Flavor Twisted Boundary Conditions on the Lattices

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Outline

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  - Lattice QCD and systematic errors.
- The issue of quantized momenta on finite volume due to the periodic boundary conditions.
  - The limitation of extracting the nucleon magnetic moment on the lattices.
- Twisted boundary conditions on the lattices.
  - The ability to induce continuous momentum transfer.
  - Finite volume effects: pion EM form factors and nucleon isovector form factors.
- Conclusions.
Introduction

Quantum Chromodynamics (QCD) is believed to be the correct theory for strong interaction.

QCD has been successful in understanding the hadronic physics in many strong interaction experiments.

Asymptotic Freedom (due to gluons self-interaction)

\[ \alpha_s(q^2) = \frac{12\pi}{(11N_C - 2N_f) \ln\left(\frac{q^2}{\Lambda^2}\right)} , \quad q^2 \gg \Lambda^2. \]

\( \alpha_s(q^2) \) becomes small at short-range. \( \Rightarrow \) Perturbative techniques.

\( \alpha_s \sim 1 \) at long-range. \( \Rightarrow \) To study the low energy regime of QCD, a non-perturbative approach is required.
The only known first principles non-perturbative approach to QCD is the lattice QCD.

Lattice QCD has made dramatic progress in understanding the non-perturbative regime of QCD.

- The increasing computing resource and power.
- The development of numerical algorithms.

Unphysically large quark masses, finite extent of box size and non-vanishing lattice spacing.

It is important to quantify the systematic errors arising in lattice calculations due to above technique difficulties.

To connect the lattice QCD results with the real world ⇒ using Chiral Perturbation Theory (χPT) to extrapolate the lattice data to the physical point.
Today, the use of lattice data in conjunction with $\chi$PT enables us to study the hadronic physics quantitatively from first principles calculations.

In the foreseeable future, the combination of lattice QCD and $\chi$PT can even make first principles predictions.
Quantized Momentum on the Lattices

- A further limitation encountered in lattice simulation: the available momentum modes.

- With periodic boundary conditions, the momentum modes are quantized.

- For a lattice with uniform spatial size $L$, the quantized momentum modes: $2\pi n/L$, where $n$ is a triplet of integers.

- $\chi$PT can be used to investigate the momentum behavior of certain observables:
  - Pion electromagnetic form factors.
  - Nucleon isovector form factors and axial form factors.

- For current dynamical lattices, the lowest non-zero momentum mode: $450\text{ MeV} \sim 500\text{ MeV}$.

- Within the applicability of $\chi$PT?
The nucleon magnetic moment can be calculated from the nucleon magnetic form factor by extrapolating the lattice data of this form factor to zero momentum transfer.

\[ F_2(q^2) = G^p_M(q^2) - G^n_M(q^2) = \mu_I + f(q^2/4m^2_\pi). \]

In particular, for small momentum transfer \( q^2 \ll m^2_\pi \): \( F_2(q^2) \) is linear in \( q^2 \).

To determine the range where the extrapolation is reliable → Deviation from linearity: \( \Delta F_2(q^2) = \frac{F_2(q^2) - F_2(0)}{q^2 F_2(0)} \).
For current lattices: $5\% \sim 10\%$ corrections to the linearity for $q^2 < 0.15\text{GeV}^2$.

Recoil correction: $q^2/M^2 \sim 20\%$ contributes to the deviation from linearity.

Therefore, the lowest available momentum mode $q \sim 450\text{MeV}$ is still away beyond the applicability of $\chi$PT.
In order to reliably extract quantities requiring non-zero momentum transfer such as charge radii and electromagnetic moments:

one must increase the lattice volume and thus generate new gauge configurations → an extremely costly solution!

Another solution: the use of Twisted Boundary Conditions.
Partially Quenched QCD

Quenched Approximation: Ghost quarks

\[
\frac{1}{A_1} + \frac{1}{A_2} = 0
\]

\text{aCourtesy D. Arndt}
Partially quenched theory: Ghost and Sea quarks

Convention: $j \leftrightarrow u$ and $r \leftrightarrow s$.

