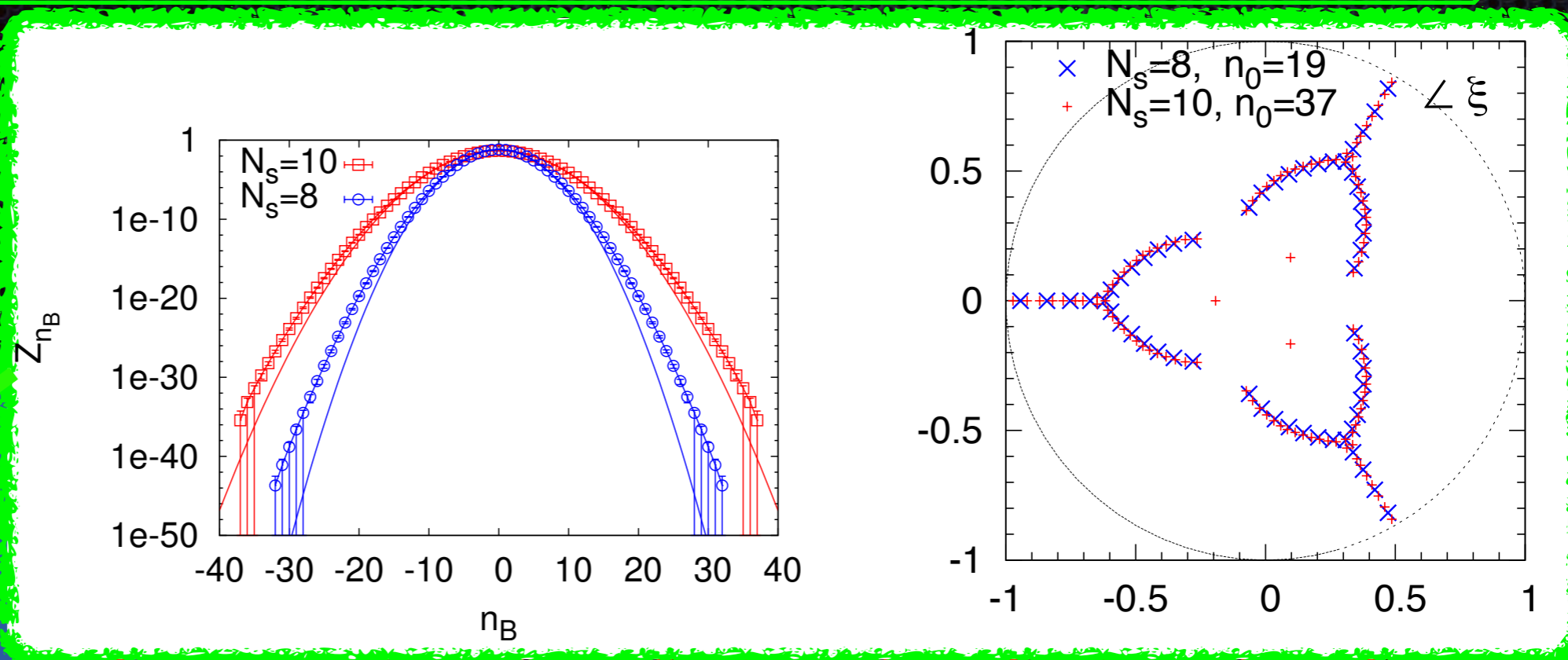
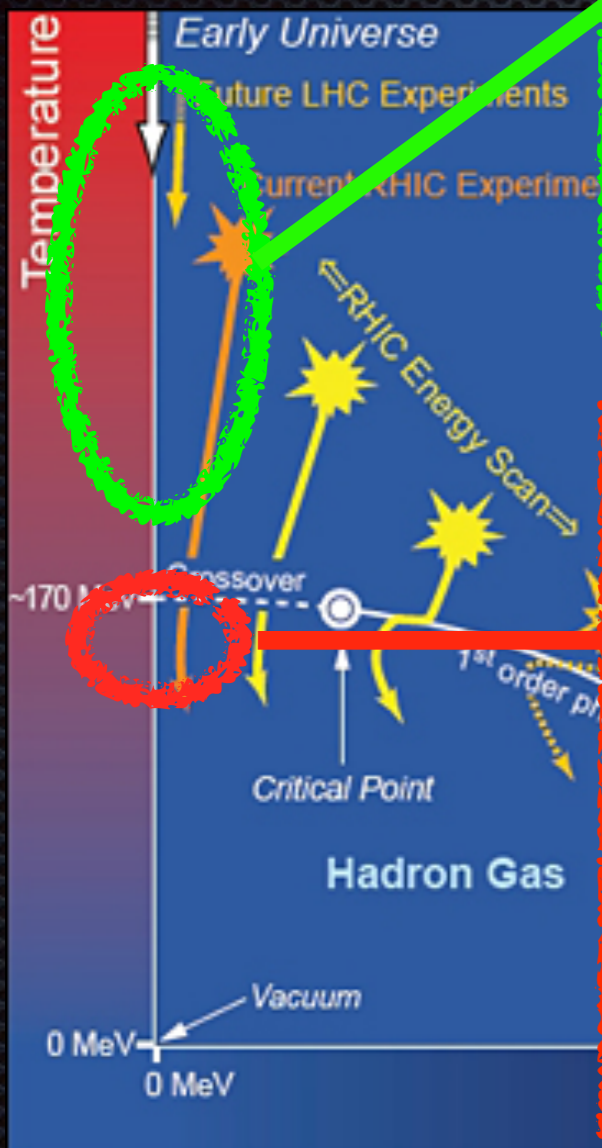
Gaussian behavior

**Theta
function**



**Roberge-Weiss
phase transition**

Summary

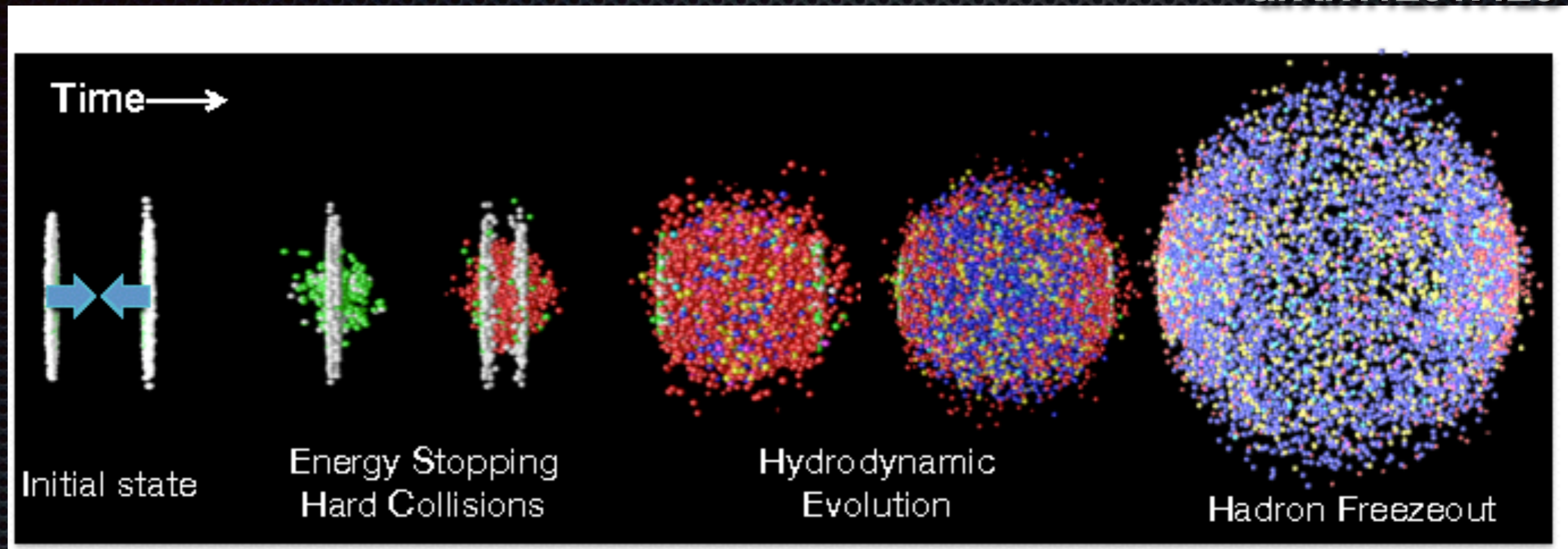


preliminary

Summary

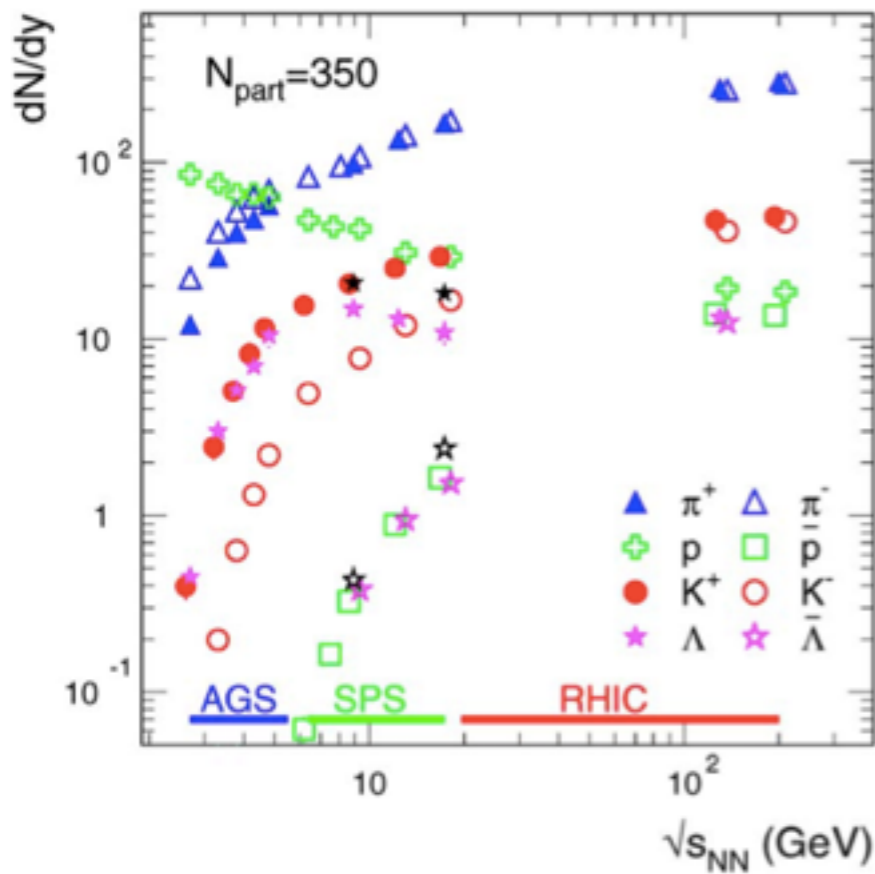
- **Canonical approach**
 - provides a way to extend data obtained at a certain μ/T to other values of μ/T .
 - can be applied not only to lattice QCD but also to experimental data.
- We showed that the net baryon number follows
 - Gaussian distribution at high temperatures
 - Gaussian shape is an indication of RW phase transition (high T)
- Lee-Yang zeros are sensitive to a shape of the canonical partition functions.

Applications to Beam energy scan experiment



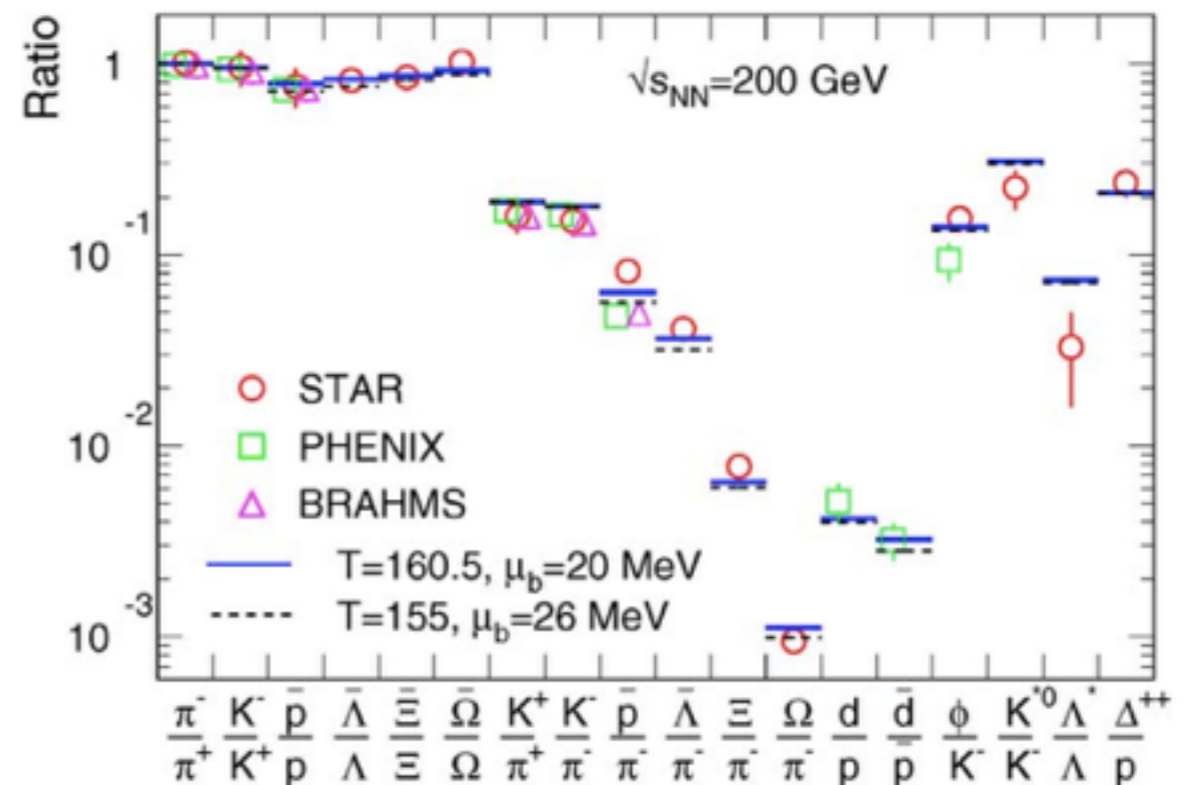
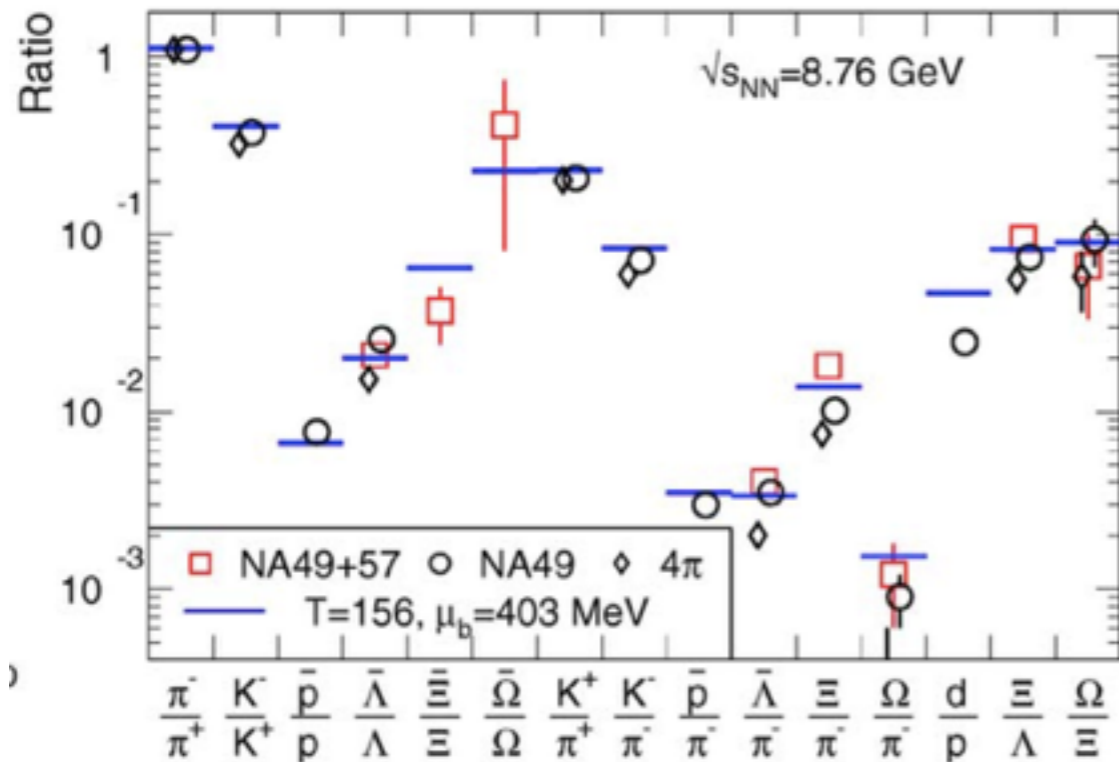
- ✦ **Number of hadrons**
 - ✦ **fixed at a time when inelastic process ceases**
 - > **chemical freeze-out**
- ✦ **Number of hadrons provide information at the freeze-out time**

