

Peeking into the θ vacuum of 4d SU(2) Yang-Mills theory

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in collaboration with

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Introduction

- Many interesting subjects related to the θ term or topology of YM theory e.g.) strong CP, axion, EDM, fate of $U_A(1)$, ...

Focus on the θ dependence of free energy density in 4d SU(2) YM

Free energy density: $f(\theta)$

$$e^{-Vf(\theta)} = \frac{Z(\theta)}{Z(0)}$$

Where $Z(\theta) = \int \mathcal{D}U e^{-S_{\text{YM}} + i\theta Q}$

$$Q = \int d^4x q(x) \quad \text{and} \quad q(x) = \frac{1}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a$$

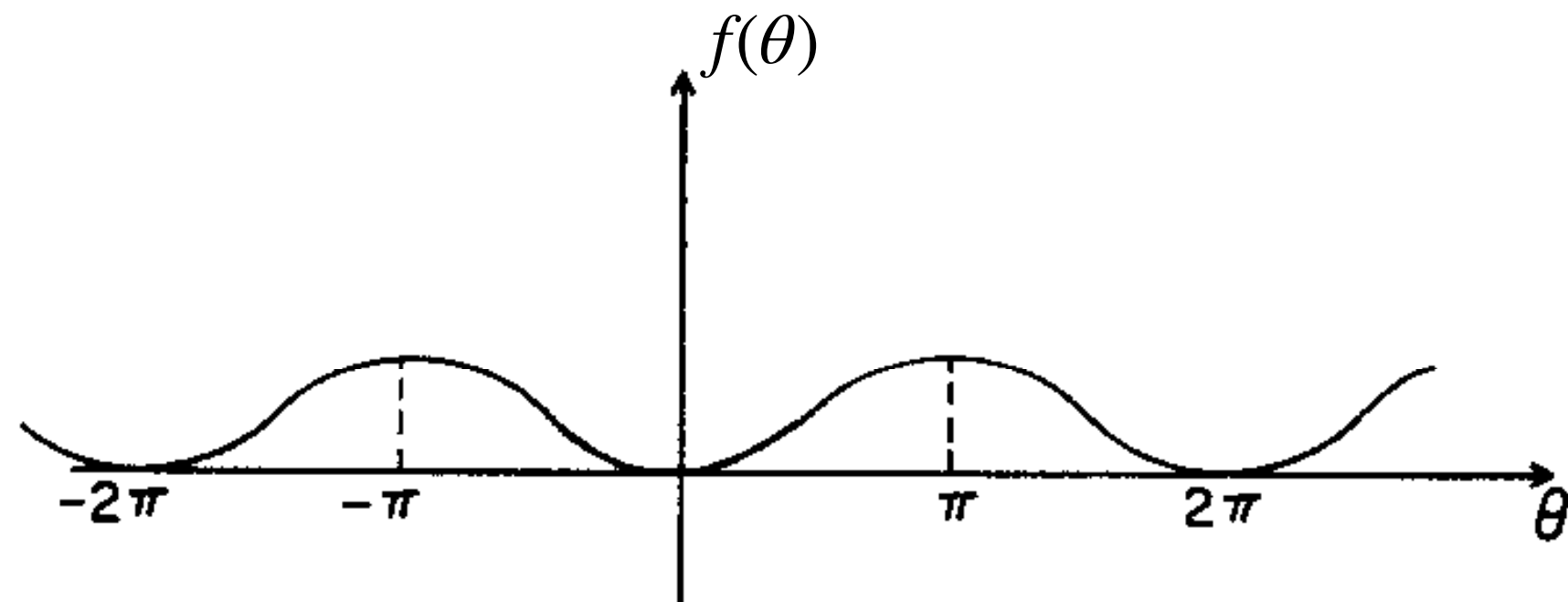
For $SU(N)$ YM theory,

$$\left. \begin{array}{l} Q \in \mathbb{Z} \Rightarrow Z(\theta) = Z(\theta + 2\pi) \Rightarrow f(\theta) = f(\theta + 2\pi) \\ S_{\text{YM}} \text{ is CP even} \Rightarrow Z(\theta) = Z(-\theta) \Rightarrow f(\theta) = f(-\theta) \end{array} \right\} f(\pi - \theta') = f(\pi + \theta')$$

θ dependence and CP violation

Dilute instanton gas approximation (DIGA)

$$\Rightarrow f(\theta) = \chi(1 - \cos \theta)$$

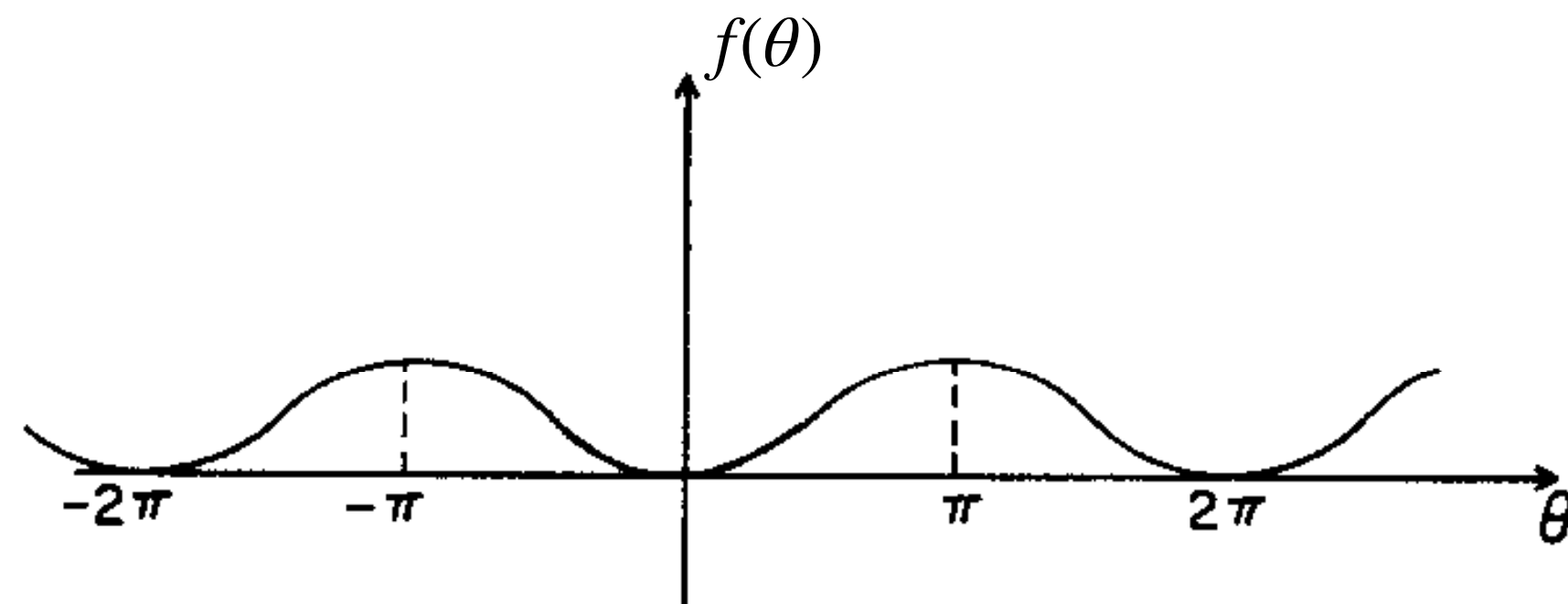


- a single branch
- smooth everywhere

θ dependence and CP violation

Dilute instanton gas approximation (DIGA)

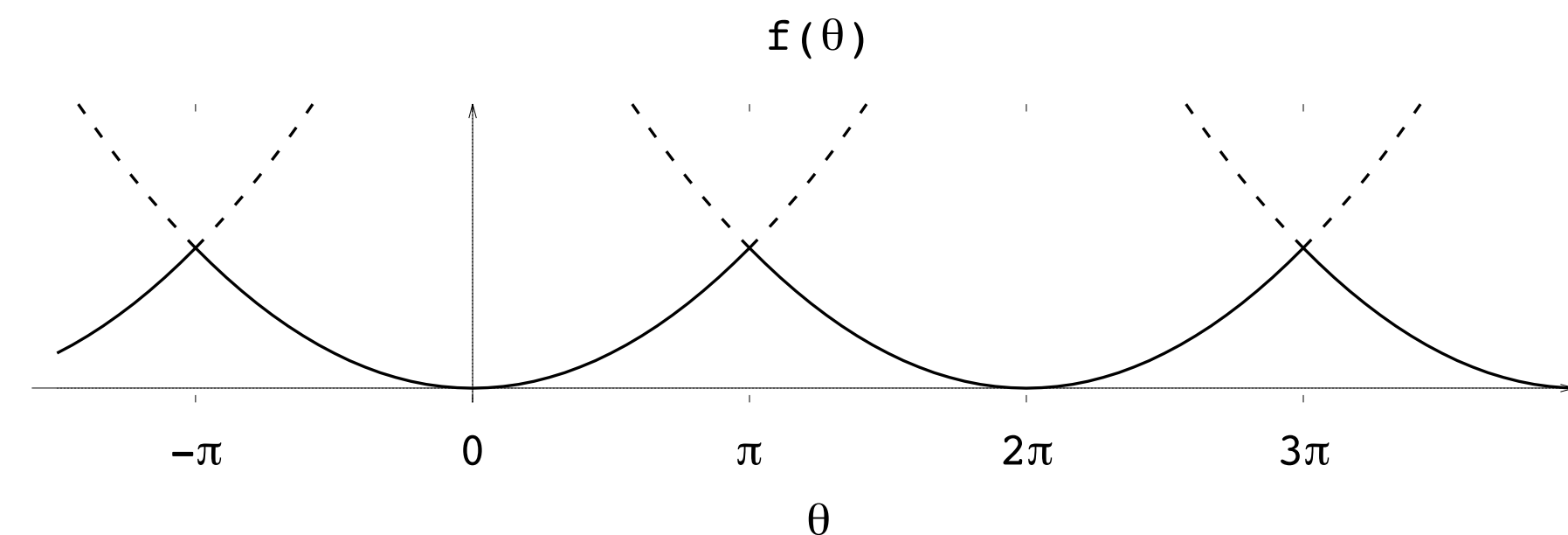
$$\Rightarrow f(\theta) = \chi(1 - \cos \theta)$$



- a single branch
- smooth everywhere

Large N argument [Witten (1980, 1998)]

$$\Rightarrow f(\theta) = \chi/2 \min_{k \in \mathbb{Z}} (\theta + 2\pi k)^2 + O(1/N^2)$$

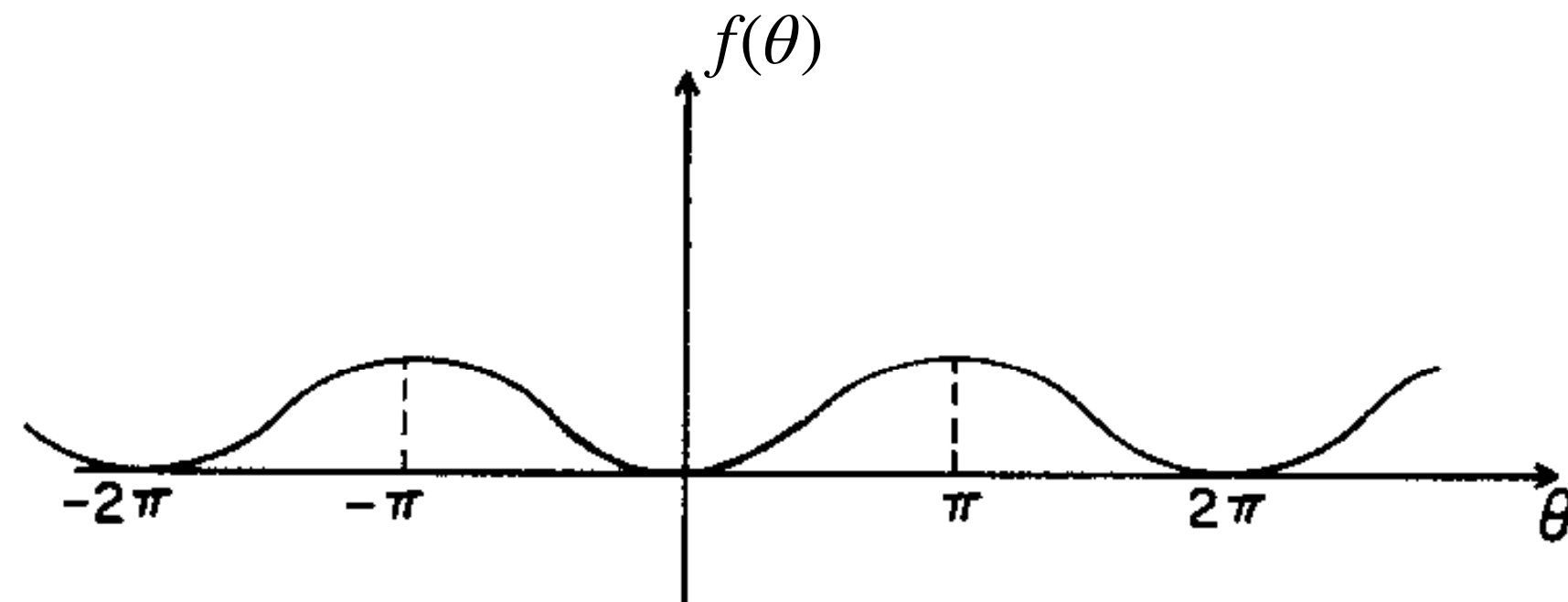


- several branches crossing
- spontaneous CPV (1st order PT) at $\theta = \pi$ with the order parameter $df(\theta)/d\theta = -i\langle q(x) \rangle$

θ dependence and CP violation

Dilute instanton gas approximation (DIGA)

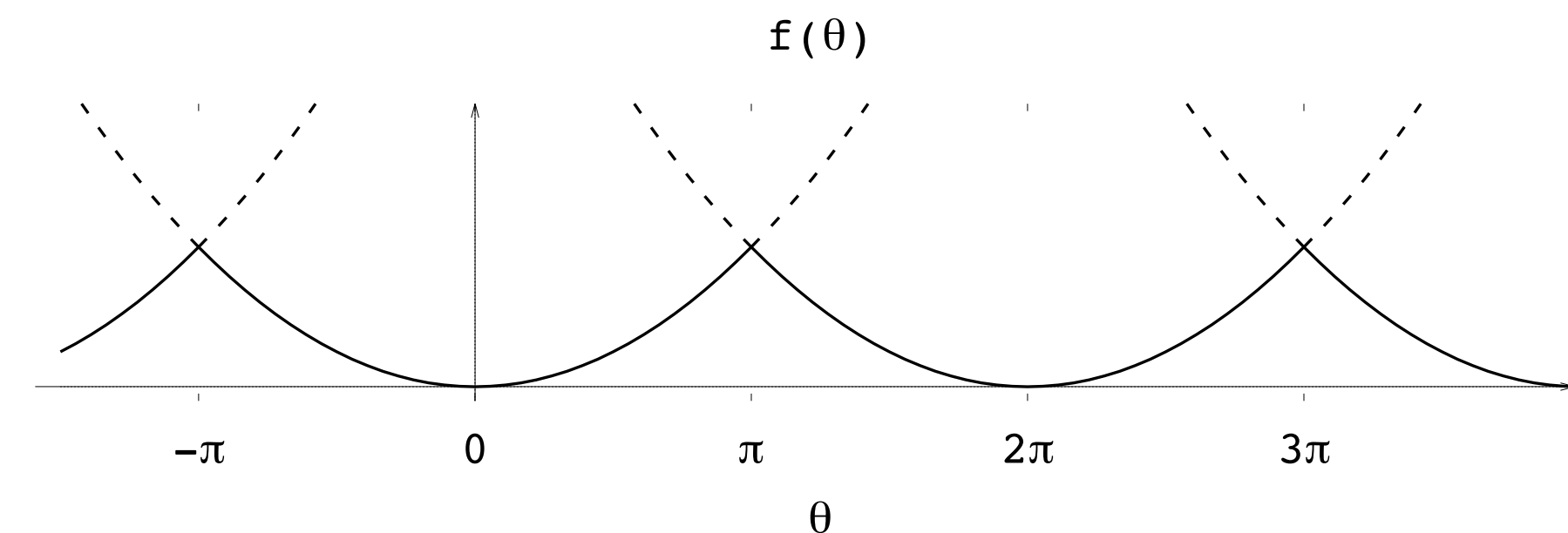
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Interested in $f(\theta)$ around $\theta \approx \pi$ in 4d $SU(N)$ YM theory.

Learning from 2d CP^{N-1} model

$$\mathcal{L} = \frac{N}{2g} \overline{D_\mu z} D_\mu z - i\theta q$$

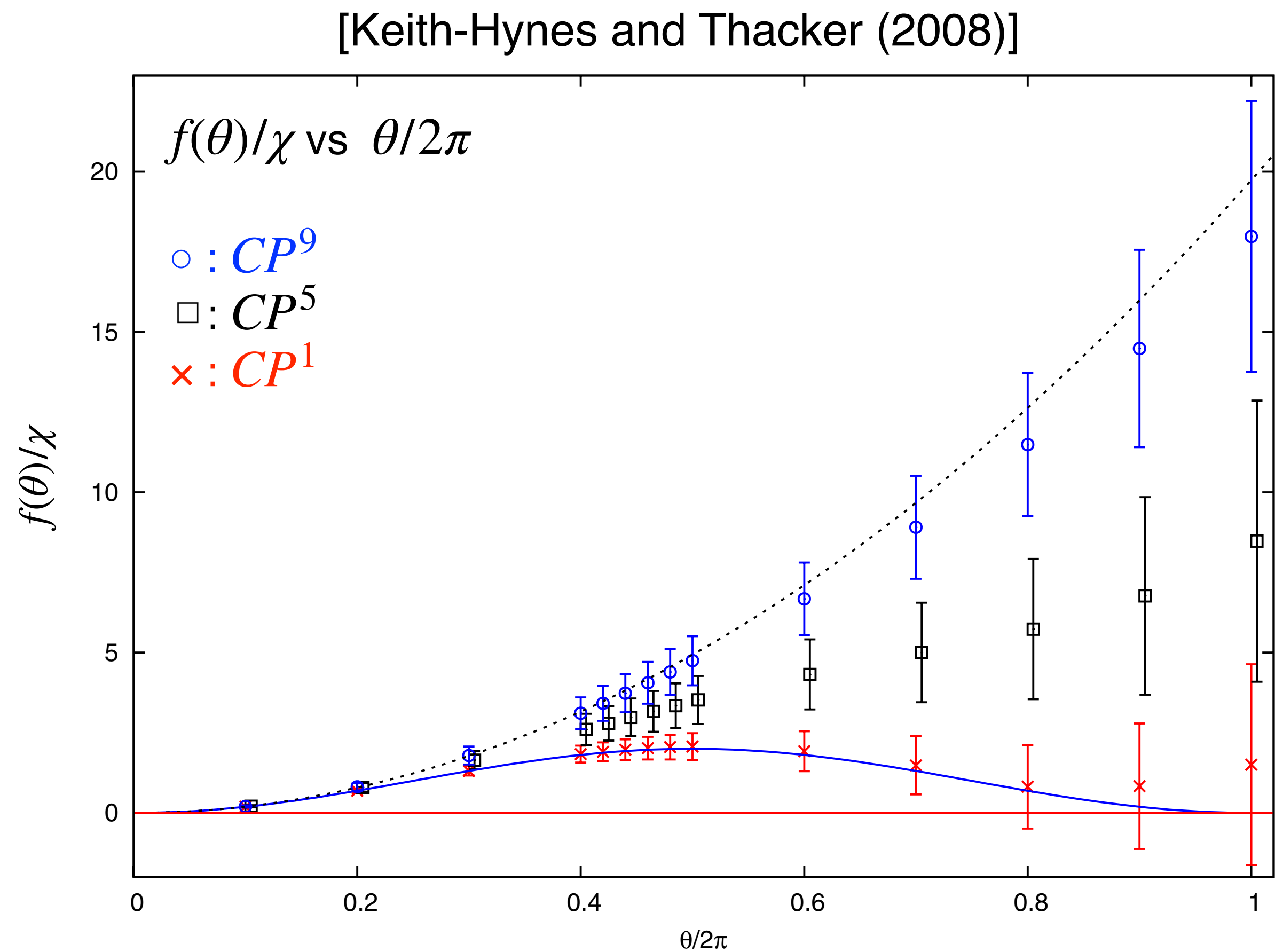
z : N-component complex scalar field with $\bar{z}z = 1$

$$D_\mu = \partial_\mu + iA_\mu, \quad A_\mu = i\bar{z}\partial_\mu z$$

$$q(x) = \frac{1}{2\pi} \epsilon_{\mu\nu} \partial_\mu A_\nu = \frac{i}{2\pi} \epsilon_{\mu\nu} \overline{D_\mu z} D_\nu z$$

- Good testing ground for 4d $SU(N)$ because of many similarities [asymptotic freedom, dynamical mass gap, instanton, $1/N$ expandable, ...]
- Gapped and CP broken at $\theta = \pi$ for $N \geq 3$.
- **But CP^1 (i.e. $N = 2$) is exceptional !**
 \Rightarrow gapless and no CPV at $\theta = \pi$ (\iff Haldane conjecture)

$f(\theta)$ in 2d CP^{N-1} model (lattice results)



$$e^{-V_{\text{sub}} f_{\text{sub}}(\theta)} = \frac{1}{Z[0]} \int \mathcal{D}z \mathcal{D}\bar{z} e^{-S_{CP(N-1)} - i\theta Q_{\text{sub}}}$$

$$= \langle e^{-i\theta Q_{\text{sub}}} \rangle$$

$$Q_{\text{sub}} = \int_{x \in V_{\text{sub}}} d^2x \frac{1}{2\pi} \epsilon_{\mu\nu} \partial_\mu A_\nu \rightarrow Q_{\text{sub}}^{\text{lat}} = \frac{-i}{2\pi} \sum_{x \in V_{\text{sub}}} \ln P_x$$

(P_x : plaquette)

CP^1 is indeed consistent with the DIGA,
 $f(\theta) = \chi(1 - \cos \theta)$
 while others indicate CPV.

Previous Lattice calculations of 4d $SU(N)$

$$\mathcal{L}_\theta = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a - \underline{i\theta q}$$
$$q(x) = \frac{g^2}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a$$

- Sign problem makes direct lattice calculation difficult/impossible.

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- Sign problem makes direct lattice calculation difficult/impossible.

