Peeking into the θ vacuum of 4d Yang-Mills theory

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in collaboration with
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[Ref. JHEP02, 073 (2021)]

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Goal

Clarify the θ dependence of free energy density $f(\theta)$ of 4d YM

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

where $Z(\theta) = \int \mathcal{D}U\, e^{-S_{\rm YM}+i\theta Q}$, $Q = \int d^4x\, q(x)$ and $q(x) = \frac{1}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma}$

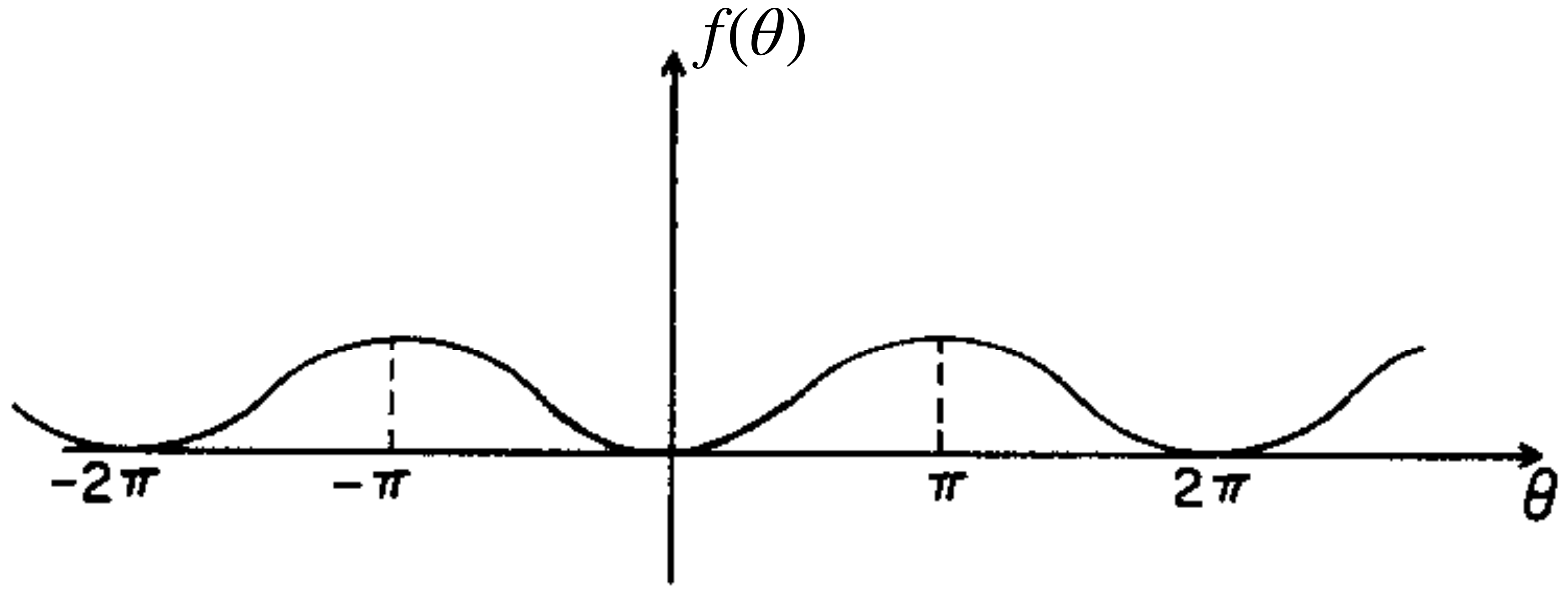
For $SU(N)$ YM theory,

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

θ dependence and CP violation

Dilute instanton gas approximation (DIGA)

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



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- smooth everywhere

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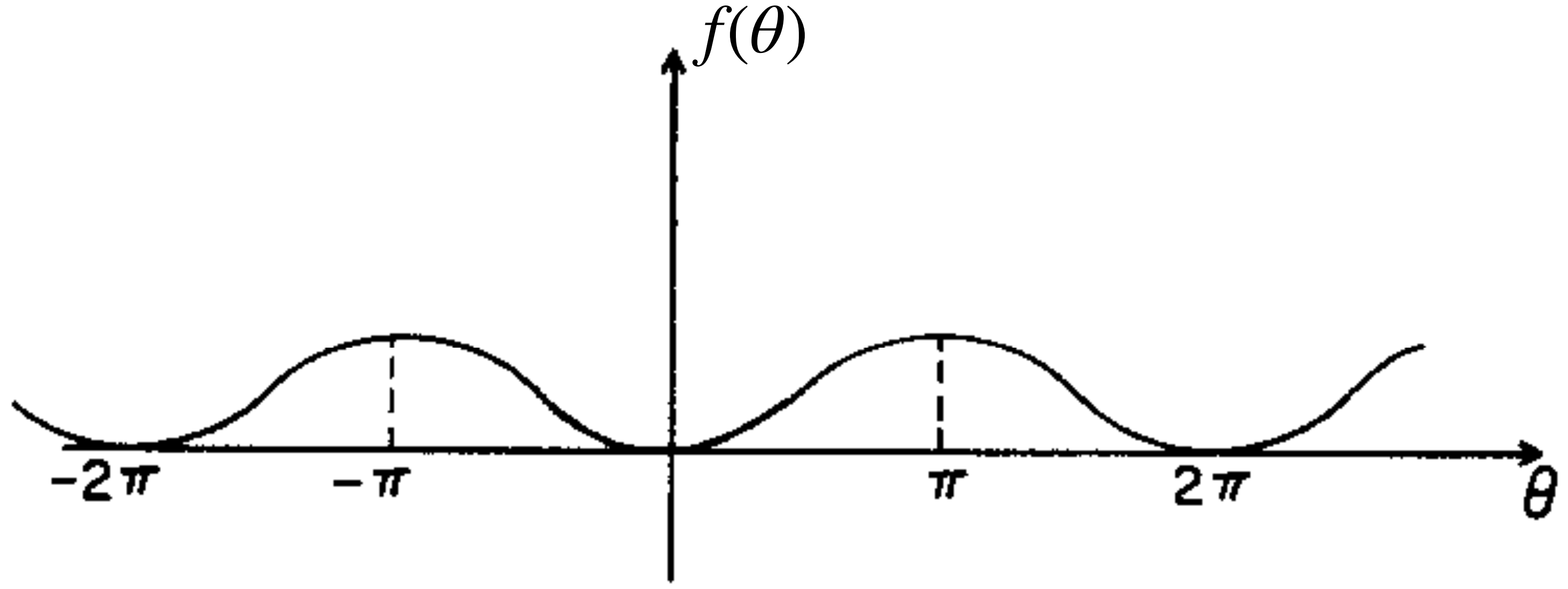

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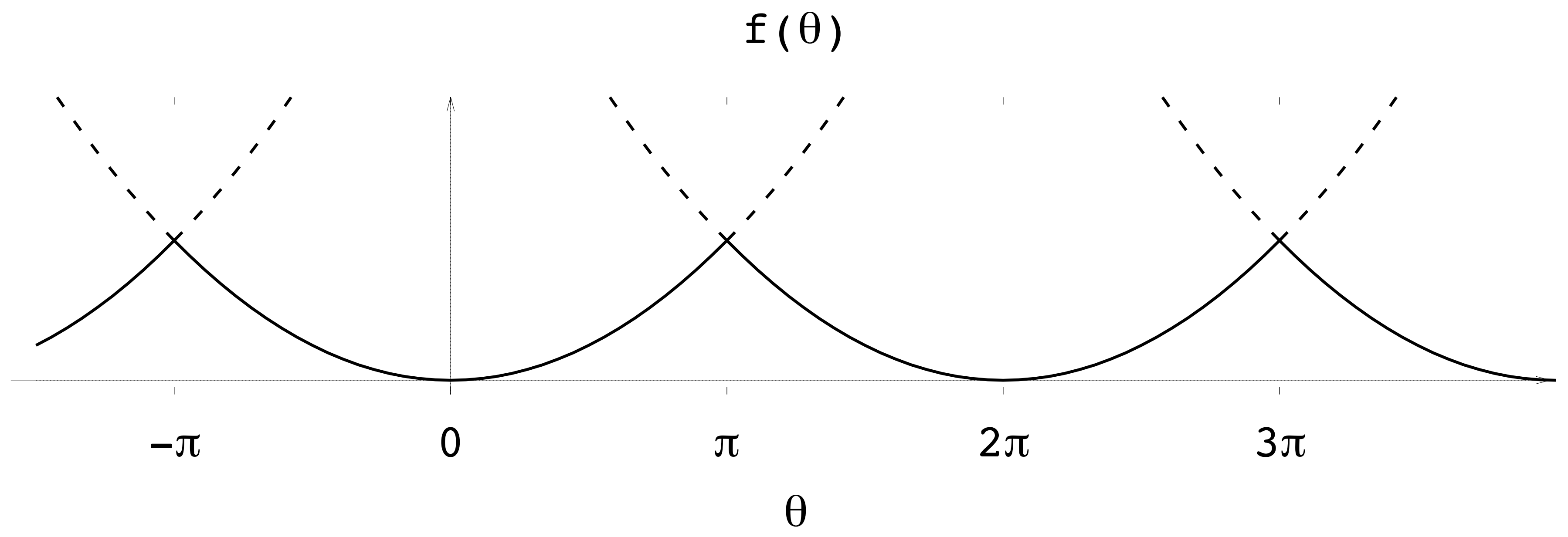
Large N argument [Witten (1980, 1998)]

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



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

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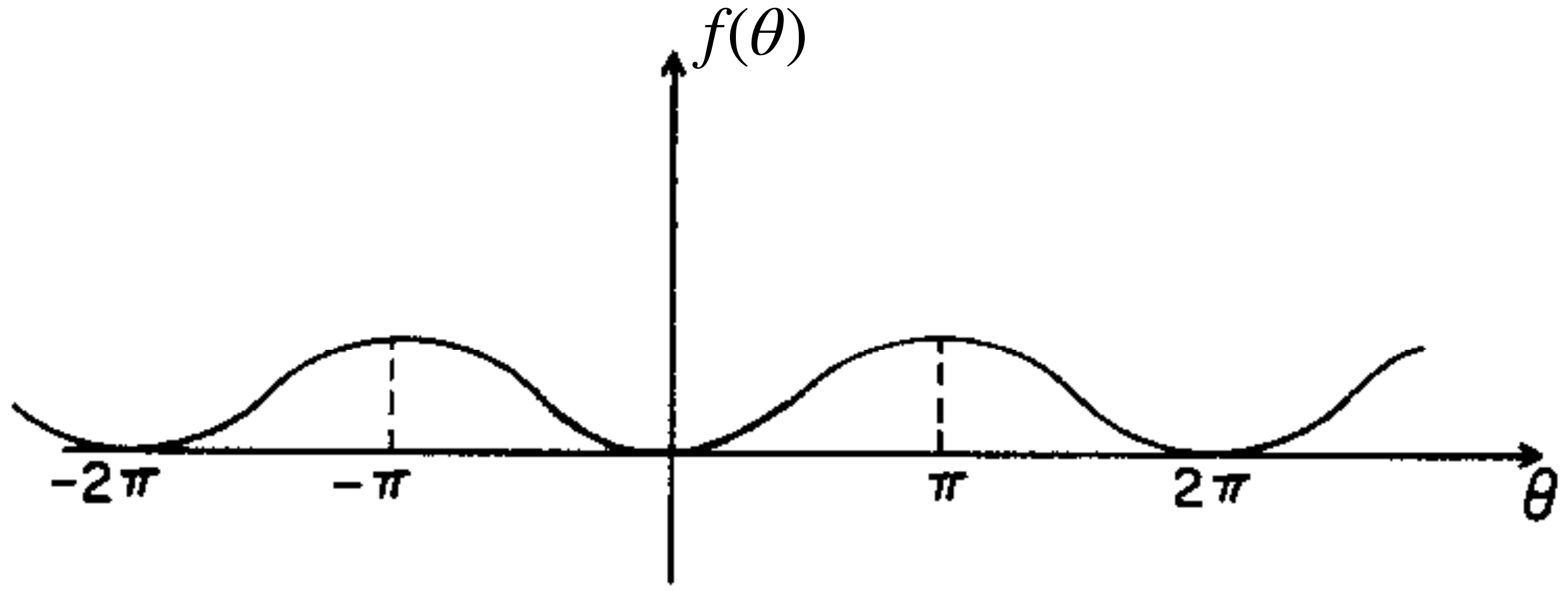

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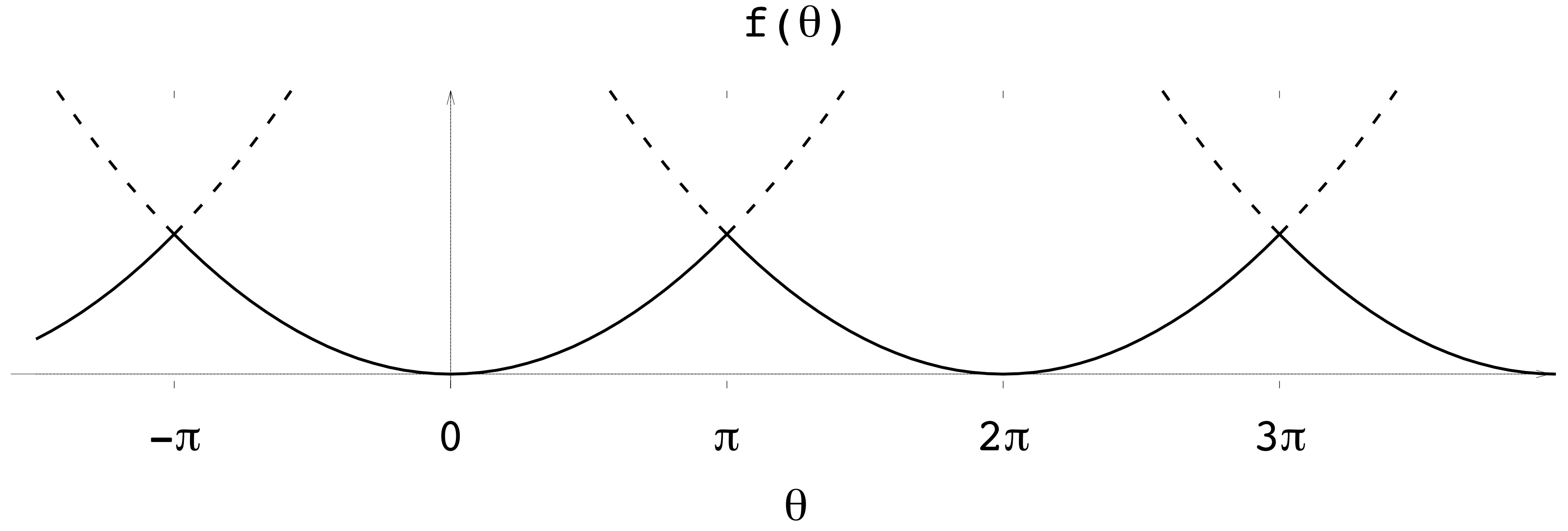

