Practical approach to the sign problem at finite theta-vacuum angle

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Sign problem vs. Theta vacuum

$$\mathcal{L}_{\mathrm{QCD}} = \bar{q}_f(\gamma_\nu D_\nu + m_f)q_f + \frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu} - i\theta\frac{1}{64\pi^2}\epsilon_{\mu\nu\sigma\rho}F^a_{\mu\nu}F^a_{\sigma\rho}$$

- Topological effect
- Complex

$\mathrm{U_A}(1)$ transformation

$$\mathcal{L}'_{\mathrm{QCD}} = \bar{q}'_f(\gamma_\nu D_\nu + m_f(\theta))q'_f + \frac{1}{4}F^a_{\mu\nu}F^a_{\mu\nu}$$

This parity-odd term
makes fermion determinant complex.

Lattice QCD simulation

- Taylor expansion around $\theta = 0$.
- Analytic continuation from imaginary θ region.

Suggestion

$$\mathcal{L}_{QCD} = \sum_{l=u,d} \bar{q}'_l \mathcal{M}_l(\theta) q'_l + \bar{q}'_s \mathcal{M}_s q'_s + \frac{1}{4} F^a_{\mu\nu} F^a_{\mu\nu}$$

$$\mathcal{M}_l(\theta) \equiv \gamma_\nu D_\nu + m_l \cos(\theta/2) + m_l i\gamma_5 \sin(\theta/2),$$

$$\mathcal{M}_s \equiv \gamma_\nu D_\nu + m_s.$$

$$\mathcal{M}'_l(\theta) \equiv \gamma_\nu D_\nu + m_l \cos(\theta/2)$$

Neglect the P-odd mass

Reweighting Method

$$\langle \mathcal{O} \rangle = \int \mathcal{D}A \, \mathcal{O}' \underbrace{(\det \mathcal{M}'_l(\theta))^2 \det \mathcal{M}_s e^{-S_g}}_{\text{Free from the sign problem}}$$

$$\mathcal{O}' \equiv \mathcal{O} \frac{(\det \mathcal{M}_l(\theta))^2}{(\det \mathcal{M}'_l(\theta))^2} \approx \mathcal{O}$$

$\det \mathcal{M}'_l(\theta)$: Fermion determinant without P odd mass

T. S., J. Takahashi, Y. Sakai, H. Kouno, and M. Yahiro, Phys. Rev. D**85** 056009 (2012)

In this work

We evaluate the validity of our reweighting method with the average reweighting factor.

1. We formulate in the 2 flavor PNJL model to concentrate on the light flavor sector.

2. Apply three reference systems
   - Simply neglect the P-odd mass (Reference A)
   - Add a higher order correction (Reference B and C)

3. Estimate the effect of mesonic fluctuation.

PNJL model

2 flavor Polyakov-loop extended Nambu-Jona-Lasinio model

$$\mathcal{L} = \bar{q}(\gamma_\nu D_\nu + m_0)q - G_1 \sum_{a=0}^{3}[(\bar{q}\tau_a q)^2 + (\bar{q}i\gamma_5\tau_a q)^2]$$

$$- 8G_2[e^{i\theta}\det \bar{q}_R q_L + e^{-i\theta}\det \bar{q}_L q_R] + \mathcal{U}(T, \Phi, \Phi^*)$$

$$\Phi = \frac{1}{3}\mathrm{tr_c}(L)$$

$$L = \exp(iA_4/T)$$

Kobayashi-Maskawa-'t Hooft interaction

- breaks the $U_A(1)$ symmetry explicitly
- Determinant is taken in the flavor space.

- Quarks are interacting by point interaction.
- Gluon is treated as back ground field.
- Potential $\mathcal{U}$ controls the back ground and determined to reproduce pure YM LQCD data.