Partially quenched generalization of $SU(N)$: $SU(N + M|N)$.

\[ \frac{1}{A_1} + \frac{1}{A_2} + \frac{1}{A_3} = \frac{1}{A_4} \]

\(^a\)Courtesy D. Arndt
Lattice Simulations

Physical (Unquenched) Theories

\[ \frac{m_{\text{Valence}}}{m_{\text{Strange}}} \]

\[ \frac{m_{\text{Sea}}}{m_{\text{Strange}}} \]

QCD

PQ Chiral Pert. Theory

\[ m_{\text{Valence}} = m_{\text{Sea}} \]

\[ \frac{m_{\text{Sea}}}{m_{\text{Strange}}} = \frac{1}{4} \]

\[ \frac{m_{\text{Sea}}}{m_{\text{Strange}}} = \frac{1}{2} \]

\[ \frac{m_{\text{Sea}}}{m_{\text{Strange}}} = 1 \]

\[ \frac{m_{\text{Valence}}}{m_{\text{Strange}}} = 1 \]

\[ \text{aCourtesy Ruth Van de Water} \]
Twisted Boundary Conditions on the lattice

Quantized momenta arise on finite volume is due to the use of periodic boundary condition (PBC).

→ defines the theory on a torus and the fields are single valued.

The use of PBC is not mandated. It is sufficient to require that the observables are single valued ⇒ the action itself is single valued on the torus.

\[ \phi(x_i + L) = U_i \phi(x_i) \quad i = 1, 2, 3, \quad U \text{ is the symmetry of the action.} \]

Consider the following Fermionic Euclidean QCD Lagrangian:

\[ \mathcal{L} = \bar{q}(x)(D + M)q(x). \]

\[ q(x_i + L) = U_i q(x_i) = \exp\left(i\theta_i^a T^a\right) q(x_i) = \exp(i\Theta_i) q(x_i) \]

\( T^a \)'s are the generators of the Cartan subalgebra of the flavor group commuting with the quark mass matrix \( M \).

Define new quark fields \( \tilde{q} \) by:

\[ \tilde{q}(x) = \exp\left(-i\frac{\Theta_i}{L} x_i\right) q(x). \]
\( \tilde{q}(x_i) \) is periodic:

\[
\tilde{q}(x_i + L) = \tilde{q}(x_i)
\]

In terms of \( \tilde{q} \), the Lagrangian can be written as:

\[
\mathcal{L} = \tilde{q}(x)(\tilde{D} + M)\tilde{q}(x),
\]

where \( \tilde{D}_\mu = D_\mu + iB_\mu \), \( B_i = \frac{\Theta_i}{L} \) for \( i = 1, 2, 3 \) and \( B_0 = 0 \).

\[
\tilde{S}(x) \equiv \langle \tilde{q}(x) \tilde{q}(0) \rangle = \int \frac{dk_4}{2\pi} \frac{1}{L^3} \sum \frac{e^{ik\cdot x}}{i(k^4 + \beta) + M}.
\]

→ The momentum in the denominator is boosted.
The Effective Lagrangian With TwBC’s.

- Same form of Chiral Lagrangian

- The long-distance physics from TwBC’s can be effectively described by coupling the periodic fields to uniform $U(1)$ gauge field $B_\mu$.

- The mesons and baryons acquire flavor-dependent momentum boost via the external uniform $U(1)$ field $B_\mu$:

$$\tilde{D}_\mu \tilde{\Sigma} \equiv \partial_\mu \tilde{\Sigma} + i [B_\mu, \tilde{\Sigma}],$$

$$\tilde{D}_\mu \tilde{B}^{ijk} = D_\mu \tilde{B}^{ijk} + i (B_\mu^i + B_\mu^j + B_\mu^k) \tilde{B}^{ijk}.$$

- In particular, each flavor of quark receives its own twist angle $\theta_\mu = B_\mu L$. 

Flavor Twisted Boundary Conditions on the Lattices – p.16/41
Dispersion Relation and Isospin Breaking With TwBC

- Since $B_\mu$ is diagonal, $\pi^0$ does not receive any boost.
- Only the charged pions and nucleons will receive momentum boost.
- TwBC introduces a particular direction:
  - The dispersion relations of charged pions as well as the nucleons are no longer hypercubic invariant in the Fourier momentum:
    $$E_{\pi^+} = \sqrt{m_{\pi}^2 + B_{\pi}^2}, \quad B_{\pi^+} = B_u - B_d \rightarrow$$
    twisting flavors differently to get momentum transfer!
    $$E_p = M_p + B_p^2/(2M_p), \quad B_p = 2B_u + B_d \rightarrow B_u \neq -B_d$$
    to induce momentum transfer.
- TwBC modifies the long distance physics at boundary and is flavor dependent:
  - Isospin is broken.
  - The degeneracy among $\pi^\pm$ and $\pi^0$ as well as nucleons are lifted by volume effects.
The isospin splitting between charged and neutral pions is given by

\[ \Delta m^2 = \delta_L \left( m^2_{\pi^\pm} \right) - \delta_L \left( m^2_{\pi^0} \right) = \frac{m^2_{\pi}}{f^2} \left[ \mathcal{I}_{1/2}(0, m^2_{\pi}) - \mathcal{I}_{1/2}(\theta_{\pi^+/L}, m^2_{\pi}) \right] \]

