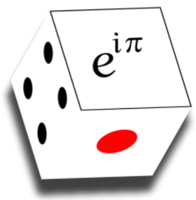
A Reduction Formula for Fermion Determinant



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in XQCD-J collaboration

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New Type of Fermions on Lattice,

2012/02/16 at YITP

Det (D) is a key in fd LQCD

- *Fermion determinant det D(mu)*
  - *chemical potential*
  - *sign problem*

- *Techinques in fdLQCD need the evaluation of det D(mu)*

- *Determinant calculation is heavy*
  - *Time O(N^3) for NxN matrix*
  - *Memory O(N^2)*

N. E. C. O.

An idea

- *There is a formula*
  - *to perform the temporal part of det D(mu) by hand*
  - *and reduce the rank of the determinant*

- *The rank of the determinant is reduced, and difficulty of the determinant evaluation is relaxed*
  - *CPU time and memory is suppressed ~ 1/Nt^2*

References

- *Derivation for Staggered type*
  - *Gibbs, PLB 172, 53 ('86). Hasenfratz &Toussaint, NPB371, 539('92).*
- *Derivation for Wilson type*

  –*Borici, PTP. Suppl. 153, 335 ('04). Alexandru &Wenger, PRD83, 034502 ('11). KN&AN, PRD82,094027 ('10).*
- *Derivation for continuum case*
  - *Adams, PRL92, 162002 ('04), PRD70, 045002 ('04).*
- *Application*

  – *reweighting : Glasgow group e.g., Barbour&Bell, Nucl.Phys. B372 (1992) 385-402. Fodor & Katz, JHEP 0203 (2002) 014.*

  – *canonical formalism : Hasenfratz &Toussaint('92). de Forcrand & Kratochivila, hep-lat/0509143.*

  –*Hadron spectrum. Fodor, Szabo & Toth, JHEP 0708, 092('07).*

  – *see also refs in KN&AN, PRD82,094027 ('10).*

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Basic concept of the reduction formula

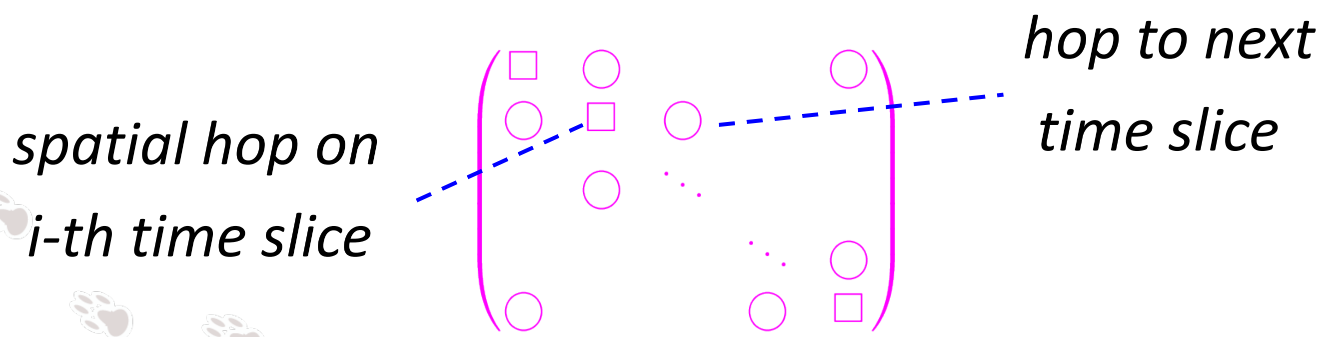
- *Fermion matrix as t-t matrix*
  - *spatial (diag), temporal (n.n + b.c)*
  - *temporal hop accompanies chemical potential*
- *Performing temporal determinant by hand*
  - *rank reduces to N/Nt (memory & CPU time ~1/Nt^2.)*
  - *det D is an analytic function of mu.*
- *Reduction formula*
  - *suppress CPU time and memory 1/Nt^2*
  - *provides an analytic form of mu-dependence*
- *Limitation*
  - *direct method is heavy*
  - *limited to small lattice size*

Focus on temporal part of quark action

$$\Delta(\mu) = I - \kappa(\text{spatial hop} + \text{clover})$$
$$- \kappa[e^{\mu a}(1-\gamma_4)U_4(x)\delta_{x',x+\hat{4}} + e^{-\mu a}(1+\gamma_4)U_4^+(x')\delta_{x',x-\hat{4}}]$$

- *Quark action as t-t matrix*
  - *temporal hop accompanies chemical potential*
  - *spatial (diag), temporal (n.n + b.c)*

$$\overline{\psi}\gamma^0\psi \to \overline{\psi}\gamma^4\psi$$



D(mu) in t-t matrix

Reduced matrix

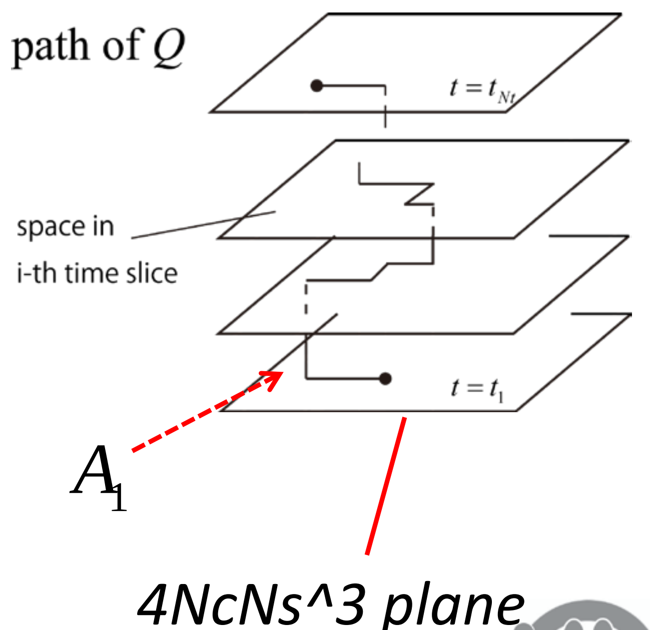
- *After calculating temporal part of determinant*

$$\det \Delta(\mu) = C_0 \xi^{-Nr} \det(Q + \xi),$$

$$Q \sim A_1 A_2 \cdots A_{Nt}$$

$$\xi = e^{-\mu/T} = e^{-\mu a N_t}$$

- *reduced matrix Q*
  — *propagation from a point at initial time to a point at final time*
  — *rank Nr= 4 Nc x Ns^3, (= full size/Nt)*
  — *independent of mu*
- *overall factor C0*
  — *spatial loops*
  — *independent of mu*



two expressions of det D(mu)

- *Calculating the eigenvalues of Q* $\det(Q - \lambda I) = 0$

$$\det\Delta(\mu) = C_0 \xi^{-Nr/2} \det(Q + \xi),$$

$$\det\Delta(\mu) = C_0 \xi^{-Nr/2} \prod_{n=1}^{Nr} (\lambda_n + \xi)$$

$$\begin{pmatrix} \lambda_1 + \xi & & & \\ & \lambda_2 + \xi & & \\ & & \ddots & \\ & & & \lambda_{N_r} + \xi \end{pmatrix}$$

Q : (Nr, Nr) matrix

Nr=4Nc Ns^3

- *Fugacity expansion*

$$\det\Delta(\mu) \sim \sum_{n=-Nr/2}^{Nr/2} c_n \ \xi^n$$

ev's or cn determine the mu-dependence of det D(mu)

