O($\alpha^2$) cutoff effects in Wilson fermion simulations

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I will discuss $O(a^2)$ lattice artifacts affecting physical observables when quarks are regularized as Wilson fermions.

I will be dealing with
- Maximally twisted fermions, either clover or not
- Standard Wilson fermion, either clover or not

Ideas of this kind have been put forward
- in $\chi$PT $\rightarrow$ Scorzato - Sharpe and Wu
- in the present context $\rightarrow$ Frezzotti @ Ringberg Castle
Outline of the talk

- Symanzik expansion
  - Symanzik LEL
  - Critical mass

- Pion mass and $O(a^2)$ effects in Mtm-LQCD
  - Neutral pion
  - Charged pion

- Pion mass and $O(a^2)$ effects with standard Wilson fermions
  - $M_{ct}$ from the vanishing of $m_{PCAC}|_L$
  - Using the optimal critical mass from Mtm-LQCD
Overview: Symanzik low energy Lagrangian - I

- Most general Wilson LQCD action

\[ S_L = S_{YM}^L + \bar{\chi} \left[ \gamma \cdot \vec{\nabla} - \frac{a}{2} \nabla^* \nabla + ic_{SW} \frac{a}{4} \sigma \cdot F + m_0 + \mu i \gamma_5 \tau_3 \right] \chi \]

- Symanzik LEL

\[ L_{\text{Sym}} = L_4 + \delta L_{\text{Sym}}, \quad \delta L_{\text{Sym}} = a L_5 + a^2 L_6 + O(a^3) \]

  - \( O(a^0) \)

\[ L_4 = L_{YM}^L + \bar{\chi} [D + m + i \gamma_5 \tau_3] \chi \]

  - \( O(a) \)

\[ L_5 = b_5 \bar{\chi} i \sigma \cdot F \chi + \delta_1 \bar{\chi} \chi + O(m, \mu) \]

  - \( O(a^2) \)

\[ L_6 = \sum_{i=1}^{3} b_6;i \Phi_{6;i}^{\text{glue}} + b_{6;4} \bar{\chi} \gamma_{\mu} (D_{\mu})^3 \chi + \sum_{i=5}^{14} b_6;i \Phi_{6;i} + \delta_2 \bar{\chi} \chi + O(m, \mu) \]

- \( \delta_{2p+1} \propto \Lambda_{\text{QCD}}^{2p+2}, p = 0, 1, ... \)

\( O(a^2) \) cutoff effects in Wilson fermion simulations
Overview: Symanzik low energy Lagrangian - II

- Four-quark operators in $L_6$
  
  $\Phi_{6;5} = (\bar{\chi}\chi)(\bar{\chi}\chi)$,
  $\Phi_{6;7} = - (\bar{\chi}\gamma_5\chi)(\bar{\chi}\gamma_5\chi)$,
  $\Phi_{6;9} = (\bar{\chi}\gamma_\lambda\chi)(\bar{\chi}\gamma_\lambda\chi)$,
  $\Phi_{6;11} = (\bar{\chi}\gamma_\gamma\gamma_5\chi)(\bar{\chi}\gamma_\gamma\gamma_5\chi)$,
  $\Phi_{6;13} = (\bar{\chi}\sigma_{\lambda\nu}\chi)(\bar{\chi}\sigma_{\lambda\nu}\chi)$,
  $\Phi_{6;6} = (\bar{\chi}\tau^b\chi)(\bar{\chi}\tau^b\chi)$,
  $\Phi_{6;8} = - (\bar{\chi}\gamma_5\tau^b\chi)(\bar{\chi}\gamma_5\tau^b\chi)$,
  $\Phi_{6;10} = (\bar{\chi}\gamma_\lambda\tau^b\chi)(\bar{\chi}\gamma_\lambda\tau^b\chi)$,
  $\Phi_{6;12} = (\bar{\chi}\gamma_\gamma\gamma_5\tau^b\chi)(\bar{\chi}\gamma_\gamma\gamma_5\tau^b\chi)$,
  $\Phi_{6;14} = (\bar{\chi}\sigma_{\lambda\nu}\tau^b\chi)(\bar{\chi}\sigma_{\lambda\nu}\tau^b\chi)$.