Hadron yields and thermal statistical model

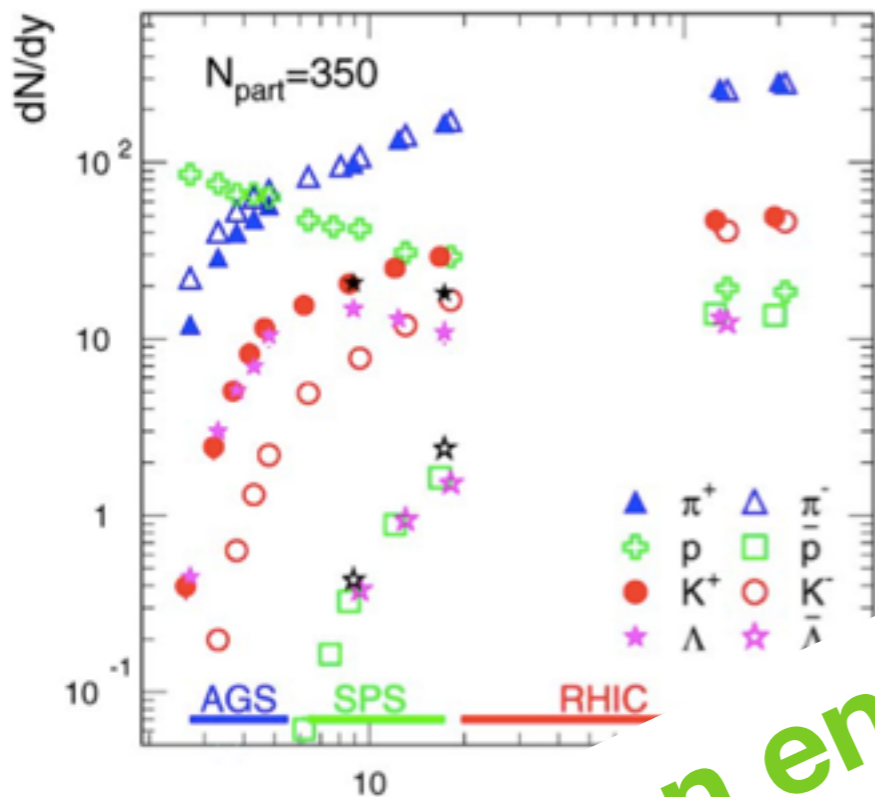


$$n_i = N_i/V = -\frac{T}{V} \frac{\partial \ln Z_i}{\partial \mu} = \frac{g_i}{2\pi^2} \int_0^\infty \frac{p^2 dp}{\exp[(E_i - \mu_i)/T] \pm 1}$$

Andronic, et., al, (2005)



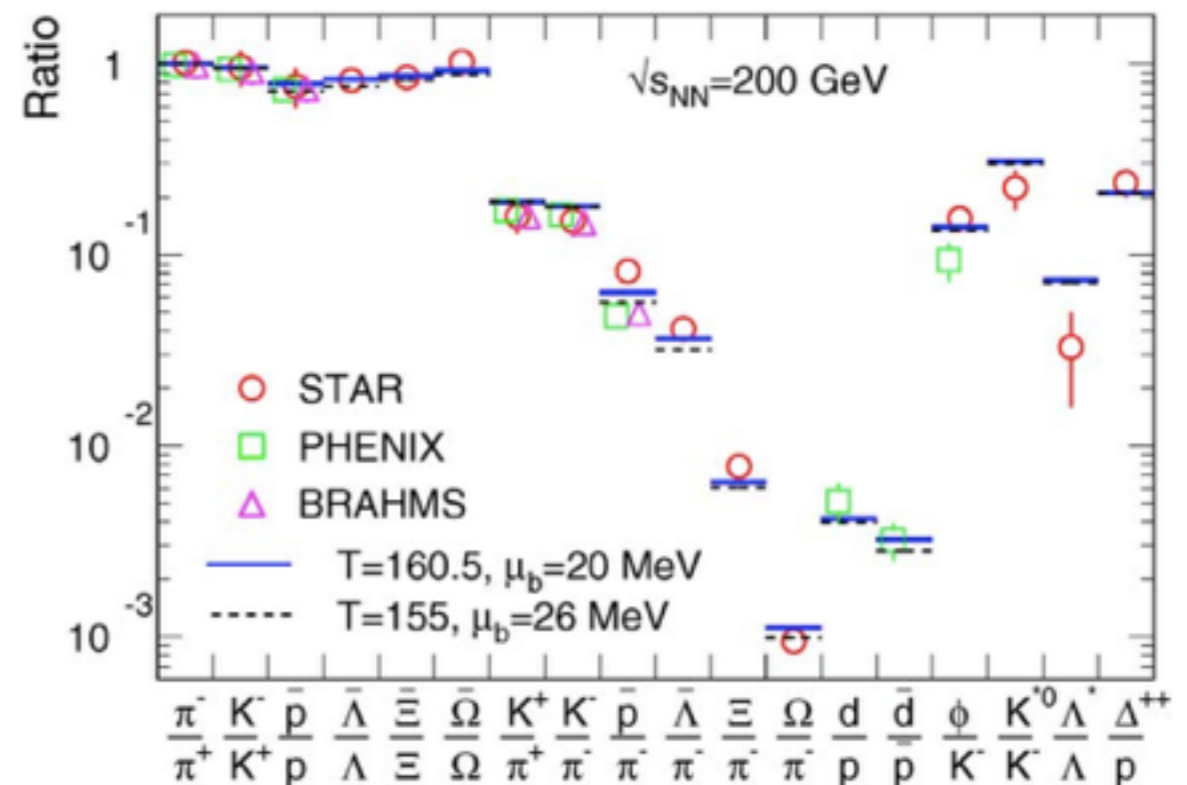
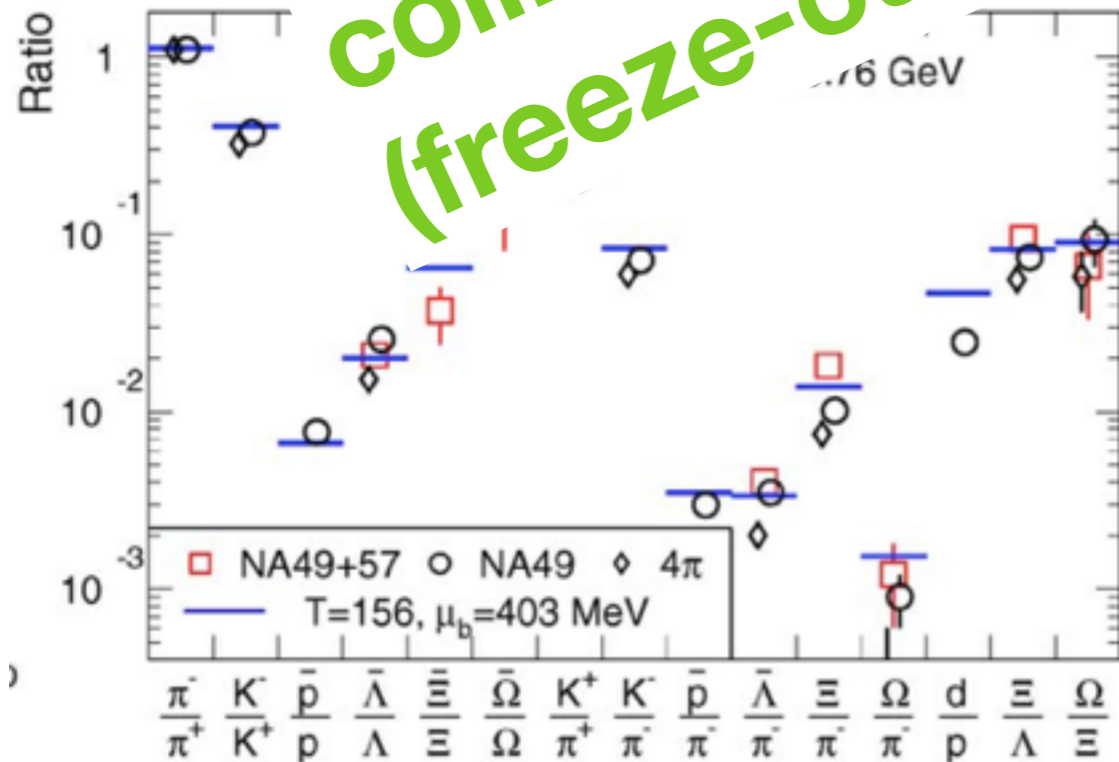
Hadron yields and thermal statistical model



$$n_i = N_i/V = -\frac{T}{V} \frac{\partial \ln Z_i}{\partial \mu} = \frac{g_i}{2\pi^2} \int_0^\infty \frac{p^2 dp}{\exp[(E_i - \mu_i)/T] \pm 1}$$

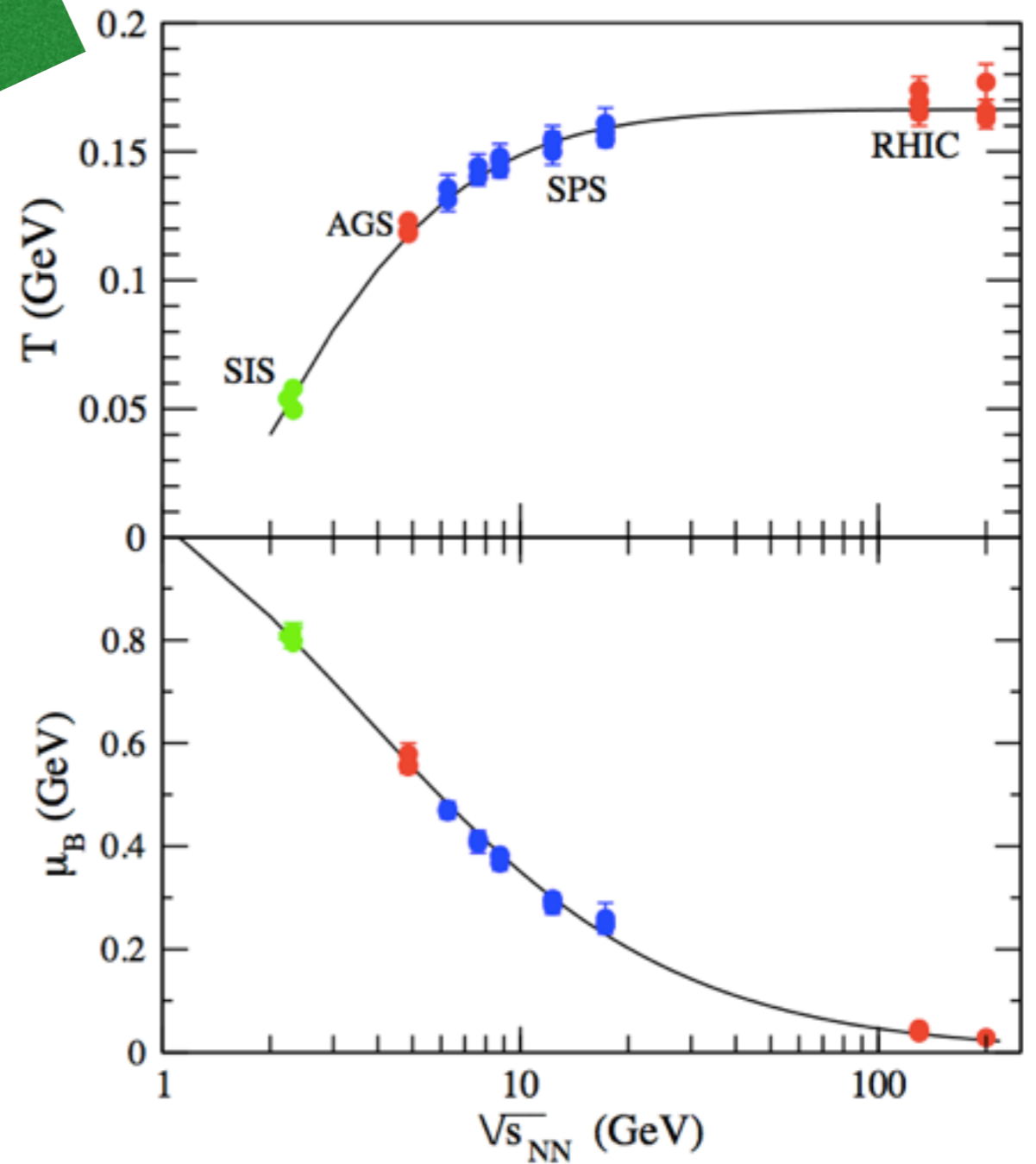
collision energy $\sim \mu, T$
(freeze-out parameters)

Andronic, et., al, (2005)