NJL model

2 flavor NJL model with theta parameter

$$\mathcal{L} = \bar{q}(\gamma_\nu D_\nu + m_0)q - G_1 \sum_{a=0}^{3}[(\bar{q}\tau_a q)^2 + (\bar{q}i\gamma_5\tau_a q)^2]$$

$$- 8G_2[\underline{e^{i\theta}} \det \bar{q}_R q_L + \underline{e^{-i\theta}} \det \bar{q}_L q_R] + \mathcal{U}(T, \Phi, \Phi^*)$$

Chiral transformation

$$q = e^{i\gamma_5 \frac{\theta}{4}} q'$$

$$\mathcal{L} = \bar{q}'(\gamma_\nu D_\nu + \underline{m(\theta)})q' - G_+[(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2]$$

$$- G_-[(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2] + \mathcal{U}$$

$$G_\pm = G_1 \pm G_2$$

$$m(\theta) = m_0\cos(\theta/2) + \boxed{m_0 i\gamma_5 \sin(\theta/2)}$$

Cause the sign problem

Reweighting factor

Reweighting Method

$$\langle \mathcal{O} \rangle = \int \mathcal{D}A \; \mathcal{O} \det \mathcal{M}(\theta) e^{-S_g}$$

$$= \int \mathcal{D}A \; \mathcal{O}' \det \mathcal{M}_{\mathrm{ref}}(\theta) e^{-S_g}$$

$$\mathcal{O}' \equiv R(\theta)\mathcal{O}$$

$$R(\theta) \equiv \frac{\det \mathcal{M}(\theta)}{\det \mathcal{M}_{\mathrm{ref}}(\theta)}$$: Reweighting factor

Average reweighting factor

The expectation value of $R(\theta)$ in the reference theory

$$\langle R(\theta) \rangle = \frac{Z}{Z_{\mathrm{ref}}}$$

J. O. Andersen, L. T. Kyllingstad, and K. Splittroff, J. High Energy Phys. **01**, 055 (2010).

Average reweighting factor in the NJL model

Saddle point approximation

$$\langle R(\theta)\rangle \approx \sqrt{\frac{\det H_{\mathrm{ref}}}{\det H}}\, e^{-\beta V(\Omega-\Omega_{\mathrm{ref}})}$$

Hessian matrix

$$H_{ij} = \frac{\partial^2 \Omega}{\partial \phi_i' \partial \phi_j'} \qquad \{\phi_i'\} \equiv \{\sigma', \eta', a_i', \pi_i'\}$$

Ω: Thermodynamic potential

Volume size

For the $N_x^3 \times N_\tau$ lattice,

$$\beta V = \left(\frac{N_x}{N_\tau}\right)^3 \frac{1}{T^4} \qquad N_x/N_\tau = 4$$

Reference theories

$$\mathcal{L} = \bar{q}'(\gamma_\nu D_\nu + m(\theta))q' - G_+[(\bar{q}'q')^2 + (\bar{q}'i\gamma_5\vec{\tau}q')^2] - G_-[(\bar{q}'\vec{\tau}q')^2 + (\bar{q}'i\gamma_5 q')^2] + \mathcal{U}$$

Original theory

$$m(\theta) = m_0\cos(\theta/2) + m_0 i\gamma_5\sin(\theta/2)$$

Reference theory A

$$m(\theta) \to m_0\cos(\theta/2)$$

$\mathrm{O}(m_0^2)$ and P-even correction

Reference theory B, C

$$m(\theta) \to m_0\cos(\theta/2) + \frac{1}{\alpha}\{m_0\sin(\theta/2)\}^2$$

α is a parameter with mass dimension.

