locality and multi-level sampling of hadronic correlators

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Scattering Amplitudes and Resonance Properties from Lattice QCD
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references

based on work with L. Giusti and S. Schaefer

- Phys. Rev. D **93** (2016) 094507 [arXiv:1601.04587]
- PoS(LATTICE2016)263 [arXiv:1612.06424]
- Phys. Rev. D **95** (2017) 034503 [arXiv:1609.02419]
- EPJ Web Conf. **175** (2018) 01003 [arXiv:1710.09212]
- EPJ Web Conf. **175** (2018) 11005 [arXiv:1711.01592]

and ongoing work, not discussed in this talk

motivations

fermions in Monte Carlo simulations

the path integral of Euclidean, lattice-regulated QCD

$$\mathcal{Z} = \int \mathcal{D}[U,\psi,\bar{\psi}] \exp\left\{ -S_{\mathrm{g}}[U] - \int \mathrm{d}^4x\, \bar{\psi} D \psi \right\}$$

to apply Monte Carlo methods, fermions are integrated out analytically

$$\mathcal{Z} = \int \mathcal{D}[U] \det D \exp\left\{ -S_{\mathrm{g}}[U] \right\}$$

with $\det D$ typically simulated with pseudofermions [Weingarten 1981]

$$\det\left\{ D^\dagger D \right\} \sim \int \mathcal{D}\left[\phi,\phi^\dagger\right] \exp\left\{ -\int \mathrm{d}^4x \left| D^{-1}\phi \right|^2 \right\}$$

and Wick's theorem applies to fermionic observables, e.g.

$$\langle [\bar{\psi}\gamma_5\psi](x)[\bar{\psi}\gamma_5\psi](0) \rangle_{U,\psi,\bar{\psi}} = \left\langle D^{-1}(0,x)\gamma_5 D^{-1}(x,0)\gamma_5 \right\rangle_U$$

$\Rightarrow$ locality is not manifest

- the fermion determinant $\det D$ is a non-local functional of the gauge field U
- fermion propagators D^{-1} are non-local functionals of the gauge field U

fermions in Monte Carlo simulations

in the non-singlet pseudoscalar meson sector ($P(x) = [\bar{\psi}\gamma_5\psi](x)$)

$$\sum_{\vec{x}} \langle P(x)P(0)\rangle \sim \mathrm{e}^{-M_\pi|x_0|} \qquad \text{for } x_0 \to \infty$$

while the variance behaves like a $\pi\pi$ state

$$\sigma^2_{PP} = \sum_{\vec{x},\vec{y}} \langle P(x)P(0)P(y)P(0)\rangle - \Big[\sum_{\vec{x}} \langle P(x)P(0)\rangle\Big]^2 \sim \mathrm{e}^{-2M_\pi|x_0|}$$

$\Rightarrow$ special rôle of pions: no signal-to-noise ratio (S/N) problem
compare e.g. correlators of gluon operators, or Wilson loops, that have constant variance with distance
$\Rightarrow$ the quark propagator decays with distance on every single gauge configuration

[Parisi 1984]

$$\left\|D^{-1}\right\|(x,0) = \left[D^{\dagger -1}D^{-1}\right]^{1/2}(x,0) \sim \mathrm{e}^{-M_\pi/2|x|}$$

fermions in Monte Carlo simulations

still, S/N problem in other fermionic observables [Parisi 1984; Lepage 1989]

- pseudoscalar mesons with non-zero momentum
- vector current correlator, e.g. $g-2$ hadronic vacuum polarization computation
- flavour-singlet mesons: the variance of disconnected contributions is not suppressed with distance
- nucleon propagator: $S/N \sim \exp\left\{-[M_N - 3/2 M_\pi]\left|x_0\right|\right\}$
  $\Rightarrow$ worsening towards physical pion masses
  $\Rightarrow$ connection to sign problem at positive baryon chemical potential
- heavy-light mesons

solution for bosonic theories: multi-level Monte Carlo integration

[Parisi, Petronzio, Rapuano 1983; Lüscher, Weisz 2001; Meyer 2003; Giusti, Della Morte 2008, 2010]

with fermions, giving up manifest locality

$\Rightarrow$ multi-level method are not straightforward to apply

multi-level Monte Carlo integration

introduced for bosonic theories as the multihit algorithm [Parisi, Petronzio, Rapuano 1983]
then generalized as the multi-level algorithm [Lüscher, Weisz 2001; Meyer 2003]

