

Preweighting method in Monte-Carlo sampling with complex action – Strong-Coupling Lattice QCD with $1/g^2$ correction, as an example –

Akira Ohnishi¹ and Terukazu Ichihara^{1,2}
1. YITP, Kyoto U., 2. Kyoto U.

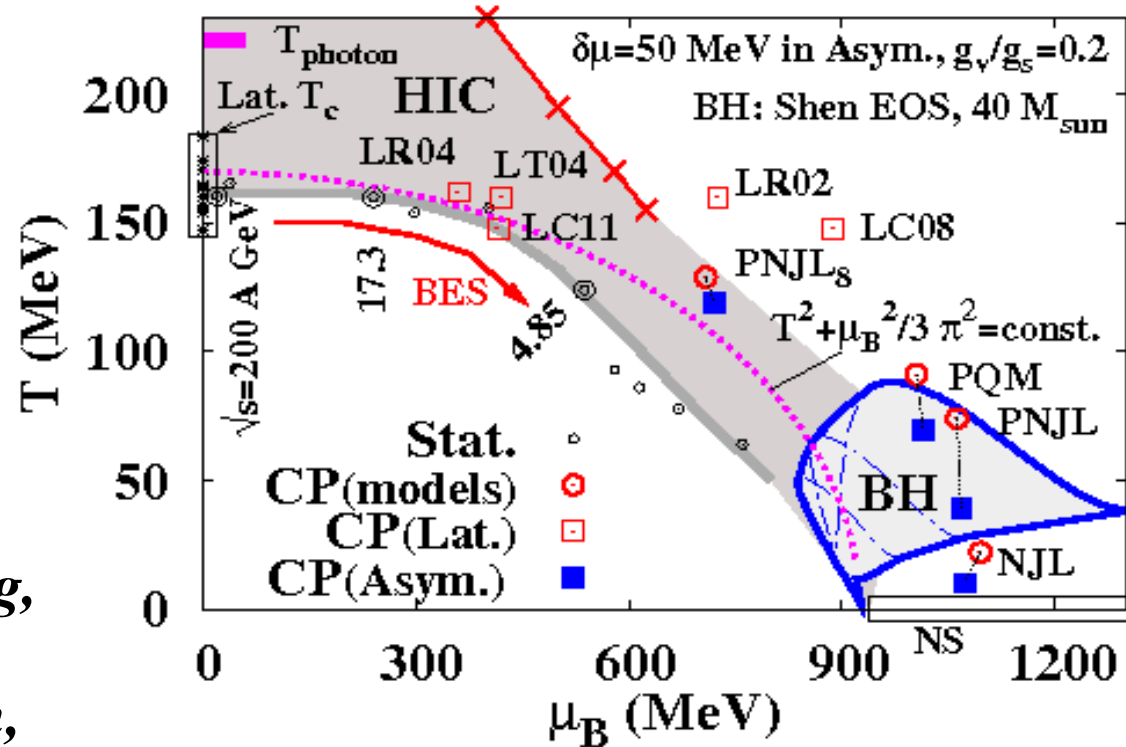
*The 33rd Int. Symp. on Lattice Field Theory,
Kobe, Japan, Jul.14-18, 2015*



QCD phase diagram and Sign Problem

AO, PTPS193('12)1.

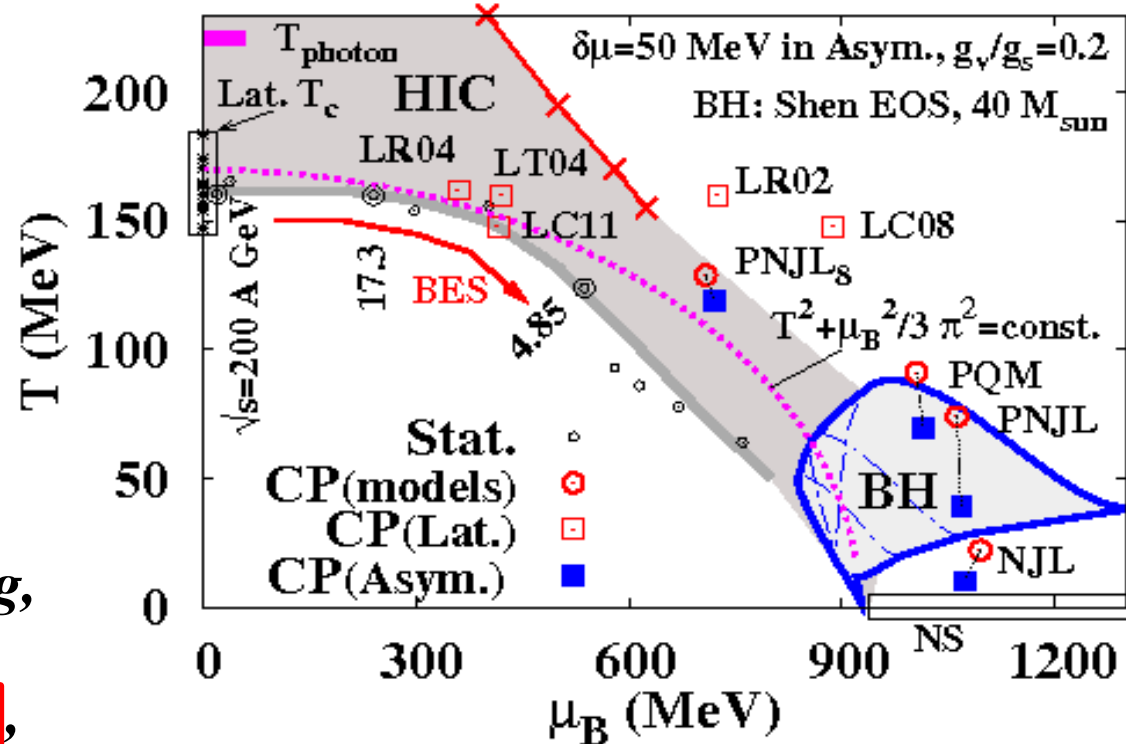
- Finite density QCD
 - Critical Point,
 - Nuclear Matter EOS,
 - Compact Stars, ...
 - Obstacle
 - = Sign problem at finite μ .
 - Many methods proposed.
 - Taylor expansion, Re-weighting,*
 - Imag. $\mu+AC$,*
 - Canonical, Fugacity expansion,*
 - Histogram method,*
 - Complex Langevin,*
 - Lefschetz thimble,*
 - Strong Coupling,*
 - ...
- but it is still difficult to attack low T.



QCD phase diagram and Sign Problem

AO, PTPS193('12)1.

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



Many Talks During Lattice 2015 !

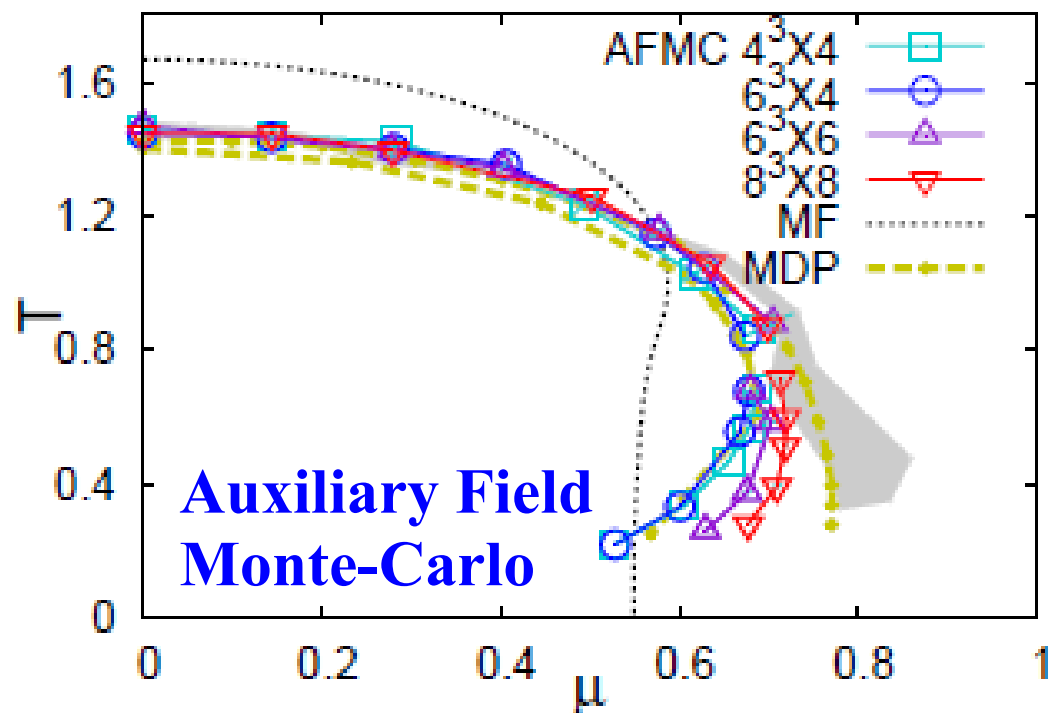
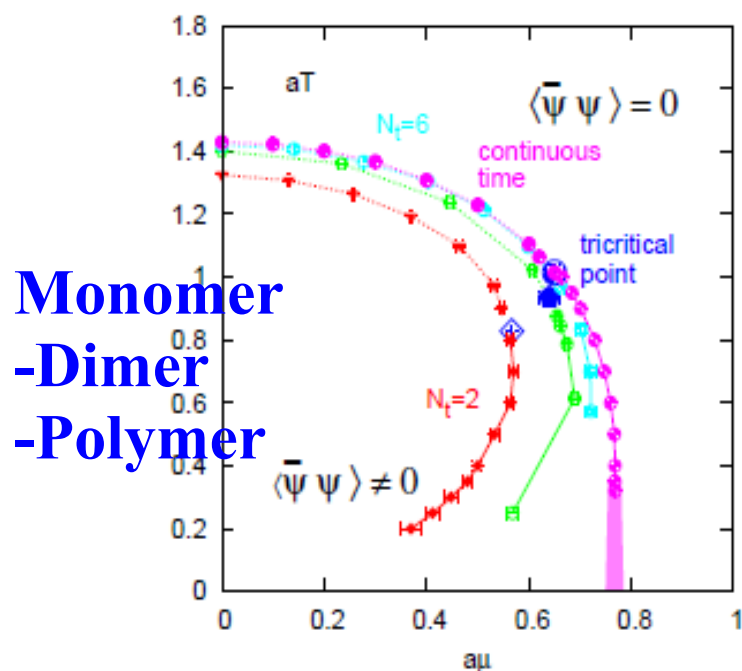
Less Popular but some in Lattice 2015.

but it is still difficult to attack low T .

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), ...

