Preweighting method in Monte-Carlo sampling with complex action

– Strong-Coupling Lattice QCD with $1/g^2$ correction, as an example –

Akira Ohnishi[1] and Terukazu Ichihara[12]

1. YITP, Kyoto U., 2. Kyoto U.

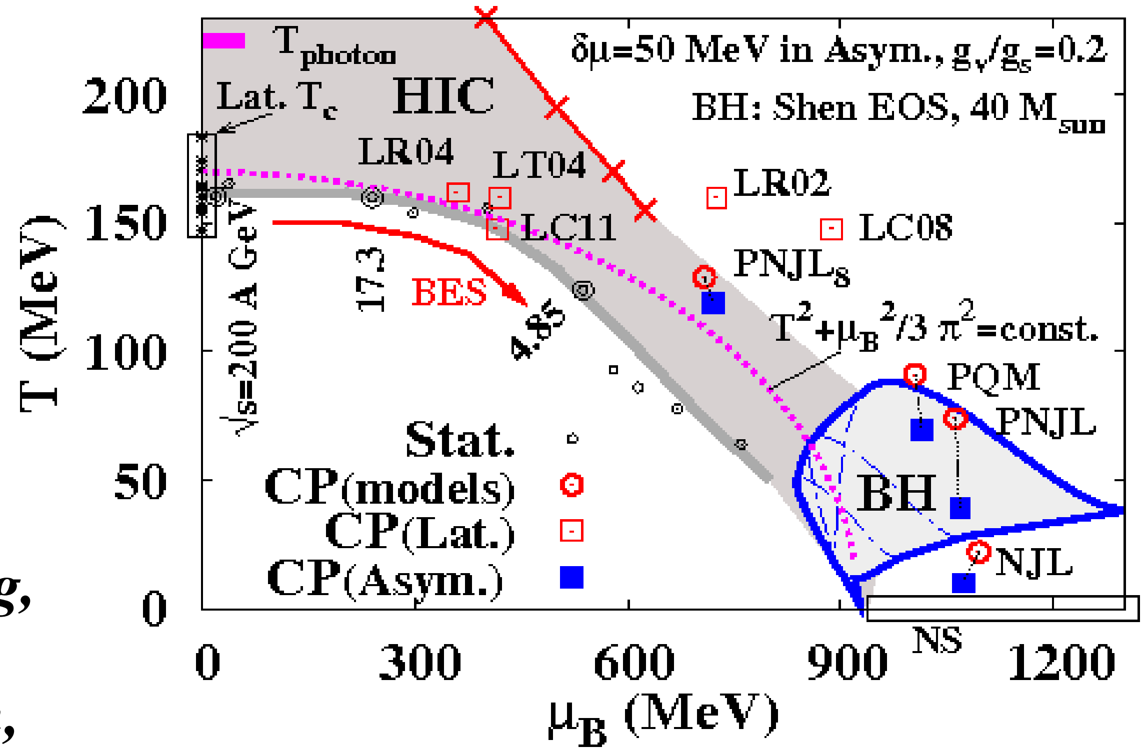
The 33rd Int. Symp. on Lattice Field Theory, Kobe, Japan, Jul.14-18, 2015

T. Ichihara, AO, work in prog.

QCD phase diagram and Sign Problem

- **Finite density QCD**
  Critical Point,
  Nuclear Matter EOS,
  Compact Stars, …

AO, PTPS193('12)1.



- **Obstacle**
  = Sign problem at finite μ.
- **Many methods proposed.**
  Taylor expansion, Re-weighting,
  Imag. μ+AC,
  Canonical, Fugacity expansion,
  Histogram method,
  Complex Langevin,
  Lefschetz thimble,
  Strong Coupling,
  …

but it is still difficult to attack low T.

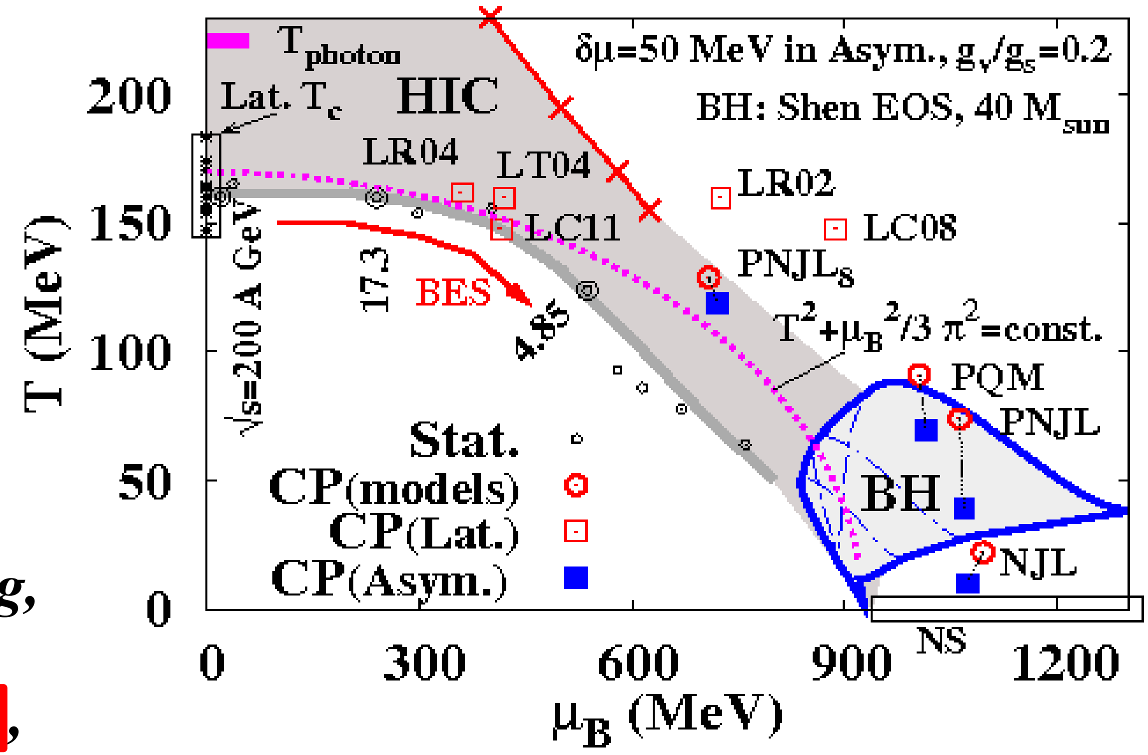
See also T. Ichihara's work on cumulants [Sat. 401, arXiv:1507.04527 [hep-lat]]

QCD phase diagram and Sign Problem

- **Finite density QCD**
  Critical Point,
  Nuclear Matter EOS,
  Compact Stars, …
- **Obstacle**
  = Sign problem at finite μ.
- **Many methods proposed.**
  Taylor expansion, Re-weighting,
  Imag. μ+AC,
  Canonical, Fugacity expansion,
  Histogram method,
  Complex Langevin,
  Lefschetz thimble,
  Strong Coupling,
  …

but it is still difficult to attack low T.

AO, PTPS193('12)1.



Many Talks During Lattice 2015 !

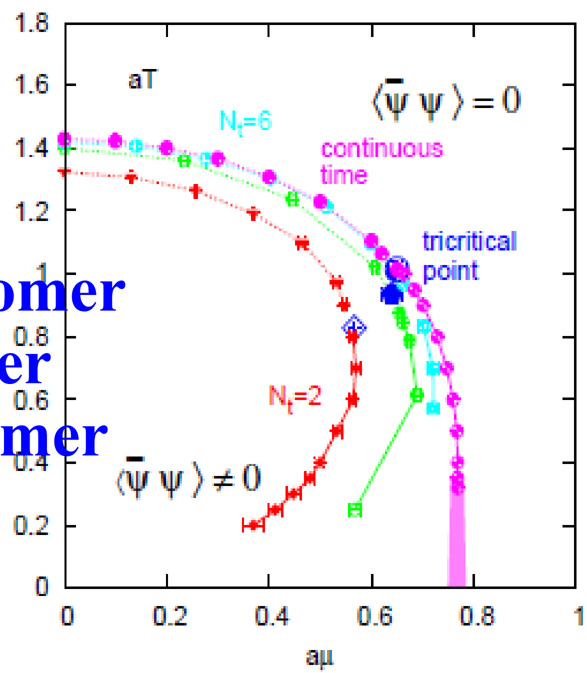
Less Popular but some in Lattice 2015.

See also T. Ichihara's work on cumulants [Sat. 401, arXiv:1507.04527 [hep-lat]]

Strong Coupling Lattice QCD

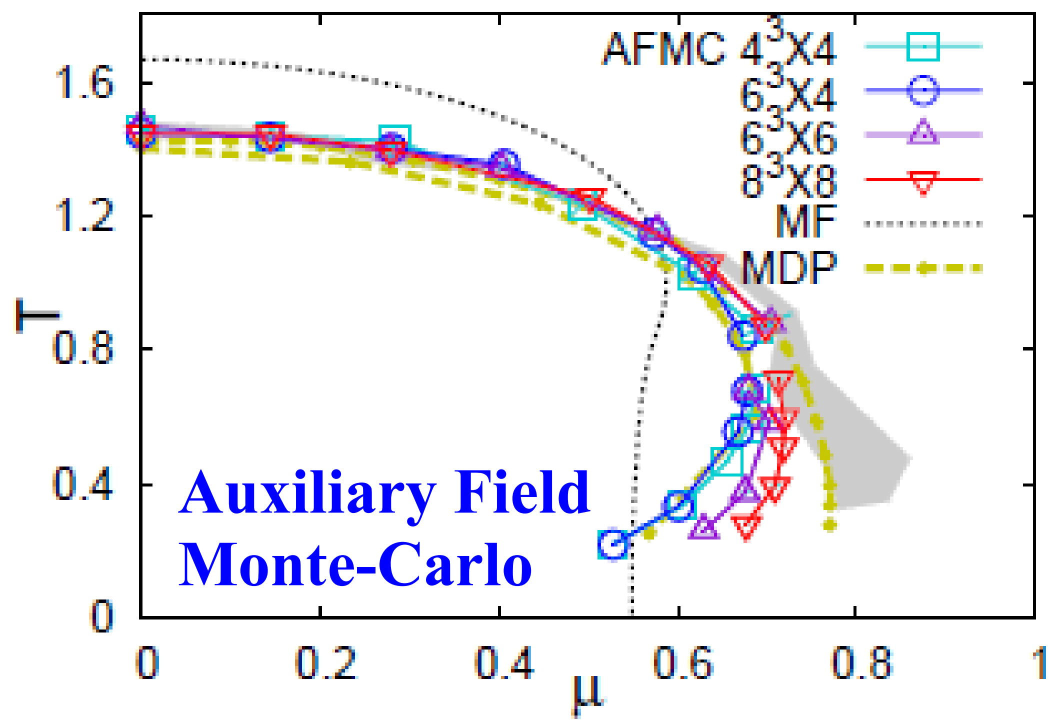
Wilson ('74), Kawamoto ('80), Kawamoto, Smit ('81), Aoki ('84), Damagaard, Hochberg, Kawamoto ('85), Bilic, Karsch, Redlich ('92), Fukushima ('03), Nishida ('03), Kawamoto, Miura, AO, Ohnuma ('07). Miura, Nakano, AO, Kawamoto ('09), Nakano, Miura, AO ('10), Mutter, Karsch ('89), de Forcrand, Fromm ('10), de Forcrand, Unger ('11), Misumi, Nakano, Kimura, AO('12), Misumi, Kimura, AO('12), AO, Ichihara, Nakano ('12), Ichihara, Nakano, AO ('14), Tomboulis ('13), ...

- **Integrate links first, and fermions later → Milder sign prob.**
- **Two indep. methods give consistent phase diagram in the *Strong Coupling Limit*.**



Monomer -Dimer -Polymer

de Forcrand, Fromm ('10), de Forcrand, Langelage, Philipsen, Unger ('14)



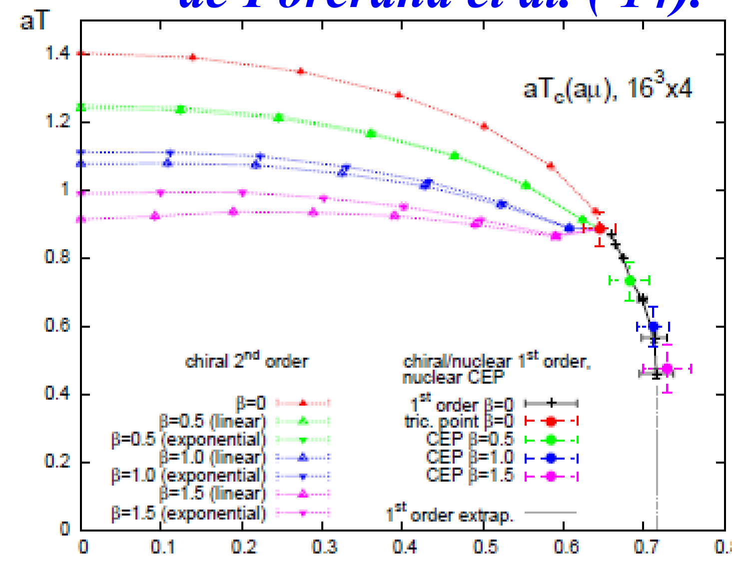
Auxiliary Field Monte-Carlo

T.Ichihara, AO, T.Z.Nakano, PTEP2014,123D02.