- domain decomposition of the lattice:
  thick time slices $0, 1, 2, \ldots$

- factorization of the action $S_g[U] = S[U_0] + S[U_1] + S[U_2] + S[U_3] + \ldots$

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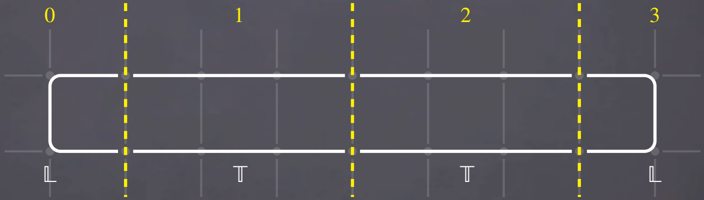

- factorization of the action $S_{\mathrm{g}}[U] = S[U_0] + S[U_1] + S[U_2] + S[U_3] + \ldots$
- factorization of $W(C) = \mathbb{L}[U_0]\mathbb{T}[U_1]\mathbb{T}[U_2]\mathbb{L}[U_3]$

$$\langle W(C)\rangle = \langle\, \mathbb{L} \quad \mathbb{T} \quad \mathbb{T} \quad \mathbb{L} \,\rangle$$

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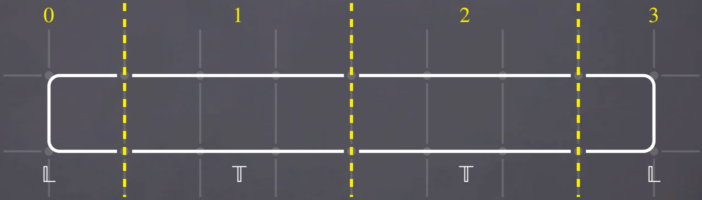


- factorization of the action $S_{\mathrm{g}}[U] = S[U_0] + S[U_1] + S[U_2] + S[U_3] + \dots$
- factorization of $W(C) = \mathbb{L}[U_0]\mathbb{T}[U_1]\mathbb{T}[U_2]\mathbb{L}[U_3]$

$$\langle W(C) \rangle = \langle [\mathbb{L}]_0 [\mathbb{T}]_1 [\mathbb{T}]_2 [\mathbb{L}]_3 \rangle$$

- n_1 level-1 Monte Carlo updates and average $[\,\cdot\,]_i$ in thick time slice i

multi-level Monte Carlo integration

- at level-0 the whole lattice is sampled ⇒ standard MC average
- level-1 average

$$[\mathbb{T}]_i \sim \exp\{-\sigma_1 L T_i\}, \quad \sigma_{\mathbb{T}}^2 = \mathcal{O}(1/n_1)$$

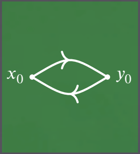
- the more the Wilson loop extends,
  the more independent thick time slices contribute to the averaging
- exponential noise reduction with larger Wilson loops

⇒ with the right setup, the S/N problem is solved

however, locality of the action and of the observables is assumed
but in the theory with fermions, locality is not manifest

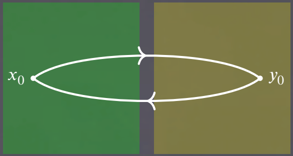
⇒ no straightforward application

multi-level Monte Carlo with fermions

$C_\Gamma(y_0, x_0) =$ 

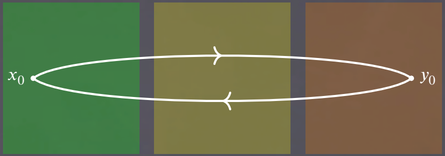
number of samples n_1 $= n_1$

multi-level Monte Carlo with fermions

$C_\Gamma(y_0, x_0) =$ 

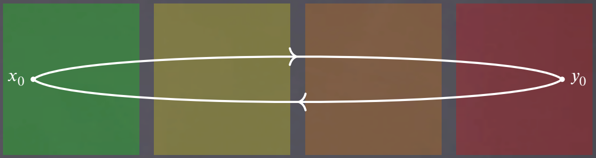
number of samples $n_1 \cdot n_1 \quad = n_1^2$

multi-level Monte Carlo with fermions

$C_\Gamma(y_0, x_0) =$ 

number of samples $n_1 \cdot n_1 \cdot n_1 \quad = n_1^3$

multi-level Monte Carlo with fermions

$C_\Gamma(y_0, x_0) =$ 

number of samples $n_1 \cdot n_1 \cdot n_1 \cdot n_1 = n_1^4$

$\Rightarrow$ the error is reduced with distance exponentially

$$\sigma_{C_\Gamma} \sim \left(n_1^{-1/2}\right)^{\frac{|x_0-y_0|}{\Delta}} \mathrm{e}^{-M_\pi|x_0-y_0|} = \mathrm{e}^{-\left(M_\pi+\frac{\ln n_1}{2\Delta}\right)|x_0-y_0|}$$