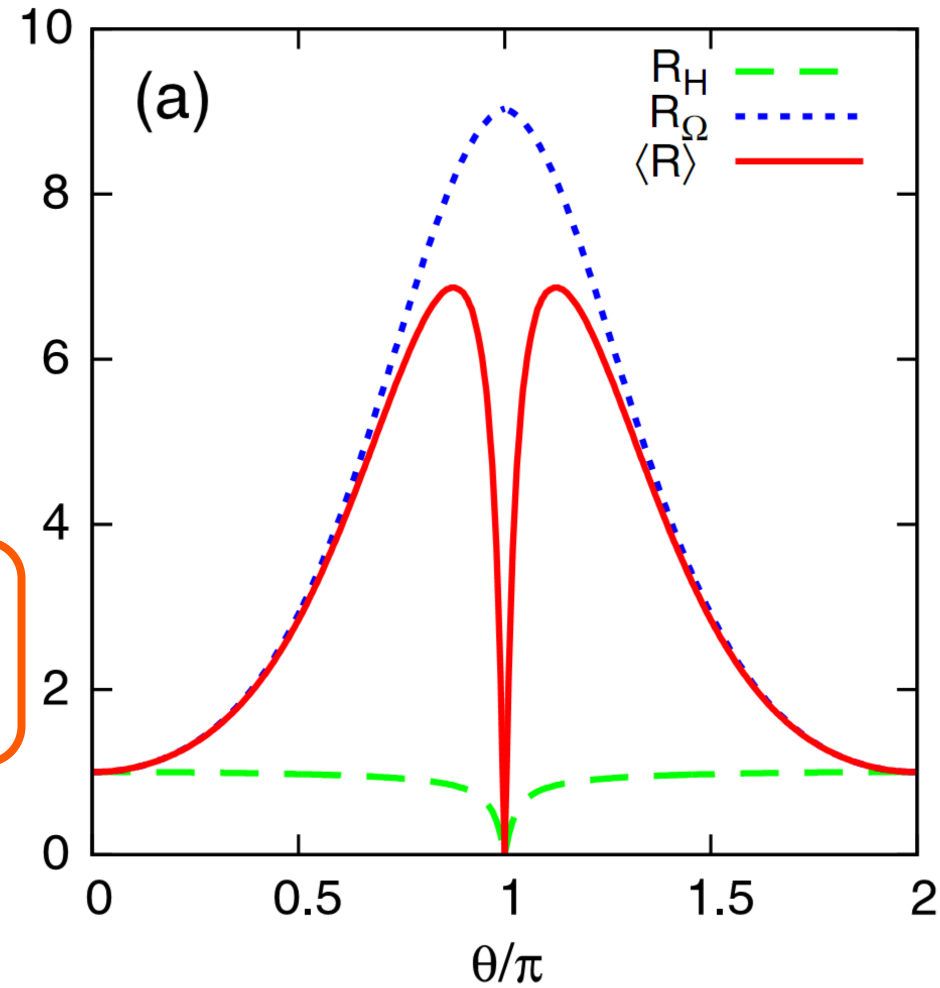
Reference A

$$m_{\mathrm{A}} = m_0 \cos(\theta/2)$$

$$\langle R(\theta) \rangle = R_{\mathrm{A}} R_{\mathrm{B}}$$

$$R_{\mathrm{A}} = \sqrt{\frac{\det H_{\mathrm{ref}}}{\det H}}$$

$$R_{\mathrm{B}} = e^{-\beta V(\Omega - \Omega_{\mathrm{ref}})}$$



The amplitude is large.
$\langle R(\theta) \rangle$ becomes 0 at $\theta = \pi$.

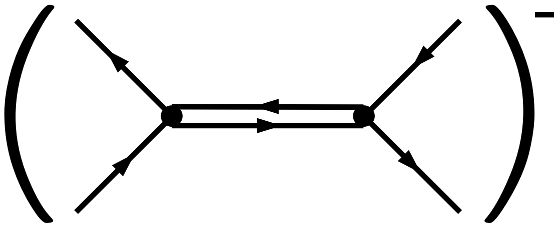
<u>Safety region</u>

$$0.5 \lesssim \langle R(\theta) \rangle \lesssim 2 \Longleftrightarrow |\theta| \lesssim 1.2$$

"Pion" mass

$$m_{\mathrm{A}} = m_0 \cos(\theta/2)$$

$\tilde{M}_\pi$ is the lowest pole mass in the isovector channel.