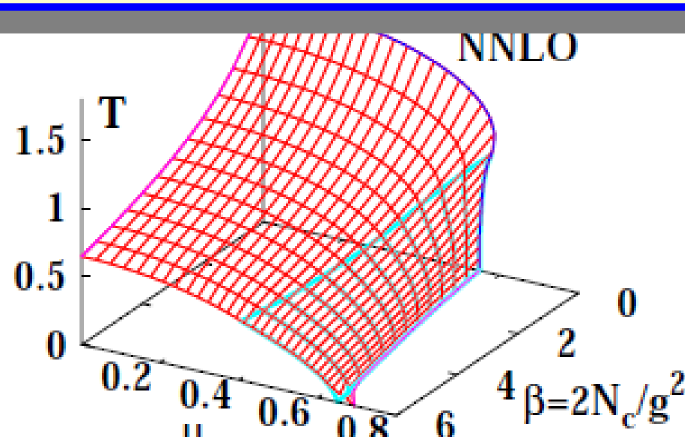
Finite coupling corrections

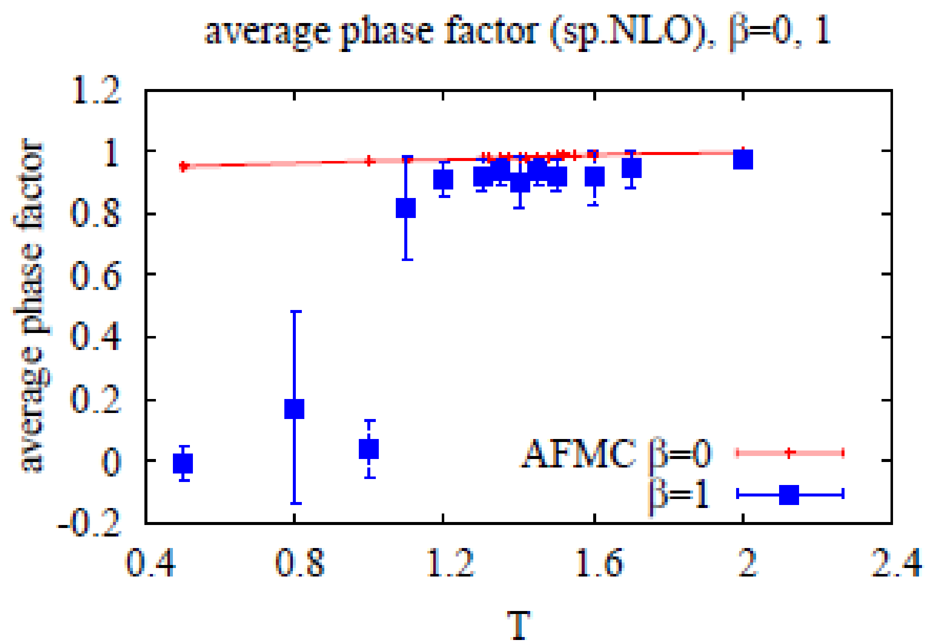
- **Mean field results: No sign prob.**
- **Monomer-Dimer-Polymer: Phase diagram by reweighting**
  de Forcrand, Langelage, Philipsen, Unger ('14)
- **Auxiliary Field Monte-Carlo: Severe weight cancellation at finite $1/g^2$**
  T.Ichihara, T.Z.Nakano, AO, Lattice 2014

de Forcrand et al. ('14).



Direct sampling method is not yet fully developed.





AO, Miura, Nakano, Kawamoto (Lattice 2009), Nakano, Miura, AO ('10, '11)

T.Ichihara, T.Z.Nakano, AO, Lattice 2014

Contents

- **Introduction**
- **Strong coupling lattice QCD with fluctuation and $1/g^2$ correction**
  - **Strong coupling expansion and Effective action**
  - **Bosonized action and Auxiliary Field**
  - **Sign problem and Shifting integration path**
  - **Phase diagram in SC-LQCD with fluctuation and $1/g^2$ effects**
- **Preweighting**
  - **Histogram method.**
  - **Can we include the cancellation effect in advance ?**
- **Summary**

Strong-Coupling Lattice QCD including Fluctuation and $1/g^2$ Effects

Lattice QCD action

- **Lattice QCD action (unrooted staggered fermion)**

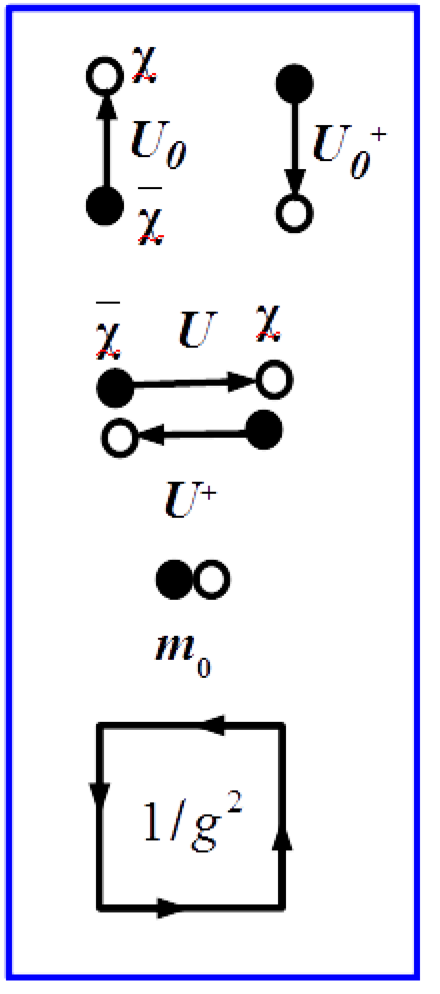
$$L=\frac{1}{2}\sum_x \left[V_x^+ - V_x^-\right] + \frac{1}{2\gamma}\sum_{x,j}\eta_j(x)\left[\bar{\chi}_x U_j(x)\chi_{x+\hat{j}} - \bar{\chi}_{x+\hat{j}} U_j^+(x)\chi_x\right]$$

$$+\frac{m_0}{\gamma}\sum_x \bar{\chi}_x\chi_x + \frac{2N_c}{g^2}\left[\gamma S_\tau^{\rm plaq} + \frac{1}{\gamma} S_s^{\rm plaq}\right]$$

$$S_\alpha^{\rm plaq} = \sum_{P_\alpha}\left[1-\frac{1}{N_c}\,\mathrm{Re}\,\mathrm{Tr}\,U_{P_\alpha}\right]$$

$$V_x^+ = \bar{\chi}_x U_0(x) e^{\mu/\gamma^2}\chi_{x+\hat{0}},\quad V_x^- = \bar{\chi}_{x+\hat{0}} U_0^+(x) e^{-\mu/\gamma^2}\chi_x$$

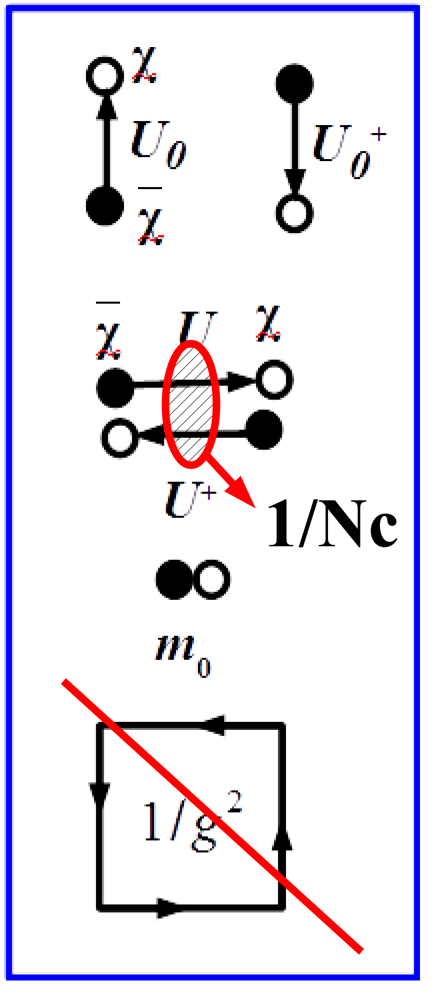
- **Staggered sign factor**
  $\eta_j(x)=(-1)^{**}(x_0+...+x_{j-1})$
- **$U(1)_L$ x $U(1)_R$ chiral sym.**
  $\chi_x \rightarrow \exp[i\,\theta\varepsilon(x)]\,\chi_x$, $\varepsilon(x)=(-1)^{**}(x_0+x_1+x_2+x_3)$
- **Anisotropy parameter γ ($T=\gamma^2/N_\tau$)** *E.g. Bilic et al. ('92)*



- **Strong coupling limit**
  Damgaard, Kawamoto, Shigemoto ('84), Jolicoeur, Kluberg-Stern, Lev, Morel, Petersson ('84).
  Spatial link integral→ Fermion action with four-Fermi int. (LO in 1/d expansion)

$$S_{\rm eff}^{\rm (SCL)} = \frac{1}{2}\sum_x \left[V_x^+ - V_x^- \right] + \frac{m_0}{\gamma}\sum_x M_x$$

$$-\frac{1}{4N_c\gamma^2}\sum_{x,j} M_x M_{x+\hat{j}} \qquad \left(M_x = \bar{\chi}_x \chi_x \right)$$



Strong Coupling Lattice QCD

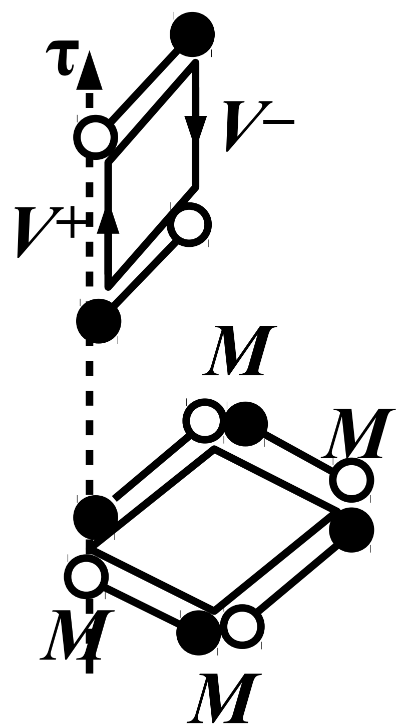
- **Strong coupling limit**
  Damgaard, Kawamoto, Shigemoto ('84), Jolicoeur, Kluberg-Stern, Lev, Morel, Petersson ('84).
  Spatial link integral→ Fermion action with four-Fermi int. (LO in 1/d expansion)

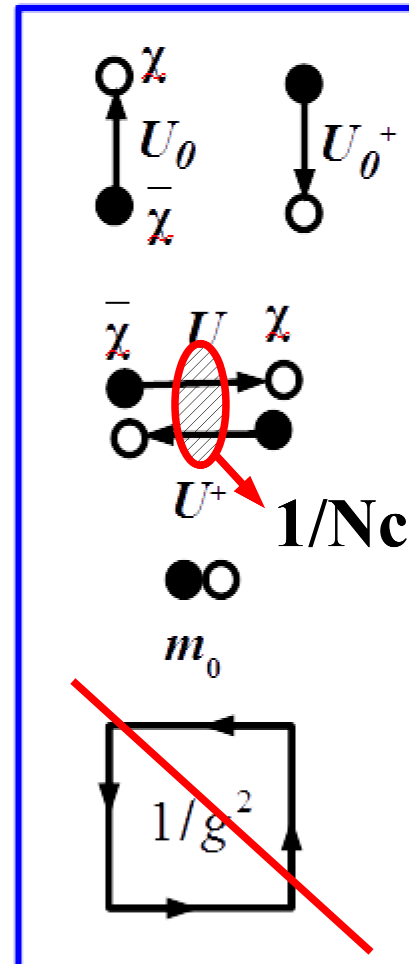
$$S_{\rm eff}^{\rm (SCL)} = \frac{1}{2}\sum_x \left[V_x^+ - V_x^-\right] + \frac{m_0}{\gamma}\sum_x M_x - \frac{1}{4N_c\gamma^2}\sum_{x,j} M_x M_{x+\hat{j}} \quad \left(M_x = \bar{\chi}_x \chi_x\right)$$

- **Eff. Action with $1/g^2$ correction**
  Faldt, Petersson ('86), Miura, Nakano, AO, Kawamoto ('09)

$$S_{\rm eff}^{\rm (NLO)} = S_{\rm eff}^{\rm (SCL)} + \frac{\beta_\tau}{2}\sum_{x,j}\left[V_x^+ V_{x+\hat{j}}^- + V_{x+\hat{j}}^+ V_x^-\right] - \frac{\beta_s}{\gamma^4}\sum_{x,k,j,k\neq j} M_x M_{x+\hat{j}} M_{x+\hat{k}} M_{x+\hat{k}+\hat{j}}$$

$$\beta_\tau = 1/2N_c^2 g^2 \gamma, \quad \beta_s = 1/16 N_c^4 g^2 \gamma$$





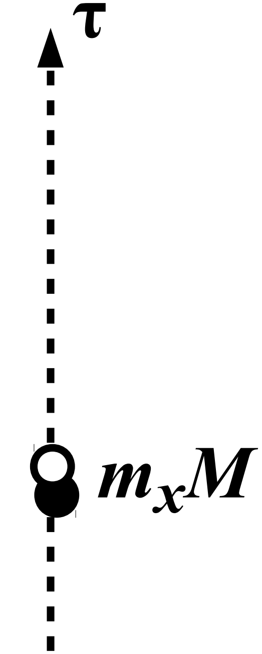
Extended Hubbard-Stratonovich Transformation

- **Extended HS transf.** $\exp(\alpha AB) = \int d\varphi\, d\varphi^*\, \exp(-\alpha[\varphi^*\varphi + \varphi^* A + \varphi B])$
- **Bosonized Effective Action**

$$S_{\rm eff}^{\rm (EHS)} = \frac{1}{2}\sum_x (\quad V_x^+ - \quad V_x^-) + \frac{1}{\gamma}\sum_x m_x M_x + S_{\rm AF}$$

$$m_x = m_0 + \frac{1}{4N_c}\sum_j (\sigma + i\varepsilon\pi)_{x\pm\hat{j}}$$

$$S_{\rm AF} = \frac{L^3}{4N_c}\sum_{\mathbf{k},\tau,f(\mathbf{k})>0} f(\mathbf{k})\left[\sigma^*_{\mathbf{k},\tau}\sigma_{\mathbf{k},\tau} + \pi^*_{\mathbf{k},\tau}\pi_{\mathbf{k},\tau}\right]$$