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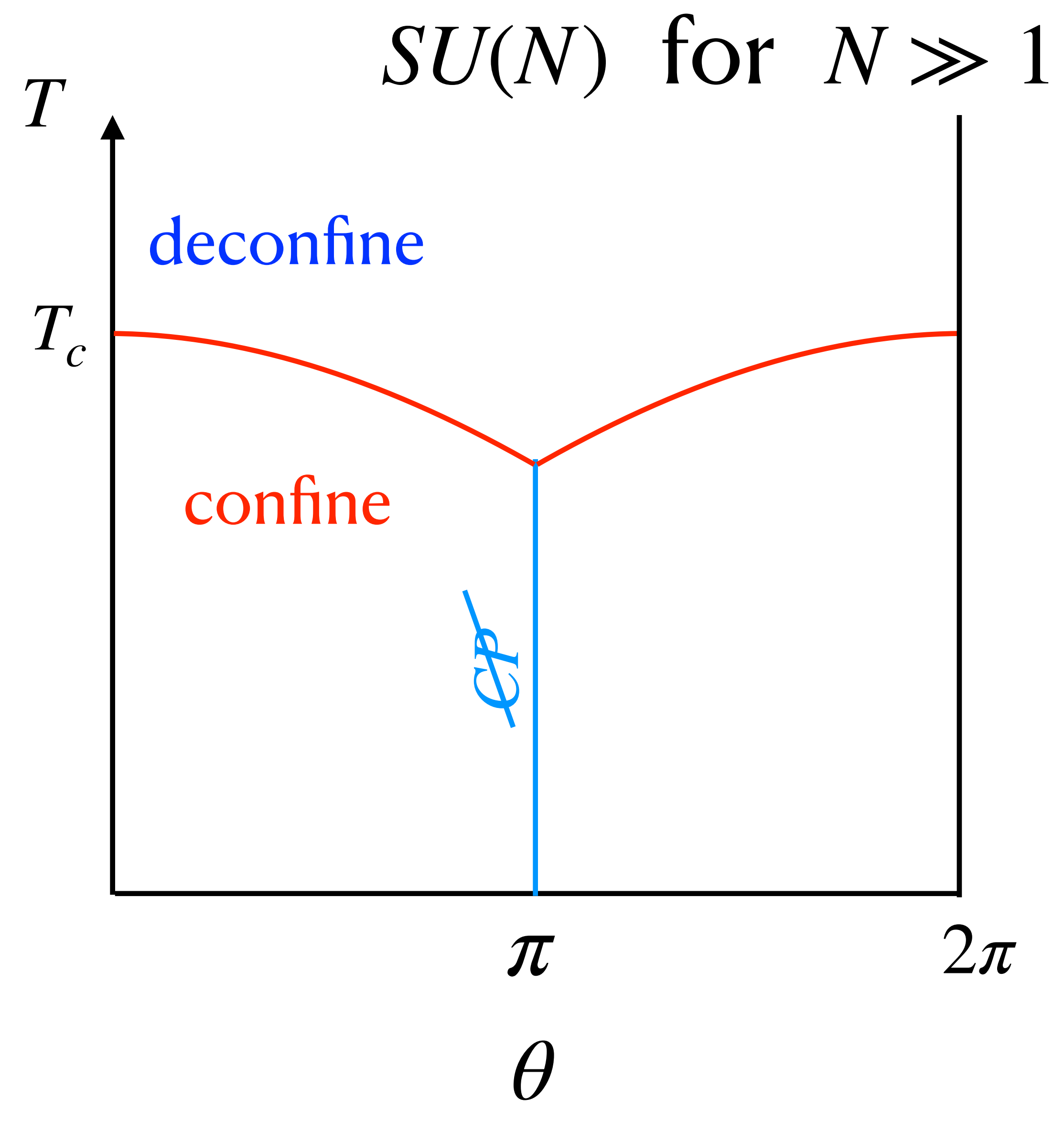
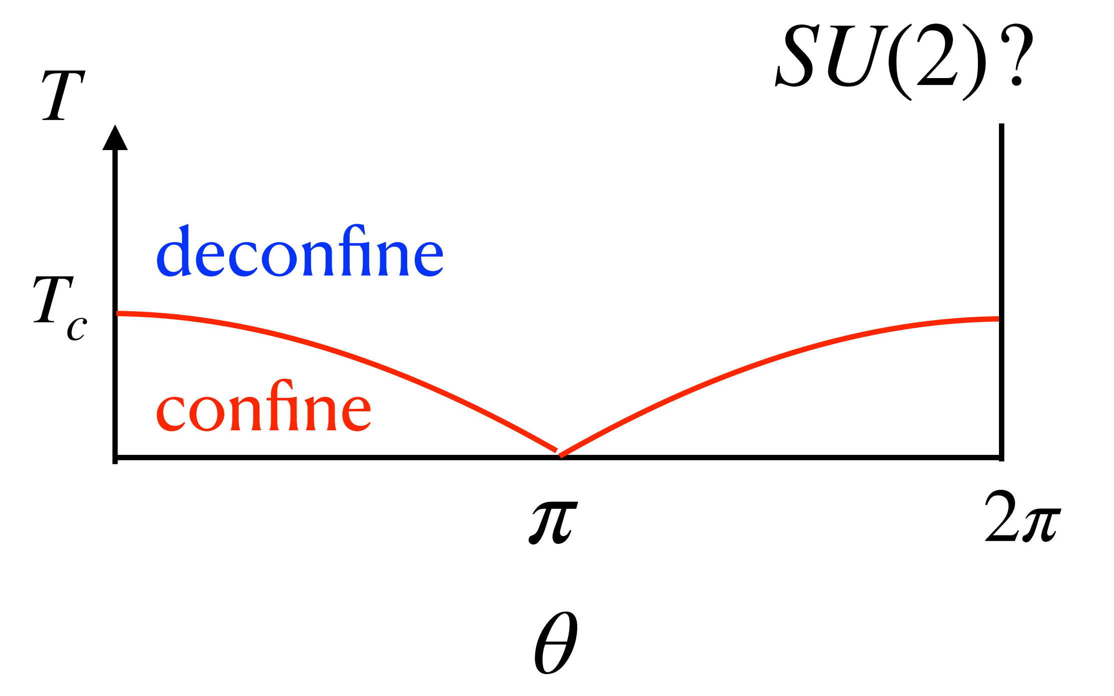
Interested in $f(\theta)$ around $\theta \approx \pi$ in 4d $SU(N)$ YM theory.

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

- Large N argument seems robust $\Rightarrow$ CPV at $\theta = \pi$ for large N
- Formal arguments tell that, 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)]
- Some numerical evidences of *CPV* for $N \geq 3$
- What happens to the possible smallest N, i.e. $SU(2)$ YM ?
  Is it like "large N" or "2d CP^1" ?

$\Rightarrow$ Lattice numerical simulations (difficult due to sign problem)





New method without any expansion

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

Generate configurations with $\theta = 0$

Define sub-volume $V_{\mathrm{sub}} = l^4$ and $Q_{\mathrm{sub}} = \sum_{x \in V_{\mathrm{sub}}} q(x) \quad \notin \mathbb{Z}$

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

$$f_{\mathrm{sub}}(\theta) = -\frac{1}{V_{\mathrm{sub}}} \ln \langle \cos(\theta Q_{\mathrm{sub}}) \rangle$$

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

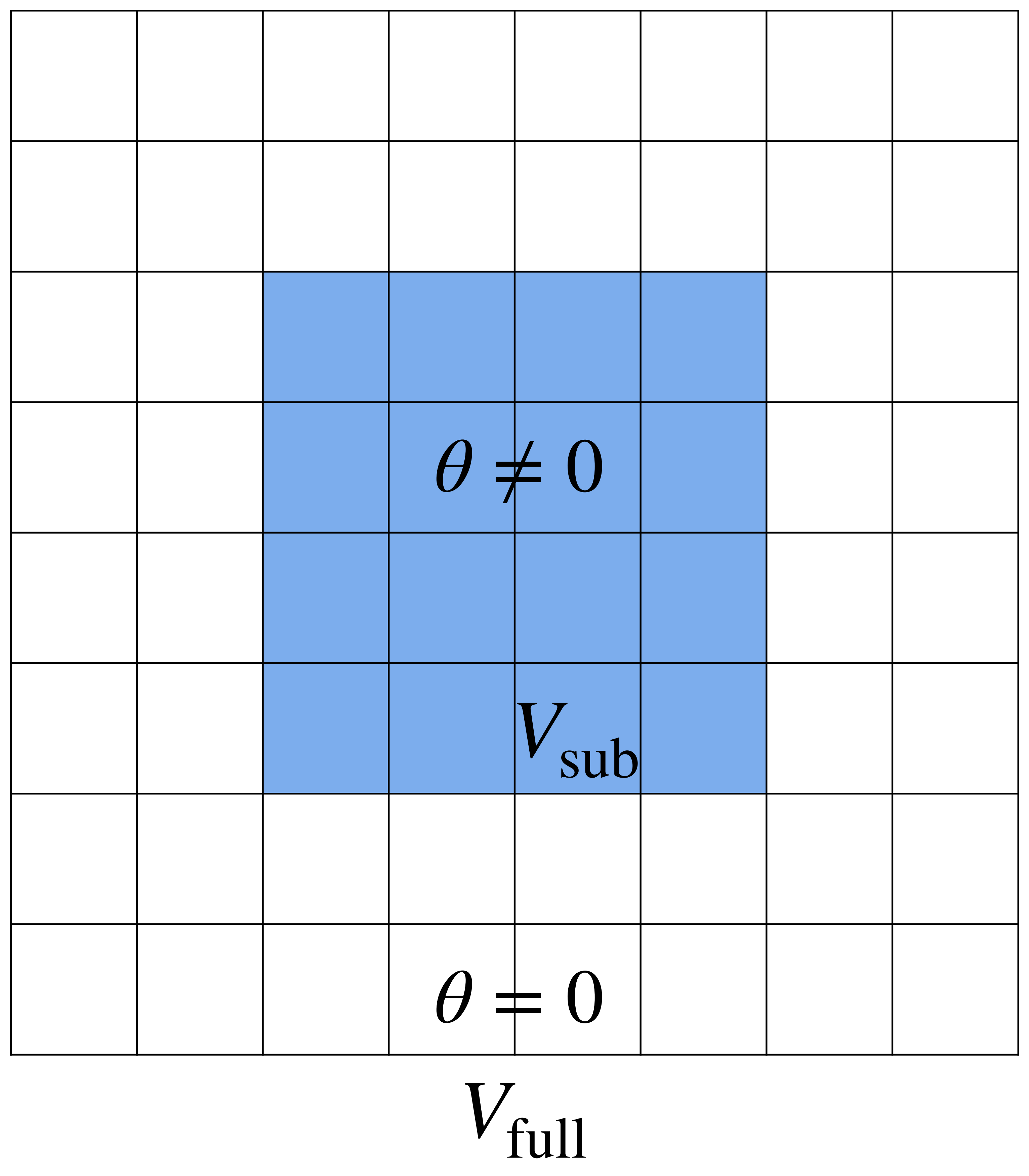
cf) string tension

with $l_{\mathrm{dyn}}^4 \ll V_{\mathrm{sub}} \ll V_{\mathrm{full}}$ (l_{dyn} : dynamical length scale)

$s(\theta)$: surface tension

"sub-volume method"

cf) 2d CP^1 by [Keith-Hynes and Thacker (2008)]



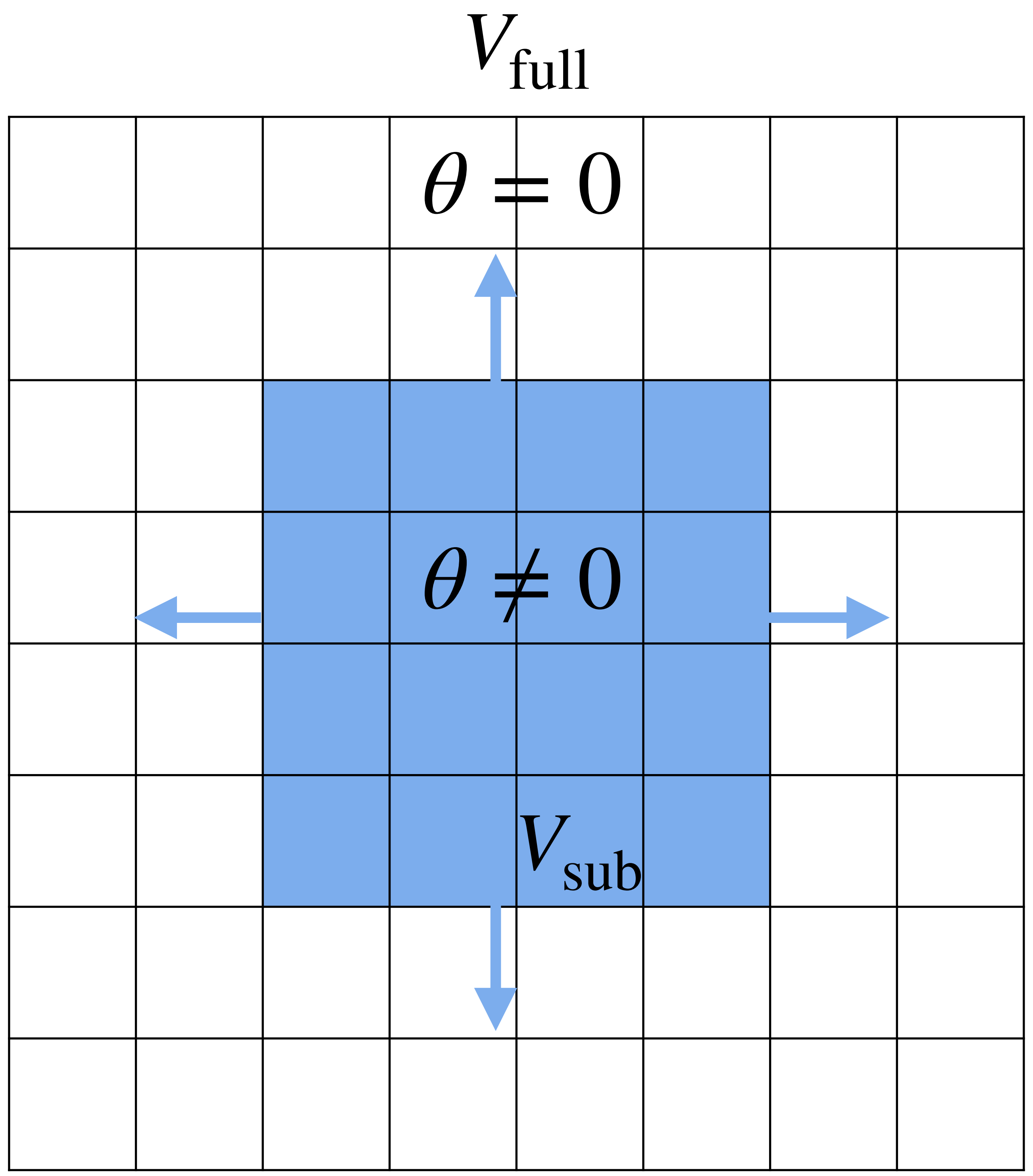
Lattice parameters and observables

- $SU(2)$ YM theory by Symanzik improved gauge action
- $\beta = \dfrac{4}{g^2} = 1.975$ (relatively fine: $1/(aT_c) = 9.50$)
- $V_{\rm full} = 24^3 \times \{48,\ 6,\ 8\}$ ($T = 0,\ 1.2T_c,\ 1.6T_c$)
- Periodic boundary condition in all directions
- # of configs = { 68000 , 10000 , 10000 }
- Calculate $Q_{\rm sub} = \sum_{x \in V_{\rm sub}} q(x)$ and estimate