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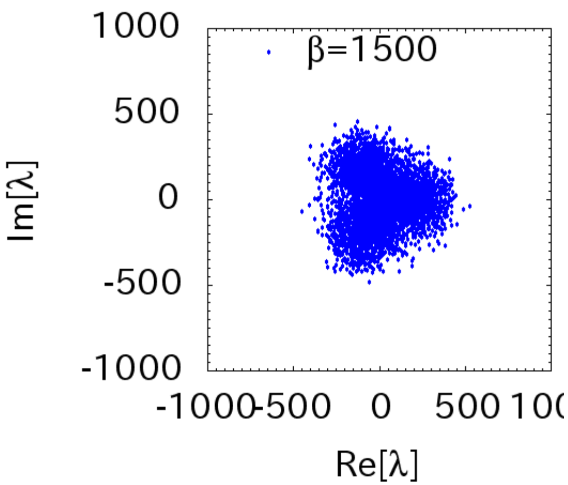
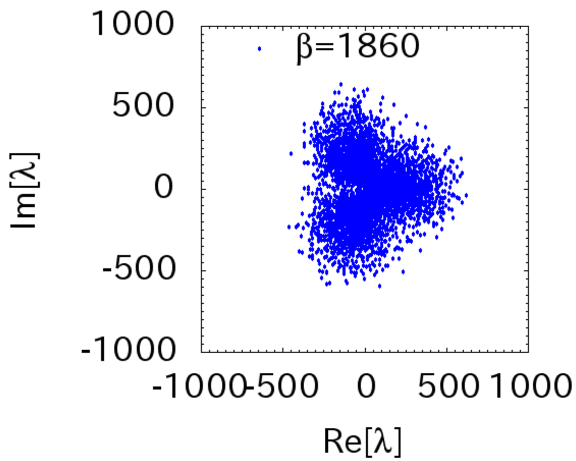
Temperature(beta) dependence 1

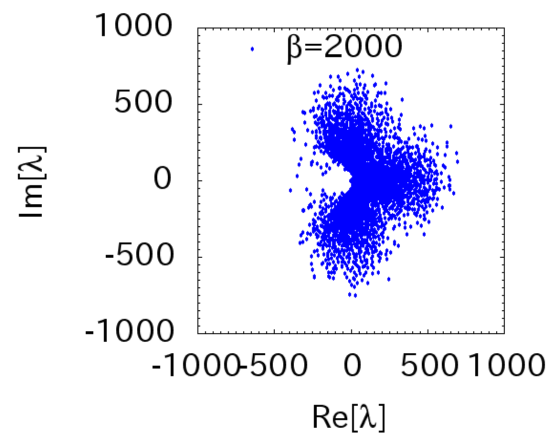
T<Tc



T=Tc



T>Tc



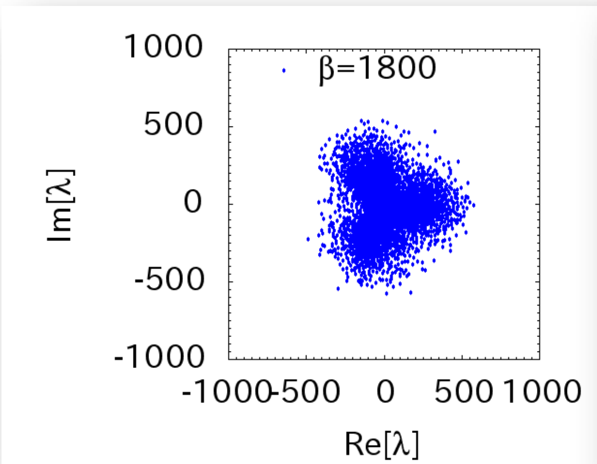
- *At low T : Z3-like distribution*
- *At high T : breaking of Z3 and broadening*
- *Blank observed at high T is related to the Polyakov loop (Alexandu&Wenger , PRD83, 034502('11).*

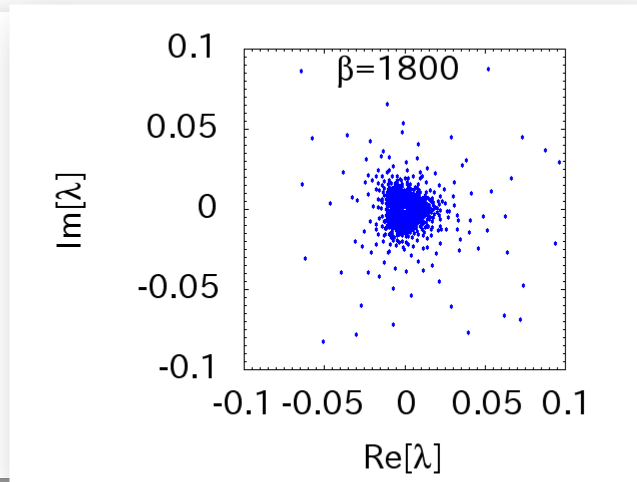
N. E. C. O.

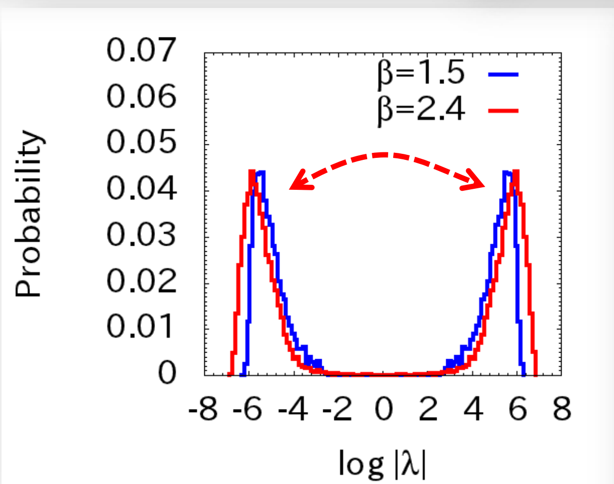
Symmetry of eigenvalues

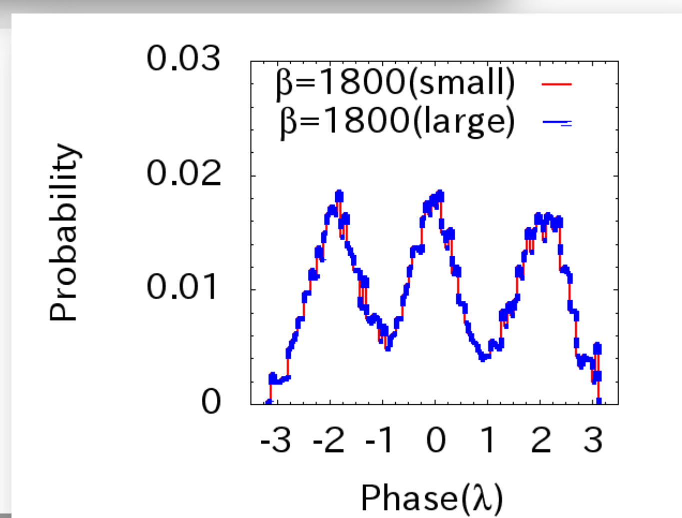
$$\lambda \leftrightarrow \frac{1}{\lambda^*}$$

clover-Wilson + RG-gauge(Nf=2)
Volume : 8^3x4
quark mass : mps/mV ~ 0.8
Configurations : HMC at mu=0