Extended Hubbard-Stratonovich Transformation

- **Extended HS transf.** $\exp(\alpha AB) = \int d\varphi\, d\varphi^* \exp(-\alpha[\varphi^*\varphi + \varphi^* A + \varphi B])$
- **Bosonized Effective Action**

$$S_{\mathrm{eff}}^{(\mathrm{EHS})} = \frac{1}{2}\sum_x \left(Z_x^- V_x^+ - Z_x^+ V_x^-\right) + \frac{1}{\gamma}\sum_x m_x M_x + S_{\mathrm{AF}}$$

$$m_x = m_0 + \frac{1}{4N_c}\sum_j (\sigma + i\varepsilon\pi)_{x\pm\hat{j}} + \beta_s \sum_j \left\{\varphi_x^{(j)*}(\Theta_x^{(j)})^{1/2} + \varphi_{x-\hat{j}}^{(j)*}(\Theta_{x-\hat{j}}^{(j)})^{1/2}\right\}$$

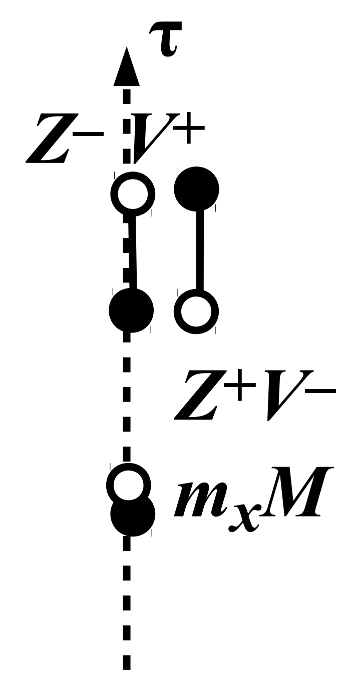
$$S_{\mathrm{AF}} = \frac{L^d}{4N_c} \sum_{\mathbf{k},\tau,f(\mathbf{k})>0} f(\mathbf{k})\left[\sigma_{\mathbf{k},\tau}^*\sigma_{\mathbf{k},\tau} + \pi_{\mathbf{k},\tau}^*\pi_{\mathbf{k},\tau}\right]$$

$$+ \beta_s L^3 \sum_{\mathbf{k},\tau,f^{(j)}(\mathbf{k})>0} f^{(j)}(\mathbf{k})\left[\sigma_{\mathbf{k},\tau}^{(j)*}\sigma_{\mathbf{k},\tau}^{(j)} + \pi_{\mathbf{k},\tau}^{(j)*}\pi_{\mathbf{k},\tau}^{(j)}\right] + \beta_s \sum_{x,j}\varphi_x^{(j)*}\varphi_x^{(j)}$$

$$+ \beta_\tau L^3 \sum_{\mathbf{k},\tau,f(\mathbf{k})>0} f(\mathbf{k})\left[\Omega_{\mathbf{k},\tau}^*\Omega_{\mathbf{k},\tau} + \omega_{\mathbf{k},\tau}^*\omega_{\mathbf{k},\tau}\right] .$$

$$\Theta_x^{(j)} = \sum_{k,k\neq j} (\sigma^{(j)} + i\varepsilon\pi^{(j)})_{x\pm\hat{k}}$$

$$Z_x^- = 1 + \beta_\tau \sum_j (\omega - \varepsilon\Omega)^*_{x\pm\hat{j}} , \quad Z_x^+ = 1 + \beta_\tau \sum_j (\omega + \varepsilon\Omega)_{x\pm\hat{j}}$$



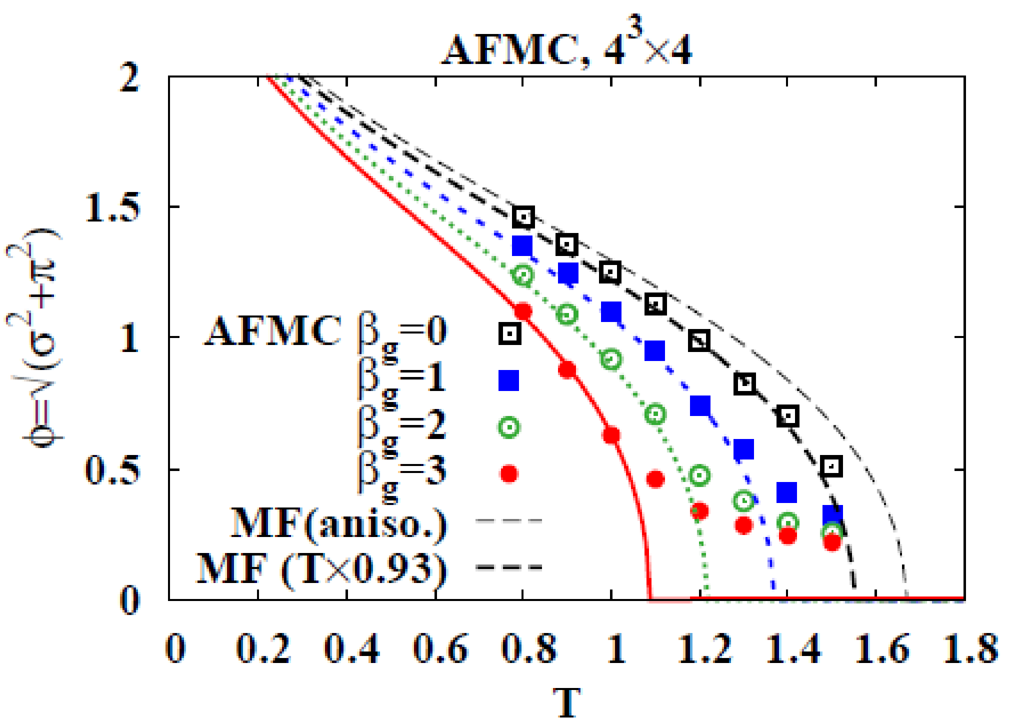
SCL+1/g² corr. → x dep. mass + mod. of temporal coef.

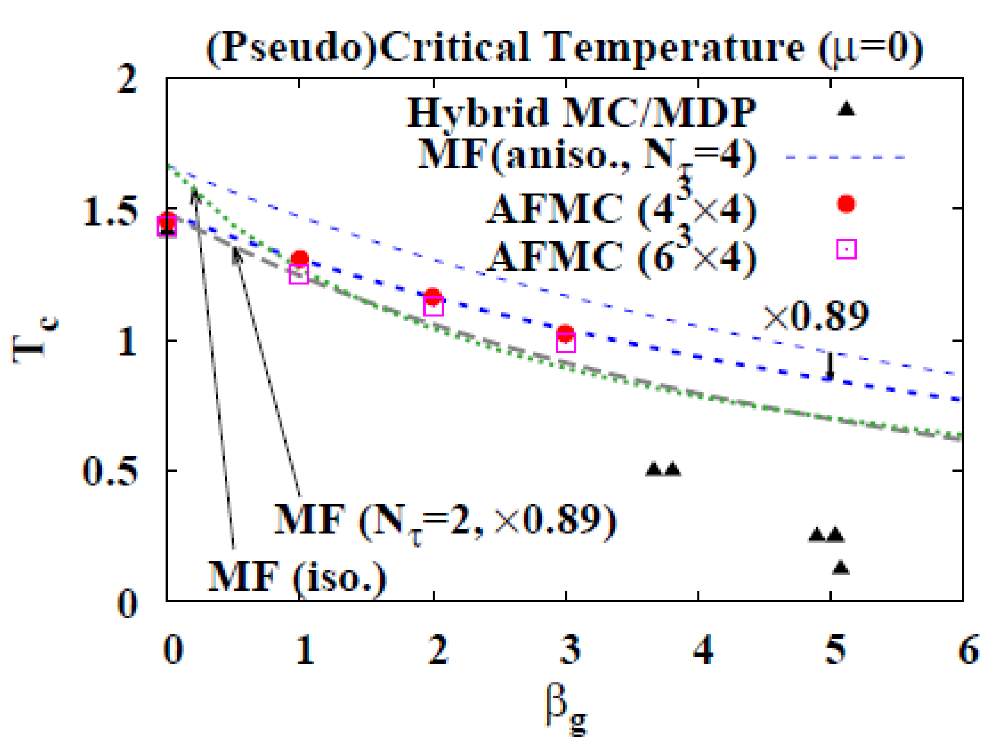
Lattice Setup

- **One species of unrooted starggered fermion**
  - **$N_f = 4$ in the continuum limit**
  - **Chiral limit → Chiral symmetry: $U(1)_L$ x $U(1)_R$**
- **Strong coupling expansion to $1/g^2$ order.**
  - **LO (strong coupling limit), NLO ($1/g^2$ correction)**
  - **Spatial link: LO in 1/d expansion (no spatial baryon hopping)**
  - **Temporal link : exact**
- **$\beta_g=2N_c/g^2 = 0, 1, 2, 3$**
- **Lattice size : 4^3 x 4, 6^3 x 4**
- **Auxiliary Field Monte-Carlo**

Phase Transition at μ=0

- Suppression of transition T from mean field results on anisotropic lattice with N_τ=4 by ~ 10 % for β_g=0~3.
  - Tc (aniso. MF, N_τ=4) > Tc (aniso. MF, N_τ=2), Tc (iso. MF)
- Tc from max. -dσ/dT

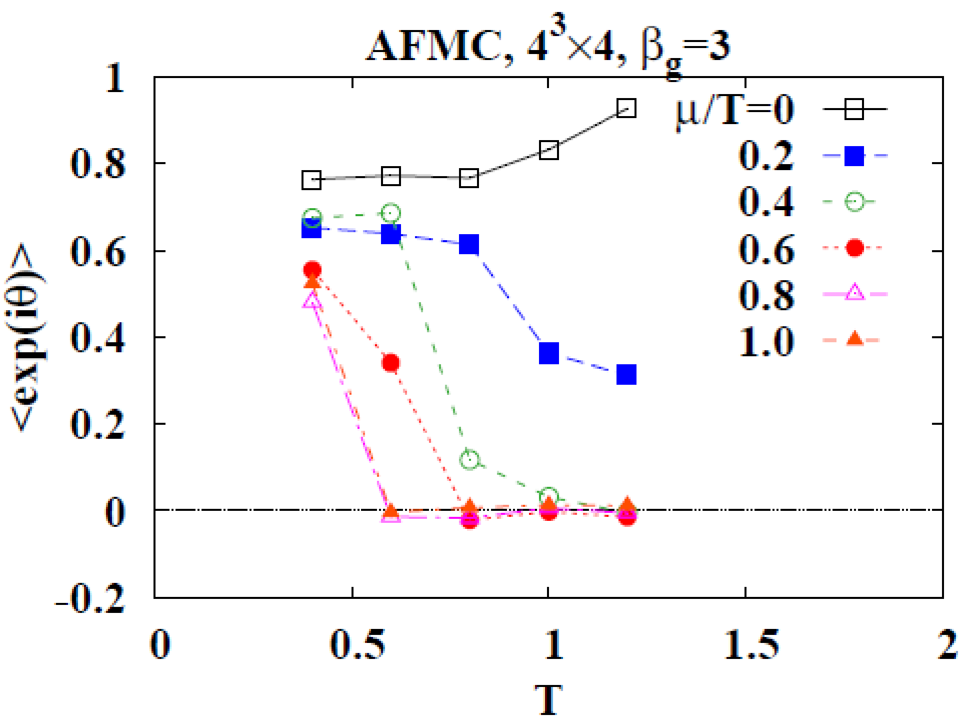


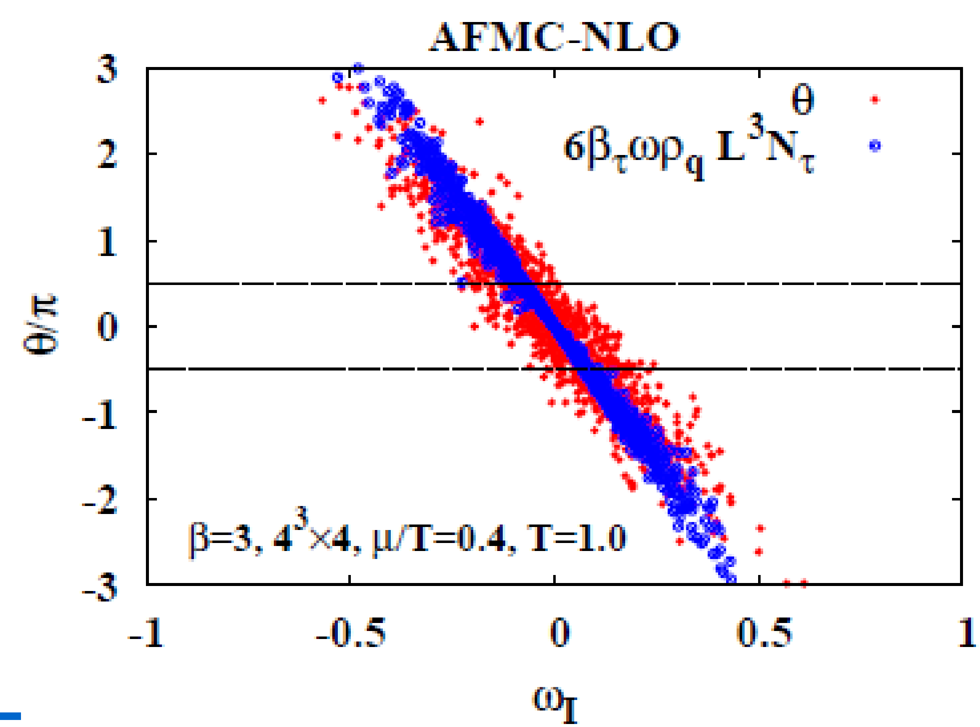


Finite μ (β_g=3)