- Relies on Taylor expansion around $\theta = 0$

$$f(\theta) = \frac{\chi}{2} \theta^2 (1 + b_2 \theta^2 + b_4 \theta^4 + \dots)$$

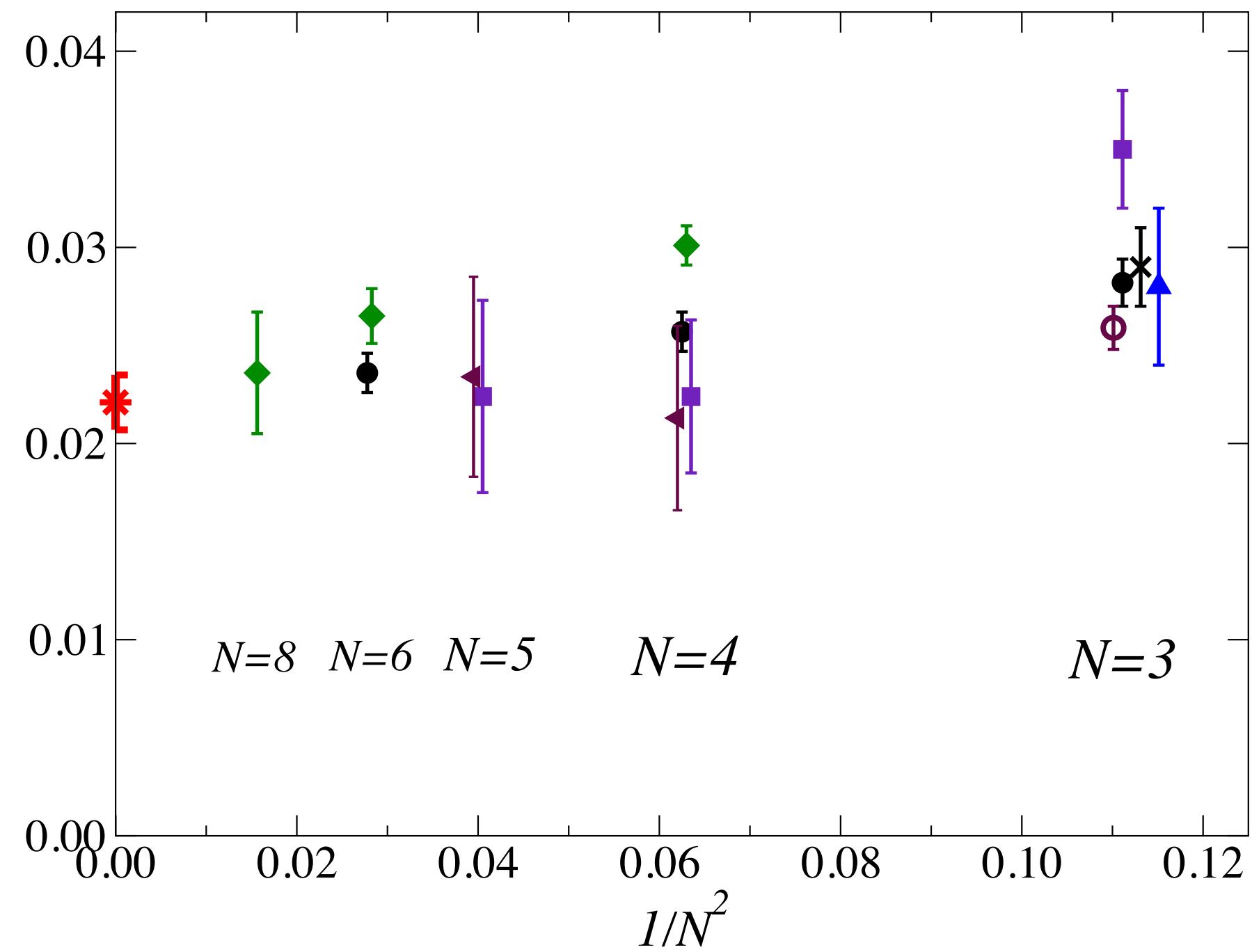
and determines each coefficient on the lattice by

$$\chi = \frac{\langle Q^2 \rangle_{\theta=0}}{V}$$
$$b_2 = - \frac{\langle Q^4 \rangle_{\theta=0} - 3 \langle Q^2 \rangle_{\theta=0}^2}{12 \langle Q^2 \rangle_{\theta=0}}$$
$$b_4 = \frac{\langle Q^6 \rangle_{\theta=0} - 15 \langle Q^2 \rangle_{\theta=0} \langle Q^4 \rangle_{\theta=0} + 30 \langle Q^2 \rangle_{\theta=0}^3}{360 \langle Q^2 \rangle_{\theta=0}}$$
$$\vdots$$

First two coefficients

[Review by Vicari and Panagopoulos (2018)]

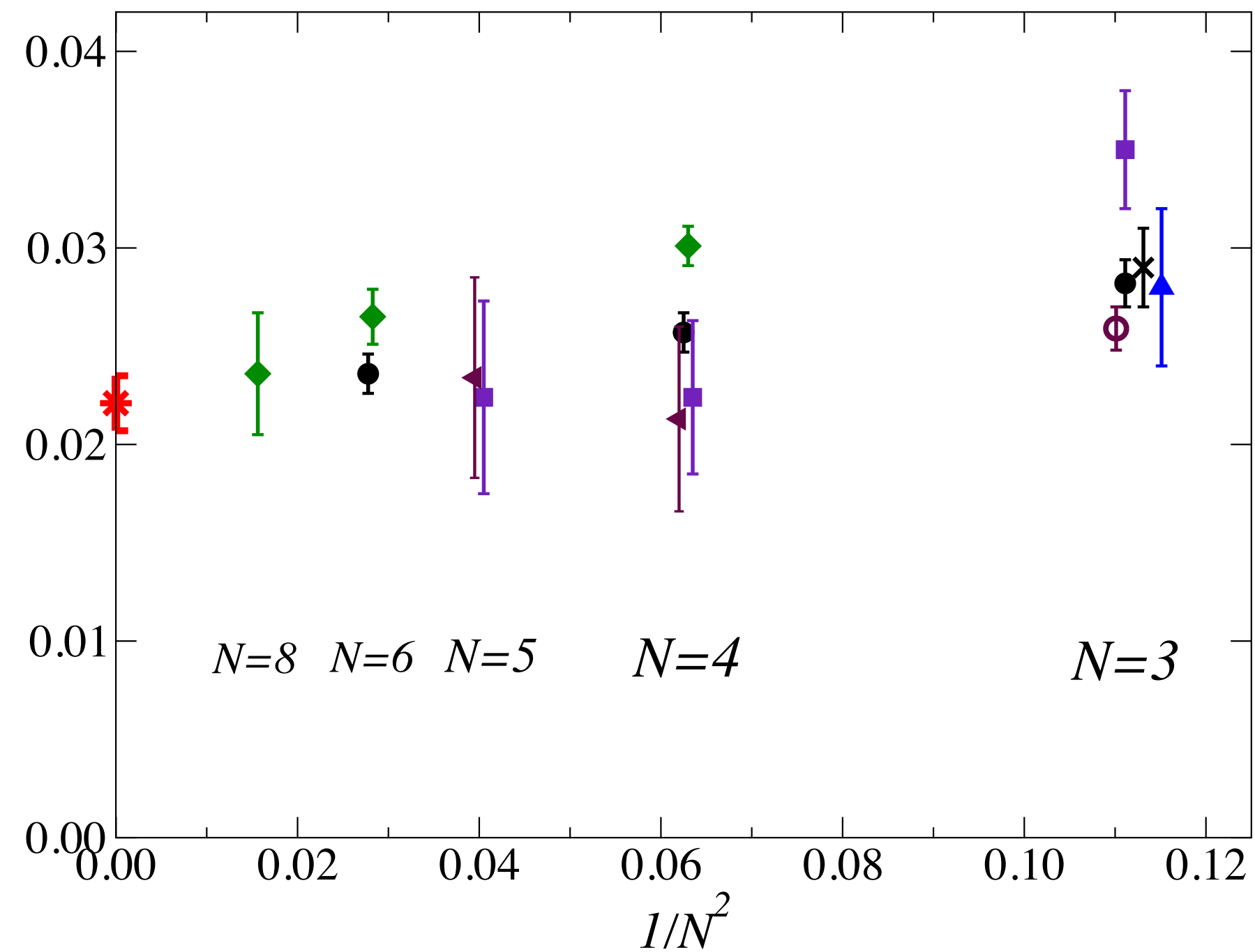
$$\chi/\sigma^2 = C_\infty + \frac{c_2}{N^2} + O(1/N^4)$$



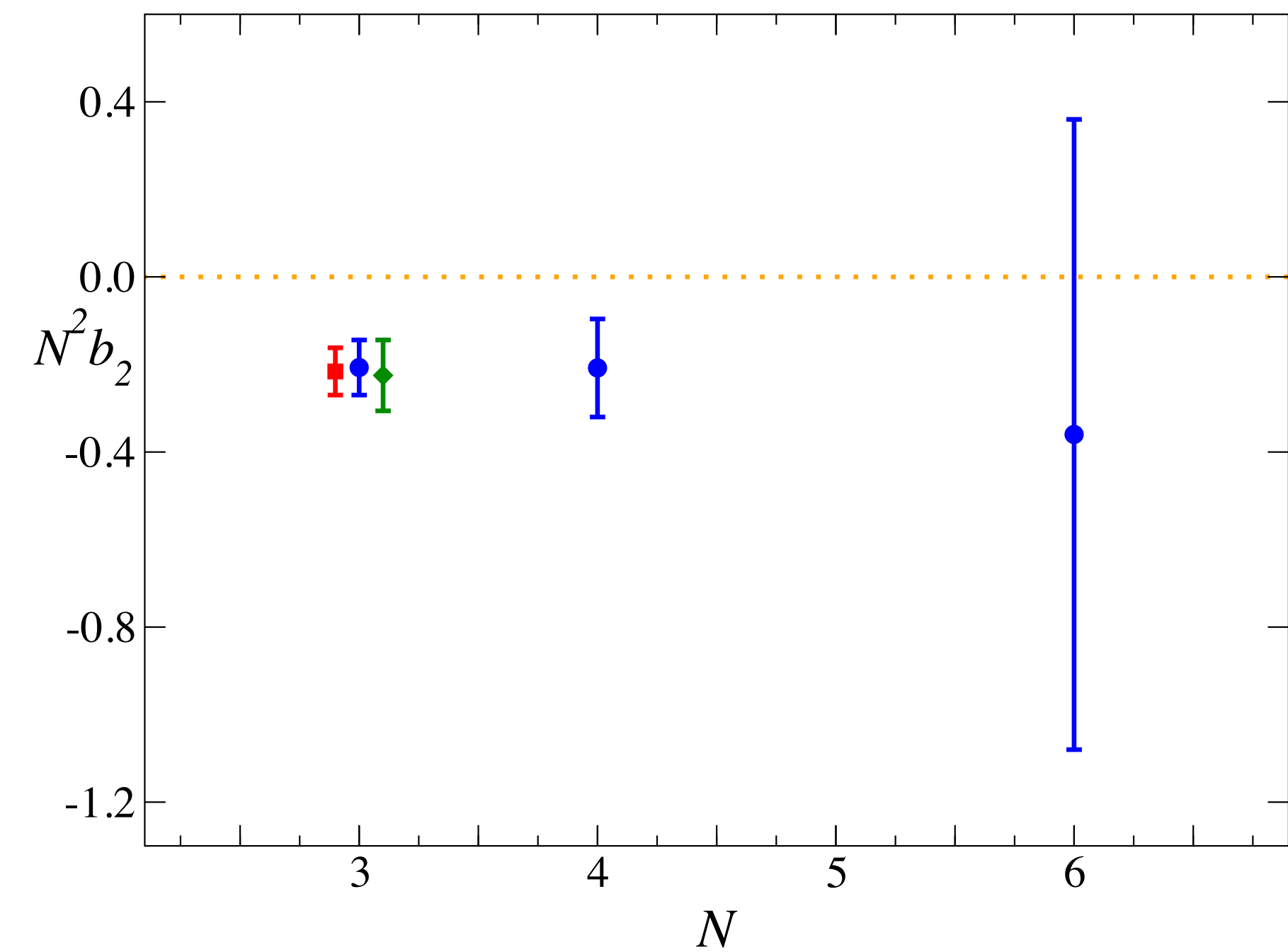
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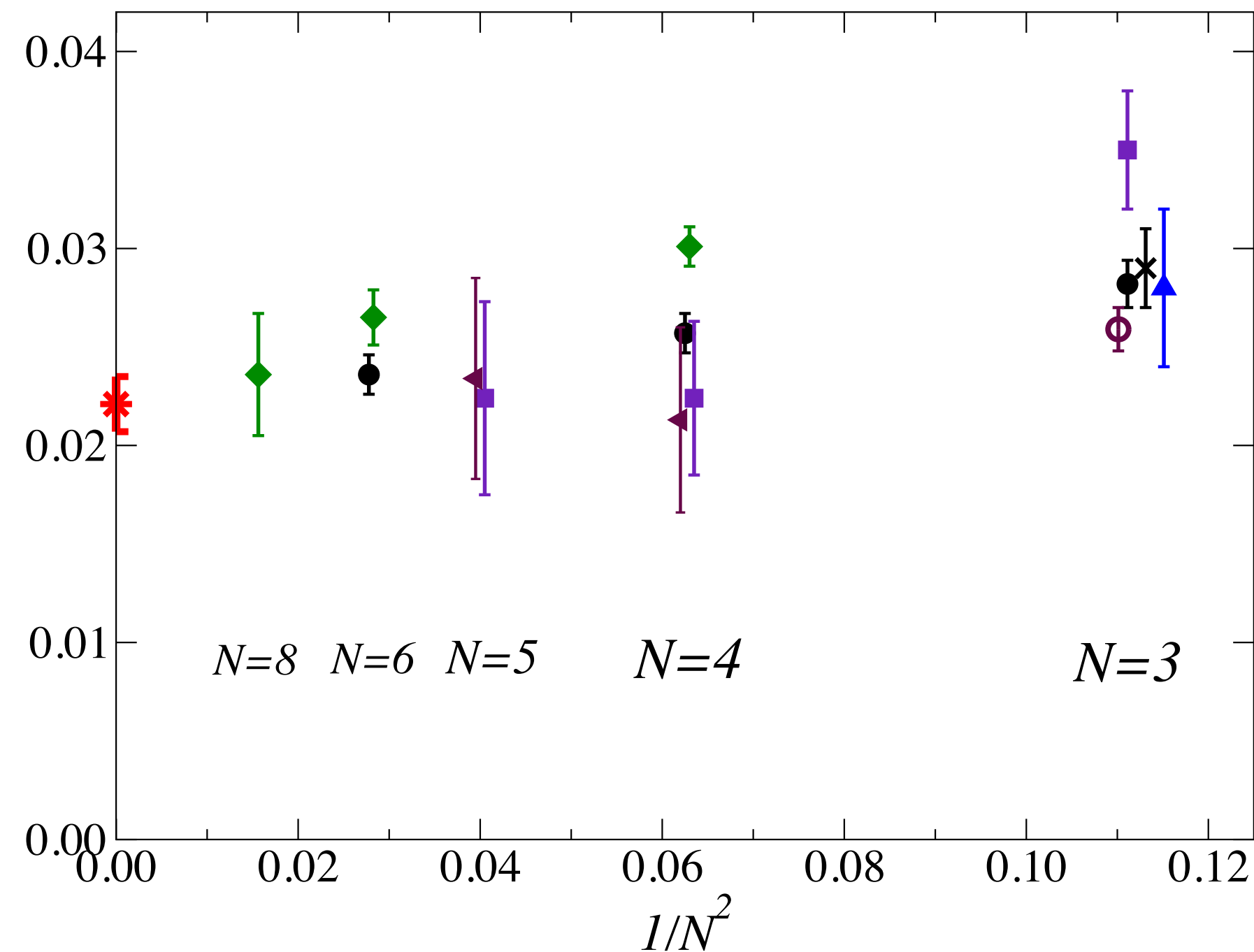
$$b_2 = \frac{\bar{b}_2}{N^2} + O(1/N^4)$$



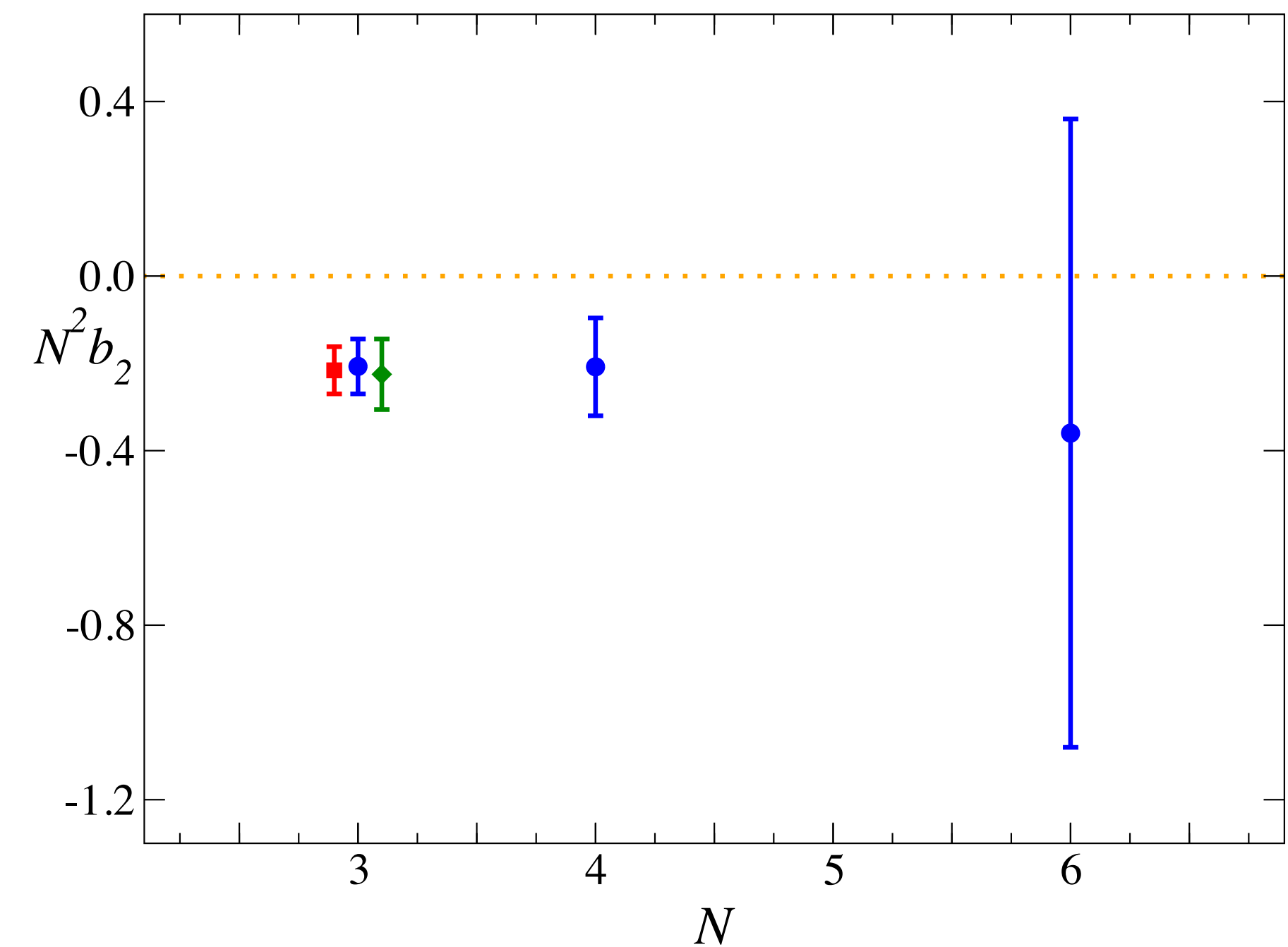
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$$b_2 = \frac{\bar{b}_2}{N^2} + O(1/N^4)$$



only small corrections to the large N limit indicates **CPV** for $N \geq 3$.
(No $SU(2)$ calculation)

Finite temperature

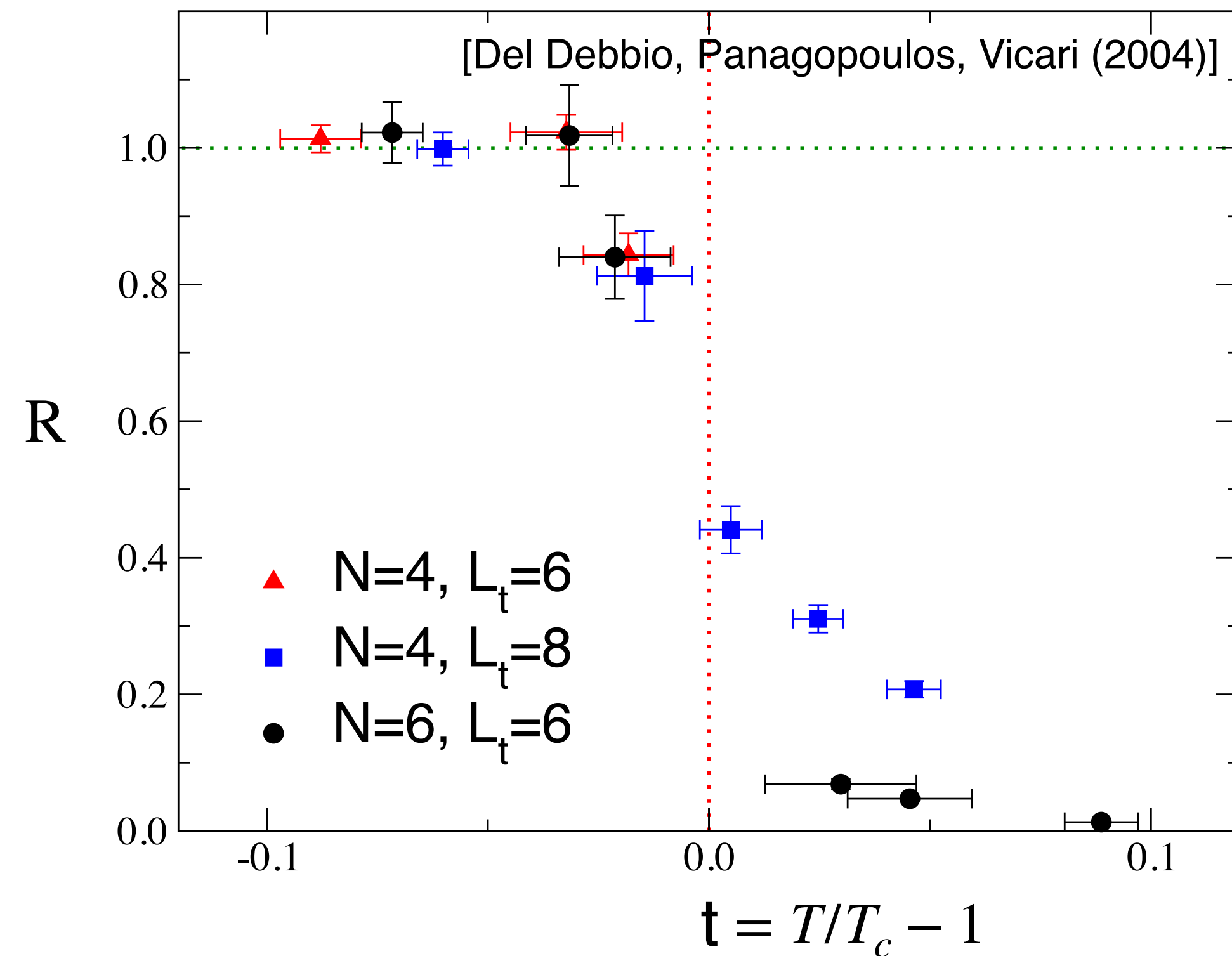
$$\text{DIGA: } f(\theta) \sim T^4 \exp\left(-\frac{8\pi^2}{g^2(T)}\right) (1 - \cos \theta) \sim \underbrace{T^{4-\frac{11N}{3}} \Lambda^{\frac{11N}{3}}}_{\propto \chi(T)} \underbrace{(1 - \cos \theta)}_{= \theta^2/2(1 + b_2\theta^2 + b_4\theta^4 + \dots)}$$

