Multi-boson block factorization of fermions

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Lattice 2017 - Granada June $19^{\rm th}$ 2017







Based on M. Cè, LG and S. Schaefer, PRD 93 (2016) 094507 [1601.04587], PRD 95 (2017) 034503 [1609.02419]

Outline



► Goal:

$$\{\det Q[U]\}^2 = \int \mathcal{D}\phi \dots \exp\left\{-S_0[\underline{U}_{\Omega_0^*},\dots] - S_1[\underline{U}_{\Lambda_1},\dots] - S_2[\underline{U}_{\Omega_1^*},\dots]\right\}$$

Motivation

► How:

Numerical tests

- domain decomposition
- multi-boson

► Conclusions & outlook

Signal/noise ratio: nucleon

The variance of the nucleon propagator

$$C_N(y_0, x_0) = \langle W_N(y_0, x_0) \rangle \propto e^{-M_N |y_0 - x_0|}$$

when $|y_0 - x_0| \rightarrow \infty$ goes as [Parisi 84; Lepage 89]

$$\sigma_N^2(y_0, x_0) \propto e^{-3M_\pi |y_0 - x_0|}$$





► Time distances of 1 fm or so are state of the art. For precise and accurate determinations of M_N, g_A,..., ⟨x⟩_{u-d}, ..., ChPT suggests that ~1.5 fm and ~2.5 fm are needed for two- and three-point functions respectively (see Bär's and Chang's plenary talks) [Tiburzi 09, 15; Bär 15-17; Hansen, Meyer 16]

Vector-vector correlator (See Lehner's plenary talk)

$$\frac{n_{\rm cnf} C_\rho^2}{\sigma_\rho^2} \propto n_{\rm cnf} \, e^{-2(M_\rho - M_\pi)|y_0 - x_0}$$

if m_{ρ} lighter than two-pion states. Relevant for ρ , g - 2, screening masses at finite T, \ldots

[Della Morte et al. 17]



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Non-zero momentum correlators

$$\frac{n_{\rm cnf}C_{\pi,\vec{p}}^2}{\sigma_{\pi,\vec{p}}^2} \propto n_{\rm cnf} \, e^{-2(E_{\pi}(\vec{p})-M_{\pi})|y_0-x_0|}$$

relevant for semi-leptonic decays, baryons, ...

[Della Morte et al. 17]



[Della Morte et al. 12] $q^2 = 2$ 0.75 0.5 0.25 0.250



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Static and static-light correlators [Lepage 92]

$$\frac{n_{\rm cnf} C_B^2}{\sigma_B^2} \propto n_{\rm cnf} \, e^{-2(E_{\rm stat}-M_\pi/2)|y_0-x_0}$$

relevant for $B \rightarrow I\nu, B \rightarrow \pi(K) I\nu, B \rightarrow K(K^*) II, \ldots$

Similar or worse problem for many other correlators, e.g. η' , glueballs, disconnected, \ldots





[Della Morte et al. 15]



Multi-level integration

[Parisi, Petronzio, Rapuano 83; Lüscher, Weisz 01; ...; Meyer 02; LG, Della Morte 08 10, ...]

 If also the observable can be factorized

$$O[U] = O_0[U_{\Omega_0^*}] imes O_2[U_{\Omega_1^*}]$$

then

$$\langle \mathcal{O}[\mathcal{U}] \rangle = \langle \langle \langle \mathcal{O}_0[\mathcal{U}_{\Omega_0^*}] \rangle \rangle_{\Lambda_0} \times \langle \langle \mathcal{O}_2[\mathcal{U}_{\Omega_1^*}] \rangle \rangle_{\Lambda_2} \rangle$$

where

$$\langle\!\langle O_0[U_{\Omega_0^*}]\rangle\!\rangle_{\Lambda_0} = \frac{1}{Z_{\Lambda_0}} \int \mathcal{D}U_{\Lambda_0} e^{-S_0[U_{\Omega_0^*}]} O_0[U_{\Omega_0^*}]$$

- Two-level integration:
 - n_0 configurations U_{Λ_1}
 - n_1 configurations U_{Λ_0} and U_{Λ_2} for each U_{Λ_1}
- If ⟨⟨·⟩⟩_{Λ_i} can be computed efficiently with a statistical error comparable to its central value, then the prefactor in the signal/noise ratio changes as

$$n_{
m cnf}
ightarrow n_0 n_1^2$$

at the cost of generating approximatively $n_0 n_1$ level-0 configurations



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 Λ_0

 $\dot{\Omega_0^*}$

 Λ_1

 Λ_2

 $\tilde{\Omega}_{1}^{*}$

• With more active blocks, at the cost of approximatively $n_0 n_1$ level-0 configurations,

$$n_{\rm cnf}
ightarrow n_0 n_1^{n_{\rm block}}$$

and the gain increases exponentially with the distance since $n_{\rm block} \propto |y_0 - x_0|$. For the same relative accuracy of the correlator, the computational effort would then increase approximatively linearly with the distance