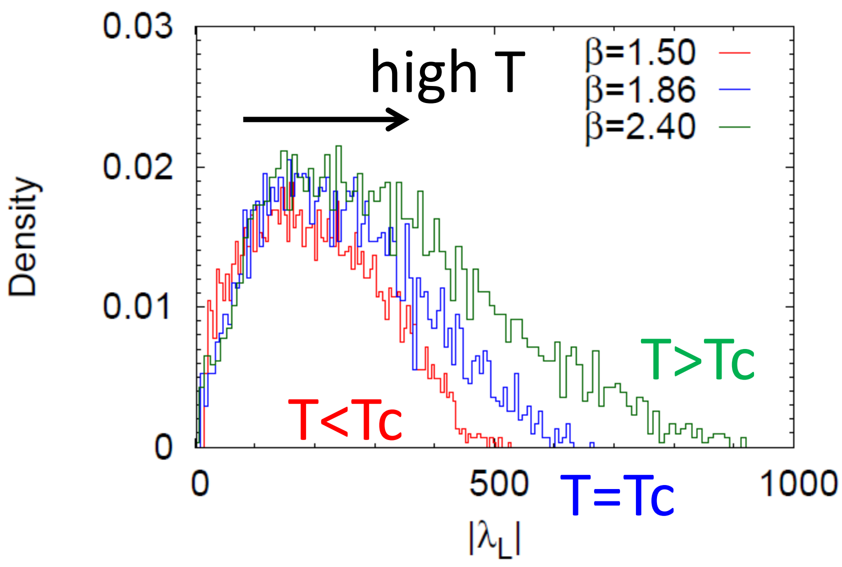


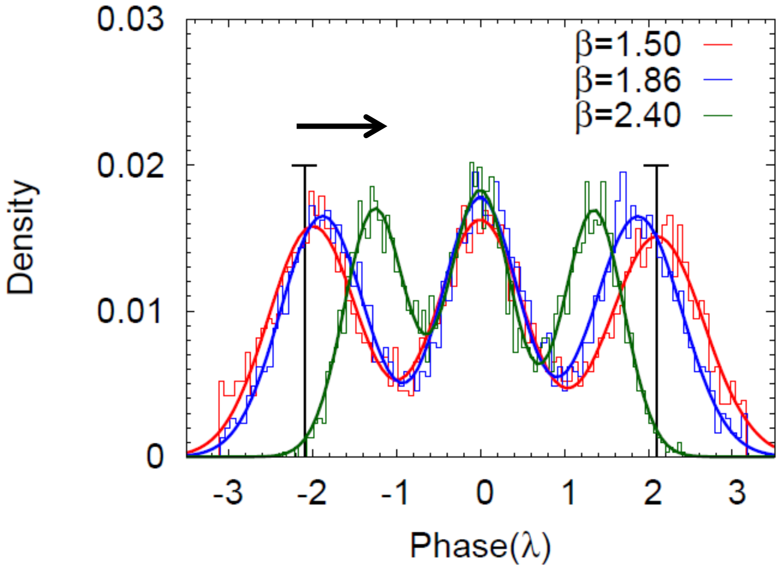




Temperature(beta) dependence 2

Histogram : Absolute (left) and phase (right)



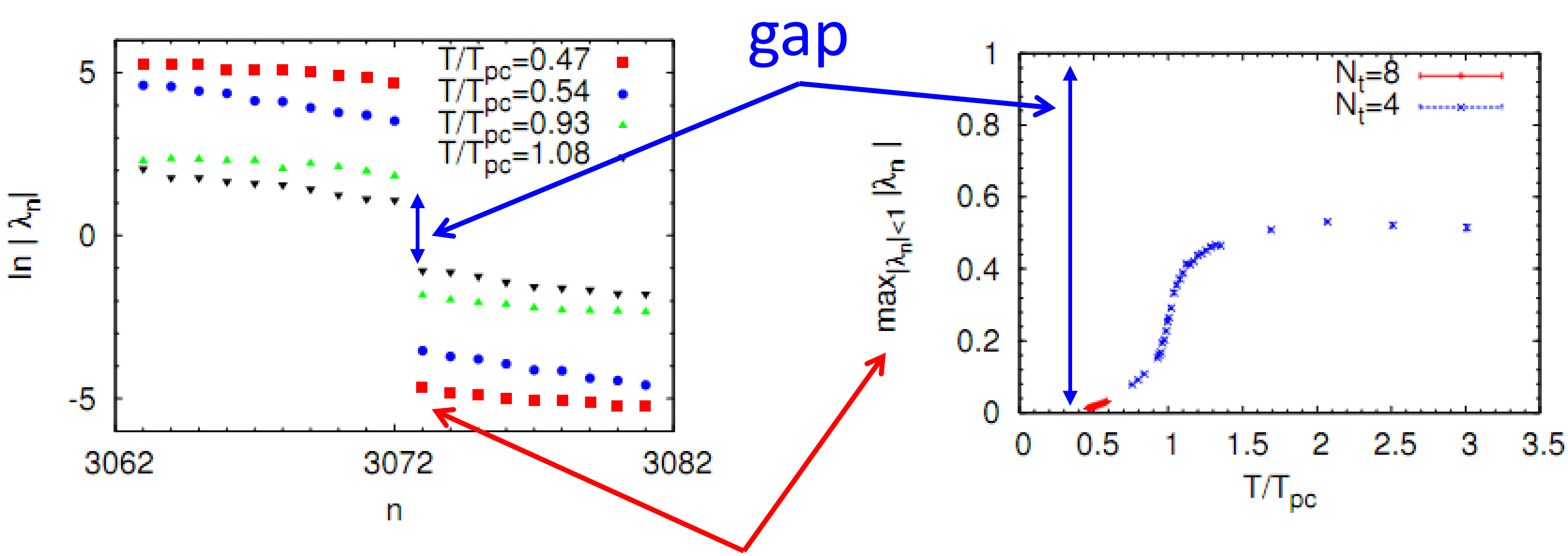


- *At low T : Z3-like distribution*
- *At high T : breaking of Z3 and broadening*

Gap of ev's near unit circle

Left : eigenvalues close to unity

Right : max. ev among the smaller half



$$\ln \max_{|\lambda_n|<1} |\lambda_n|$$

The gap decreases as T increases.