$\Rightarrow b_2 = -1/12, \dots$

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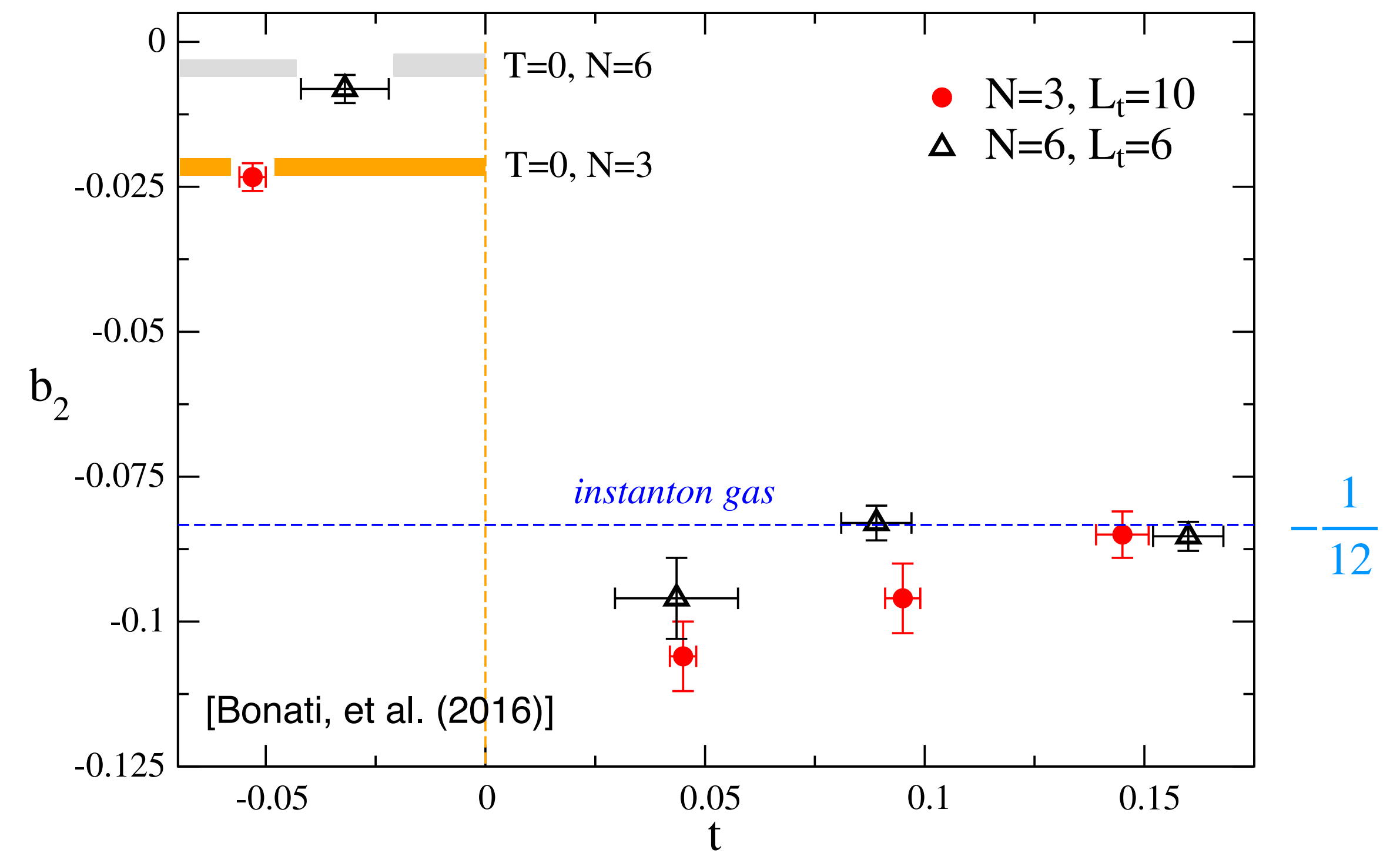
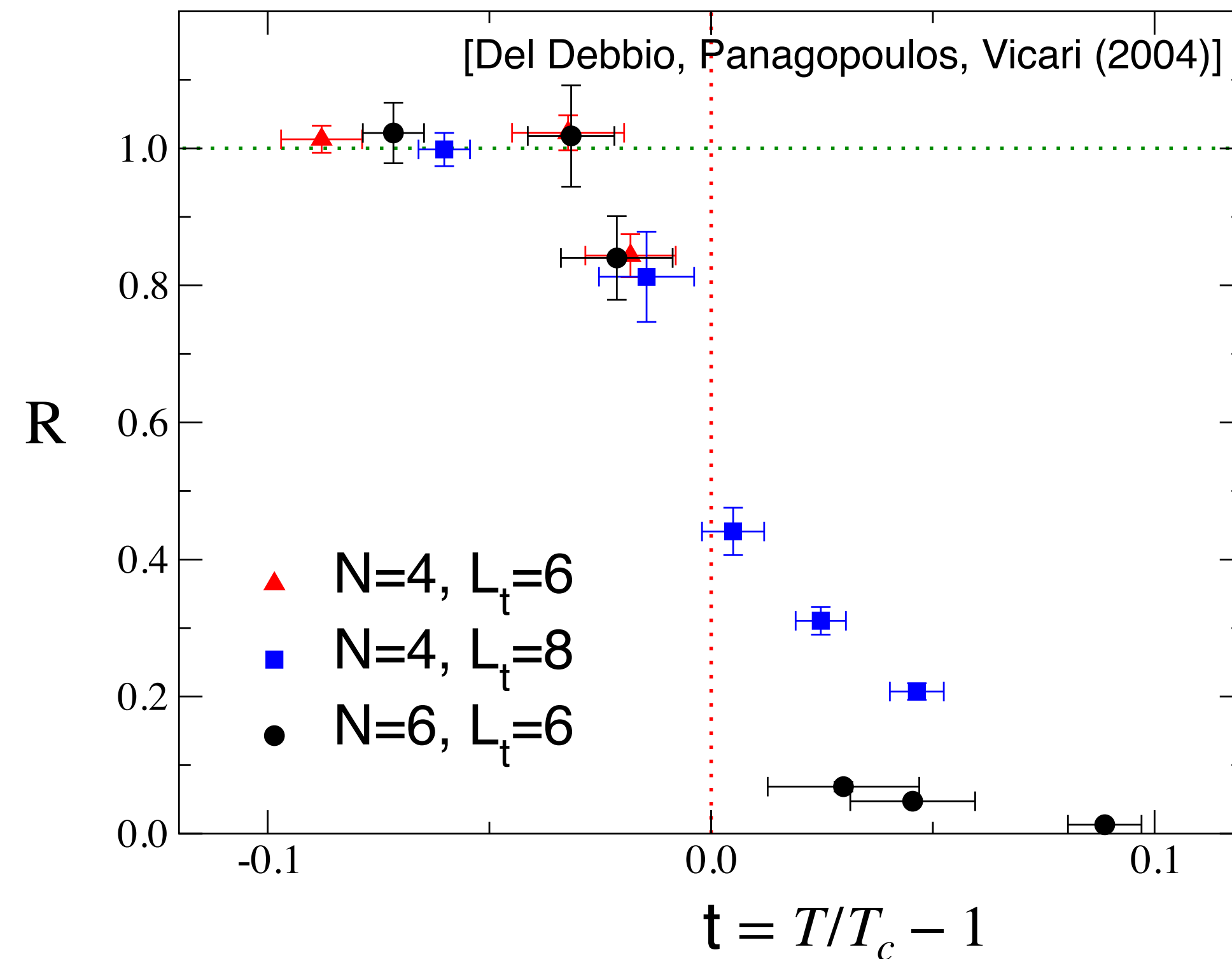
$$R(T) = \chi(T)/\chi(T=0) \Rightarrow b_2 = -1/12, \dots$$



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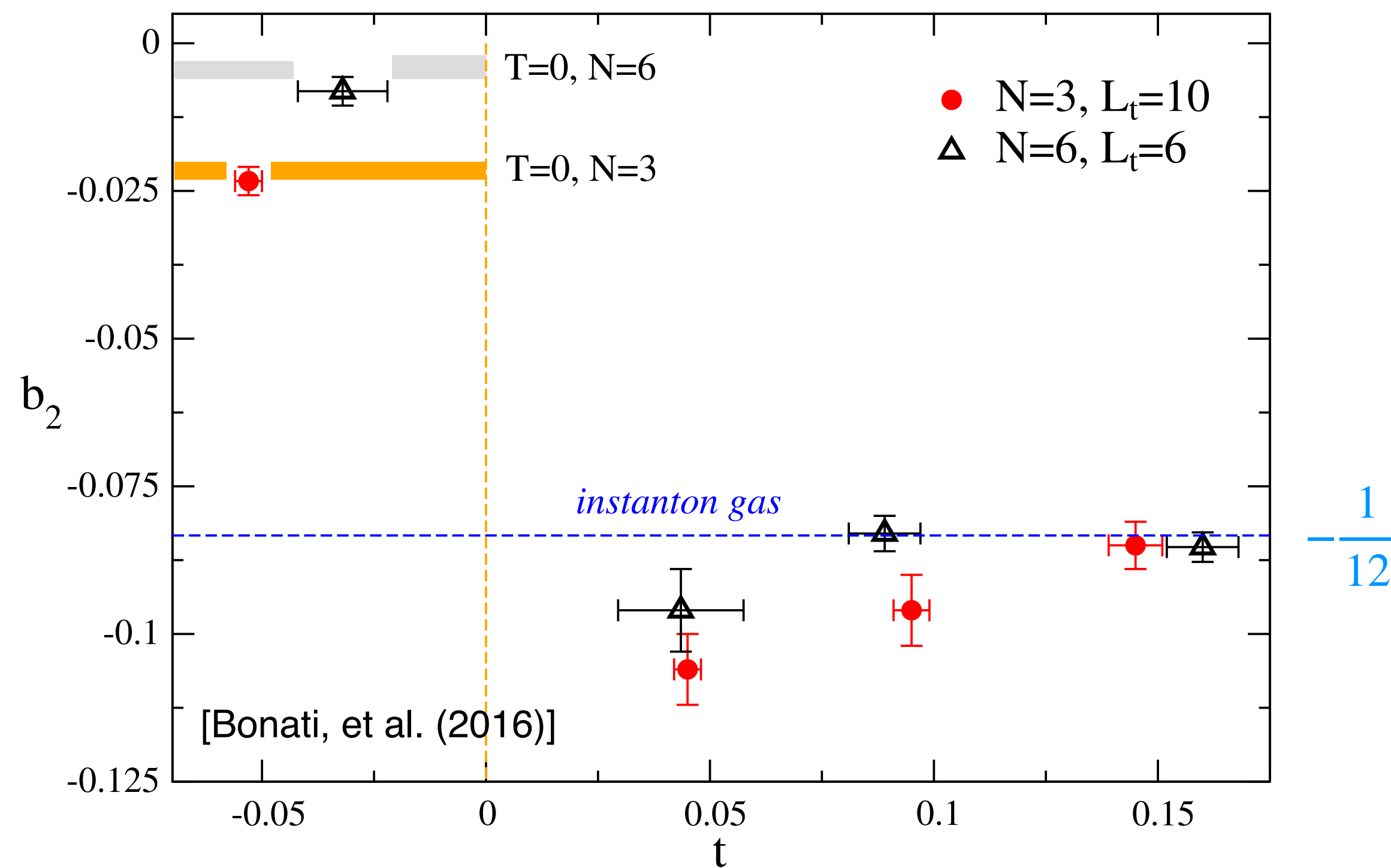
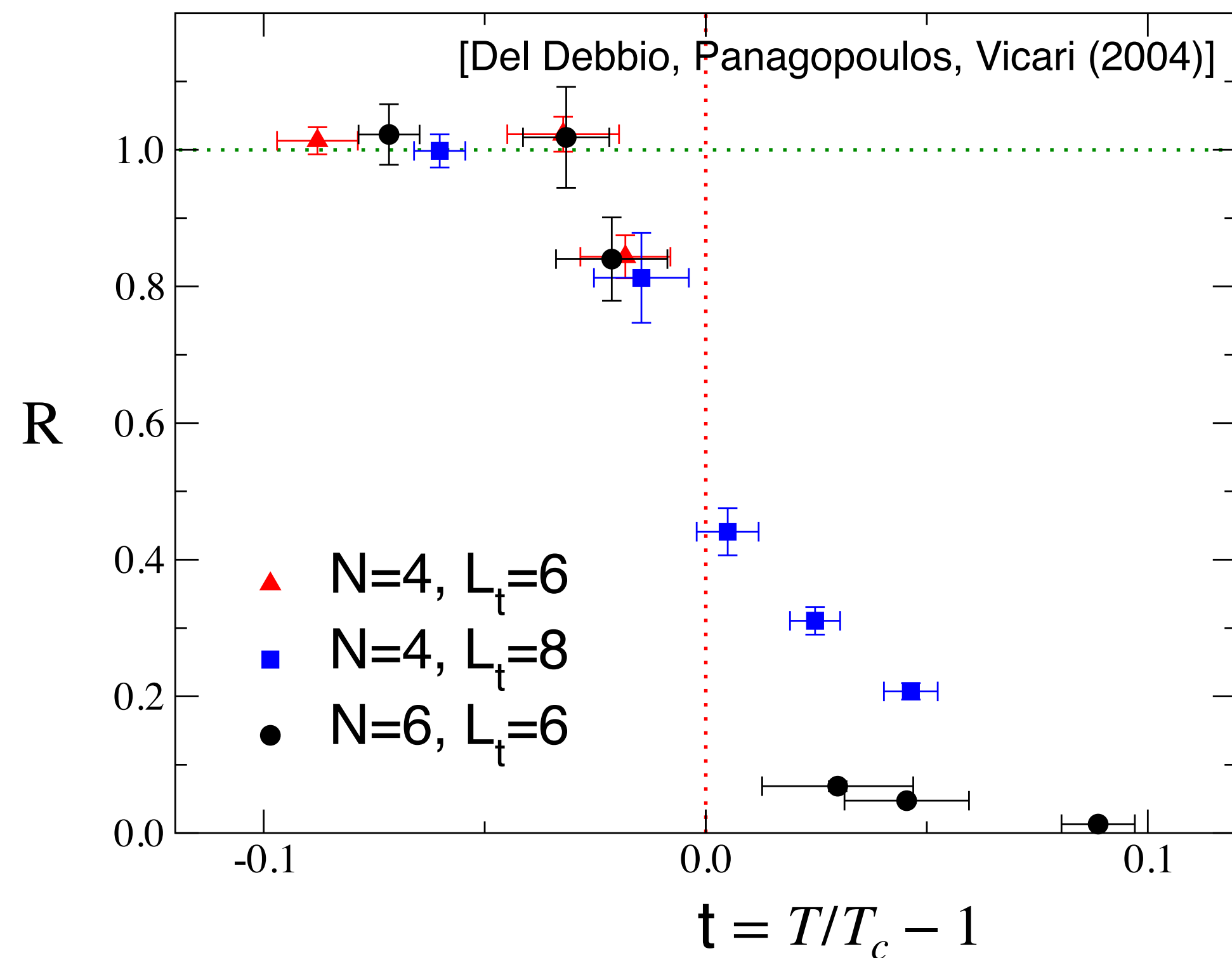
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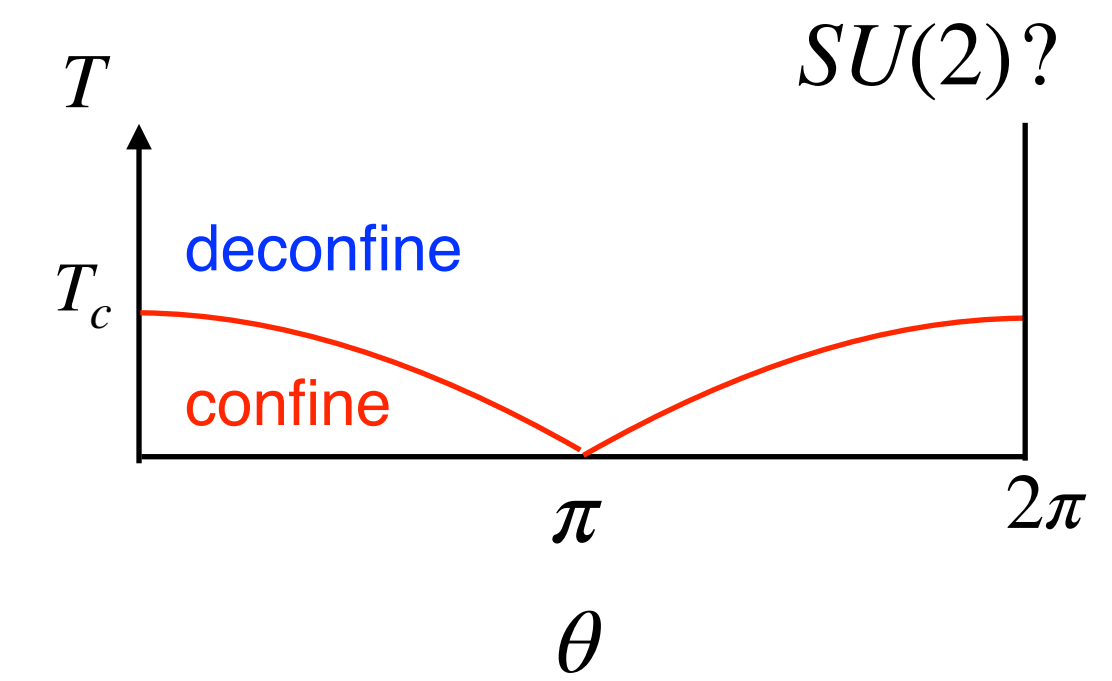
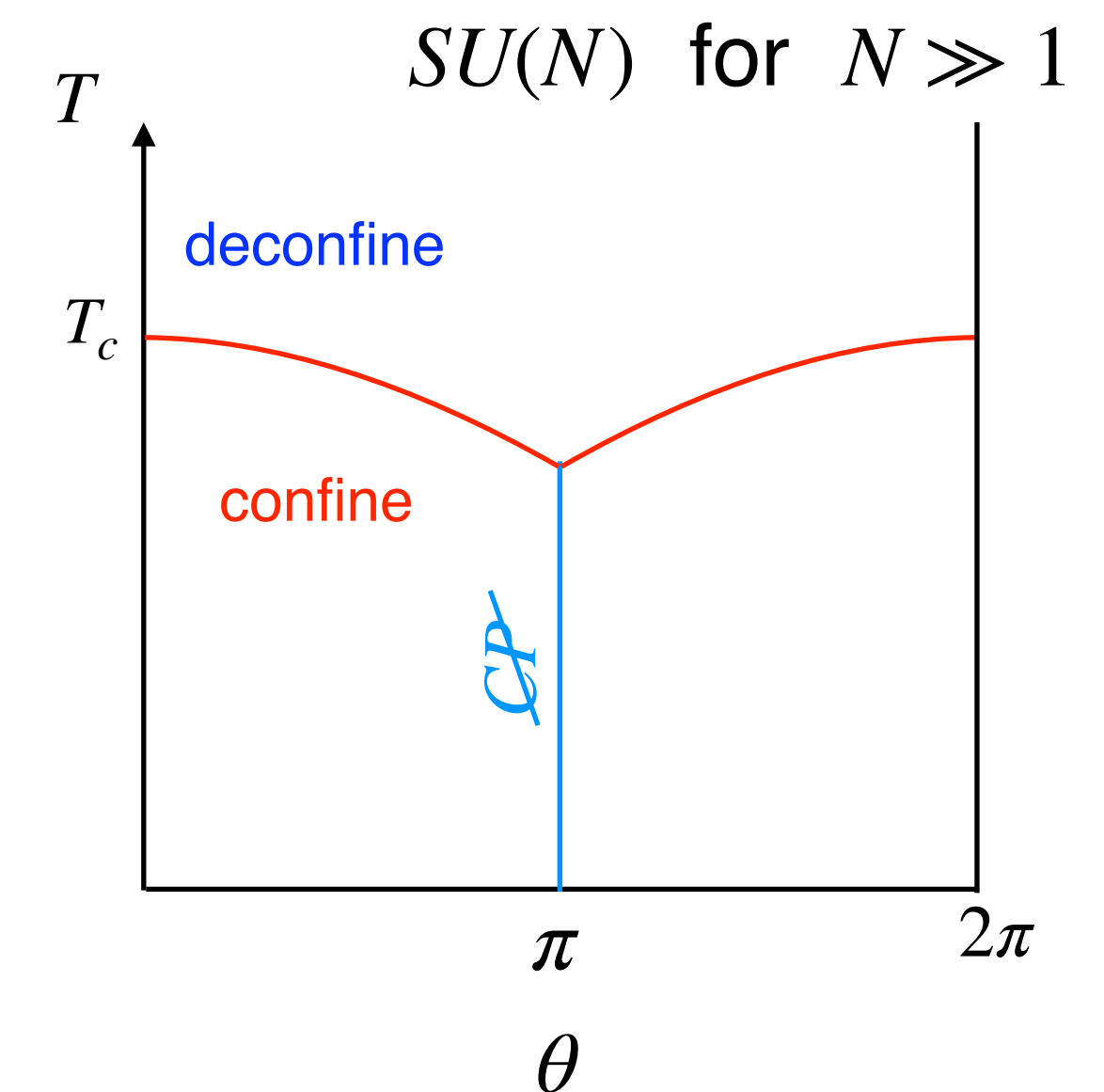
$$R(T) = \chi(T)/\chi(T=0) \Rightarrow b_2 = -1/12, \dots$$



DIGA works for $T > 1.15 T_c$ (No $SU(2)$ calculation)

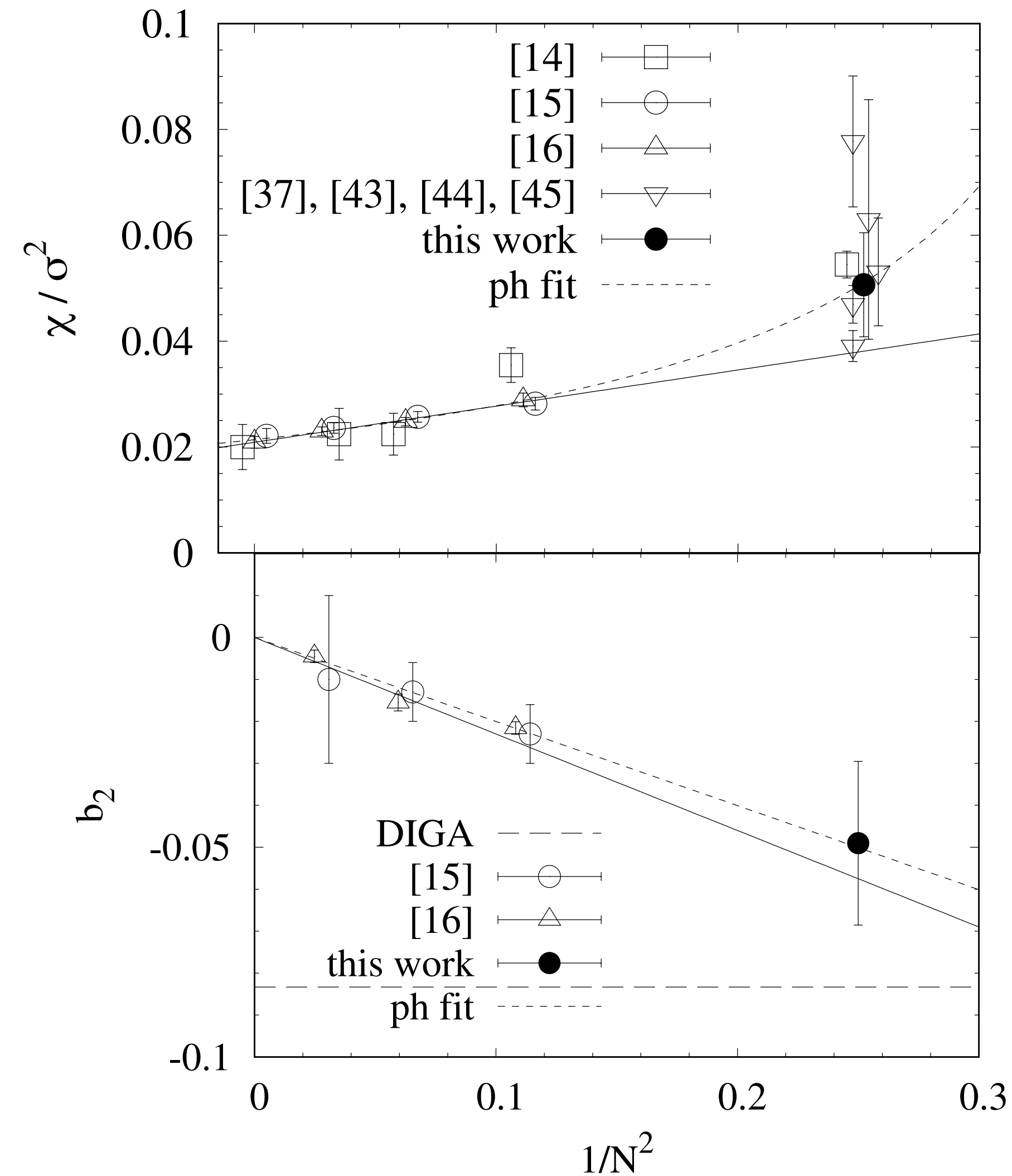
Summary of previous results on $f(\theta)$

- Large N argument seems robust \Rightarrow CPV at $\theta = \pi$ and large N
- Formal arguments tell “For general N , CP has to be broken at $\theta = \pi$ if the vacuum is in the confining phase.”
[Gaiotto, et al.(2017)], [Kitano, Suyama, NY(2017)]
- Numerical evidences of CPV for $N \geq 3$
- What happens to the possible smallest N , i.e. $SU(2)$?
Is it like “large N ” or “2d CP^1 ” ?
 \Rightarrow Lattice numerical simulations