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



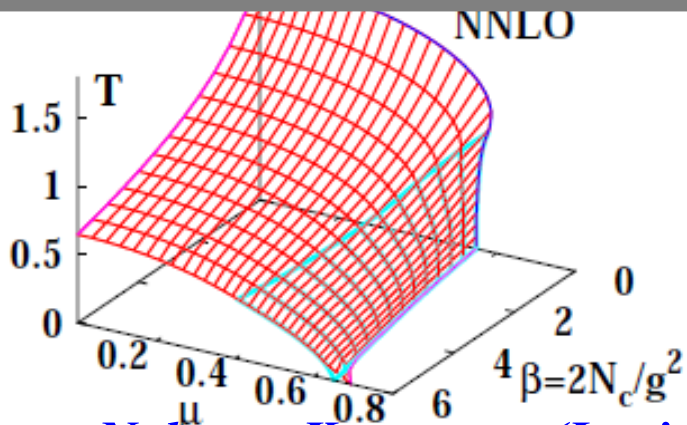
de Forcrand, Fromm ('10), de Forcrand, Langelage, Philipsen, Unger ('14)

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

Finite coupling corrections

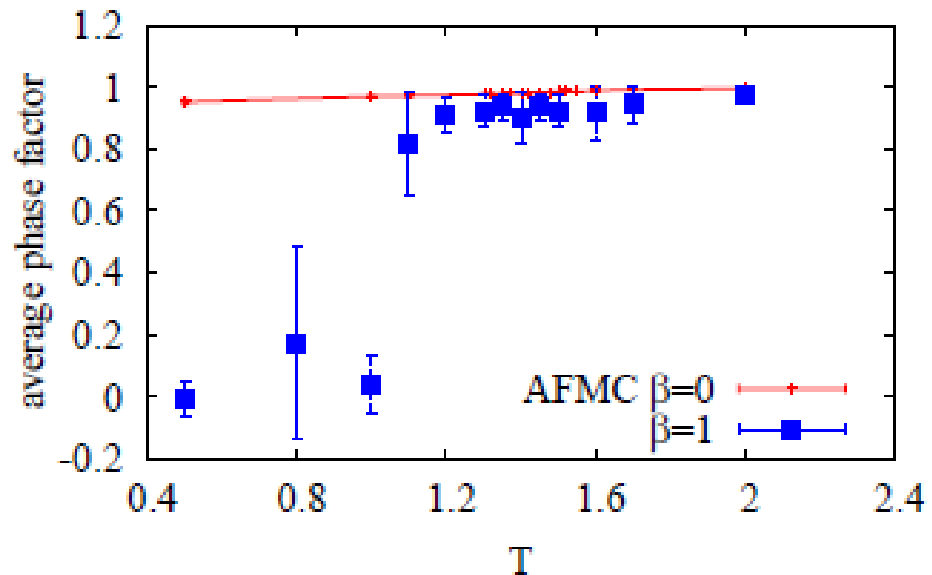
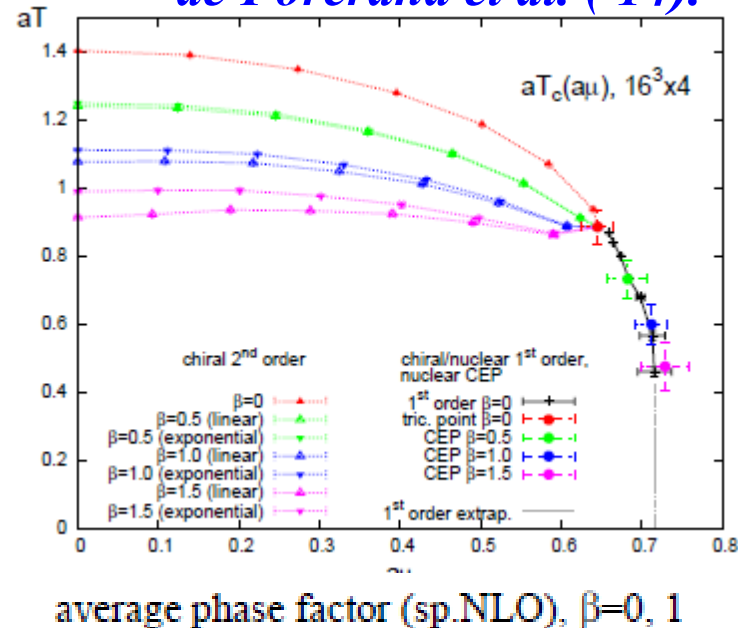
- Mean field results: No sign prob.
- Monomer-Dimer-Polymer: Phase diagram by reweighting *de Forcrand, Langelage, Philipsen, Unger ('14)*
- Auxiliary Field Monte-Carlo: Severe weight cancellation at finite $1/g^2$ *T.Ichihara, T.Z.Nakano, AO, Lattice 2014*

Direct sampling method is not yet fully developed.



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

de Forcrand et al. ('14).



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)

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

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

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

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

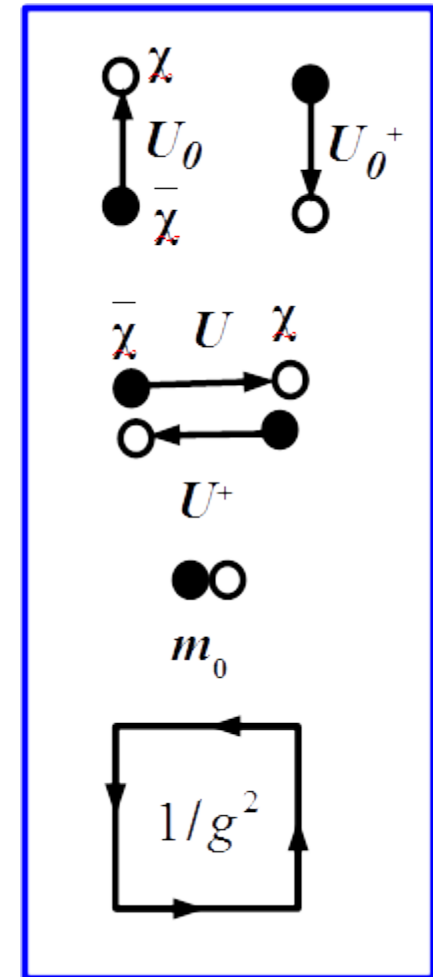
● Staggered sign factor

$$\eta_j(\mathbf{x}) = (-1)^{x_0 + \dots + x_{j-1}}$$

● $U(1)_L \times U(1)_R$ chiral sym.

$$\chi_x \rightarrow \exp[i\theta \varepsilon(\mathbf{x})] \chi_x, \quad \varepsilon(\mathbf{x}) = (-1)^{x_0 + x_1 + x_2 + x_3}$$

● Anisotropy parameter γ



Strong Coupling Lattice QCD

■ Strong coupling limit

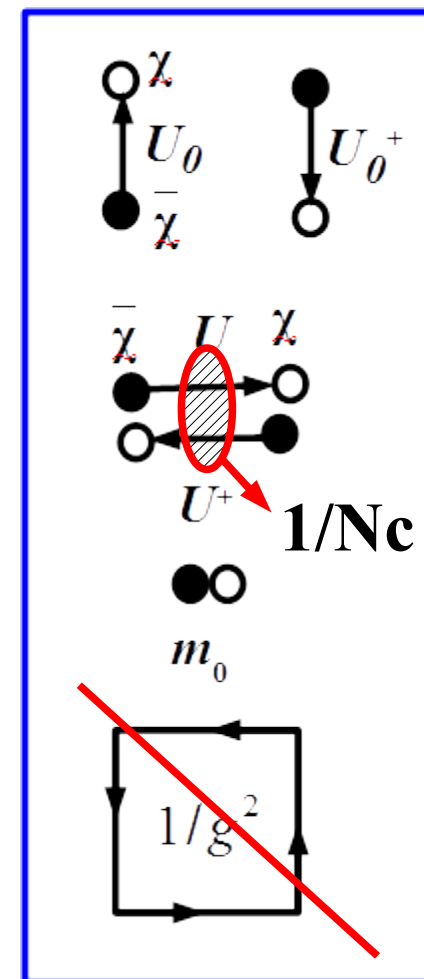
Damgaard, Kawamoto, Shigemoto ('84), Jolicoeur, Kluberg-Stern, Lev, Morel, Petersson ('84).

Spatial link integral → Fermion action with four-Fermi int.

(LO in 1/d expansion)

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

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



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)

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

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

Eff. Action with 1/g² correction

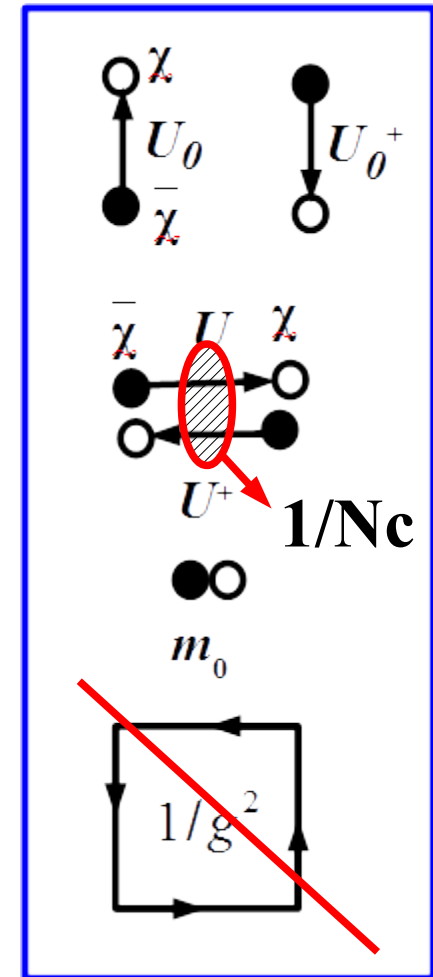
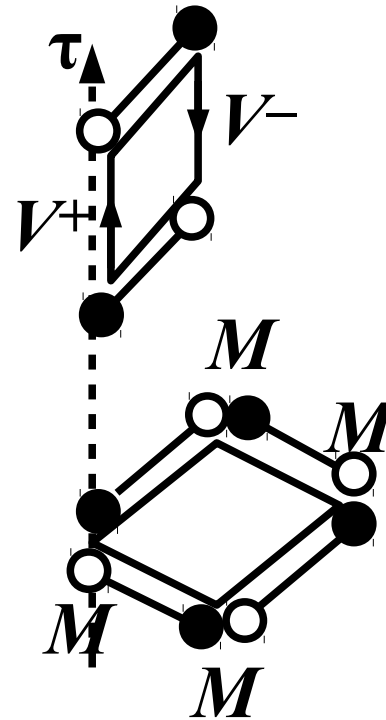
Faldt, Petersson ('86), Miura, Nakano, AO,

Kawamoto ('09)

$$S_{\text{eff}}^{(\text{NLO})} = S_{\text{eff}}^{(\text{SCL})} + \frac{\beta_\tau}{2} \sum_{x,j} [V_x^+ V_{x+\hat{j}}^- + V_{x+\hat{j}}^+ V_x^-]$$

$$- \frac{\beta_s}{\gamma^4} \sum_{x,k,j,k \neq j} M_x M_{x+\hat{j}} M_{x+\hat{k}} M_{x+\hat{k}+\hat{j}}$$

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



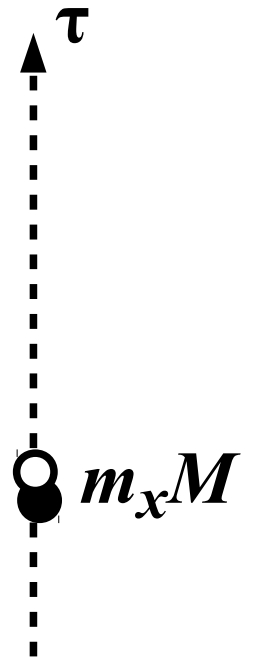
Extended Hubbard-Stratonovich Transformation

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

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

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

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



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

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

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

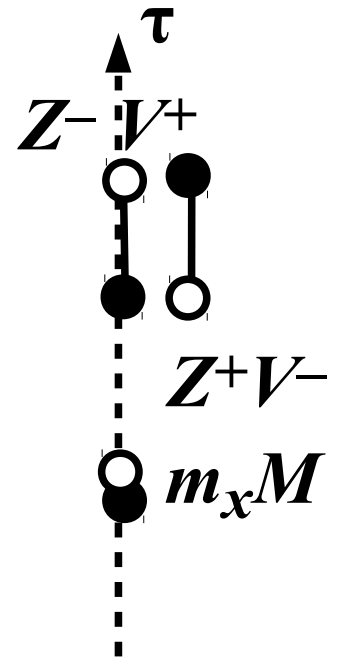
$$S_{\text{AF}} = \frac{L^d}{4N_c} \sum_{\mathbf{k}, \tau, f(\mathbf{k}) > 0} f(\mathbf{k}) \left[\sigma_{\mathbf{k}, \tau}^* \sigma_{\mathbf{k}, \tau} + \pi_{\mathbf{k}, \tau}^* \pi_{\mathbf{k}, \tau} \right]$$