- only up to the extent that there is a S/N problem

how? we need a factorization at the block level of

- $\det D$, the quark determinant
- D^{-1}, the quark propagator

locality of the Dirac operator

using the LDU block-decomposition the (Wilson-)Dirac operator

$$D = \begin{pmatrix} D_0 & D_{01} \\ D_{10} & D_1 \end{pmatrix} = \begin{pmatrix} \mathbb{1} & \\ D_{10} D_0^{-1} & \mathbb{1} \end{pmatrix} \begin{pmatrix} D_0 & \\ & D/D_0 \end{pmatrix} \begin{pmatrix} \mathbb{1} & D_0^{-1} D_{01} \\ & \mathbb{1} \end{pmatrix}$$

- ultralocal operator $\Rightarrow$ D_{01}, D_{10} are supported on the boundaries
- $D/D_0 = D_1 - D_{10} D_0^{-1} D_{01}$ is the Schur complement of the block D_0

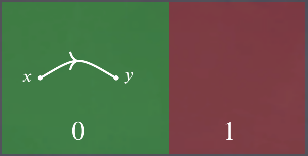
the inverse is block-decomposed in

$$D^{-1} = \begin{pmatrix} D_0^{-1} - D_0^{-1} D_{01} [D/D_0]^{-1} D_{10} D_0^{-1} & -D_0^{-1} D_{01} [D/D_0]^{-1} \\ -[D/D_0]^{-1} D_{10} D_0^{-1} & [D/D_0]^{-1} \end{pmatrix}$$

note: the inverse of D/D_0 is a block in the inverse of D

$$[D/D_0]^{-1} = P_1 D^{-1} P_1$$

quark propagator factorization



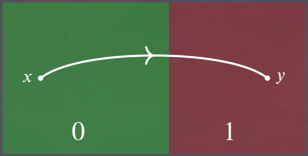
$$D^{-1} = \begin{pmatrix} D_0^{-1} - D_0^{-1} D_{01} D^{-1} D_{10} D_0^{-1} & -D_0^{-1} D_{01} D^{-1} P_1 \\ -P_1 D^{-1} D_{10} D_0^{-1} & P_1 D^{-1} P_1 \end{pmatrix}$$

two cases:

1. source x and sink y inside region $0 \Rightarrow$ disconnected contributions

$$D^{-1}(y,x) = D_0^{-1}(y,x) - \sum_{z,w \in \partial o} \left[D_0^{-1} D_{01} \right](y,z) D^{-1}(z,w) \left[D_{10} D_0^{-1} \right](w,x)$$

quark propagator factorization



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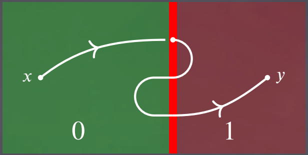
2. source x in region 0, sink y in region 1

$$D^{-1}(y,x) = - \sum_{z \in \partial o} D^{-1}(y,z) \left[D_{10} D_0^{-1} \right](z,x)$$

quark propagator factorization, 2.



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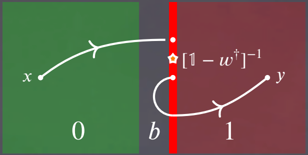


$$D^{-1}(y,x) = -\sum_{z\in\partial 1} D^{-1}(y,z)\left[D_{1b}D_{\bar{0}}^{-1}\right](z,x)$$

or equivalently

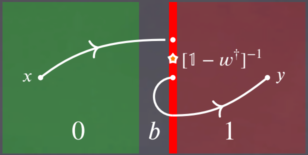
$$D^{-1}(y,x) = -\sum_{z\in\partial 1} D_{\bar{1}}^{-1}\left[\mathbb{1} - w^\dagger\right]^{-1}(y,z)\left[D_{1b}D_{\bar{0}}^{-1}\right](z,x)$$

- overlapping regions: $\bar{0} = 0 \cup b$, $\bar{1} = 1 \cup b$
- $w = D_{\bar{1}}^{-1} D_{b0} D_{\bar{0}}^{-1} D_{b1}$ is 'small', $\mathcal{O}(\mathrm{e}^{-M_\pi \|b\|})$

[Phys. Rev. D **95** (2017) 034503]

$\Rightarrow$ the Neumann series converges

quark propagator factorization, 2.