- **Sudden collapse of the average phase factor, < exp (i θ) >, where quark number density becomes finite.**
- **Strong correlation is found btw θ and one of the aux. field, ω_I = Im(ω (k=0)). → O(V^2) effect !**

$$\theta \sim 6 \beta_\tau \rho_q \omega_I L^3 N_\tau$$

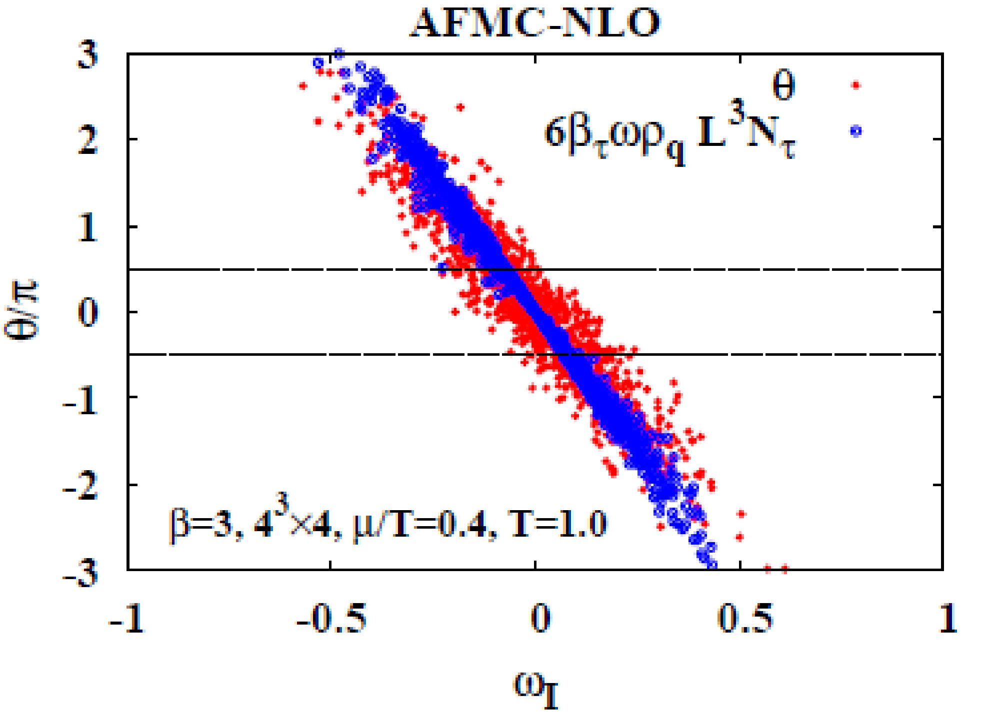




Why do we have a large complex phase ?

- **Effective action terms including ω_I(k=0)**

$$S_{\omega_I} = \frac{1}{2} C L^3 \omega_I^2 + i C \omega_I N_q$$

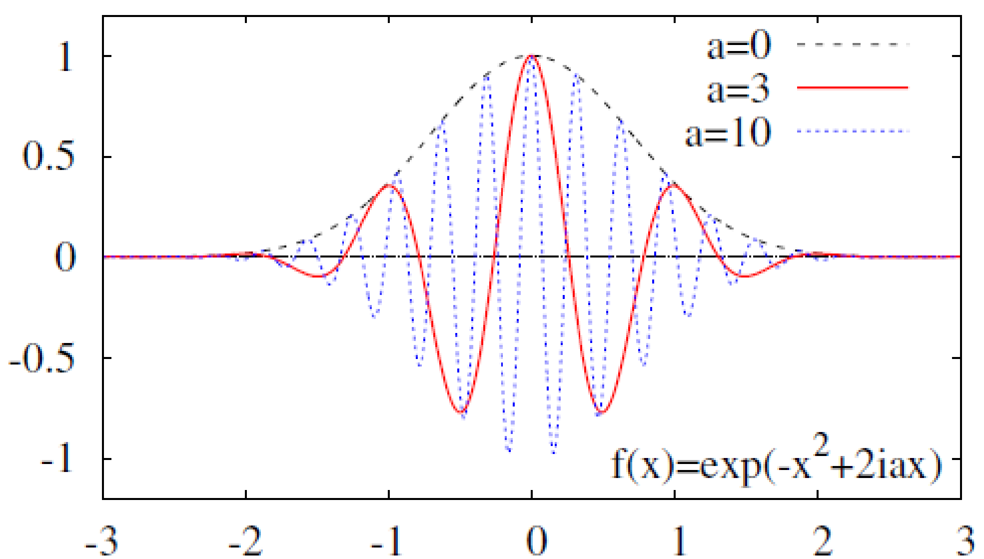


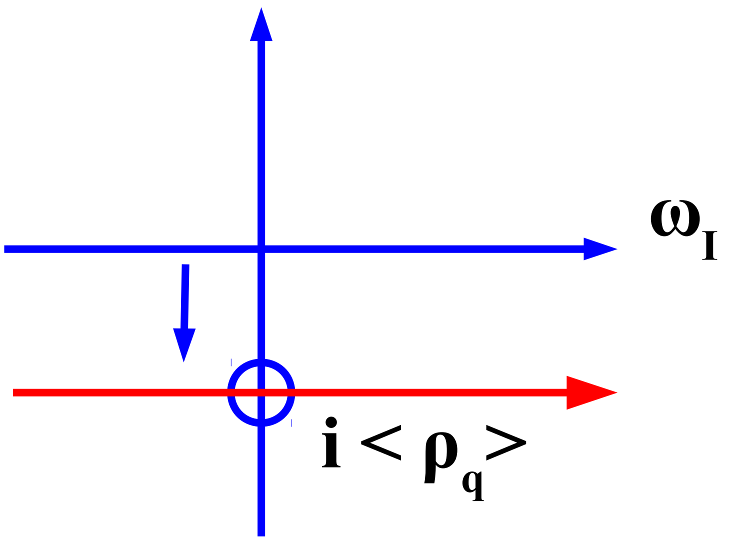
Q: Why ? A: Repulsive Vector Potential

- **Effective action terms including $\omega_I(k=0)$**

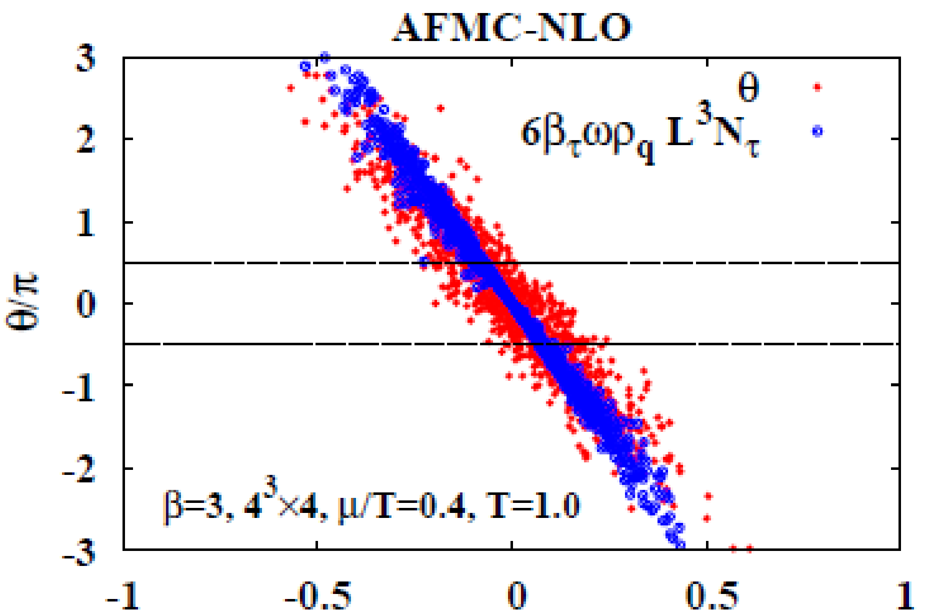
$$S_{\omega_I} = \frac{1}{2} C L^3 \omega_I^2 + i C \omega_I N_q = \frac{1}{2} C L^3 (\omega_I^2 + i \rho_q)^2 + \frac{1}{2} C L^3 \rho_q^2$$

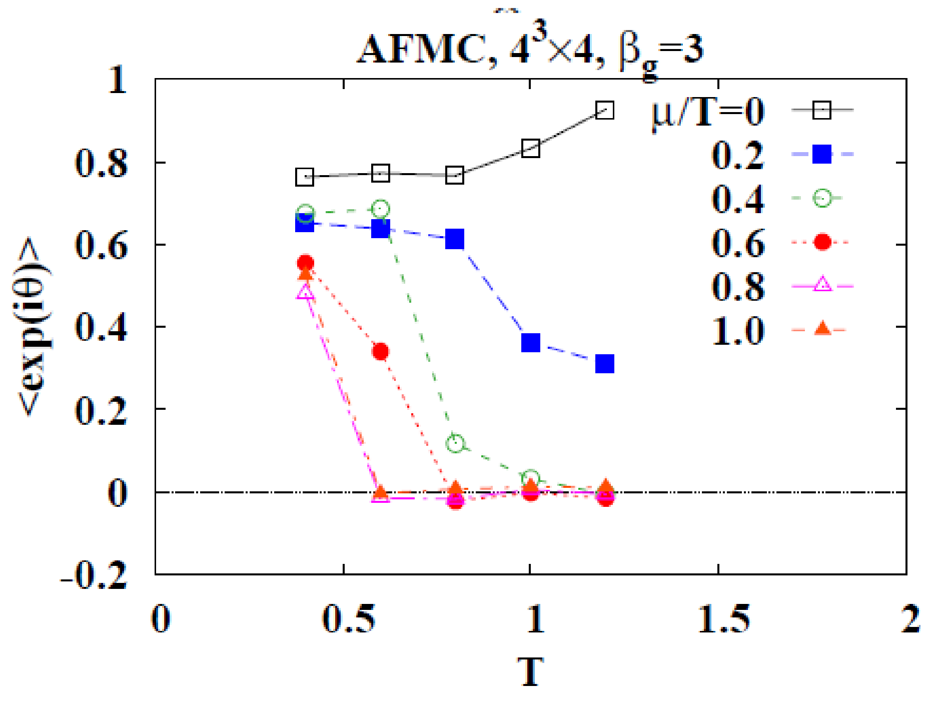
→ Textbook example of the sign problem,
and we know the answer !
→ Shift the integral path to imaginary direction.