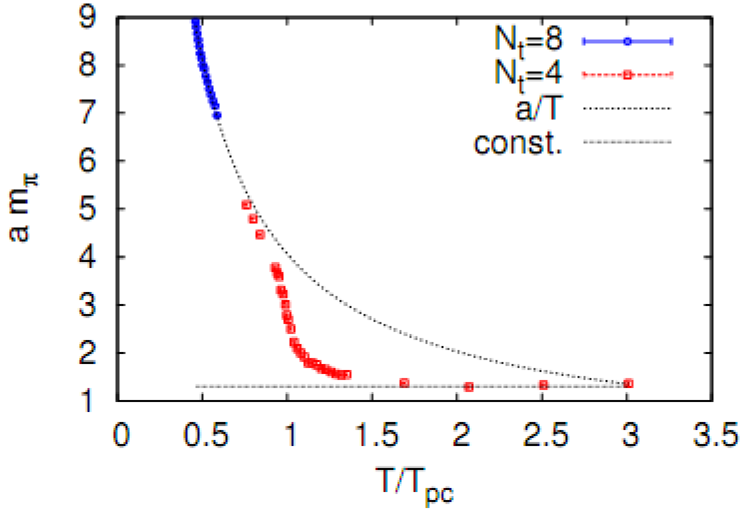
Gap is related to pion mass

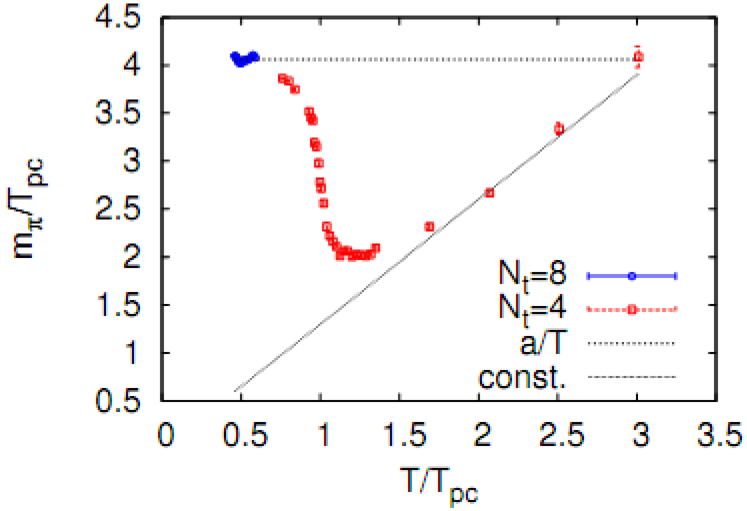
$$am_\pi = -\frac{1}{Nt}\ln \max_{|\lambda_n|<1} |\lambda_n|^2$$

Gibbs('86). Eigenvalues and mpi

See also, Fodor, Szabo, Toth ('06). Eigenvalues and hadron spectrum

Left : mpi/T. Right : mpi/Tpc



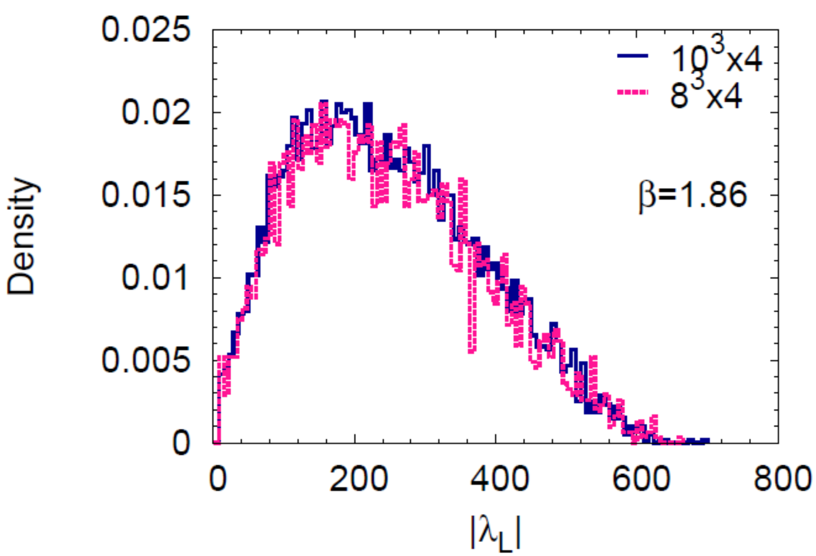


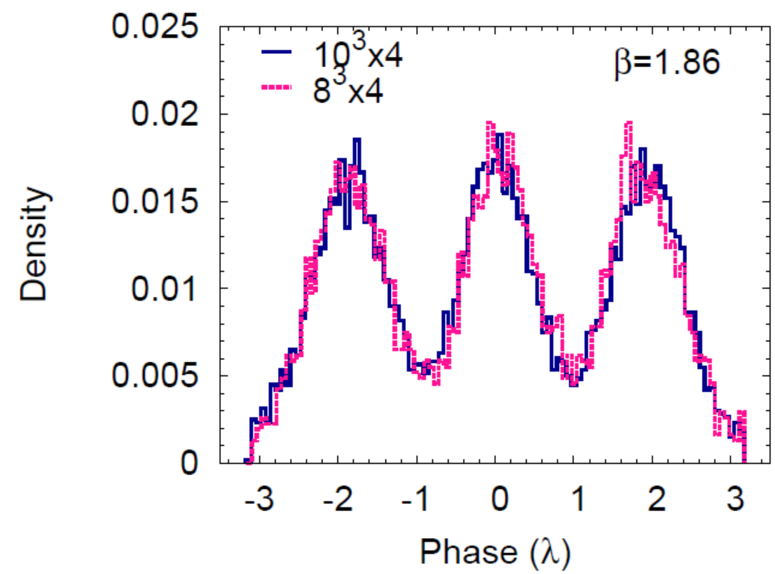
- *At low T, mpi/T is well fitted with a/T, a = 4 Tpc (mq heavy)*
- *At high T, mpi approaches to a constant*

Check 1. Volume dependence

Histograms : |ev| (Left), arg(ev) (Right)

blue : 10^3 x4, red : 8^3 x 4



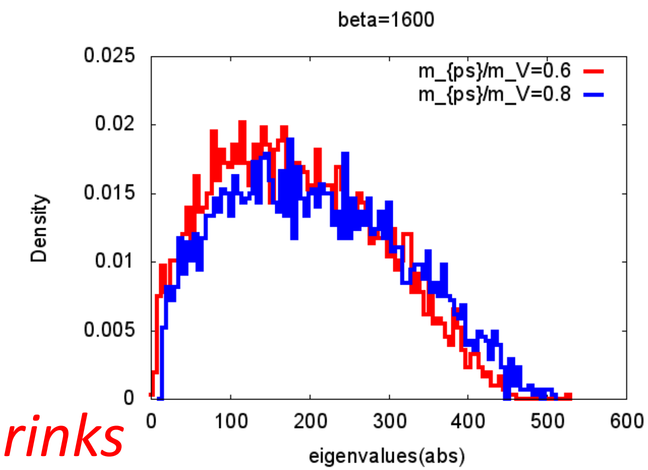


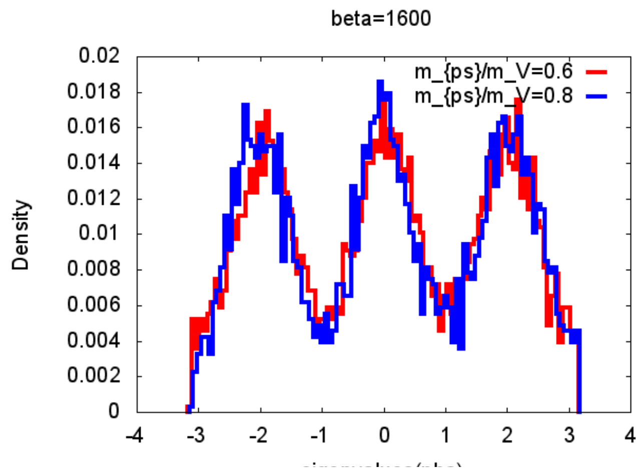
- *The small V-dependence suggests long distance propagations are small*
- *Further investigation for small quark mass is important*