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

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

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

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



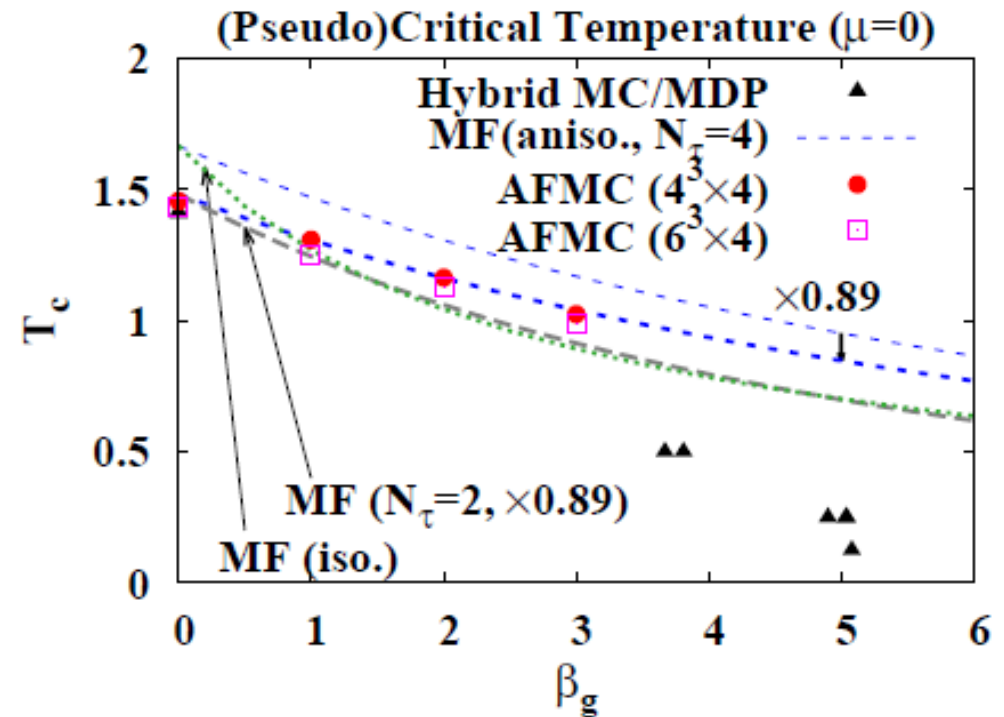
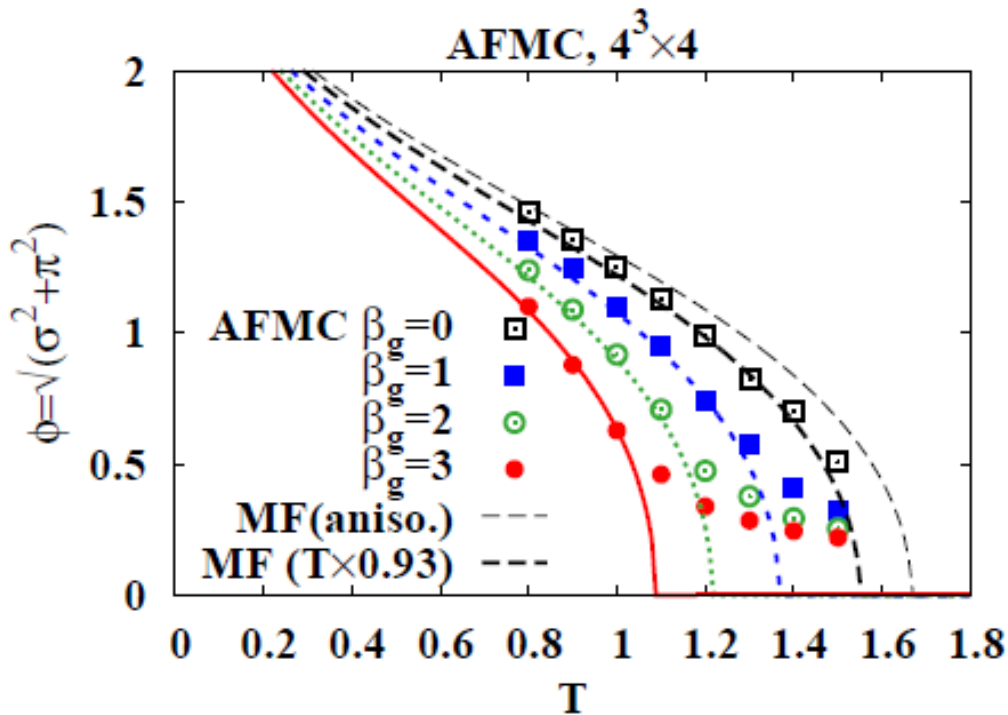
SCL+1/g² corr. → x dep. mass + mod. of temporal coef.

Lattice Setup

- One species of unrooted staggered fermion
 - $N_f = 4$ in the continuum limit
 - Chiral symmetry: $U(1)_L \times U(1)_R$
- 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 : $4^3 \times 4, 6^3 \times 4$
- Auxiliary Field Monte-Carlo

Phase Transition at $\mu=0$

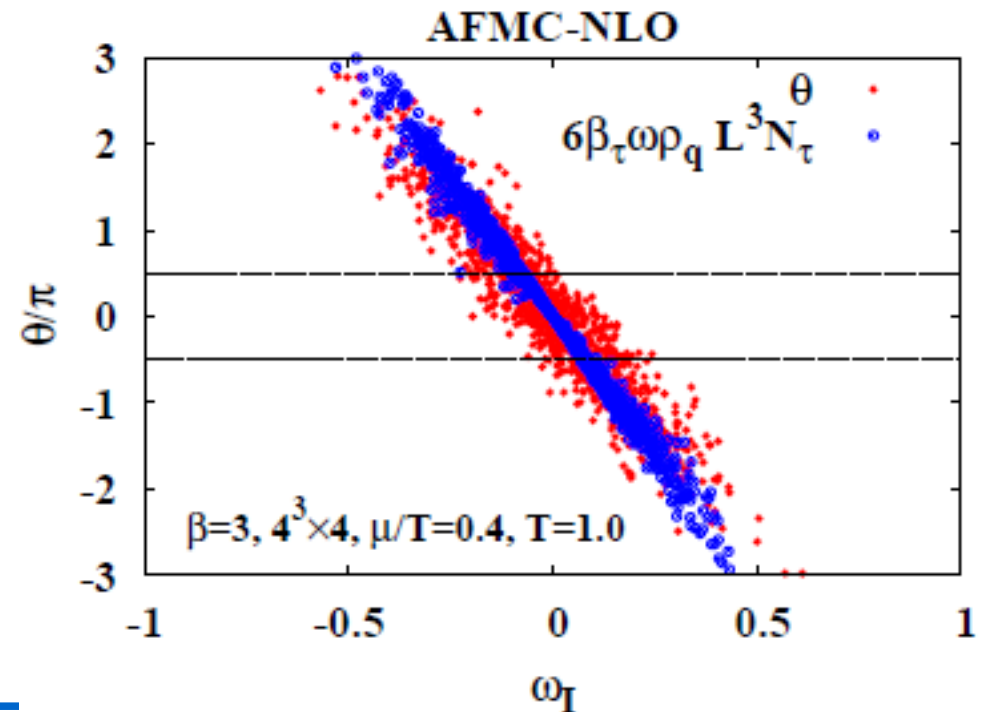
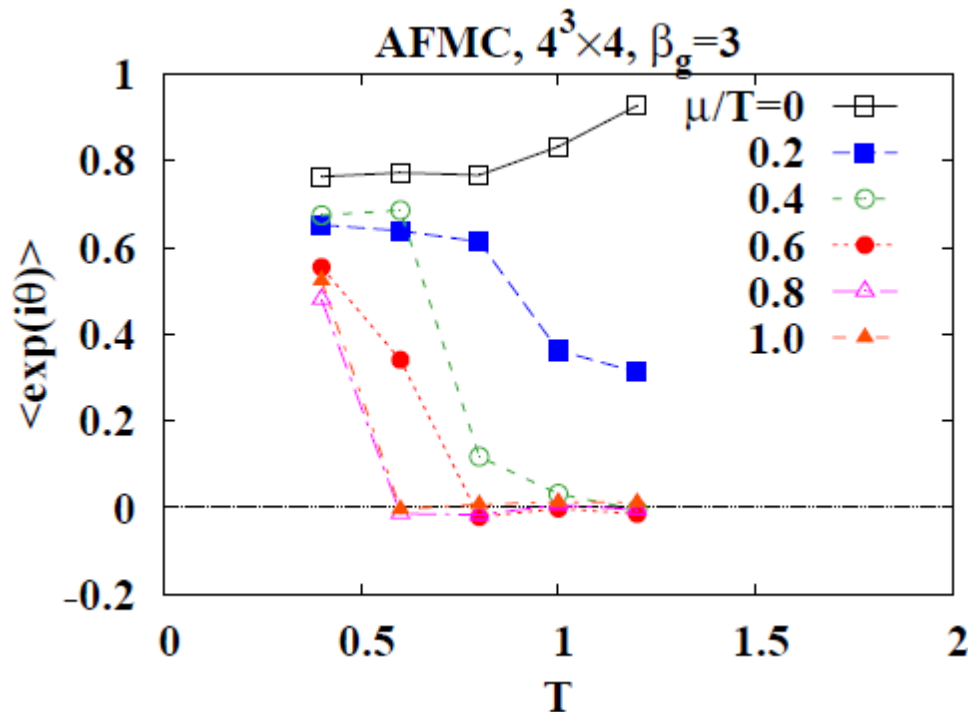
- Suppression of transition T from mean field results on anisotropic lattice with $N_\tau=4$ by $\sim 10\%$ for $\beta_g=0\sim 3$.
 - $T_c(\text{aniso. MF}, N_\tau=4) > T_c(\text{aniso. MF}, N_\tau=2), T_c(\text{iso. MF})$
- T_c from max. $-d\sigma/dT$



Finite μ ($\beta_g=3$)

- Sudden collapse of the average phase factor, $\langle \exp(i\theta) \rangle$, where quark number density becomes finite.
- Strong correlation is found btw θ and one of the aux. field, $\omega_I = \text{Im}(\omega(k=0))$. $\rightarrow O(V^2)$ effect !

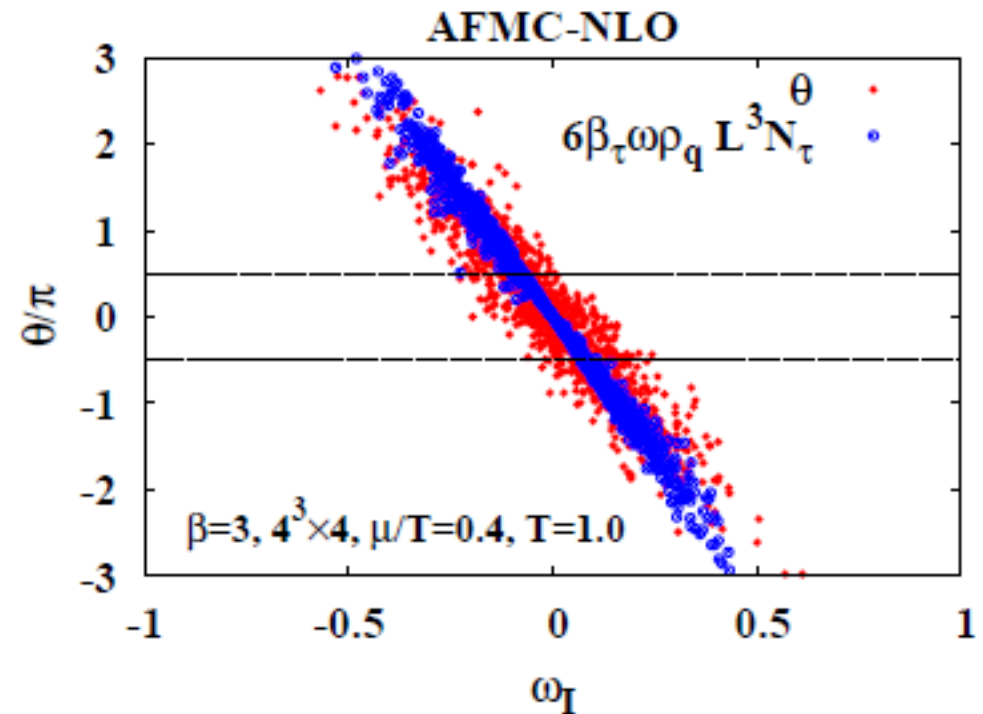
$$\theta \sim 6\beta_\tau \rho_q \omega_I L^3 N_\tau$$



Why do we have a large complex phase ?

