Domain decomposition and multilevel integration for fermions II

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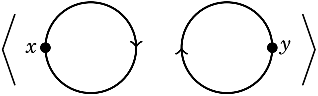
Case I: disconnected correlation functions

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



Factorization:

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

`see talk by Schaefer`

$\Rightarrow$ disconnected two point function splits in four contributions

$$\begin{aligned}
&\left\langle [\mathrm{tr}\,\gamma_5 D^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D^{-1}(y,y)] \right\rangle \\
&= \left\langle [\mathrm{tr}\,\gamma_5 D_{\Gamma}^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)] \right\rangle \\
&+ \left\langle [\mathrm{tr}\,\gamma_5 D_{\Gamma}^{-1}(x,x)][\mathrm{tr}\,\gamma_5 \delta D_{\Gamma^*}^{-1}(y,y)] \right\rangle \\
&+ \left\langle [\mathrm{tr}\,\gamma_5 \delta D_{\Gamma}^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)] \right\rangle \\
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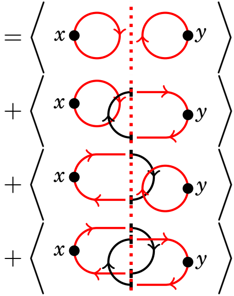
\end{aligned}$$



Numerical test

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

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

64×24^3 lattice with open boundary conditions in time

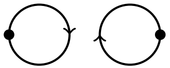
Two-level Monte Carlo:

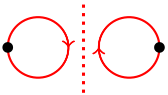
- $n_0 = 200$ level-0 configurations
- domain decomposition in two thick time slices
- $n_1 = 100$ level-1 configurations

Estimation of $\mathrm{tr}\,\gamma_5 D^{-1}$:

- Stochastic volume sources
- Hopping parameter expansion to reduce UV noise

Note: to be computed only

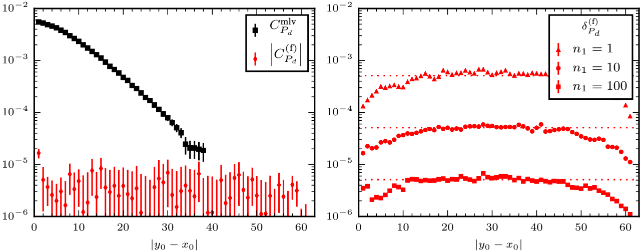




Contributions to propagator: factorized

$$\langle[\mathrm{tr}\,\gamma_5 D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)]\rangle$$
$$+\langle[\mathrm{tr}\,\gamma_5 D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 \delta D_{\Gamma^*}^{-1}(y,y)]\rangle + \langle[\mathrm{tr}\,\gamma_5 \delta D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)]\rangle$$
$$+\langle[\mathrm{tr}\,\gamma_5 \delta D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 \delta D_{\Gamma^*}^{-1}(y,y)]\rangle$$

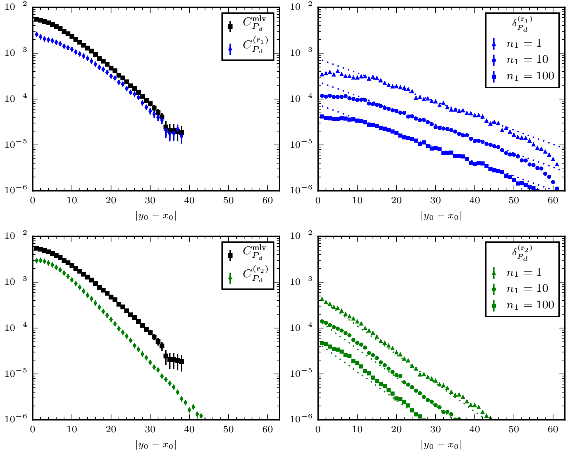
Factorized contribution $\Rightarrow$ independent averaging over level-1 configs