Toward (the dream of) simulating large lattices

- Simulating large lattices by updating sub-lattices independently (see Lüscher's plenary talk)
- For example the lattices

 320^4 , a = 0.05 fm, L = 16 fm

 24×640^3 , a = 0.05 fm, L = 32 fm, T = 164 MeV

can split in 4096 48^4 and 24×48^3 overlapping blocks

This would open new perspectives for:

-

- Multi-baryon states
- Multi-particle scattering states
- Form factors at small momenta
- Gas of many hadrons at finite T





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Signal/noise ratio: the rôle of pions

• By defining $Q = \gamma_5 D$ and

$$W_{\pi}(y_0, x) = \sum_{\vec{y}} \operatorname{Tr} \left\{ Q^{-1}(y, x) [Q^{-1}(y, x)]^{\dagger} \right\}$$



at large time distances the pion propagator and its variance goes as

$$C_{\pi}(y_{0}, x_{0}) = \langle W_{\pi}(y_{0}, x) \rangle \propto e^{-M_{\pi}|y_{0} - x_{0}|} \qquad \sigma_{\pi}^{2}(y_{0}, x_{0}) \propto e^{-2M_{\pi}|y_{0} - x_{0}|}$$

and therefore the signal/noise ratio is (almost) constant

Indeed, when $|y - x| \rightarrow \infty$, numerical simulations confirm that

$$\operatorname{Tr}\left\{Q^{-1}(y,x)[Q^{-1}(y,x)]^{\dagger}\right\} \propto e^{-M_{\pi}|y-x|}$$

for every background field in the representative ensemble. The size of each quark line, $\exp\{-M_{\pi}|y-x|/2\}$, is responsible for large fluctuations in other connected correlators (See also Grabowska, Kaplan, Nicholson 13; Kaplan 13; Wagman, Savage 17)

The suppression of the propagator with the distance between source and sink, however, is also the clue for the solution





By defining the Schur complement as usual

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

and by choosing $\Gamma = \Lambda_2$ and $\Gamma^* = \Omega_0^*$, the inverse can be written as

$$Q^{-1} = \begin{pmatrix} & \dots & & & \\ & & \dots & & \\ & & \dots & & Q_{\Omega_0^*}^{-1} + Q_{\Omega_0^*}^{-1} Q_{\Lambda_{1,2}} S_{\Lambda_2}^{-1} Q_{\Lambda_{2,1}} Q_{\Omega_0^*}^{-1} \end{pmatrix}$$

► The dependence from the gauge field in Λ_2 stems from the second contribution in the 22 element, a term which is suppressed $\propto e^{-M_{\pi}\Delta}$ for large values of the thickness Δ of Λ_1

What about the gauge-field dependence of Q⁻¹(y, x) when x ∈ Λ₀ and y ∈ Λ₂ ?



- What about the gauge-field dependence of Q⁻¹(y, x) when x ∈ Λ₀ and y ∈ Λ₂ ?
- Again DD $[\Gamma = \Lambda_0 \text{ and } \Gamma^* = \Omega_1^*]$

$$Q^{-1} = \begin{pmatrix} S_{\Lambda_0}^{-1} & \dots & \\ & & \\ -Q_{\Omega_1^*}^{-1} Q_{\Lambda_{1,0}} S_{\Lambda_0}^{-1} & \dots & \end{pmatrix}$$

The 11 element and previous result give

$$S_{\Lambda_{\mathbf{0}}}^{-1} = P_{\Lambda_{\mathbf{0}}} Q^{-1} P_{\Lambda_{\mathbf{0}}} = P_{\Lambda_{\mathbf{0}}} Q_{\Omega_{\mathbf{0}}^{*}}^{-1} P_{\Lambda_{\mathbf{0}}} + \dots$$

which together with the 21 term leads to

$$Q^{-1}(y,x) = -Q^{-1}_{\Omega_1^*}(y,\cdot)Q_{\Lambda_{1,0}}Q^{-1}_{\Omega_0^*}(\cdot,x) + \dots$$



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Let us understand it better.....