N. E. C. O.

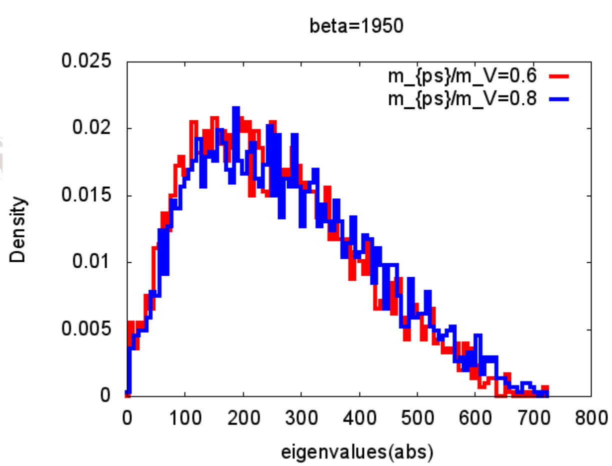
Check 2. quark mass dependence

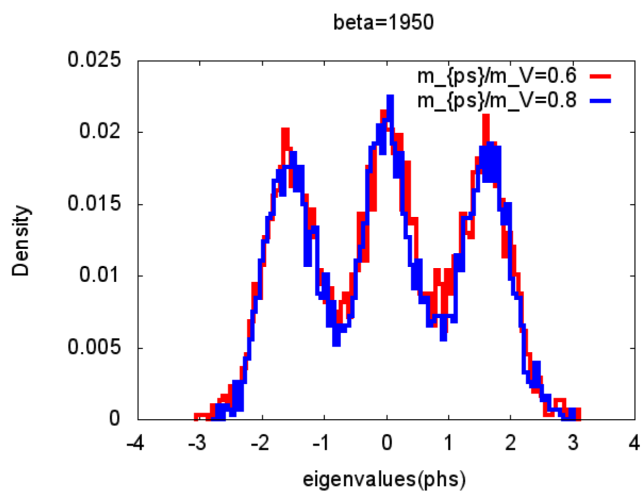
mps / mv = 0.6 (red), 0.8 (blue)
Histograms : |ev| (Left), arg(ev) (Right)
confinement (top), deconfinement(bottom)





Gap shrinks

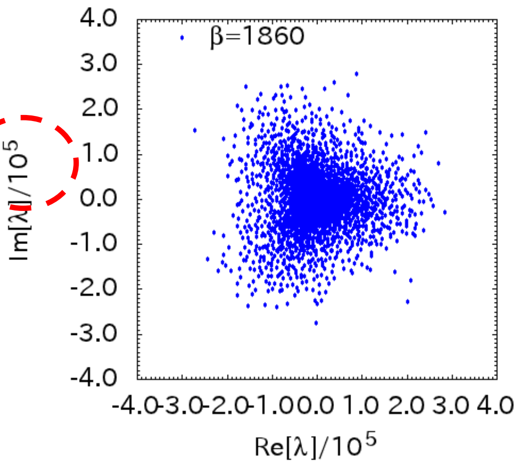




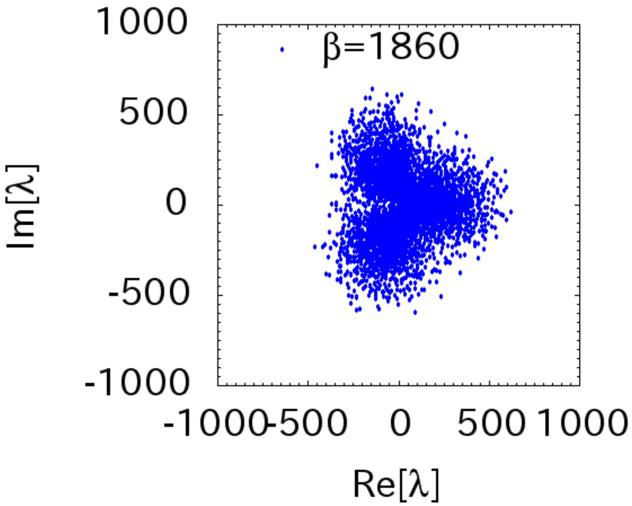
Temperature(Nt) dependence

Nt=8(T/Tc=0.5)

10^5



Nt=4 (T/Tc=1)

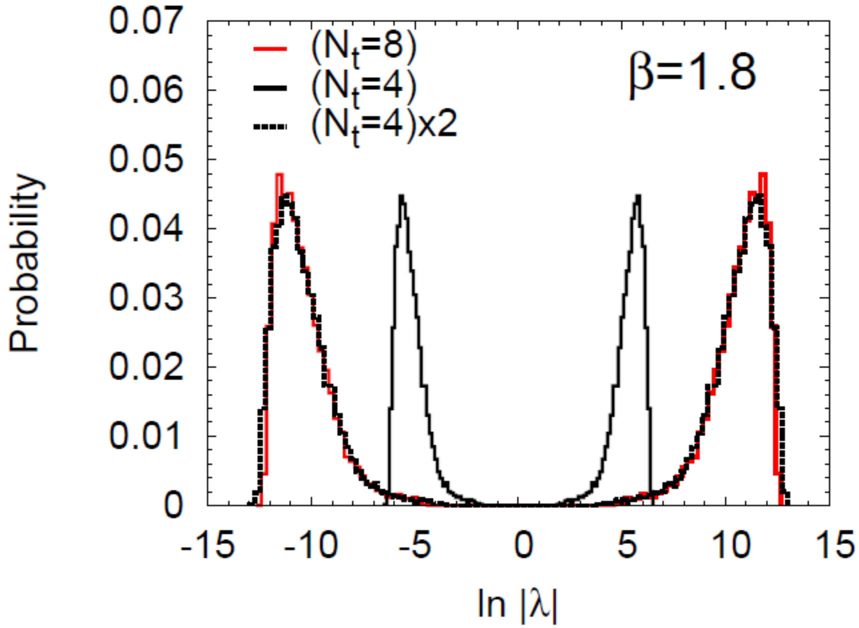


- *As Nt increases (T decrease)*
  - *— larger half of ev's become larger*
  - *— smaller half of ev's become smaller*

$$\lambda \leftrightarrow \frac{1}{\lambda^*}$$

Temperature(Nt) dependence 2

Power-law of ev's with an exponent Nt



$$|\lambda_{N_t=4}|^2 = |\lambda_{N_t=8}|$$

$$|\lambda| = l^{Nt}$$

- *Q is a product of Nt-matrices* $Q \sim A_1 A_2 \cdots A_{Nt}$
- *In equilibrium, it is expected* $A_i = \overline{A} + \delta A_i$
- *Power law* $Q \sim \overline{A}^{N_t}$

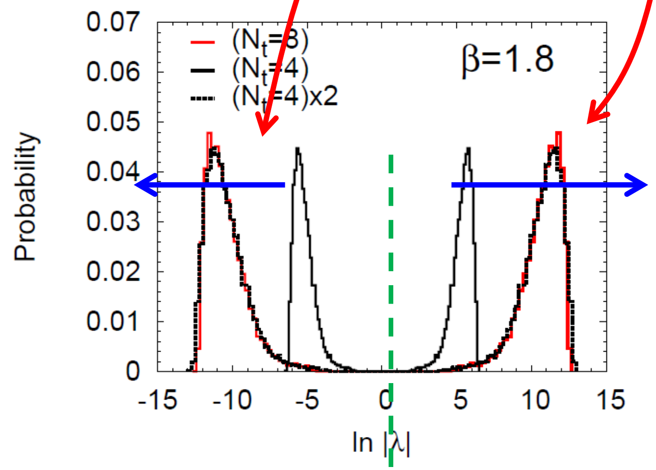
N. E. C. O.