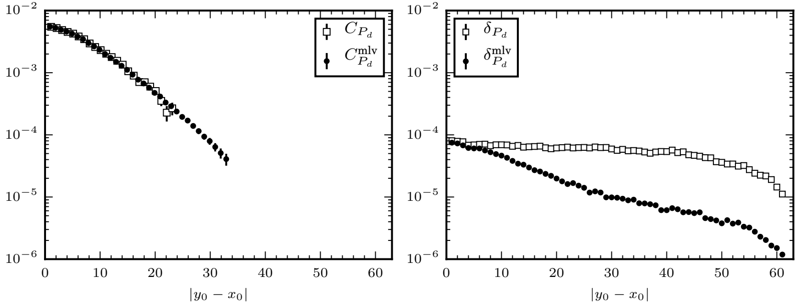
- first term carries almost no signal, only noise
- Note that $\langle \mathrm{tr}\,\gamma_5 D_\Gamma^{-1}(x,x)] \rangle = 0$
- Multilevel works at full potentiality to reduce the variance

Contributions to propagator: correction

$$\langle[\mathrm{tr}\,\gamma_5 D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)]\rangle$$
$$+\langle[\mathrm{tr}\,\gamma_5 D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 \delta D_{\Gamma^*}^{-1}(y,y)]\rangle+\langle[\mathrm{tr}\,\gamma_5 \delta D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 D_{\Gamma^*}^{-1}(y,y)]\rangle$$
$$+\langle[\mathrm{tr}\,\gamma_5 \delta D_\Gamma^{-1}(x,x)][\mathrm{tr}\,\gamma_5 \delta D_{\Gamma^*}^{-1}(y,y)]\rangle$$



Summary: disconnected



short-distance: error dominated by the first correction

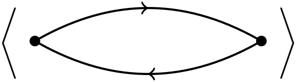
long-distance: error dominated by the factorized contribution

$\Rightarrow$ **Factorization and multilevel integration works**

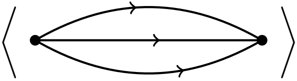
- error decreases exponentially
- maintain signal for additional 1 fm

Case II: connected correlation functions

- meson propagator



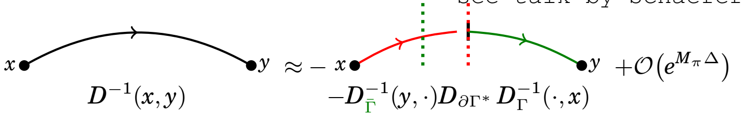
- baryon propagator



Factorization less obvious. Two steps:

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

`see talk by Schaefer`



2. factorization of the hadron two-point function

With the factorized propagator:

3. multilevel integration

Numerical test

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

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

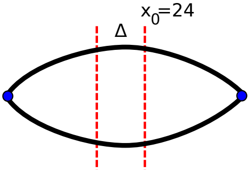
64×24^3 lattice with open boundary conditions in time

Test of quark propagator factorization:

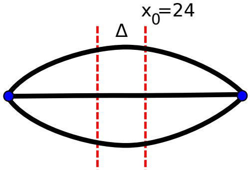
- stochastic sources on time slice $x_0 = 4a$
- first cut at $x_0 = 24a$
- $\Delta = 8a,\ 12a$ and $16a \Rightarrow$ second cut at $24a - \Delta$

Contraction of two or three quark lines:

- **pseudoscalar** propagator

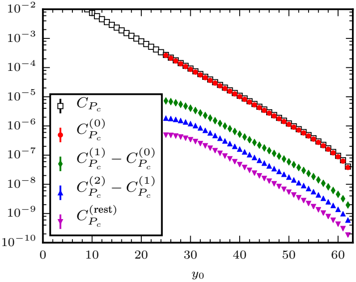


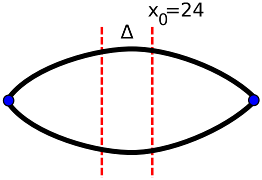
- **nucleon** propagator



Meson

Pseudoscalar two-point function



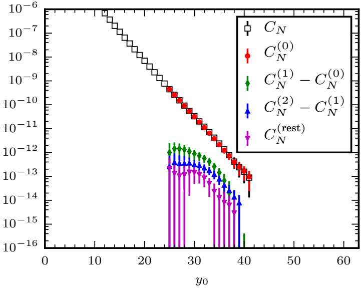


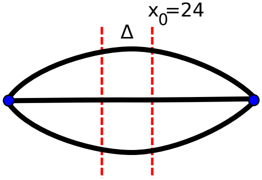
$$C_{P_c} = C_{P_c}^{(0)} + \left[C_{P_c}^{(1)} - C_{P_c}^{(0)}\right] + \left[C_{P_c}^{(2)} - C_{P_c}^{(1)}\right] + C_{P_c}^{(\mathrm{rest})}$$