The splitting vanishes when the twist angles preserve isospin, \( \theta_u = \theta_d \).
\[ \theta_{\pi^+} = (\pi, \pi, \pi). \]

- Isospin splitting is less than 1\% for pion masses \( \sim 0.3 \text{GeV} \) in a 2.5fm box.
- For current dynamical lattices, the isospin breaking effect among pions due to the TwBCs is negligible in practice.
The isospin breaking of nucleon is given by

\[
M_n - M_p = -\frac{1}{2f^2} \left( \frac{1}{6} g_{\pi NN}^2 \left[ K(m_{\pi}, B_d, 0) - K(m_{\pi}, B_u, 0) \right] - \frac{2}{9} g_{\Delta N}^2 \left[ K(m_{\pi}, B_d, \Delta) - K(m_{\pi}, B_u, \Delta) \right] \right)
\]

\[
g_{\pi NN}^2 = 8g_A^2 + 4g_A g_1 - g_1^2.
\]

The isospin breaking between neutron and proton due to the TwBCs can be safely ignored in reality.

For current dynamical lattices, the effect of isospin breaking is less than 3\%.
Few Remarks of TwBCs

- Flavor singlet form factor (operator self-contraction): TwBCs are of no avail because the BC chosen for the quarks in the current do not affect the momenta of the external states.

- Flavor non-singlet current (such as flavor changing current) can be accessed at continuous momentum transfer.

- A conceptually clear way to see this is as follows
  - An incoming quark with twist angle $\theta \rightarrow$ an outgoing quark with twist angle $\theta'$: momentum transfer $(\theta - \theta')/L$ will be induced.
  - In the infinite volume limit, the BC is irrelevant and the current thus produces momentum transfer by striking a single quark.

- Rest frame : $\theta = 0$.
- Breit frame : $\theta' = -\theta$. 

Flavor Twisted Boundary Conditions on the Lattices – p.21/41
The usefulness of TwBCs lies on:

- In a partially quenched theory, for the calculations related to the flavor non-singlet currents, one can twist the valence (ghost) quarks and use periodic sea quarks.

- The twist angle $\theta$ can be implemented on the lattices by modifying the links:
  $$U_j(x) \rightarrow U_j(x)e^{i\theta q_j/L}.$$ 

- Since the sea quarks are not twisted, the existing gauge configurations can be post-multiplied by the $U(1)$ gauge potential $\theta/L$ in order to catch the effects from the use of the TwBCs.

- **No need to generate new gauge configurations!**
The pion EM form factor $G_\pi(q^2)$ arises in the charged pion matrix element of EM current $J_\mu^{\text{em}}$

$$\langle \pi^+(p') | J_\mu^{\text{em}} | \pi^+(p) \rangle = (p' + p)_\mu e G_\pi(q^2),$$

with $q = p' - p$.

The charge radius $< r_\pi^2 >$ is defined through

$$< r_\pi^2 > = -6 \frac{d}{dq^2} G_\pi(q^2) \bigg|_{q^2=0}. $$
Finite volume formula for the relevant matrix element:

\[
\langle \pi^+ (p') | J_{4}^{em} | \pi^+ (p) \rangle = i \left( [E_{\pi^+} (p') + E_{\pi^0} (p)] [G_{\pi} (Q^2) + G_{FV}] \\
+ [E_{\pi^+} (p') - E_{\pi^0} (p)] [G_{iso}^{FV} + (p' + B_{\pi^+} + p) \cdot G_{rot}^{FV}] \right),
\]

\[
E_{\pi^0} (p)^2 = p^2 + m_{\pi^0}^2 + \delta_L (m_{\pi^0}^2), \quad B_{\pi^+} = B_u - B_d,
\]

\[
E_{\pi^+} (p)^2 = (p + B_{\pi^+} + K)^2 + m_{\pi}^2 + \delta_L (m_{\pi^+}^2), \quad Q = q + B_{\pi^+}.
\]

