DOMAIN DECOMPOSITION AND
MULTILEVEL INTEGRATION FOR FERMIONS II

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Lattice 2016, July 27th, 2016
Case I: disconnected correlation functions

\[ \left\langle \left[ \text{tr} \gamma_5 D^{-1}(x, x) \right] \left[ \text{tr} \gamma_5 D^{-1}(y, y) \right] \right\rangle = \left\langle x \quad y \right\rangle \]

**Factorization:**

use quark propagator factorization, case I (sink close to source)

\[ \Rightarrow \text{disconnected two point function splits in four contributions} \]

\[ \left\langle \left[ \text{tr} \gamma_5 D^{-1}(x, x) \right] \left[ \text{tr} \gamma_5 D^{-1}(y, y) \right] \right\rangle \]

\[ = \left\langle \left[ \text{tr} \gamma_5 D^{-1}_\Gamma(x, x) \right] \left[ \text{tr} \gamma_5 D^{-1*}_\Gamma(y, y) \right] \right\rangle \]

\[ + \left\langle \left[ \text{tr} \gamma_5 D^{-1}_\Gamma(x, x) \right] \left[ \text{tr} \gamma_5 \delta D^{-1}_\Gamma(y, y) \right] \right\rangle \]

\[ + \left\langle \left[ \text{tr} \gamma_5 \delta D^{-1}_\Gamma(x, x) \right] \left[ \text{tr} \gamma_5 D^{-1*}_\Gamma(y, y) \right] \right\rangle \]

\[ + \left\langle \left[ \text{tr} \gamma_5 \delta D^{-1}_\Gamma(x, x) \right] \left[ \text{tr} \gamma_5 \delta D^{-1*}_\Gamma(y, y) \right] \right\rangle \]
Numerical test

Wilson plaquette action $\beta = 6 \Rightarrow a \approx 0.093 \text{ fm}$

Wilson fermions $\kappa = 0.1560 \Rightarrow m_\pi \approx 450 \text{ MeV}$

$64 \times 24^3$ lattice with open boundary conditions in time

Two-level Monte Carlo:
- $n_0 = 200$ level-0 configurations
- Domain decomposition in two thick time slices
- $n_1 = 100$ level-1 configurations

Estimation of $\text{tr} \, \gamma_5 D^{-1}$:
- Stochastic volume sources
- Hopping parameter expansion to reduce UV noise

Note: to be computed only
Contributions to propagator: factorized

\[ \langle [\text{tr} \gamma_5 D^{-1}_\Gamma(x, x)] [\text{tr} \gamma_5 D^{-1}_{\Gamma^*}(y, y)] \rangle \\
+ \langle [\text{tr} \gamma_5 D^{-1}_\Gamma(x, x)] [\text{tr} \gamma_5 \delta D^{-1}_{\Gamma^*}(y, y)] \rangle \\
+ \langle [\text{tr} \gamma_5 \delta D^{-1}_\Gamma(x, x)] [\text{tr} \gamma_5 D^{-1}_{\Gamma^*}(y, y)] \rangle \\
+ \langle [\text{tr} \gamma_5 \delta D^{-1}_\Gamma(x, x)] [\text{tr} \gamma_5 \delta D^{-1}_{\Gamma^*}(y, y)] \rangle \]

Factorized contribution ⇒ independent averaging over level-1 configs

- first term carries almost no signal, only noise
- Note that \( \langle \text{tr} \gamma_5 D^{-1}_\Gamma(x, x) \rangle = 0 \)
- Multilevel works at full potentiality to reduce the variance
Contributions to propagator: correction

\[
\langle [\text{tr} \gamma_5 D^{-1}_\Gamma (x, x)][\text{tr} \gamma_5 D^{-1}_\Gamma^* (y, y)] \rangle 
+ \langle [\text{tr} \gamma_5 D^{-1}_\Gamma (x, x)][\text{tr} \gamma_5 \delta D^{-1}_\Gamma (y, y)] \rangle 
+ \langle [\text{tr} \gamma_5 \delta D^{-1}_\Gamma (x, x)][\text{tr} \gamma_5 D^{-1}_\Gamma^* (y, y)] \rangle 
+ \langle [\text{tr} \gamma_5 \delta D^{-1}_\Gamma (x, x)][\text{tr} \gamma_5 \delta D^{-1}_\Gamma^* (y, y)] \rangle
\]
Summary: disconnected

short-distance: error dominated by the first correction

long-distance: error dominated by the factorized contribution

⇒ **Factorization and multilevel integration works**
  - error decreases exponentially
  - maintain signal for additional 1 fm
Case II: connected correlation functions