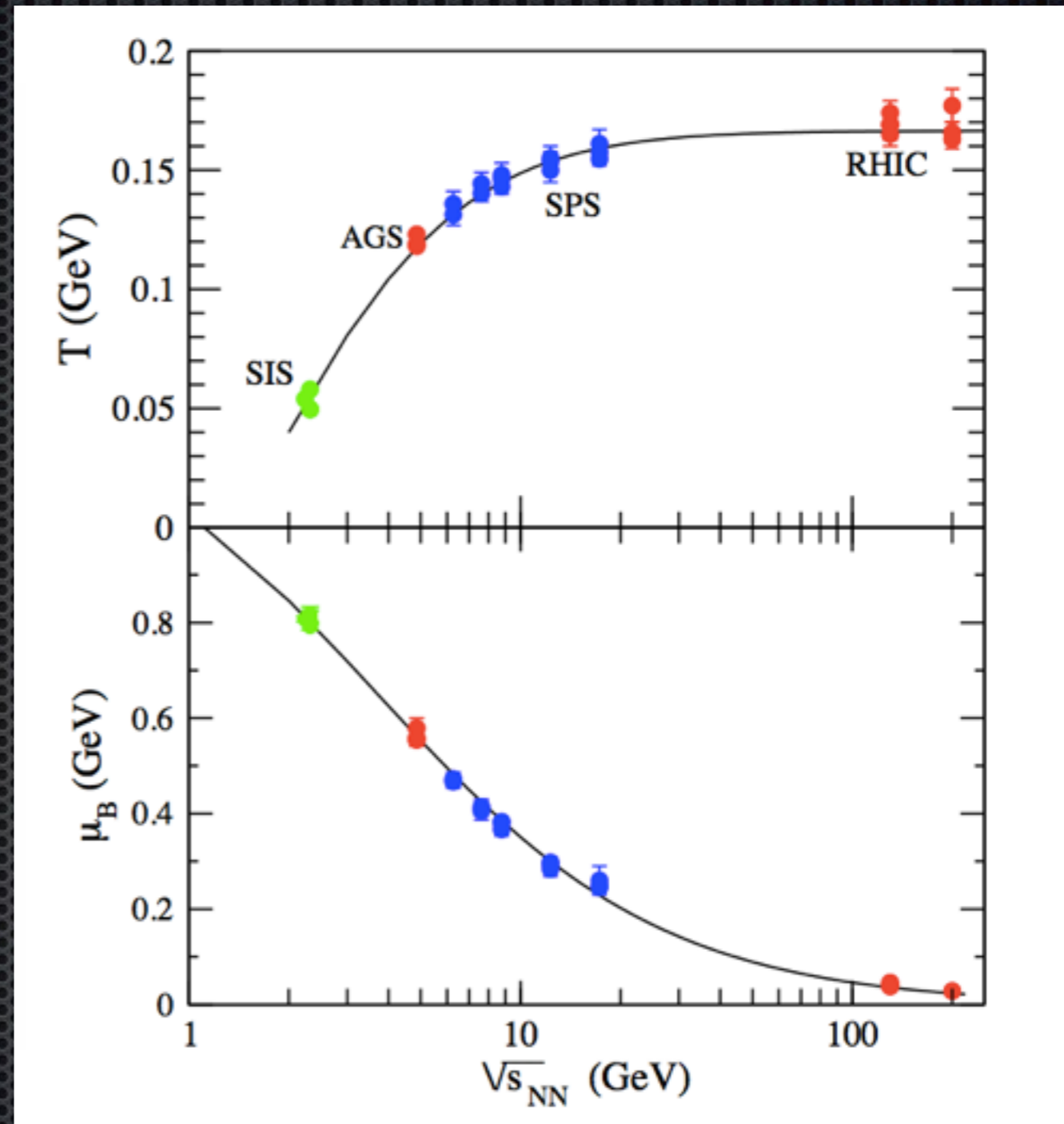
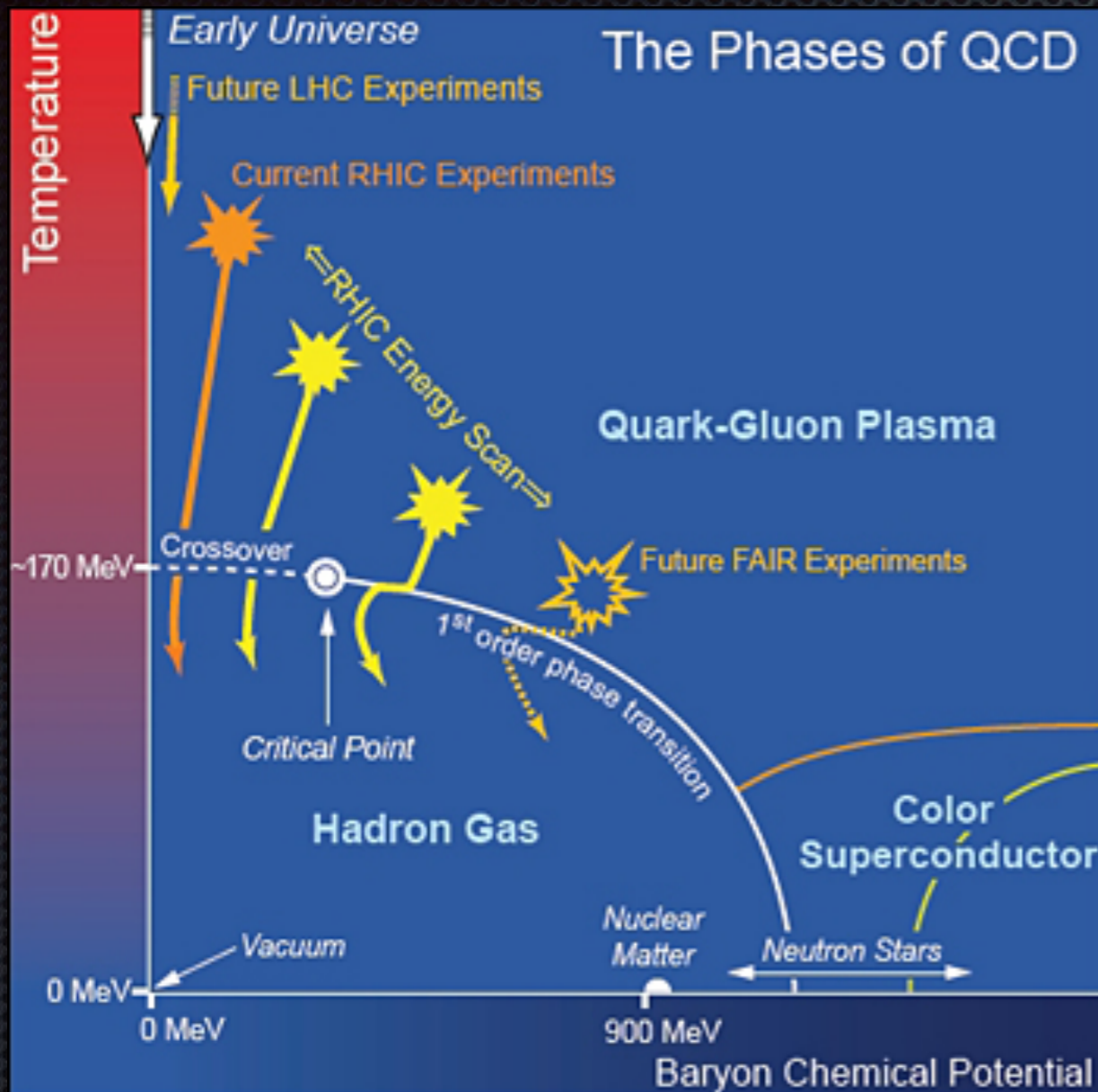
Energy dependence of freeze-out parameters

Freeze-out points are located on a line ~ freeze-out line



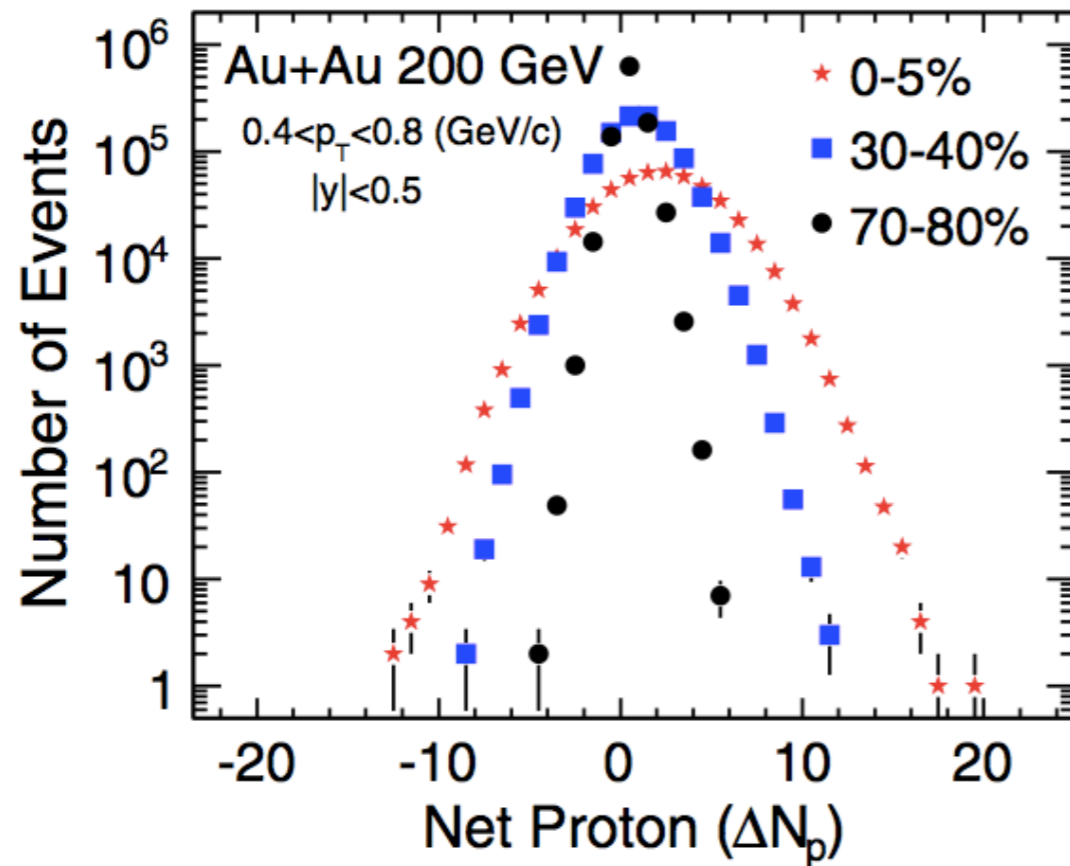
Cleymans et. al.

Energy dependence of freeze-out parameters



Cleymans et. al.

Fluctuation



Aggarwal et al. STAR,
PRL105, 022302('10)

Probability distribution for some hadrons are obtained. This is used to obtain event-by-event fluctuation at a freeze-out point.

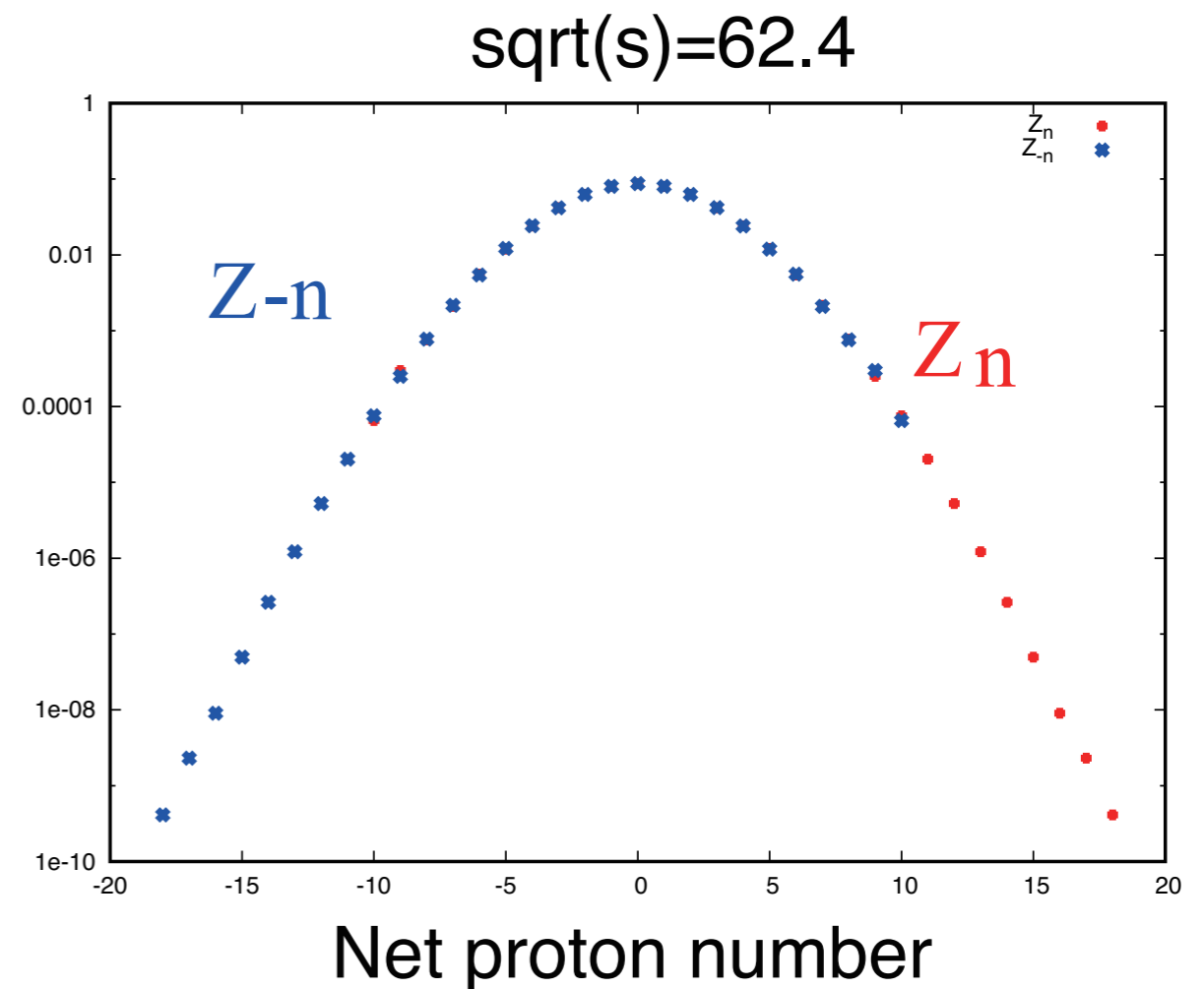
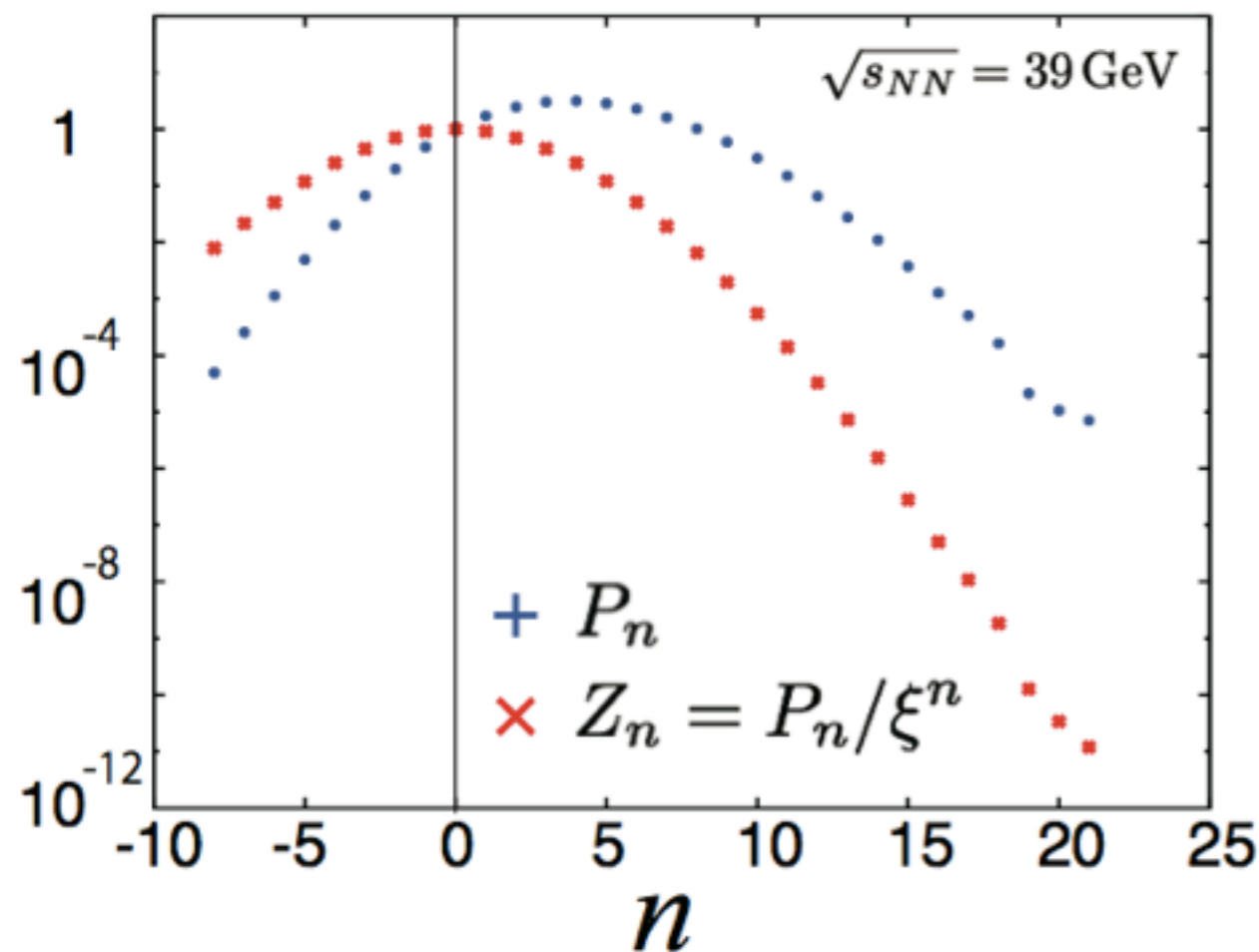
Extension of data to wide range of μ