- For \( \pi^+ \), the field momentum \( B_{\pi^+} \) receives additive renormalization \( K \).
- \( G_{\pi} (Q^2) \) is the pion EM form factor in the infinite volume limit.
- \( G_{FV} \) is the finite volume modification to \( G_{\pi} \) and remains even without TwBC.
- \( G_{iso}^{FV} \) is due to the isospin breaking arising from TwBC. It vanishes when \( B_u = B_d \).
- \( G_{rot}^{FV} \) arises from the breaking of hypercubic invariance and vanishes only with \( B_u = B_d = 0 \).
To understand the impact of the TwBCs on the extraction of pion charge radius from the lattices data:

- $B^d = 0$ and $B^u = (0, |B|, 0)$, with $|B| = \theta / L$.
- Project the sink and source onto zero Fourier momentum,
- Investigate the related difference between the finite volume form factor and the infinite volume form factor:

$$
\delta_L[G_\pi(Q^2) - 1] = \frac{1}{-\sqrt{2}(p'_4 + p_4)} \langle \pi^+(0) | J^+_4 | \pi^0(0) \rangle - G_\pi(Q^2) \frac{G_\pi(Q^2) - 1}{G_\pi(Q^2) - 1}.
$$

- In particular, for small twist angles, one has

$$
\lim_{\theta \to 0} \delta_L[G_\pi(Q^2) - 1] \equiv \delta_L[< r^2_\pi >] = \frac{< r^2_\pi >_L - < r^2_\pi >_\infty}{< r^2_\pi >_\infty}.
$$
From the figure, one sees for current lattices, the finite volume effects is negligible.

For example, for $m_\pi = 250\text{MeV}$ in a 2.5fm box, the finite volume effects is less than 2%.
The Breit Frame Calculations

- Our results so far are done in the rest frame.

- Most lattice calculations of pion EM form factor are implemented in the Breit Frame.
  - At finite volume, the initial and final state quarks are distinct because a given field can only have one BC.
  - The lattice action relevant to the Breit frame must be described by a theory with an enlarged valence flavor group.

- In addition to the usual valence up and down quark $u_1$ and $d_1$, one needs to introduce 2 fictitious valence up and down quarks $u_2$, $d_2$ which only differ by their BC into the theory.
To calculate the pion EM form factor on the lattices using TwBCs in the Breit frame, two separate current insertions are required:

- In the first insertion, the current strikes the up quark.
- In the second insertion, the current strikes the anti-down quark.

\[
\langle u_2 d_1(0) | J^1_\mu | u_1 d_1(0) \rangle \bigg|_{\theta_d=0} + \langle u_2 d_2(0) | J^2_\mu | u_2 d_1(0) \rangle \bigg|_{\theta_u=0}
\]

\[L \to \infty \langle \pi^+( -p) | J_\mu | \pi^+( p) \rangle, \]

\[p = \theta / L, \quad J^1_\mu = q_u \bar{u}_2 \gamma_\mu u_1, \quad J^2_\mu = q_d \bar{d}_1 \gamma_\mu d_2.\]

To study the long-distance effects from TwBCs in the Breit frame:

- One must formulate the relevant effective field theory.
- Matching above quark level operators onto the effective theory.
The corresponding low-energy theory is $SU(6|4) \chi$PT.

The form factor is calculated from the fourth component of the current as is done in the real lattice simulations.

We work in $p$-regime with time treated as infinite in extent.

In the infinite volume limit, the results obtained from $SU(6|4) \chi$PT agree with those from usual $SU(4|2) \chi$PT.

In particular, the well-known infinite volume $SU(2) \chi$PT results are recovered from the $SU(6|4) \chi$PT results when $m_j = m_u$. 
Finite Volume Effects in the Breit Frame

Finite volume modification: \( \delta \mathcal{M}(L) \equiv \mathcal{M}(L) - \mathcal{M}(L = \infty) \).

\[
\delta \mathcal{M}(L) = 2E_{\pi}(\theta) \frac{1}{f^2} \int_0^1 dx \left[ -I_{1/2} \left( \frac{\theta}{L}, m_{ju}^2 \right) 
+ I_{1/2} \left( (1 - 2x) \frac{\theta}{L}, m_{ju}^2 + 4x(1 - x) \frac{\theta^2}{L^2} \right) \right]
\]

\[
E_{\pi}(\theta) = \sqrt{m_{\pi}^2 + \frac{\theta^2}{L^2}}.
\]

