Domain decomposition and multilevel integration for fermions I

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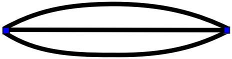
Based on: Cè, Giusti, S.S, Phys.Rev. D93 (2016) 094507

Motivation

Exponential signal-to-noise problem. `Parisi'83, Legage'89`

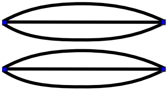
Nucleon two-point function

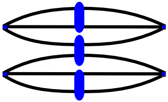
$$C_{\rm n}(x_0) \propto e^{-m_N x_0}$$



Variance has contribution from three pion state

$$\mathrm{var}(C_{\rm n}) \propto e^{-3m_\pi x_0}$$





Signal-to-noise ratio

$$\frac{C_{\rm n}(x_0)}{\delta C_{\rm n}(x_0)} \propto \sqrt{N} e^{-(m_{\rm n} - \frac{3}{2} m_\pi) x_0}$$

Becomes a problem at small pion masses

Lattice computations involving baryons highly unreliable.

Motivation

Larger distances need more averaging

$$\frac{C(x_0)}{\delta C(x_0)} \propto \sqrt{N} e^{-\alpha x_0}$$

Quark-line disconnected correlators

$\rightarrow$ contribution from the vacuum, error constant with distance.

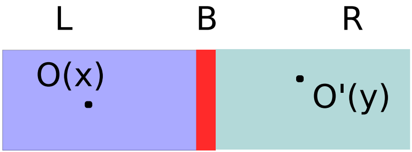
Use locality of the theory

Regions far away from each other are more and more independent

$\rightarrow$ can update them independently

Multilevel integration

General idea



Decompose lattice in regions

Action needs to decompose into independent contributions from these regions.

Write observable in product of region's contribution

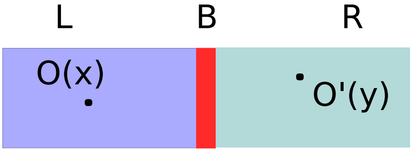
Classical examples

Multihit — Parisi, Petronzio, Rapuano'83

Multilevel for Wilson loops — Lüscher & Weisz '01

General idea

Two-Level algorithm



Level-0

N_0 realizations of boundary field B

Level-1

For each of the N_0 B fields: N_1 gauge fields in L and R

$\rightarrow$ Cost $\propto N_0 \times N_1$

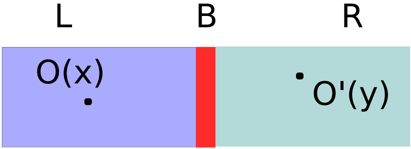
Construction of $N_0 \times N_1^2$ configurations.

In best case: signal-to-noise ratio $\propto \sqrt{N_0} \times N_1$

More slices: get effectively $N_1^{N_{\mathrm{slice}}}$ configs

see also: `Meyer'02, Giusti, Della Morte'08,'10`

General idea



Start with set of N_0 level-0 gauge field configurations

Define the boundary field U_B

$$\langle\{O(x)-\bar{O}\}\{O'(y)-\bar{O}'\}\rangle$$
$$=\frac{1}{Z_B}\int[dU_B]e^{-S_B[U_B]}[\{O(x)-\bar{O}\}]_L(U_B)[\{O'(y)-\bar{O}'\}]_R(U_B)$$

Estimate integrals over variables in L and R with N_1 configs per U_B

$$[O(x)]_L(U_B)=\frac{1}{Z_L}\int[dU_L]e^{-S(U_B,U_L)}O(x)$$
$$[O(y)]_R(U_B)=\frac{1}{Z_R}\int[dU_R]e^{-S(U_B,U_R)}O'(y)$$

Requirements

For multi-level to work we need two ingredients

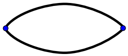
1) Factorized observable

2) Factorized action

Since we have used Wick's theorem, this is not obvious for observables and for the QCD action

Quark-line connected

$$\langle P^{ud}(x)P^{du}(y)\rangle = -\frac{1}{Z}\int [dU]\,\mathrm{det}\,D\,e^{-S_g[U]}\,\mathrm{tr}\left[\frac{1}{D_{m_u}}(x,y)\gamma_5\frac{1}{D_{m_d}}(y,x)\gamma_5\right]$$



Quark-line disconnected

$$\langle P^{uu}(x)P^{dd}(y)\rangle = \frac{1}{Z}\int [dU]\,\mathrm{det}\,D\,e^{-S_g[U]}\,\mathrm{tr}\left[\frac{1}{D_{m_u}}(x,x)\gamma_5\right]\mathrm{tr}\left[\frac{1}{D_{m_d}}(y,y)\gamma_5\right]$$

Approximate observables

Classical methods assume exact factorization of observable.

For fermions: only approximate observable factorizable.

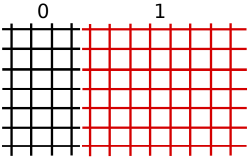
$$\langle \mathcal{O} \rangle = \langle \mathcal{O}_{\text{approx}} \rangle + \langle \mathcal{O} - \mathcal{O}_{\text{approx}} \rangle$$

$\langle \mathcal{O}_{\text{approx}} \rangle$: Use multilevel algorithm

$\langle \mathcal{O} - \mathcal{O}_{\text{approx}} \rangle$: standard estimate of correction term

Task: Find an excellent approximation to observable.