The probability distribution of net baryon number

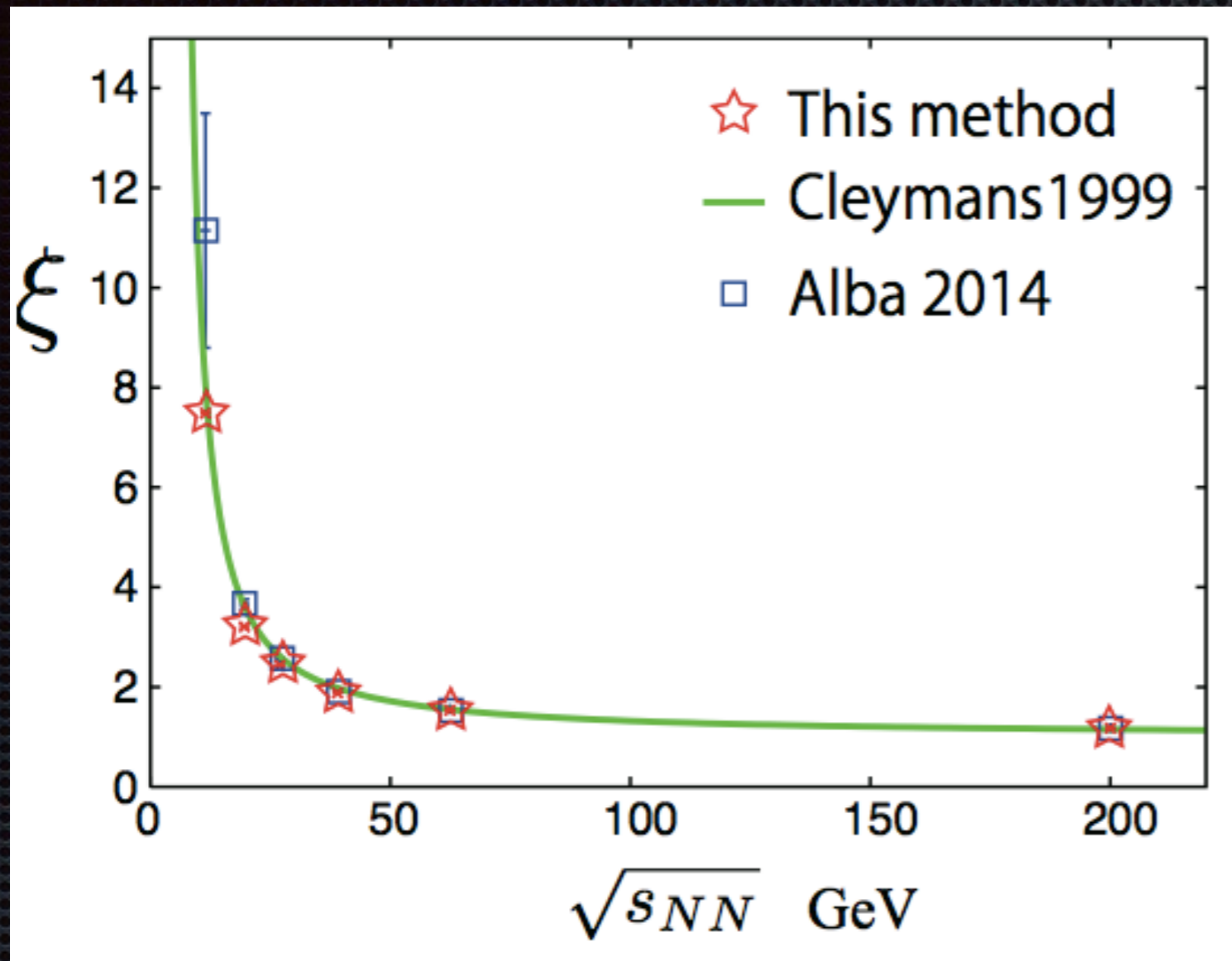
(here we use the proton number as an approximation)

$$P_n \propto Z_n e^{n\mu/T}$$

μ/T is determined from CP invariance : $Z(n) = Z(-n)$



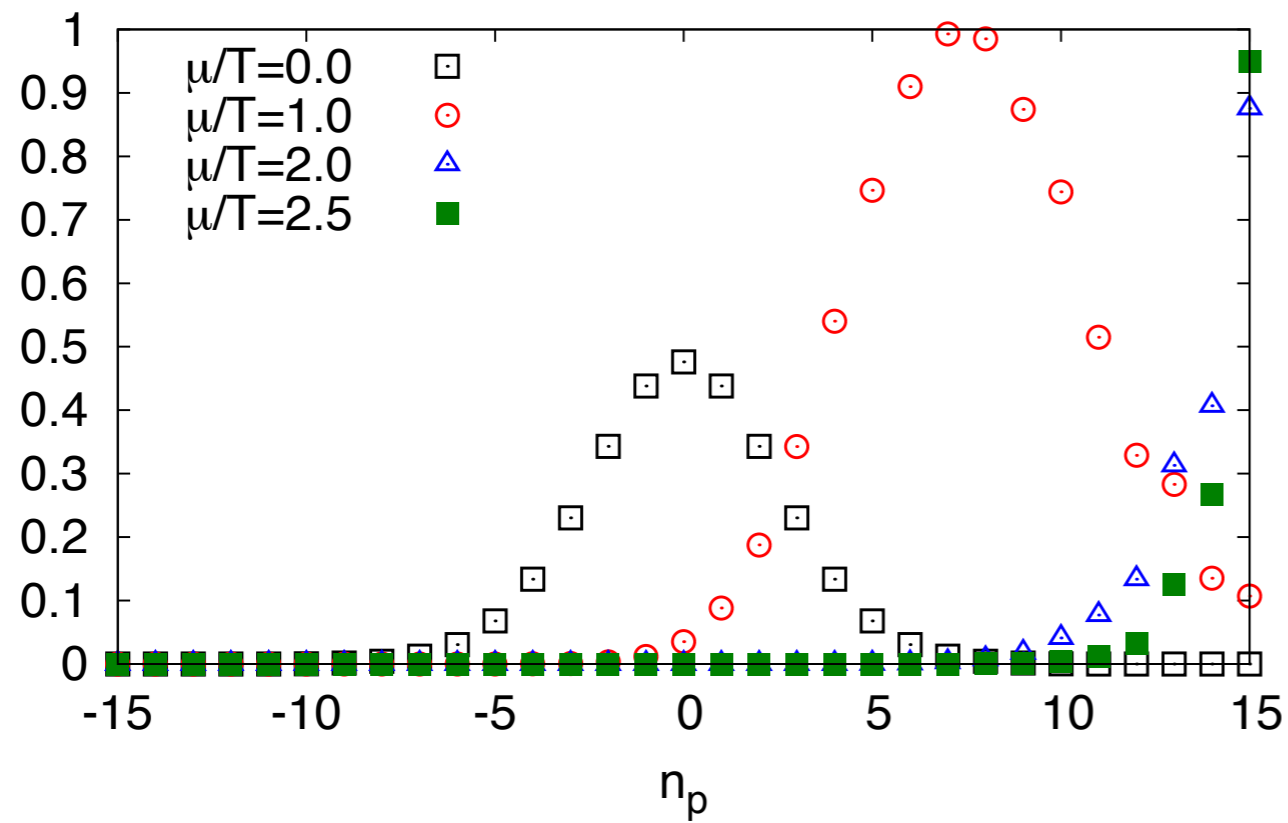
Extension of data to wide range of μ



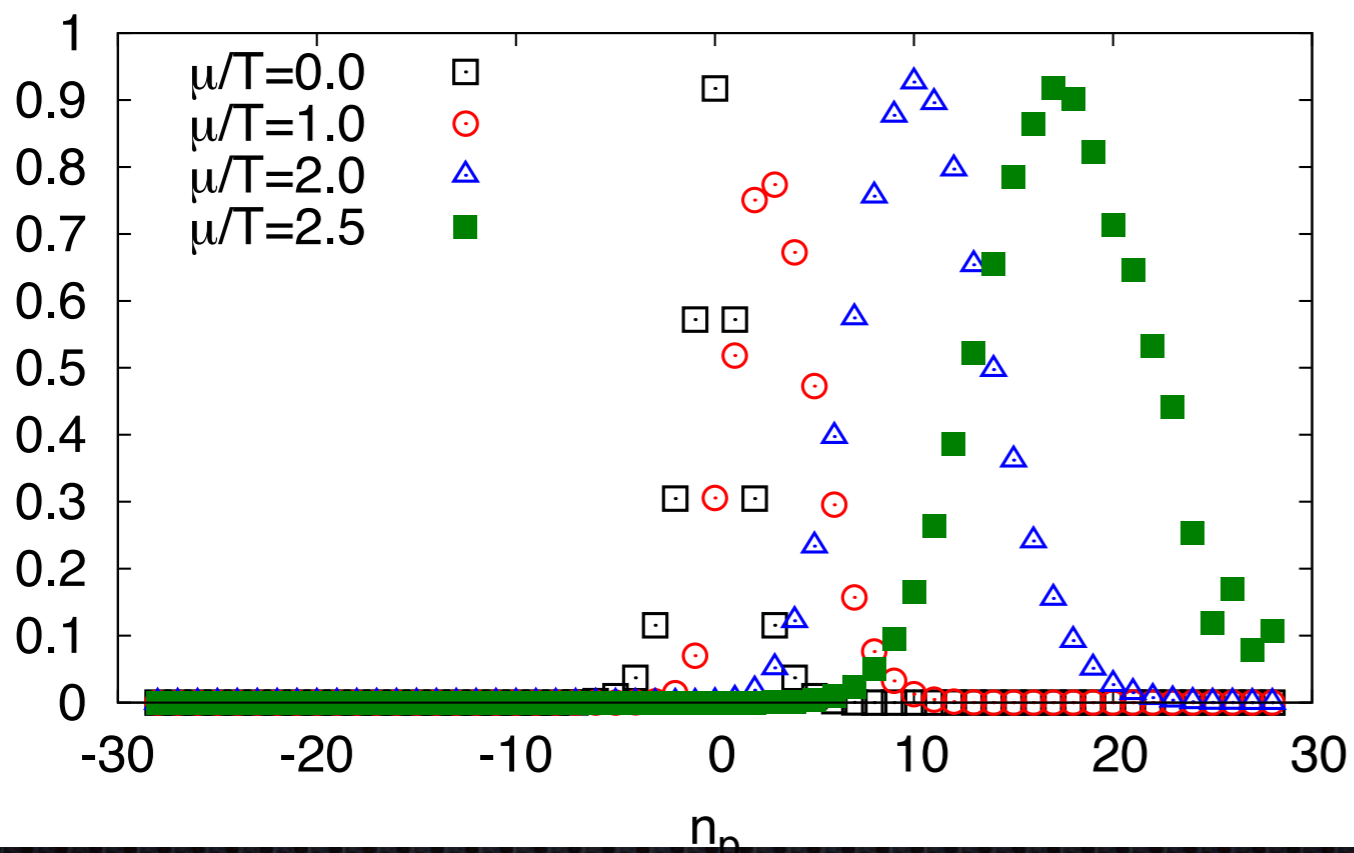
$$\xi = \exp(\mu/T)$$

- ✦ μ/T obtained from CP invariance agree with those obtained from thermal statistical model for wide range of collision energies.

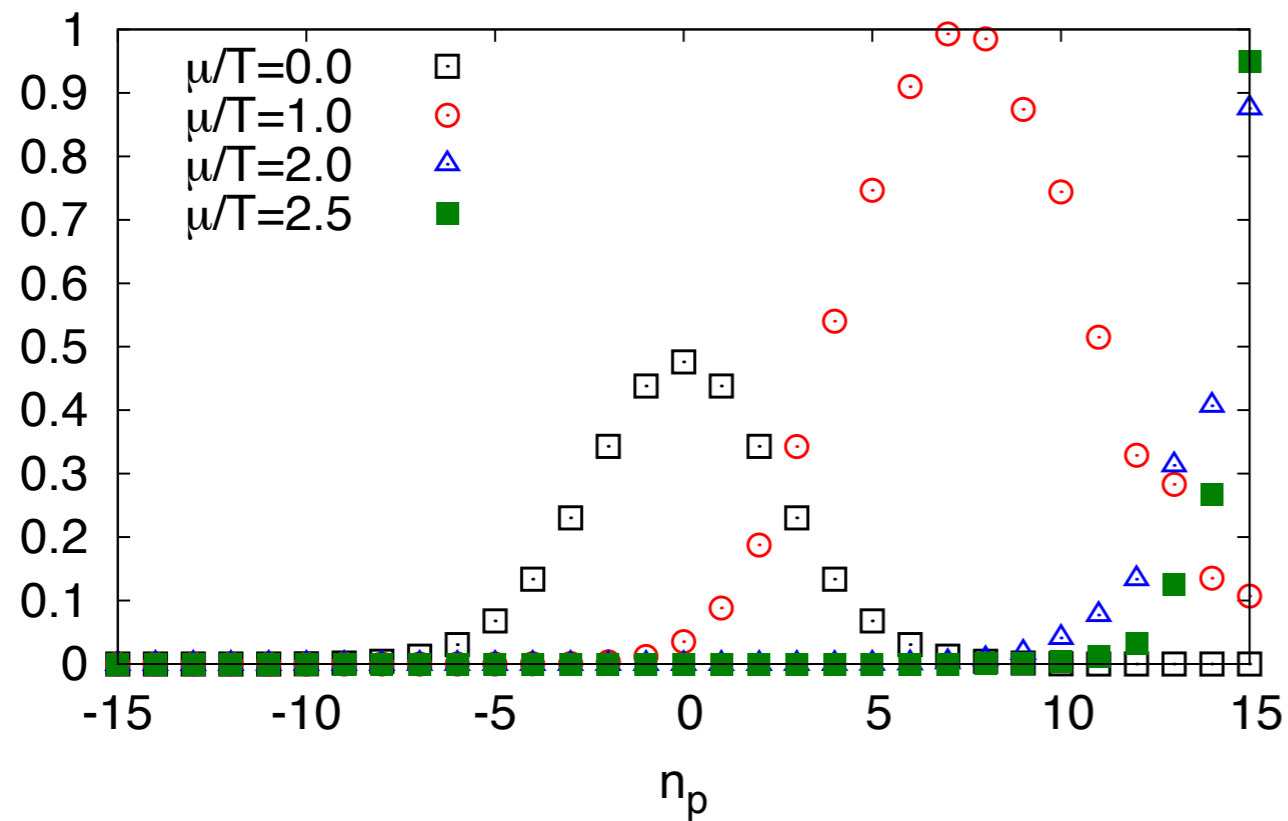
$Z(n_p) e^{n_p \mu/T}$, $\text{sqrts}_{NN}=200$