By introducing the matrix

$$\omega = P_{\partial \Lambda_{\mathbf{0}}} Q_{\Omega_{\mathbf{0}}^*}^{-1} Q_{\Lambda_{\mathbf{1},\mathbf{2}}} Q_{\Omega_{\mathbf{1}}^*} Q_{\Lambda_{\mathbf{1},\mathbf{0}}}$$

which :

- Acts on one boundary only
- Is suppressed (exp.) in Δ
- Has factorized field dependence



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• The exact propagator for $x \in \Lambda_0$ and $y \in \Lambda_2$ is given by [Lüscher 16; Cè, LG, Schaefer 17]

$$Q^{-1}(y,x) = -Q_{\Omega_1^*}^{-1}(y,\cdot)Q_{\Lambda_{\mathbf{1},\mathbf{0}}} \frac{1}{1-\omega} Q_{\Omega_{\mathbf{0}}^*}^{-1}(\cdot,x)$$

and analogously for the other components

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$$Q^{-1}(y,x) = -Q_{\Omega_{\mathbf{1}}^{\mathbf{1}}}^{-1}(y,\cdot)Q_{\Lambda_{\mathbf{1},\mathbf{0}}} \sum_{n=0}^{\infty} \omega^n Q_{\Omega_{\mathbf{0}}^{\mathbf{1}}}^{-1}(\cdot,x)$$

and analogously for the other components

Full gauge dependence factorized. Built by quarks looping around the boundaries, each loop bringing a suppression factor ∝ e^{-M_πΔ}. Merit of SAP with overlapping domains

A crucial test on the spectrum of ω

 Wilson glue with two-flavours of O(a)improved Wilson quarks

$$\beta = 5.3$$
, $c_{_{\rm SW}} = 1.90952$, $k = 0.13625$

$$(T/a) \times (L/a)^3 = 64 \times 32^3$$
, $a = 0.065$ fm

 $n_{\rm cnf} = 200 \quad aM_{\pi} = 0.1454 \,, \quad M_{\pi} = 440 \,\,{\rm MeV}$

Computed 60 eigenvalues with largest norm

$$\omega \mathbf{v}_{i} = \mathbf{\delta}_{i} \mathbf{v}_{i}$$

 $\Delta = 12a$



 $\bar{\delta} = \exp\{-M_{\pi}\Delta\}$

Δ/a	$\overline{\delta}$	$\langle max_i \ket{\delta_i} angle$	$\sigma(max_i \delta_i)$	$\max\max_i \delta_i $
8	0.3273	0.2886	0.0616	0.5130
12	0.1710	0.1692	0.0453	0.3193
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30 25 20 15 10 5 0 0.05 0.10 0.15 0.20 0.25 0.30 0.35 max, [\delta]

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For the matrix (1 − ω) the spectral gap ε is large (as expected). For Δ = 12a ~ 0.8 fm is ε ~ 0.7 or so. The Neumann series converges very fast!

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▶ We start again from

$$Q = \left(egin{array}{cc} Q_{\Gamma} & Q_{\partial\Gamma} \ Q_{\partial\Gamma^*} & Q_{\Gamma^*} \end{array}
ight)$$





$$\det \ Q = \frac{1}{\det \ Q_{\Gamma^*}^{-1} \det \ S_{\Gamma}^{-1}}$$



$$\det Q = \frac{1}{\det Q_{\Gamma^*}^{-1} \det [P_{\Gamma} Q^{-1} P_{\Gamma}]}$$

▶ By first choosing $\Gamma^* = \Lambda_1$ and $\Gamma = \Lambda_0 \cup \Lambda_2$, and then iterating once more in Γ

$$\det \ Q = \frac{1}{\det \ Q_{\Lambda_{1,1}}^{-1} \det \left[P_{\Lambda_{2}} \ Q_{\Omega_{1}^{*}}^{-1} \ P_{\Lambda_{2}} \right] \det \left[P_{\Lambda_{0}} \ Q^{-1} \ P_{\Lambda_{0}} \right]}$$

Determinant factorizes in 3 terms, but last factor still depends on gauge field everywhere

By remembering again that

$$P_{\Lambda_{\mathbf{0}}} Q^{-1} P_{\Lambda_{\mathbf{0}}} = P_{\Lambda_{\mathbf{0}}} Q_{\Omega_{\mathbf{0}}^{*}}^{-1} P_{\Lambda_{\mathbf{0}}} + \dots$$





$$\det Q = \frac{1}{\det Q_{\Lambda_{1,1}}^{-1} \det \left[P_{\Lambda_{0}} Q_{\Omega_{0}^{-1}}^{-1} P_{\Lambda_{0}} \right] \det \left[P_{\Lambda_{2}} Q_{\Omega_{1}^{+}}^{-1} P_{\Lambda_{2}} \right]} \det \left(1 - \omega \right)$$