- Maximally twisted fermions
  
  $\mu = O(a^0)$, $m_0 = M_{cr} \to m = 0$ in $L_4$

  Physical basis $\to \chi = \exp(-i\frac{\pi}{4}\gamma_5\tau^3)\psi$, $\bar{\chi} = \bar{\psi}\exp(-i\frac{\pi}{4}\gamma_5\tau^3)$

- Standard Wilson fermions
  
  $\mu = 0$, $m_0 = M_{cr} + m \to m$ in $L_4$

$O(a^2)$ cutoff effects in Wilson fermion simulations
Overview: determining the critical mass

- In twisted mass LQCD fix $m_0$ (at decreasing $\mu$) such that FMPR

$$\alpha^3 \sum_{\vec{x}} \left< (\bar{\psi}_0 \tau^2 \psi)(\vec{x}, t)(\bar{\psi}_5 \tau^1 \psi)(0) \right>_L = 0$$

- $O(\alpha^{-1}) \implies m = 0 \text{ in } L_4 \rightarrow$ restoration of parity and flavour sym's

$$\left. \int d^3 x \left< (\bar{\psi}_0 \tau^2 \psi)(\vec{x}, t)(\bar{\psi}_5 \tau^1 \psi)(0) \right> \right|_{\text{cont}} = 0$$

- $O(\alpha) \implies \xi_\pi \equiv \langle \Omega | L_5^{\text{Mtm}} | \pi^3(\vec{0}) \rangle \bigg|_{\text{cont}} = O(\mu)$

$$\left. \int d^3 x \int d^4 y \langle [b_{5;SW} \bar{\psi}_5 \tau^3 \sigma \cdot F \psi + \delta_1 \bar{\psi}_i \gamma_5 \tau^3 \psi](y) V_0^2(x) P^1(0) \rangle \right|_{\text{cont}} = 0$$

- $O(\alpha^2) \implies \delta_2 = 0$

$$\left. \int d^3 x \int d^4 y \langle \mathcal{L}_6^{\text{even}} + \delta_2 \bar{\psi}_i \gamma_5 \tau^3 \psi + O(\mu) \rangle \bigg|_{\text{cont}} = 0$$

- $O(\alpha^2)$ cutoff effects in Wilson fermion simulations

- and so on, for any even ($\delta_{2p} = 0$) and odd ($\delta_{2p+1}$ fixed) power of $\alpha$

- the latter described by $\alpha^{2p+1} \delta_{2p+1} \bar{\psi}_i \gamma_5 \tau^3 \psi$ in $L_{2p+1}$.
In standard Wilson fermions fix \( m_0 \) (at \( \mu \equiv 0 \)) such that

\[
\frac{\sum_{\vec{x}} \delta_\mu \langle A^b_\mu(\vec{x}, t)P^b(0) \rangle}{2 \sum_{\vec{x}} \langle P^b(\vec{x}, t)P^b(0) \rangle} \bigg|_L = m_{PCAC} \bigg|_L = 0 \quad b = 1, 2, 3
\]

- Actual estimates, \( M_{cr}^{\theta_W} \), affected by lattice artifacts of any order in \( a \).
- Described in the Symanzik LEL by \( a^k \delta_k \bar{\chi}\chi \), \( k = 1, 2, ... \) \( (\delta_k \propto \Lambda_{QCD}^{k+1}) \)
- For clover improved Wilson fermions the term with \( k = 1 \) is missing.
Pion mass in Mtm-LQCD

- At $p = 0$ and in the limit of small lattice neutral pion mass, consider

$$\Gamma_L(p) = \alpha^4 \sum_x e^{ipx} \langle P^3(x)P^3(0) \rangle \bigg|_L$$

$$\Gamma_L(0) \rightarrow \left| \frac{G_{\pi^3}}{m_{\pi^3}^2} \right|^2 \bigg|_L, \quad G_{\pi^3} \bigg|_L = \langle \Omega | P^3 | \pi^3(0) \rangle \bigg|_L$$

- Symanzik expansion of $\Gamma_L(0)$, up to orders $\alpha^2$ included

$$\Gamma_L(0) = \alpha^4 \sum_x \langle P^3(x)P^3(0) \rangle \bigg|_L = \int d^4x \langle P^3(x)P^3(0) \rangle \bigg|_{\text{cont}} +$$

$$+ \alpha^2 \int d^4x \langle \Delta_1 P^3(x) \Delta_1 P^3(0) \rangle \bigg|_{\text{cont}} + \alpha^2 \int d^4x \langle \Delta_1 P^3(x)P^3(0) \int d^4y L_5^{\text{Mtm}}(y) \rangle \bigg|_{\text{cont}} +$$

$$+ \alpha^2 \int d^4x \langle P^3(x) \Delta_1 P^3(0) \int d^4y L_5^{\text{Mtm}}(y) \rangle \bigg|_{\text{cont}} +$$

$$+ \frac{\alpha^2}{2} \int d^4x \langle P^3(x)P^3(0) \int d^4y L_5^{\text{Mtm}}(y) \int d^4y' L_5^{\text{Mtm}}(y') \rangle \bigg|_{\text{cont}} +$$

$$- \alpha^2 \int d^4x \langle \Delta_2 P^3(x)P^3(0) \rangle \bigg|_{\text{cont}} - \alpha^2 \int d^4x \langle P^3(x) \Delta_2 P^3(0) \rangle \bigg|_{\text{cont}} +$$

$$- \alpha^2 \int d^4x \langle P^3(x)P^3(0) \int d^4y L_6^{\text{Mtm}}(y) \rangle \bigg|_{\text{cont}} + O(\alpha^4) + \ldots$$
• Comments

