Multilevel integration for meson propagators

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Signal-to-noise ratio problem

Signal of a two-point function (e.g. for the \textit{rho} meson) \cite{Parisi; 1983}, \cite{Lepage; 1989}

\[ C_\rho(y_0 - x_0) \propto e^{-m_\rho |y_0 - x_0|} \]

while its variance gets contribution from

\[ \sigma_\rho^2(C_\rho(y_0 - x_0)) \propto e^{-2m_\pi |y_0 - x_0|} \]

and so the ratio is \textbf{exponentially} suppressed at large source-sink distances

\[ \frac{C_\rho(y_0 - x_0)}{\sigma_\rho(y_0 - x_0)/\sqrt{N}} \propto \sqrt{N}e^{-(m_\rho - m_\pi)|y_0 - x_0|} \]

\( \rightarrow \) particularly severe at small pion masses
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\rightarrow \text{particularly severe at small pion masses}
\]

Same problem for

nucleon correlators

\[
\frac{C_N(y_0 - x_0)}{\sigma_N(y_0 - x_0)/\sqrt{N}} \propto \sqrt{N} e^{-(m_N-\frac{3}{2}m_\pi)|y_0-x_0|} 
\]
Signal-to-noise ratio problem

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Same problem for

nonzero momentum correlators

\[ \frac{C_{\pi,p}(y_0 - x_0)}{\sigma_{\pi,p}(y_0 - x_0)/\sqrt{N}} \propto \sqrt{N} e^{-(E_\pi(p) - m_\pi)|y_0 - x_0|} \]
Multilevel integration

- A way of dealing with an exponentially vanishing signal-to-noise ratio is through a **multilevel integration scheme**
- Exploiting the locality of the theory, regions that are far away can be updated independently

Simplest case: two-level algorithm with two regions

- **Level-0**: $n_0$ realizations of boundary between two regions (later: “frozen region”)
- **Level-1**: the two regions are independently updated $n_1$ for each of the $n_0$ boundaries
- $n_0 \times n_1^2$ configurations for the cost of $n_0 \times n_1$
- $n_{\text{reg}} > 2 \rightarrow n_1^{n_{\text{reg}}}$ samples - the error goes like

$$
\delta(C) \sim n_1^{-\frac{n_{\text{reg}}}{2}} e^{-m\pi|y_0-x_0|}
$$
A way of dealing with an exponentially vanishing signal-to-noise ratio is through a **multilevel integration scheme**.

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This is feasible if **both the action and the observable can be factorized**.

Solutions in pure-gauge theory:

- multihit [Parisi, Petronzio & Rapuano; 1983]
- multilevel for Wilson loops and Polyakov loop correlators [Lüscher & Weisz; 2001]
- also [Meyer; 2002] and [Giusti & Della Morte; 2008, 2010]
After Wick’s theorem it’s not obvious how the QCD action and the observable (propagator) can be factorized.

→ breakthrough in the development of a multilevel integration scheme for fermions [Cè, Giusti & Schaefer; 2016, 2017].

→ both the determinant and the propagator can be completely factorized

Setup: overlapping domains $\Omega_0^*$ and $\Omega_1^*$
The exact propagator can be written as

\[ Q^{-1} = -Q_{\Omega_1^*}^{-1} Q_{\Lambda_1,0} \frac{1}{1 - \omega} Q_{\Omega_0^*}^{-1} \]

with \( Q = \gamma_5 D \) and where

\[ \omega = Q_{\Omega_0^*}^{-1} Q_{\Lambda_1,2} Q_{\Omega_1^*}^{-1} Q_{\Lambda_1,0} \]

Fully factorized approximation:

\[ Q^{-1} \simeq -Q_{\Omega_1^*}^{-1} Q_{\Lambda_1,0} Q_{\Omega_0^*}^{-1} \]
A new method with noise sources

A viable method is needed to compute $C_{\Gamma}^{\text{fact}}$ efficiently in a multilevel integration scheme

$$C_{\Gamma}^{\text{fact}}(y_0, x_0) = \text{Tr} \left\{ Q^{-1}_{\Omega_0^*}(\cdot, x_0) \Gamma Q^{-1}_{\Omega_0^*}(x_0, \cdot) Q_{\Lambda_1,0} Q^{-1}_{\Omega_1^*}(\cdot, y_0) \Gamma Q^{-1}_{\Omega_1^*}(y_0, \cdot) Q_{\Lambda_1,0} \right\}$$

Naively one would store $\sim (V_3)^2$ (or $(V_3)^3$ for baryons) complex numbers... $\rightarrow$ not feasible