Factorization less obvious. Two steps:

1. Factorization of the quark propagator, case II (sink far from source)

\[ D^{-1}(x, y) \approx -x \]

\[ -D_{\Gamma}^{-1}(y, \cdot)D_{\partial \Gamma^*}D_{\Gamma}^{-1}(\cdot, x) + \mathcal{O}(e^{M_\pi \Delta}) \]

2. Factorization of the hadron two-point function

With the factorized propagator:

3. Multilevel integration
Wilson plaquette action $\beta = 6 \Rightarrow a \approx 0.093 \text{ fm}$

Wilson fermions $\kappa = 0.1560 \Rightarrow m_\pi \approx 450 \text{ MeV}$

$64 \times 24^3$ lattice with open boundary conditions in time

Test of quark propagator factorization:
- stochastic sources on time slice $x_0 = 4a$
- first cut at $x_0 = 24a$
- $\Delta = 8a$, $12a$ and $16a \Rightarrow$ second cut at $24a - \Delta$

Contraction of two or three quark lines:
- **pseudoscalar** propagator
- **nucleon** propagator
Pseudoscalar two-point function

\[ C_{Pc} = C_{Pc}^{(0)} + \left[ C_{Pc}^{(1)} - C_{Pc}^{(0)} \right] + \left[ C_{Pc}^{(2)} - C_{Pc}^{(1)} \right] + C_{Pc}^{(\text{rest})} \]

\[ C^{(0)}: \Delta = 8\alpha \]
\[ C^{(1)}: \Delta = 12\alpha \]
\[ C^{(2)}: \Delta = 16\alpha \]
Nucleon two-point function

\[ C_N = C_N^{(0)} + \left[ C_N^{(1)} - C_N^{(0)} \right] + \left[ C_N^{(2)} - C_N^{(1)} \right] + C_N^{\text{(rest)}} \]

\( C^{(0)}: \Delta = 8a \quad C^{(1)}: \Delta = 12a \quad C^{(2)}: \Delta = 16a \)
Factorization of propagator in principle works

- small $\Delta$ already gives excellent approximation
- can be improved by hierarchy of $\Delta_i$

$\Rightarrow$ potential for multi-level

**Problem:**
Natural building blocks have two or three propagator on surface

$(6V^3)^2$ or $(6V^3)^3$ complex numbers

$\Rightarrow$ too much to be saved to disk
Projection of the propagator

Cut the fermion line with $P$:

$$S(y, x) = -D^{-1}_\Gamma D_{\partial \Gamma^*} \cdot P \cdot D^{-1}_\Gamma (x, y)$$

$P$ projects on lower dimensional space

$$P = \sum_{i=1}^{N} \psi_i \psi_i^\dagger$$

Reduce memory of building block $(6V_3)^2 \rightarrow N^2$

Several possibilities:

- stochastic sources $\Rightarrow$ does not seem to work, large $N$ required
- local deflation subspace
- eigenmodes of block Dirac operator
Projections: deflation subspace

Pseudoscalar two-point function with

\(P\): deflation subspace at \(x_0/\alpha = 24\)

Deflation subspace:

\(N_s = 60\) block modes, \(4^4\) blocks

\(\Rightarrow\) Virtually no difference visible

Factorization only

\(\Delta/\alpha = 8, 12, 16\)

Lüscher ’07
Projections: block eigenvectors subspace

Pseudoscalar two-point function with

\( P \): eigenvectors of Dirac operator restricted to \( x_0 \in [24 - \Delta, 24 + \Delta] \)

Block eigenvectors subspace:
\( N_{ev} = 120 \) vectors

\( \Rightarrow \) Virtually no difference visible

Factorization only
\( \Delta/a = 8, 12, 16 \)
Projections: deflation subspace

Nucleon two-point function with

\( P \): deflation subspace at \( x_0/a = 24 \)

Deflation subspace:

\( N_s = 60 \) block modes, \( 4^4 \) blocks

Lüscher '07

Factorization only

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Nucleon two-point function with

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Block eigenvectors subspace: \( N_{ev} = 120 \) vectors

Factorization only \( \Delta/a = 8, 12, 16 \)

⇒ **Surprise**: also the nucleon can be saturated by low-modes
Factorization of pion and nucleon two-point functions in principle possible.