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

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

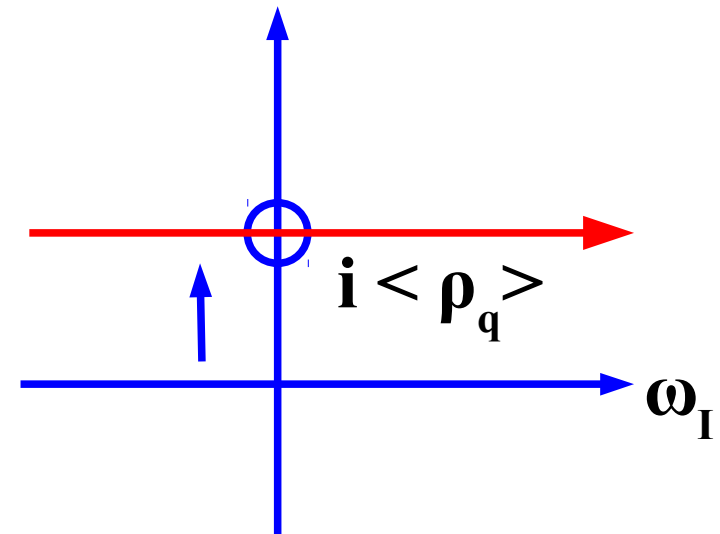
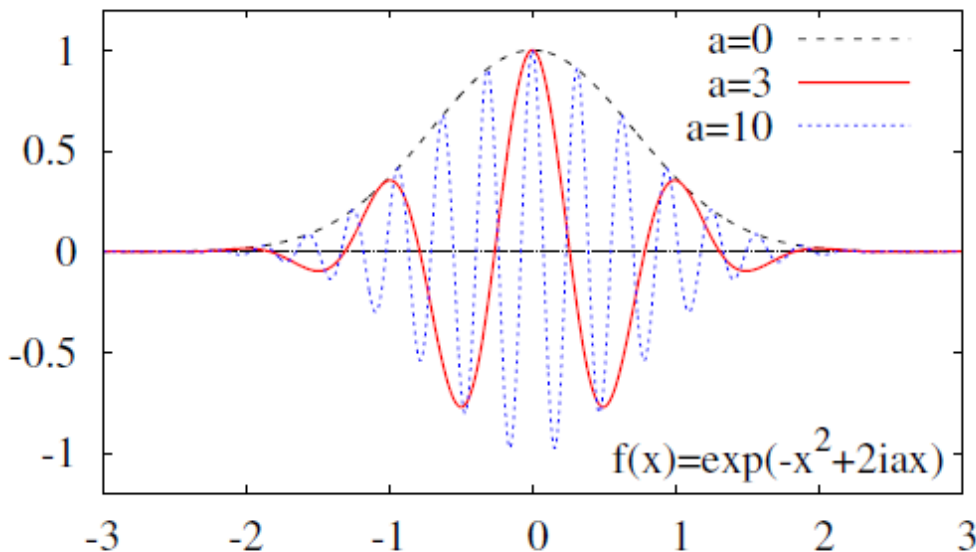


Q: Why ? A: Repulsive Vector Potential

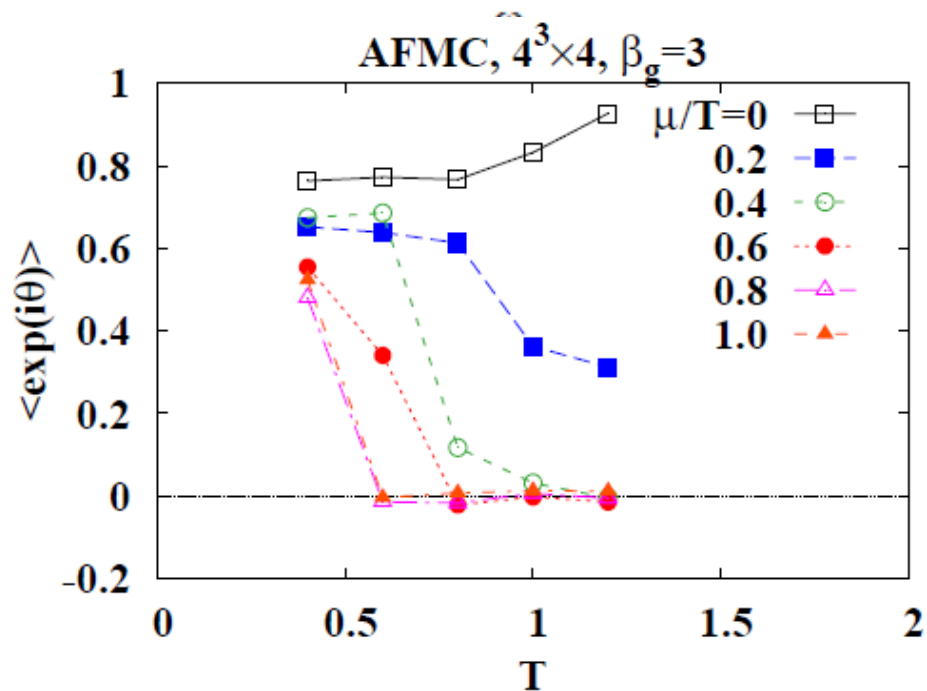
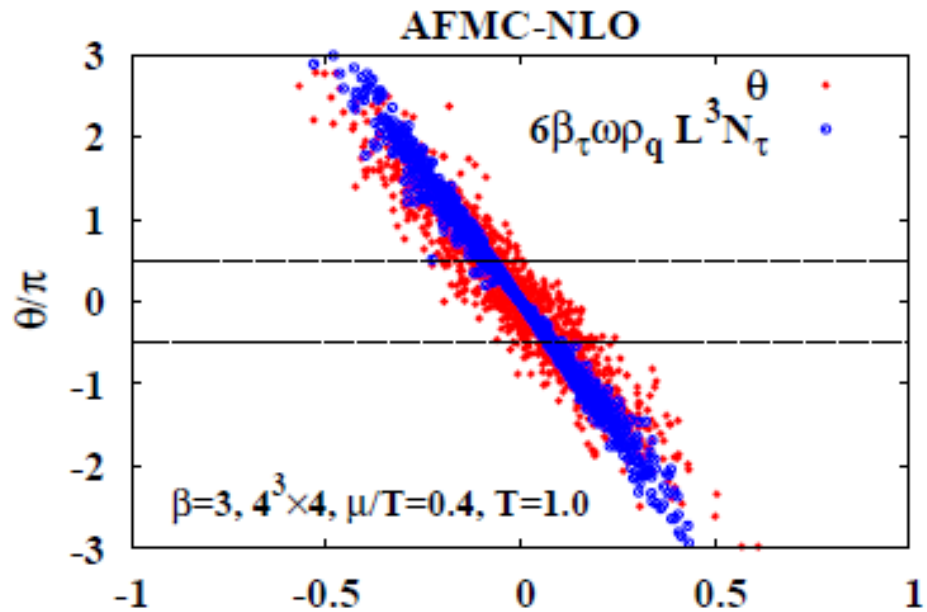
- Effective action terms including $\omega_I(k=0)$

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

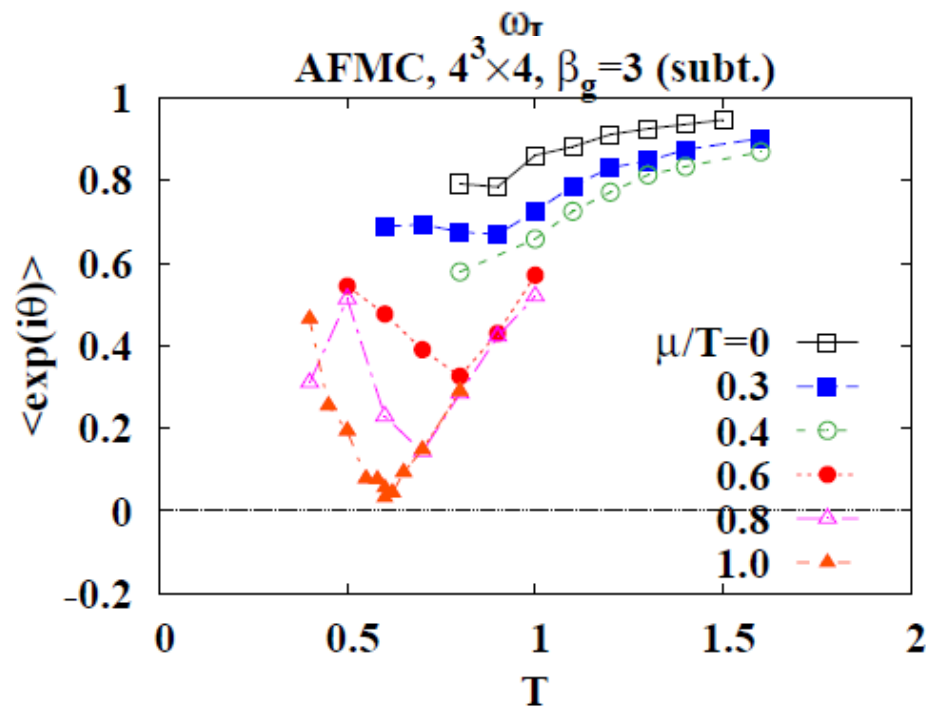
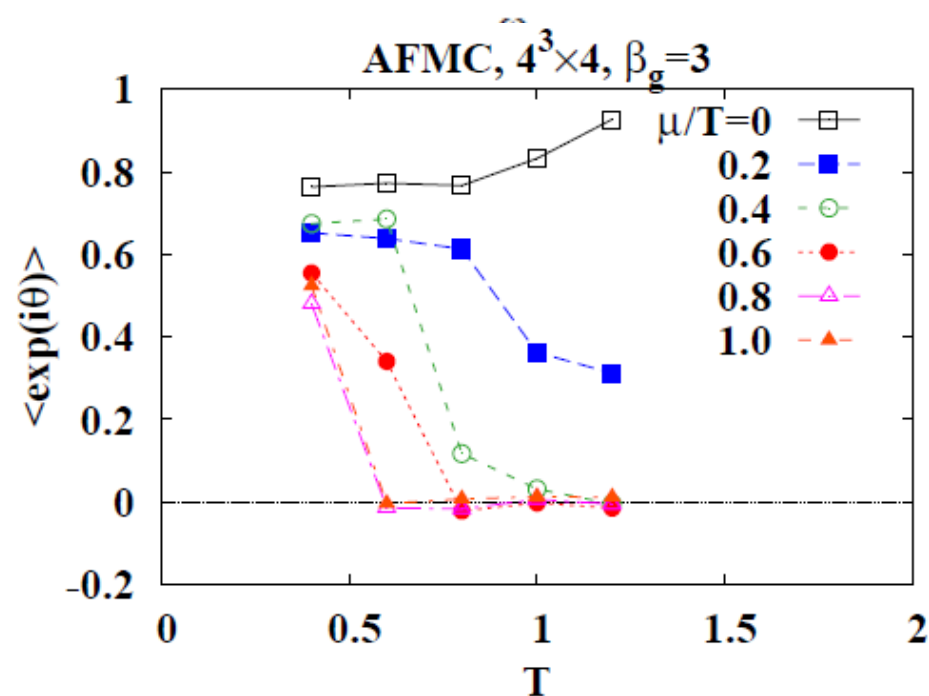
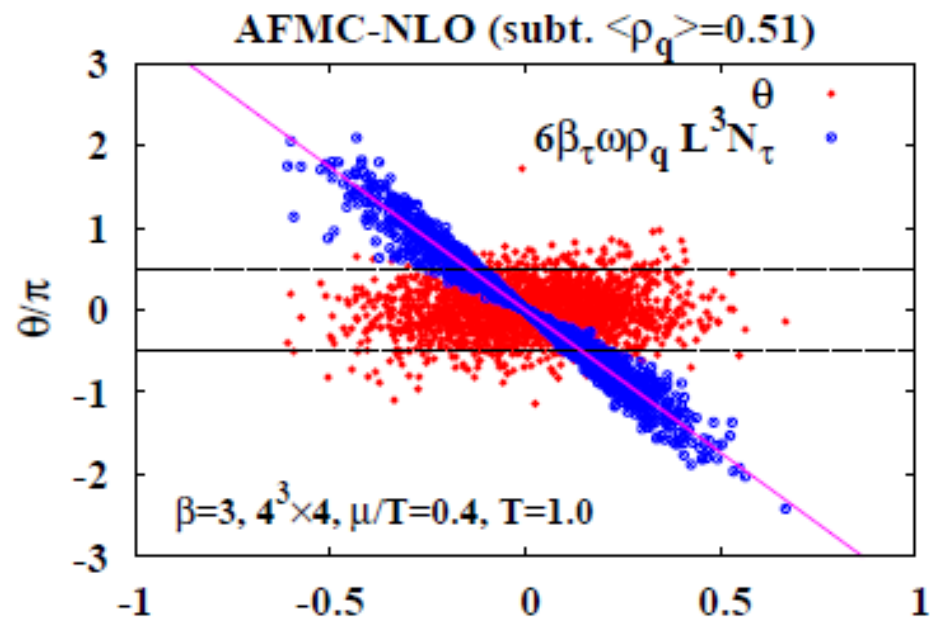
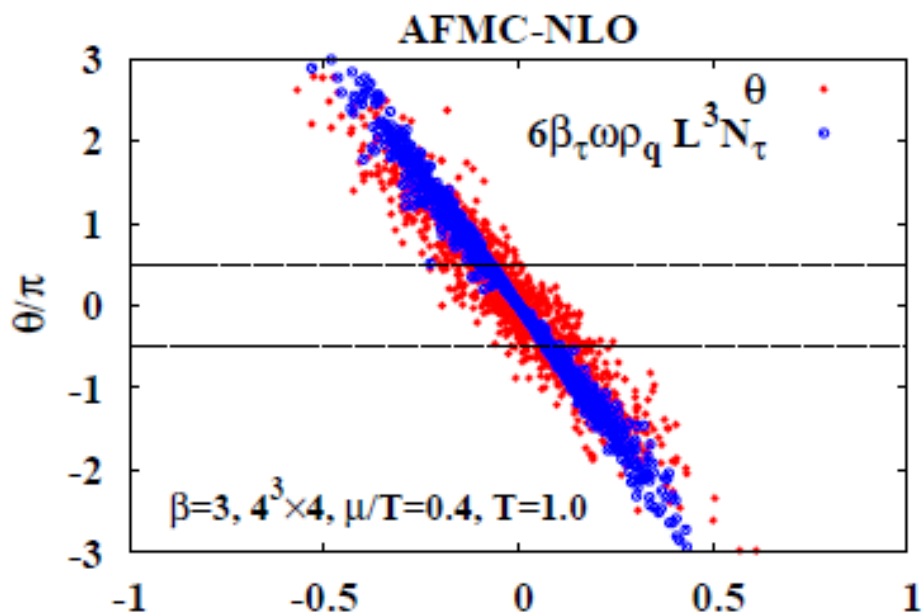
- Textbook example of the sign problem, and we know the answer !
- Shift the integral path to imaginary direction.