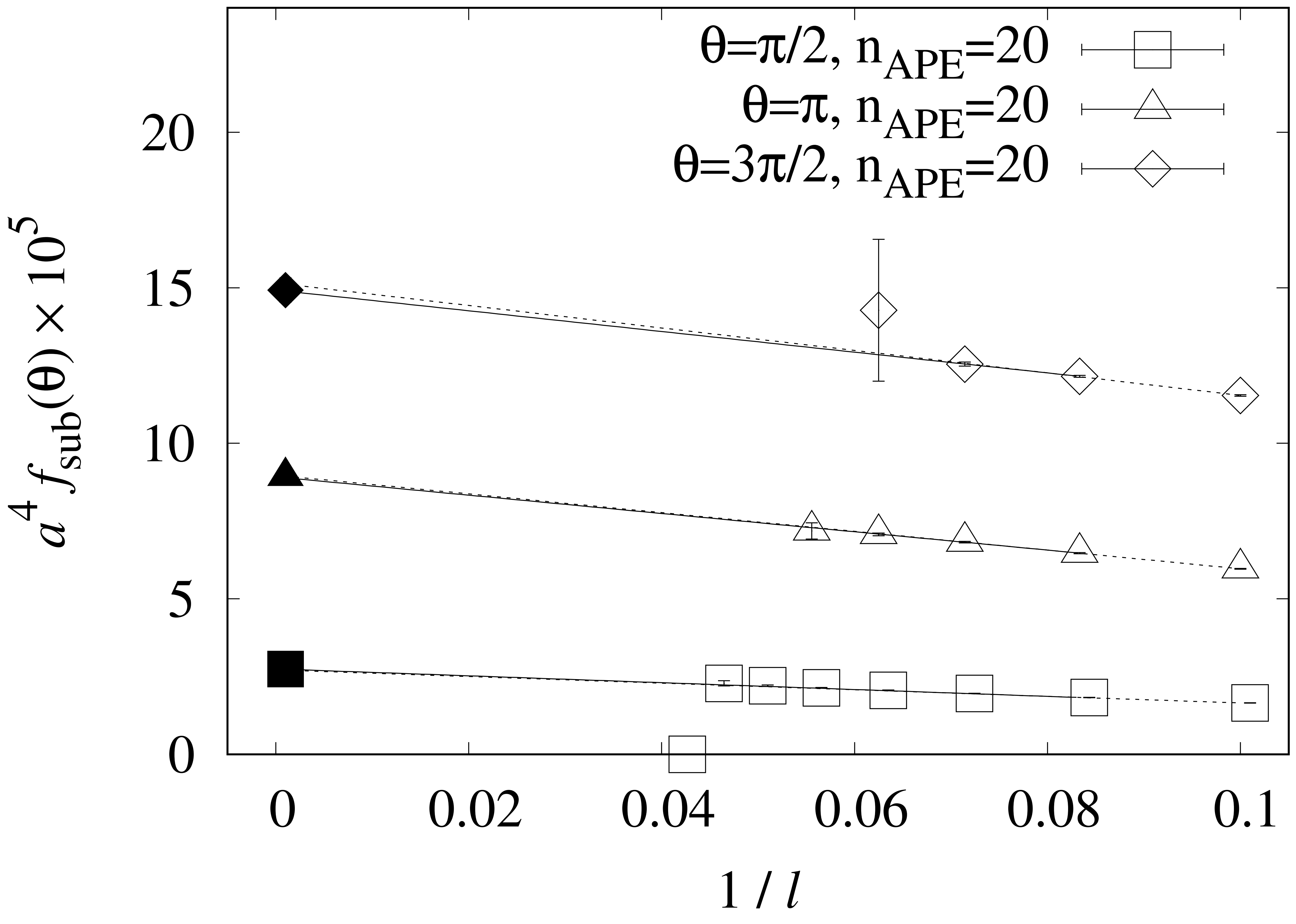
✓ $f(\theta) = -\lim_{V_{\rm sub}\to\infty} \dfrac{1}{V_{\rm sub}} \ln\langle \cos(\theta Q_{\rm sub}) \rangle$

✓ $\dfrac{df(\theta)}{d\theta} = \lim_{V_{\rm sub}\to\infty} \dfrac{1}{V_{\rm sub}} \dfrac{\langle Q_{\rm sub} \sin(\theta Q_{\rm sub}) \rangle}{\langle \cos(\theta Q_{\rm sub}) \rangle}$

which are used to crosscheck each other



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

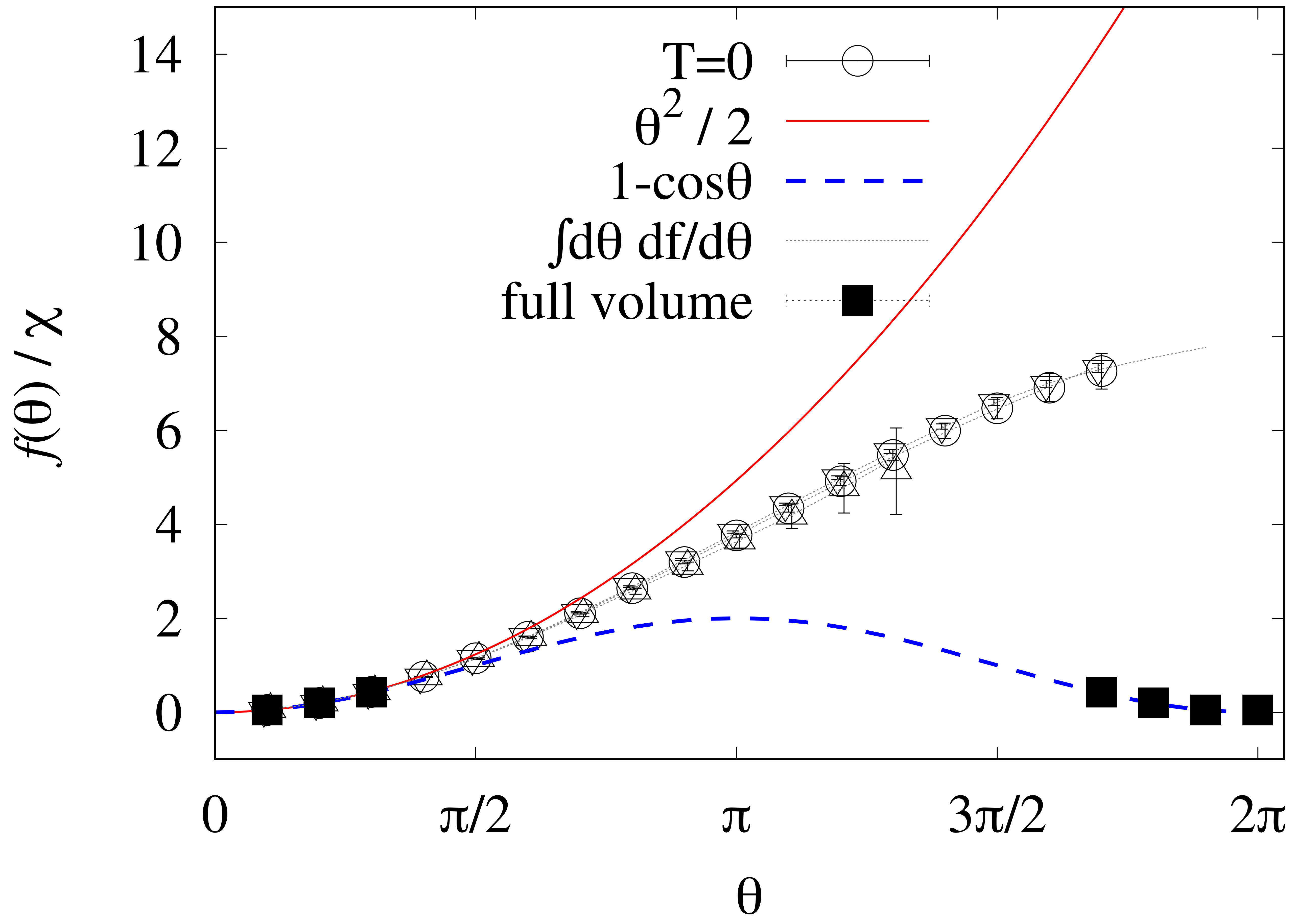


- $V_{\mathrm{sub}} = l^4$ with $l \in \{10,\ 12,\ \cdots,\ 24\}$
- Data in the range of $l_{\mathrm{dyn}}^4 \ll V_{\mathrm{sub}} \ll V_{\mathrm{full}}$ are fitted to

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

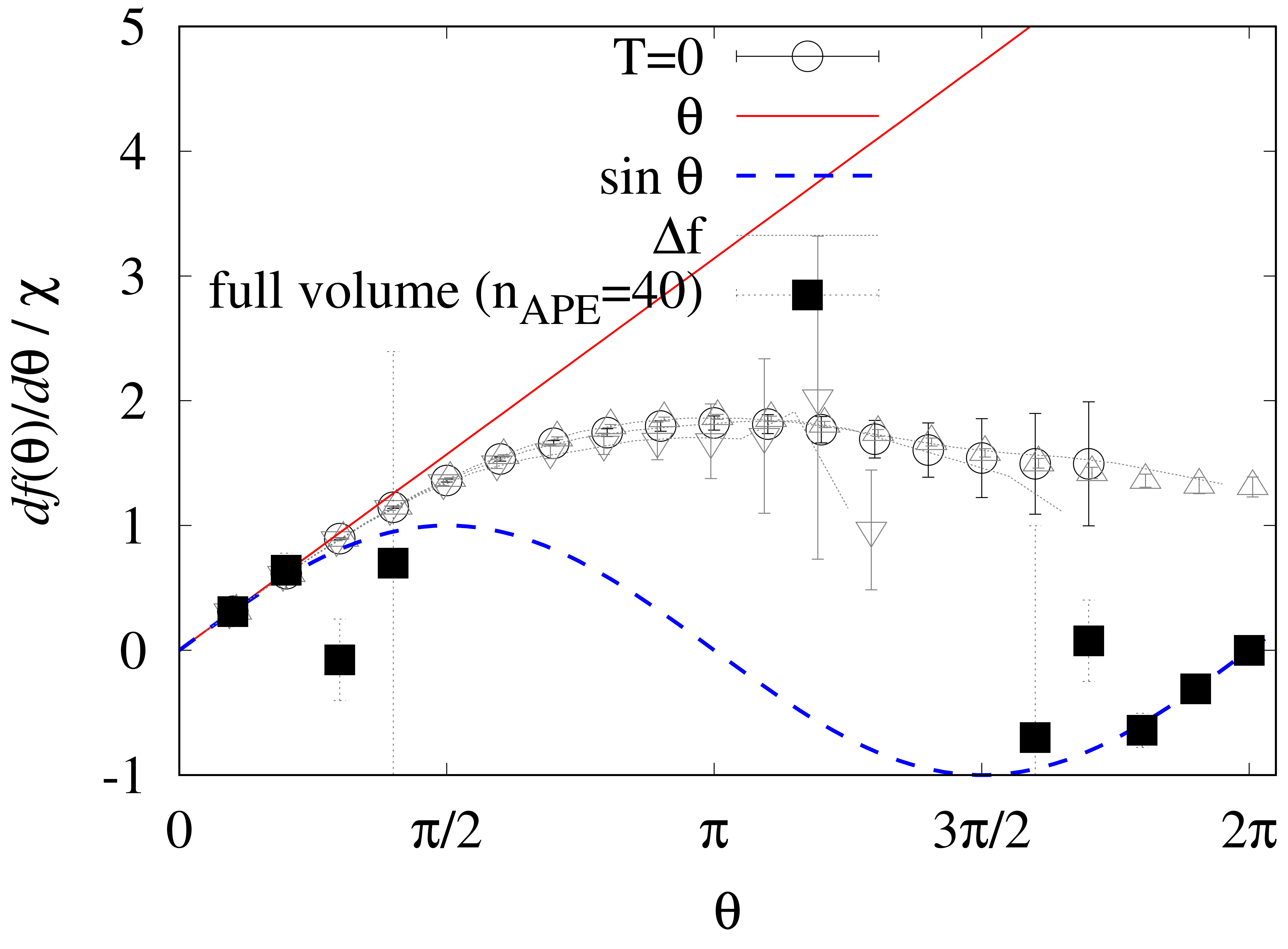
- Linear extrapolation works well.