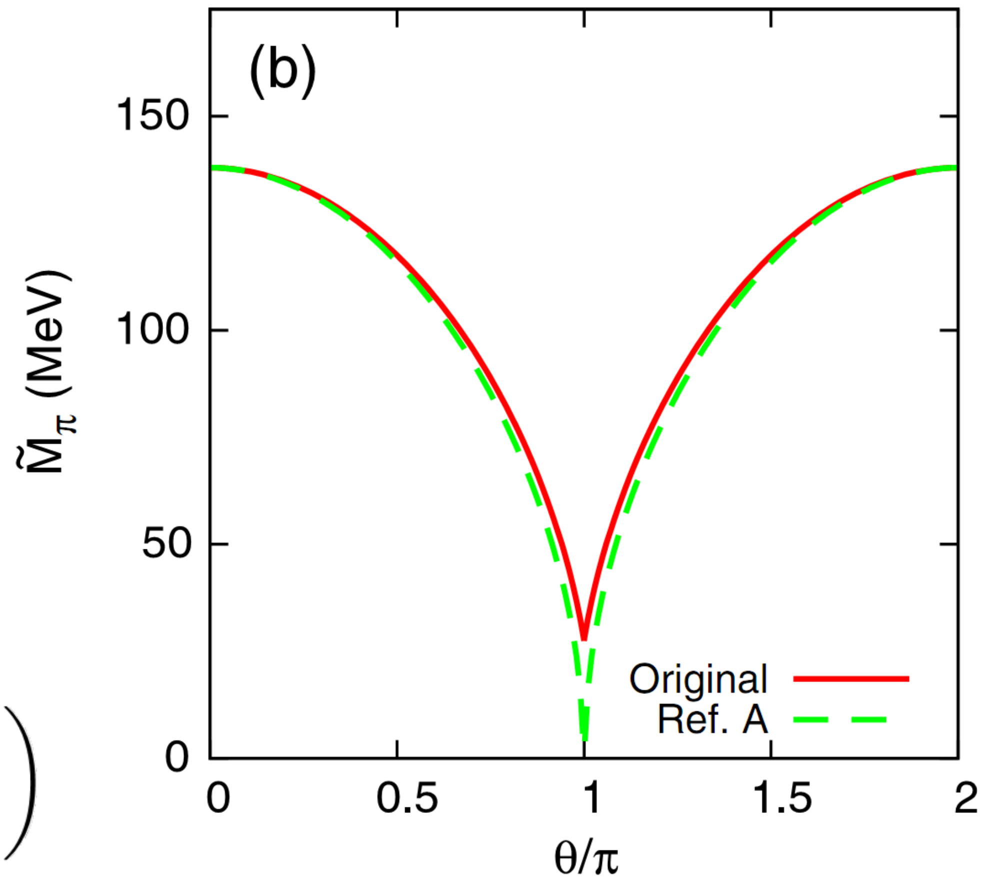


$$(\ \cdots\ )^{-1} = 0$$

$$\det[1 - 2G\Pi(\tilde{M}_\pi^2)] = 0$$

$$G = \begin{pmatrix} G_1 - G_2 & 0 \\ 0 & G_1 + G_2 \end{pmatrix}$$

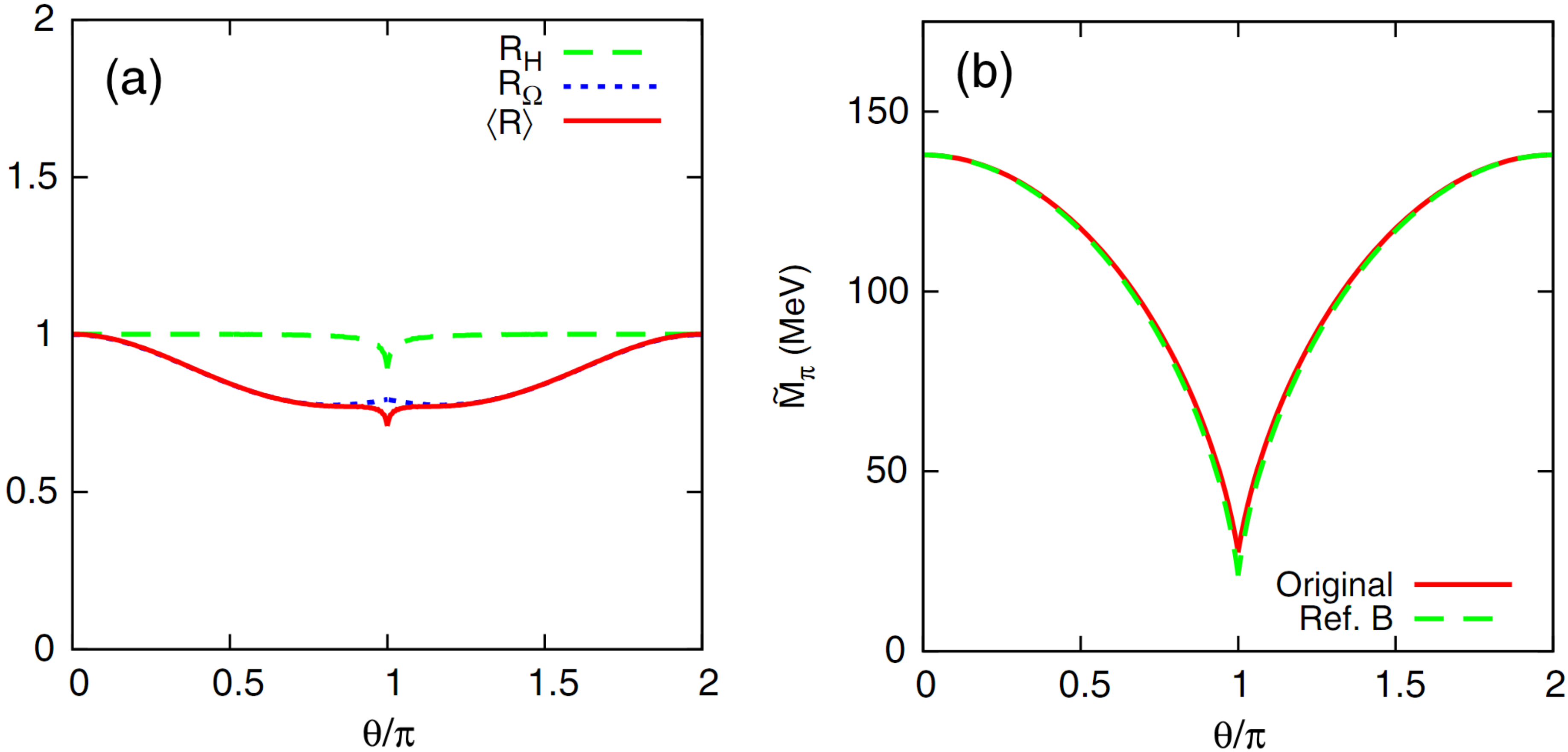
$$\Pi(q^2) = \begin{pmatrix} \Pi^{\mathrm{SS}}(q^2) & \Pi^{\mathrm{SP}}(q^2) \\ \Pi^{\mathrm{PS}}(q^2) & \Pi^{\mathrm{PP}}(q^2) \end{pmatrix}$$



In the reference A, $\tilde{M}_\pi = 0$ at $\theta = \pi$.
(corresponds to the chiral limit)

Reference B

$$m_{\mathrm{B}} = m_0 \cos(\theta/2) + \frac{1}{\alpha}\{m_0 \sin(\theta/2)\}^2 \;, \quad \alpha = M_\pi$$



The ref. B well reproduces $\tilde{M}_\pi(\theta)$ of the original system.
However $\langle R(\theta) \rangle$ is a little bit small.

Reference C

From the chiral Lagrangian with $\mathrm{O}(m_0^2)$ term [1]

$$\begin{cases} \tilde{M}_\pi^2(\theta) = \dfrac{m_0|\sigma_0|}{f_\pi^2}|\cos(\theta/2)| + \dfrac{2l_7 m_0^2 \sigma_0^2}{f_\pi^6}\sin^2(\theta/2) \\ l_7 \approx \dfrac{f_\pi^2}{2M_{\eta'}^2} \quad \text{(Large } \mathrm{N_c} \text{ estimation [2])} \end{cases}$$