  Maximal twist → only odd powers of $a$

  We look for corrections to the pion mass → double pole terms $(1/m^2_\pi)^2$

  Optimal critical mass ($\xi_\pi/m^2_\pi = O(1)$) → no contributions from $L^5_{\text{Mtm}}$

  Only the last term is relevant

• Result

\[
\left| \frac{G_{\pi^3}}{m^2_{\pi^3}} \right|_{L} = \left| \frac{G_{\pi}}{m^2_{\pi}} \right|_{\text{cont}} \left( 1 - a^2 \frac{\langle \pi^3(\vec{0})|L^6_{\text{Mtm}}|\pi^3(\vec{0}) \rangle}{m^2_{\pi}} \right)_{\text{cont}} + O\left( \frac{a^2}{m^2_{\pi}} \right)
\]

from which a simple Taylor expansion in $a^2$ yields the key formula

\[
m^2_{\pi^3}\bigg|_{L} = m^2_{\pi} + a^2 \zeta_\pi + O(a^2 m^2_{\pi}, a^4),
\]

\[
\zeta_\pi \equiv \langle \pi^3(\vec{0})|L^6_{\text{Mtm}}|\pi^3(\vec{0}) \rangle_{\text{cont}}
\]

• We would like to estimate the order of magnitude of $\zeta_\pi$

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Consider chiral non-invariant 4-fermion operators in $\mathcal{L}_6^{\text{Mtm}}$

having non-vanishing m.e.'s between $\pi^3$ states in the chiral limit

giving a non-zero contribution in the vacuum saturation (VS) approximation

Typical example is

$$O_{P3P3} = -P^3P^3 = -(\bar{\psi}\gamma_5\tau^3\psi)(\bar{\psi}\gamma_5\tau^3\psi) \quad (1)$$

In the massless limit, chiral symmetry implies the equality

$$\langle \pi^3(\vec{0})| - O_{P3P3}|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}} = \langle \pi^3(\vec{0})|O_{SS}|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}}$$

In fact, from Soft Pion Theorem's ($f_\pi \simeq 131$ MeV)

$$\langle \pi^3(\vec{0})| - O_{P3P3}|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}} = \frac{2i}{f_\pi} \langle \Omega|[Q^3_A, -O_{P3P3}]|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}} + O(m^2_\pi) \,,$$

$$\langle \pi^3(\vec{0})|O_{SS}|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}} = \frac{2i}{f_\pi} \langle \Omega|[Q^3_A, O_{SS}]|\pi^3(\vec{0})\rangle \bigg|_{\text{cont}} + O(m^2_\pi)$$

and an explicit evaluation of the commutators, eq. (??) follows.
In the VS approximation (recall $L_6^{\text{Mtm}} \sim P^3 P^3 + \ldots$)

$$\alpha^2 \zeta_\pi \sim \alpha^2 |\hat{G}_\pi|^2, \quad \hat{G}_\pi = \langle \Omega | \hat{P}^3 | \pi^3 (\vec{0}) \rangle \bigg|_{\text{cont}}$$

Two numerical estimates of the continuum quantity $\hat{G}_\pi$

- A direct lattice measurement at $\beta = 3.9, m_{\pi^\pm} |_L \sim 310 \, \text{MeV}$ yields

$$\alpha^2 \hat{G}_\pi \sim 0.06 \quad [Z_P \sim 0.39(1) \text{ has been used}]$$

- From the continuum WTI

$$2\hat{m}_q \langle \Omega | \hat{P}^3 | \pi^3 \rangle \bigg|_{\text{cont}} = f_\pi m^2_\pi + O(m_\pi^4),$$

one obtains

$$\hat{G}_\pi = \frac{f_\pi m^2_\pi}{2\hat{m}_q} \sim (570 \, \text{MeV})^2 \quad [\hat{m}_q \sim 4 \, \text{MeV} \text{ has been used from PDB}]$$