$C^{(0)}$: $\Delta = 8a$ $\quad$ $C^{(1)}$: $\Delta = 12a$ $\quad$ $C^{(2)}$: $\Delta = 16a$

Baryon

Nucleon two-point function





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

$C^{(0)}$: $\Delta = 8a$ $\quad$ $C^{(1)}$: $\Delta = 12a$ $\quad$ $C^{(2)}$: $\Delta = 16a$

Factorized propagator

Factorization of propagator in principle works

- small Δ already gives excellent approximation
- can be improved by hierarchy of Δ_i

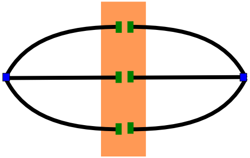
$\Rightarrow$ potential for multi-level

Problem:

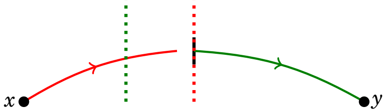
Natural building blocks have two or three propagator on surface

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

$\Rightarrow$ too much to be saved to disk



Projection of the propagator



Cut the fermion line with P:

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

P projects on lower dimensional space

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

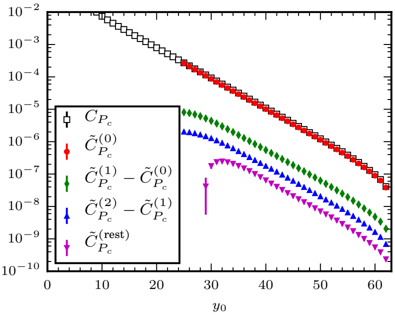
Reduce memory of building block $(6V_3)^2 \to N^2$

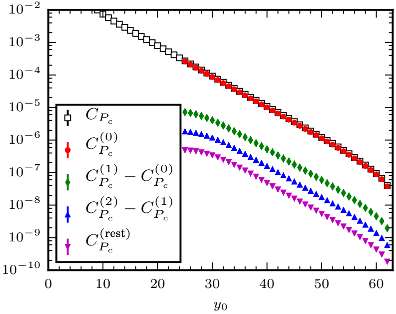
Several possibilities:

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

Pseudoscalar two-point function with

P: deflation subspace at $x_0/a = 24$





Deflation subspace:
$N_s = 60$ block modes, 4^4 blocks
Lüscher '07

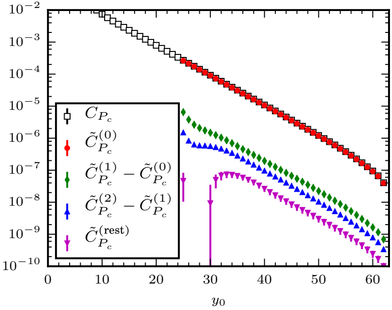
Factorization only
$\Delta/a = 8, 12, 16$

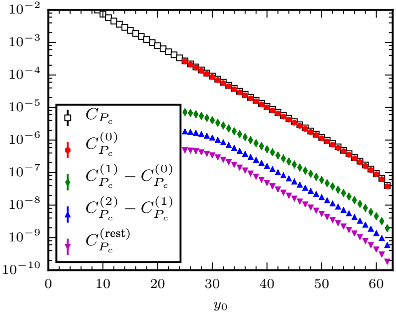
$\Rightarrow$ Virtually no difference visible

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

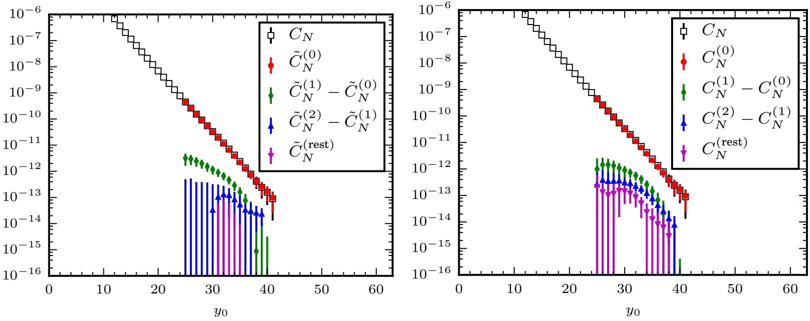
Factorization only
$\Delta/a = 8, 12, 16$