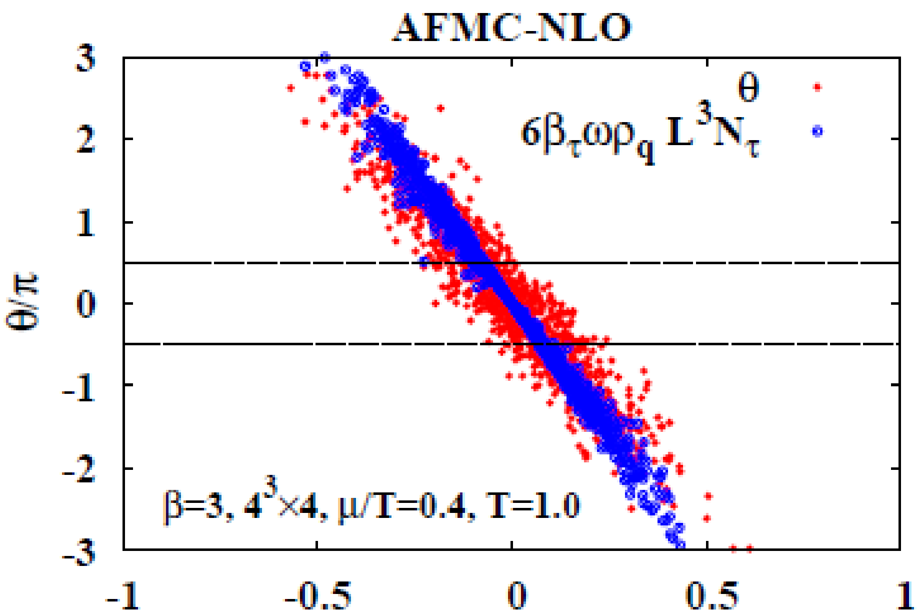


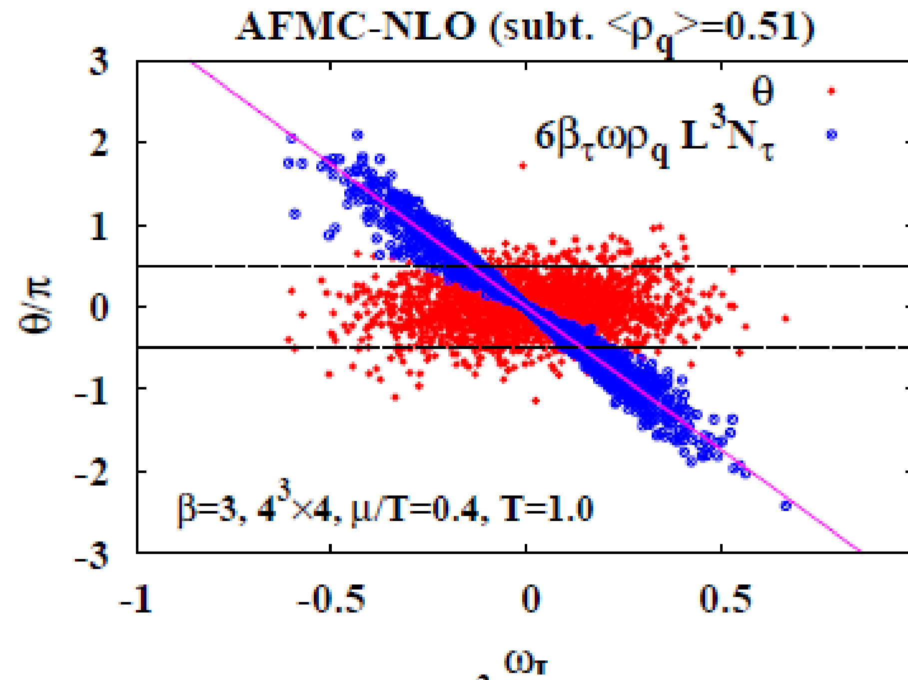
Q: Why ? A: Repulsive Vector Potential

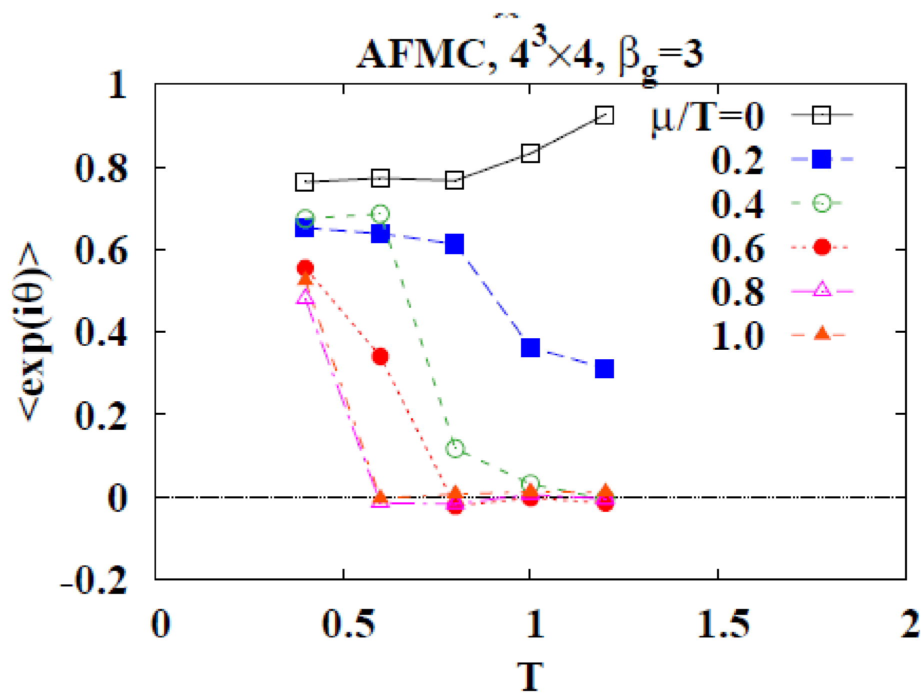


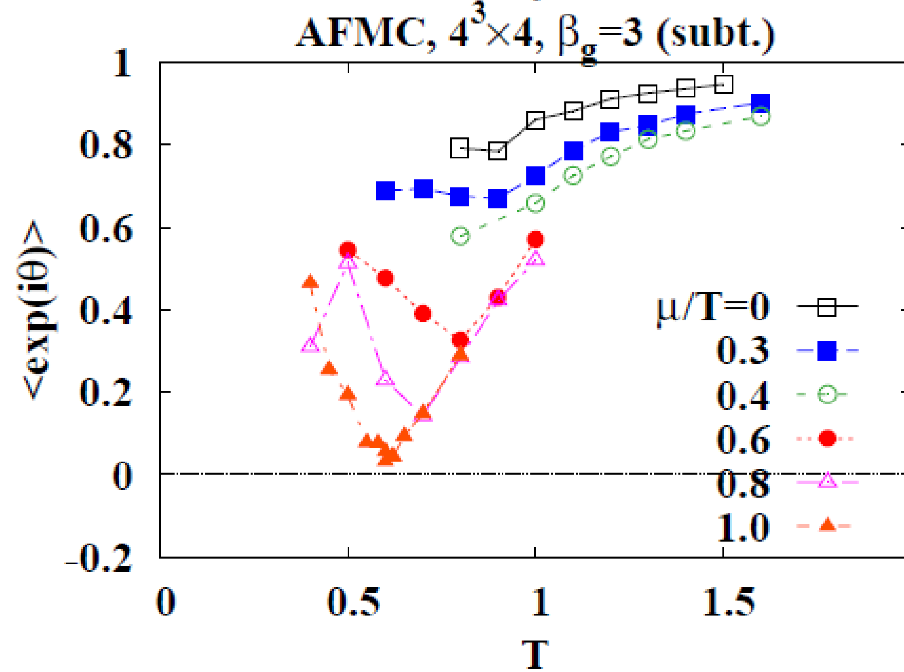


Q: Why ? A: Repulsive Vector Potential



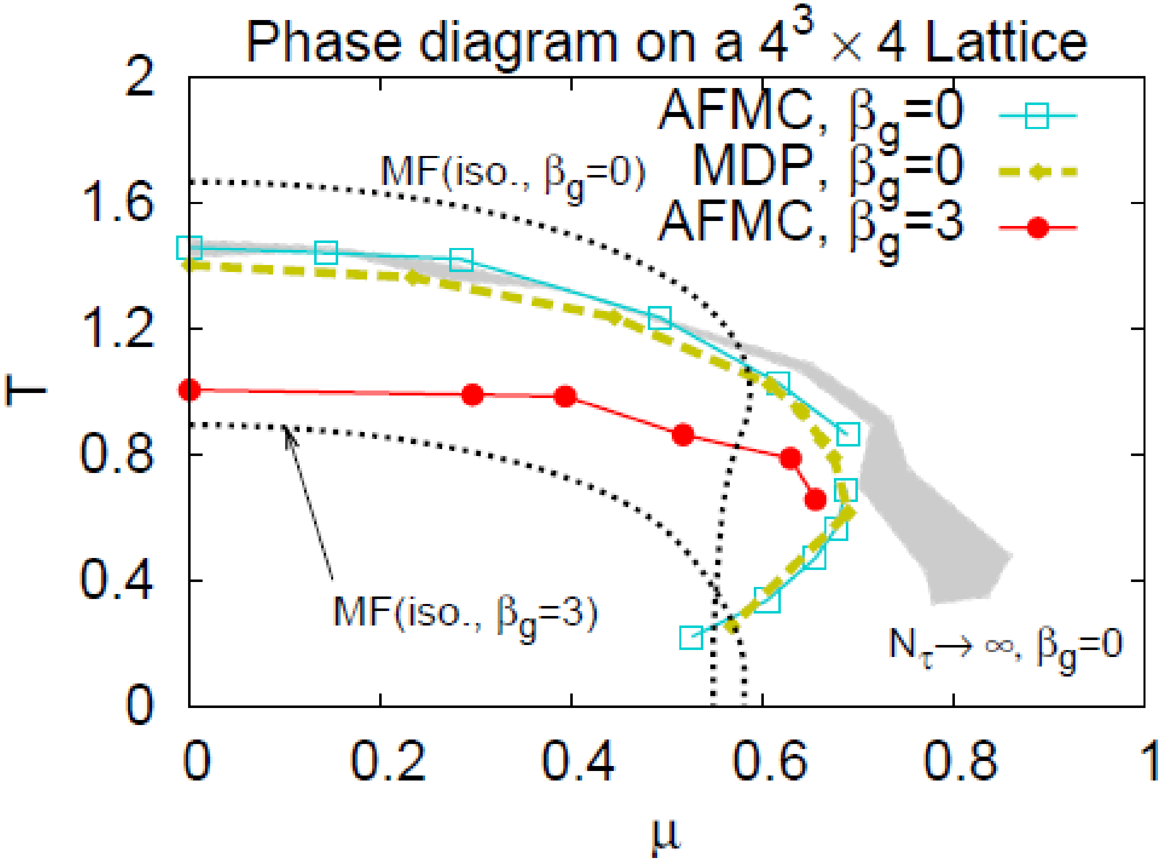






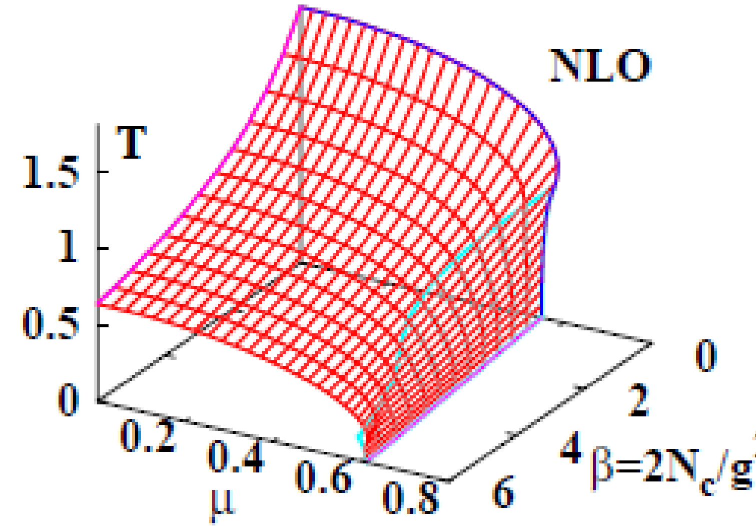
Phase diagram at finite β_g

- **Phase diagram on a 4^3 x 4 lattice at $\beta_g = 3$**
  - **Suppression of Tc(μ=0), Smaller curvature.**

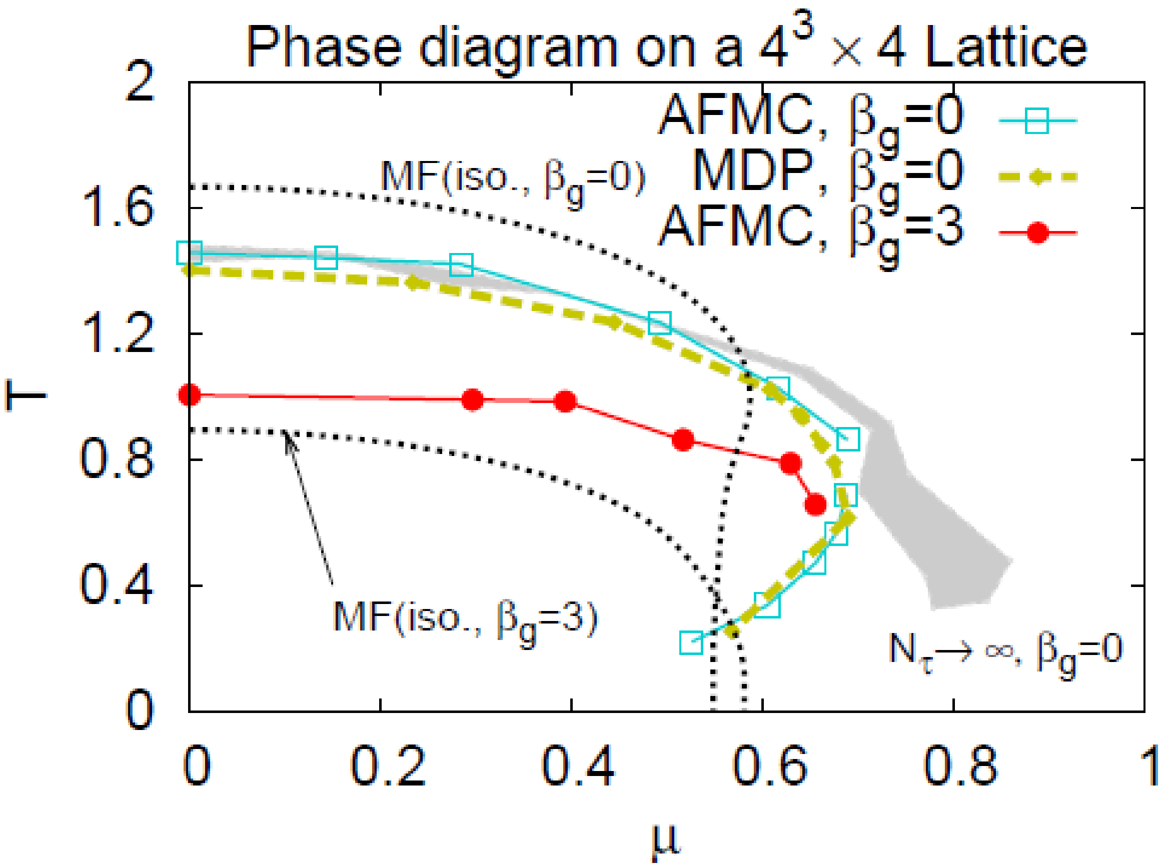


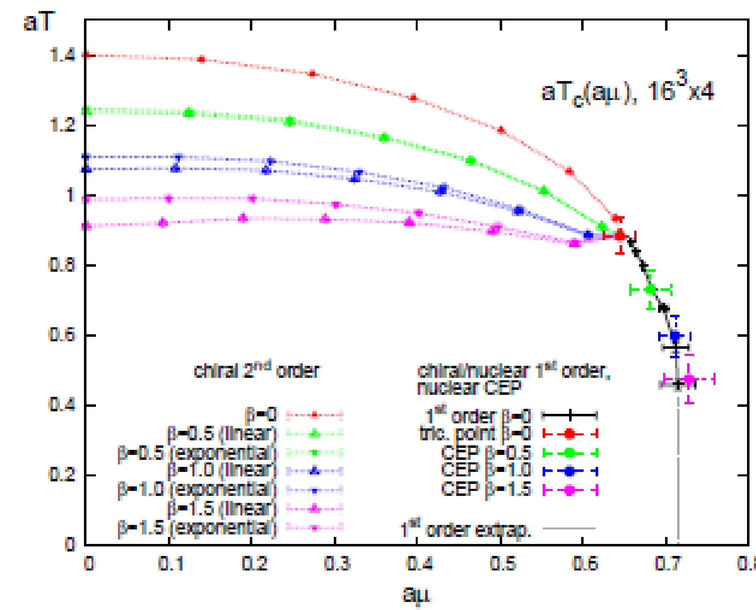
Phase diagram at finite β_g

- **Phase diagram on a 4^3 x 4 lattice at $\beta_g = 3$**
  - **Suppression of Tc(μ=0), Smaller curvature.**
  - **Different βg dep. from previous works?**