Inserting the ETMC value $\alpha^{-1} \sim 2.3 \, \text{GeV}$, the two estimates turn out to be numerically well consistent.
• For the \textit{charged} pions one similarly obtains

\[
m^2_{\pi^\pm} \bigg|_L = m^2_{\pi^\pm} + \alpha^2 \langle \pi^\pm (0) | \mathcal{L}_0^{\text{Mtm}} | \pi^\pm (0) \rangle \bigg|_\text{cont} + O(\alpha^2 m^2_{\pi}, \alpha^4)
\]

• From the invariance under the “oblique” group $\text{SU}(2)_{\text{ob}} = (Q^3_V, Q^+_A, Q^-_A)$

\[
[Q^\pm_A, \mathcal{L}^{\text{Mtm}}_{\text{Sym}}] = O(\mu) = O(m^2_{\pi}),
\]

one gets the SPT

\[
\langle \pi^\pm (0) | \mathcal{L}_0^{\text{Mtm}} | \pi^\pm (0) \rangle \bigg|_\text{cont} = \frac{2i}{f_{\pi}} \langle \Omega |[Q^\pm_A, \mathcal{L}_0^{\text{Mtm}}] | \pi^\pm (0) \rangle \bigg|_\text{cont} + O(m^2_{\pi}) = O(m^2_{\pi})
\]

• Hence

\[
m^2_{\pi^\pm} \bigg|_L = m^2_{\pi} + O(\alpha^2 m^2_{\pi}, \alpha^4)
\]

\[
\Delta m^2_{\pi} \bigg|^{\text{Mtm}}_L = m^2_{\pi^3} \bigg|_L - m^2_{\pi^\pm} \bigg|_L = \alpha^2 \zeta_{\pi} \sim \alpha^2 (570 \text{ MeV})^4 \sim (140 \text{ MeV})^2 (\alpha^{-1} \sim 2.3 \text{ GeV})
\]

\[
\Delta m^2_{\pi} \bigg|^{\text{Mtm}}_L = (180(40) \text{ Mev})^2 \text{ ETMC measured value}
\]
Consider correlators in Fourier space

There will be corrections to pole locations and residues

- **Pole locations** ↔ hadron square masses
  The relevant matrix element is $\alpha^2 \langle h | \mathcal{L}_6^{\text{Mtm}} | h \rangle |_{\text{cont}}$

- **Residues**
  - **Operators**: $\alpha^2 \mathcal{L}_6^{\text{Mtm}}$ can only correct 4-dimensional operators with (lattice) vacuum quantum numbers. These are the operators in $\mathcal{L}_4$, which anyway mix with the identity.
  - **On-shell states**: there can be (kinematically suppressed) contaminations to $|\Omega\rangle$ and $|n\pi\rangle$ states

Lin, Martinelli, Sachrajda and Testa

$$\zeta_\pi = \langle \pi^3(\vec{0}) | \mathcal{L}_6^{\text{Mtm}} | \pi^3(\vec{0}) \rangle |_{\text{cont}}$$ (practically) only matters in $m_{\pi^3}$

\[O(\alpha^2)\] cutoff effects in Wilson fermion simulations
With standard Wilson fermions one similarly gets for the pion mass

\[ m^2_{\pi} \bigg|_L = m^2_{\pi} + \alpha^2 \langle \pi(0) | L^\text{cl}_0 | \pi(0) \rangle \bigg|_{\text{cont}} + O(\alpha^2 m^2_{\pi}, \alpha^4), \]

\[ L^\text{cl}_0 = L^\text{P-even}_0 + \delta_2 \bar{\chi} \chi, \quad \delta_2 \propto \Lambda^3_{\text{QCD}} \]

Assume \( O(a) \) Symanzik improvement for easier comparison to Mtm-LQCD

Magnitude of \( L^\text{cl}_0 \) coefficients depends on how critical mass is determined

Typically one can

1. set \( m_{\text{PCAC}} \big|_L = 0 \rightarrow M_{\text{cr}}^\text{W} \)

\[ \frac{\sum \bar{x} \tilde{\delta}_\mu \langle A^b_\mu(\bar{x}, t) P^b(0) \rangle}{2 \sum \bar{x} \langle P^b(\bar{x}, t) P^b(0) \rangle} \bigg|_L = m_{\text{PCAC}} \bigg|_L, \quad b = 1, 2, 3 \]  \hspace{1cm} (2)

2. take the critical mass from Mtm-LQCD simulations \( \rightarrow M_{\text{cr}}^{\text{opt}} \)