χ and b_2 in $SU(2)$ at $T = 0$

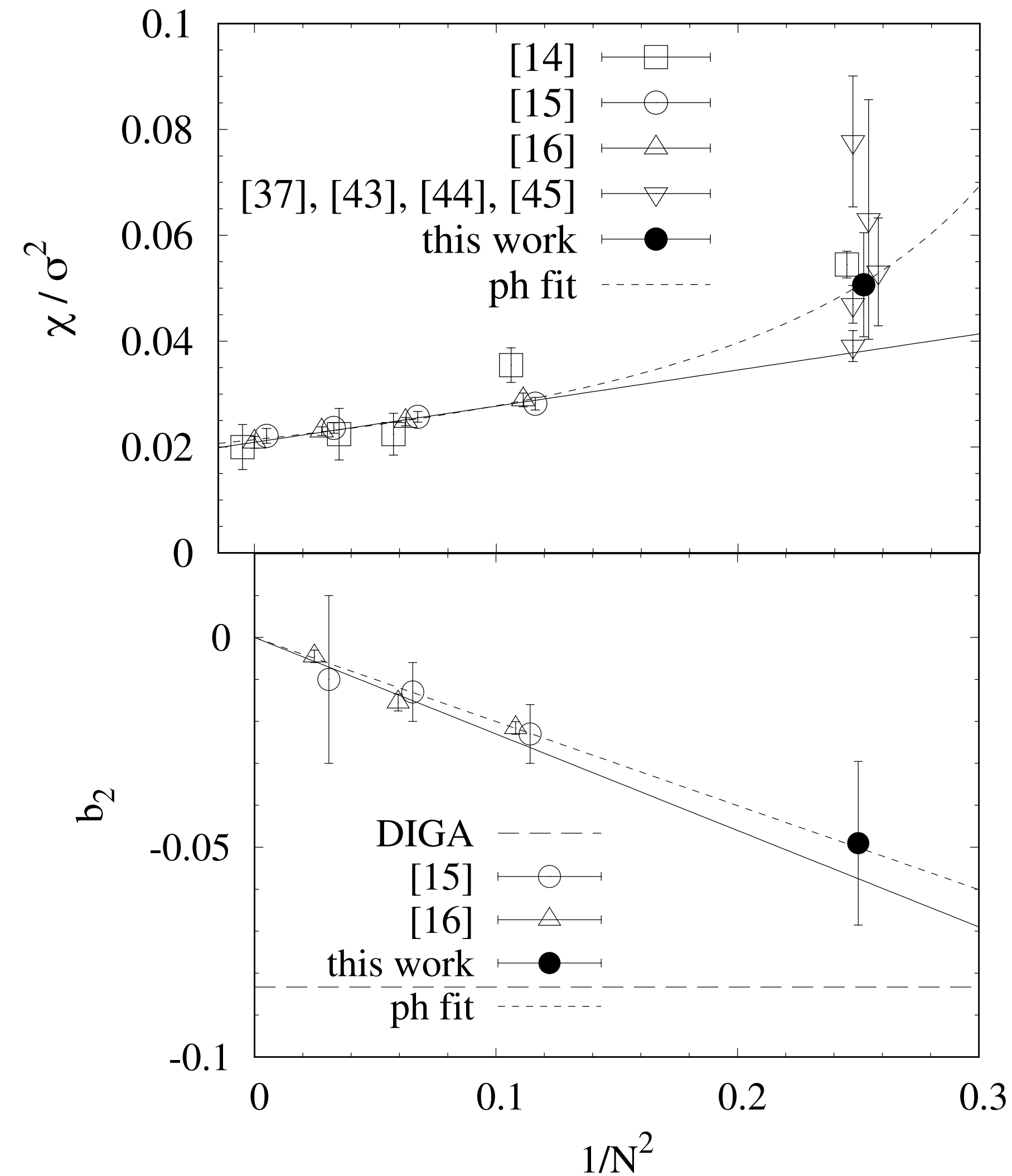
[Kitano, NY, Yamazaki (2021)]



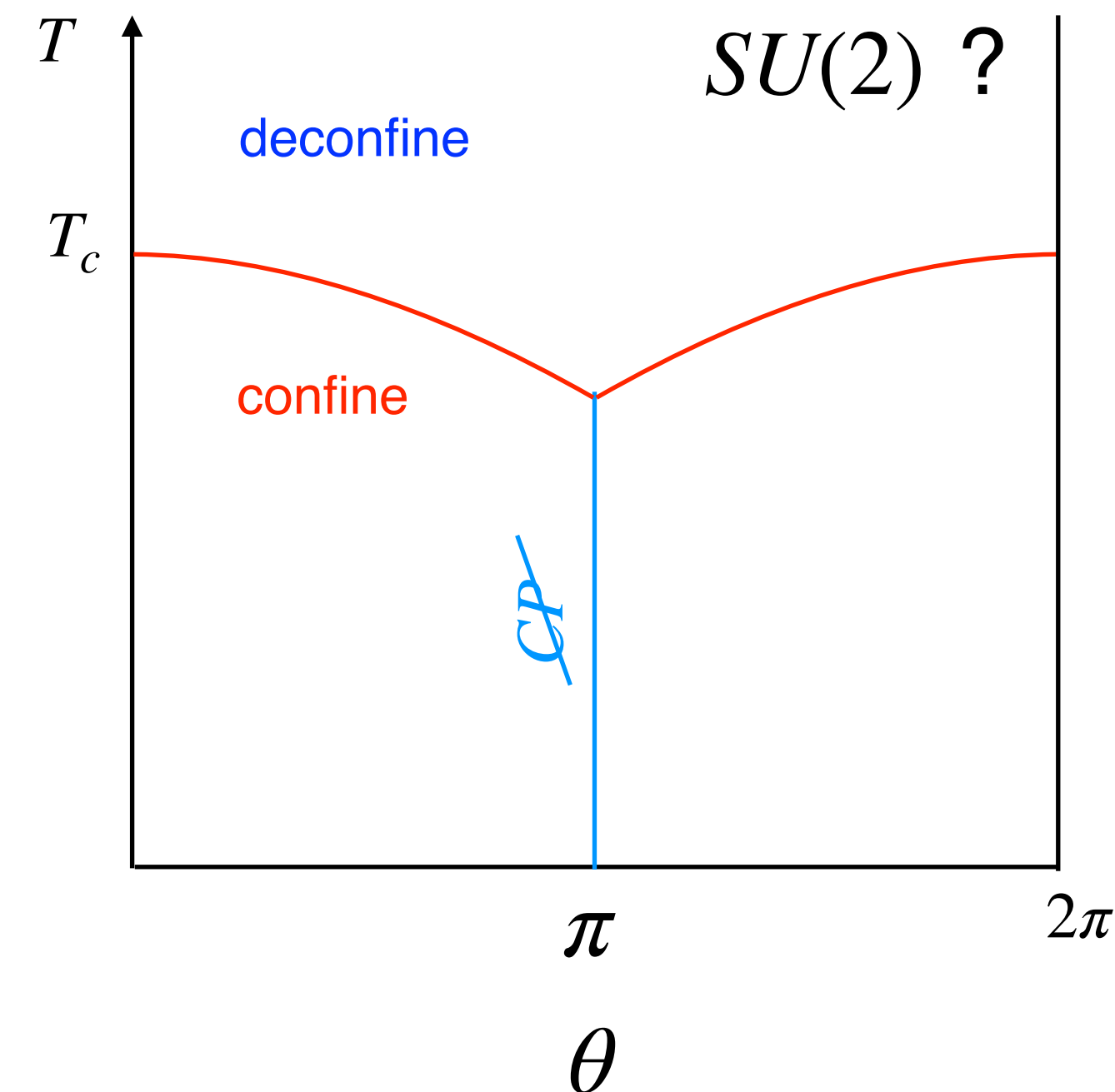
- smoothly connected to large N limit
 $\Rightarrow N \in \mathbb{Z}$ can be analytically continued to \mathbb{R}
 $\Rightarrow f(\theta)$ would be smooth function of N
- $b_2 \neq -\frac{1}{12}$ (i.e. not instanton-like)
 \Rightarrow conjectured that $SU(2)$ belongs to large N class and
CPV takes places at $\theta = \pi$.

χ and b_2 in $SU(2)$ at $T = 0$

[Kitano, NY, Yamazaki (2021)]



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New method without any expansion

[Kitano, Matsudo, NY, Yamazaki(2021)]

Introduce sub-volume $V_{\text{sub}} = l^4$ and

$$Q_{\text{sub}} = \sum_{x \in V_{\text{sub}}} q(x) \notin \mathbb{Z}$$

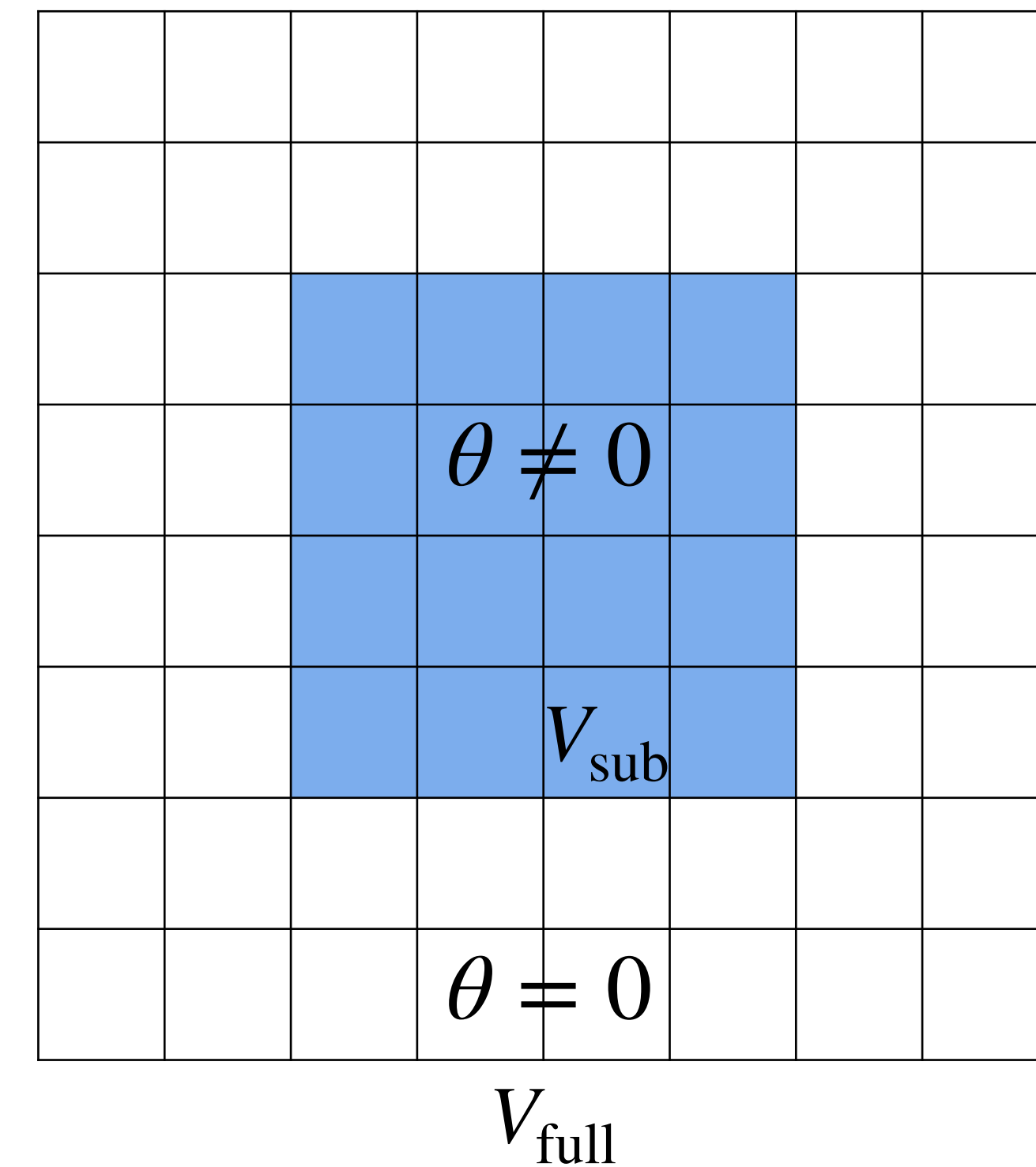
$$e^{-V_{\text{sub}} f_{\text{sub}}(\theta)} = \frac{Z(\theta)}{Z(0)} = \frac{1}{Z(0)} \int \mathcal{D}U e^{-S_g + i\theta Q_{\text{sub}}} = \langle e^{i\theta Q_{\text{sub}}} \rangle_{\theta=0}$$

$$f_{\text{sub}}(\theta) = -\frac{1}{V_{\text{sub}}} \ln \langle \cos(\theta Q_{\text{sub}}) \rangle_{\theta=0}$$

$$f(\theta) = \lim_{V_{\text{sub}} \rightarrow \infty} f_{\text{sub}}(\theta) = \lim_{l \rightarrow \infty} \left\{ f(\theta) + \frac{s(\theta)}{l} + O(1/l^2) \right\}$$

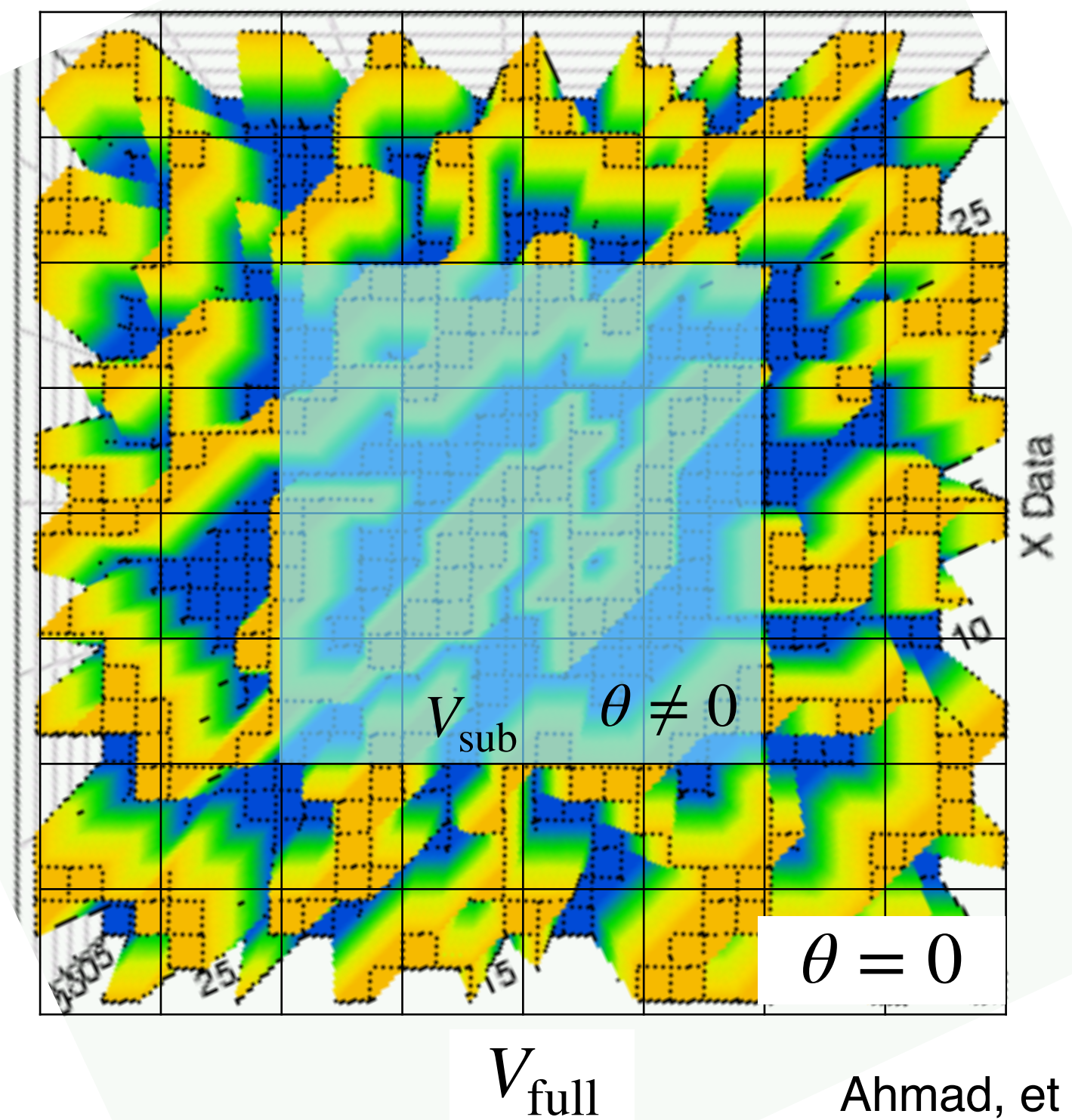
with $l_{\text{dyn}}^4 \ll V_{\text{sub}} \ll V_{\text{full}}$ (l_{dyn} : dynamical length scale)
 $s(\theta)$: surface tension

“sub-volume method”



Expected behavior of $f_{\text{sub}}(\theta)$ as a function of V_{sub}

- $V_{\text{sub}} \gg l_{\text{dyn}}^4$ would have to be satisfied.
- As long as $V_{\text{sub}} \gg l_{\text{dyn}}^4$, $f_{\text{sub}}(\theta)$ is expected to show the scaling behavior, $f_{\text{sub}}(\theta) = f(\theta) + \frac{s(\theta)}{l} + O(1/l^2)$.
- Such a behavior will end as $V_{\text{sub}} \rightarrow V_{\text{full}}$, where $Q_{\text{sub}} \rightarrow Q_{\text{full}} \in \mathbb{Z}$. Thus, $V_{\text{sub}} \ll V_{\text{full}}$ is required.
- On the other hand, the method fails when $|\theta Q_{\text{sub}}| \sim \pi$ because $f_{\text{sub}}(\theta) \propto \ln\langle \cos(\theta Q_{\text{sub}}) \rangle$ becomes ill-defined.
- **Crucial question:**
 V_{sub} satisfying $l_{\text{dyn}}^4 \ll V_{\text{sub}} \ll V_{\text{full}}$ and $|\theta Q_{\text{sub}}| < \pi$ exists ?



Ahmad, et al. (2005)

Similarity to the static potential calculation

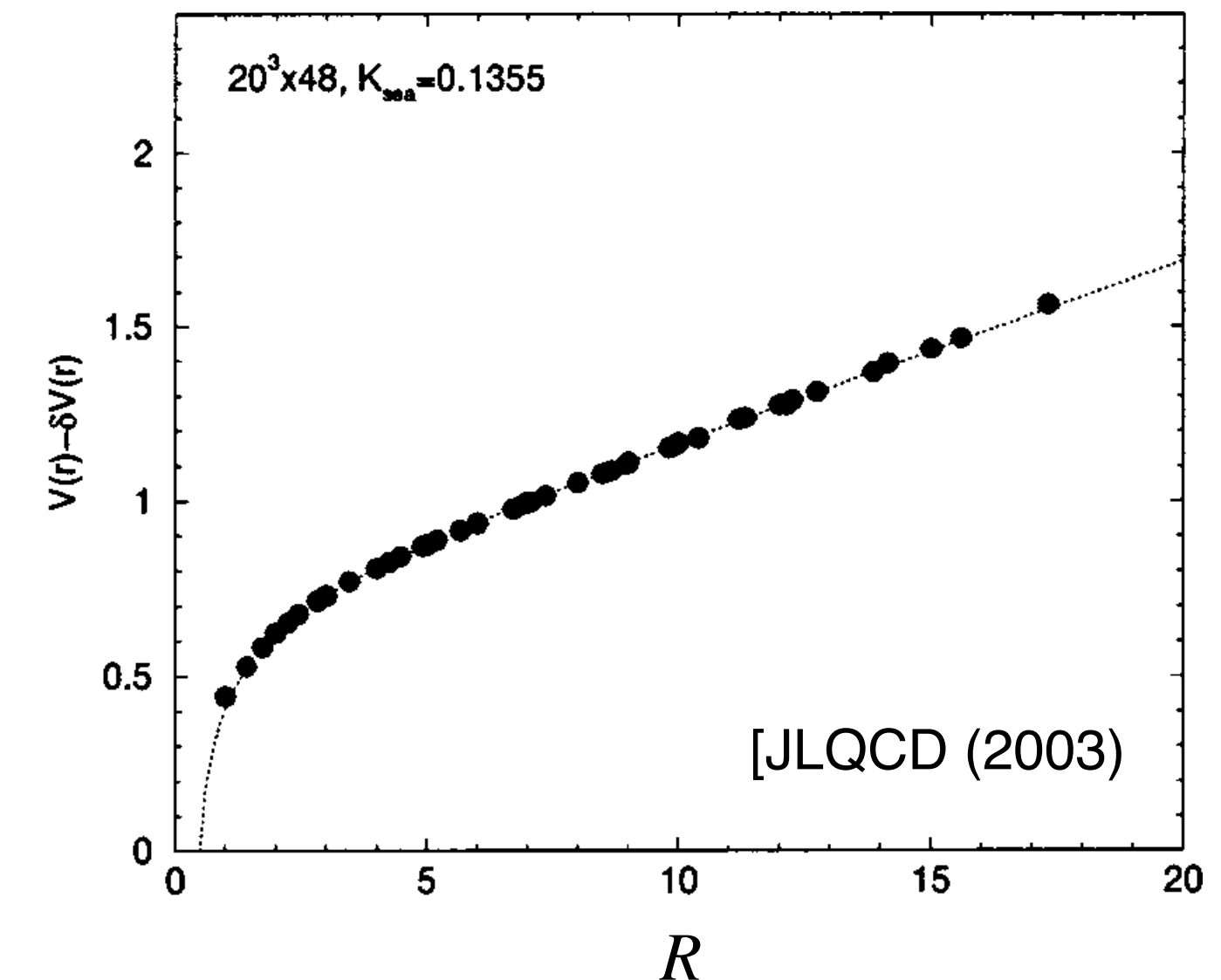
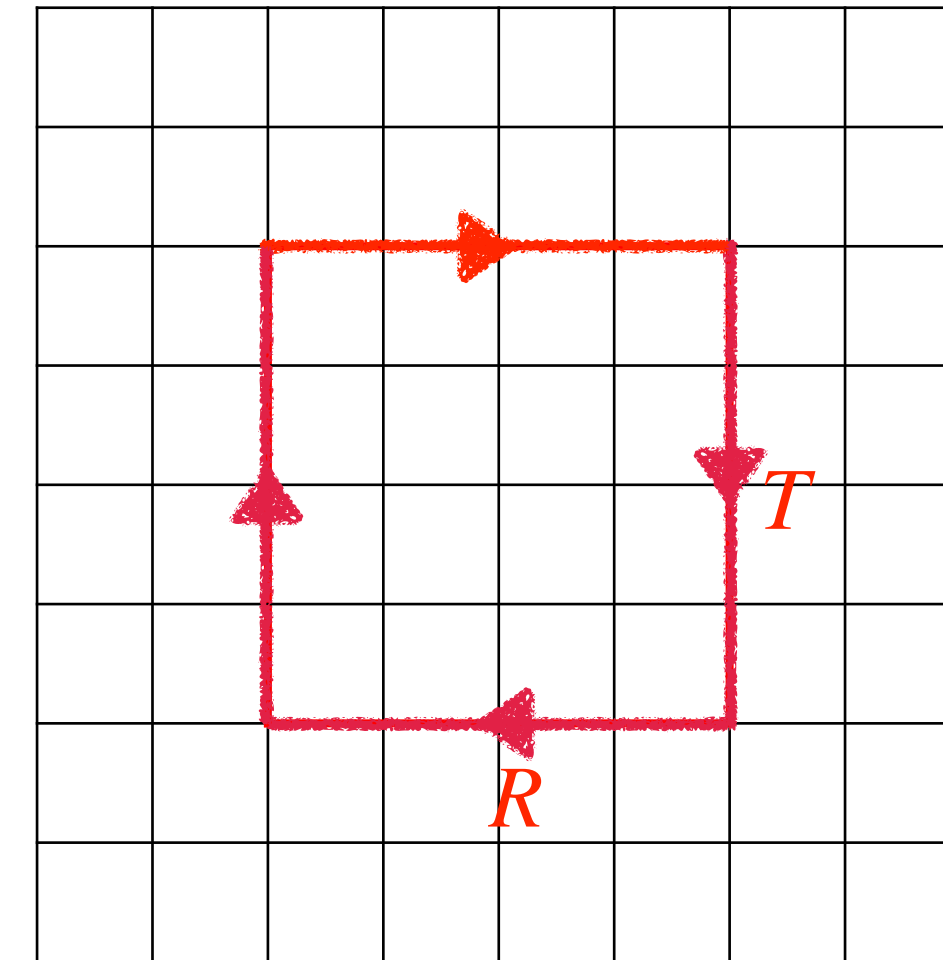
In the static potential calculation, Wilson loop is inserted.

$$\frac{Z(\square)}{Z(1)} = \frac{1}{Z(1)} \int \mathcal{D}U \operatorname{Tr}[e^{i\oint A}] e^{-S_{\text{QCD}}} = \langle \operatorname{Tr}[e^{i\oint A}] \rangle \rightarrow e^{-V(\mathcal{A})}$$

$$V(\mathcal{A}) = - \lim_{\mathcal{A} \rightarrow \infty} \ln \langle \operatorname{Tr}[e^{i\oint A}] \rangle = \sigma \mathcal{A} + \dots$$

In **sub-volume method**, instead a operator extending over subvolume is inserted.

$f(\theta)$ is analogous to σ in the static potential.