Q: Why ? A: Repulsive Vector Potential



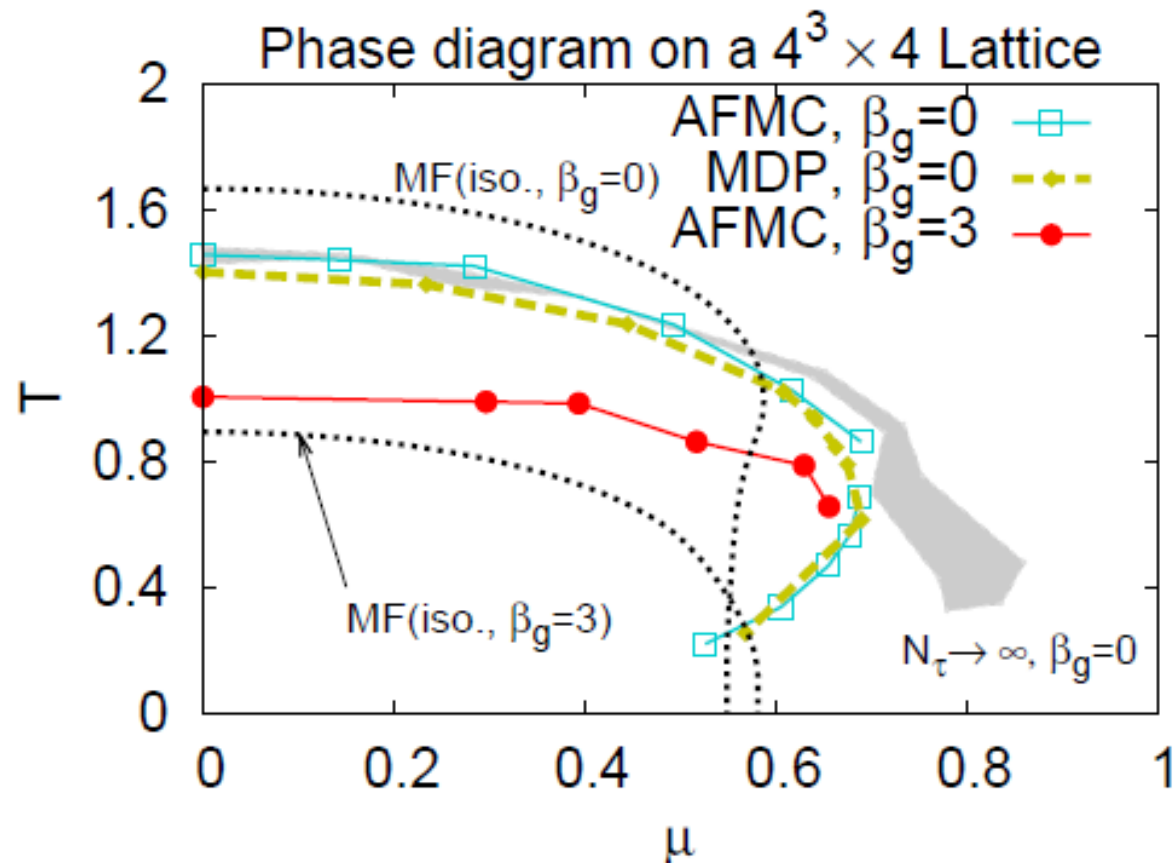
Q: Why ? A: Repulsive Vector Potential



Phase diagram at finite β_g

■ Phase diagram on a $4^3 \times 4$ lattice at $\beta_g = 3$

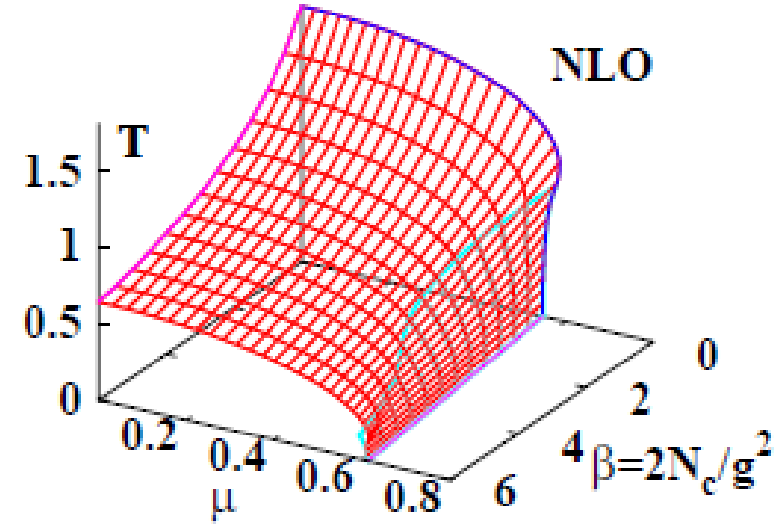
- Suppression of $T_c(\mu=0)$,
Smaller curvature.



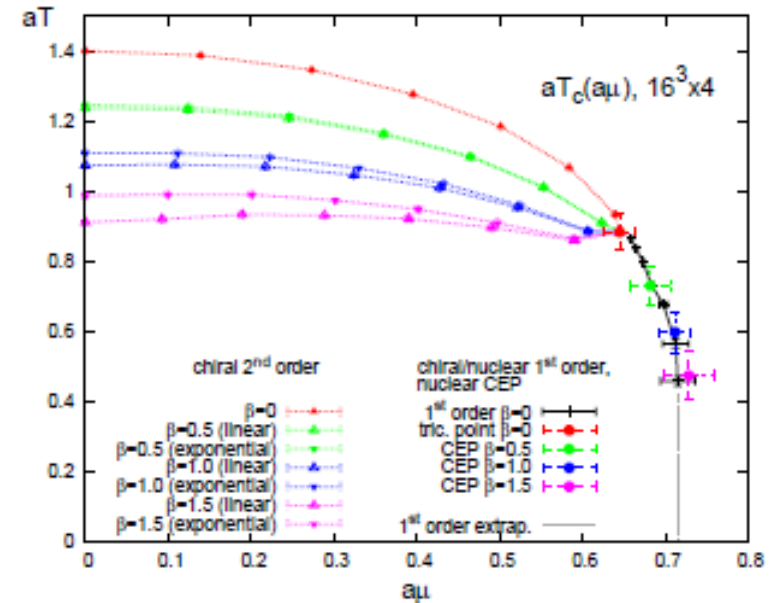
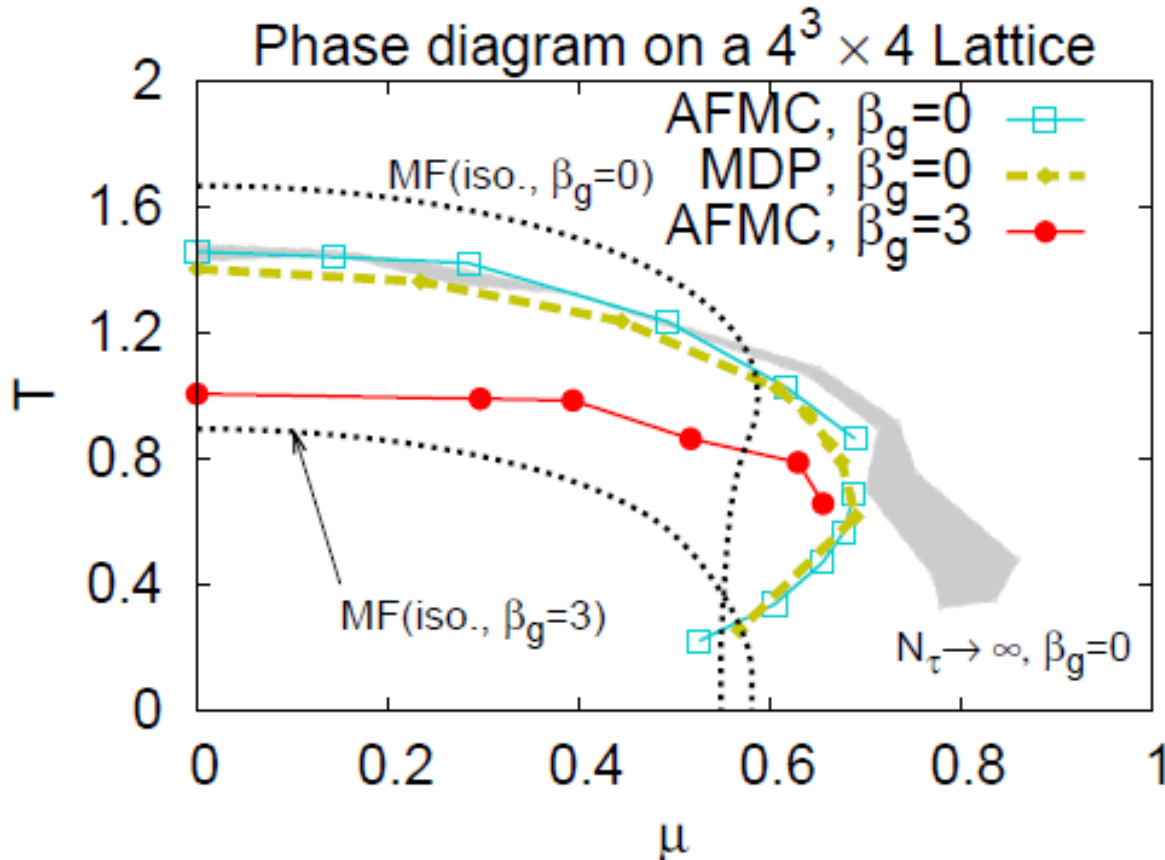
Phase diagram at finite β_g

Phase diagram on a $4^3 \times 4$ lattice at $\beta_g = 3$

- Suppression of $T_c(\mu=0)$, Smaller curvature.
- Different β_g dep. from previous works?