\( O(\alpha^2) \) cutoff effects in Wilson fermion simulations
Taking the limit $t \to \infty$ of (2), one gets the lattice formula

$$m_{\pi}^2 \frac{f_\pi}{2|G_\pi|} \bigg|_L = m_{\text{PCAC}} \bigg|_L$$

- $m_{\pi}^2 |_L$ and $m_{\text{PCAC}} |_L$ are proportional
- are affected by the same (additive $O(a^2)$) cutoff effects

I) Critical mass from $m_{\text{PCAC}} |_L = 0 \to M_{\text{cr}}^W$ (generically all powers of $a$)

- $O(a^{-1}) \to m = 0$ in $\mathcal{L}_4$
- $O(a) \to$ clover term, no condition
- $O(a^2) \to \langle \pi(\vec{0})|\mathcal{L}_6^{cl}\pi(\vec{0}) \rangle_{\text{cont}} = \langle \pi(\vec{0})|\mathcal{L}_6^{P-\text{even}} + \delta_2 \bar{\chi}\chi|\pi(\vec{0}) \rangle_{\text{cont}} = 0$

II) Critical mass from Mtm-LQCD $\to M_{\text{cr}}^{\text{opt}}$ (only odd powers of $a$)

- $O(a^{-1}) \to m = 0$ in $\mathcal{L}_4$
- $O(a) \to$ clover term, no condition
- $O(a^2) \to$ No (need for an) $a^2 \delta_2 \bar{\chi}\chi$ term $\to \mathcal{L}_6^{\text{cl}} = \mathcal{L}_6^{P-\text{even}}$

$O(a^2)$ cutoff effects in Wilson fermion simulations
Summary of the standard Wilson fermion case

- Typical alternatives as for the choice of the critical mass are
  - $M_{cr}^{\text{EW}}$
    - No $O(\alpha^2)$ effects in $m^2_\pi$, as $\langle \pi(\vec{0}) | \mathcal{L}^\text{P-even}_6 + \delta_2 \bar{\chi}\chi | \pi(\vec{0}) \rangle |_{\text{cont}} = 0$
    - $\delta_2 \neq 0$ and possibly large
    - It yields, e.g. an $\alpha^2 \delta_2 \langle h | \bar{\chi}\chi | h \rangle$ contribution to $m^2_h$
  - $M_{cr}^{\text{opt}}$
    - $m^2_\pi |_L = m^2_\pi - \alpha^2 \zeta_\pi + O(\alpha^2 m^2_\pi, \alpha^4)$
    - $\delta_2 = 0$
  - such $O(\alpha^2)$ effects are absent, e.g. in hadronic masses

Observations

- $\zeta_\pi = \langle \pi(\vec{0}) | \mathcal{L}^\text{P-even}_6 | \pi(\vec{0}) \rangle |_{\text{cont}} = -\langle \pi^3(\vec{0}) | \mathcal{L}^\text{Mtm}_6 | \pi^3(\vec{0}) \rangle |_{\text{cont}}$ (with clover term)
- Since $\langle O \int \bar{\chi}\chi \rangle |_{\text{cont}} \propto \frac{\partial \langle O \rangle |_{\text{cont}}}{\partial m}$, above $O(\alpha^2)$ effects negligible,
  - if $m$ dependence of $\langle O \rangle |_{\text{cont}}$ is weak
Conclusions

- Origin of large $O(a^2)$ lattice artifacts has been identified
- In Mtm-LQCD they only affect $m^2_{\pi}$
- With standard Wilson fermions where they appear depends on how $M_{cr}$ is determined
- For OS fermions situation is similar to Mtm-LQCD
  - pseudo scalar mass tuning is crucial for WME kinematics
  - finding a cure...work in progress
Thank you for your attention
O(\(a^2\)) cutoff effects in Wilson fermion simulations
An apparent paradox

- Two equivalent conditions - The only difference is the value of $\mu$
- Why lattice artifacts look different?

\[
\alpha^2 \langle A_0^1 P^1 L_6^{Mtm} \rangle \Bigg|_{\text{cont}} \begin{cases} 
= 0 & \text{for } m = 0, \mu > 0 \quad [P\text{-parity } \leftarrow \mathcal{L}_4] \\
\neq 0 & \text{for } m > 0, \mu = 0 \quad [\text{No } R_5 \leftarrow S\chi\text{SB}] 
\end{cases}
\]

A simple model for this behaviour

\[
\alpha^2 \langle A_0^1 P^1 L_6^{Mtm} \rangle \Bigg|_{\text{cont}} \propto \tgh \frac{m}{\sqrt{\lambda_{\text{min}}^2 + \mu^2}}
\]

- At $m > 0, \mu = 0$ one is sensitive to the underlying $S\chi\text{SB}$