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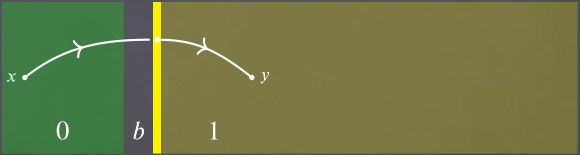
  $\Rightarrow$ the Neumann series converges
- the first term is completely factorized

$$D^{-1}(y,x) \approx -\sum_{z\in\partial o} D_{\bar{1}}^{-1}(y,z)\Big[D_{1b}D_{\bar{0}}^{-1}\Big](z,x)$$

quark propagator factorization, 2.

the extension to multiple regions is straightforward



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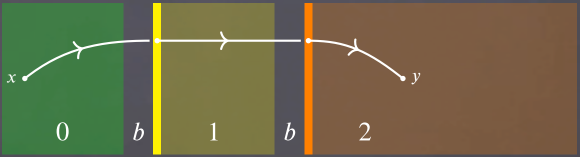
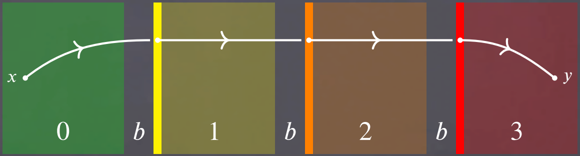


$$D^{-1}(y,x) \approx + \sum_{z \in \partial o} D_{\bar{2}}^{-1}(y,z') \left[D_{2b} D_{\bar{1}}^{-1} \right](z',z) \left[D_{1b} D_{\bar{0}}^{-1} \right](z,x)$$

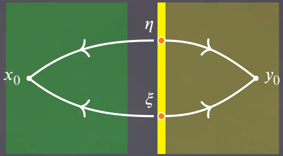
quark propagator factorization, 2.

the extension to multiple regions is straightforward



$$D^{-1}(y,x) \approx -\sum_{z\in\partial o} D_{\bar{3}}^{-1}(y,z'')\left[D_{3b}D_{\bar{2}}^{-1}\right](z'',z')\left[D_{2b}D_{\bar{1}}^{-1}\right](z',z)\left[D_{1b}D_{\bar{0}}^{-1}\right](z,x)$$

hadronic propagator factorization, implementation



$$C_\Gamma(y_0, x_0) \approx \mathrm{tr}\Big\{ \xi^\dagger D_{\bar{1}}^{-1}(\cdot, y_0)\gamma_5 \Gamma D_{\bar{1}}^{-1}(y_0, \cdot)\eta$$

$$\eta^\dagger D_{1b} D_{\bar{0}}^{-1}(\cdot, x_0)\Gamma\gamma_5 D_{\bar{0}}^{-1} D_{b1}(x_0, \cdot)\xi \Big\}$$

⇒ quark line 'cutting'

successful factorization obtained with [Phys. Rev. D **93** (2016) 094507]

- inverse iteration vectors of the Dirac operator in region b
- local deflation subspace (from openQCD)

bad volume scaling ⇒ possibly expensive, further studies needed

note: the (small) bias introduced by any approximation is corrected at level 0

alternative strategy: A. Nada, Lattice 2018 talk

numerical tests

test the multi-level in the quenched theory

$\Rightarrow$ trivial factorization of the action, negligible generation cost

with 64×24^3, OBCs in time, $a \approx 0.093\,\mathrm{fm}$, $aM_\pi \approx 0.216$

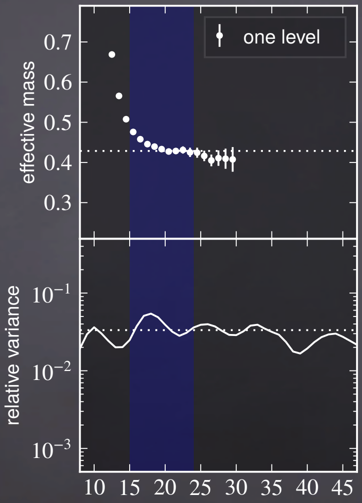
[Phys. Rev. D **93** (2016) 094507]