Miura, Nakano, AO, Kawamoto ('09), AO, Miura, Nakano, Kawamoto ('09)

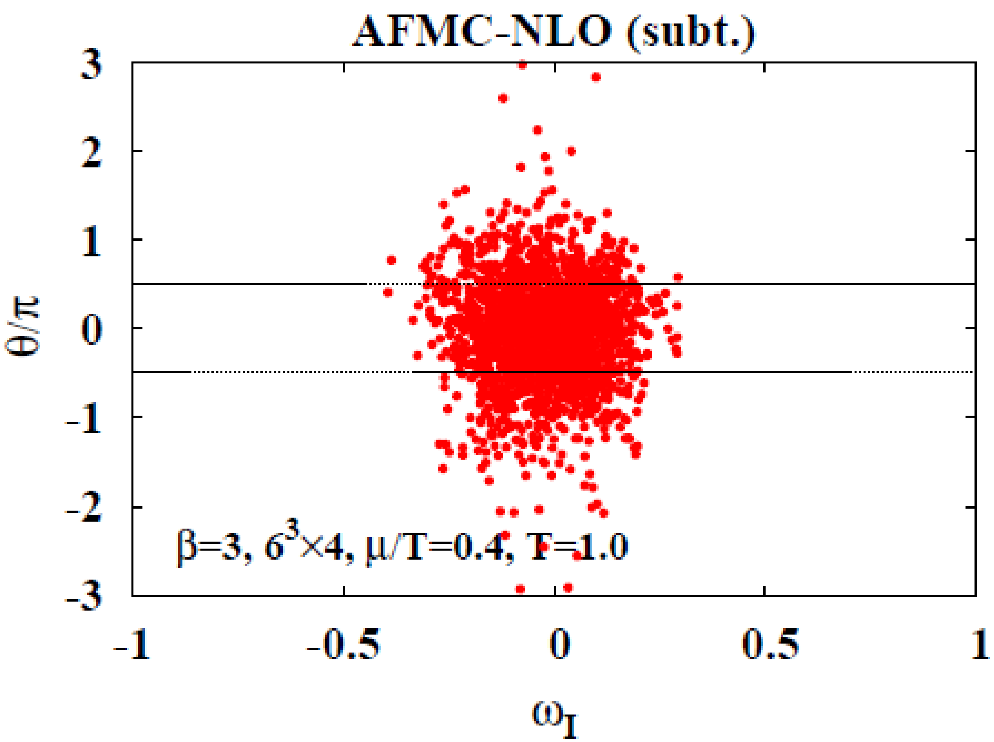


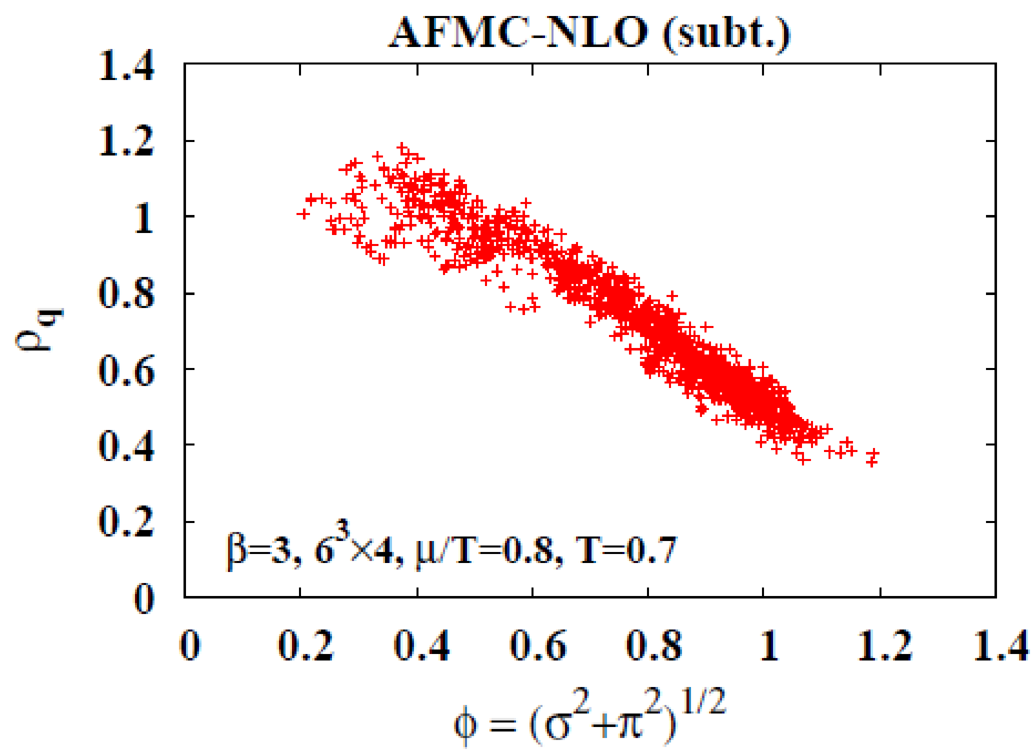


de Forcrand, Langelage, Philipsen, Unger, PRL113('14)152002

Remaining Problem

- **Larger spread of θ distribution on lager lattice.**
  How to handle it ?
- **Phase coexisting region.**
  Two local minima have different ρ_q values,
  then how can we shift the path ?





Preweighting

Preweighting

- **Histogram method (Gaussian θ dist.)**

S. Ejiri, PRD77('08)014508

$$Z=\int D\Phi d\theta e^{-S_R[\Phi]+i\theta}=\int D\Phi d\theta e^{-S'_R[\Phi]}\boxed{\frac{e^{-\theta^2/2\Delta^2[\Phi]}}{\sqrt{2\pi\Delta[\Phi]}}}e^{i\theta}$$

$$=\int D\Phi e^{-S'_R[\Phi]}\boxed{\exp(-\Delta^2[\Phi]/2)}$$

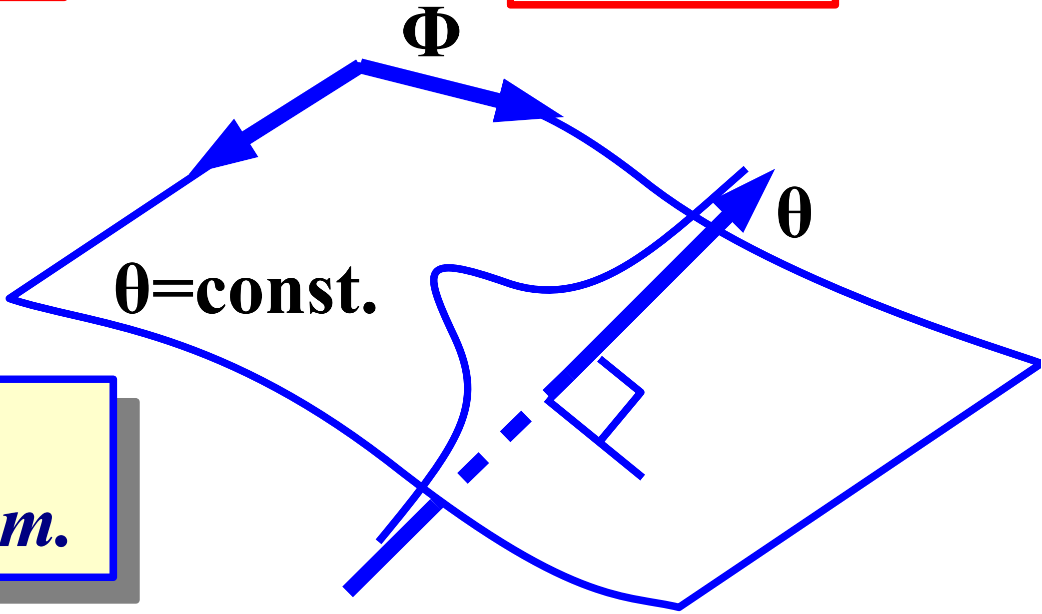
Φ dep. APF **θ-dist.**

- **Preweighting**

supp. large θ **Φ dep. supp. factor**

$$Z_{\mathrm{prew}}=\int D\Phi d\theta e^{-S_R[\Phi]}\boxed{\exp(-f(\theta))}=\int D\Phi e^{-S'_R[\Phi]}\boxed{F(\Delta[\Phi])}$$

$$F(\Delta)=\int d\theta\frac{e^{-\theta^2/2\Delta^2}}{\sqrt{2\pi\Delta}}e^{-f(\theta)}$$



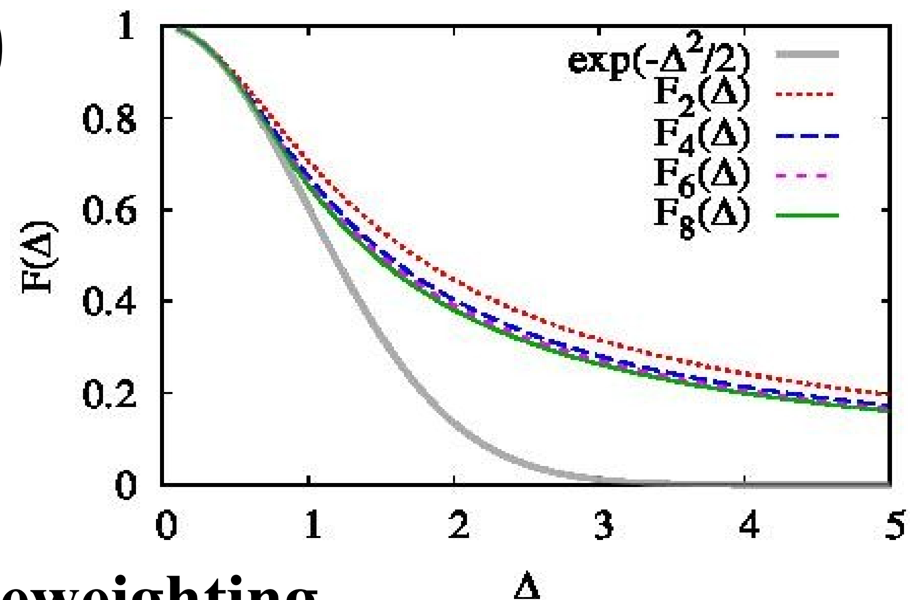
If F(Δ)=exp(-Δ²/2),
we can obtain Z w/o sign problem.

Preweighting Function

- **Can we find f(θ) which satisfies $F(\Delta)=\exp(-\Delta^2/2)$?**
  → Yes, as perturbative series of Δ

$$f(\theta) = \frac{1}{2}\theta^2 + \frac{1}{12}\theta^4 + \frac{1}{45}\theta^6 + \frac{17}{1260}\theta^8 + \mathcal{O}(\theta^{10})$$

$$\rightarrow F(\Delta) = \exp(-\Delta^2/2) + O(\Delta^{10})$$



- **But there is no free lunch.**

$$F(\Delta) = \int d\theta \frac{e^{-\theta^2/2\Delta^2}}{\sqrt{2\pi}\Delta} e^{-f(\theta)}$$

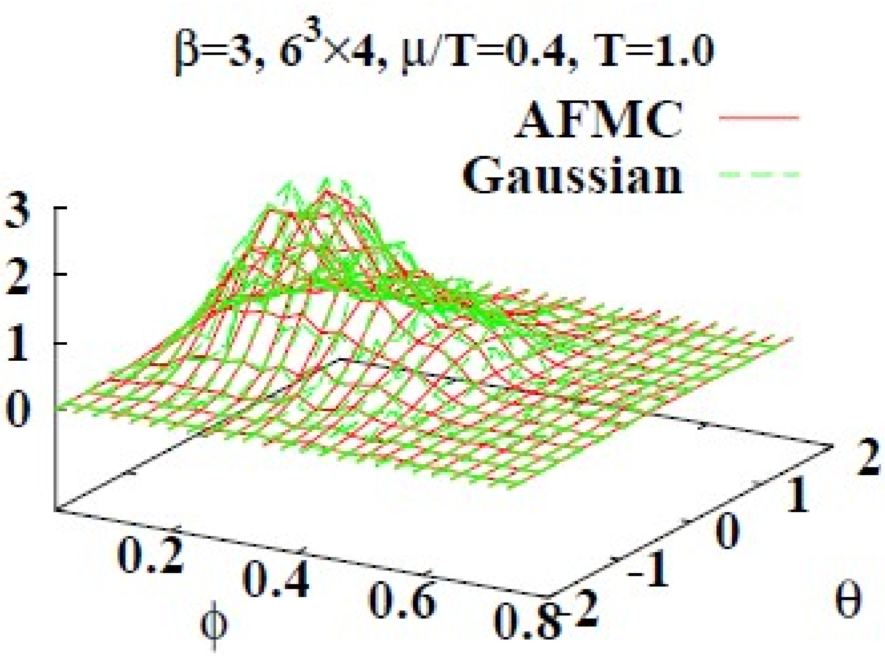
$$\rightarrow \frac{1}{\sqrt{2\pi}\Delta} \int d\theta\, e^{-f(\theta)} \quad (\Delta \rightarrow \infty)$$