Scale separation

$$\det\Delta(\mu) = C_0 \xi^{-Nr/2} \prod_{n=1}^{Nr/2} (1/\lambda_n^* + \xi) \quad \prod_{n=1}^{Nr/2} (\lambda_n + \xi)$$

$$\lambda = | l |^{Nt}$$

$$\det\Delta(\mu) = C_0 \xi^{-Nr/2} \prod_{n=1}^{Nr/2} (l_n^{*-Nt} + \xi) \prod_{n=1}^{Nr/2} (l_n^{Nt} + \xi)$$



Nt larger

$$\xi = e^{-\mu/T} = e^{-\mu a N_t}$$

low T limit

Eigenvalues at low T $T \to 0, (Nt \to \infty)$

$$\lambda_L \sim l^{Nt} \to \infty, \ \lambda_S \sim l^{-Nt} \to 0$$

Fugacity depends on T $\xi = e^{-\mu/T} = e^{-\mu a N_t}$

$$\det \Delta(\mu) = C_0 \xi^{-Nr/2} \prod_{n=1}^{Nr/2} (l_n^{*-Nt} + \xi) \prod_{n=1}^{Nr/2} (l_n^{Nt} + \xi)$$

Deriavtion of low-T limit of det D(mu) needs a careful calculation

Symmetry of Reduced matrix

$$\det \Delta(\mu) = C_0 \xi^{-Nr/2} \prod_{n=1}^{Nr/2} (l_n^{*-Nt} + \xi) \prod_{n=1}^{Nr/2} (l_n^{Nt} + \xi)$$

1. mu/T=fixed (xi=const.) $\det \Delta(\mu) = C_0 \prod_{n=1}^{Nr/2} \lambda_n^L \in R$

2. mu=fixed (xi->infty, T->0)

   a. small mu $e^{\mu a} < \bar{l}$ $\det \Delta(\mu) = C_0 \prod_{n=1}^{Nr/2} \lambda_n^L \in R$

   b. large mu $e^{\mu a} > \bar{l}$ $\det \Delta(\mu) = C_0 \xi^{-Nr/2} \det Q \in R$

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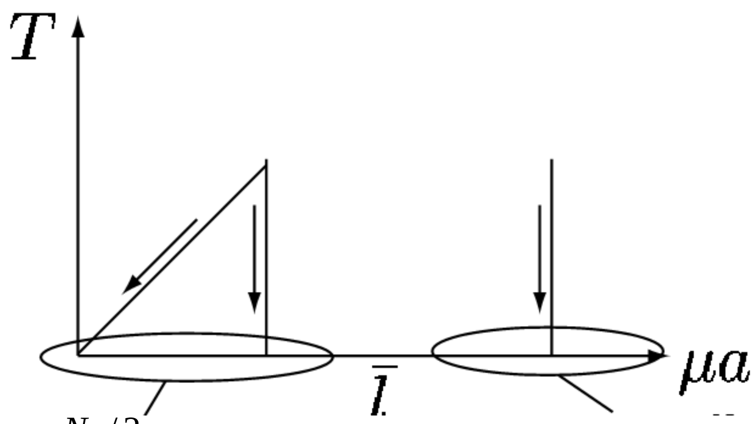
Interpretation



$$\xi^{-Nr/2} = \exp(2N_c N_f N_s^3)$$

$$\det\Delta(\mu) = C_0 \prod_{n=1}^{Nr/2} \lambda_n^L \in R$$

$$\det\Delta(\mu) = C_0 \xi^{-Nr/2} \det Q \in R$$

<n>=0

<n> = 2 Nc Nf [lattice unit]
(all states are occupied)

"Silver Blaze problem"
Independence of det D on mu at low T : Cohen, PRL91,222001 ('03)Adams, PRD70, 045002 ('04).

Lee-Yang zero

- *Lee-Yang theorem : origin of thermodynamical singularities, i.e., phase transition*

$$F = -T \ln Z(\xi), \ \frac{\partial F}{\partial \mu} \infty - T \frac{1}{Z} \frac{\partial Z}{\partial \mu}, \ \xi = \exp(-\mu / T)$$

$$Z(\xi) = 0 \Rightarrow F' \to \infty$$

N. E. C. O.

Canonical formalism of QCD

- *Grand partition function is expanded in powers of fugacity*

$$Z(\mu) = \sum_{n=-N_q}^{N_q} Z_n \xi^n$$

- *Nq (= Max. # of the quark) is given by (d.o.f x V)*
- *Negative power terms come from the anti-quark*

N. E. C. O.

Canonical formalism of QCD

Preliminary

- *We employ the Glasgow method*
  - *Reduction formula + reweighting*

$$Z_n = \left\langle \frac{c_n}{(\det \Delta(0))^2} \right\rangle_0 \quad (\det \Delta(\mu))^2 = \sum_{n=-Nr}^{Nr} c_n \, \xi^n$$

- *Approaches to improve overlap for canonical and LY*
  - *Fodor & Katz, Phys.Lett. B534 (2002) 87-92*
  - *de Forcrand & Kratochivila, hep-lat/0509143*
  - *Ejiri & Yoneyama, arXiv:0911.2257 [hep-lat]*
  - *Li, Alexandru & Liu, Phys.Rev. D84 (2011) 071503*

XQCD-J

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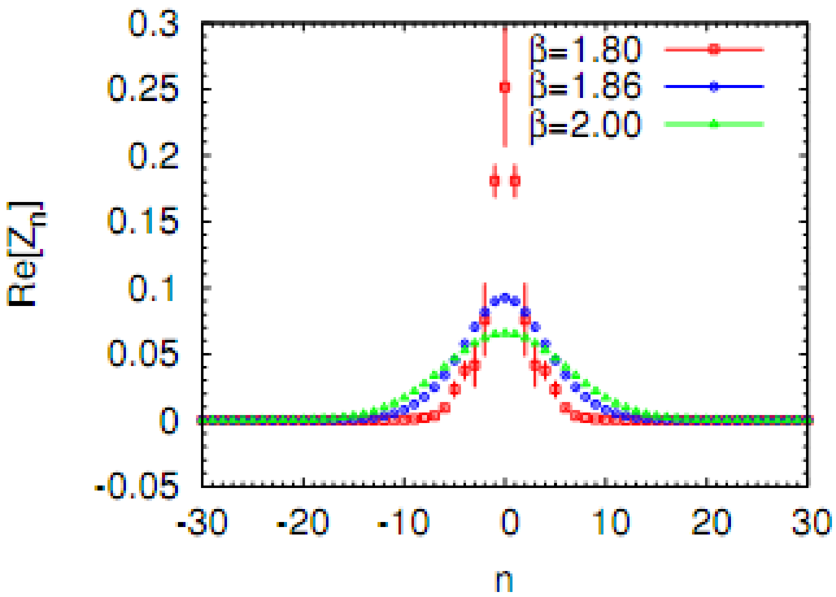
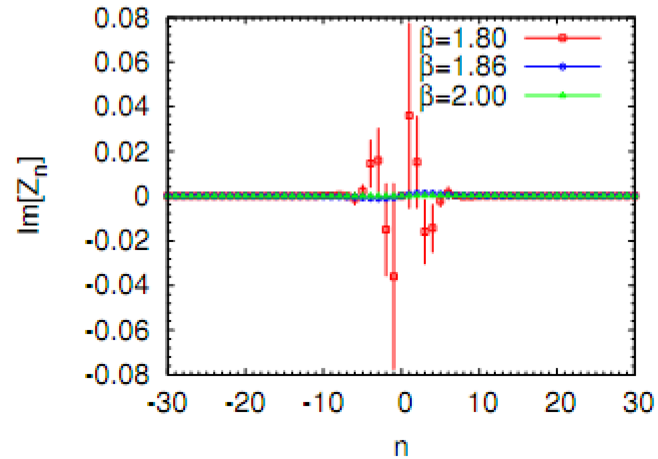
Canonical partition function