About smearing

- Need to numerically calculate $q(x) = \frac{1}{64\pi^2} \epsilon_{\mu\nu\rho\sigma} F_{\mu\nu}^a F_{\rho\sigma}^a$ on the lattice
- Raw configurations are contaminated by local lumps.
- Smearing (= smoothing a configuration) removes such short-distance artifacts.
- However, at the same time, smearing may alter relevant topological excitations, too.
- We studied this point and developed the procedure to restore relevant information.
[Kitano, NY, Yamazaki (2021)]
 - calculate an observable every 5 steps of the smearing
 - extrapolate those back to $n_{\text{APE}} \rightarrow 0$, $\langle O \rangle = \lim_{n_{\text{APE}} \rightarrow 0} \langle O(n_{\text{APE}}) \rangle$

Lattice parameters and observables

- $SU(2)$ YM theory by Symanzik improved gauge action

$$\beta = \frac{4}{g^2} = 1.975 \quad (\text{relatively fine: } 1/(aT_c) = 9.50)$$

$$\bullet V_{\text{full}} = 24^3 \times \{48, 6, 8\} \quad (T = 0, 1.2T_c, 1.6T_c)$$

- Periodic boundary condition in all directions

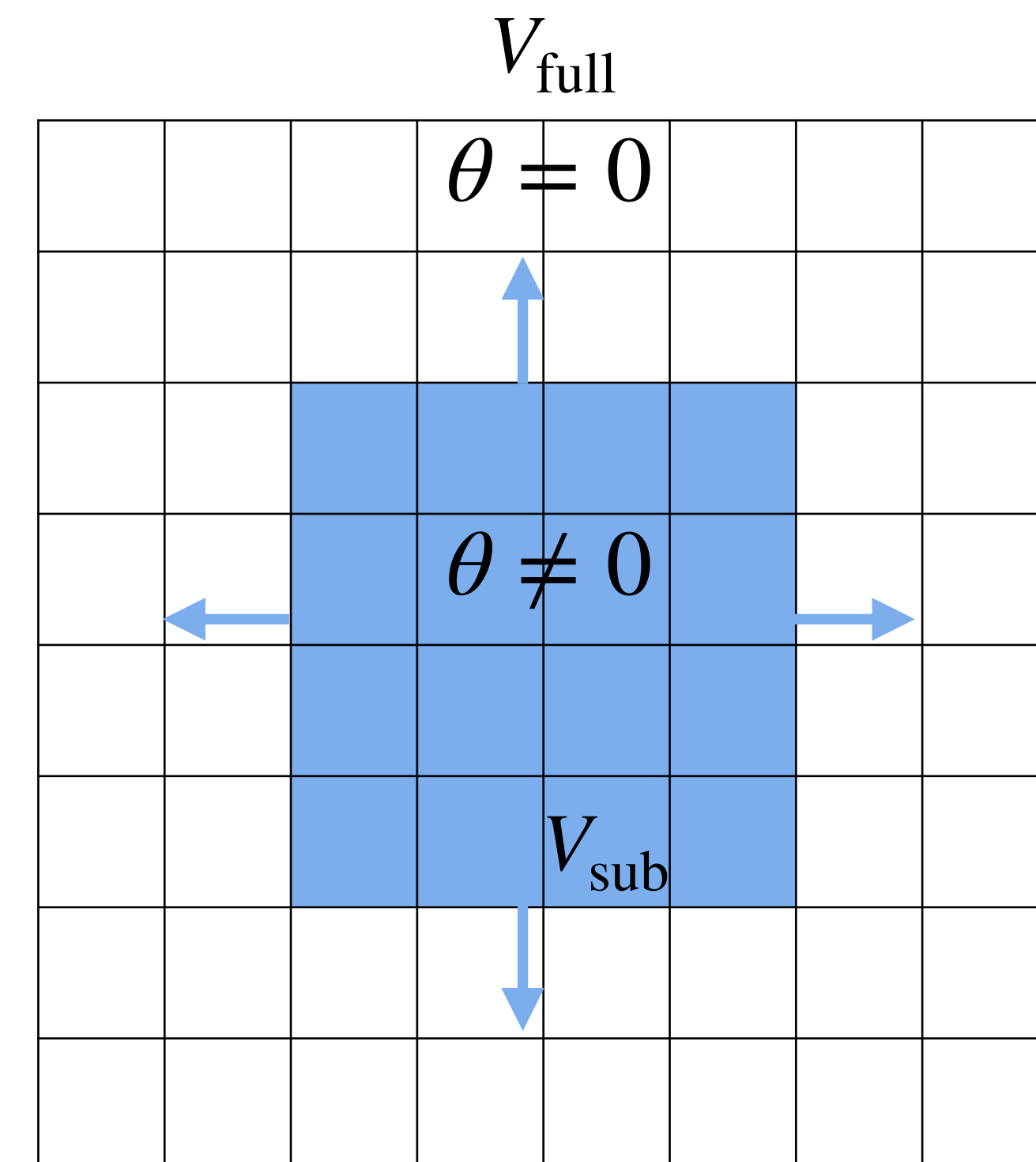
$$\bullet \# \text{ of configs} = \{ 68000, 5000, 5000 \}$$

$$\bullet \text{Calculate } Q_{\text{sub}} = \sum_{x \in V_{\text{sub}}} q(x) \text{ and estimate}$$

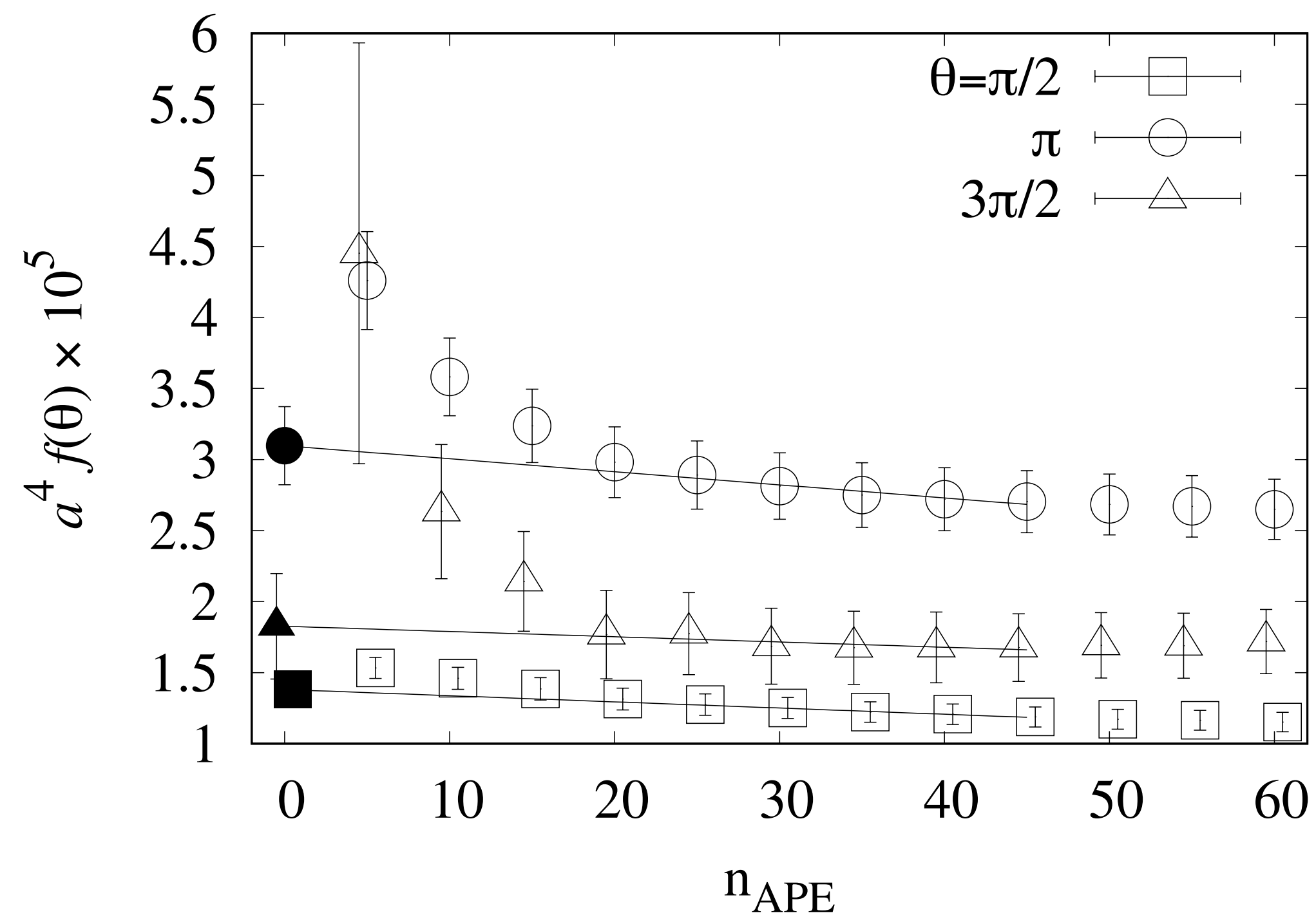
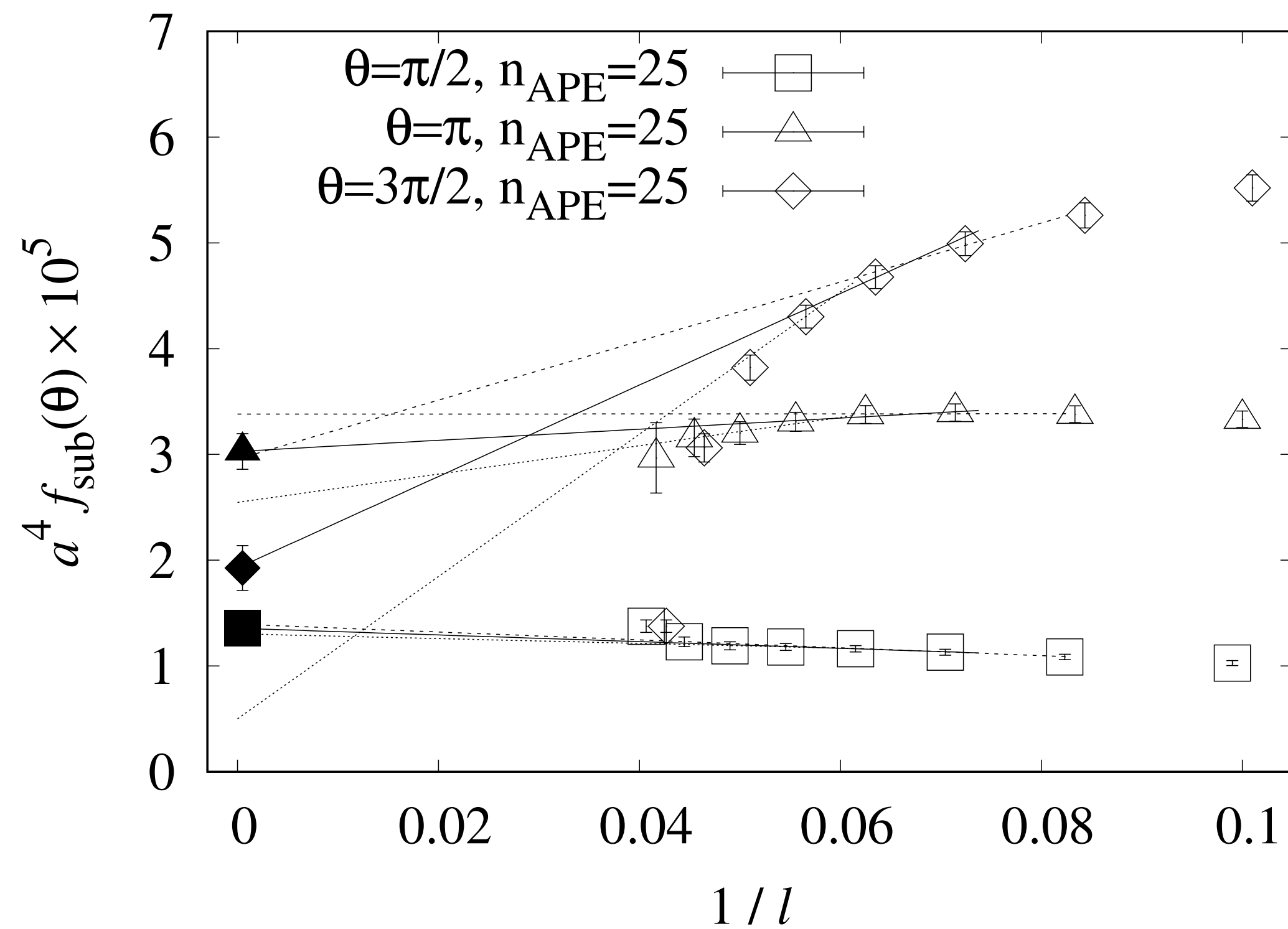
$$\checkmark f(\theta) = - \lim_{V_{\text{sub}} \rightarrow \infty} \frac{1}{V_{\text{sub}}} \ln \langle \cos(\theta Q_{\text{sub}}) \rangle$$

$$\checkmark \frac{df(\theta)}{d\theta} = \lim_{V_{\text{sub}} \rightarrow \infty} \frac{1}{V_{\text{sub}}} \frac{\langle Q_{\text{sub}} \sin(\theta Q_{\text{sub}}) \rangle}{\langle \cos(\theta Q_{\text{sub}}) \rangle}$$

which are used to crosscheck each other

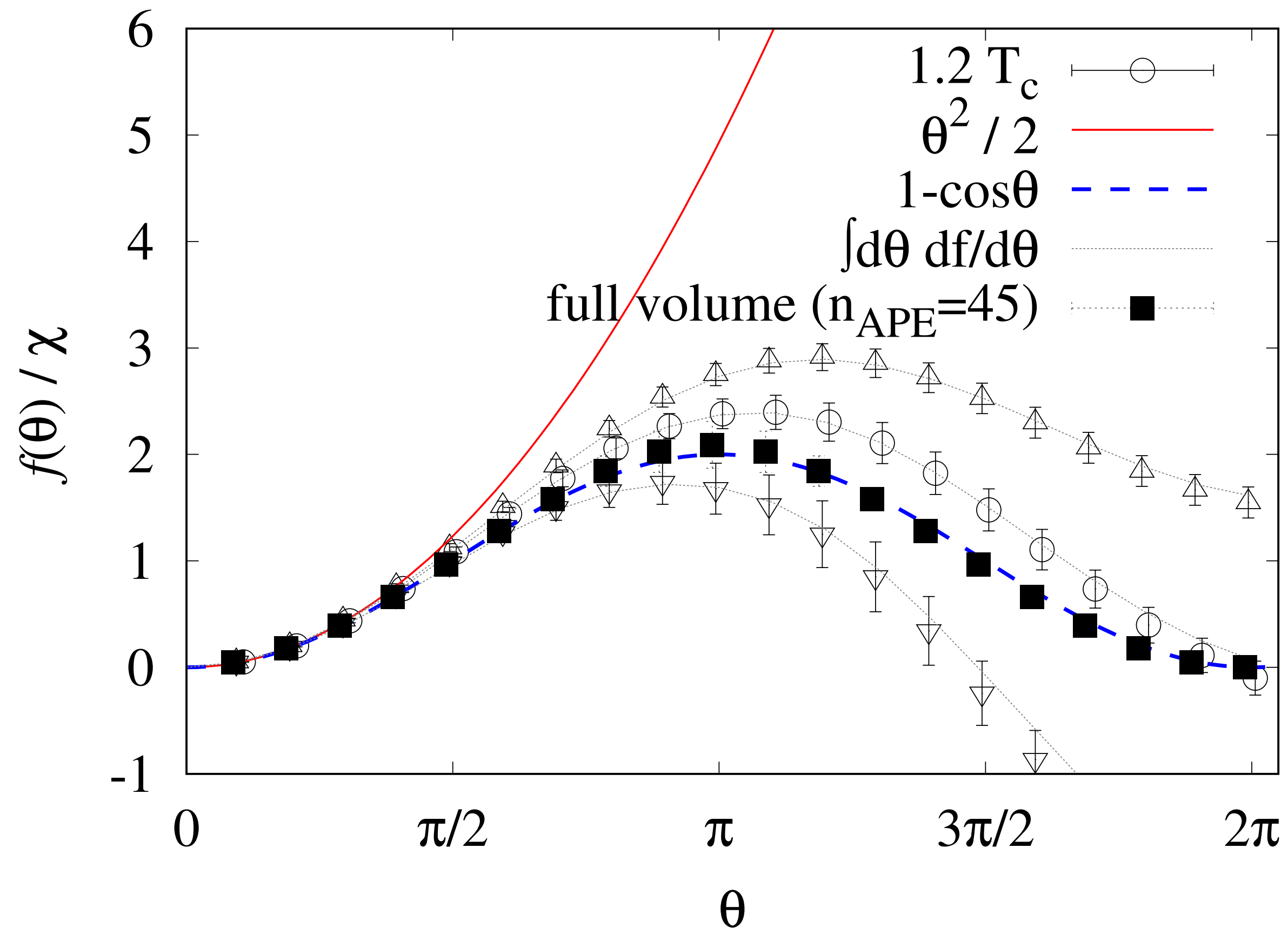


Finite temperature ($T = 1.2 T_c$)



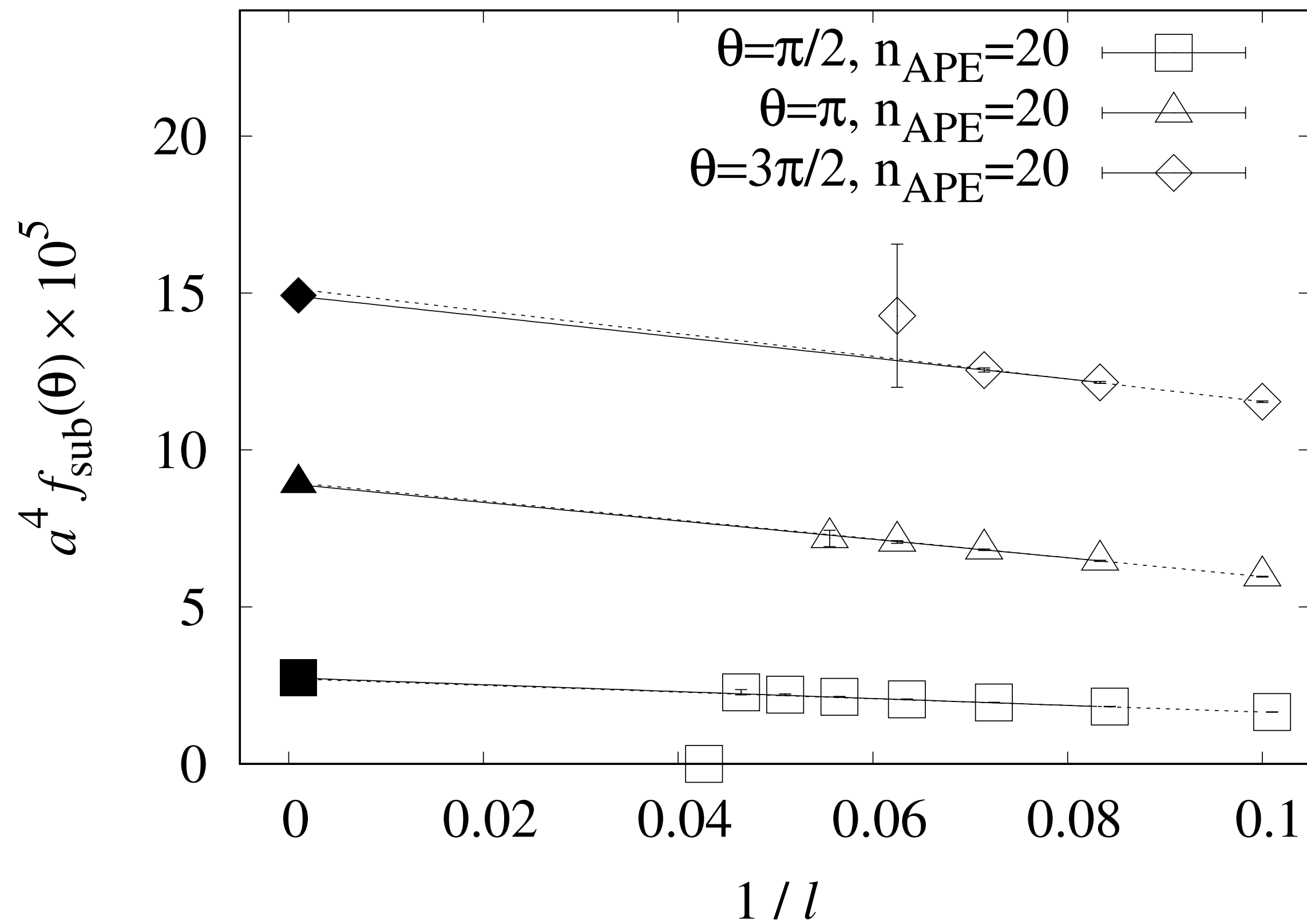
- $V_{\text{sub}} = l^3 \times 6$ with $l \in \{12, \dots, 20\}$
- Linear fit works well in either extrapolations.
- Not monotonic function, $f(\pi) > f(3\pi/2)$

θ dependence of $f(\theta)$ at $T = 1.2T_c$



- Systematic error due to ambiguity of the scaling region is large for $\theta > \pi$
- Within large uncertainty, consistent with the DIGA.
- $df(\theta)/d\theta \Big|_{\theta=\pi} \approx 0 \Rightarrow$ **no CPV** above T_c
- Numerical consistency with $\int d\theta \frac{df}{d\theta}$
- Similar results at $T = 1.6T_c$