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 $T = 0$

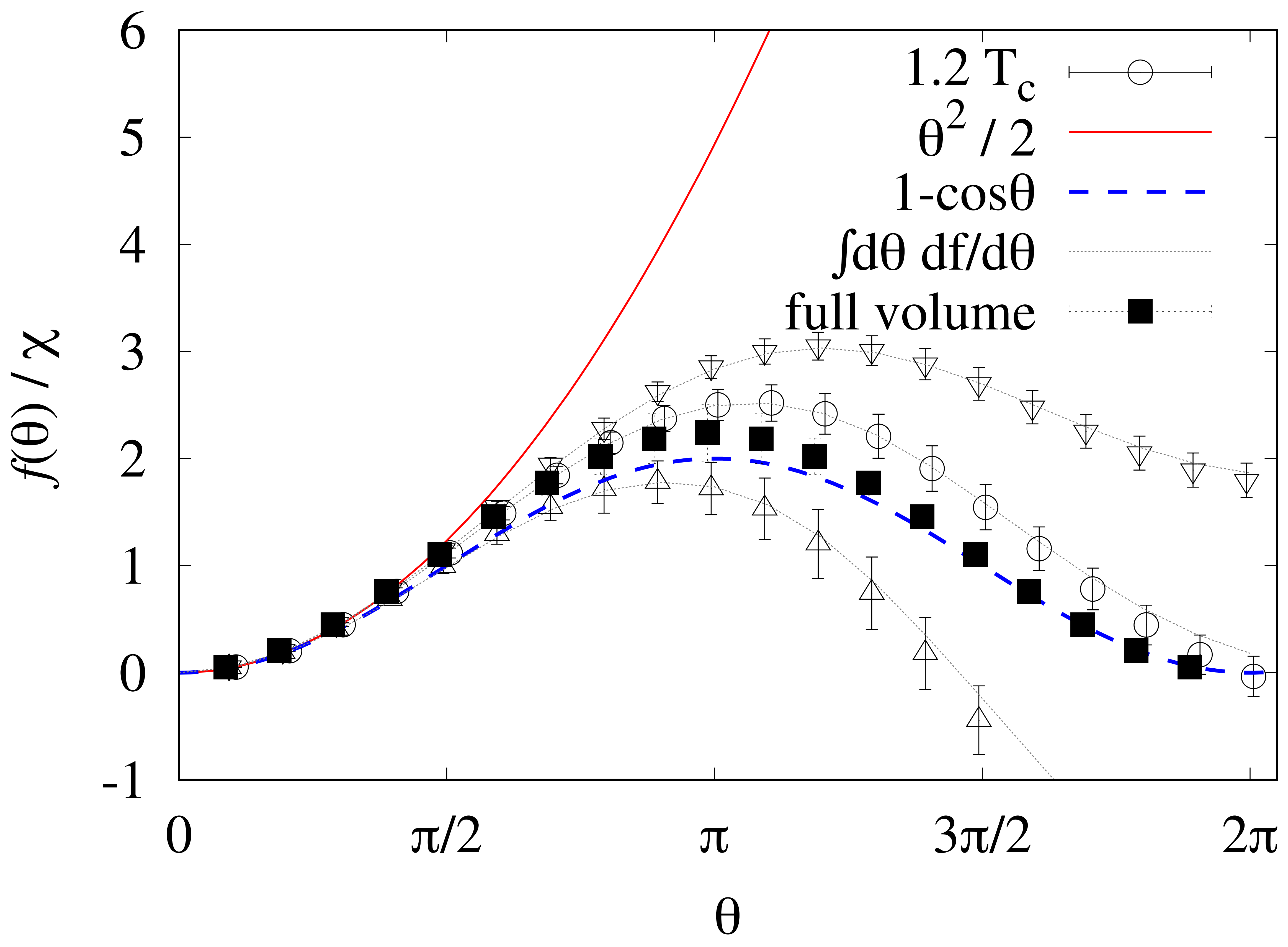


- Order parameter is non-zero

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

⇒ spontaneous CPV at $\theta = \pi$

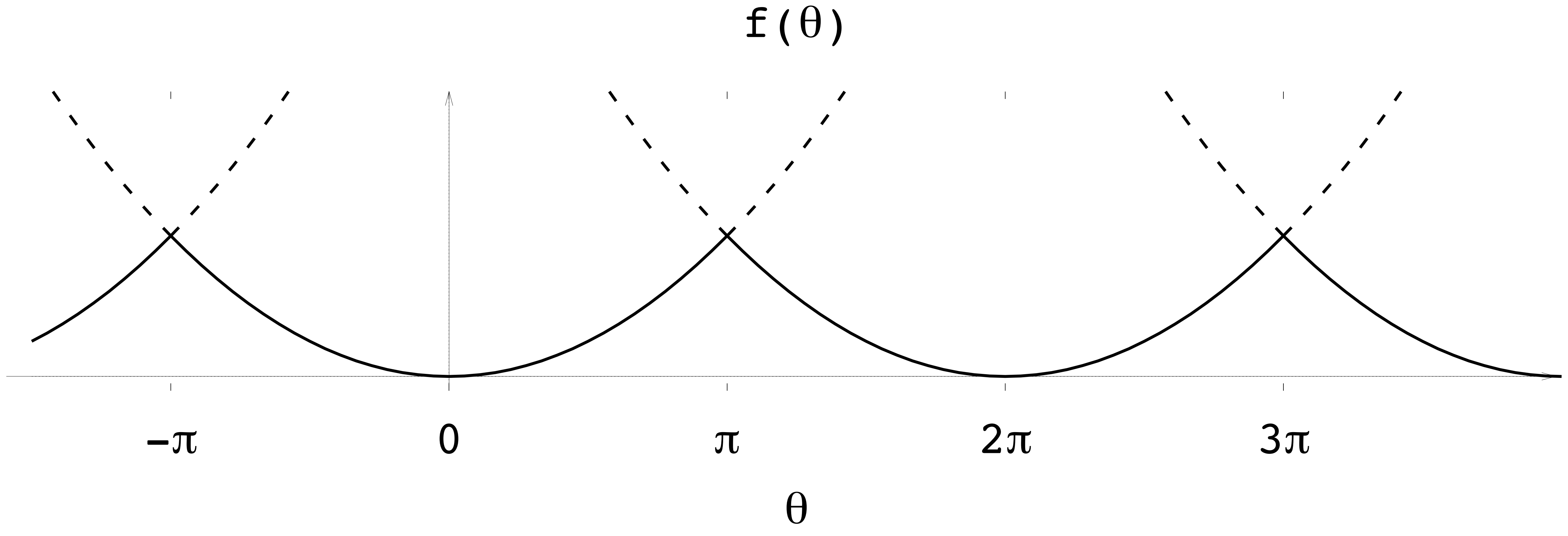
θ dependence of $f(\theta)$ at $T = 1.2T_c$



- 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 $T = 1.6\,T_c$

Discussion

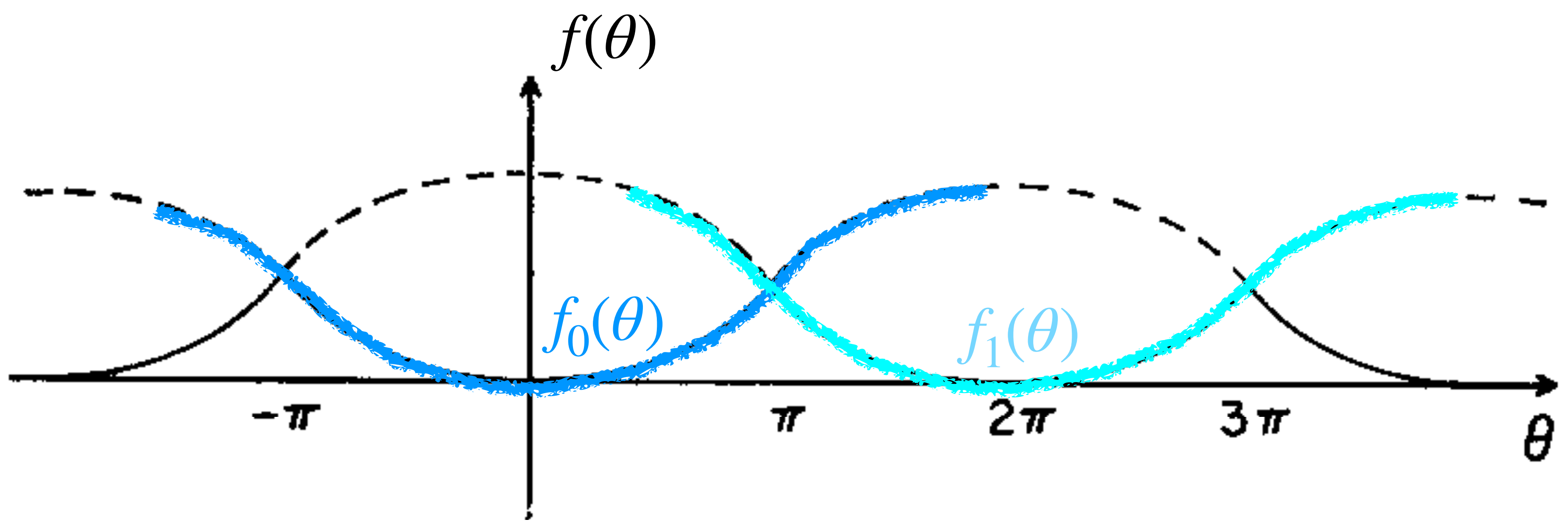
- For $T > T_c$, consistent with $f(\theta) = \chi(1 - \cos\theta)$
- At $T = 0$, $f(\pi - \theta) \neq f(\pi + \theta)$ is not satisfied and it is not like



Why ?

Interpretation

- Sub-volume method seems to trace an original branch even after the crossing point is passed.



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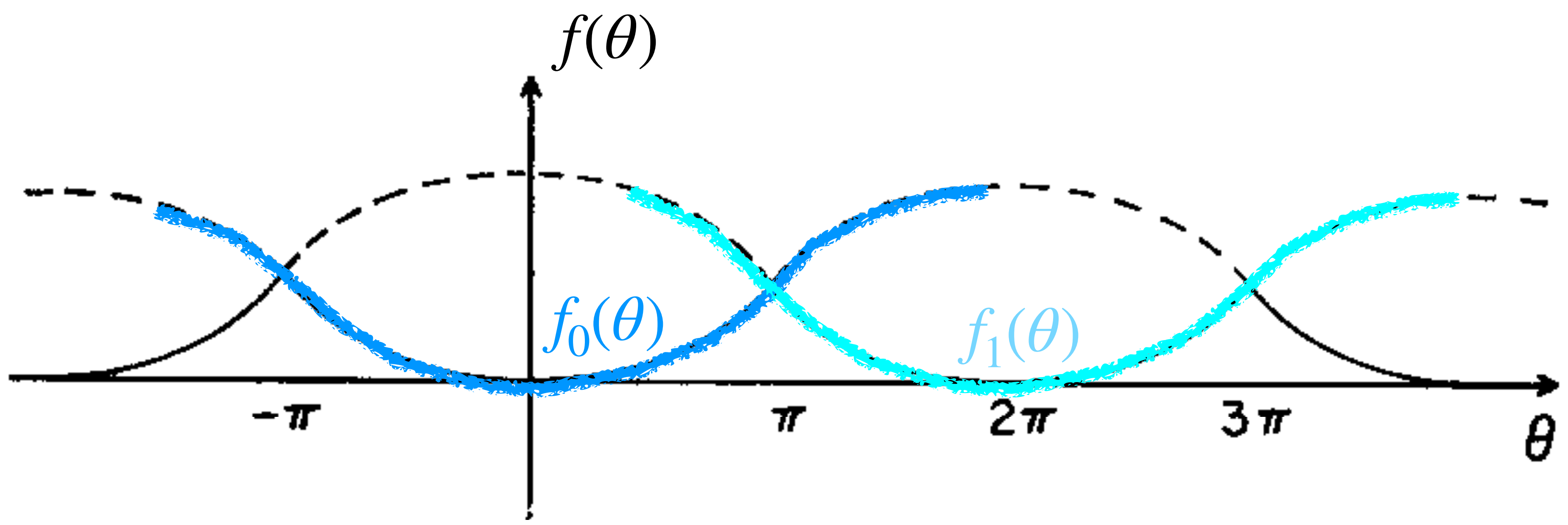
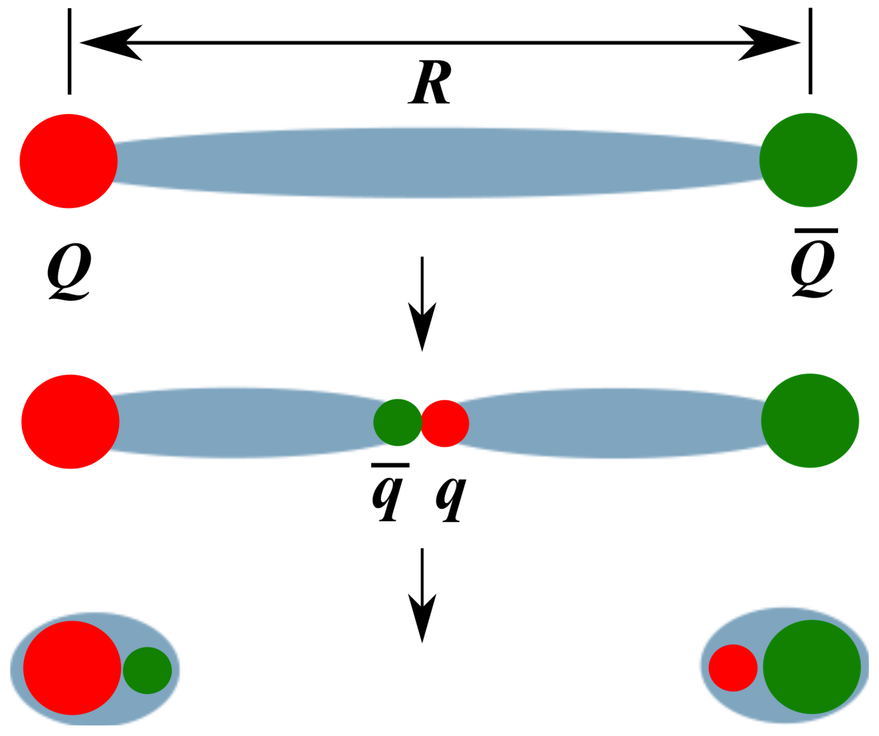
- Sub-volume method seems to trace an original branch even after the crossing point is passed.

- Similar to the calculation of the static potential, where“string breaking” should happen but never occurs.





Chernodub (2010)

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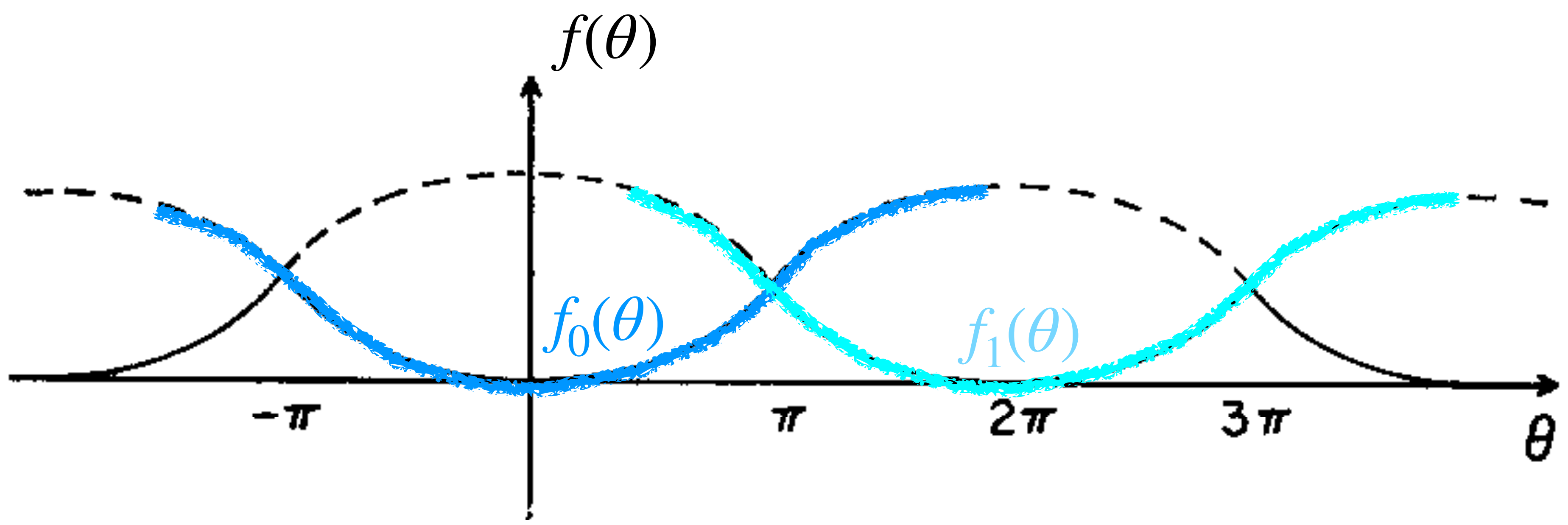