large phase fluctuation at low T

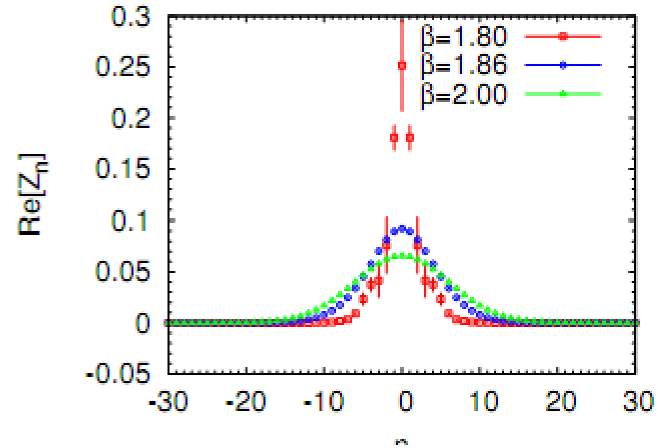
- *Zn decreases exponentially*
  - *broadening at high T : increase of effective d.o.f*
- *Zn (mod(n,3) !=3) does not vanish even in confinement phase*
  - *because of importance sampling at mu=0*
  - *including all Z3 sectors by hand leads to cancelation*

N. E. C. O.

Lee-Yang Zero 1

- *In the vinicity of mu =0, Z(mu) is dominated by terms near n=0*

$$Z(\mu) = \sum_{|n|\leq N'} Z_n \xi^n + \sum_{|n|>N'} Z_n \xi^n$$



- *The behavior of the root distribution near xi=1 can be studied by the first terms.*
- *(Density depends on N' (f(x) = 1 + x + x^2 + ... + x^N)*
- *This approximation should not be used for the study of the order of the phase.)*

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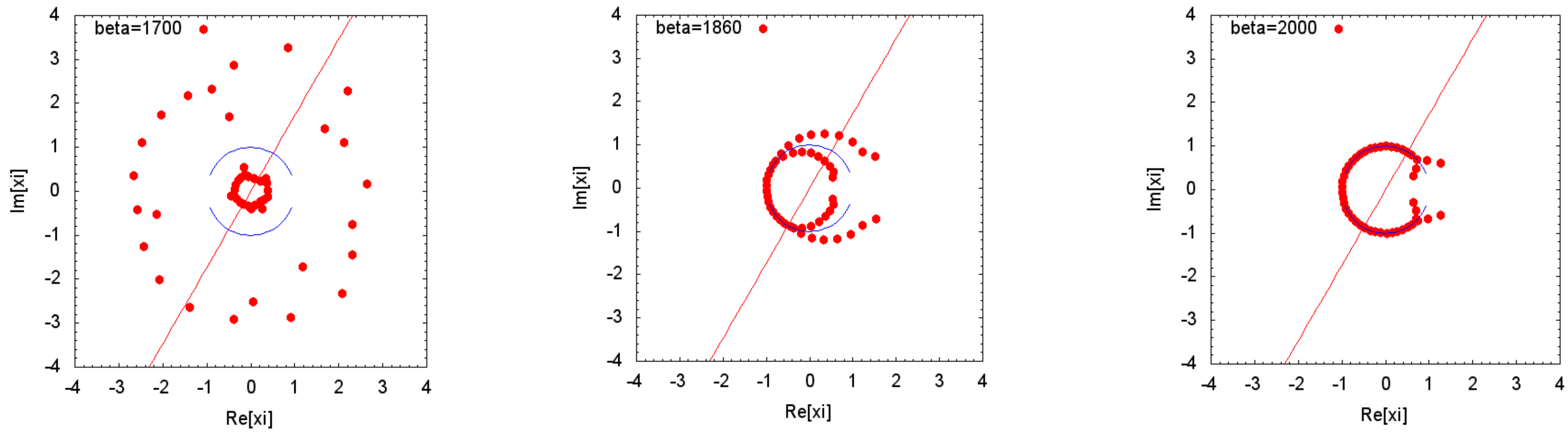
Lee-Yang Zero

$$Z(\mu) = \sum_{|n|\leq N'} Z_n \xi^n = (\xi - r_1)(\xi - r_2)\cdots$$

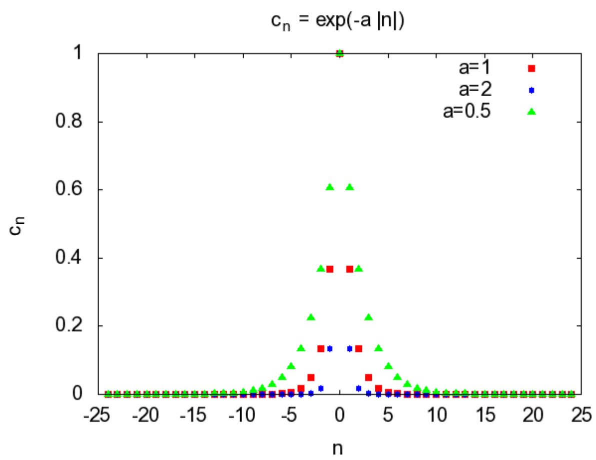
T<Tc T=Tc T>Tc

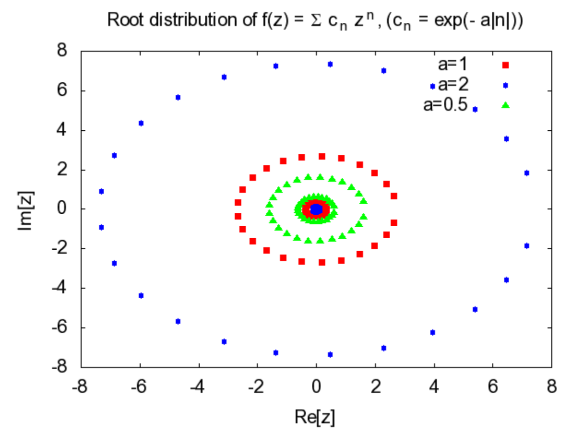


- *Root distribution shows two different behavior*
  - *at low T : two circle (Zn = exp(- a |n|))*
  - *at high T : unit circle + 3 branches (Zn = exp (-a n^2))*
  - *branch point is located at near RW endpoint*