$l \rightarrow \infty$ limit at $T = 0$

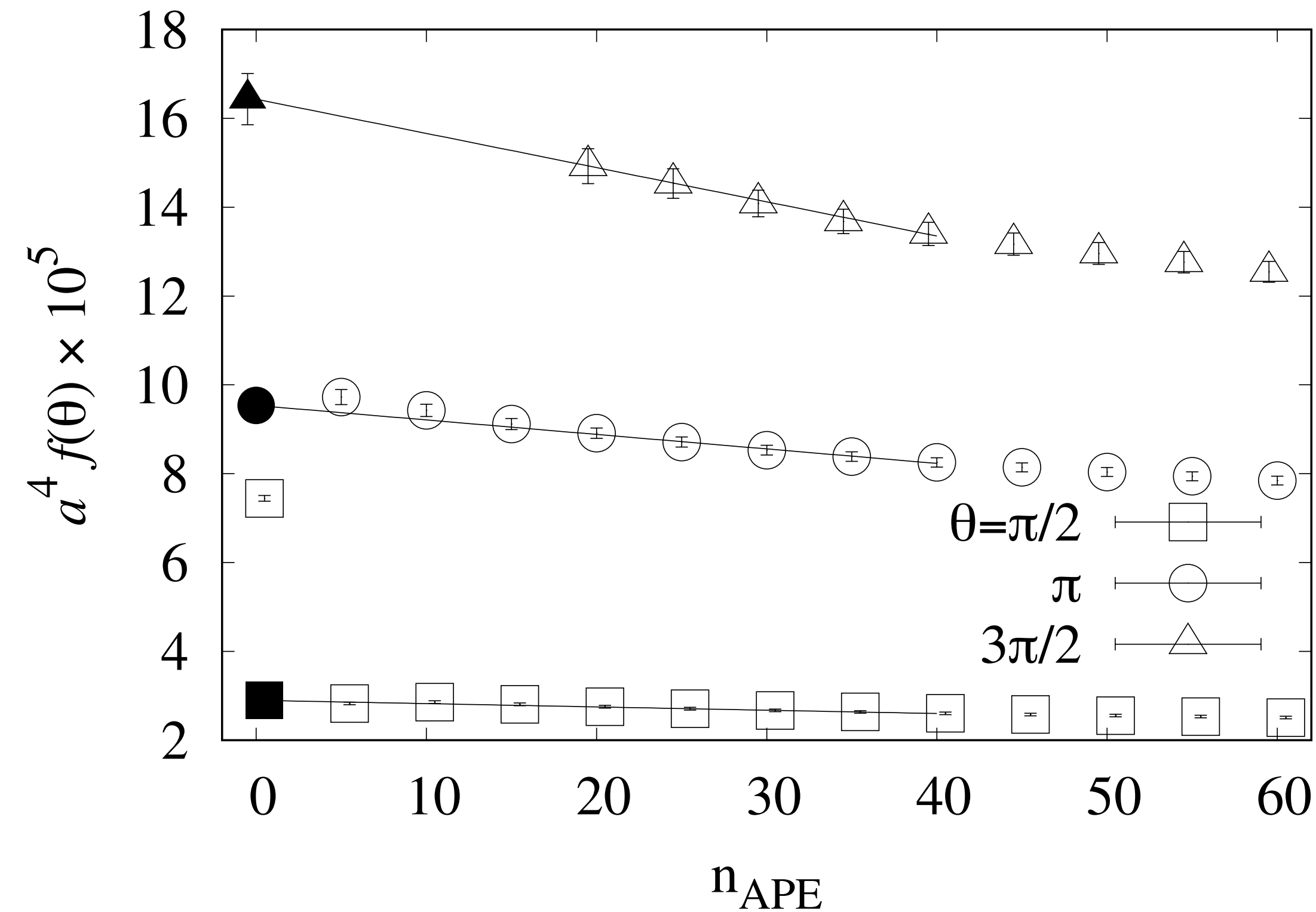


- $V_{\text{sub}} = l^4$ with $l \in \{10, 12, \dots, 20\}$
- Data in the range of $l_{\text{dyn}}^4 \ll V_{\text{sub}} \ll V_{\text{full}}$ are fitted to

$$f_{\text{sub}}(\theta) = f(\theta) + \frac{as(\theta)}{l}$$

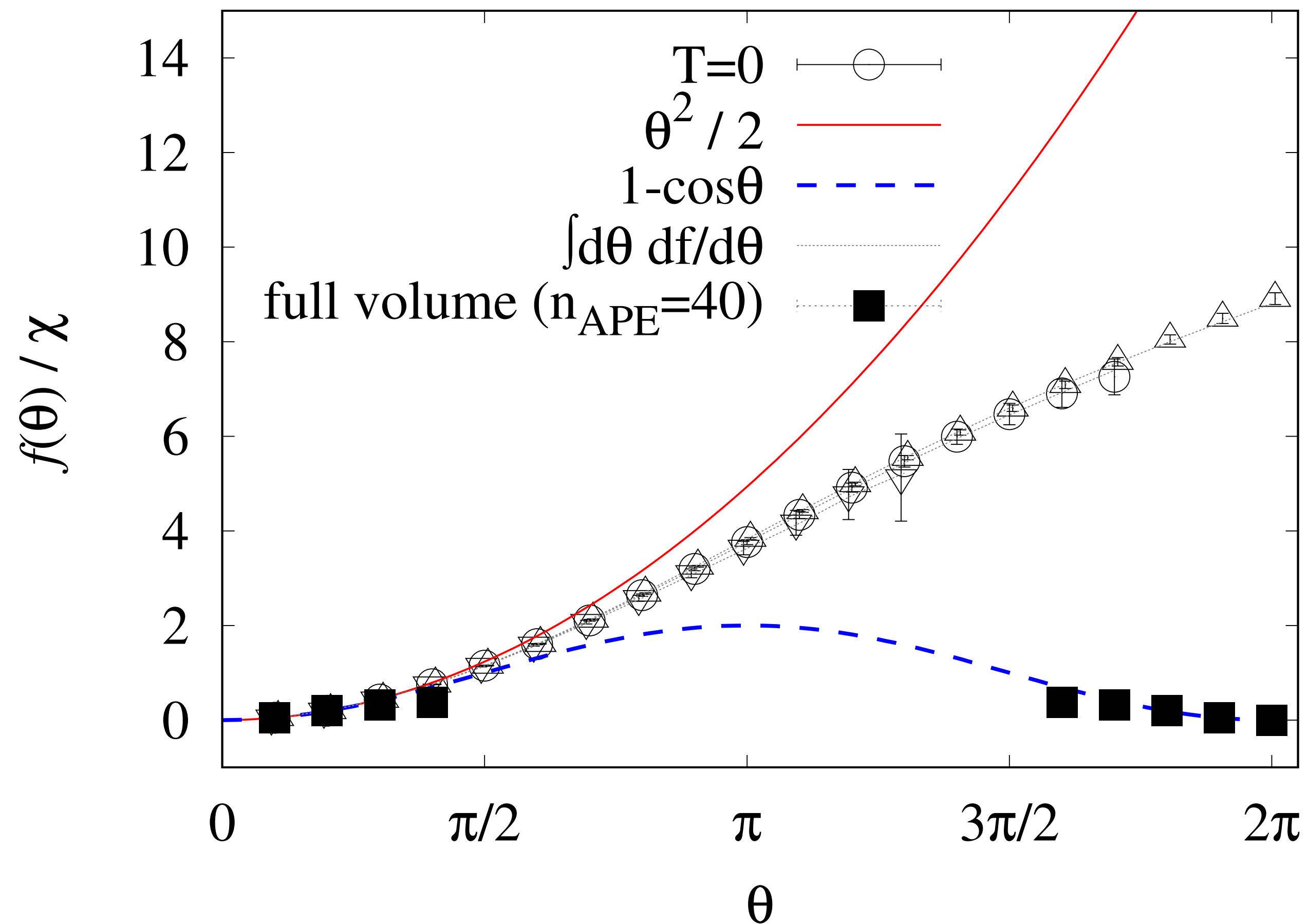
- Linear extrapolation works well.

$n_{\text{APE}} \rightarrow 0$ limit at $T = 0$



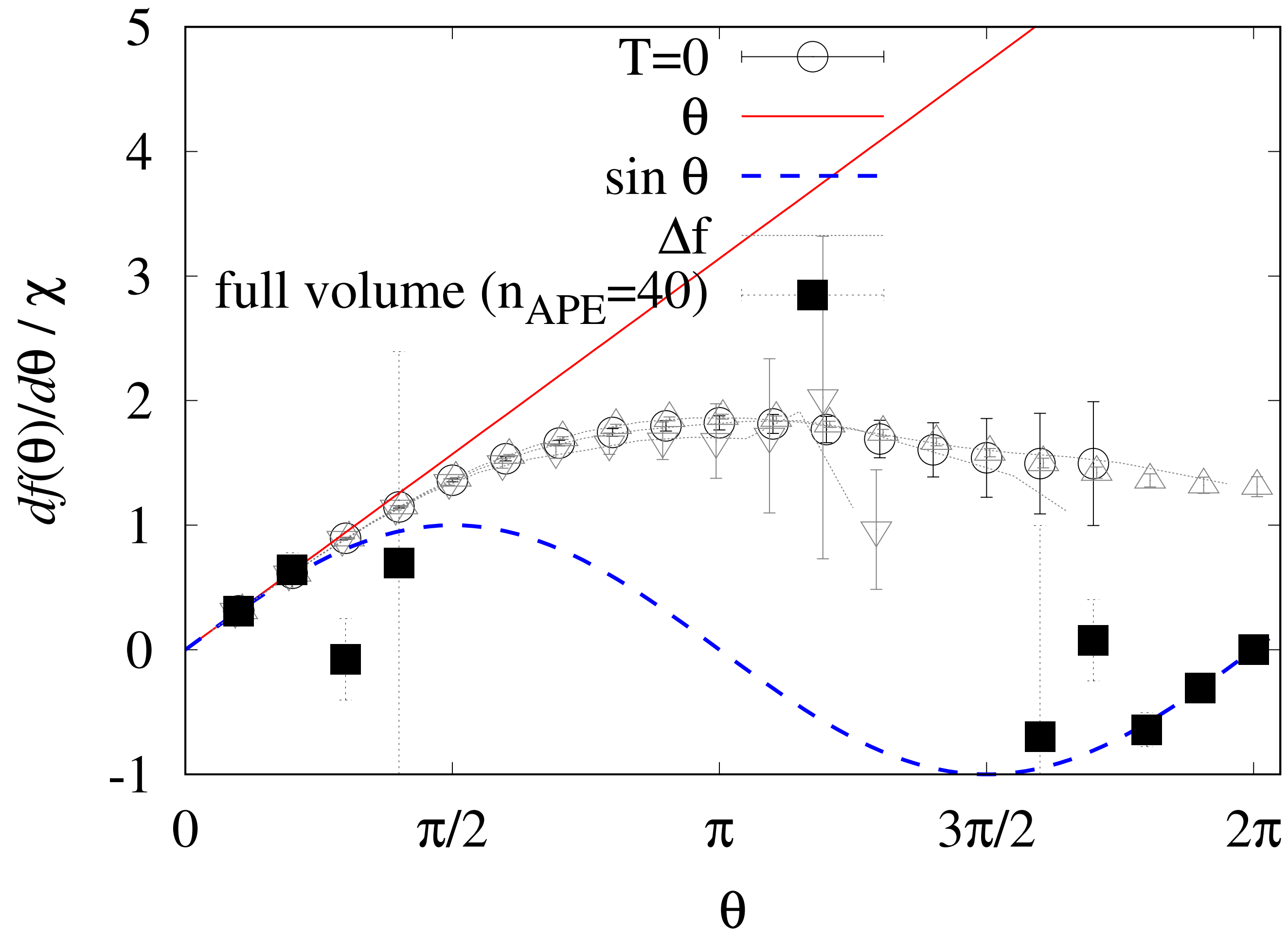
- Fit range $n_{\text{APE}} = [20, 40]$ determined in [\[Kitano, NY, Yamazaki \(2021\)\]](#).
- Linear fit works well.
- Monotonic function $f(\pi) < f(3\pi/2)$

θ dependence of $f(\theta)$ at $T = 0$



- Succeed to calculate up to $\theta \sim 3\pi/2$
- Monotonically increasing function
- Inconsistent with DIGA
- $f(\pi - \theta) \neq f(\pi + \theta)$ requires explanation.
- Re-weighting (=full volume) method works only around $\theta = 0$.
- Numerical consistency with $\int d\theta \frac{df}{d\theta}$

$df(\theta)/d\theta$ at $T = 0$



- Order parameter is non-zero

$$df(\theta)/d\theta \Big|_{\theta=\pi} = -i \langle q(x) \rangle_{\theta=\pi} \neq 0$$

\Rightarrow spontaneous CPV at $\theta = \pi$

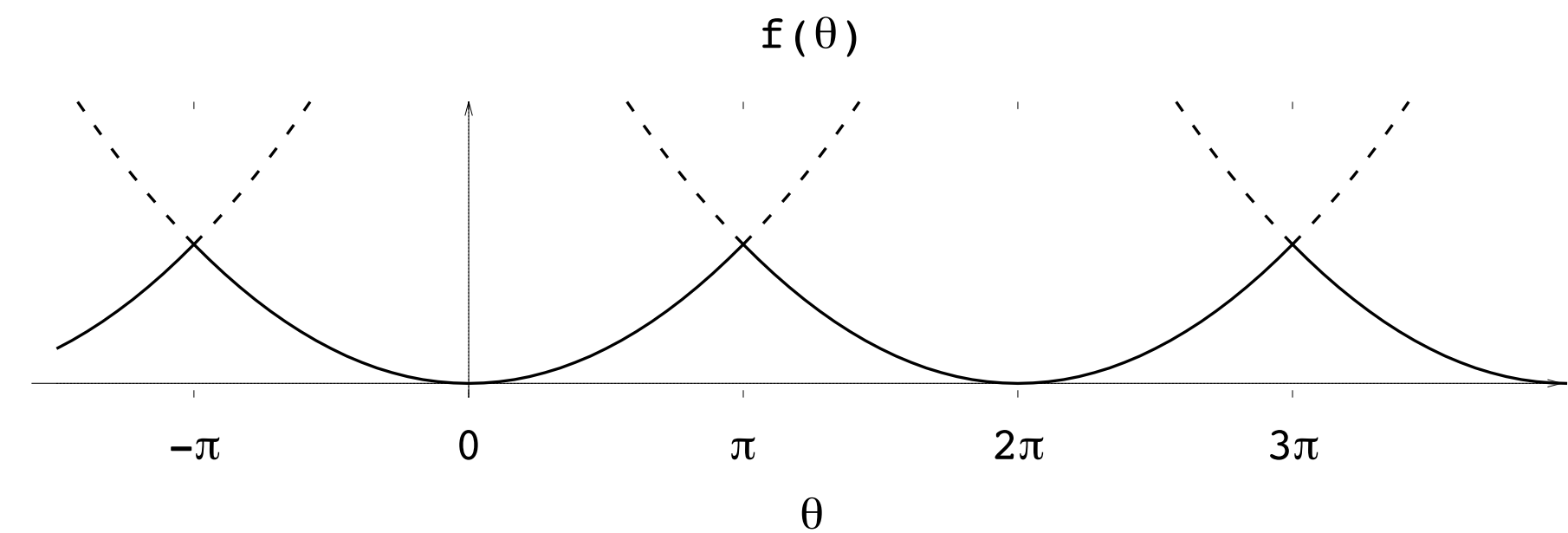
Discussion

- At $T > T_c$,

consistent with $1 - \cos \theta$ and **no CPV** as expected (though non-trivial).

- At $T = 0$,

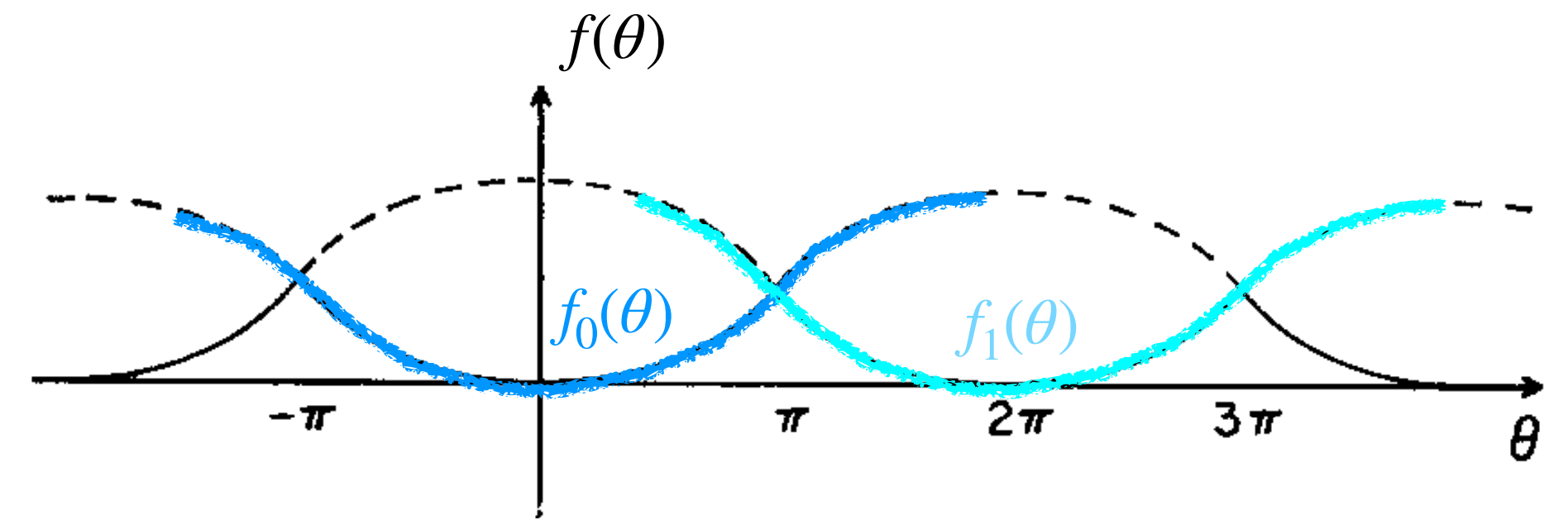
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Why ?

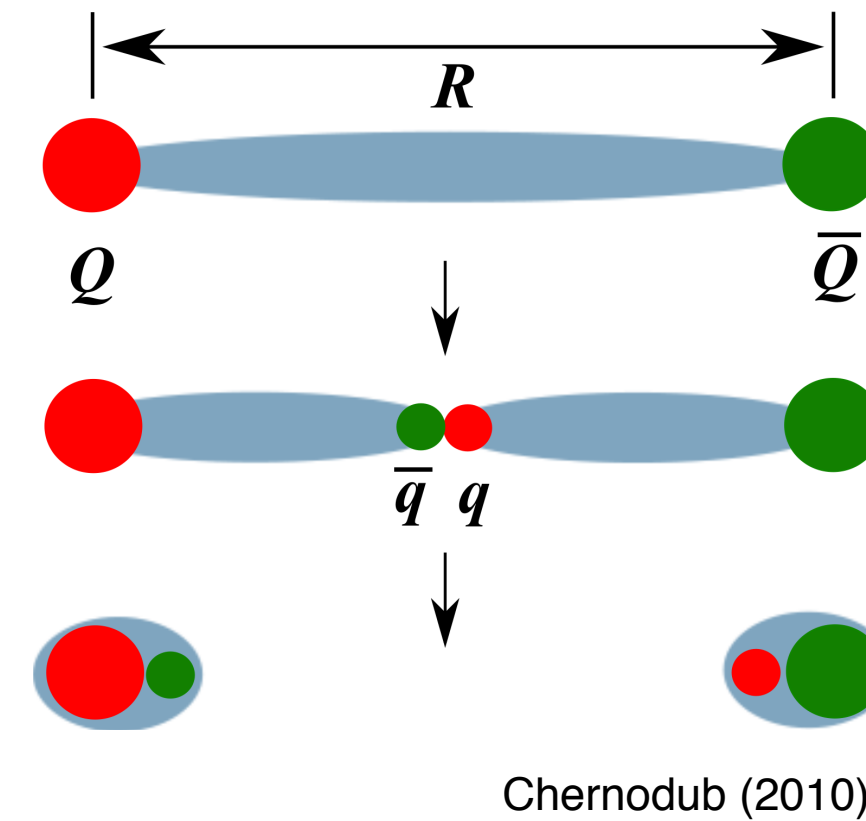
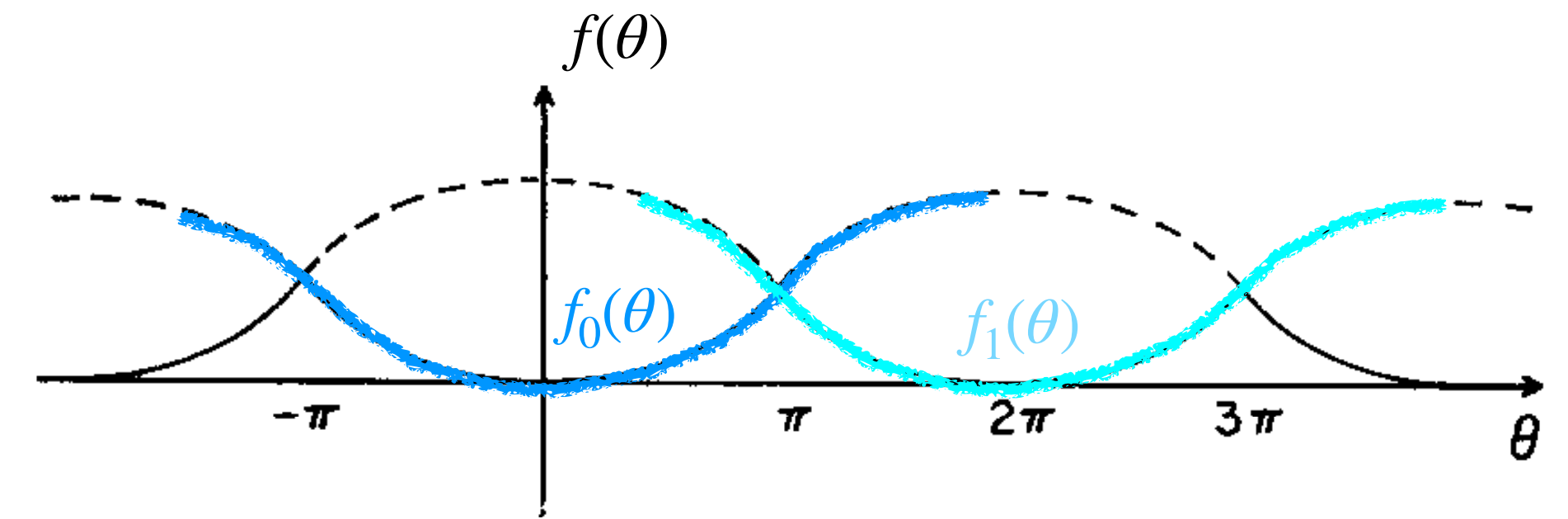
Interpretation