Factorizing the propagator



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

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

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

with the Schur complements

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

Basic strategy: substitute $S_\Gamma^{-1} \to D_\Gamma^{-1}$ in controlled manner

Case I: disconnected correlation functions

Quark-line disconnected correlation functions

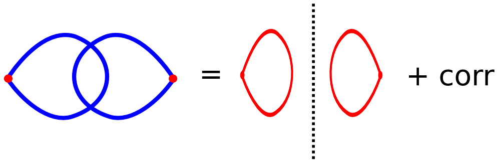
$$\langle P^{uu}(x)P^{dd}(y)\rangle = \frac{1}{Z}\int [dU] \det D\, e^{-S_g[U]} \mathrm{tr}\left[\frac{1}{D_{m_u}}(x,x)\gamma_5\right] \mathrm{tr}\left[\frac{1}{D_{m_d}}(y,y)\gamma_5\right]$$

Put boundary on time-slice between x and y.

Impose **Dirichlet boundary conditions** on surface of B.

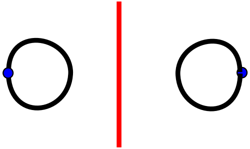
$$D^{-1}(x,x) \to D_\Gamma^{-1}(x,x)$$

Neglect contribution from links far away from x.



Quark-line disconnected

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



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

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

Approximation by imposing Dirichlet boundary conditions on B.

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

Correction term

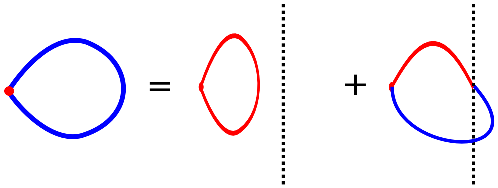
$$\frac{1}{D_\Gamma - D_{\partial\Gamma} D_{\Gamma^*}^{-1} D_{\partial\Gamma^*}} - \frac{1}{D_\Gamma}$$

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

Correction term

For diagonal elements

$$D^{-1}(x,x) = D_\Gamma^{-1} - D^{-1} D_{\partial\Gamma^*} D_\Gamma^{-1} = D_\Gamma^{-1} + \delta D_\Gamma^{-1}$$



Correction term has propagator to and from boundary.

$$\mathrm{tr}\gamma_5 \delta D^{-1}(y,y)] \propto e^{-m_\pi \Delta}$$

Full two point function split in four contributions

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

Case II: connected correlation functions

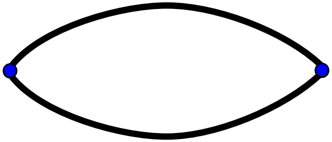
Quark-line connected correlation functions

$$\langle P^{ud}(x) P^{du}(y)\rangle$$
$$= -\frac{1}{Z}\int [dU] \det D \, e^{-S_g[u]} \mathrm{tr}\left[\frac{1}{D_{m_u}}(x,y)\gamma_5 \frac{1}{D_{m_d}}(y,x)\gamma_5\right]$$

Factorization less obvious

First factorization of the propagator

Second step factorization of two-point function



Factorization

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

Turn formula around

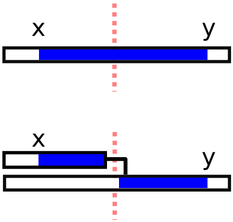
Inverse of Schur complement computed by projection of full propagator

For $x \in \Gamma$ and $y \in \Gamma^*$

$$D^{-1}(y, x)$$

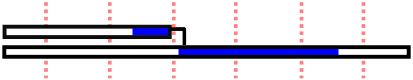
$$= -S_{\Gamma^*}^{-1}(y, \cdot)\, D_{\partial\Gamma^*}\, D_\Gamma^{-1}(\cdot, x)$$

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

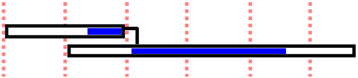


Approximation

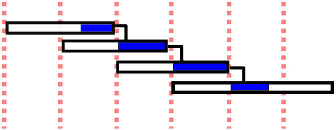
Introduce thick time slices



And **drop contributions** which are more than one time slice away by introducing Dirichelt boundary conditions



Iterate .....



$$D^{-1}(x,y) \approx (-1)^{m-l}\left[\prod_{i=l}^{m+1} D^{-1}_{\Omega_i^*} D_{\Lambda_{i,i-1}}\right](x,\cdot)\, D^{-1}_{\Omega_{m+2}}(\cdot,y)$$

Factorized propagator

Factorization of propagator in principle works.

Potential for multi-level

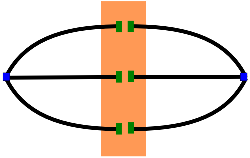
- small Δ already gives excellent approximation
- can be improved by hierarchy of Δ_i

Problem

Observable is the full correlation function

Natural building blocks have two or three propagator on surface

Problem with memory: $(6V_3)^2$ or $(6V_3)^3$ complex numbers



Summary

Multilevel methods offer a way to solve the exponential signal-to-noise problem

Need to factor observables into local contributions

For fermions it is possible to factorize approximate propagator.

Use to define approximate n-point functions $\rightarrow$ multilevel integration

Compute difference between approximate and exact observable with standard MC.

Demonstration of feasibility $\rightarrow$ following talk by M. Cè