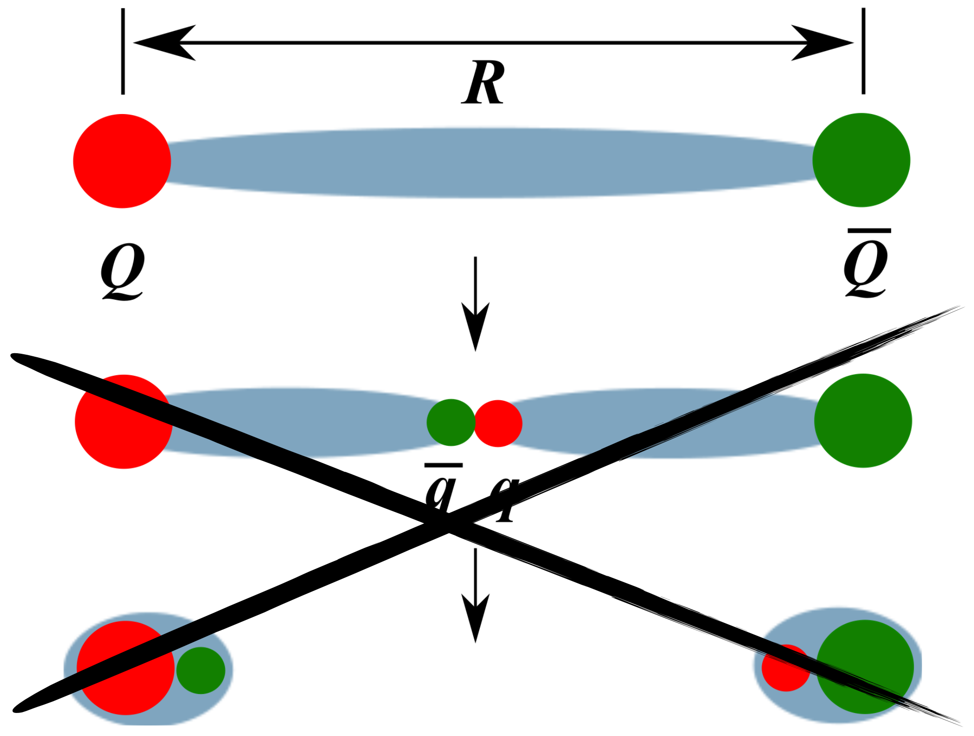

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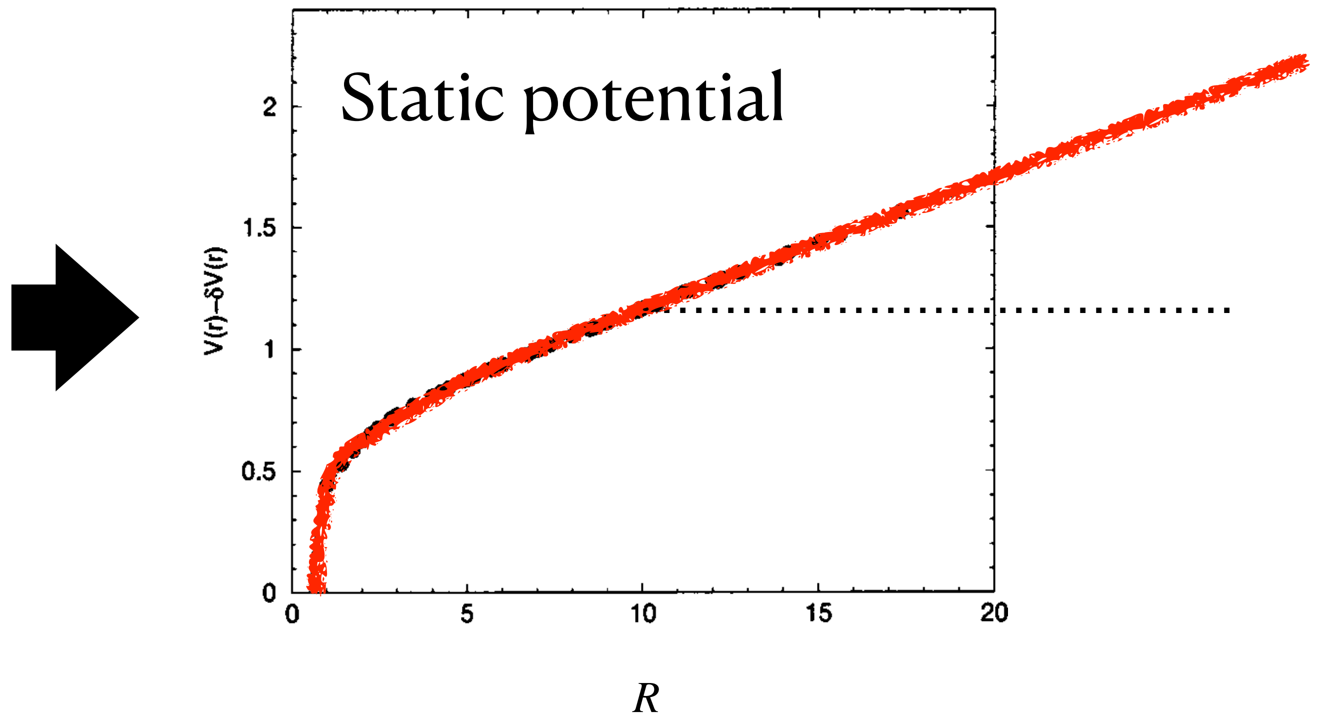

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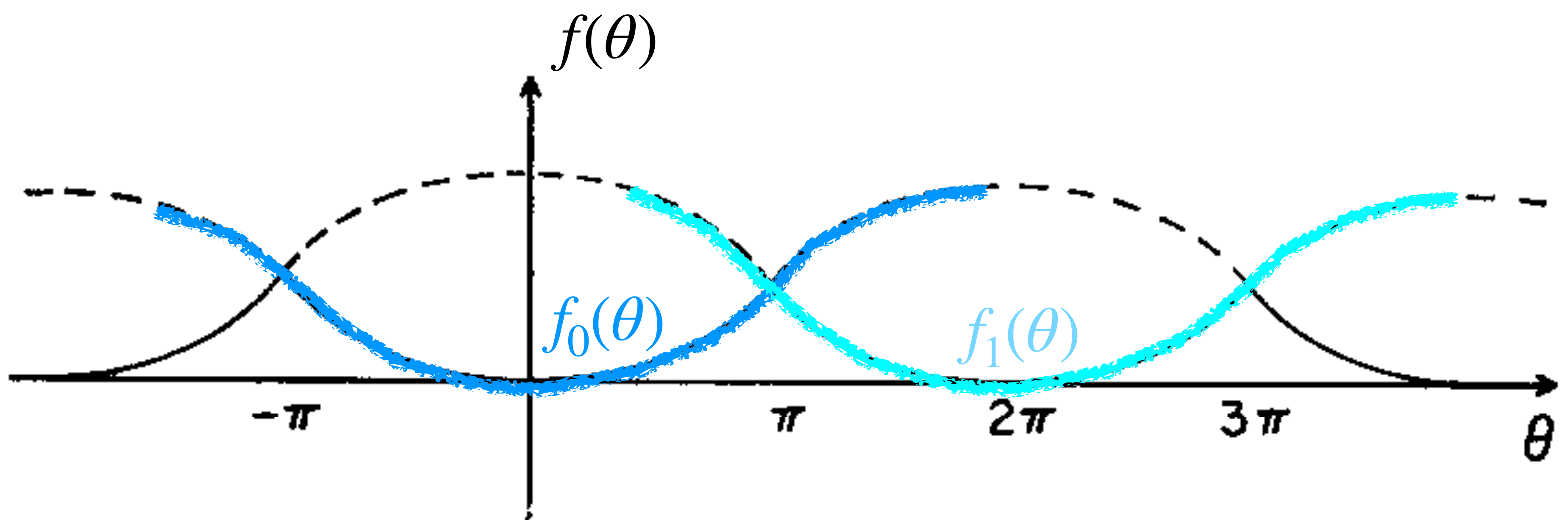

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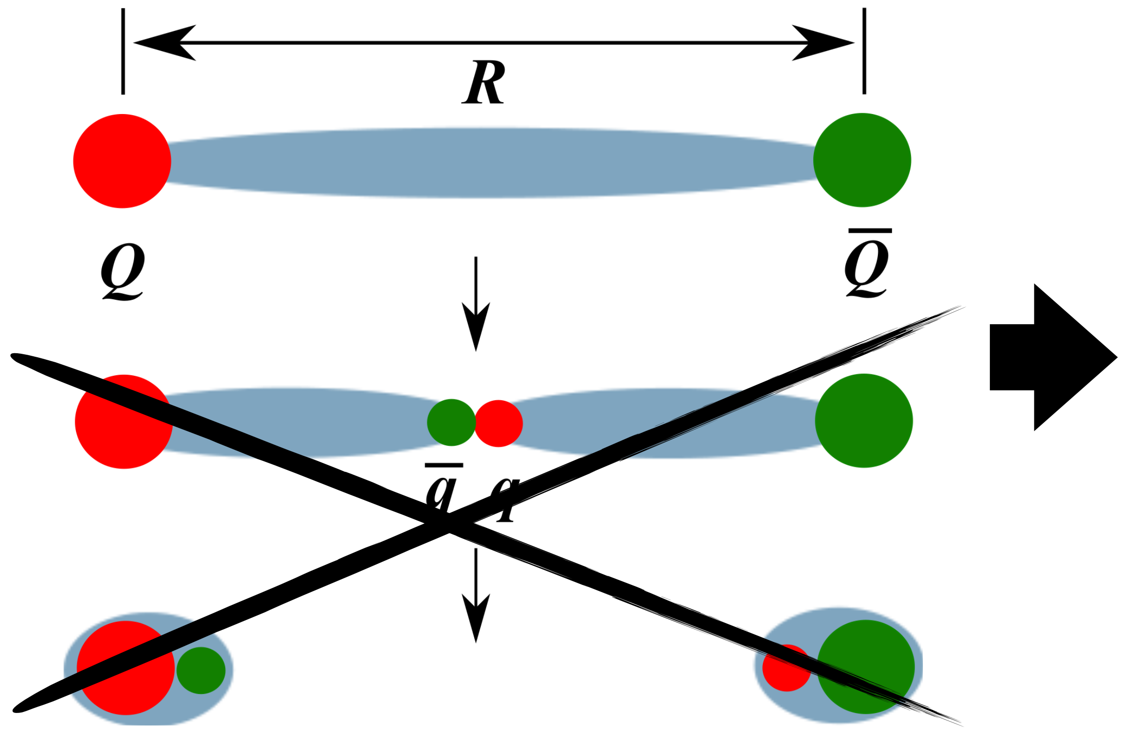

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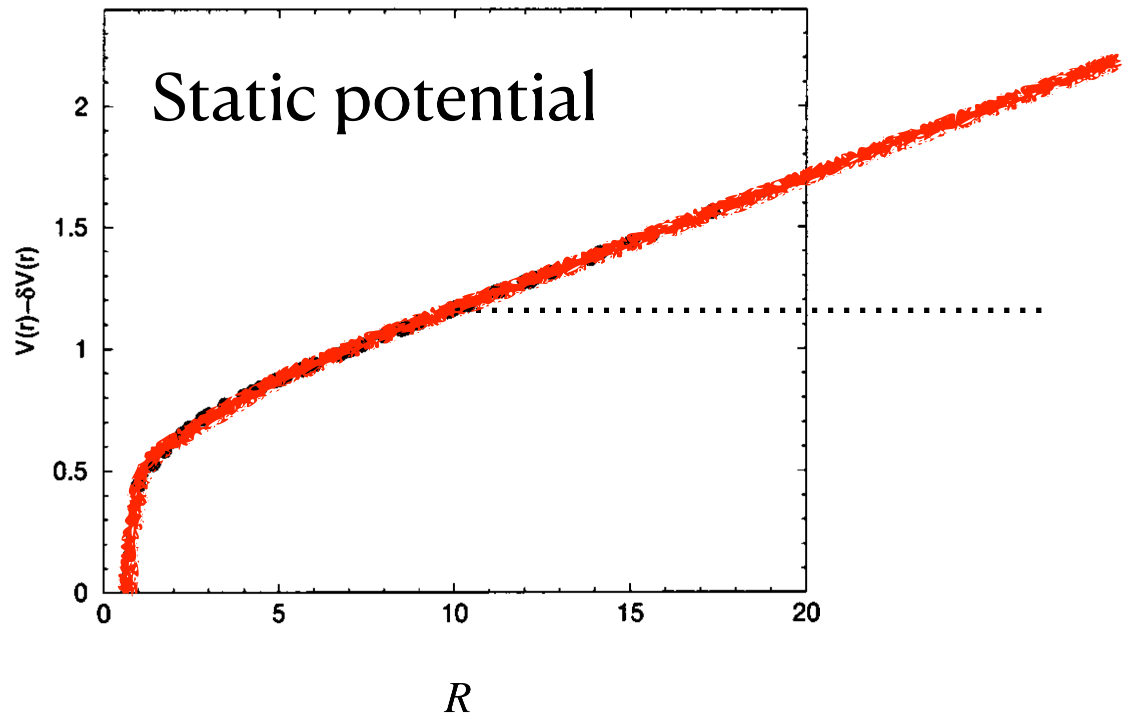

- In the present case, the domain to domain-wall transition should occur but does not in this method.