For the first 3 terms factorization of the gauge dependence achieved, e.g. for $N_f = 2$

$$\frac{1}{\det\left[P_{\Lambda_{2}} Q_{\Omega_{1}^{*}}^{-1} P_{\Lambda_{2}}\right]^{2}} = \int [d\phi_{2} d\phi_{2}^{\dagger}] e^{-|P_{\Lambda_{2}} Q_{\Omega_{1}^{*}}^{-1} \phi_{2}|^{2}}$$

• The matrix ω is the only direct coupling between the gauge field in Λ_0 and Λ_2

► Again the matrix

$$\omega = P_{\partial \Lambda_{\mathbf{0}}} Q_{\Omega_{\mathbf{0}}^*}^{-1} Q_{\Lambda_{\mathbf{1},\mathbf{2}}} Q_{\Omega_{\mathbf{1}}^*}^{-1} Q_{\Lambda_{\mathbf{1},\mathbf{0}}}$$

which is also:

- similar to ω^\dagger



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By writing also in this case

$$\det\left(1-\omega
ight)=rac{1}{\det[(1-\omega)^{-1}]}$$

Again the matrix

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We can expand again (1 − ω)⁻¹ in series [u_k = e^{i 2πk}/_{N+1}] [Lüscher 93; Borici, de Forcrand 95; Jegerlehner 95]

$$\frac{\det(1-\omega)}{\det[1-R_{N+1}(\omega)]} = \frac{1}{\det[P_N(\omega)]} \propto \prod_{k=1}^{N/2} \det^{-1}\{(u_k-\omega)^{\dagger}(u_k-\omega)\}$$

by choosing $P_N(\omega) = \sum_{n=0}^N \omega^n$ so that $|R_{N+1}(\omega)| = |\omega^{N+1}| \le (1-\epsilon)^{N+1}$

• But the gauge fields in Λ_0 and Λ_2 still both enter ω



$$rac{1}{\det[P_N(1-\omega)]} \propto \prod_{k=1}^{N/2} \det^{-1}(W_{\sqrt{u_k}}^{\dagger} W_{\sqrt{u_k}})$$



the auxiliary multi-boson fields can be introduced on both boundaries so that for $N_f = 2$ [Lüscher 93; Borici, de Forcrand 95; Jegerlehner 95]

$$rac{1}{\det[P_N(1-\omega)]^2} \propto \prod_{k=1}^N \left\{ \int [d\chi_k d\chi_k^\dagger] e^{-|W_{\sqrt{w_k}}\chi_k|^2}
ight\}$$

where, by defining $\eta_k = P_{\partial \Lambda_0} \chi_k$ and $\xi_k = P_{\partial \Lambda_2} \chi_k$,

$$|W_{z}\chi_{k}|^{2} = |P_{\partial\Lambda_{0}}Q_{\Omega_{0}^{*}}^{-1}Q_{\Lambda_{1,2}}\xi_{k}|^{2} + |P_{\partial\Lambda_{2}}Q_{\Omega_{1}^{*}}^{-1}Q_{\Lambda_{1,0}}\eta_{k}|^{2} + z(\xi_{k}, Q_{\Lambda_{2,1}}Q_{\Omega_{0}^{*}}^{-1}\eta_{k}) + \dots$$

► The dependence of the full bosonic action from the links in Λ_0 and Λ_2 is thus factorized. The (small) direct coupling, *due to quarks looping up to N times around the boundaries*, is replaced by a block-local interaction of links with N/2 multi-boson fields per flavour

Multi-level integration with fermions

A generic scheme for multi-level integration is:

$$\langle O \rangle = \frac{\langle O \, \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N} = \frac{\langle O_{\rm fact} \, \rangle_N}{\langle \mathcal{W}_N \rangle_N} + \frac{\langle O \, \mathcal{W}_N - O_{\rm fact} \rangle_N}{\langle \mathcal{W}_N \rangle_N}$$

where O_{fact} is a (rather precise) approximation of O, and $\langle O_{\text{fact}} \rangle_N$ is computed by multi-level integration with (a small number of) N multi-boson fields