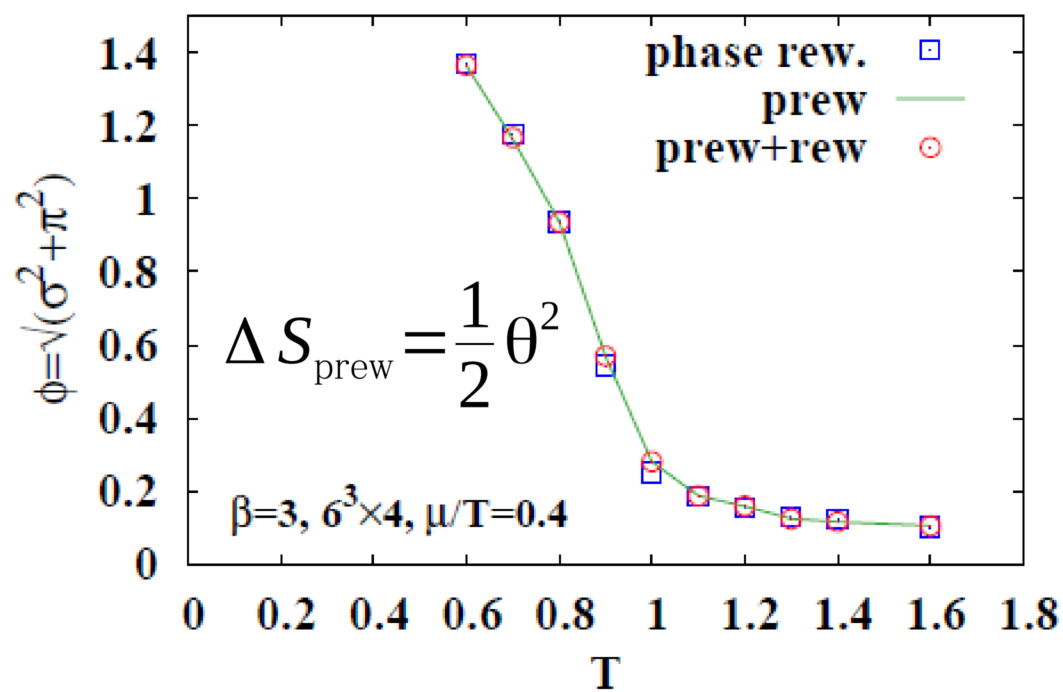
- **Practical method: Preweighting+Reweighting**
  - **MC with preweighting fn, e.g. $f(\theta)=\theta^2/2$,**
  - **Make a histogram in Φ and obtain Δ[Φ]**
  - **Give Reweighting factor $\exp(-\Delta^2/2)$ / F(Δ)**

Let us examine in SC-LQCD !

θ dist. in SC-LQCD (β_g=3, μ/T=0.4)

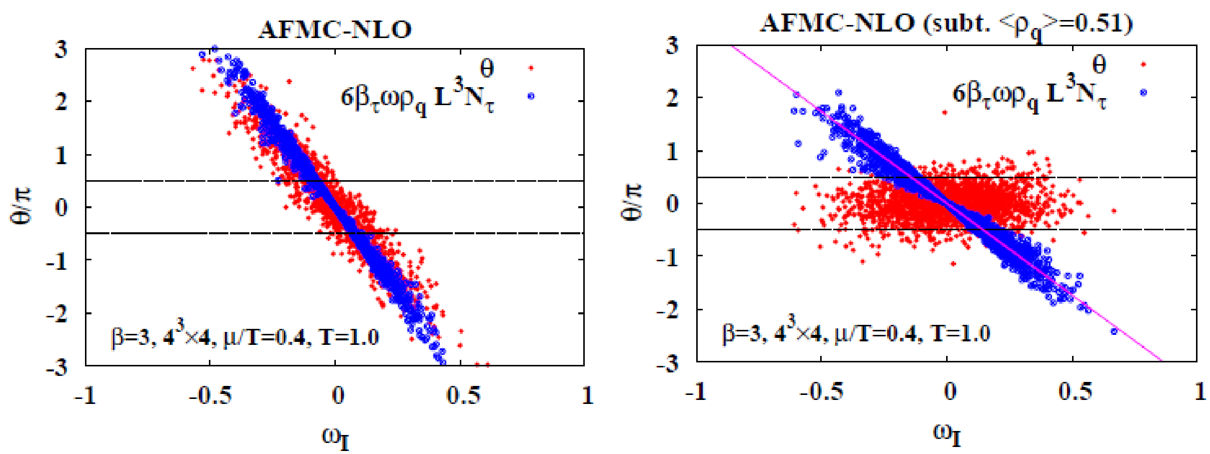
- **Chiral condensate distribution is spread, but θ distribution is well approximated by Gaussian.**
- **Observed results in**
  phase reweighting,
  preweighting, preweighting+(Gauss) reweighting
  agrees well.





Summary

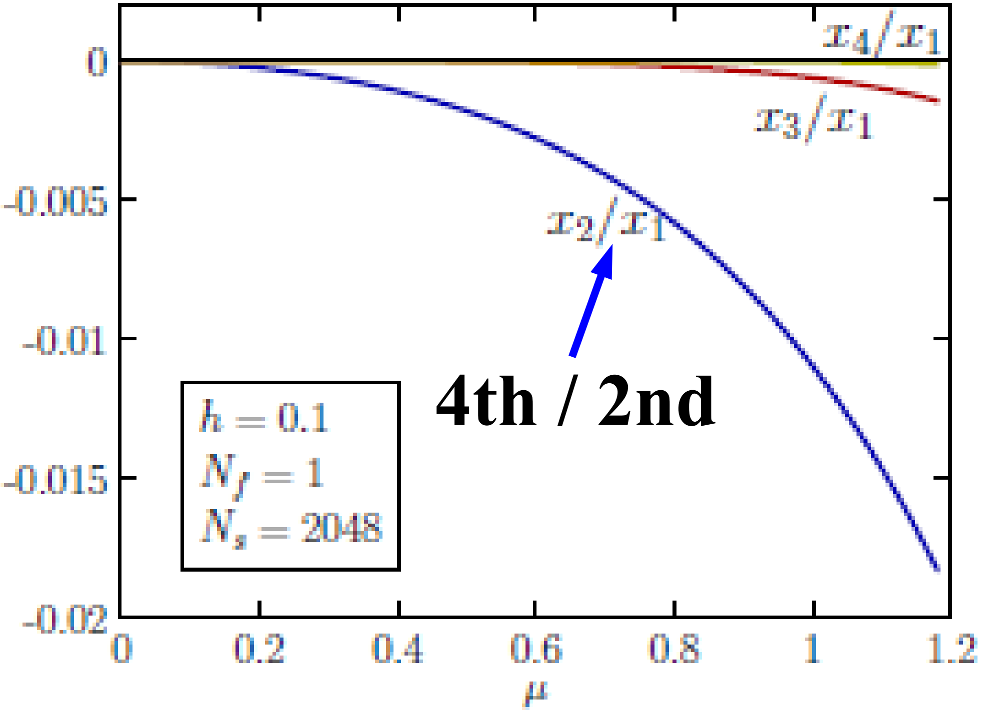
- **Strong-coupling lattice QCD including fluctuation and $1/g^2$ effects is developed, and applied to phase diagram study.**
  - **Dominant contribution to complex phase comes from the repulsive vector potential, which can be removed by shifting the integration path.**



  - **Caveat: Self-consistent subtraction is necessary for stability.**
  - **Preliminary phase diagram is obtained.**
- **Once the correlated auxiliary fields are subtracted, θ distribution seems to be well described by Gaussian. Then we can obtain observables even when APF is very small.**
  Adding preweighting action will help to enhance statistics.

Discussion & Future works

- **Non-gaussianity of θ distribution**
  - **SC & HP expansion:** ***Greensite, Myers, Splittorf, arXiv:1311.4568.***
  - **Superposed Lorenzian in the π cond. phase**
    M.P. Lombardo, K. Splittorff, J.J.M. Verbaarschot, PRD80 ('09) 054509
- **To do**
  - **Config. dep. subtraction.**
  - **Polyakov loop**
- **Application to other systems**
  - **AFMC with $1/g^2$ terms**
  - **Link MC LQCD**
    Can we remove π cond. phase ?
  - **Which variable is most closely correlated with θ ?**



Greensite, Myers, Splittorf, arXiv:1311.4568.

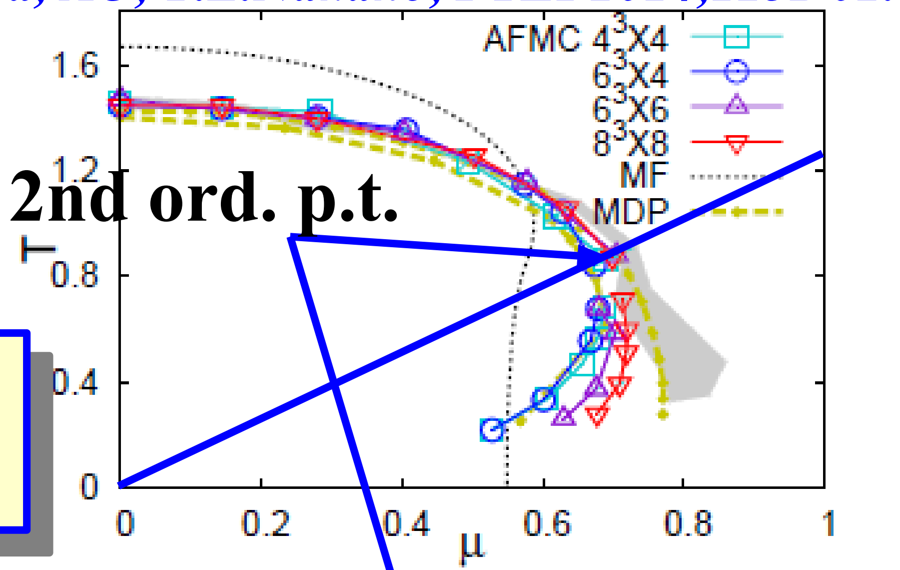
Thank you !

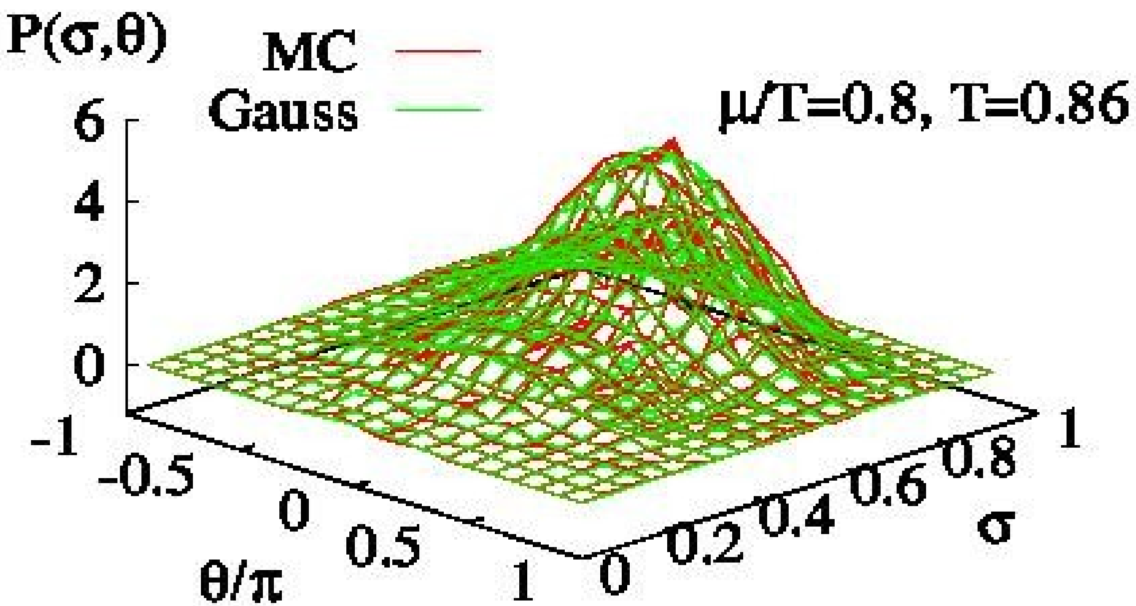
θ dist. in AFMC-SCL (μ/T=0.8)

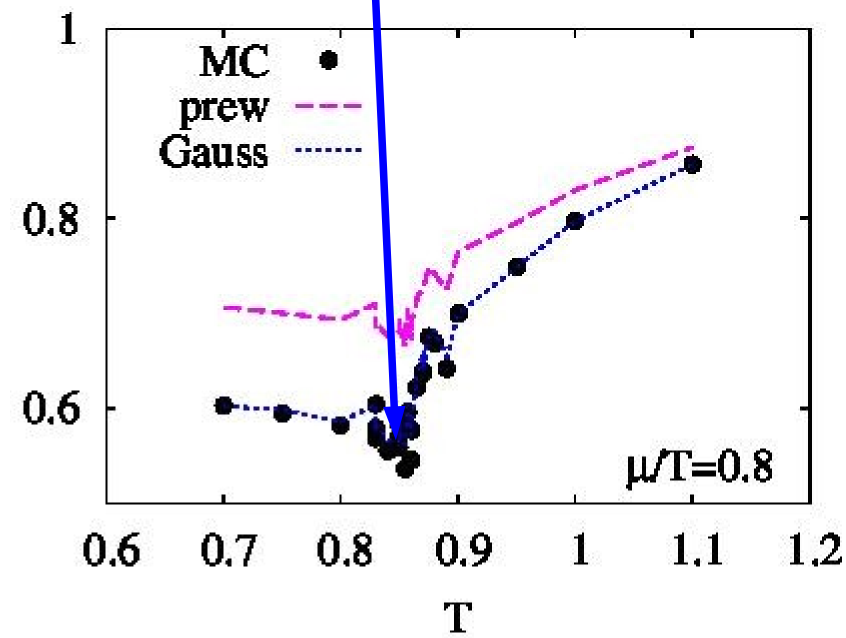
T.Ichihara, AO, T.Z.Nakano, PTEP2014,123D02.