$\Rightarrow$ Virtually no difference visible

Projections: deflation subspace

Nucleon two-point function with

P: deflation subspace at $x_0/a = 24$



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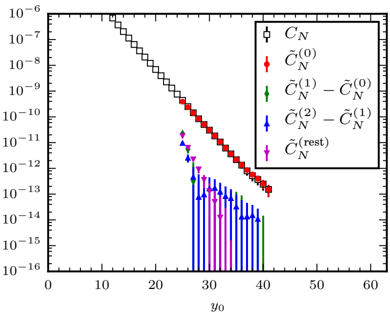
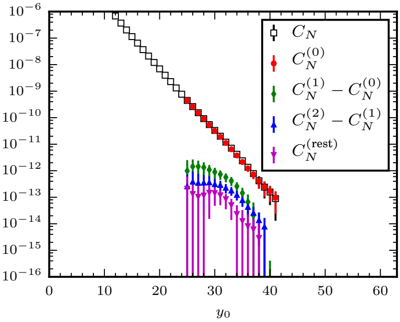




Block eigenvectors subspace:
$N_{ev} = 120$ vectors

Factorization only
$\Delta/a = 8, 12, 16$

$\Rightarrow$ **Surprise:** also the nucleon can be saturated by low-modes

Summary of factorization

Factorization of pion and nucleon two-point functions in principle possible.

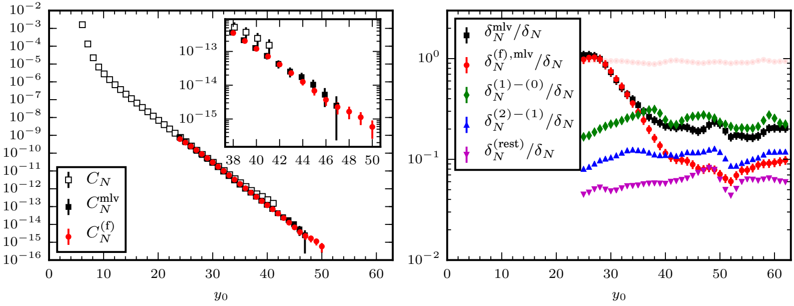
Two approximations involved:

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

Surprise: the nucleon propagator is saturated by low modes!

$\Rightarrow$ **Multilevel in quenched is possible**

Multilevel



Two-level Monte Carlo integration:

level-0 $n_0 = 50$ configurations

level-1 $n_1 = 20$ updates

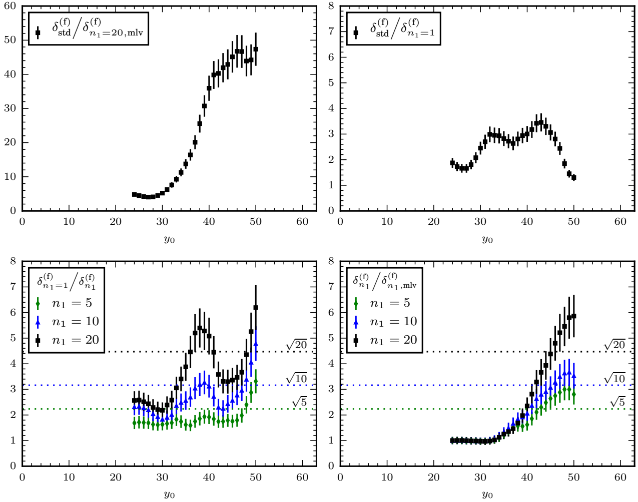
Factorized contribution with two-level algorithm

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

$$\left\langle \mathrm{tr}\left\{\Gamma\,\frac{1}{D}(x,x)\right\}\,\mathrm{tr}\left\{\Gamma\,\frac{1}{D}(y,y)\right\}\right\rangle$$

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

  `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 $\sqrt{N} \propto e^{mx_0} \longrightarrow N \propto e^{mx_0}$

$\Rightarrow$ **Number of configurations to reach target statistics**
$\sim$ **square root of the standard case**

Conclusions & Outlook

Two-level methods work:

- quark-line disconnected meson correlation functions

$$\left\langle \mathrm{tr}\left\{\Gamma\,\frac{1}{D}(x,x)\right\}\ \mathrm{tr}\left\{\Gamma\,\frac{1}{D}(y,y)\right\}\right\rangle$$