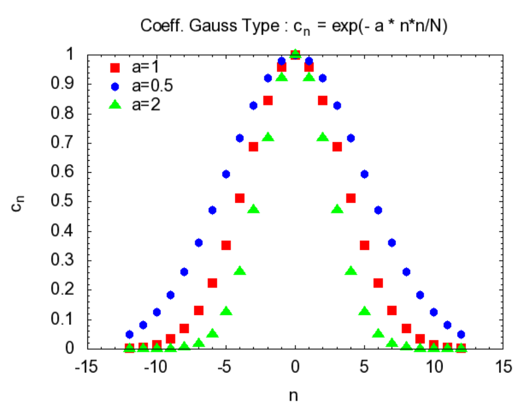
Examples for Polynomial's Root

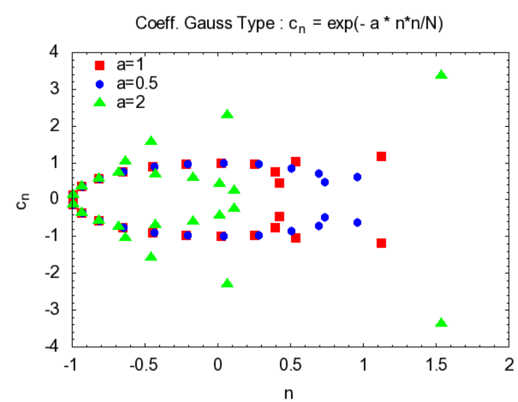
$$c_n = \exp(-a|n|)$$





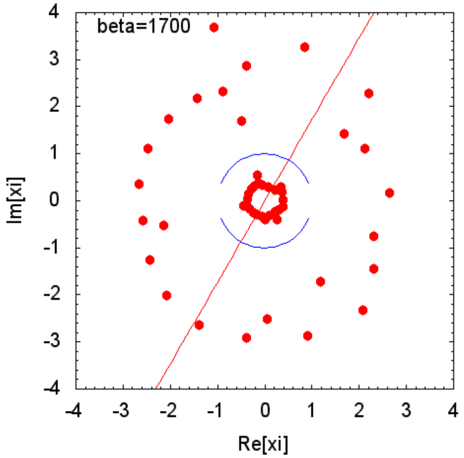
$$c_n = \exp(-an^2)$$

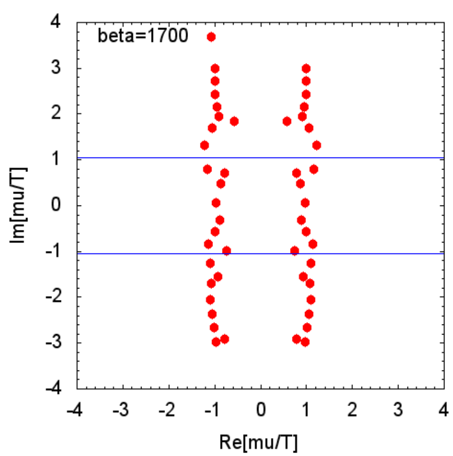




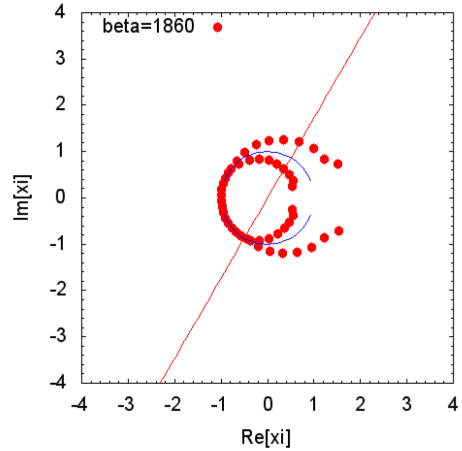
Lee-Yang Zero 2

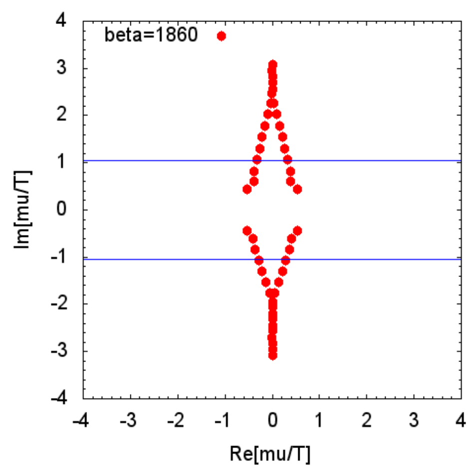
T<Tc



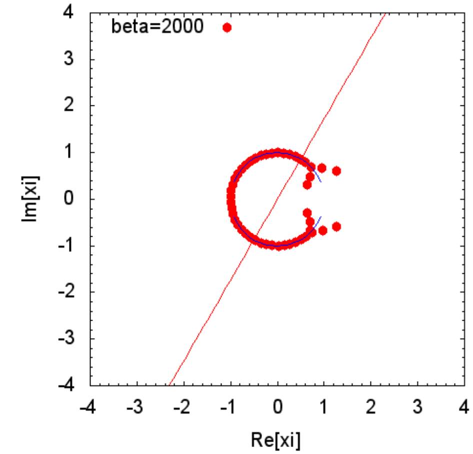


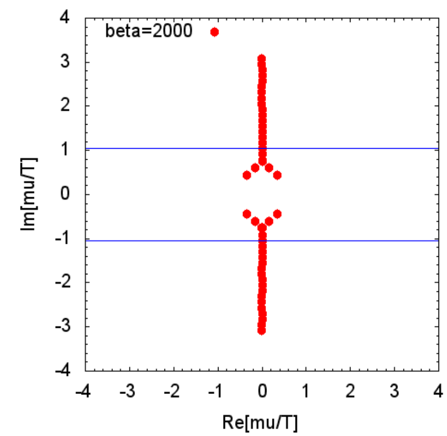
T=Tc



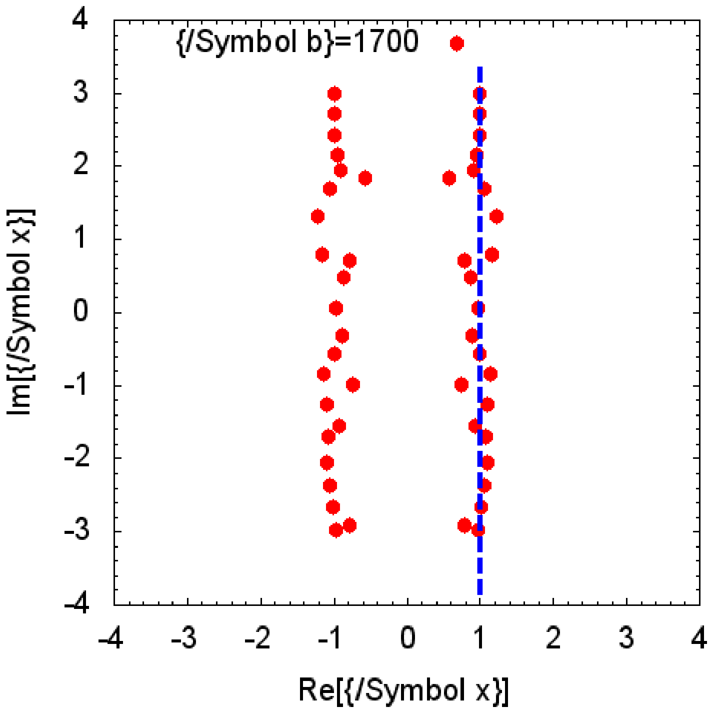


T>Tc





CEP



- *LYzeros seems to approach to real axis near mu/T = 1*
- *Further investigations are needed for*
  - *overlap problem & sign problem*
  - *thermodyanamic limit*

N. E. C. O.

Summary

- *Reduction formula*
  - *relax the difficulty to calculate fermion determinant*
  - *provides the analytic expression of det D(mu)*
  - *although it is still heavy, the formula is sometimes useful to study finite density systems.*
- *Properties of reduced matrix*
  - *angular distribution is related to Z3*
  - *gap is related to chiral symmetry breaking*
  - *the whole eigenvalues are important in overlap &sign problem*
- *In this talk, we have studied*
  - *numerical properties of transfer matrix*
  - *low-T limit of det D(mu)*
  - *canonical partition function & Lee-Yang zero*