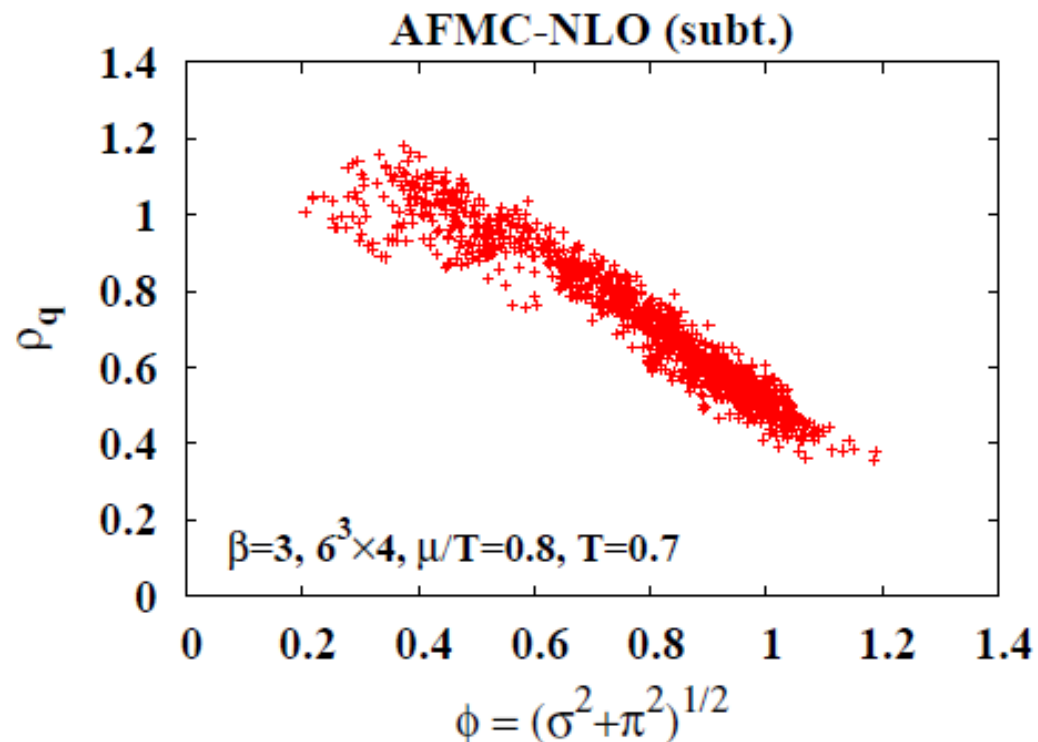
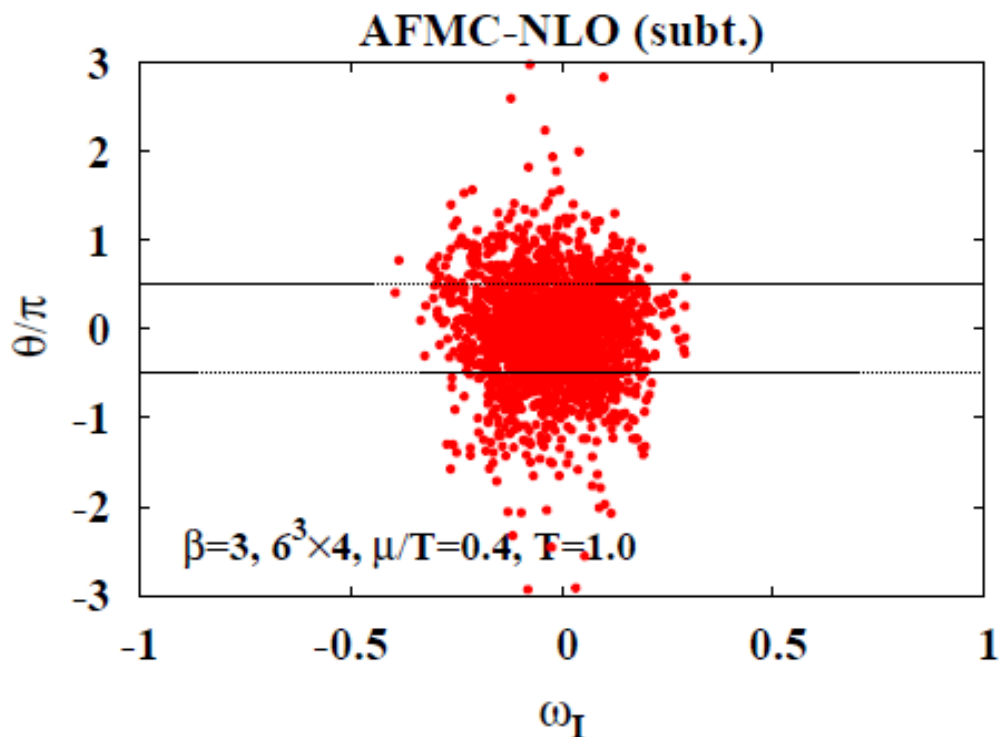
*Miura, Nakano, AO, Kawamoto ('09),
AO, Miura, Nakano, Kawamoto ('09)*



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

Remaining Problem

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



Prewighting

Prewighting

■ Histogram method (Gaussian θ dist.)

S. Ejiri, PRD77('08)014508

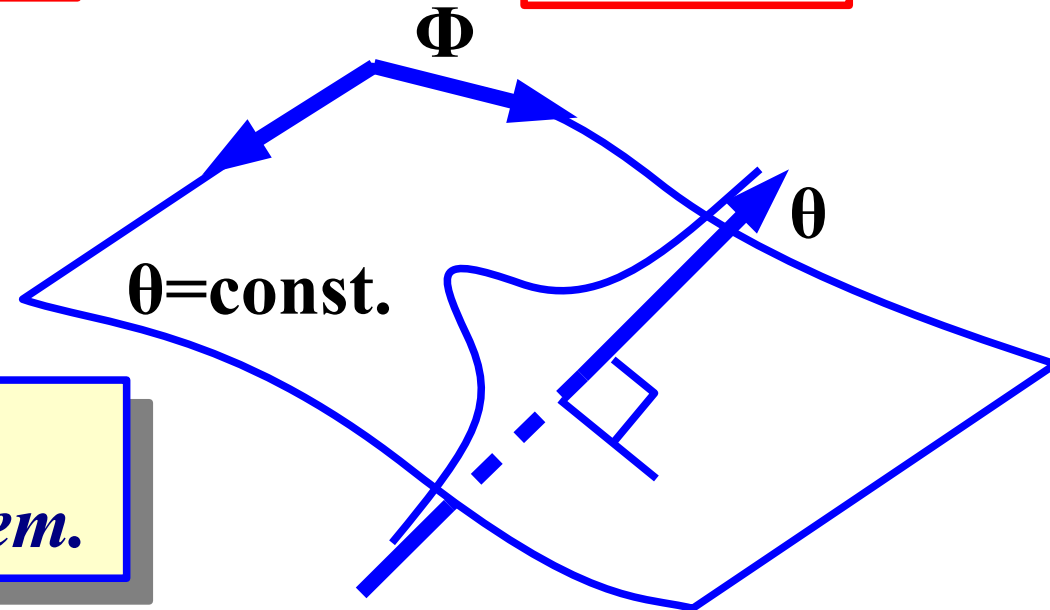
$$\begin{aligned}
 Z &= \int D\Phi d\theta e^{-S_R[\Phi] + i\theta} = \int D\Phi d\theta e^{-S'_R[\Phi]} \frac{e^{-\theta^2/2\Delta^2[\Phi]}}{\sqrt{2\pi\Delta[\Phi]}} e^{i\theta} \\
 &= \int D\Phi e^{-S'_R[\Phi]} \boxed{\exp(-\Delta^2[\Phi]/2)} \quad \Phi \text{ dep. APF} \quad \theta\text{-dist.}
 \end{aligned}$$

■ Prewighting

supp. large θ

Φ dep. supp. factor

$$\begin{aligned}
 Z_{\text{prew}} &= \int D\Phi d\theta e^{-S_R[\Phi]} \boxed{\exp(-f(\theta))} = \int D\Phi e^{-S'_R[\Phi]} \boxed{F(\Delta[\Phi])} \\
 F(\Delta) &= \int d\theta \frac{e^{-\theta^2/2\Delta^2}}{\sqrt{2\pi\Delta}} e^{-f(\theta)}
 \end{aligned}$$



*If $F(\Delta) = \exp(-\Delta^2/2)$,
we can obtain Z w/o sign problem.*

Prewighting Function

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

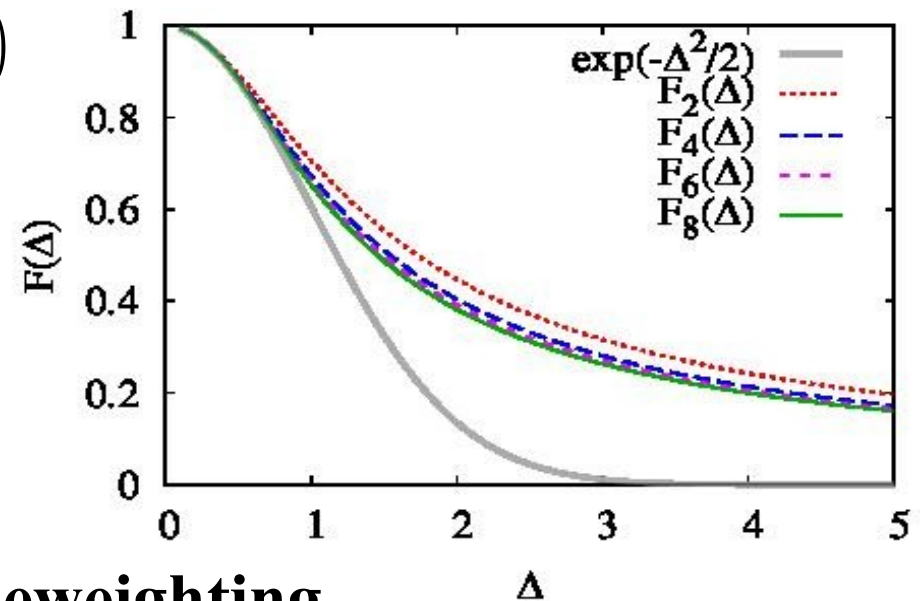
$$f(\theta) = \frac{1}{2}\theta^2 + \frac{1}{12}\theta^4 + \frac{1}{45}\theta^6 + \frac{17}{1260}\theta^8 + \mathcal{O}(\theta^{10})$$

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

- But there is no free lunch.