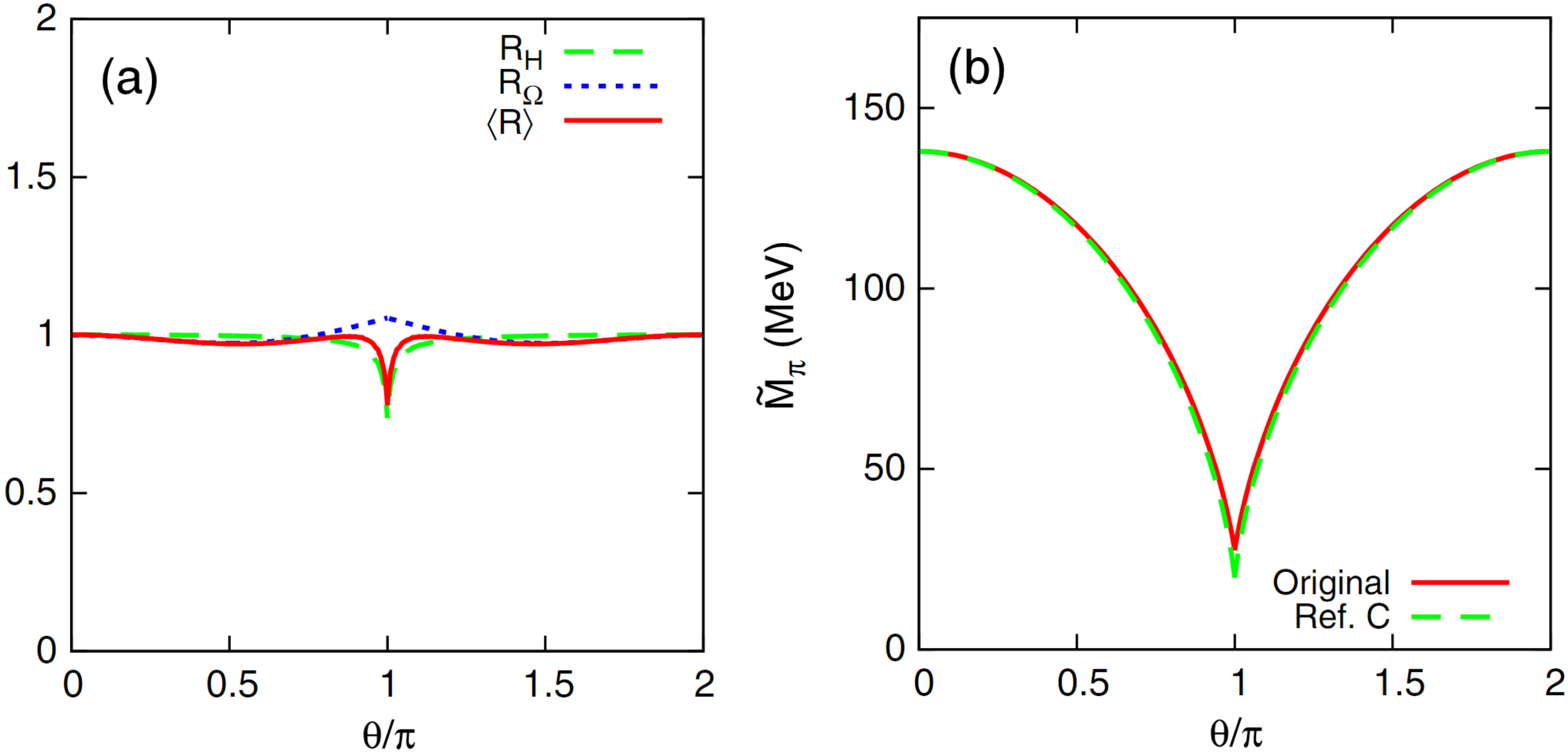
$$\tilde{M}_\pi^2(\theta) = \frac{|\sigma_0|}{f_\pi^2} \underbrace{\left[m_0|\cos(\theta/2)| + \frac{m_0 M_\pi^2}{M_{\eta'}^2}\sin^2(\theta/2) \right]}_{\text{Interpret as } m(\theta)}$$

$$m_C(\theta) = m_0\cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2}\sin^2(\theta/2)$$

[1] M.A. Metlitski and A.R. Zhitnitsky, Phys. Lett. B **633**, 721 (2006).
[2] A. V. Smilga, Phys. Rev. D **59**, 114021 (1999).