Two approximations involved:

- approximate factorization of propagator
- projection to low-mode subspace

**Surprise:** the nucleon propagator is saturated by low modes!

⇒ **Multilevel in quenched is possible**
Two-level Monte Carlo integration:

level-0  \( n_0 = 50 \) configurations

level-1  \( n_1 = 20 \) updates

Factorized contribution with two-level algorithm

Correction term with source at \( x_0 = 4a \) only on level-0
Detailed improvement

**Total**

**Source average**

**Ord. \( n_1 \) avg.**

**Two-level**
Conclusions & Outlook

Two-level methods work:

- quark-line disconnected meson correlation functions
  \[
  \left\langle \text{tr} \left\{ \Gamma \frac{1}{D}(x,x) \right\} \text{tr} \left\{ \Gamma \frac{1}{D}(y,y) \right\} \right\rangle
  \]

- also gluonic correlation functions
  \[\langle \bar{q}(x_0)q(y_0) \rangle\]

Garcia-Vera, Schaefer '16

For quark line connected there is hope:

- correlation functions shown to be factorizable.
- two-level is only partial solution
- signal-to-noise require \( \sqrt{N} \propto e^{mx_0} \rightarrow N \propto e^{mx_0} \)

\[\Rightarrow \text{Number of configurations to reach target statistics} \sim \text{square root of the standard case}\]
Two-level methods work:

- quark-line disconnected meson correlation functions

\[
\left\langle \text{tr} \left\{ \Gamma \frac{1}{D}(x, x) \right\} \text{tr} \left\{ \Gamma \frac{1}{D}(y, y) \right\} \rightangle
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Outlook:

- generalize quark line factorization to multilevel
- factorization of the fermion determinant
Thanks for your attention!
Backup
Quark propagator factorization, case I

Two regions: \( \Gamma \cup \Gamma^* \). The Dirac operator is

\[
D = \begin{pmatrix}
D_\Gamma & D_{\partial \Gamma} \\
D_{\partial \Gamma^*} & D_{\Gamma^*}
\end{pmatrix}
\]

For the Wilson Dirac operator, \( D_{\partial \Gamma} \) and \( D_{\partial \Gamma^*} \) act on the boundaries only.

The propagator is

\[
D^{-1} = \begin{pmatrix}
S_\Gamma^{-1} & -S_\Gamma^{-1}D_{\partial \Gamma}D_{\Gamma^*}^{-1} \\
-D_{\Gamma^*}^{-1}D_{\partial \Gamma^*}S_\Gamma^{-1} & S_{\Gamma^*}^{-1}
\end{pmatrix}
\]

with the Schur complements

\[
S_\Gamma = D_\Gamma - D_{\partial \Gamma}D_{\Gamma^*}^{-1}D_{\partial \Gamma^*} \quad S_{\Gamma^*} = D_{\Gamma^*} - D_{\partial \Gamma^*}D_{\Gamma}^{-1}D_{\partial \Gamma}
\]

Dirichlet boundary conditions: \( D_{\partial \Gamma} = D_{\partial \Gamma^*} = 0 \)

\[
D^{-1} \approx \begin{pmatrix}
D_\Gamma^{-1} & 0 \\
0 & D_{\Gamma^*}^{-1}
\end{pmatrix}
\]