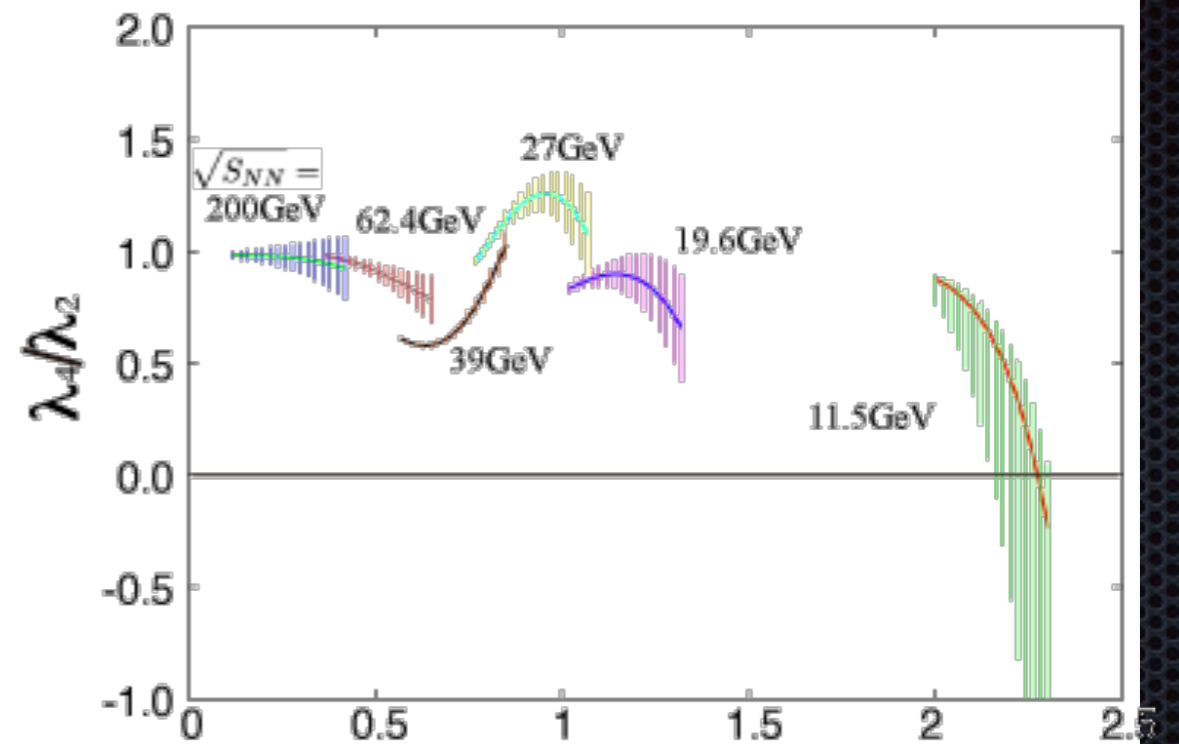
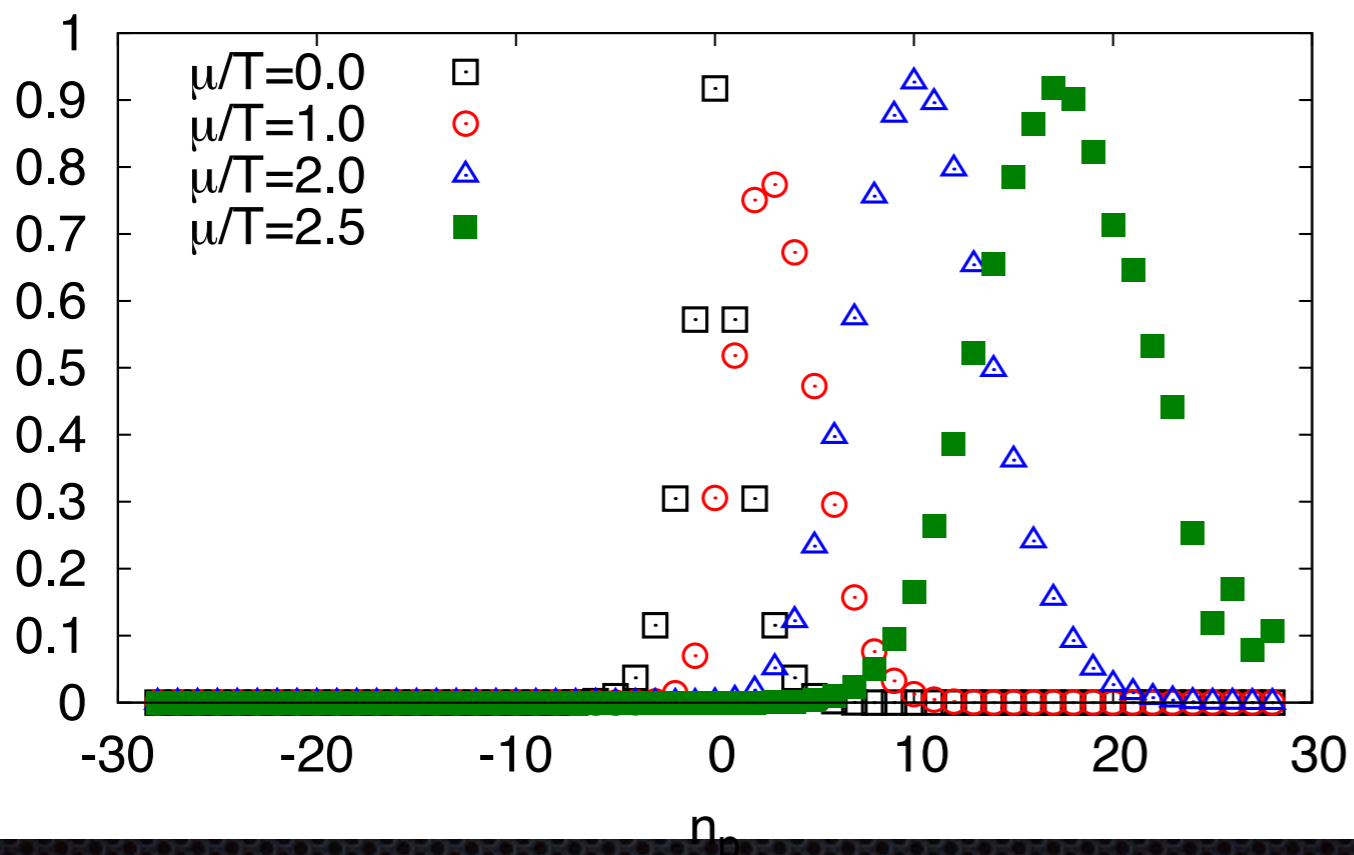
$Z(n_p) e^{n_p \mu/T}$, $\text{sqrts}_{NN}=11.5$



$Z(n_p) e^{n_p \mu/T}$, $\sqrt{s_{NN}}=200$



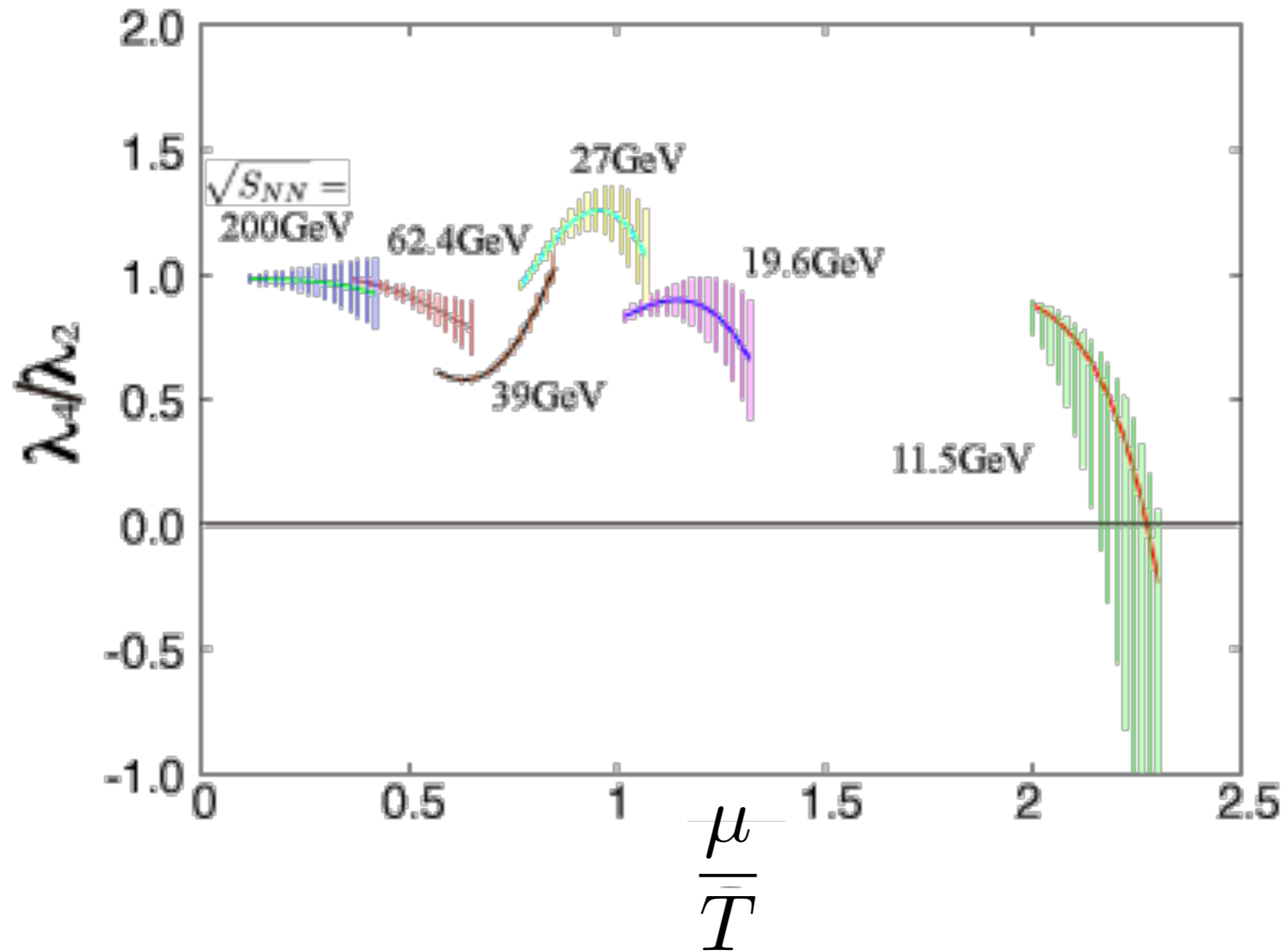
$Z(n_p) e^{n_p \mu/T}$, $\sqrt{s_{NN}}=11.5$



$$\lambda_n \propto (\partial/\partial\mu)^n \ln Z(\mu)$$

RHIC Data

Kurtosis $\frac{\lambda_4}{\lambda_2}$ as a function of $\frac{\mu}{T}$

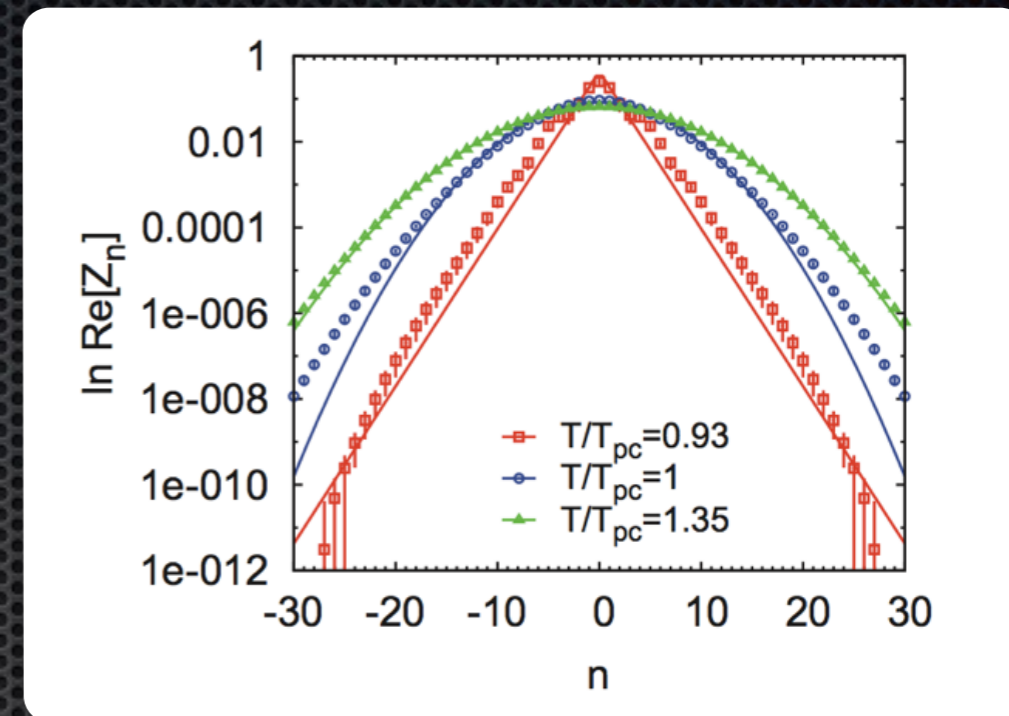


Buck up slides

How to achieve LY zeros ?

- Calculation of Z_n : truncation is inevitable

$$Z(\mu) = \sum_{n=-\infty}^{\infty} Z_n e^{n\mu/T}$$
$$\rightarrow \sum_{n=-n_0}^{n_0} Z_n e^{n\mu/T}$$



Calculation of Lee-Yang zeros

Lee-Yang零点を2通りの方法で計算します。

- Zeros of the fugacity polynomial

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

- Cancellation of the free energy

$$Z = e^{-V f_I/T} + e^{-V f_{II}/T}$$

1. Cancellation of free-energy

Free energy is different in different RW phases

- RW phases are distinguished by the argument of Pol.
- The $\arg(\text{Pol})$ is translated into A_4 .

$$\mathcal{L}_4 = \bar{\psi}(\gamma_4(igA_4 + \mu))\psi$$

$$\mu \rightarrow \mu + igA_4 = \mu + i\omega T$$

- This modifies the free energy as

$$f_{\text{I}} = -T^4(c_0 + c_2(\mu/T)^2 + c_4(\mu/T)^4),$$

$$f_{\text{II}} = -T^4(c_0 + c_2(\mu'/T)^2 + c_4(\mu'/T)^4), \mu' = \mu + i\omega T$$

$$\mu, \mu' \in \mathbb{C}$$

1. Cancellation of free-energy

Cancellation of two types of free energy allows $Z=0$

- Cancellation of free energies [Biskup et al('01)]

$$Z = e^{-V f_I/T} + e^{-V f_{II}/T}$$

$$\begin{cases} \operatorname{Re}[f_I - f_{II}] = 0 \\ \frac{V}{T} \operatorname{Im}[f_I - f_{II}] = (2k - 1)\pi, (k \in \mathbb{Z}) \end{cases}$$

- Approximate solution for $c_2 \gg c_4$

$$(\mu_R, \mu_I) = \left(\frac{3(2k - 1)}{4VT^3 c_2}, -\pi/3 \right)$$

- Possible to solve it with c_4
- f_I and f_{III} , and f_{II} and f_{III} .