- No isospin breaking terms.
- No discrete rotational symmetry breaking terms.
- Symmetry under \( \theta \rightarrow -\theta \).
Finite Volume Effects in the Breit Frame

The finite volume effect to the pion EM form factor in the Breit frame can be investigated through:

\[ \delta_L [G_\pi(Q^2) - 1] = \frac{\delta M(L)/2E_\pi(\theta)}{G_\pi(Q^2) - 1}, \]

\[ Q^2 = 4\theta^2/L^2, \quad E_\pi(\theta) = \sqrt{m_\pi^2 + \theta^2/L^2}. \]
\[ L = 2.5\text{fm} \]

Volume corrections are at percent level and become non-negligible only for light pions with small twist angles.
In the real lattice calculations, only the active quark, namely, the quark “attached” to the “photon”, will be twisted.

The relevant theory is $SU(7|5)$ partially quenched QCD.

The relevant low-energy effective field theory is $SU(7|5)\chi$PT.
Finite Volume Effects to Nucleon Electric Form Factor From TwBCs

\[
\Delta G_E^v(Q^2, L) = \frac{G_E^v(Q^2, L) - G_E^v(Q^2)}{G_E^v(Q^2)} \quad \text{and} \quad G_E^v(Q^2, L) - G_E^v(Q^2) = \delta_L[G_E^v(Q^2)]
\]

\[
\delta_L[G_E^v(Q^2)] = \frac{1}{f^2} \int_0^1 dx \left[ I_{1/2}(m_\pi P_\pi, xQ) - \frac{1}{2} I_{1/2}(m_\pi, 0) - \frac{1}{2} I_{1/2}(m_\pi, B') \right]
\]

\[
- \frac{3}{2 f^2} \left\{ g_A^2 \left[ \overline{J}(m_\pi, 0, 0) + \overline{J}(m_\pi, B', 0) \right] \right. \\
\left. - \frac{4}{9} g_{\Delta N}^2 \left[ \overline{J}(m_\pi, 0, \Delta) + \overline{J}(m_\pi, B', \Delta) \right] \right\}
\]

\[
+ \frac{3}{f^2} \int_0^1 dx \left[ g_A^2 J(m_\pi P_\pi, 0, Q, xQ, 0) - \frac{4}{9} g_{\Delta N}^2 J(m_\pi P_\pi, 0, Q, xQ, \Delta) \right],
\]

(1)
$L = 2.75\text{fm}$

$m_\pi = 0.25 \text{ [GeV]}$
\[
\Delta G_M^v(Q^2, L) = \frac{\delta_L[G_M^v(Q^2)]}{G_M^v(Q^2)},
\]

\[
\delta_L[G_M^v(Q^2)] = \frac{-2M_N}{B' f^2} (g_A^2 + g_{A1}^2) K^2(m_\pi, B' \hat{y}, 0)
\]

\[
+ \frac{3M_N}{f^2} \int_0^1 dx \left[ g_A^2 L^{33}(m_\pi P_\pi, 0, B' \hat{y}, xB' \hat{y}, 0) \right.
\]

\[
+ \left. \frac{2}{9} g_{\Delta N}^2 L^{33}(m_\pi P_\pi, 0, B' \hat{y}, xB' \hat{y}, \Delta) \right].
\]
\[ L = 2.75 \text{fm}, \quad -2 \leq g_1 \leq 2.\]

\[ m_\pi = 0.30 \text{ [GeV]} \]
A Comment on the Breit Frame Calculations

- The use of Breit frame can simplify the calculations of the finite volume shift to the pion EM form factor significantly.

- Unlike the pion case, the Breit frame does not eliminate the complication of the calculations for the nucleon isovector form factors.

- The main contribution to the finite volume effects to the nucleon magnetic form factor is from $\kappa$, which is odd in $\theta'$, hence the use of Breit frame even doubles the finite volume effects.
Conclusion

- The flavor TwBC provides a promising technique to overcome the restriction of quantized momenta on the lattices.

- The finite volume effects (due to the use of TwBC) are under theoretical control on pion observables and the nucleon electric form factor.

- The finite volume effect to the nucleon magnetic form factor are sizable for certain values of twist angles.

- For better controlled extractions of the pion charge radius, nucleon magnetic moment and nucleon charge radii, the formulae presented here are important.

- Nucleon axial form factor, pseudoscalar decay constants.....

- This technique is employing on the lattices (calculations) vigorously.
This figure is from UKQCD collaboration.
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