- θ dist. ~ Gaussian
- average prew. factor ~ 0.7
- average phase factor ~ 0.5-0.6

Preweighting accounts for a large part of weight cancellation !



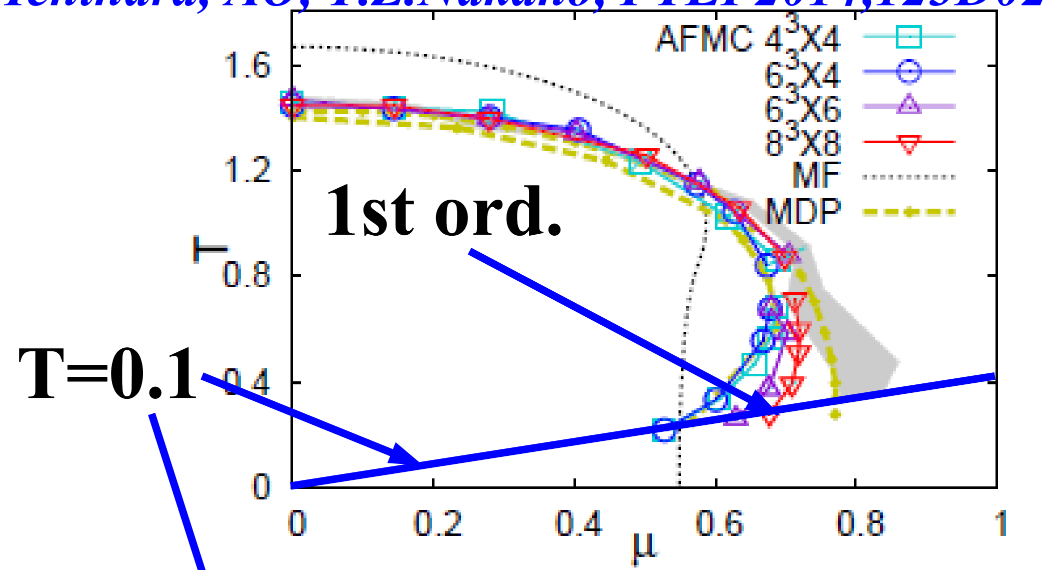


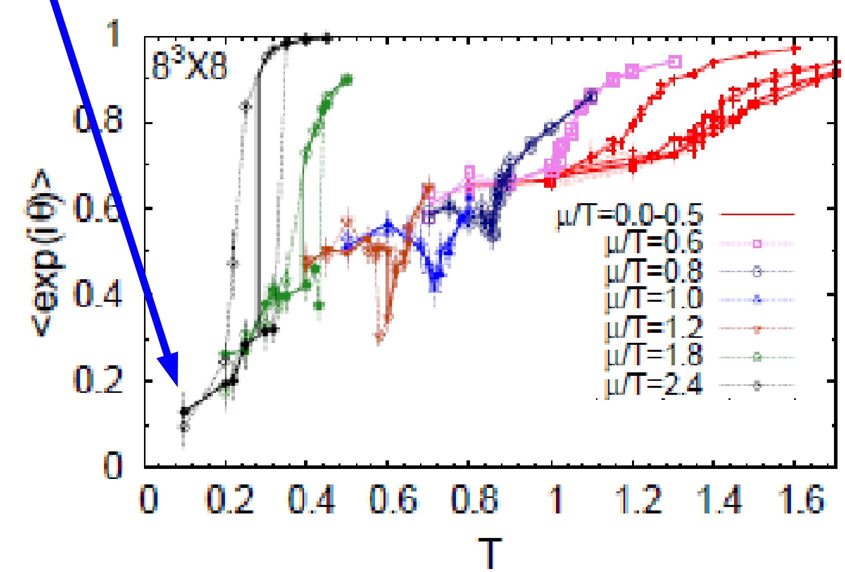


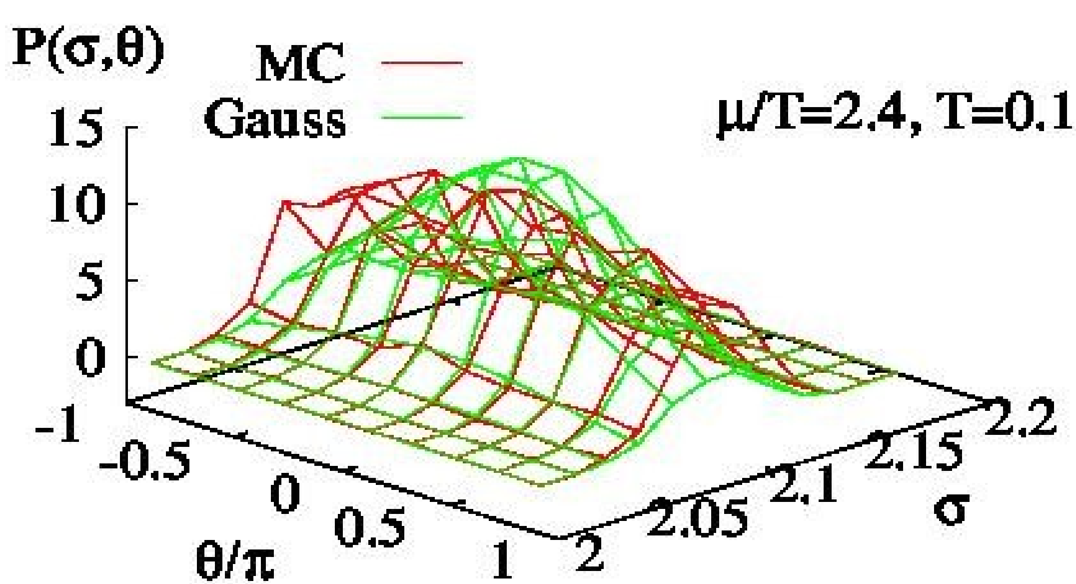
θ dist. in AFMC-SCL (μ/T=2.4)

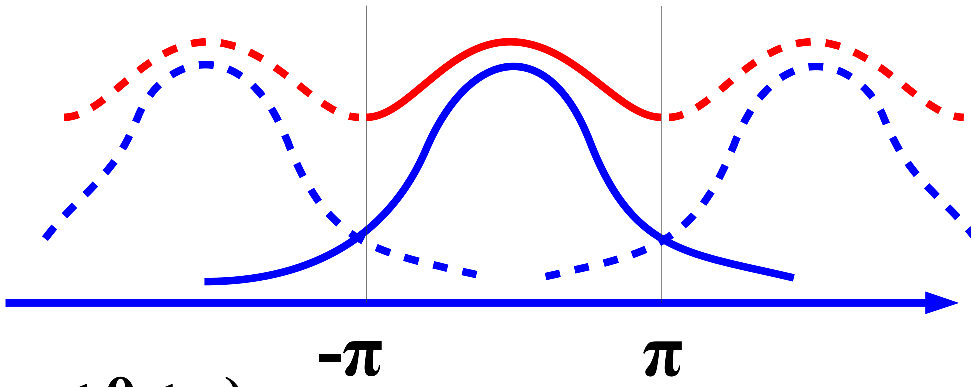
T.Ichihara, AO, T.Z.Nakano, PTEP2014,123D02.

- **θ dist. ≠ Gaussian**
  - **θ distribution well extends around θ ~ π.**
    → We need to consider *mirror* contributions.





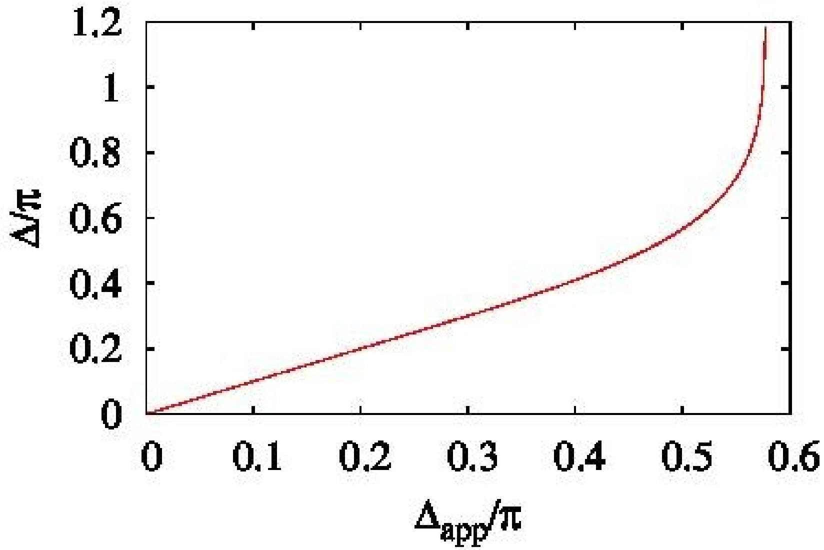


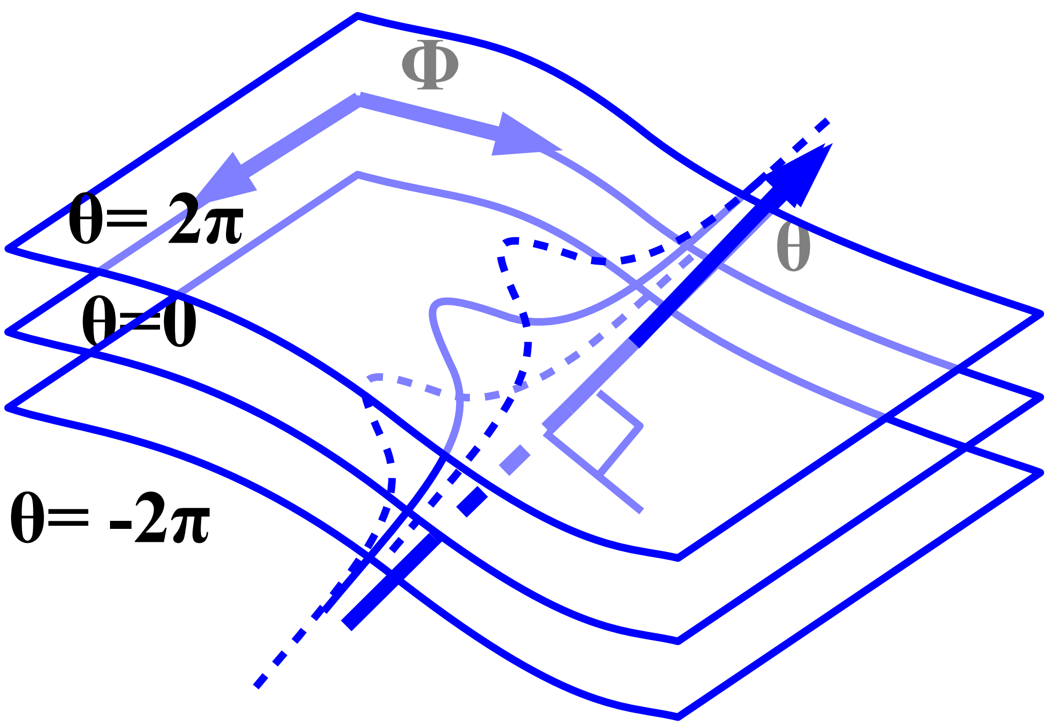


- **Mirrored Gaussian**

$$P(\theta)=\frac{1}{\sqrt{2\pi\Delta}}\sum_n \exp\left(-\frac{(\theta-2\pi n)^2}{2\Delta^2}\right)$$

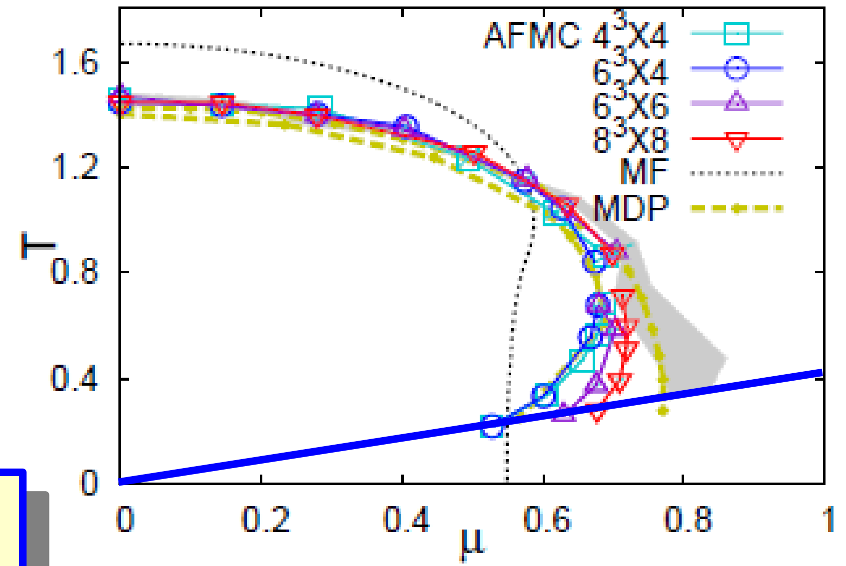
  - **Apparent std. dev. Δ (obtained in –π< θ< π)**
    → Actual Δ (defined in -∞< θ < ∞)
  - **Alternative**
    Obtain θ in -∞ < θ < ∞ (Ejiri)





θ dist. in AFMC-SCL (μ/T=2.4, again)

- **θ dist. ~ Mirrored Gaussian**
  - **APF is also well explained with Mirrored Gaussian.**
  - **average prew. factor ~ (0.4-0.6)**
  - **average phase factor ~ (0.1-0.3)**



Preweighting accounts for around half of weight cancellation !