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

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



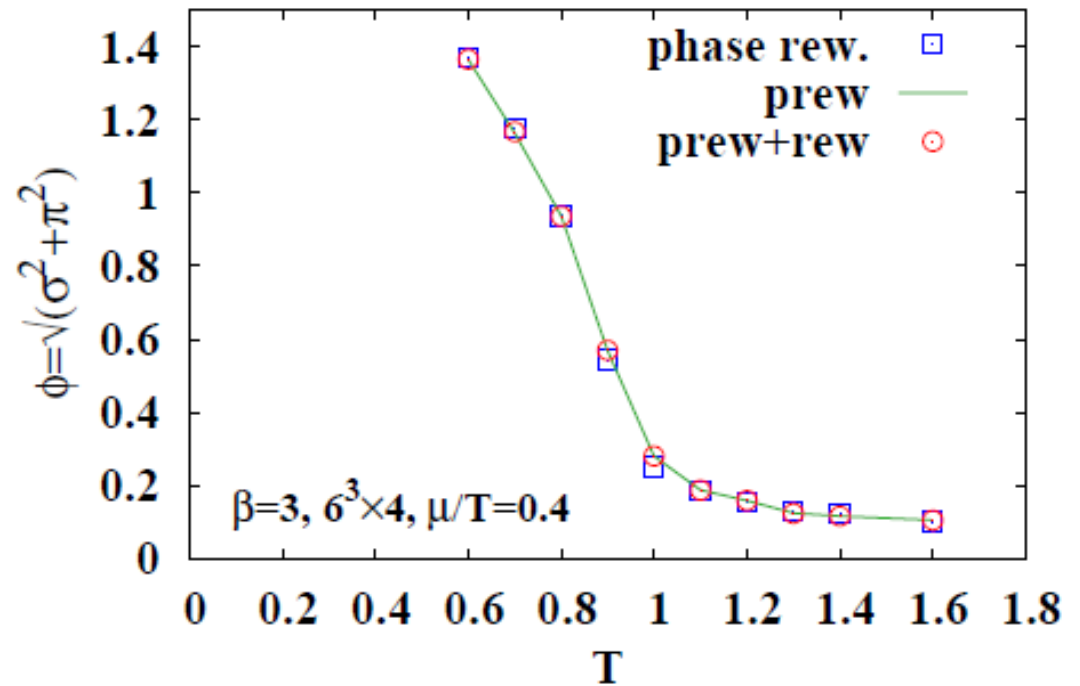
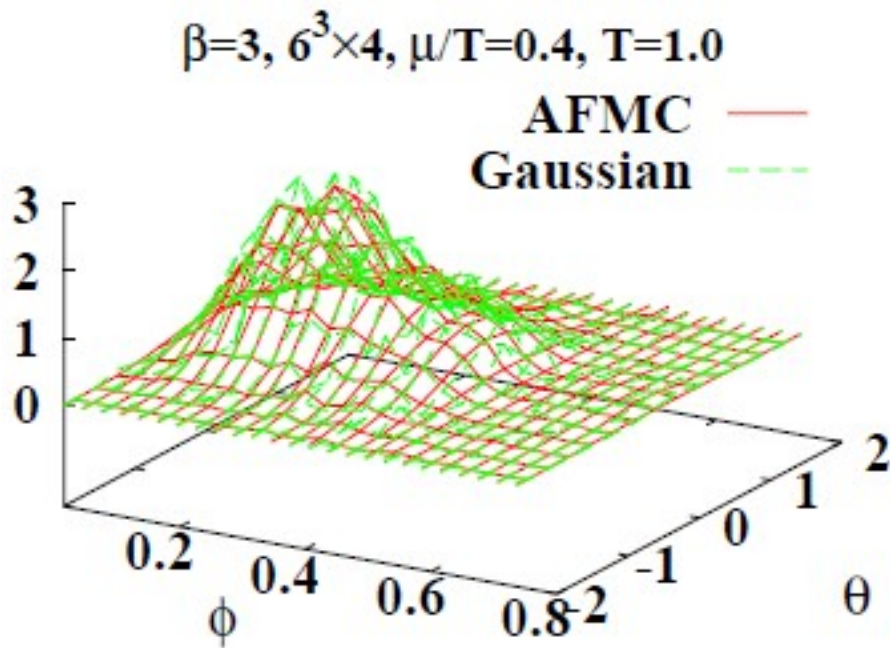
- Practical method: Prewighting+Reweighting

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

*Let us examine
in SC-LQCD !*

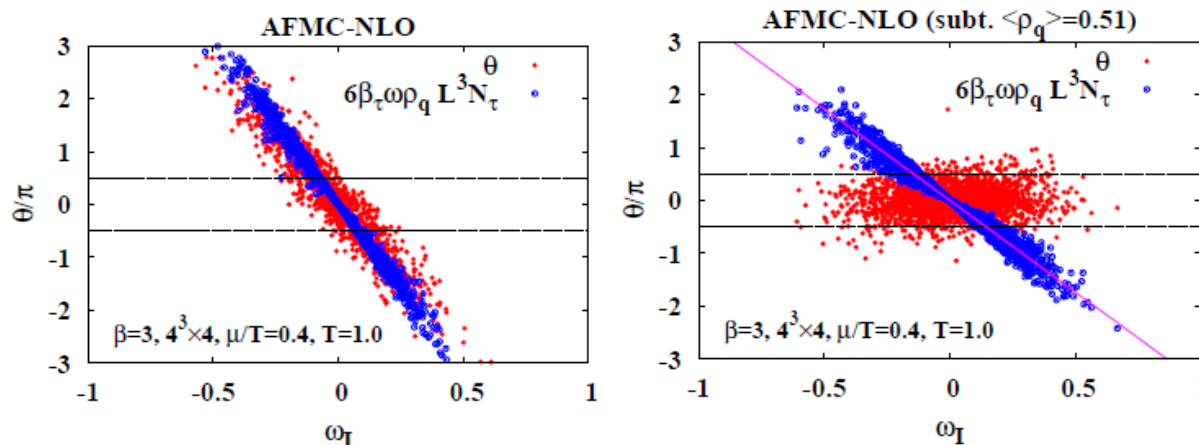
θ dist. in SC-LQCD ($\beta_g=3, \mu/T=0.4$)

- 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 function will help to enhance statistics.

Discussion & Future works

■ Non-gaussianity of θ distribution

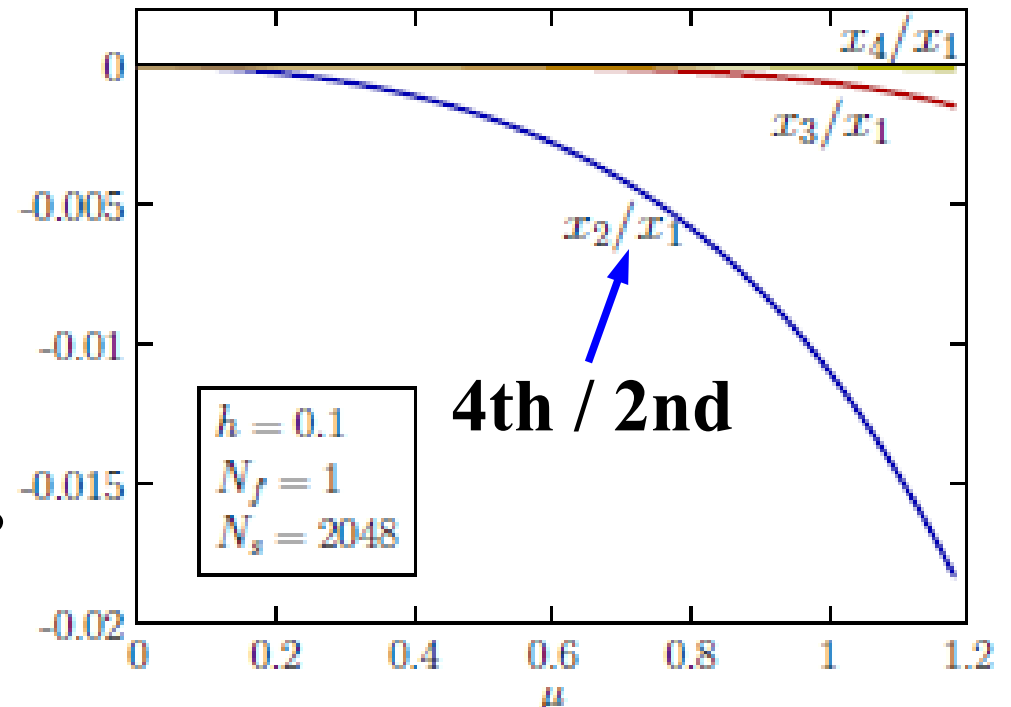
- SC & HP expansion: *Greensite, Myers, Splittorf, arXiv:1311.4568.*
- Superposed Lorentzian in the π cond. phase
M.P. Lombardo, K. Splittorff, J.J.M. Verbaarschot, PRD80 ('09) 054509

■ To do

- Configg. 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 !

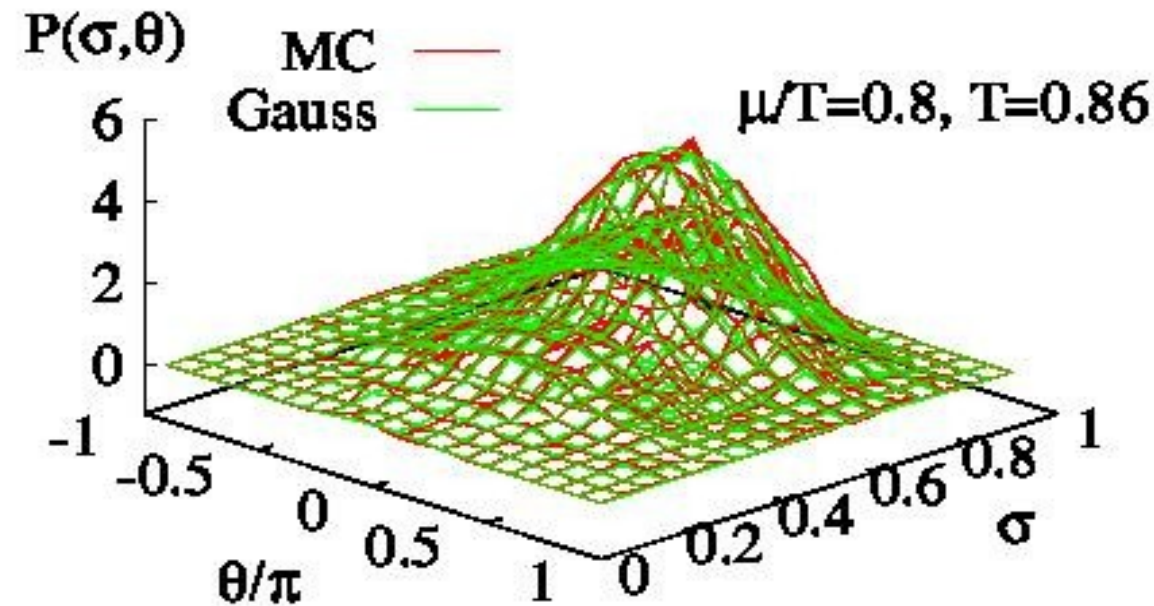
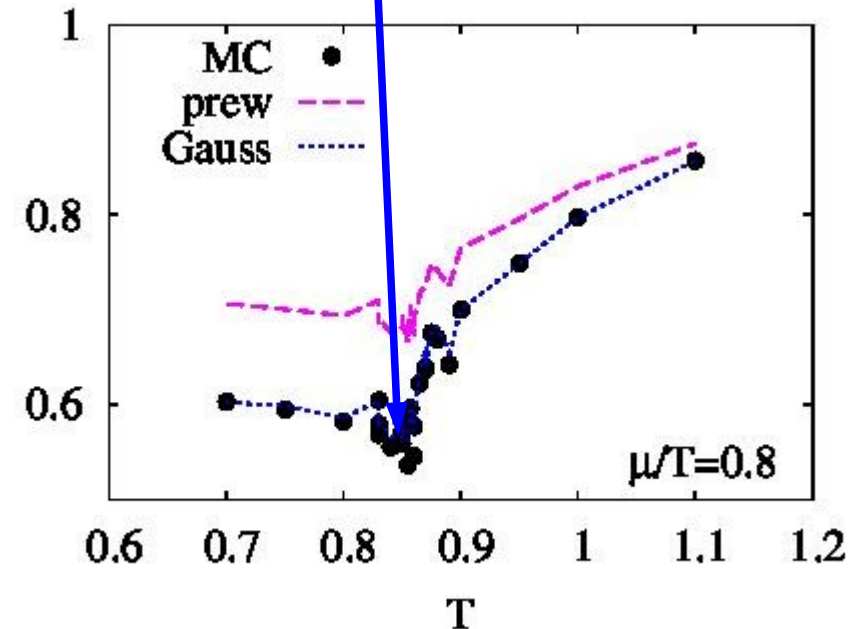
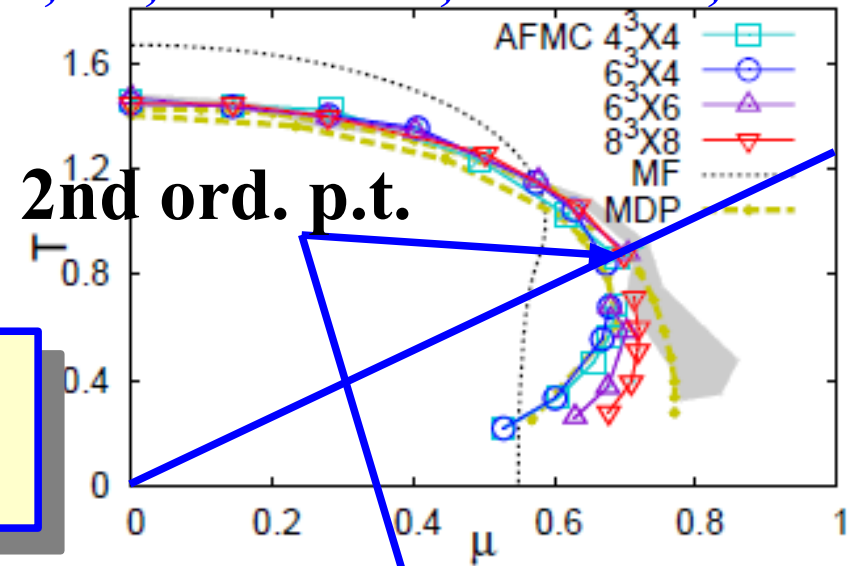


θ dist. in AFMC-SCL ($\mu/T=0.8$)

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

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

Prewighting accounts for a large part of weight cancellation !