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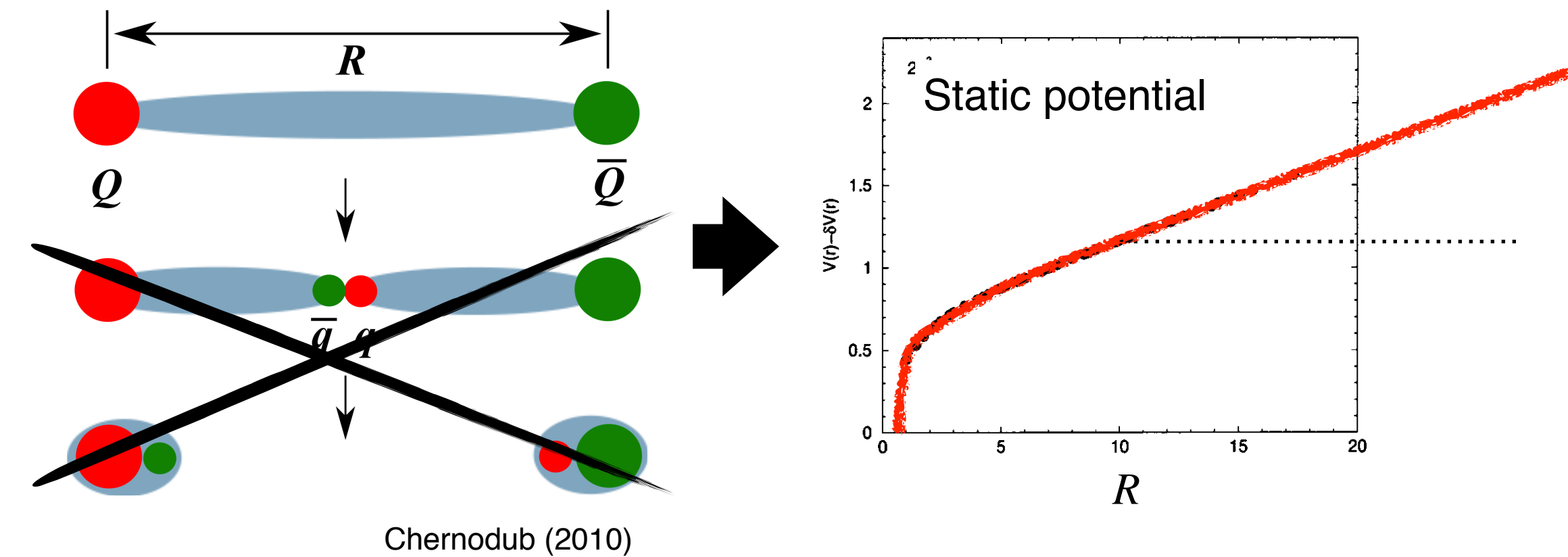
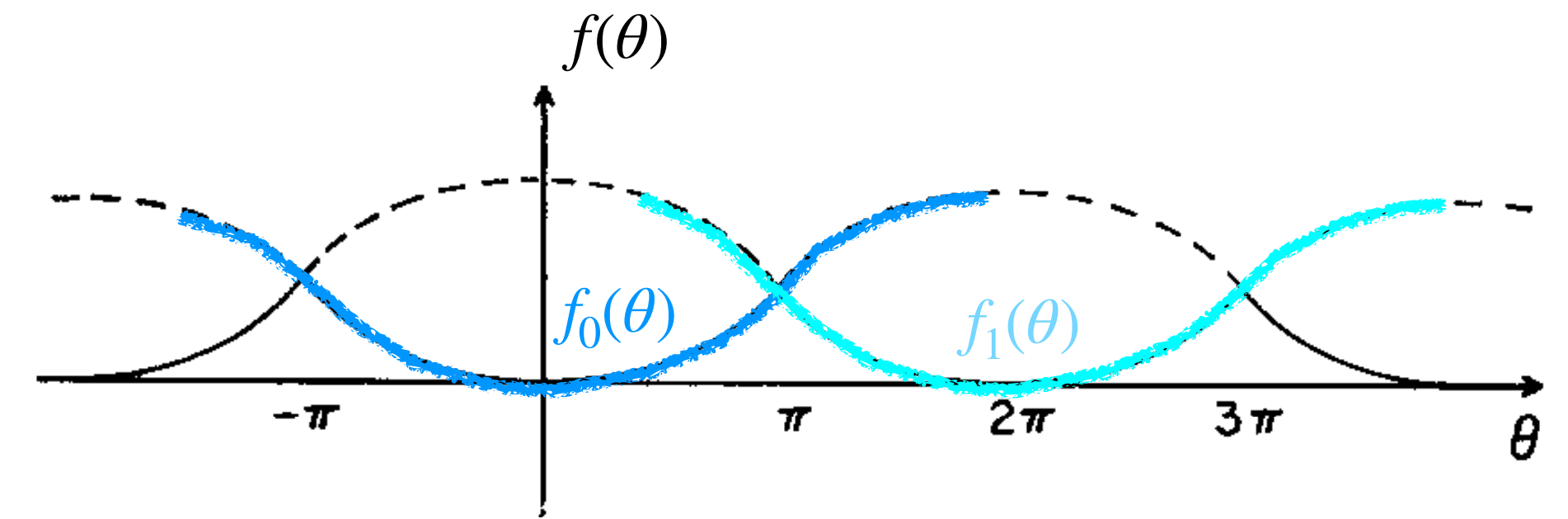
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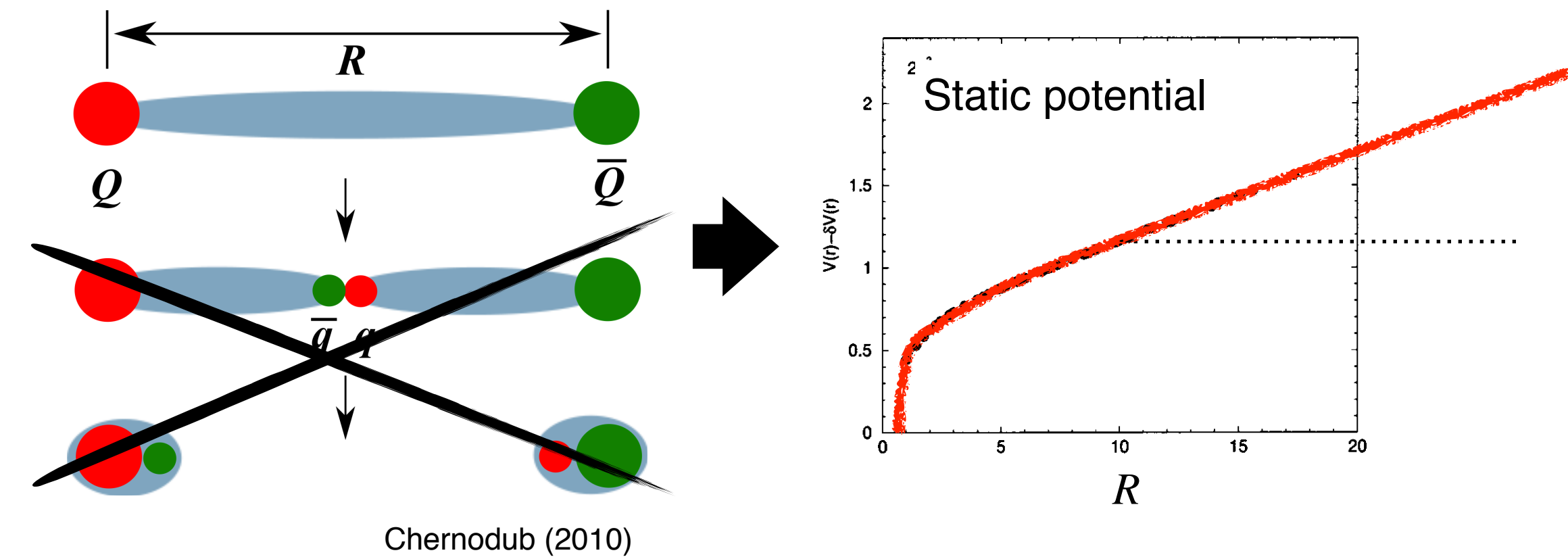
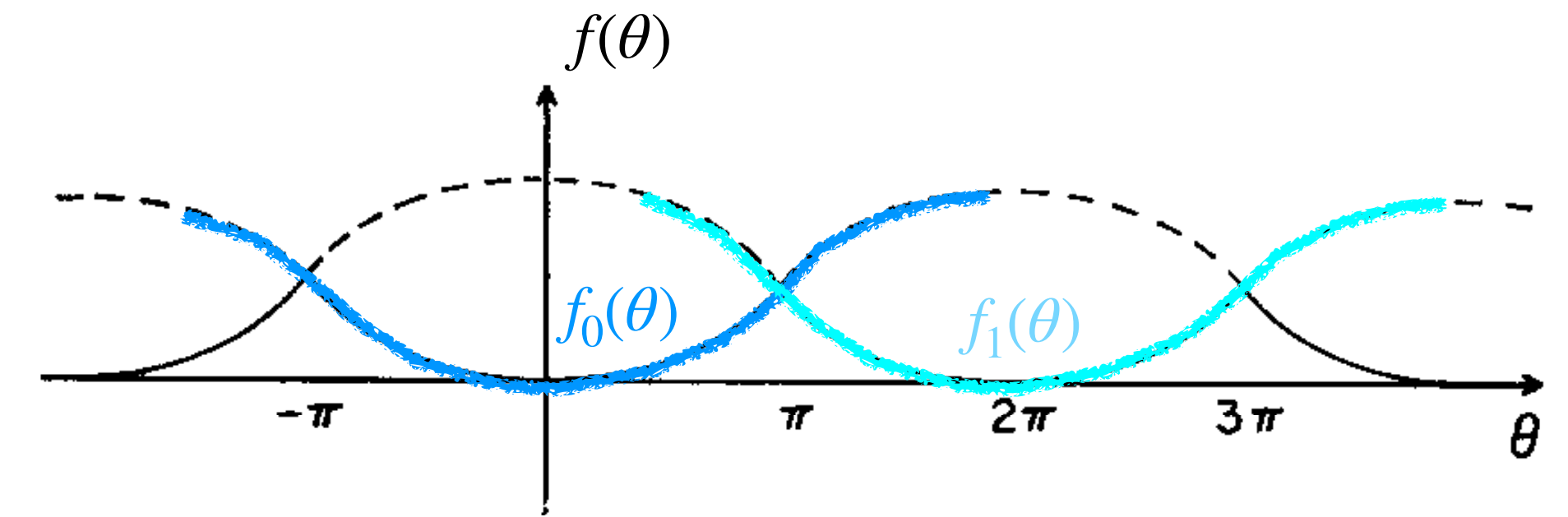
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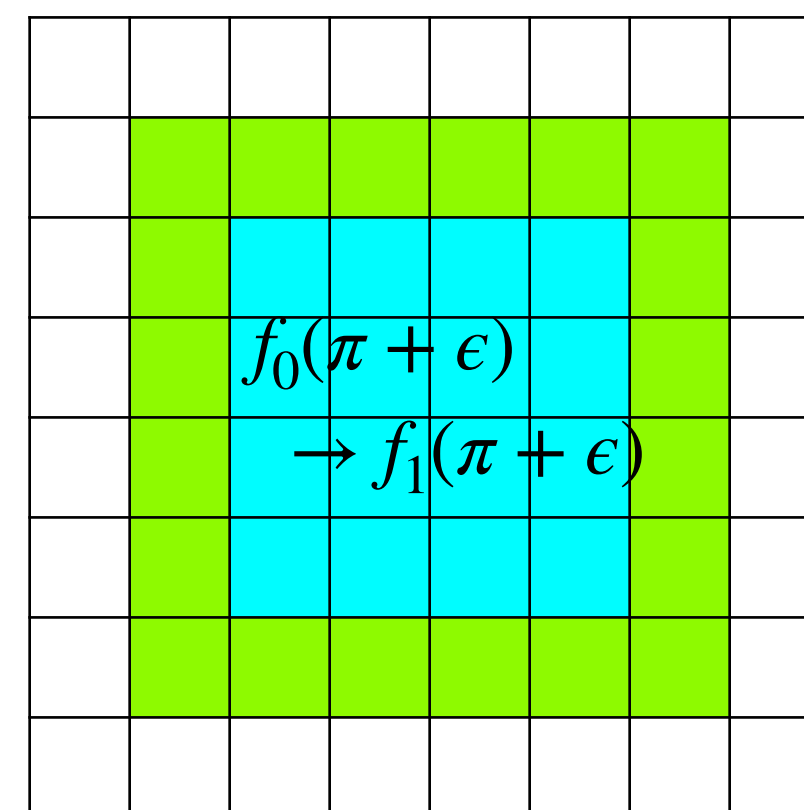
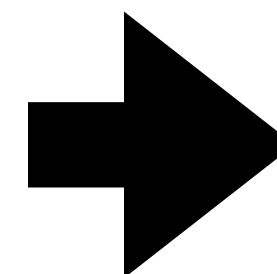
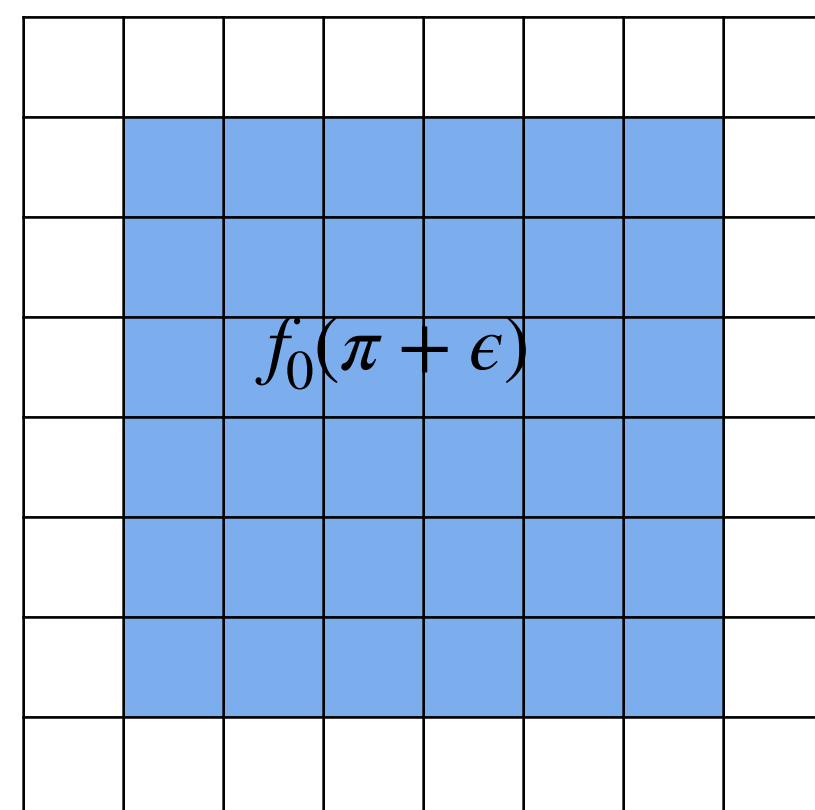
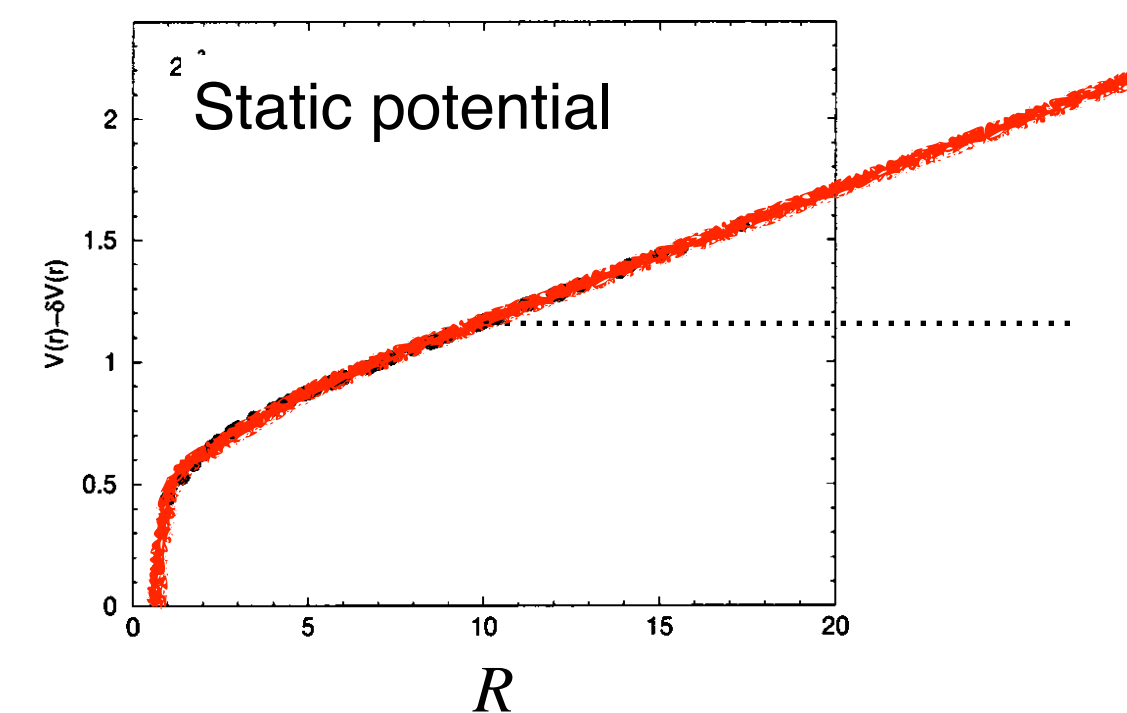
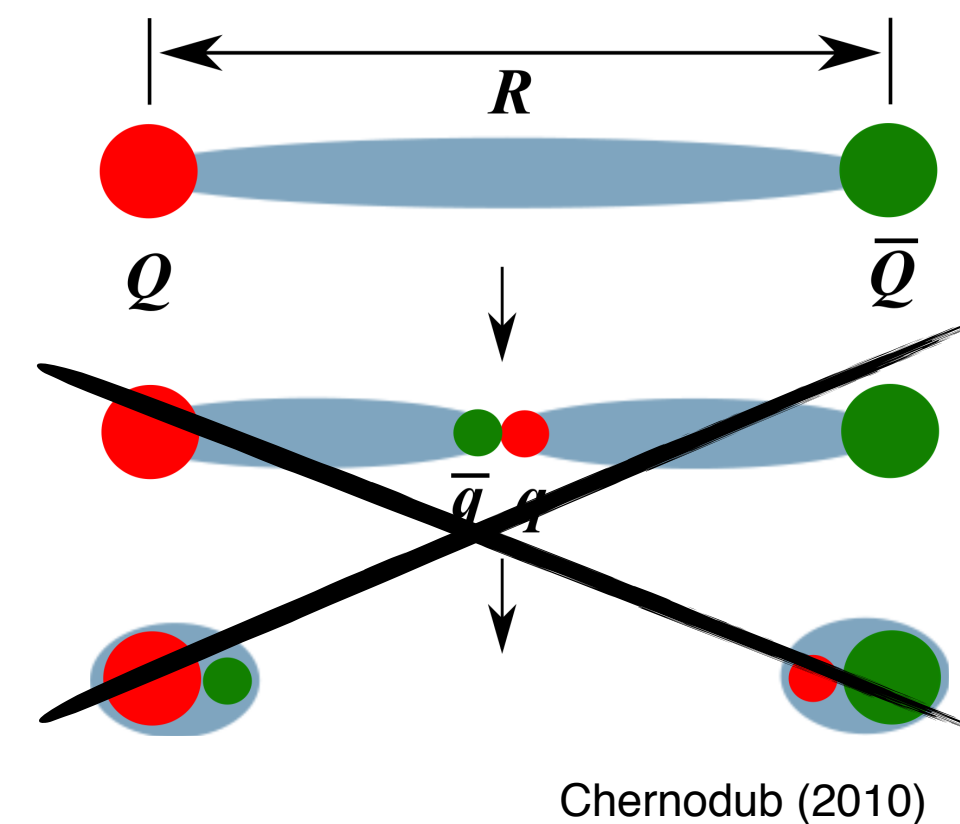
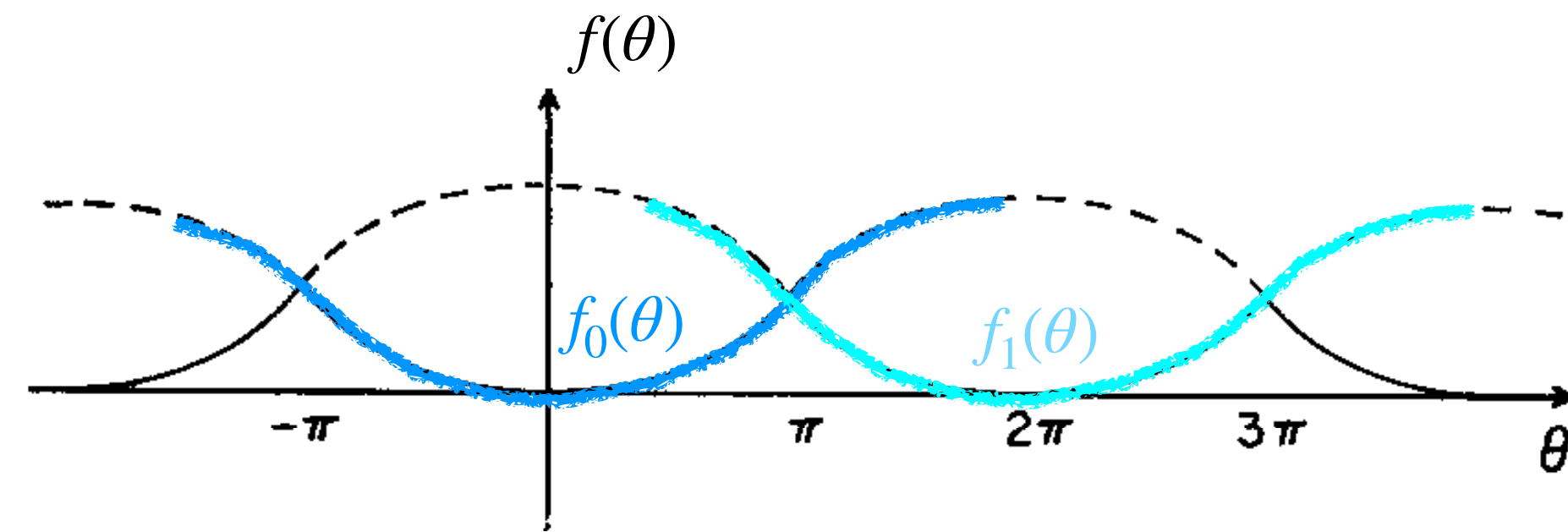
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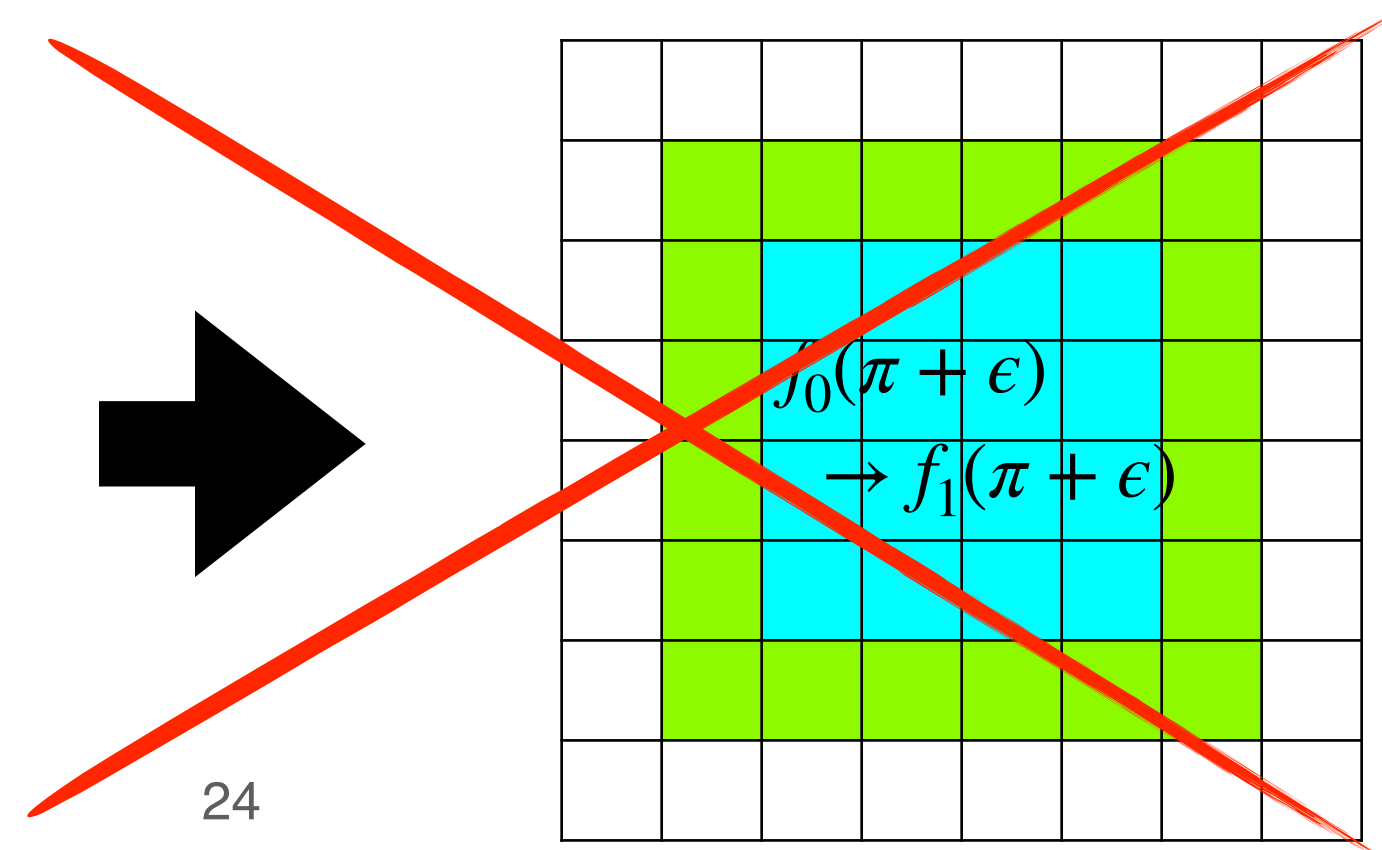
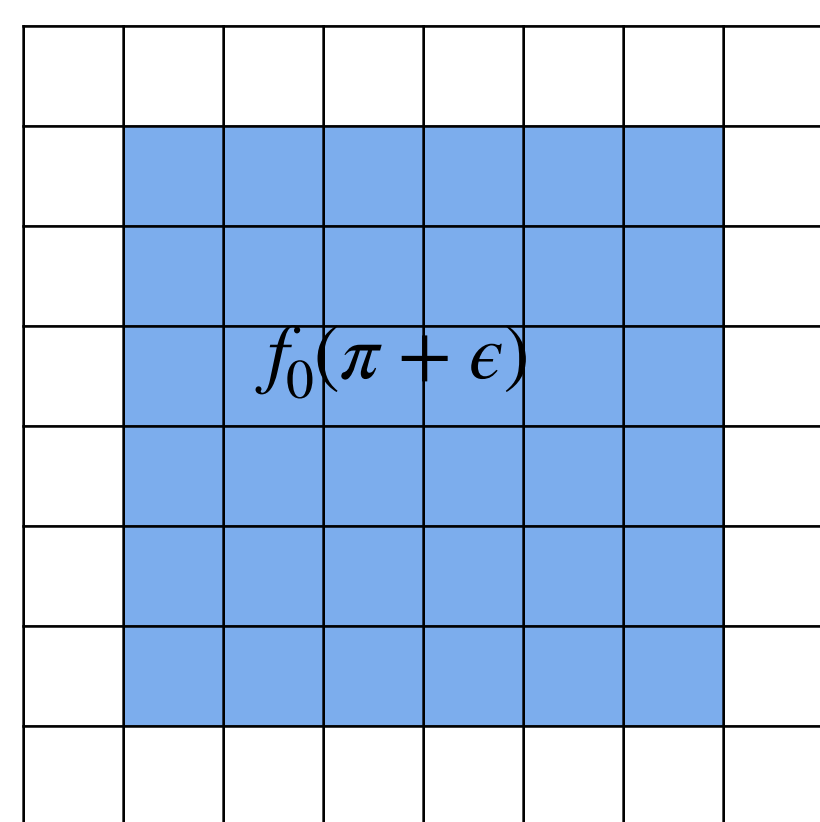
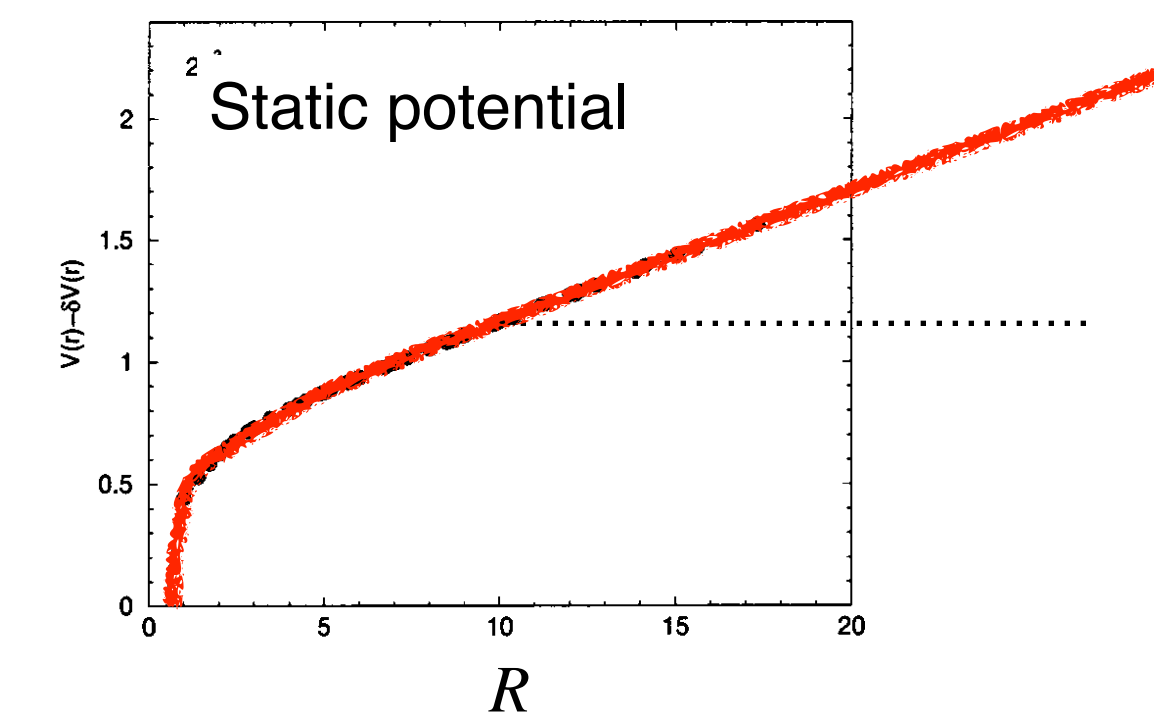
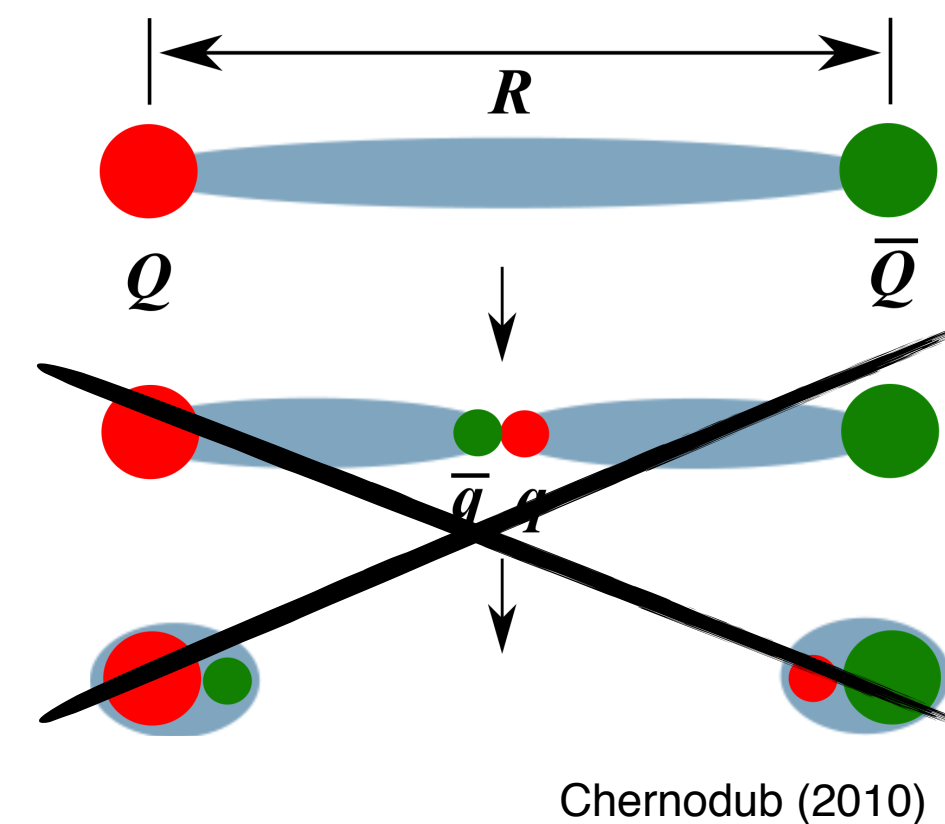
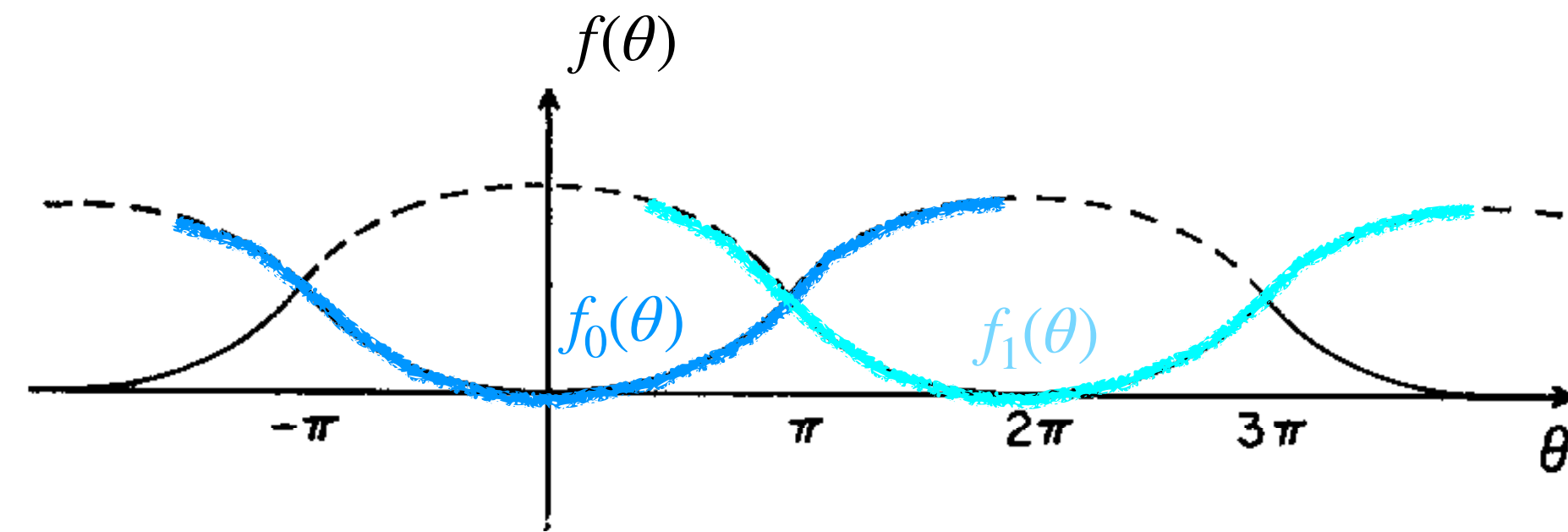
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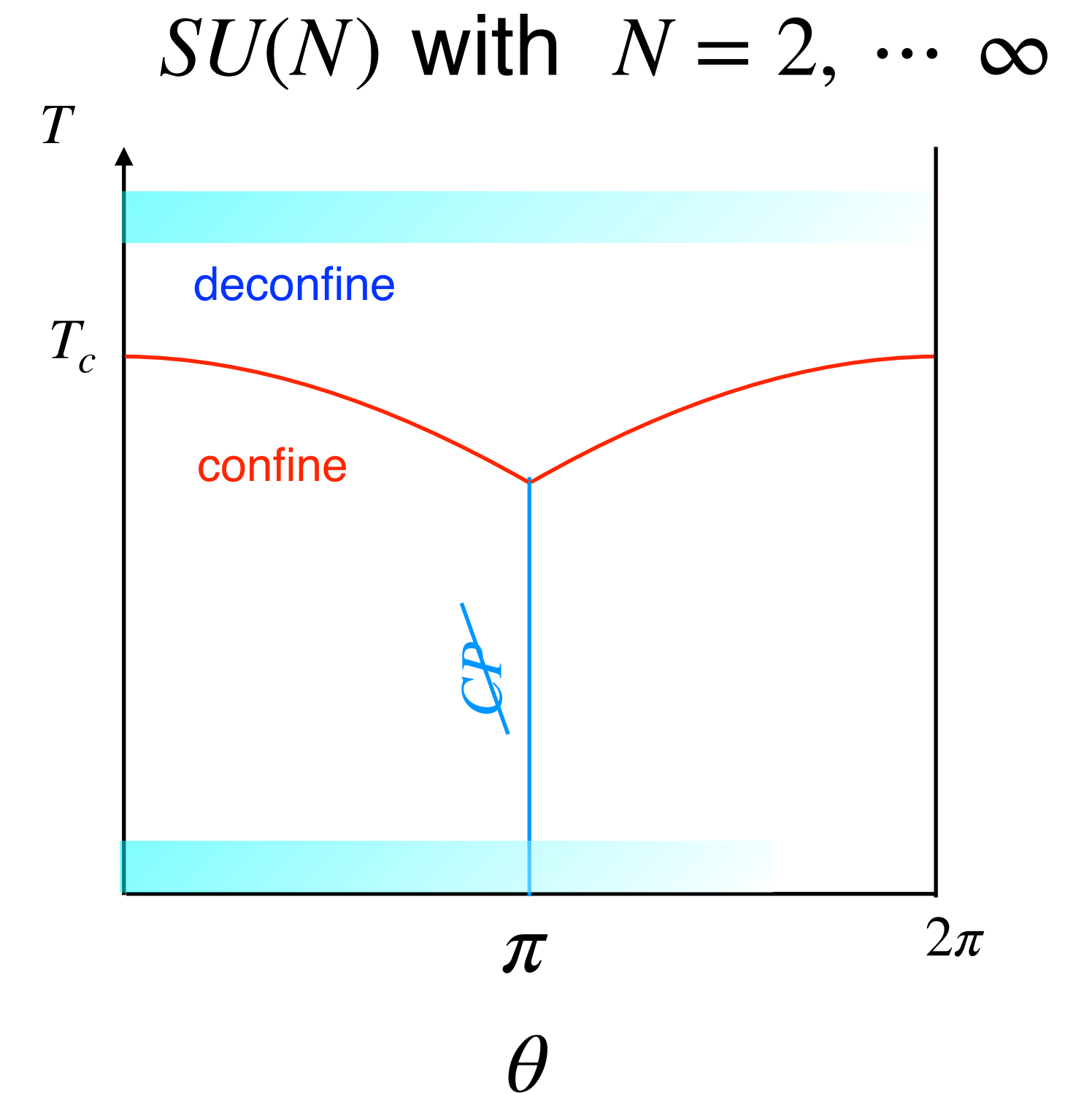
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Summary and conclusion