Correction term:

\[
\delta D_\Gamma^{-1} = \frac{1}{D_\Gamma - D_{\partial \Gamma}D_{\Gamma^*}^{-1}D_{\partial \Gamma^*}} - \frac{1}{D_\Gamma}
\]

\[
= \frac{1}{D_\Gamma - D_{\partial \Gamma}D_{\Gamma^*}^{-1}D_{\partial \Gamma^*}}D_{\partial \Gamma}D_{\Gamma^*}^{-1}D_{\partial \Gamma^*} \frac{1}{D_\Gamma} = -D_\Gamma^{-1}D_{\partial \Gamma^*}D_{\Gamma}^{-1}
\]
Quark propagator factorization, case I

Graphically:

\[ D^{-1} = D^{-1}_\Gamma - D^{-1}D_{\partial \Gamma^*}D^{-1}_\Gamma \]

or

\[ \text{Correction term } \delta D^{-1}_\Gamma \text{ has propagator to and from boundary} \]

\[ \text{Tr} \gamma_5 \delta D^{-1}_\Gamma \propto e^{-m_\pi \Delta} \]
Quark propagator factorization, case II

see talk by Schaefer

\[ D^{-1} = \begin{pmatrix} S_{\Gamma}^{-1} & -S_{\Gamma}^{-1}D_{\partial\Gamma}D_{\Gamma*}^{-1} \\ -S_{\Gamma*}D_{\partial\Gamma*}D_{\Gamma}^{-1} & S_{\Gamma*}^{-1} \end{pmatrix} \]

Now take \( x \in \Gamma \) and \( y \in \Gamma^* \), in different domains:

\[
\begin{align*}
D^{-1}(x, y) &= -x \cdot y \\
&= -D^{-1}(y, \cdot)D_{\partial\Gamma*}D_{\Gamma}^{-1}(\cdot, x)
\end{align*}
\]
Quark propagator factorization, case II

see talk by Schaefer

\[ D^{-1} = \begin{pmatrix} S^{-1}_\Gamma & -S^{-1}_\Gamma D_{\partial \Gamma} D^{-1}_\Gamma^* \\ -S_{\Gamma^*} D_{\partial \Gamma^*} D^{-1}_\Gamma & S^{-1}_{\Gamma^*} \end{pmatrix} \]

Now take \( x \in \Gamma \) and \( y \in \Gamma^* \), in different domains:

Approximation with a second Dirichlet b.c. cut
\( \Rightarrow \) correction \( \approx e^{M_\pi \Delta/2} \)
Some error analysis

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\[ \hat{A} = \frac{1}{N_0} \sum_{i=1}^{N_0} \sum_{j=1}^{N_1} \sum_{k=1}^{N_1} O^{ij} O'^{ik} \]

Specialize to \( \langle O \rangle = \langle O' \rangle = 0 \); connected contribution.

\[ \sigma_A^2 = \frac{1}{N_0 N_1^2} \langle \text{Var}_L(O) \text{Var}_R(O') \rangle_B + \frac{1}{N_0} \left( \langle [O]^2 [O']^2 \rangle_B - \bar{A}^2 \right) \]

\[ + \frac{1}{N_0 N_1} \langle \text{Var}_L(O) [O']^2_R + \text{Var}_R(O') [O]^2_L \rangle_B \]

\[ \text{Var}_L(O) = [O^2]_L - [O]^2_L \]
Some error analysis

\[ \sigma_A^2 = \frac{1}{N_0 N_1^2} \langle \text{Var}_L(O) \text{Var}_R(O') \rangle_B \rightarrow \text{const} \]
\[ + \frac{1}{N_0 N_1} \langle \text{Var}_L(O) [O']^2_R + \text{Var}_R(O') [O]^2_L \rangle_B \rightarrow e^{-2m\Delta} \]
\[ + \frac{1}{N_0} \left( \langle [O]^2_L [O']^2_R \rangle_B - A^2 \right) \rightarrow e^{-2m\Delta} \]

Contributions which do not profit from multilevel inevitable.
These decay exponentially with the distance from the boundary \( \Delta \).

Difference between \([O(x)]_L(U_B)\) and \(\langle O \rangle = \langle [O(x)]_L \rangle_B\)

\[ \langle ([O]_L - \langle O \rangle)^2 \rangle_B = \langle ([O^t]_R - \langle O^t \rangle)([O]_L - \langle O \rangle) \rangle_B \propto e^{-m|x_0-y_0|} \]
...assuming time-slice boundary.