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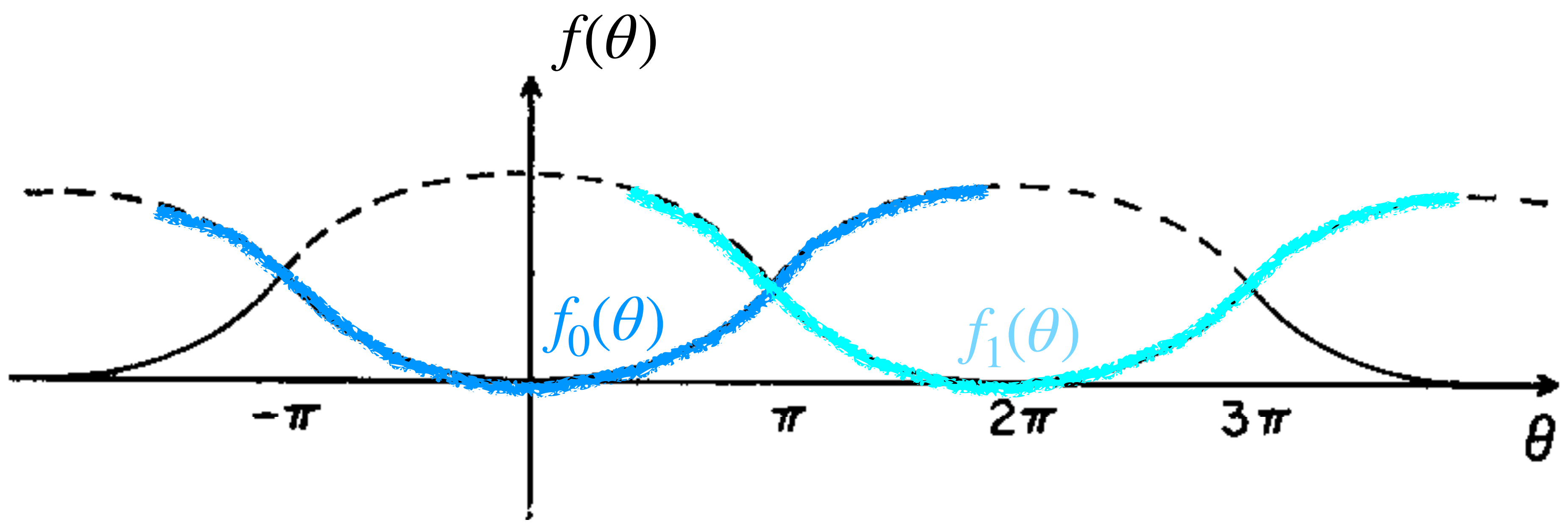

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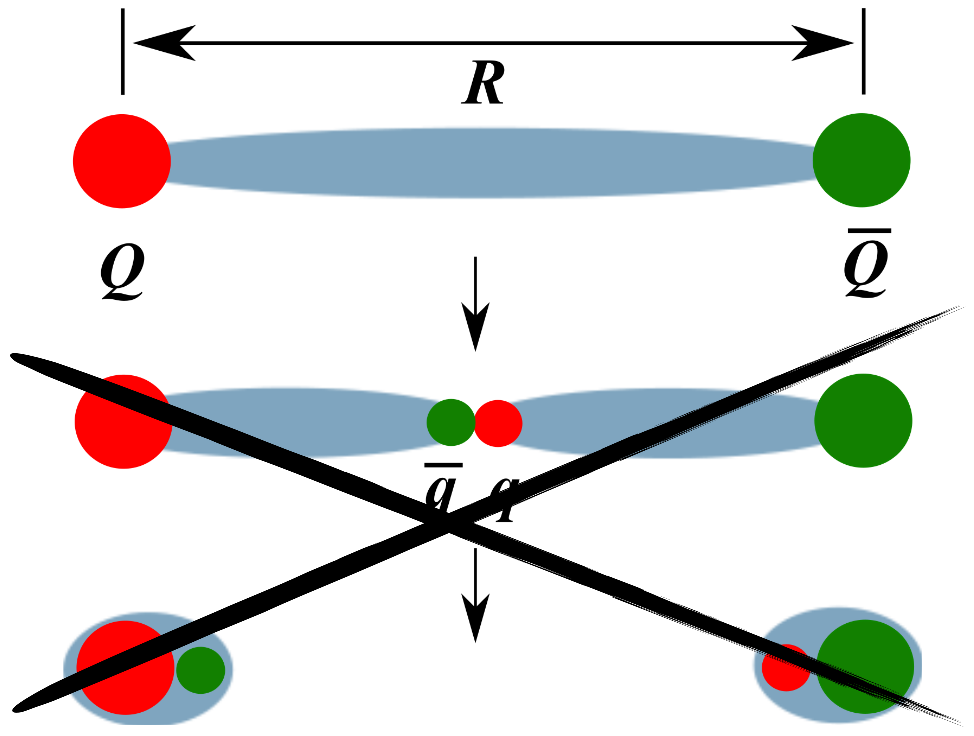

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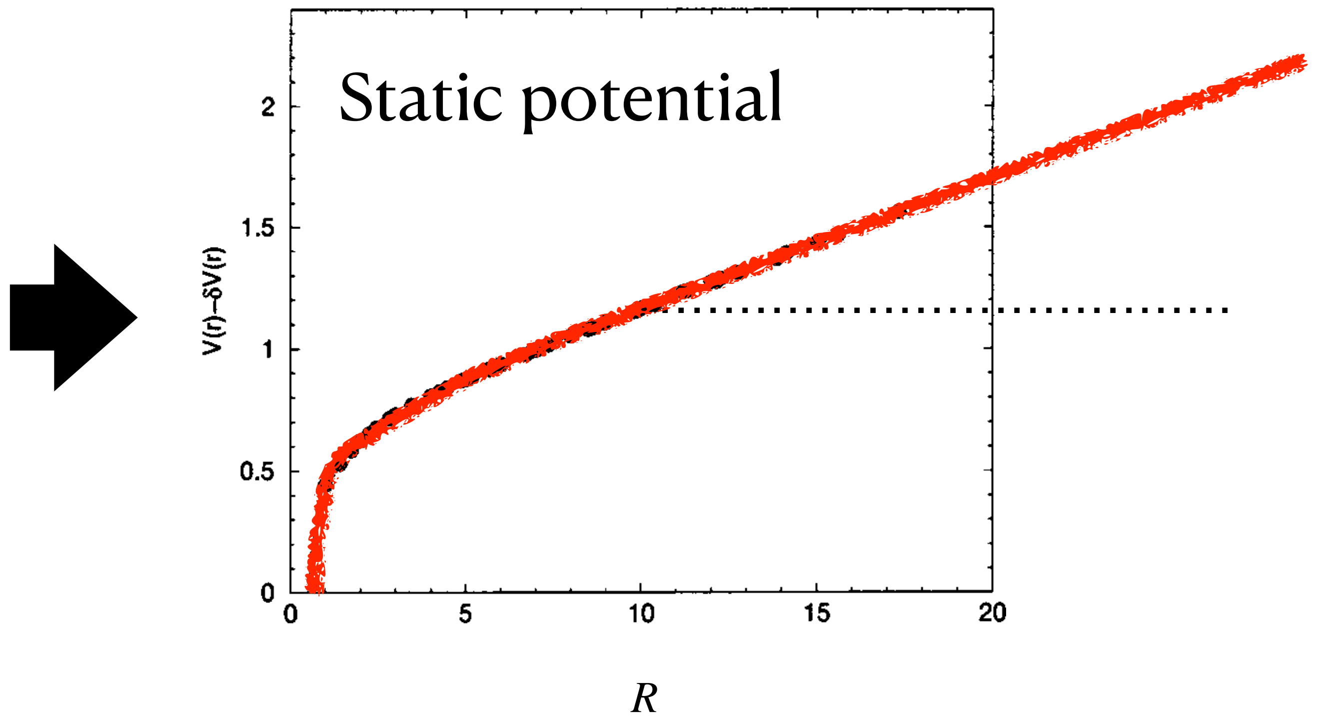

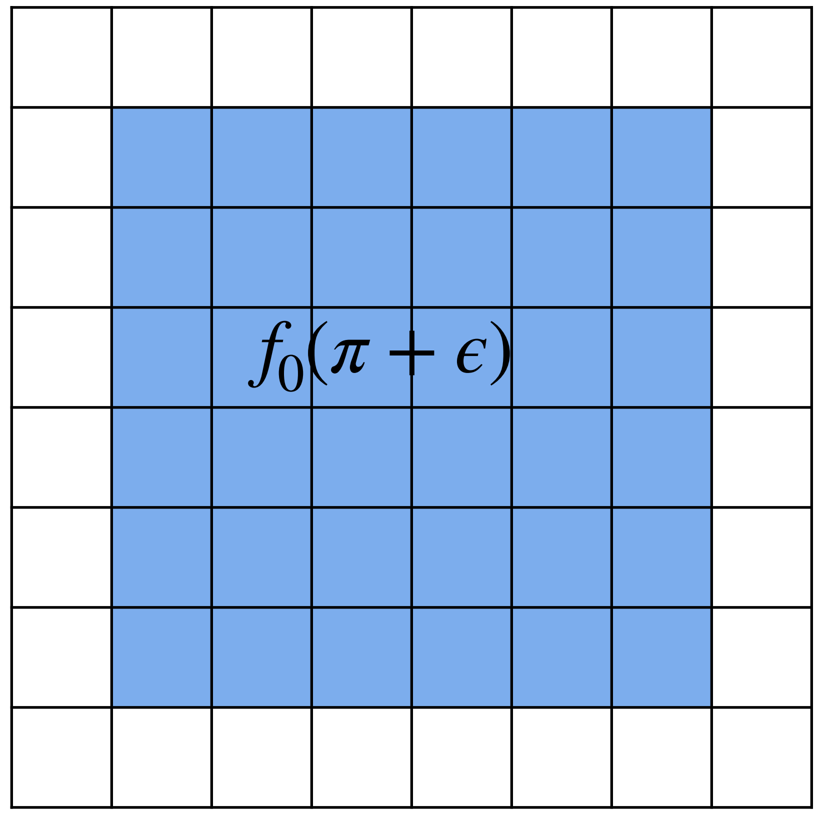

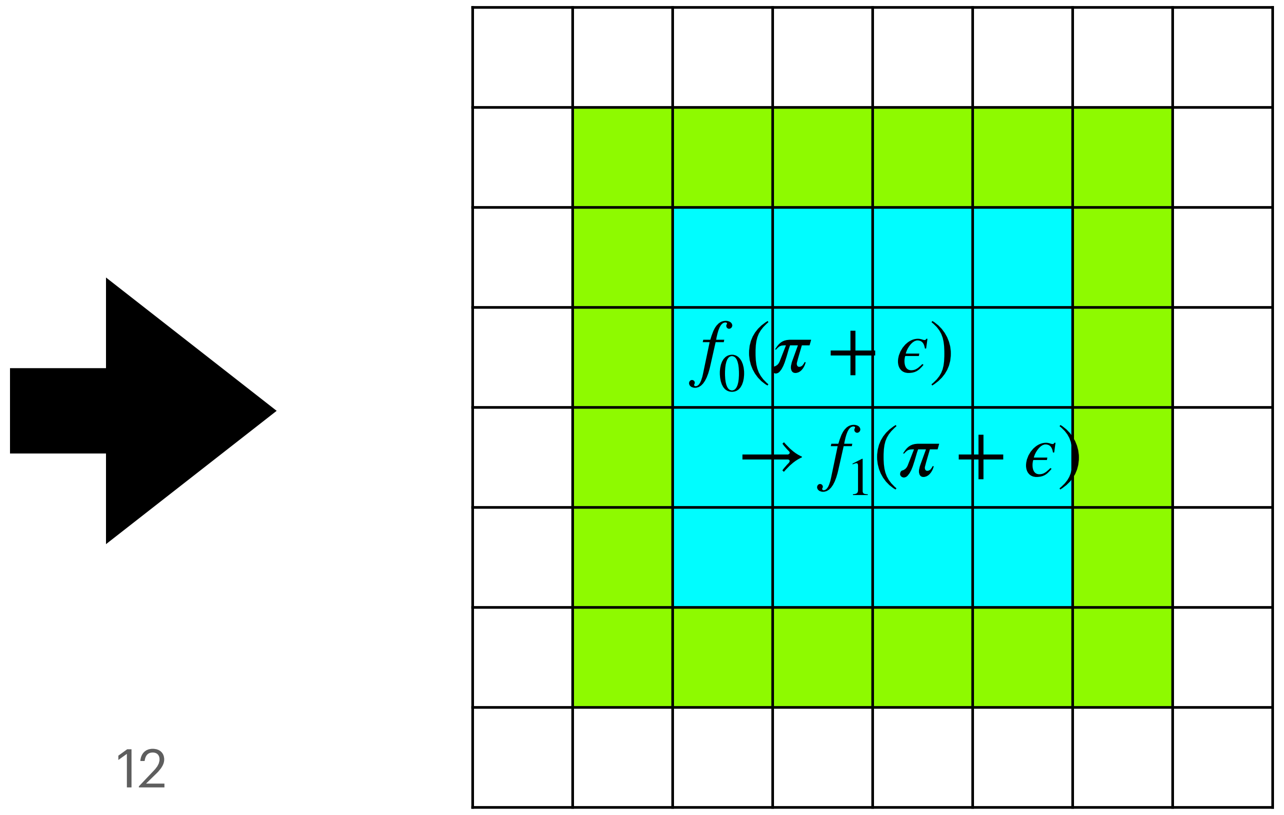

4d SU(N) YM has an topological object called a bag or a domain-wall [Luscher (1978)].

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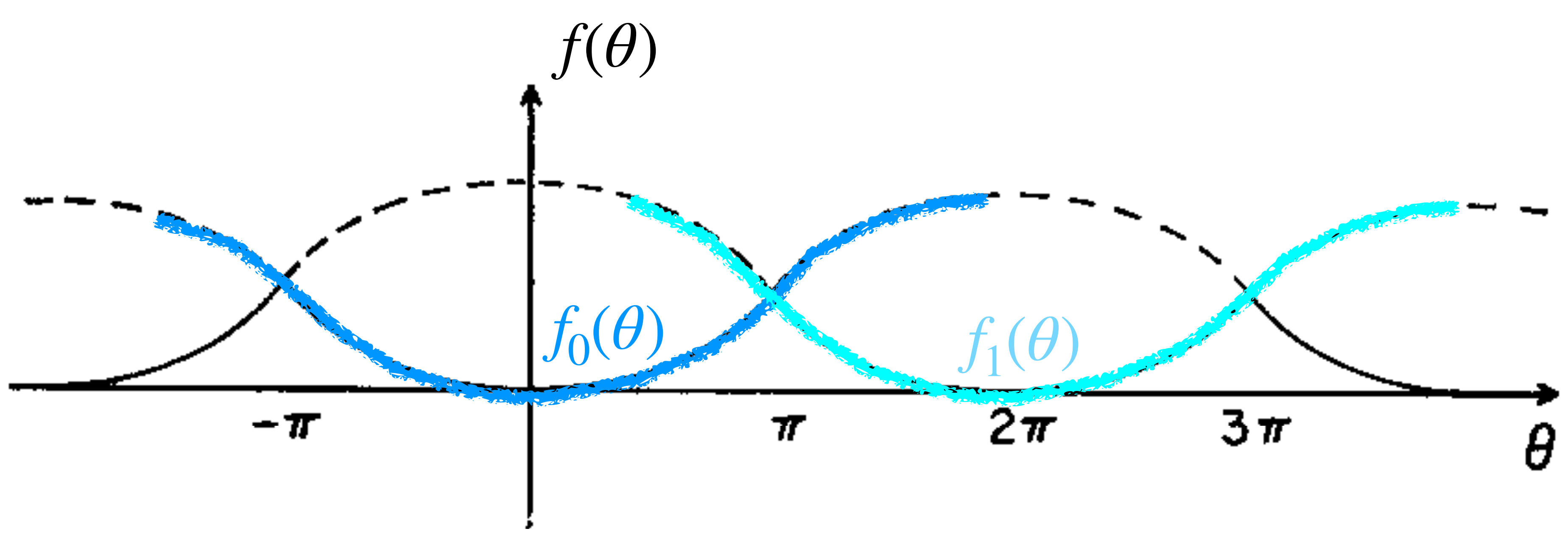