2. Zeros of the fugacity polynomial

We show that the fugacity polynomial of high T QCD is well approximated by a well-known polynomial.

$$Z(\mu) = \sum_{n=-N}^N Z_n e^{n\mu/T}$$

- ✦ **We need Z_n . : Fourier integral with the free energy as input (analytic)**
- ✦ **(We use the fugacity expansion in lattice simulation.)**

First, we derive Z_n using the Fourier transformation.

$$Z(\mu) = \sum_{n=-N}^N Z_n e^{n\mu/T}$$

Z_n from the Fourier transformation

$$Z_n = \int Z(\theta) e^{in\theta} d\theta, \quad \mu/T = i\theta, (\theta \in \mathbb{R})$$

$$f = -\frac{T}{V} \ln Z(\mu)$$

- We use the quartic form of $f(\mu)$ as input.
- $f(\mu)$ is obtained for real μ . On the other hand, the Fourier integral requires complex μ .

Next, we use the RW periodicity

$$Z_n = \int Z(\theta) e^{in\theta} d\theta, \quad \mu/T = i\theta, \quad (\theta \in \mathbb{R})$$

We decompose the integral into three domains.

$$Z_n = \int_{-\pi/3}^{\pi/3} e^{-Vf(\theta)/T} e^{in\theta} \frac{d\theta}{2\pi} + \int_{\pi/3}^{\pi} e^{-Vf(\theta-2\pi/3)/T} e^{in\theta} \frac{d\theta}{2\pi} \\ + \int_{\pi}^{5\pi/3} e^{-Vf(\theta-4\pi/3)/T} e^{in\theta} \frac{d\theta}{2\pi},$$

Shift of θ leads to

$$Z_n = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} e^{-Vf(\theta)/T} e^{in\theta} d\theta, \quad n \equiv 0 \pmod{3}$$

(This relation holds for any temperature, regardless of the RW phase transition)

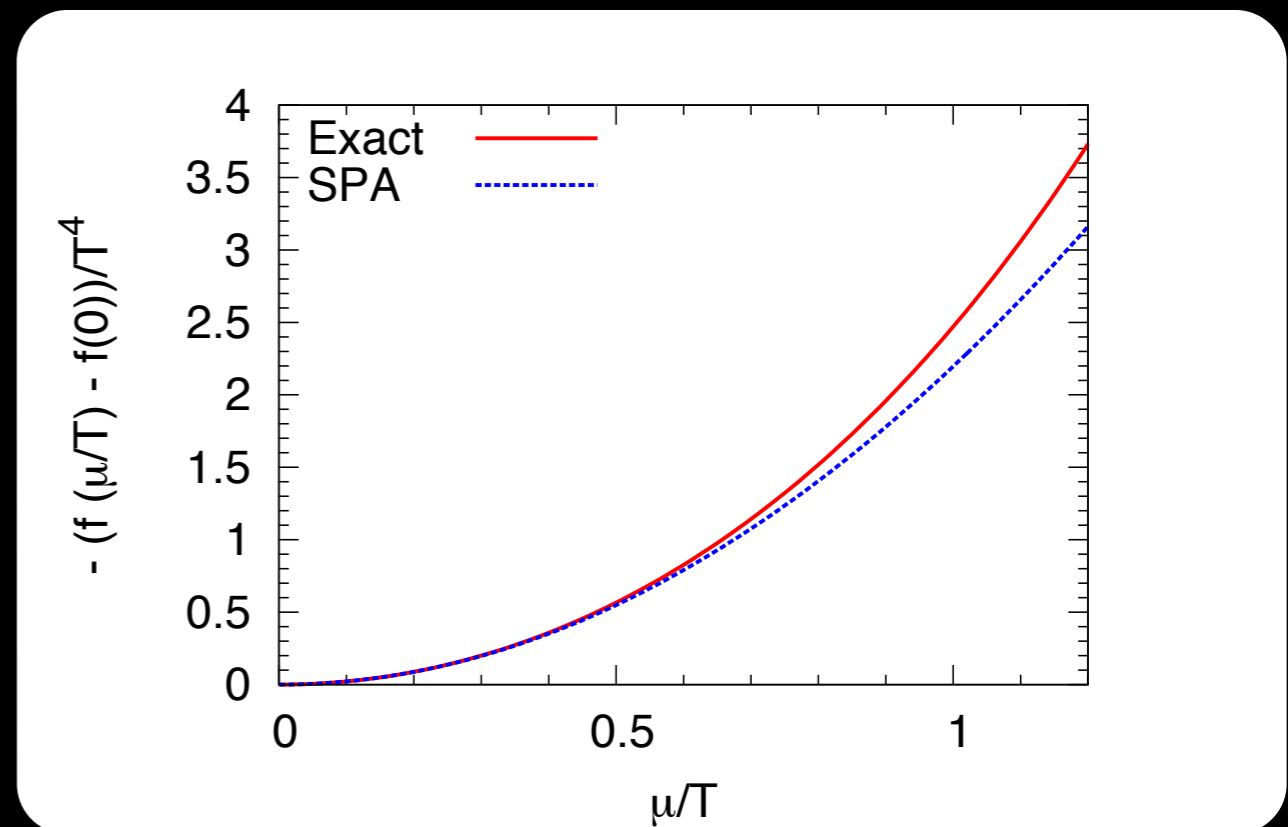
Now, we use the quartic expression of $f(\mu)$ and SPA

$$Z_n = \frac{3}{2\pi} \int_{-\pi/3}^{\pi/3} e^{VT^3(c_0 - c_2\theta^2 + c_4\theta^4)} e^{in\theta} d\theta, \quad n \equiv 0 \pmod{3}$$

At $T/T_c > 1.1 \sim 1.2$, $c_2/c_4 \sim 10$. We use the saddle point approximation.

$$Z_n = C e^{-n^2/(4T^3 V c_2)}, \quad (n \equiv 0 \pmod{3})$$

- ✦ We assume the Gaussian Z_n is valid for large n .
- ✦ SPA is valid for small $\text{Re}[\mu]$



If Z_n is Gaussian, then $Z(\mu)$ is a Jacobi-theta function.

$$Z(\mu) = C \sum_{n_B=-\infty}^{\infty} e^{-9n_B^2 / (4T^3 V c_2) + 3n_B \mu / T}$$

Theta function

$$\vartheta(z, \tau) = \sum_{n=-\infty}^{\infty} e^{-\pi i n^2 \tau + 2\pi i n z}$$

$$\begin{aligned} i\pi\tau &= 9 / (4T^3 V c_2), \\ 2\pi i z &= 3\mu / T \end{aligned}$$

Zeros of theta function

$$\vartheta(z, \tau) = 0 \Leftrightarrow z = l + k\tau + \frac{1}{2} + \frac{\tau}{2}, (k, l \in \mathbb{Z})$$

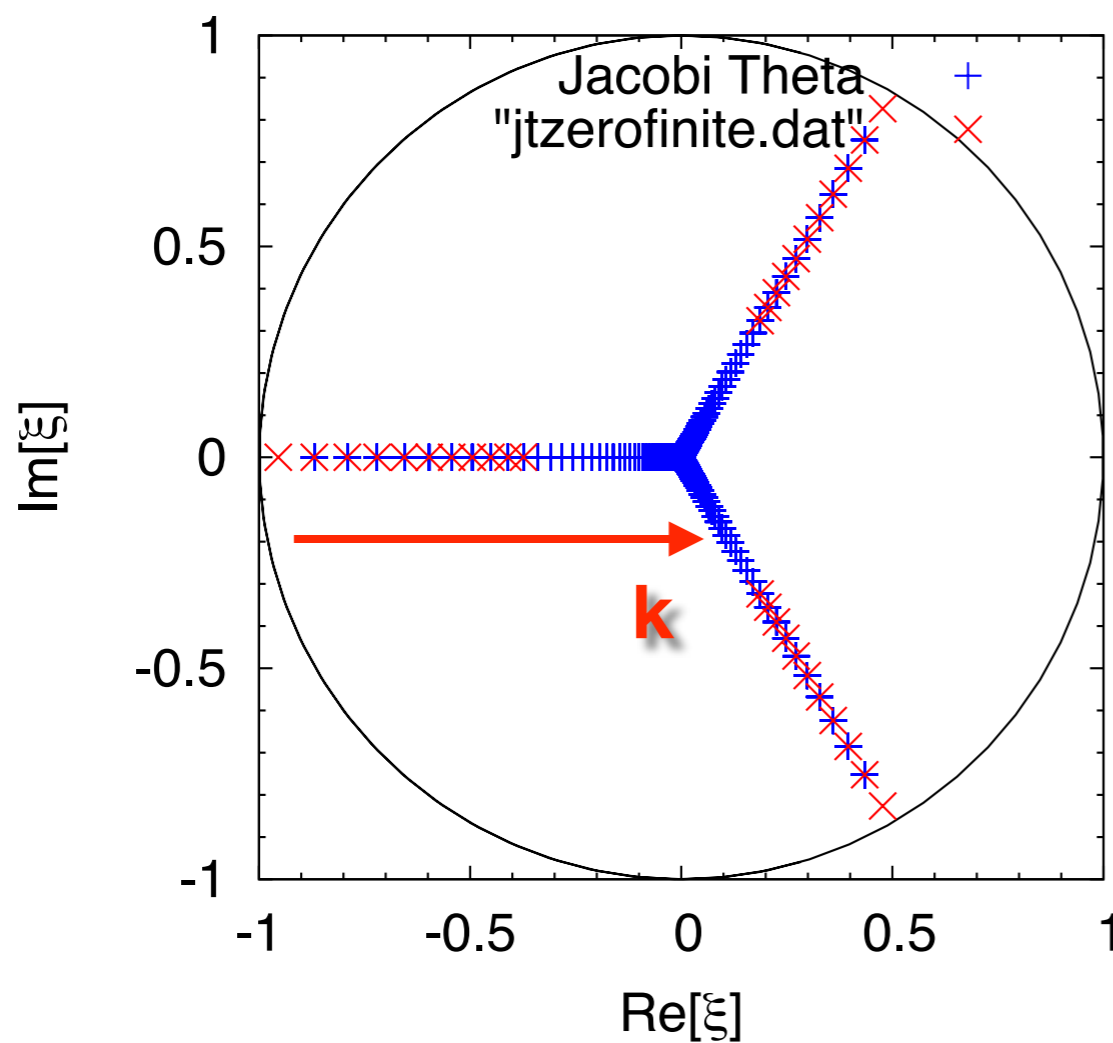
$$\frac{\mu}{T} = \frac{(2l + 1)\pi i}{3} - \frac{3(2k + 1)}{4VT^3 c_2}$$

$$(\mu_R, \mu_I) = \left(\frac{3(2k - 1)}{4VT^3 c_2}, -\pi/3 \right)$$

Method1

Lee-Yang zero distribution of theta function

$$\frac{\mu}{T} = \frac{(2l+1)\pi i}{3} - \frac{3(2k+1)}{4VT^3 c_2}$$



**Zeros approaches to the RW transition point as $1/N$.
Spacing of zeros is a prediction**

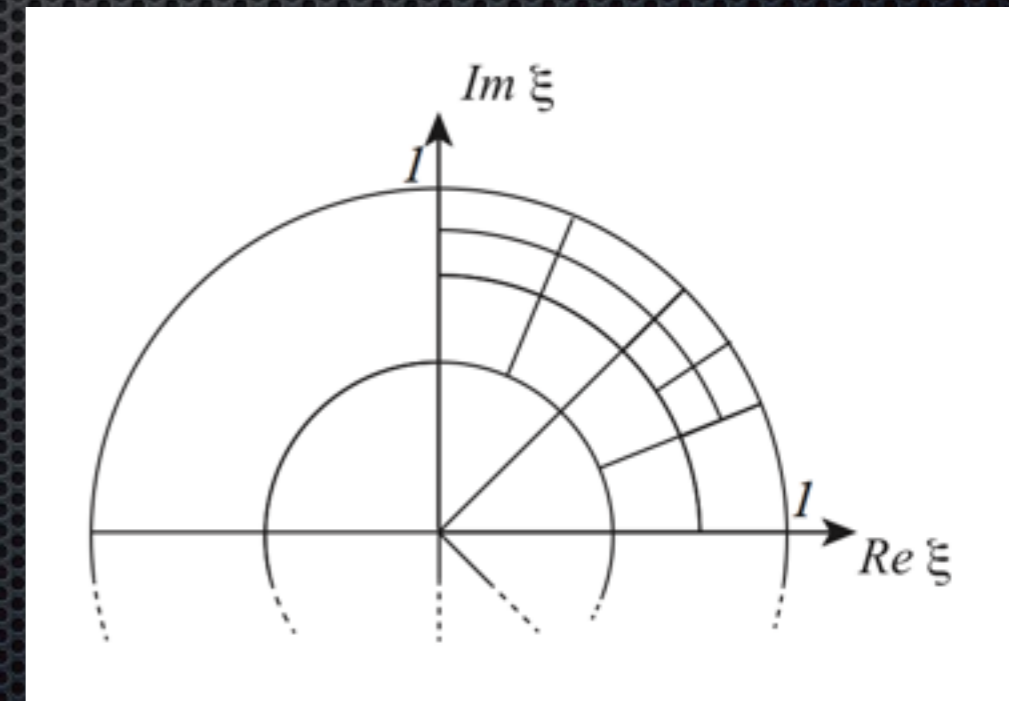
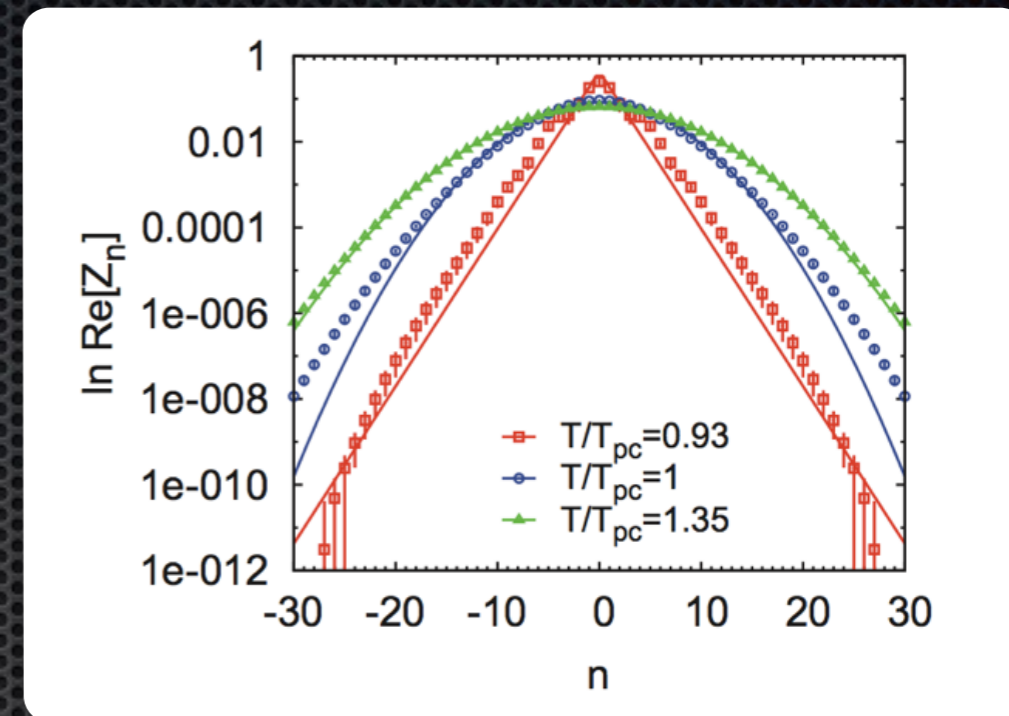
How to achieve LY zeros ?