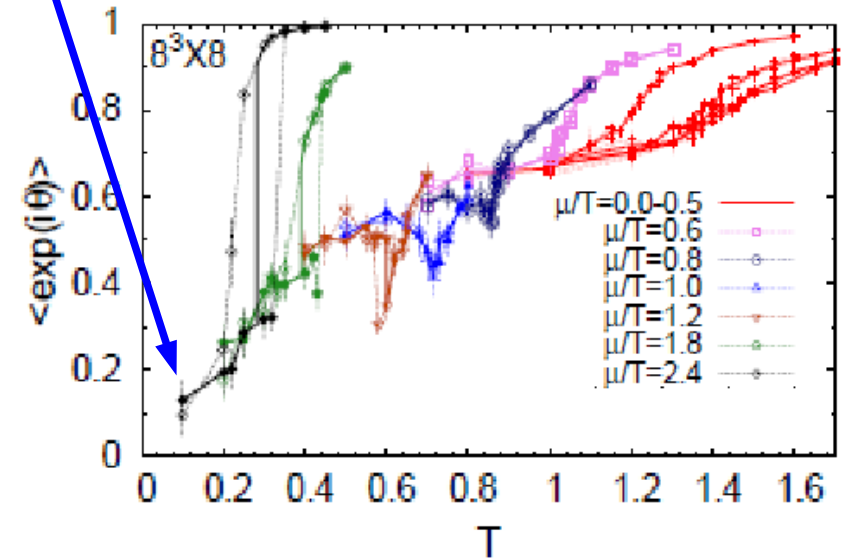
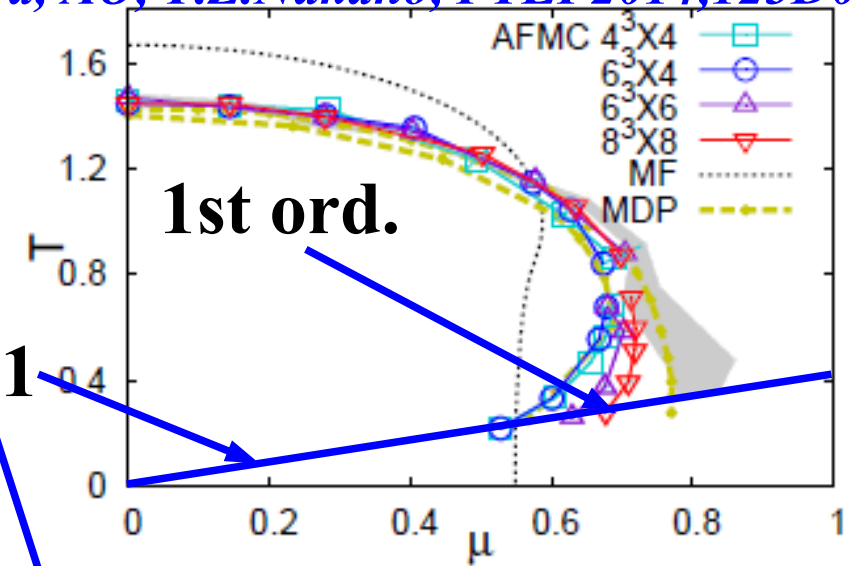
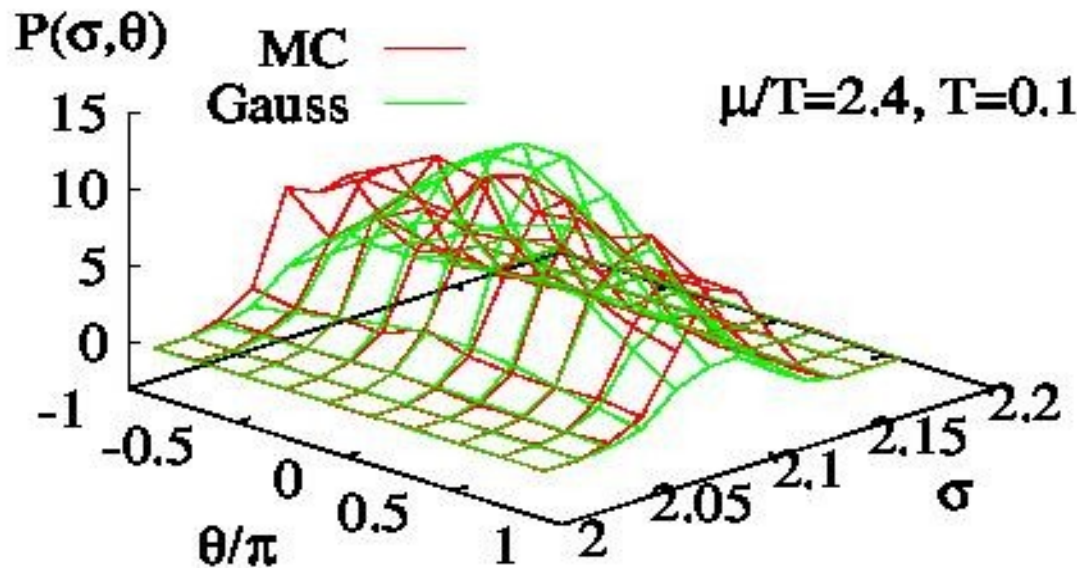
θ dist. in AFMC-SCL ($\mu/T=2.4$)

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

■ θ dist. \neq Gaussian

- θ distribution well extends around $\theta \sim \pi$.

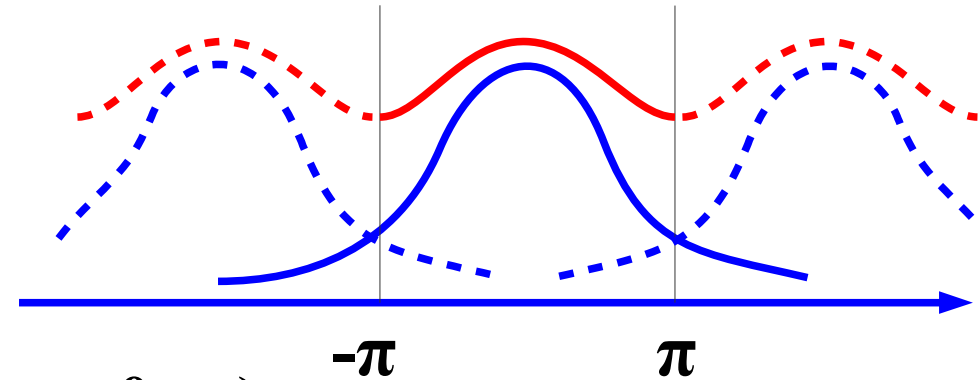
→ We need to consider *mirror* contributions.



Mirror contributions

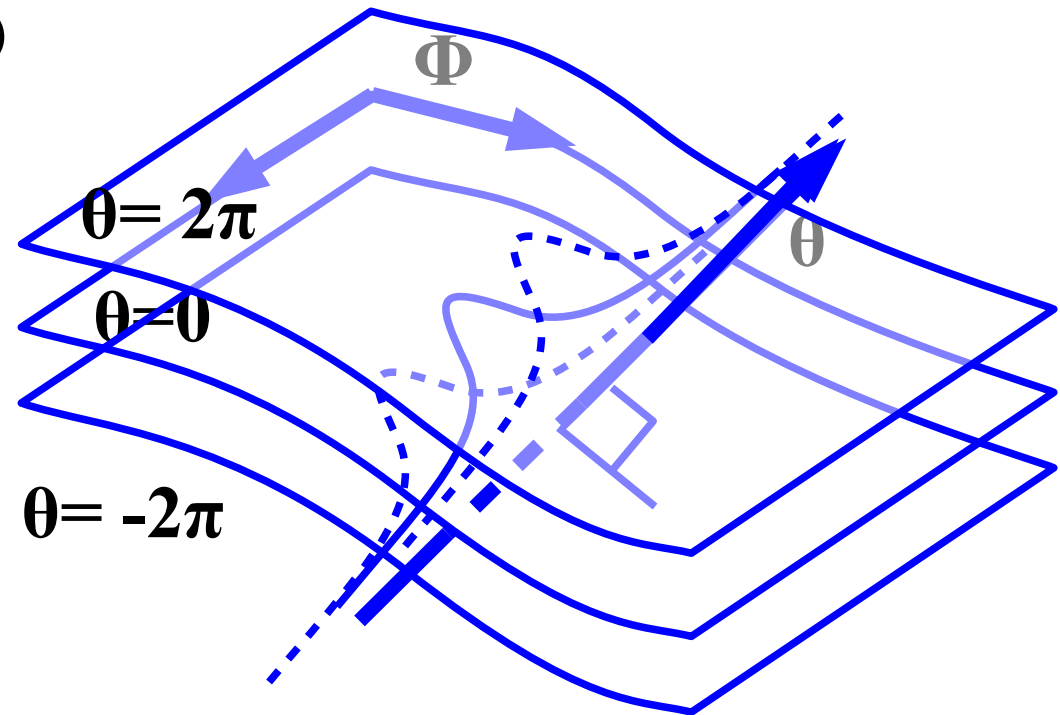
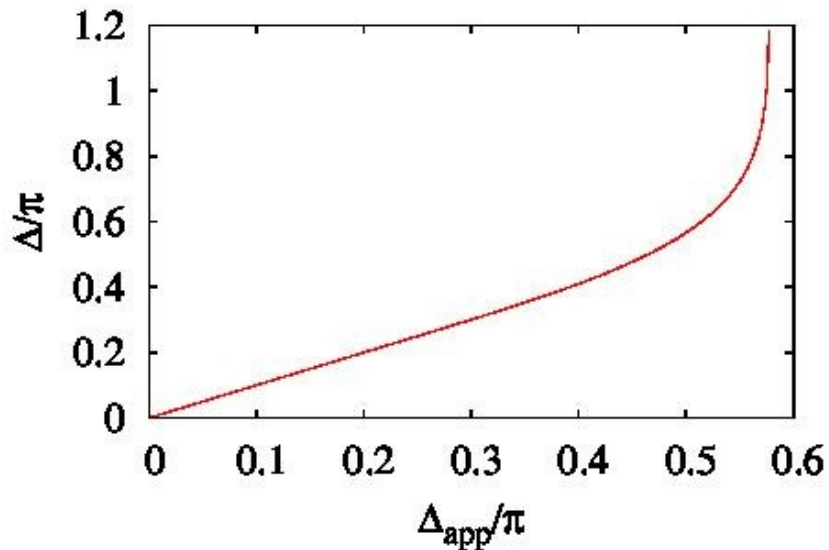
■ Mirrored Gaussian

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



- Apparent std. dev. Δ (obtained in $-\pi < \theta < \pi$)
 \rightarrow Actual Δ (defined in $-\infty < \theta < \infty$)

- Alternative
 Obtain θ in $-\infty < \theta < \infty$ (Ejiri)



θ dist. in AFMC-SCL ($\mu/T=2.4$, again)

■ θ dist. \sim Mirrored Gaussian

- APF is also well explained with Mirrored Gaussian.
- average prew. factor \sim (0.4-0.6)
- average phase factor \sim (0.1-0.3)

Prewighting accounts for around half of weight cancellation !