Our new proposal exploits the newly factorized observable by putting noise sources in the middle of the lattice

$\rightarrow$ right next to the boundary of the frozen region, i.e.

$$C_{\Gamma}^{\text{fact}}(y_0, x_0) = \frac{1}{N_\eta} \sum_{i}^{N_\eta} \text{Tr} \left\{ Q^{-1}_{\Omega_0^*}(\cdot, x_0) \Gamma Q^{-1}_{\Omega_0^*}(x_0, \cdot) \eta_i \eta_i^\dagger Q_{\Lambda_1,0} Q^{-1}_{\Omega_1^*}(\cdot, y_0) \Gamma Q^{-1}_{\Omega_1^*}(y_0, \cdot) Q_{\Lambda_1,0} \right\}$$

$\rightarrow$ the meson propagator can be computed sequentially $\rightarrow$ only $\sim V_3$ complex numbers to be saved
$$\text{Tr} \left\{ Q_{\Omega_1}^{-1} Q_{\Lambda_{1,0}} Q_{\Omega_0}^{-1} \Gamma Q_{\Omega_0}^{-1} \eta \eta^\dagger Q_{\Lambda_{1,0}} Q_{\Omega_1}^{-1} \Gamma \right\}$$
\[ \text{Tr} \left\{ Q_{\Omega_1}^{-1} Q_{\Lambda_1,0} Q_{\Omega_0}^{-1} \Gamma Q_{\Omega_0}^{-1} \eta \eta^\dagger Q_{\Lambda_1,0} Q_{\Omega_1}^{-1} \Gamma \right\} \]
\[ \text{Tr} \left\{ Q_{\Omega_1^*}^{-1} Q_{\Lambda,0} Q_{\Omega_0^*}^{-1} \Gamma Q_{\Omega_0^*}^{-1} \eta \eta^\dagger Q_{\Lambda,0} Q_{\Omega_1^*}^{-1} \Gamma \right\} \]
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\[ \text{Tr} \left\{ Q_{\Omega_1}^{-1} Q_{\Lambda_{1,0}}^{-1} \Gamma Q_{\Omega_0}^{-1} \eta \eta^\dagger Q_{\Lambda_{1,0}}^{-1} Q_{\Omega_1}^{-1} \Gamma \right\} \]
A test in quenched QCD

The quenched theory suffers from the S-N ratio problem as well → perfect playground for a multilevel test

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$L/a$</th>
<th>$T/a$</th>
<th>$\kappa$</th>
<th>$c_{SW}$</th>
<th>$m_{PS}$ (MeV)</th>
<th>$a$ (fm)</th>
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</thead>
<tbody>
<tr>
<td>6.2</td>
<td>32</td>
<td>96</td>
<td>0.1352</td>
<td>1.61375</td>
<td>580</td>
<td>0.068</td>
</tr>
</tbody>
</table>

→ periodic boundary conditions

Multilevel simulation with

- two active regions connected by two frozen regions of width $\Delta = 8a$
- $n_0 = 50$ level-0 updates $\times$ $n_1 = 16$ level-1 updates
- $N_\eta = 40$ noise sources
- $\Gamma = \gamma_i$ with $i = 1, 2, 3$

The factorized meson propagator is an approximation: also the rest (whose size depends on $\Delta$) has to be computed. Strategy of the calculation:

$$\langle C_\rho \rangle = \langle C_{\rho}^{\text{fact}} \rangle_{\text{ML}} + \langle C_{\rho}^{\text{ex}} - C_{\rho}^{\text{fact}} \rangle_{\text{SMC}}$$
Vector-vector correlator

\[ x_0 = 24a \quad \Delta = 8a \]

\[ C_{\text{vector}}(y_0/a) \]

\[ \begin{array}{cccc}
10^{-12} & 10^{-11} & 10^{-10} & 10^{-9} \\
40 & 48 & 56 & 64 & 72 & 80 & 88 \\
\end{array} \]

\[ C^{(\text{exact})}_{\text{SMC}} \quad C^{(\text{fact})}_{\text{ML}} \]

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Vector-vector correlator: ML gain

\[ \sigma^2_{\text{ML}} / \sigma^2_{\text{SMC}} \]

\[ y_0 / a = 24a \quad \Delta = 8a \]

ML gain

\[ 1/16 \]

0.00 0.25 0.50 0.75 1.00 1.25

\[ 40 48 56 64 72 80 88 \]
The correction term

\[ x_0 = 24a \quad \Delta = 8a \]

\[ \frac{C_{\text{vector}}(y_0/a)}{a} = 24a \]

\[ C^{(\text{fact})} - C^{(\text{exact})} \]