- Calculation of Z_n : truncation is inevitable

$$Z(\mu) = \sum_{n=-\infty}^{\infty} Z_n e^{n\mu/T}$$
$$\rightarrow \sum_{n=-n_0}^{n_0} Z_n e^{n\mu/T}$$

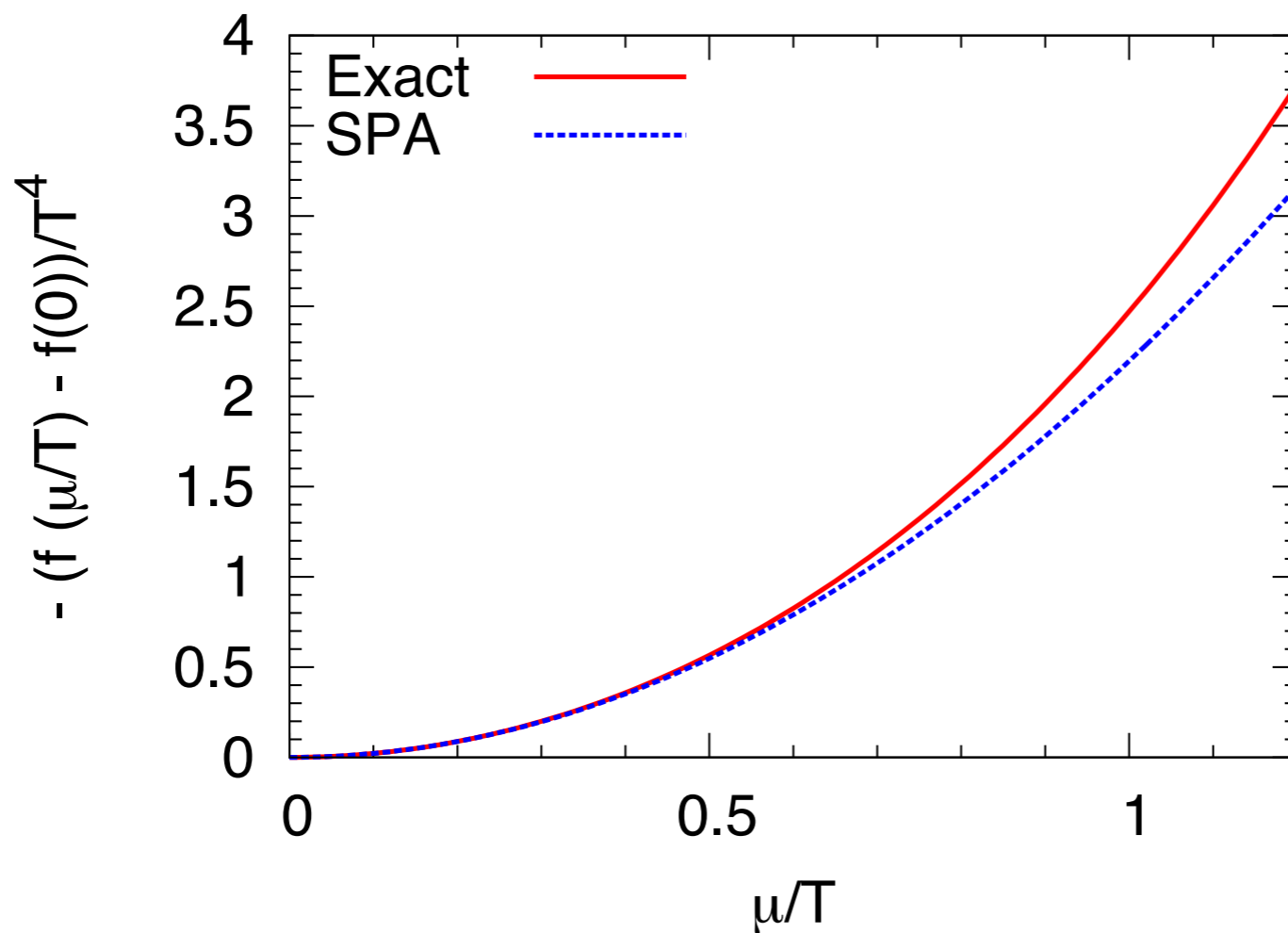
- Cauchy integral + recursive division + multi-precision arithmetic

$$Z(\mu) = \sum Z_n e^{n\mu/T} \rightarrow \prod (1 - \xi/\xi_i)$$

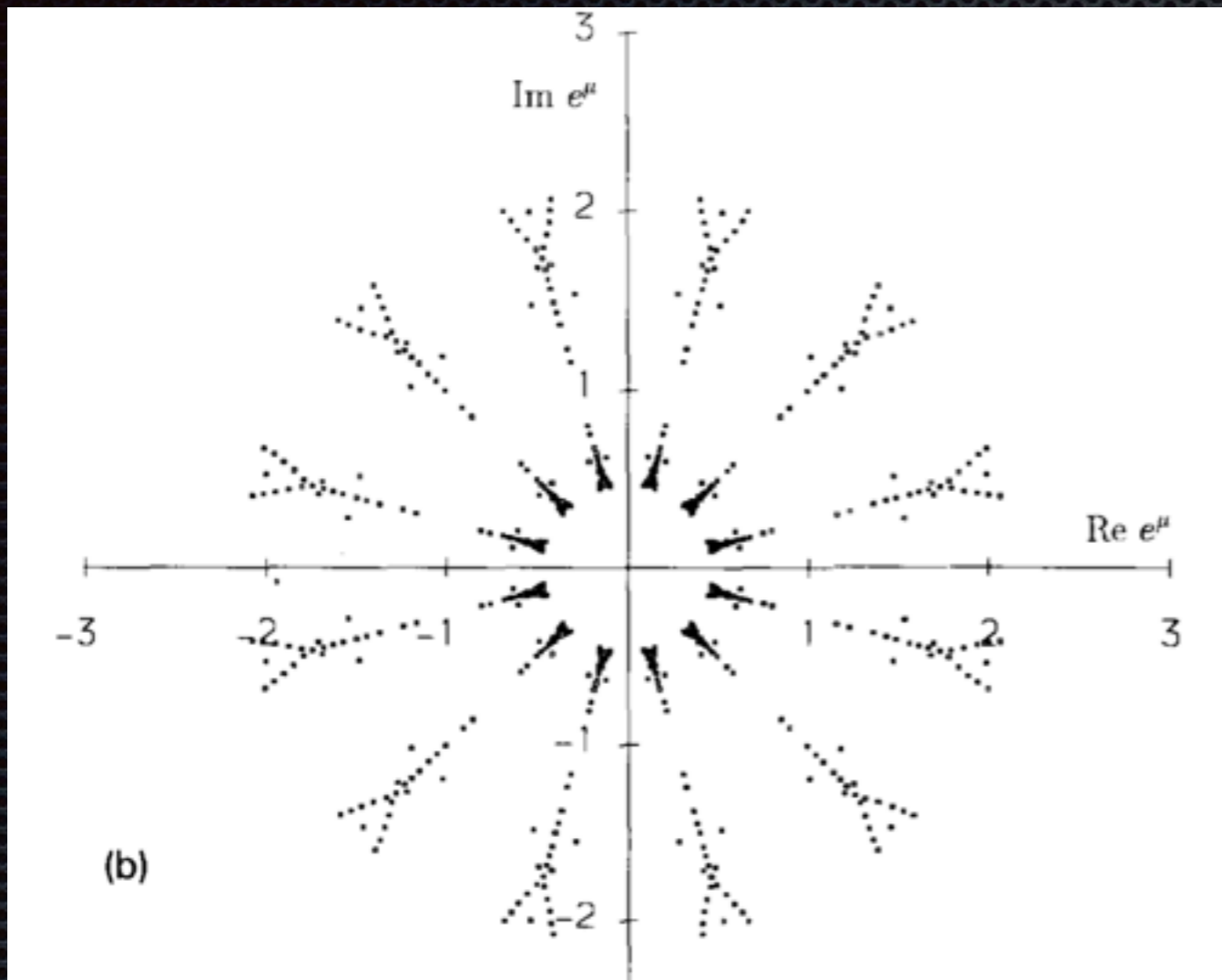


Validity of SPA

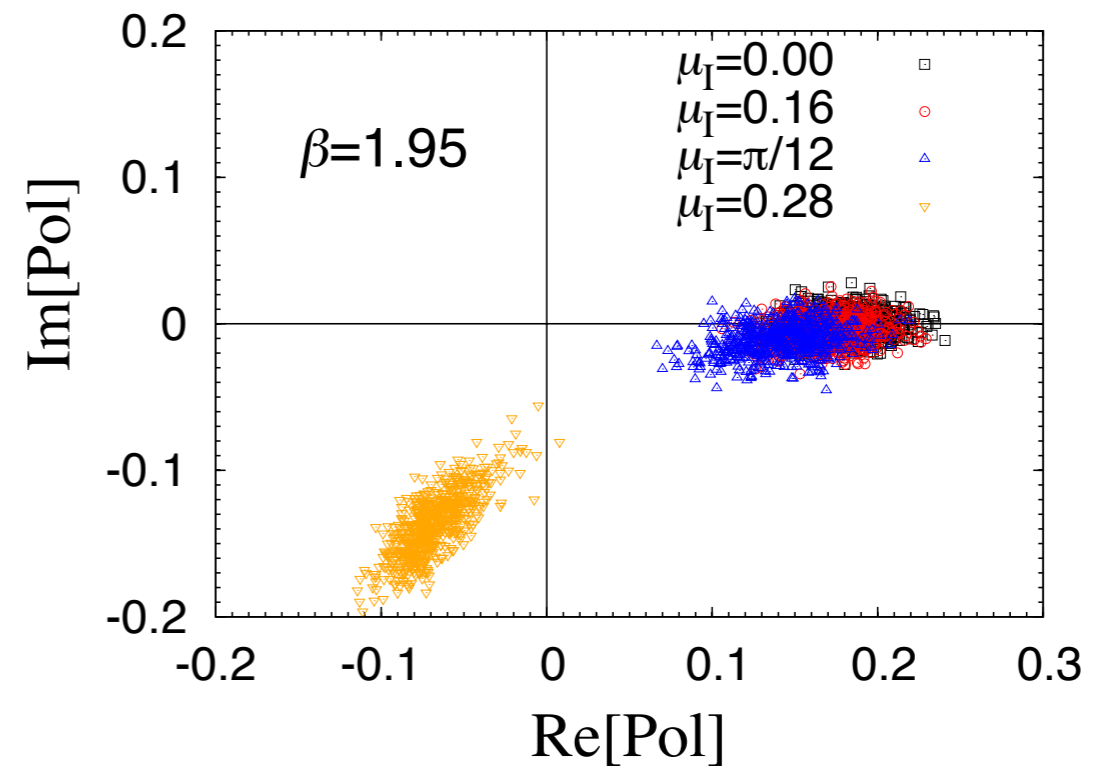
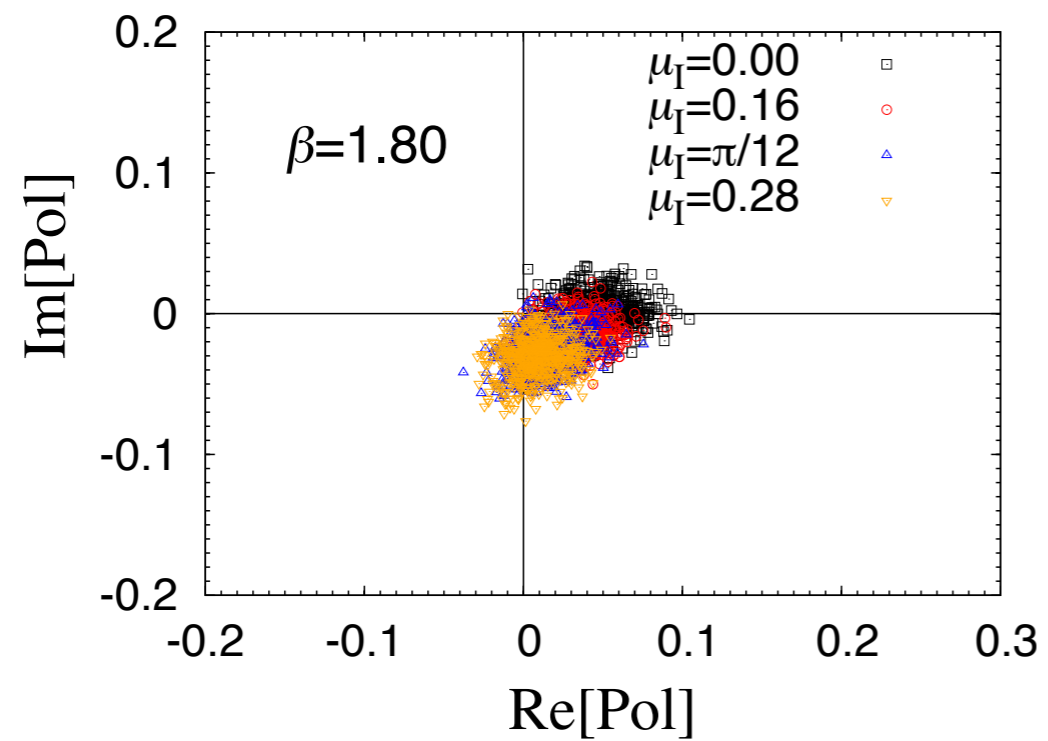
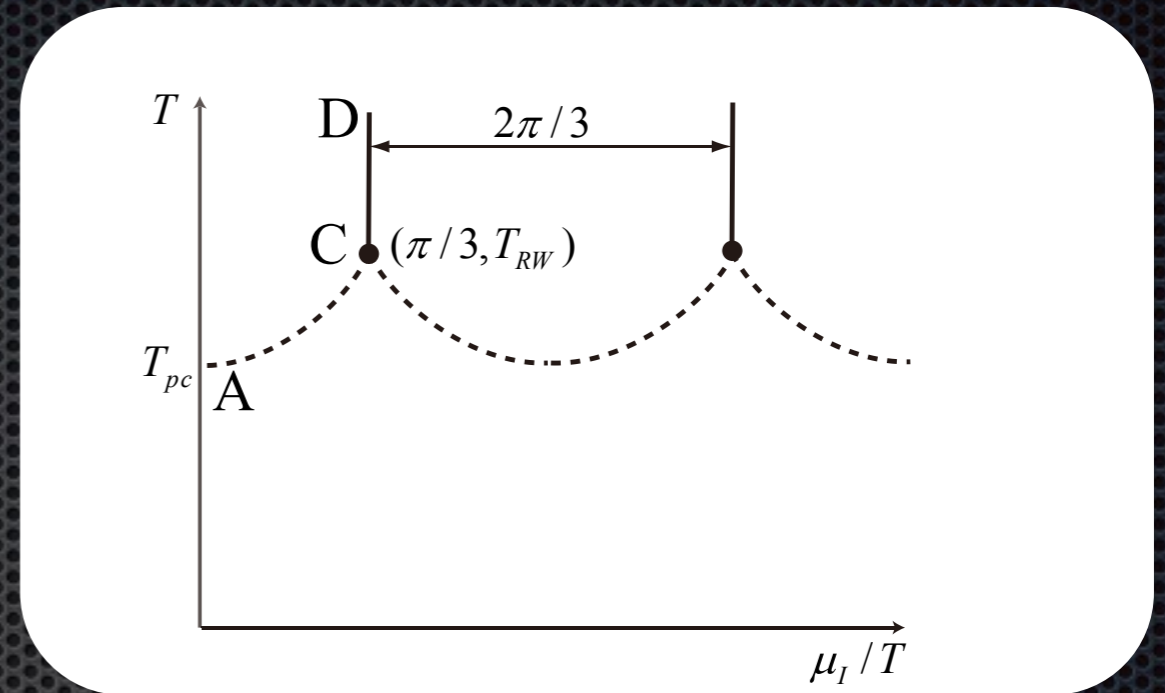
$$Z(\mu) = C \sum e^{-9n^2 / (4VT^3 c_2) + 3n\mu/T}$$
$$= C\vartheta(z, \tau)$$