Reference C

$$m_{\mathrm{C}}(\theta) = m_0 \cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2} \sin^2(\theta/2)$$



- In the ref. C, $\tilde{M}_\pi(\theta)$ is a little bit smaller than that in the original system.
- $\langle R(\theta) \rangle$ is almost 1 for all theta.

Meson fluctuation

$$m(\theta) = m_0 \cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2} \sin^2(\theta/2)$$

$$\langle R(\theta) \rangle \approx \sqrt{\frac{\det H_{\mathrm{ref}}}{\det H}} e^{-\beta V(\Omega - \Omega_{\mathrm{ref}})}$$

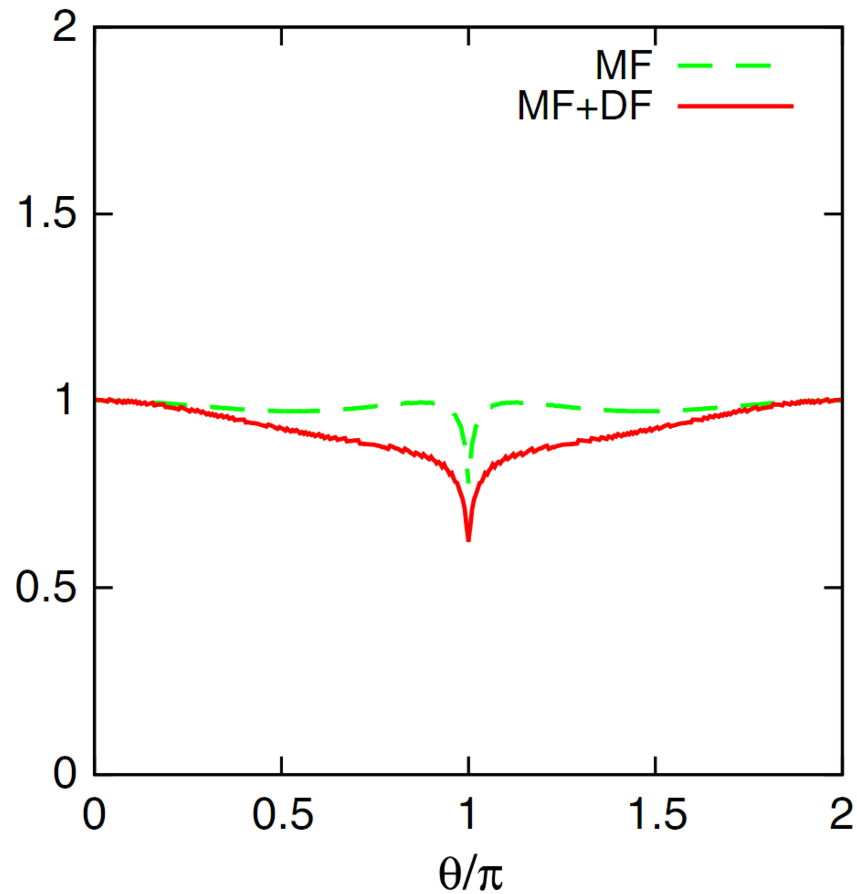
Meson fluctuation is included with free gas approximation.

$$\Omega = \Omega_{\mathrm{MF}} + \Omega_{\mathrm{DF}}$$

$$\Omega_{\mathrm{DF}} = 3 \int \frac{d^3 p}{(2\pi)^3} T \ln\left(1 - e^{-\beta E_\pi}\right)$$

$$E_\pi = \sqrt{\vec{p}^2 + \tilde{M}_\pi^2},$$

Average reweighting factor



Although $\langle R(\theta) \rangle$ decreases by the fluctuation, the effect is not serious.

Summary

We have evaluated the average reweighting factor
for finite theta-vacuum angle with the 2 flavor PNJL model.

The effect of pion fluctuation is not serious for the estimation.

Our best reference theory

$$m(\theta) = m_0 \cos(\theta/2) + m_0 i\gamma_5 \sin(\theta/2)$$

$$\Rightarrow \quad m_{\mathrm{C}}(\theta) = m_0 \cos(\theta/2) + \frac{m_0 M_\pi^2}{M_{\eta'}^2} \sin^2(\theta/2)$$