<table>
<thead>
<tr>
<th>Value</th>
<th>x-axis</th>
</tr>
</thead>
<tbody>
<tr>
<td>40</td>
<td></td>
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<tr>
<td>48</td>
<td></td>
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<td>88</td>
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</tbody>
</table>
The correction term: error

\( x_0 = 24a \quad \Delta = 8a \)

\[
\begin{align*}
\text{error} & / a \\
x_0 & = 24a \\
\Delta & = 8a \\
\delta & \text{(fact)} \\
\delta & \text{(fact)ML} \\
\delta & \text{(corr)}
\end{align*}
\]
Conclusions

- new method to directly compute the factorized form of the connected propagator \textit{sequentially} (with 2 active regions)

- clear improvement with respect to previous method (projection to deflated modes)

- theoretical gain of multilevel ($\sim 16$ in the cost) reached far away enough from the frozen region

- the rest of the propagator is computed with standard MC $\rightarrow$ in this case it is quite small $\sim 3 - 5\%$ for $\Delta = 8$

- if it is large and/or with large error $\rightarrow$ multilevel also on the rest

- next: advancements for disconnected propagator by Tim
Thanks for your attention!
Factorization of the quark propagator

- Decomposition of Hermitian Wilson-Dirac operator $Q = \gamma_5 D$ [Lüscher; 2003]

$$Q = \begin{pmatrix} Q\Gamma & Q\partial\Gamma \\ Q\partial\Gamma^* & Q\Gamma^* \end{pmatrix}$$

- Schur complement

$$S\Gamma = Q\Gamma - Q\partial\Gamma Q\Gamma^* Q\partial\Gamma^*$$

If $\Gamma = \Lambda_0$ and $\Gamma^* = \Omega_1^*$ we can write

$$Q^{-1} = \begin{pmatrix} S^{-1}_{\Lambda_0} - S^{-1}_{\Lambda_0} Q\Lambda_{1,0} Q\Omega_{1,0}^* Q\Omega_{1,0}^* & -S^{-1}_{\Lambda_0} Q\Lambda_{1,0} Q\Omega_{1,0}^* \\ -Q^{-1}_{\Omega_1^*} Q\Lambda_{1,0} S^{-1}_{\Lambda_0} & Q^{-1}_{\Omega_1^*} + Q^{-1}_{\Omega_1^*} Q\Lambda_{1,0} S^{-1}_{\Lambda_0} Q\Lambda_{1,0} Q\Omega_{1,0}^* \end{pmatrix}$$

and noting that

$$S^{-1}_{\Lambda_0} = P_{\Lambda_0} Q^{-1} P_{\Lambda_0} = P_{\Lambda_0} Q^{-1}_{\Omega_0} P_{\Lambda_0} + ...$$

we get (bottom left element)

$$Q^{-1} \approx -Q^{-1}_{\Omega_1^*} Q\Lambda_{1,0} Q\Omega_{1,0}^*$$
Vector-vector correlator

\[ x_0 = 32a \quad \Delta = 8a \]

\[
\begin{array}{cccccc}
10^{-12} & 10^{-11} & 10^{-10} & 10^{-9} & 10^{-8} & 10^{-7} \\
40 & 48 & 56 & 64 & 72 & 80 & 88
\end{array}
\]

\( C^{(\text{exact})}_{\text{SMC}} \)

\( C^{(\text{fact})}_{\text{ML}} \)

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Vector-vector correlator: ML gain

\[ \frac{\sigma^2_{ML}}{\sigma^2_{SMC}} \]

\[ y_0 / a \quad x_0 = 32a \quad \Delta = 8a \]

\[ 0.00 \quad 0.25 \quad 0.50 \quad 0.75 \quad 1.00 \quad 1.25 \]

\[ 40 \quad 48 \quad 56 \quad 64 \quad 72 \quad 80 \quad 88 \]

Alessandro Nada (DESY)
Factorizing the two–point function was previously attempted in different ways:

- placing two different noise sources to cut the two quark lines → in practice the variance is extremely large, due to the presence of disconnected diagrams which do not benefit from volume averaging

- cut the two lines with $N$ orthonormal vectors which can be used to project the propagator → memory problem under control ($V_3^2 \rightarrow N^2$

- it is a viable (but expensive) possibility. successfully implemented using
  - local deflation subspace
  - generating eigenvectors of the Dirac operator restricted to a block of width $2\Delta$