• For $N_f = 2$, the reweighting factor is

$$\mathcal{W}_{N} = \det\{1 - R_{N+1}(1-\omega)\}^{2} = \frac{\int [d\eta] [d\eta^{\dagger}] e^{-|(1-R_{N+1})^{-1}\eta|^{2}}}{\int [d\eta] [d\eta^{\dagger}] e^{-\eta^{\dagger}\eta}}$$

where $R_{N+1}(1-\omega) = \omega^{N+1}$

- Given the large spectral gap of (1ω) , and depending on the target statistical error, W_N can be neglected with $N \sim 10$ or so. Not a big number!
- In practice $\Delta \sim 0.5$ fm or so may be already sufficient for ω to be suppressed enough

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Correlation functions of gluonic operators

We have computed the gluonic fields

$$\begin{split} \bar{e}(x_0) &= \frac{1}{4} \sum_{\vec{x}} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x) \\ \bar{q}(x_0) &= \frac{1}{64\pi^2} \sum_{\vec{x}} \epsilon_{\mu\nu\rho\sigma} F^a_{\mu\nu}(x) F^a_{\rho\sigma}(x) \end{split}$$

and the expectation values

$$C_{e}(x_{0}) = \frac{1}{L^{3}} \langle \bar{e}(x_{0}) \rangle$$
$$C_{qq}(y_{0}, x_{0}) = \frac{1}{L^{3}} \langle \bar{q}(y_{0}) \, \bar{q}(x_{0})$$

Blocking with two level integration in Λ₀ and Λ₂

$$\Lambda_0$$
: $x_0 \in [0, 23a]$, Λ_1 : $x_0 \in [24a, 35a]$

 Λ_2 : $x_0 \in [36a, 63a]$, a = 0.065 fm, N = 12

the gain turns out to be the best possible one



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• Blocking with two level integration in Λ_0 and Λ_2 $\Lambda_0 : x_0 \in [0, 23a]$, $\Lambda_1 : x_0 \in [24a, 35a]$ $\Lambda_2 : x_0 \in [36a, 63a]$, a = 0.065 fm, N = 12the gain turns out to be the best possible one



Multi-level for nucleon two-point function

Wilson glue with quenched Wilson quarks

$$\beta = 6.0$$
, $k = 0.1560$, $(T/a) \times (L/a)^3 = 64 \times 24^3$

 $a = 0.093 \, {
m fm}$ $a M_{\pi} = 0.215$, $M_{\pi} = 455 \, {
m MeV}$

 $n_{\rm cnf} = 1000$, $n_0 = 50$, $n_1 = 20$

The Wick contraction is decomposed as

$$W_N(y_0, x_0) = W_N^{\text{fact}}(y_0, x_0) + W_N^r(y_0, x_0)$$





Multi-level for nucleon two-point function

Wilson glue with quenched Wilson quarks

$$\beta = 6.0, \quad k = 0.1560, \quad (T/a) \times (L/a)^3 = 64 \times 24^3$$

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- At large time distances the multi-level works at its best. The (signal/noise)² is proportional to n₁² (as opposed to n₁) until it hits the green curve
- Refined definitions of $W_N^{\text{fact}}(y_0, x_0)$ are desirable to make computation even cheaper ...
- For similar results in other channels (vector-vector, pion with $\vec{p} \neq 0,...$) see (M. Cè parallel talk on Thursday)

Conclusions & Outlook



- The effective quark interaction among the gauge field at distant points can be factorized out in (L)QCD by exploiting a decomposition of the space-time in overlapping domains
- By introducing (a small number of) multi-boson auxiliary fields, the resulting action is local in the block scalar and gauge fields and can be efficiently simulated

$$\{\det Q[U]\}^2 = \int \mathcal{D}\phi \dots \exp\left\{-S_0[U_{\Omega_0^*},\dots] - S_1[U_{\Lambda_1},\dots] - S_2[U_{\Omega_1^*},\dots]\right\}$$

When combined with the factorization of Wick contractions, these results pave the way for multi-level integration in the presence of fermions, opening new perspectives in LGT

Conclusions & Outlook



The computations of many interesting quantities are expected to profit: baryons (g_A,..., < x >_{u−d}), g − 2, leptonic, semi-leptonic and hadronic decays, ρ,η',

- Domains need neither to have a particular shape nor to be connected. What matters is the minimum distance between Λ₀ and Λ₂. 4D decomposition attractive for large volumes
- Two key ingredients: locality of the Dirac operator and the fast decrease of its inverse with the distance between sink and source. The factorization may, therefore, be applicable to very different theories with fermions if they enjoy these very basic properties