Lee-Yang zeros - 20 years

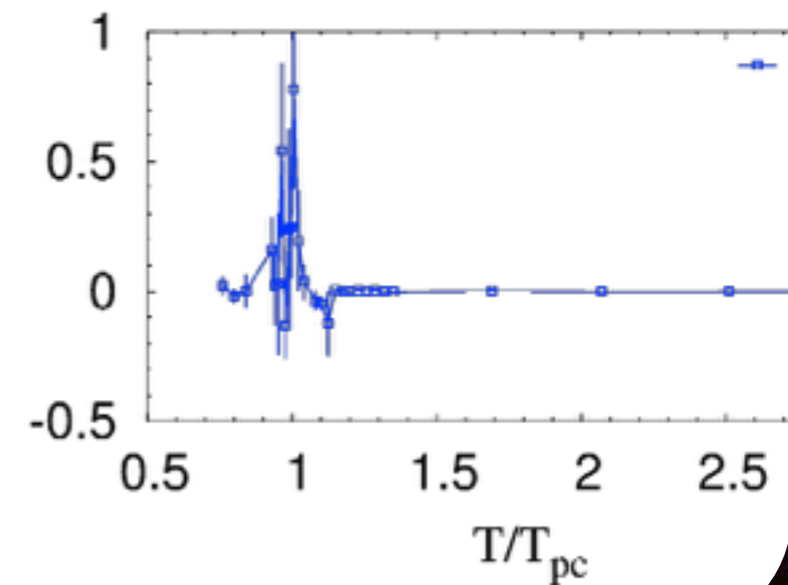
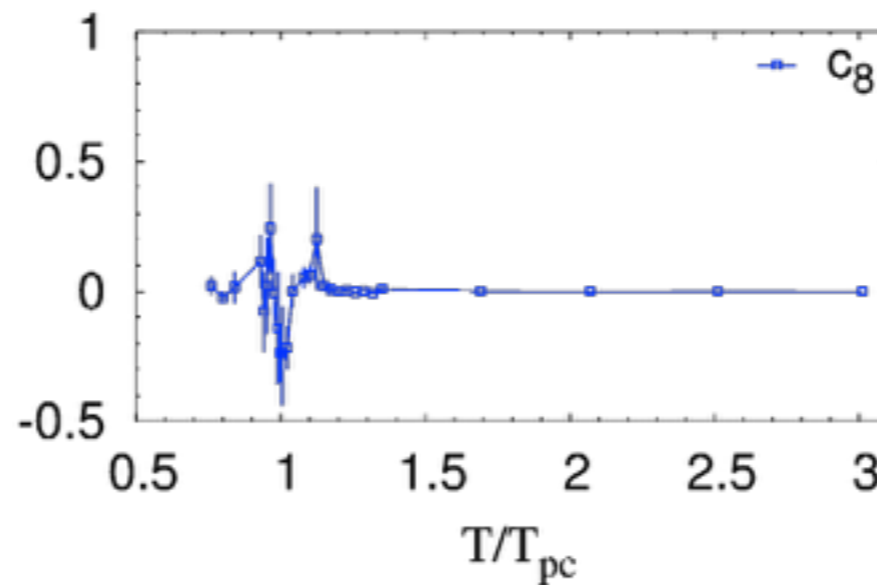
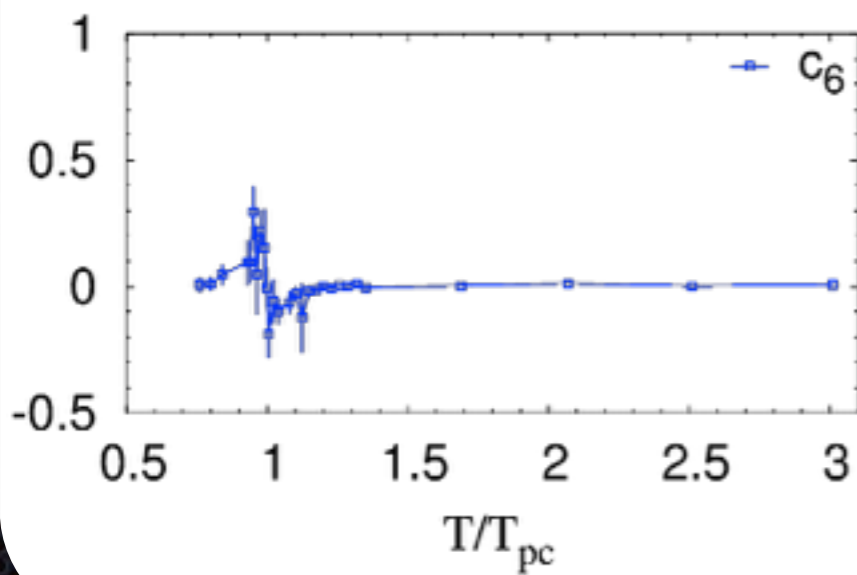
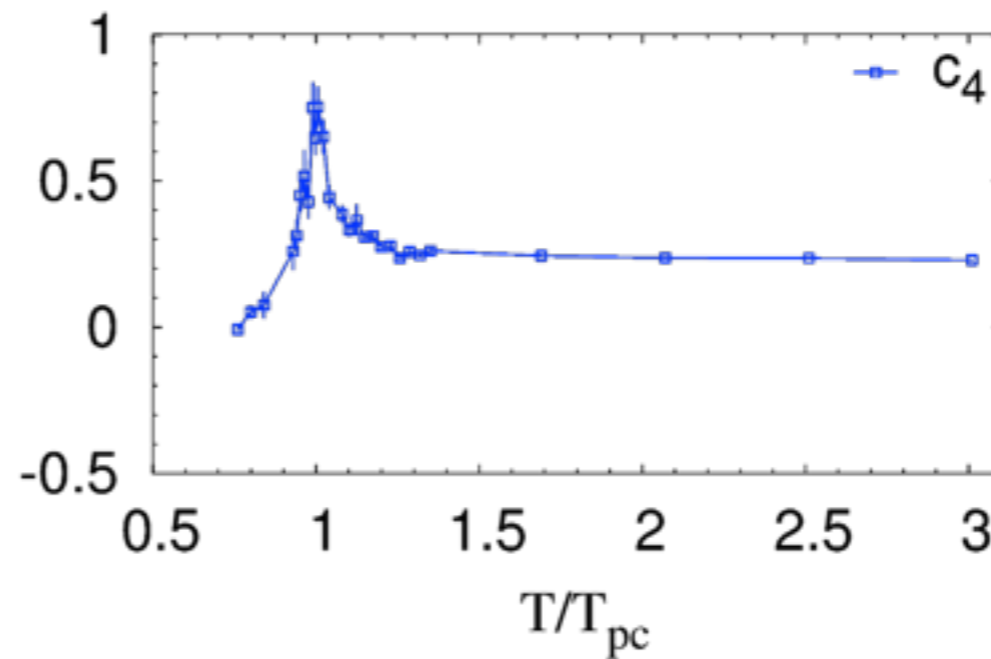
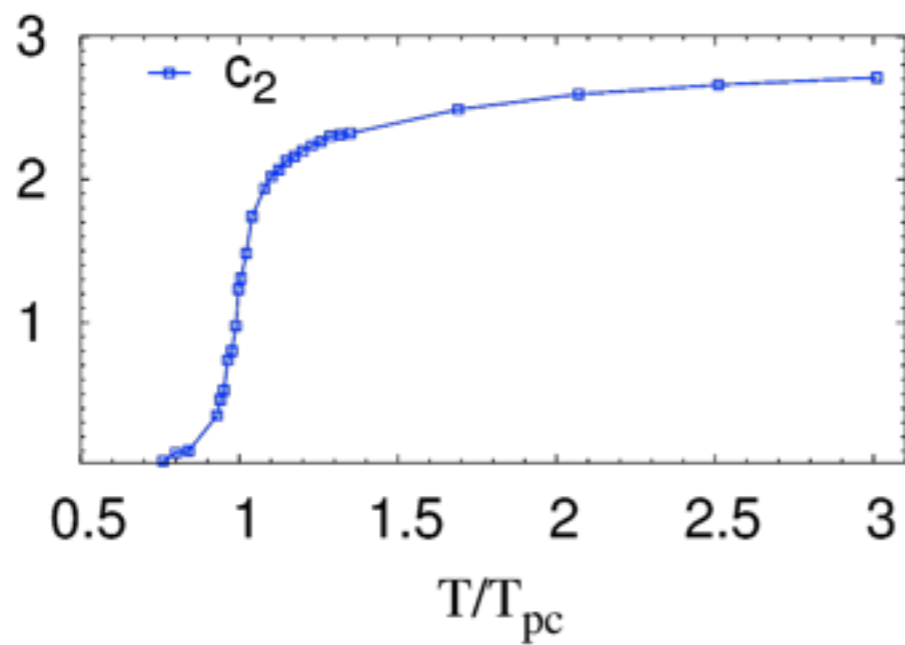


RW periodicity & phase transition



Taylor coefficients of free energy

$$-\frac{f}{T^4} = \sum_{n=0} c_{2n} (\mu/T)^{2n}$$

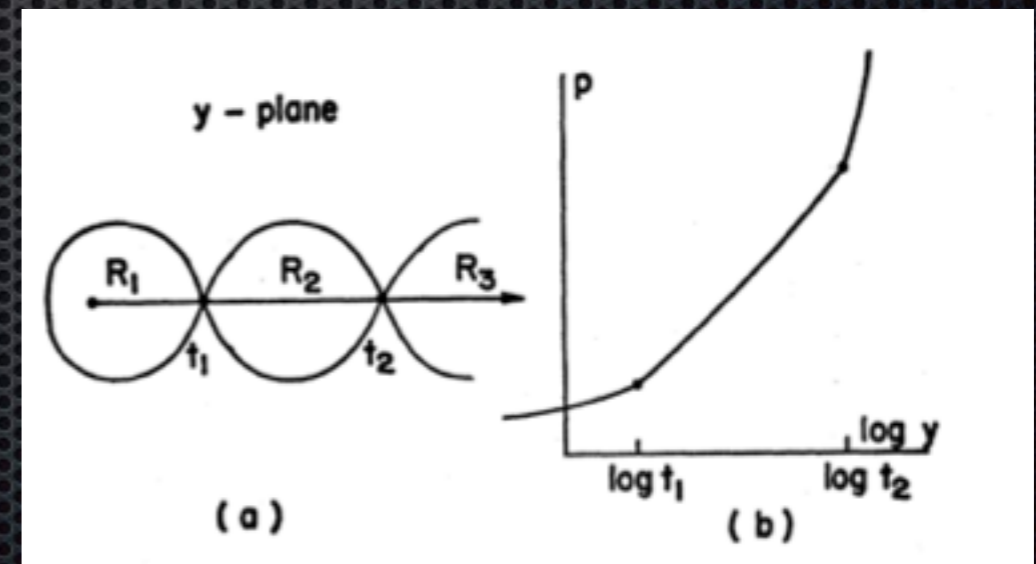
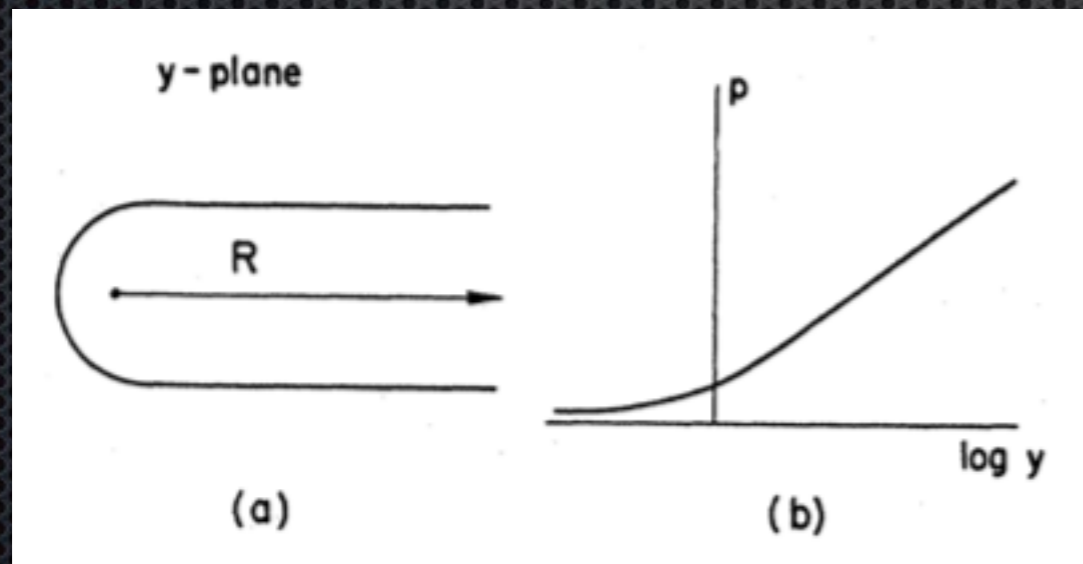


Lee-Yang zeros : from CPF to Phase transition

- Lee-Yang zeros [Lee & Yang 1952]

$$Z(\mu) = \sum Z_n e^{n\mu/T}$$
$$\propto \prod (1 - \xi/\xi_i)$$

- $Z(\mu) = 0$ is an origin of a thermodynamic non-analyticity



Convergence on the negative real axis

- **Infinite sum of higher order terms is bounded on the negative real axis.**

$$\begin{aligned} |Z(\mu) - \sum_{|n| < N} Z_n \xi^n| &= \left| \sum_{|n| \geq N} Z_n \xi^n \right| \\ &< |Z_N \xi^N| \end{aligned}$$

- c.f. Leibnitz's test for an alternating series

$$1/2 - 1/3 + 1/4 - 1/5 + 1/6 + \dots < 1/2$$