- We have developed a sub-volume method, which enables us to calculate $f(\theta)$ up to $\theta \sim 3\pi/2$ in SU(2) Yang-Mills theory.
- Combining with the theory requirement $f(\pi - \theta) = f(\pi + \theta)$, our result provides with the evidence for **spontaneous CPV** at $\theta = \pi$ and at $T = 0$ and the existence of a bag-like object.
 \Rightarrow N=2 belongs to large N class (not like CP^1 model).
- The same method roughly reproduces the DIGA result, $f(\theta) \sim \chi(1 - \cos \theta)$, above T_c , which makes the above result more confident.

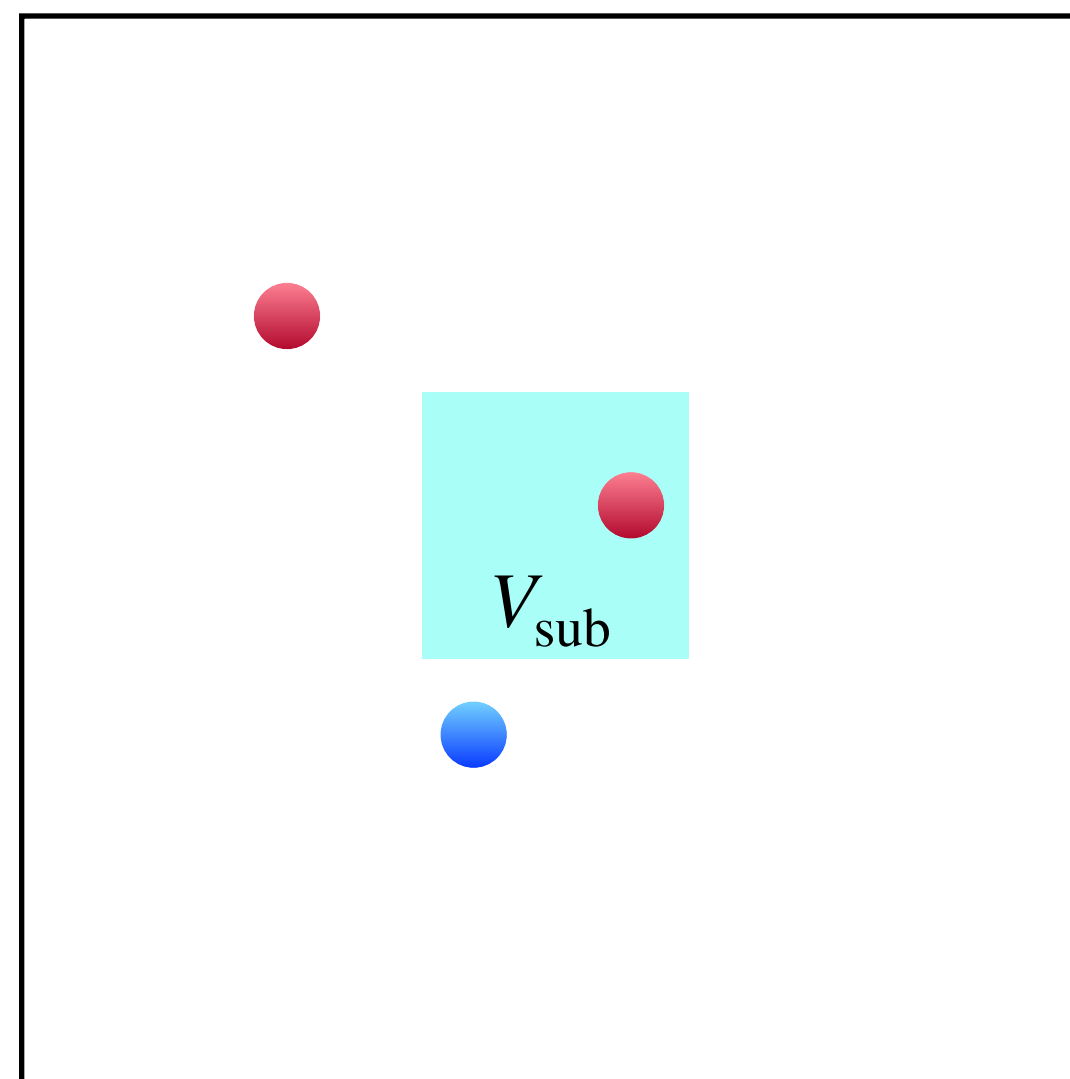
Future studies

- exploring the location of $T_c(\theta)$
- Suppose that $T_c(\theta)$ depends on θ . Then, does it mean that the β -function depend on θ ?
- Also interesting to apply the sub-volume method to the finite density system.

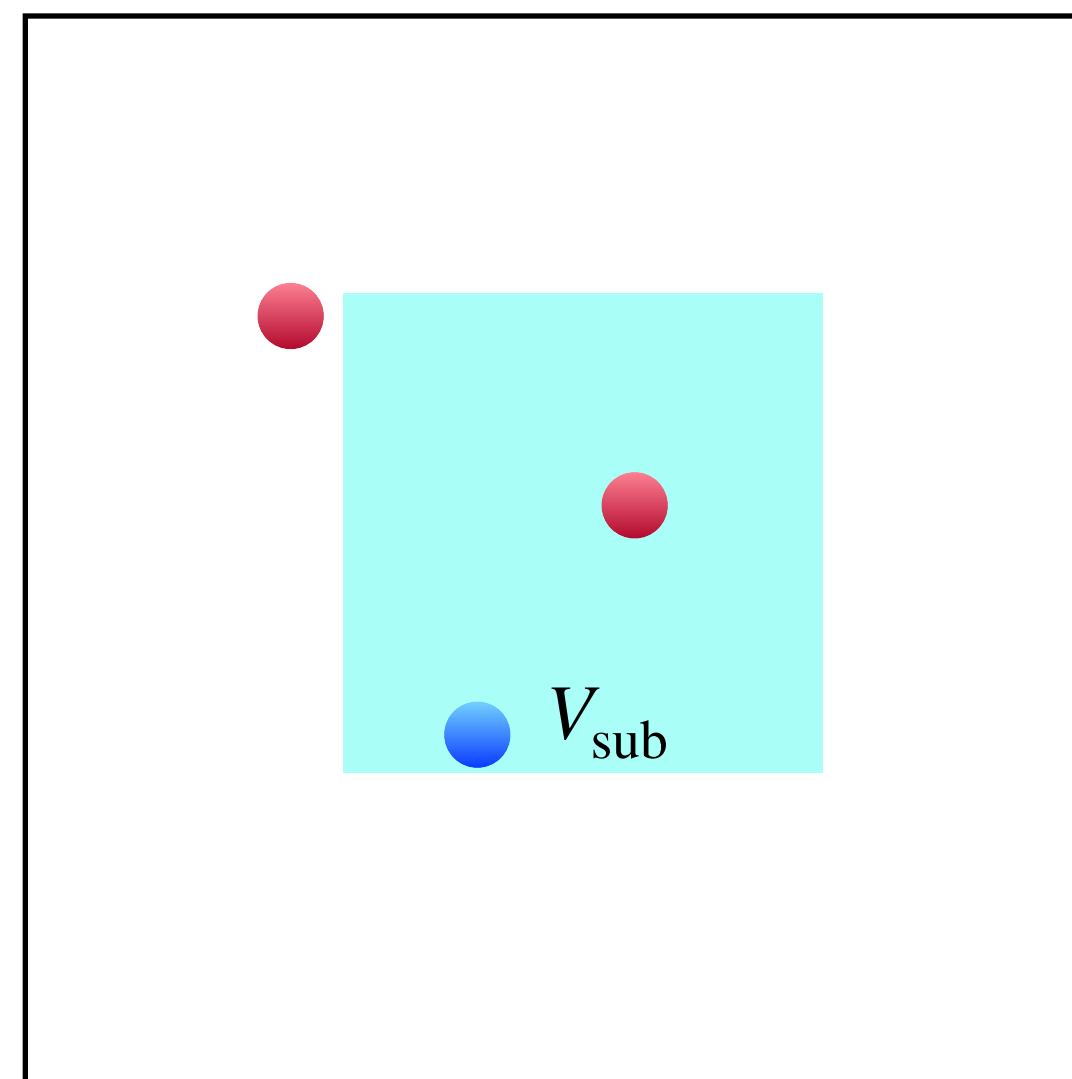


Intuitive understanding of periodic behavior of $f(\theta)$

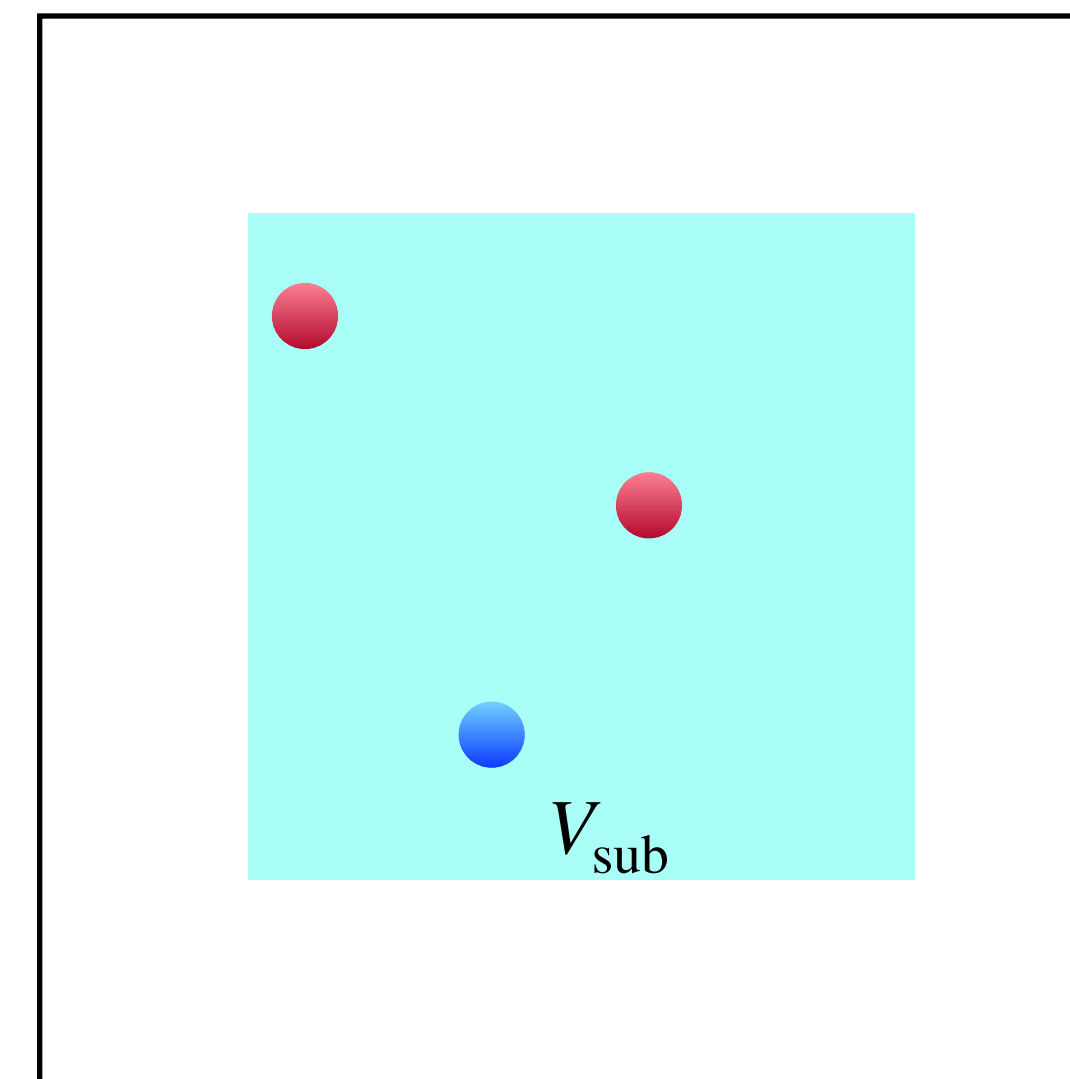
$$f(\theta) = - \lim_{V_{\text{sub}} \rightarrow \infty} \frac{1}{V_{\text{sub}}} \ln \langle e^{-i\theta Q_{\text{sub}}} \rangle = - \lim_{V_{\text{sub}} \rightarrow \infty} \frac{1}{V_{\text{sub}}} \ln \langle \cos(\theta Q_{\text{sub}}) \rangle$$



$Q_{\text{sub}} = +1$



$Q_{\text{sub}} = 0$



$Q_{\text{sub}} = +1$

- : instanton
- : anti-instanton

In this case, Q_{sub} is almost always integer if $\rho_{\text{instanton}}^4 \ll V_{\text{sub}}$.

$\Rightarrow f(\theta) \Big|_{\theta \approx 2\pi} \sim 0 \Rightarrow 2\pi\text{-periodicity can be expected.}$

θ -vacuum

- The vacuum can have an integer winding number, labeled by $|n\rangle$.
- But, this label is changed by gauge transformation, e.g. $U_{(1)}|n\rangle \rightarrow |n+1\rangle$.

- Define $|\theta\rangle = \sum_{n=-\infty}^{+\infty} e^{in\theta} |n\rangle \iff U_{(1)}|\theta\rangle = e^{-i\theta} |\theta\rangle$

- $\langle\theta_+|\theta_-\rangle_J = \sum_{m,n} e^{in\theta} e^{-im\theta} \langle m_+|n_-\rangle_J = \sum_Q e^{i\theta Q} \sum_m \langle m_+|m_-+Q\rangle_J$

$$= \sum_Q \int_{\epsilon \in Q} \mathcal{D}A e^{-S_g + i\theta Q + \int J \cdot A} \delta \left(Q - \frac{g^2}{32\pi^2} \int d^4x G \tilde{G} \right)$$

$$= \int \mathcal{D}A e^{-S_g + i\theta Q + \int J \cdot A}$$