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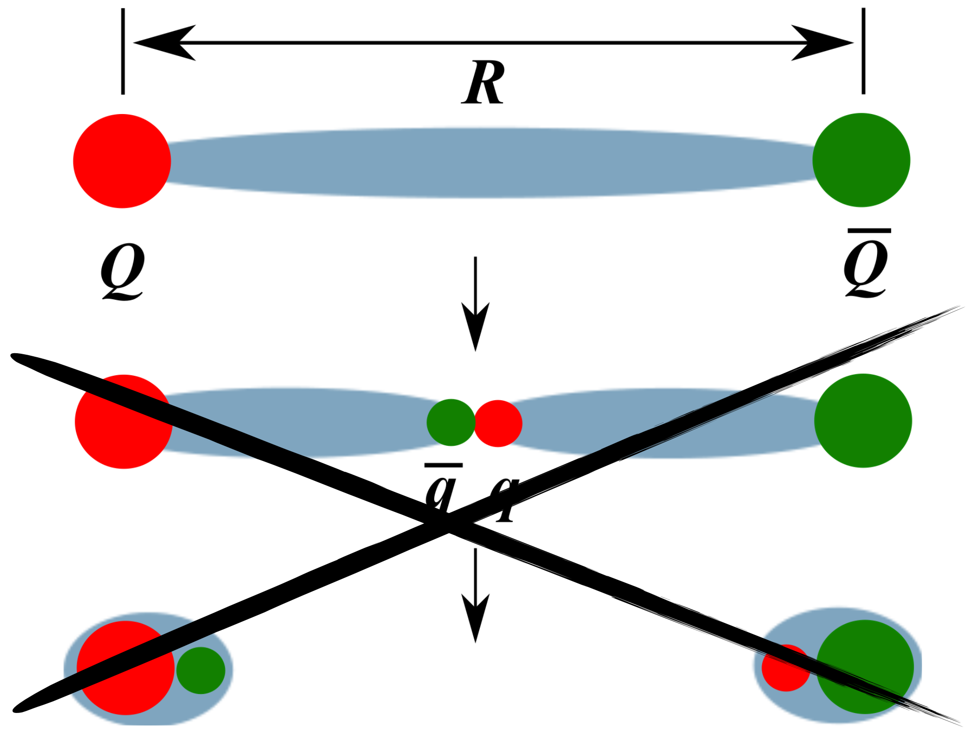

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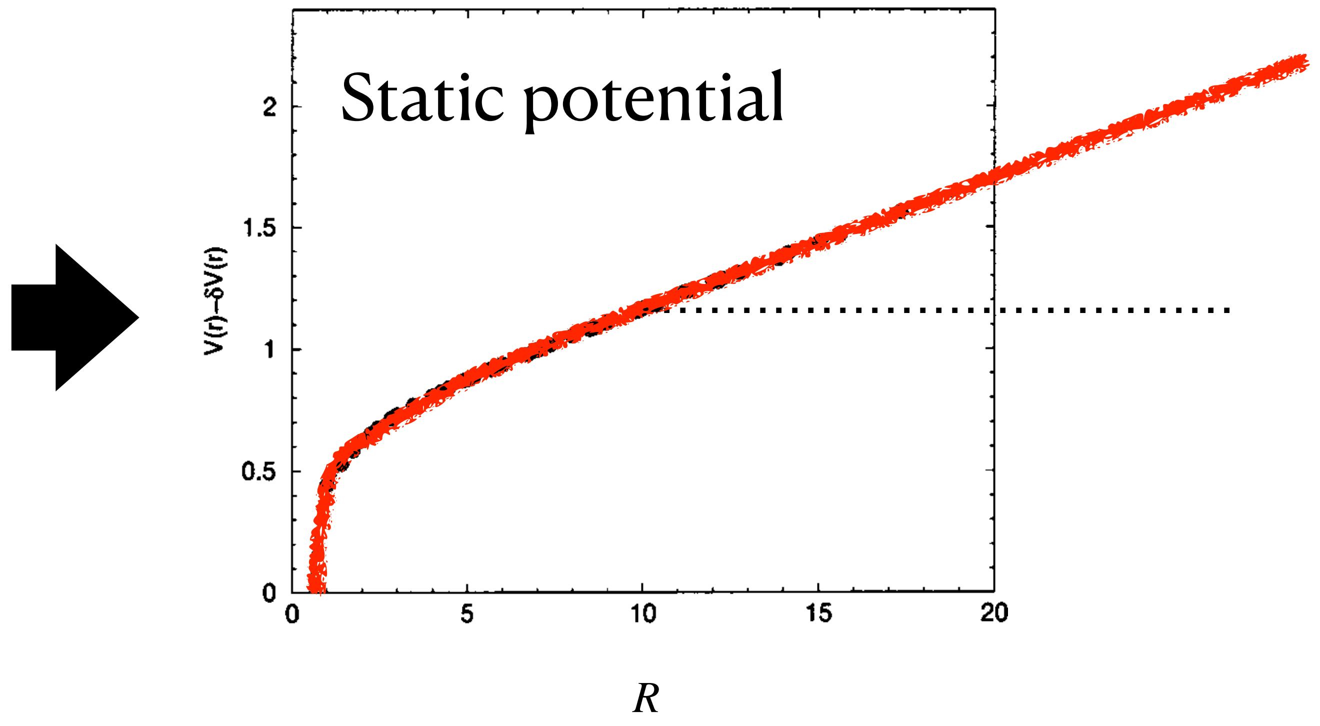

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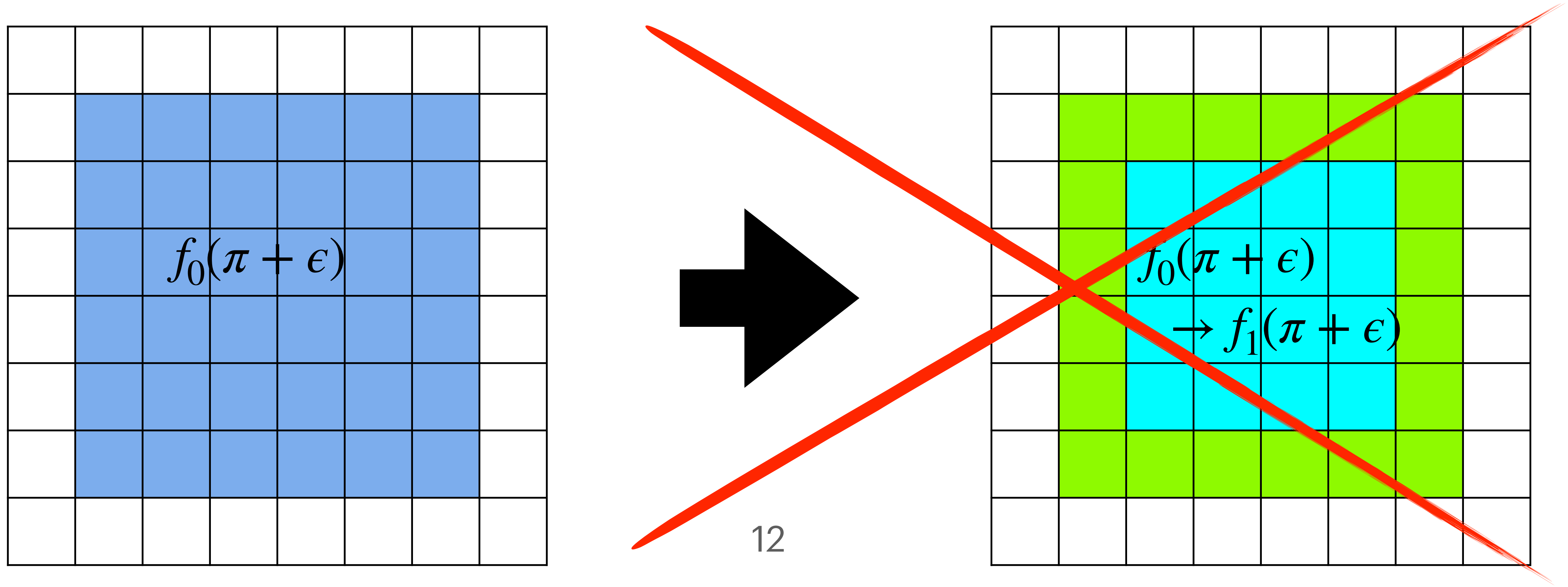

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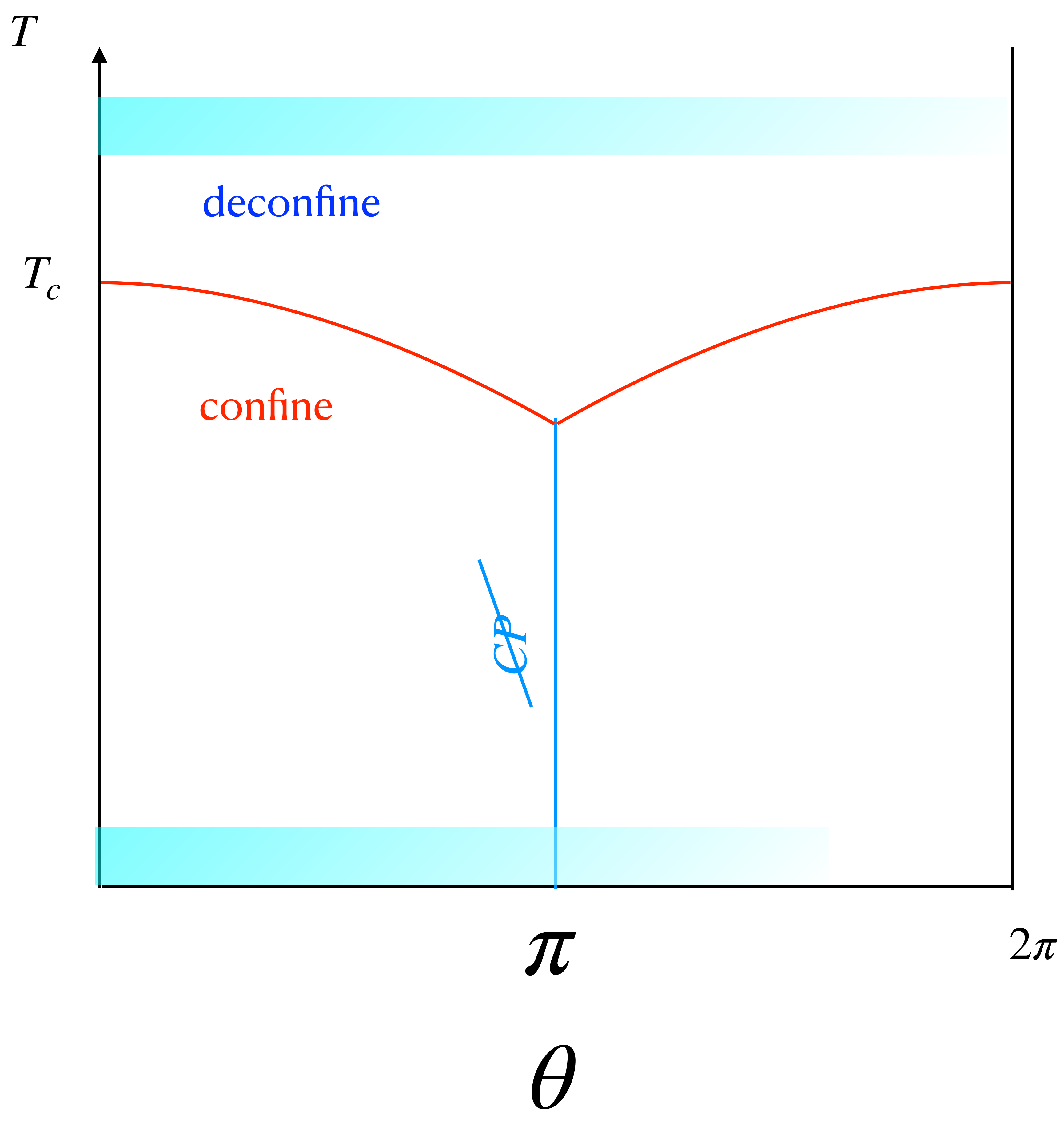
Summary and conclusion

- 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 $T = 0$.
  $\Rightarrow$ ***SU(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 $T_c(\theta)$
- applying the sub-volume method to the finite density system.