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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

$$S_\Gamma = D_\Gamma - D_{\partial\Gamma} D_{\Gamma^*}^{-1} D_{\partial\Gamma^*} \qquad S_{\Gamma^*} = D_{\Gamma^*} - D_{\partial\Gamma^*} D_\Gamma^{-1} D_{\partial\Gamma}$$

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

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

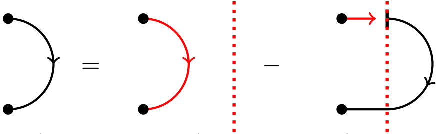
Correction term:

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

$$= \frac{1}{D_\Gamma - D_{\partial\Gamma} D_{\Gamma^*}^{-1} D_{\partial\Gamma^*}} D_{\partial\Gamma} D_{\Gamma^*}^{-1} D_{\partial\Gamma^*} \frac{1}{D_\Gamma} = -D^{-1} D_{\partial\Gamma^*} D_\Gamma^{-1}$$

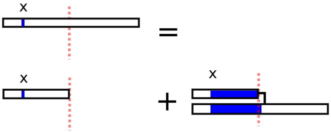
Quark propagator factorization, case I

Graphically: see talk by Schaefer



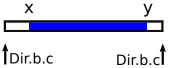
$$D^{-1} = D_\Gamma^{-1} - D^{-1} D_{\partial\Gamma^*} D_\Gamma^{-1}$$

or



Correction term δD_Γ^{-1} has propagator to and from boundary

$$\mathbf{Tr}\,\gamma_5 \delta D_\Gamma^{-1} \propto e^{-m_\pi \Delta}$$

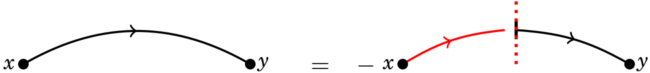


Quark propagator factorization, case II

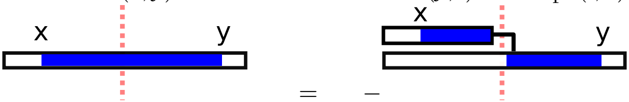
see talk by Schaefer

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

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



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



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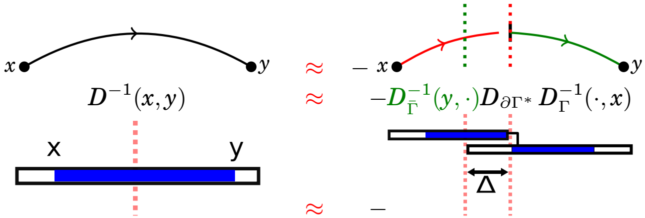
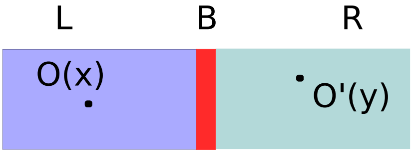


Approximation with a second Dirichlet b.c. cut
$\Rightarrow$ correction $\approx e^{M_\pi \Delta/2}$

Some error analysis

Garcia-Vera, Schaefer '16



$$\hat{A} = \frac{1}{N_0}\sum_{i=1}^{N_0}\frac{1}{N_1^2}\sum_{j=1}^{N_1}\sum_{k=1}^{N_1}\mathcal{O}^{ij}\mathcal{O}'^{ik}$$

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

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

$$\mathrm{Var}_L(\mathcal{O}) = \left[\mathcal{O}^2\right]_L - [\mathcal{O}]_L^2$$

Some error analysis

$$
\begin{aligned}
\sigma_A^2 = {} & \frac{1}{N_0 N_1^2} \langle \mathrm{Var}_L(\mathcal{O}) \mathrm{Var}_R(\mathcal{O}') \rangle_B && \to \text{const} \\
& + \frac{1}{N_0 N_1} \langle \mathrm{Var}_L(\mathcal{O}) [\mathcal{O}']_R^2 + \mathrm{Var}_R(\mathcal{O}') [\mathcal{O}\ ]_L^2 \rangle_B && \to e^{-2m\Delta} \\
& + \frac{1}{N_0} \left(\langle [\mathcal{O}]_L^2 [\mathcal{O}']_R^2 \rangle_B - \bar{A}^2 \right) && \to e^{-2m\Delta}
\end{aligned}
$$

Contributions which do not profit from multilevel inevitable.

These decay exponentially with the distance from the boundary Δ.

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.