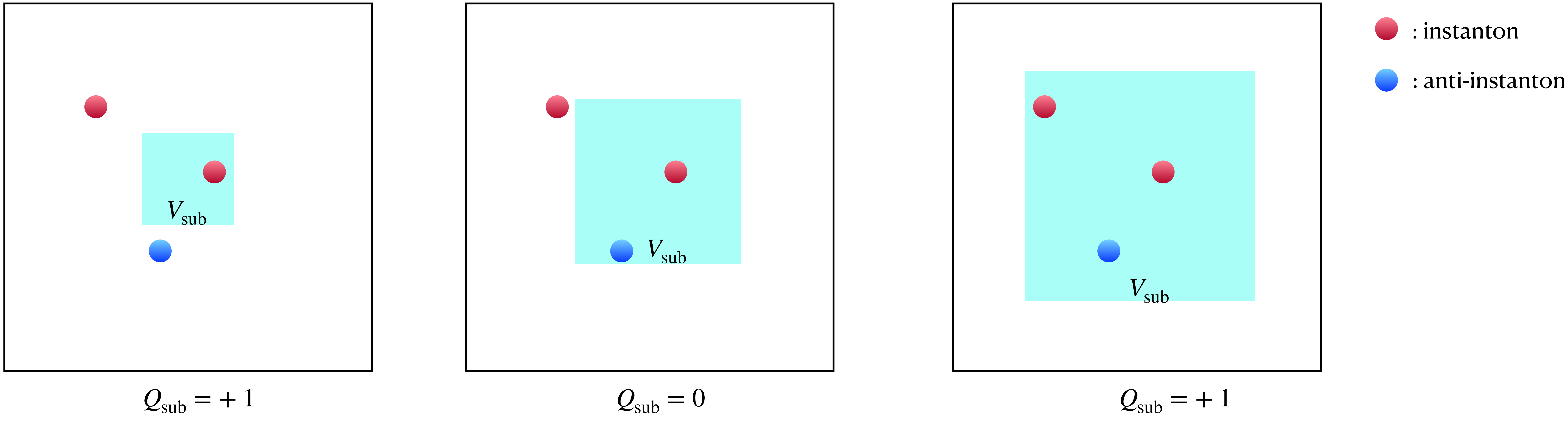
$SU(N)$ with $N = 2, \cdots \infty$



Backup slides

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

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



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

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

θ-vacuum

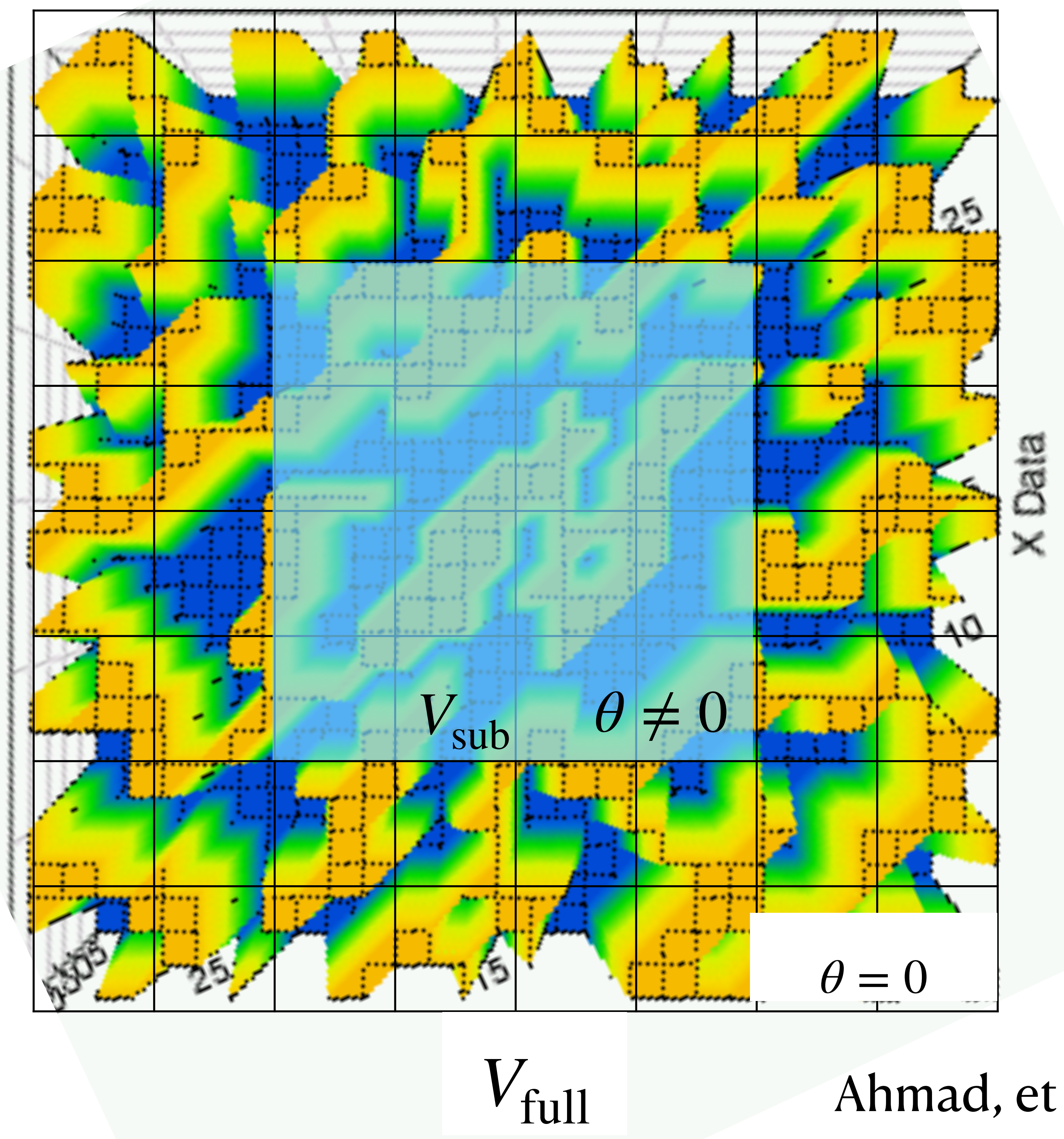
- The vacuum can have an integer winding number, labeled by $|n\rangle$.
- But, this label is changed by gauge transformation, e.g. $U_{(1)}|n\rangle \to |n+1\rangle$.
- Define $|\theta\rangle = \sum_{n-\infty}^{+\infty} e^{in\theta}|n\rangle \iff U_{(1)}|\theta\rangle = e^{-i\theta}|\theta\rangle$
- $\langle\theta_+|\theta_-\rangle_J = \sum_{m,n} e^{in\theta}e^{-im\theta}\langle m_+|n_-\rangle_J = \sum_Q e^{i\theta Q}\sum_m \langle m_+|m_- + Q\rangle_J$

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

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

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

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



Ahmad, et al. (2005)

Similarity to the static potential calculation

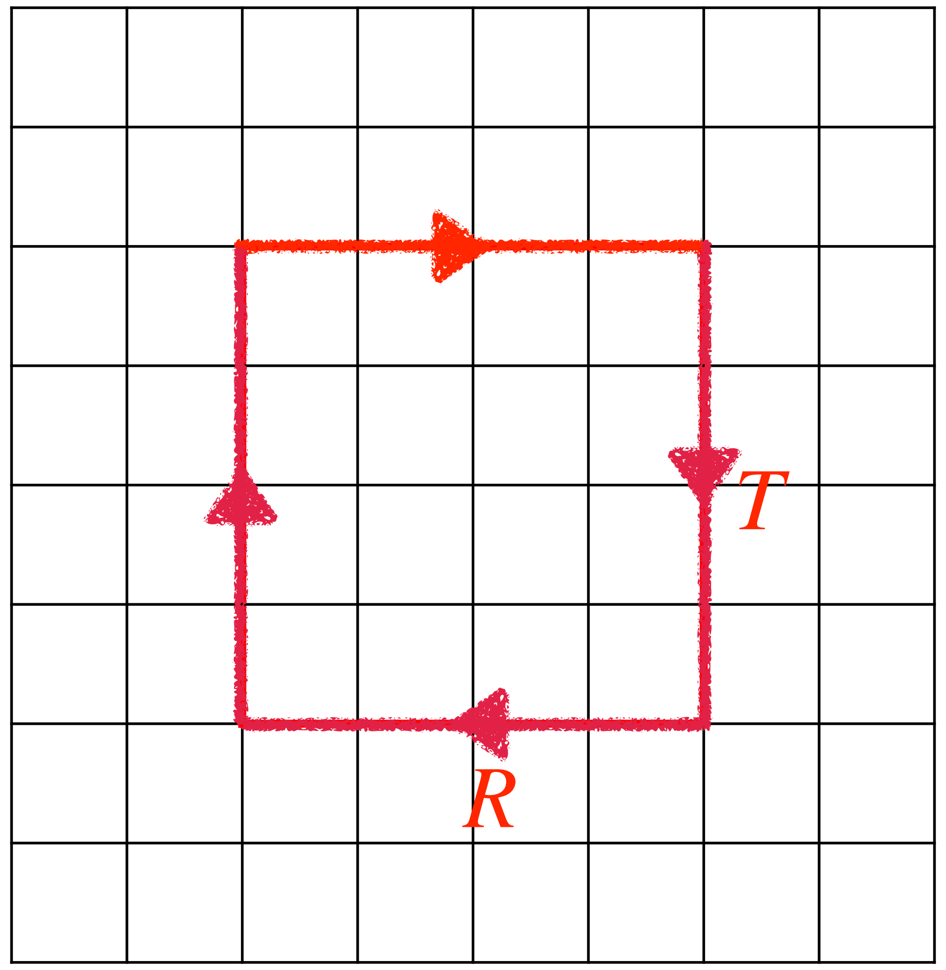
In the static potential calculation, Wilson loop is inserted.

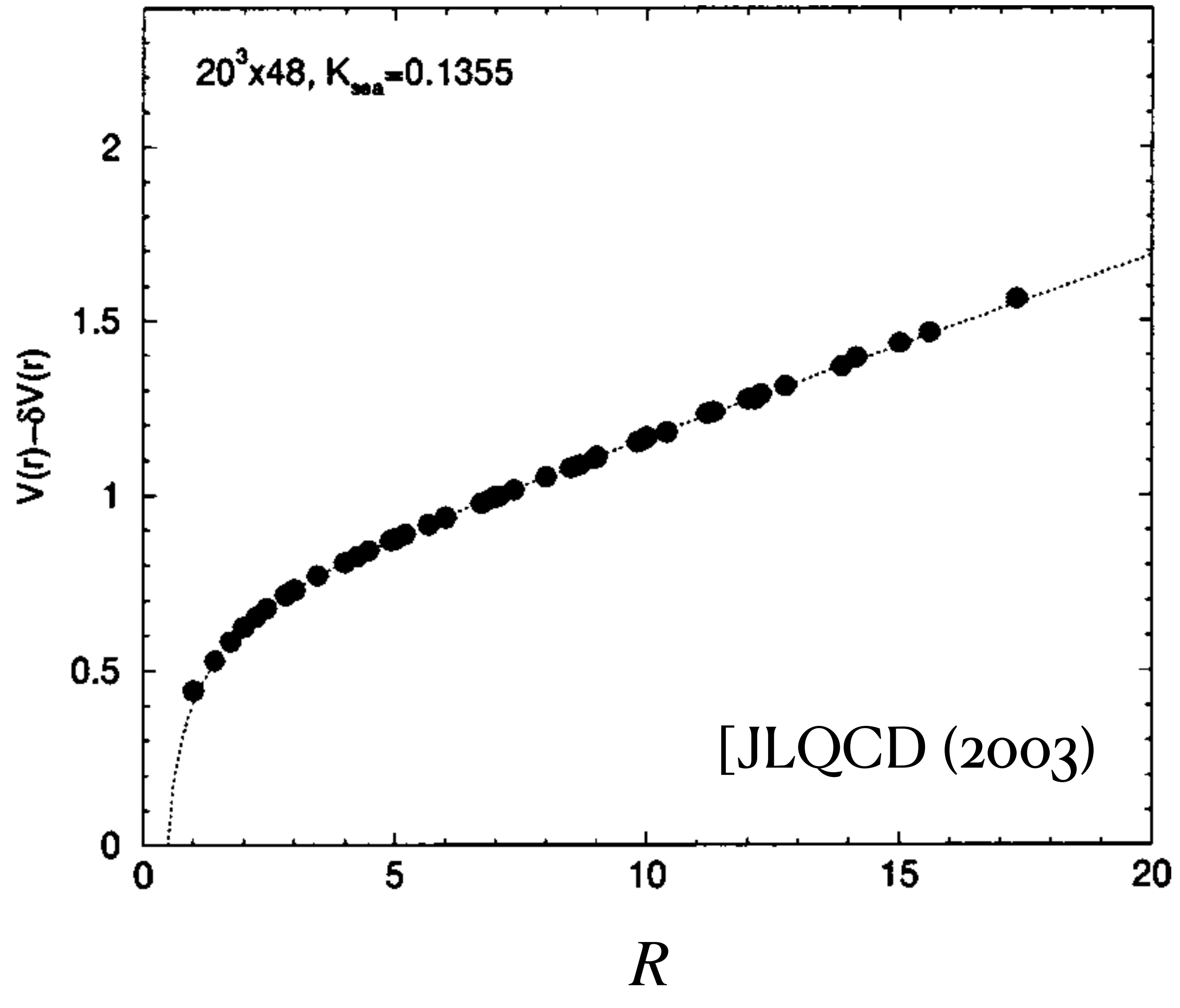
$$\frac{Z(\Box)}{Z(1)} = \frac{1}{Z(1)}\int \mathscr{D}U \ \mathrm{Tr}\left[e^{i\oint A}\right]e^{-S_{\mathrm{QCD}}} = \langle \mathrm{Tr}\left[e^{i\oint A}\right]\rangle \to e^{-V(\mathscr{A})}$$

$$V(\mathscr{A}) = -\lim_{\mathscr{A}\to\infty} \ln\langle \mathrm{Tr}\left[e^{i\oint A}\right]\rangle = \sigma\mathscr{A} + \cdots$$

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

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

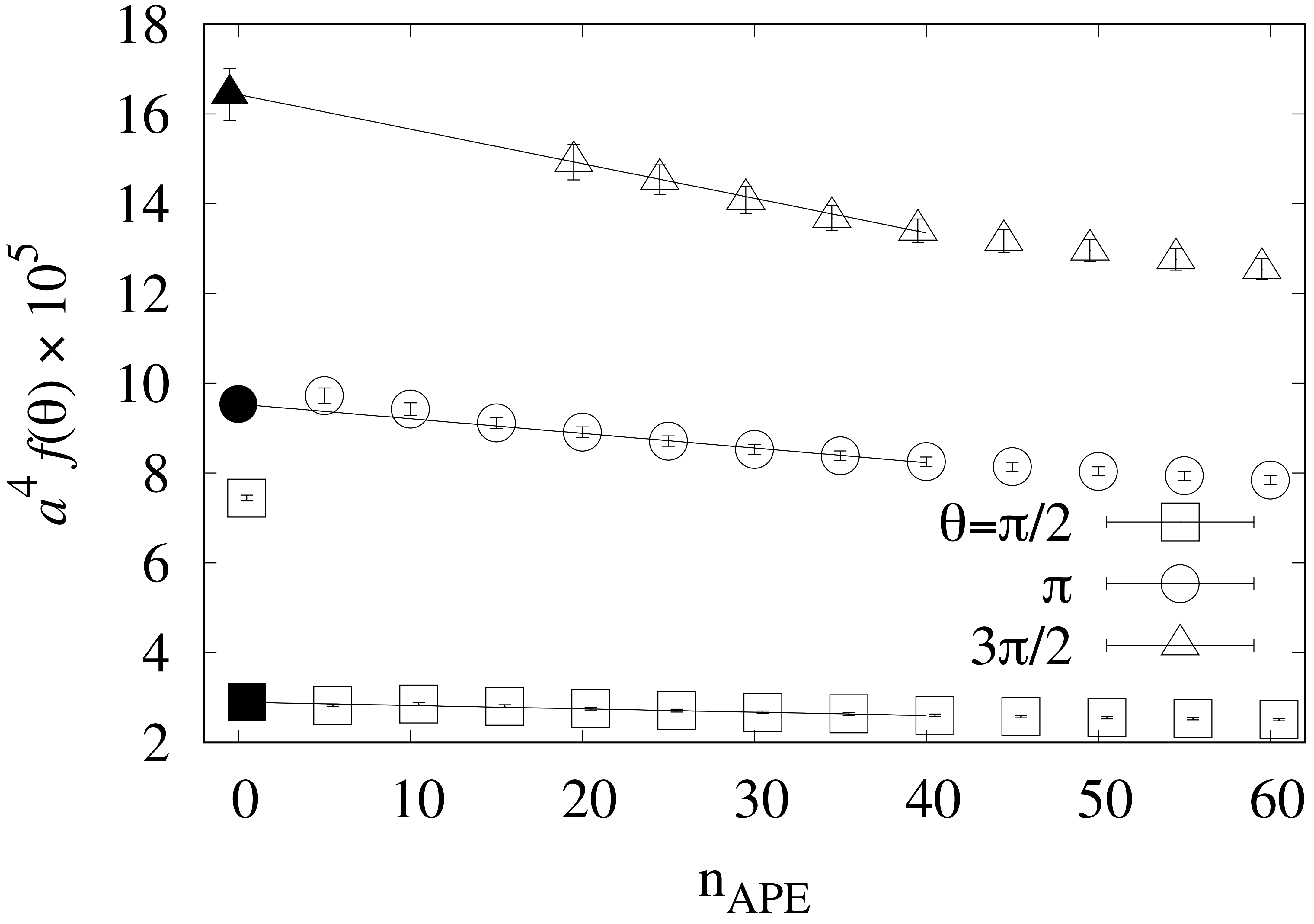




About smearing

- Need to numerically calculate $q(x) = \frac{1}{64\pi^2}\epsilon_{\mu\nu\rho\sigma}F^a_{\mu\nu}F^a_{\rho\sigma}$ 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 $n_{\mathrm{APE}} \to 0$, $\langle O \rangle = \lim_{n_{\mathrm{APE}} \to 0} \langle O(n_{\mathrm{APE}}) \rangle$

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



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