$n_0 = 50$ global updates and $n_1 = 30$ independent updates of two regions

region $0 = \{x : x_0 \in (0, 15)\}$ region $1 = \{x : x_0 \in (24, T)\}$

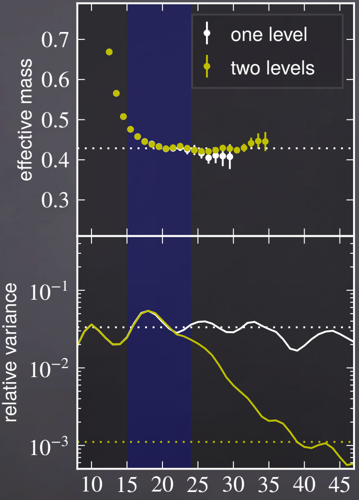
while gauge links in region $b = \{x : x_0 \in (16, 23)\}$ are frozen

pseudoscalar correlator with $p^2 = 2$



- $n_0 = 50$, $n_1 = 30$
- stochastic $3d$-volume sources on time-slice $x_0 = 8a \in$ region 0
- S/N decaying with $\sqrt{M_\pi^2 + p^2} - M_\pi \approx 0.213/a$
- single level average
  $\Rightarrow$ standard reduction of variance $\propto 1/n_1$

pseudoscalar correlator with $p^2 = 2$



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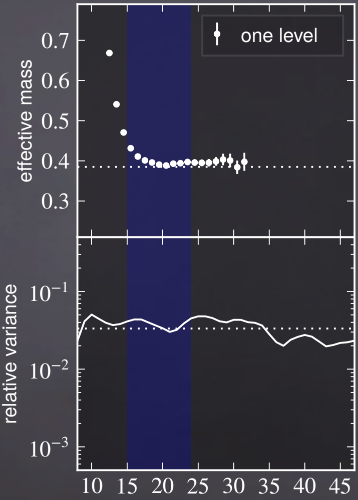
- two levels average $\Rightarrow$ improved variance reduction, $\propto 1/n_1^2$ for $y_0 \in$ region 1

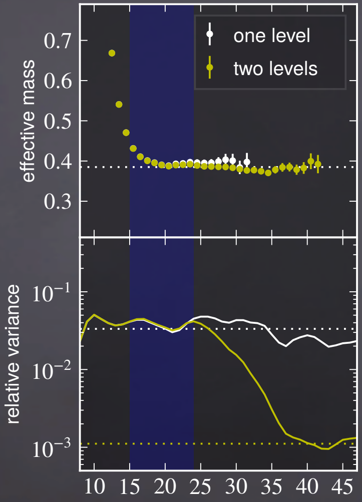
vector correlator



- $n_0 = 50$, $n_1 = 30$
- stochastic $3d$-volume sources on time-slice $x_0 = 8a \in$ region 0
- S/N decaying with

  $M_\rho - M_\pi \approx 0.170/a$
- single level average
  $\Rightarrow$ standard reduction of variance $\propto 1/n_1$

vector correlator



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- S/N decaying with

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- single level average
  $\Rightarrow$ standard reduction of variance
  $\propto 1/n_1$
- two levels average
  $\Rightarrow$ improved variance reduction,
  $\propto 1/n_1^2$ for $y_0 \in$ region 1

$\approx 1\,\mathrm{fm}$ gain, stopping at $n_1 = 30$

$\Rightarrow$ space for more gain

conclusions

using the locality of the Dirac operator and the fast decrease of its inverse

- hadronic propagator factorization, including disconnected contributions
- determinant factorization
  ⇒ multiboson domain-decomposed HMC algorithm
- gradient flow observables [García Vera, Schaefer 2016]

the theory is ‘local enough’ for multi-level methods to be applied

- exponential increase in S/N w.r.t. standard techniques

having a local formulation has implications beyond S/N and multi-level methods

- factorization in space domains
- ‘master field’ simulations [Lüscher 2017]
- reduced communications on parallel computers

thanks
for your attention!

questions?

backup

factorization of fermion determinant

locality at the level of a single gauge link is not needed

it is enough to be able to update extended regions of the lattice independently

[Phys. Rev. D **95** (2017) 034503, EPJ Web Conf. **175** (2018) 11005]

given a decomposition in multiple thick time slices,

using that $\left\| D^{-1}(x,0) \right\| \sim \mathrm{e}^{-M_\pi |x|/2}$ on every gauge configuration

we can factorize the gauge-link dependence of the determinant of $Q = \gamma_5 D$

with a combination of two main ideas

- domain decomposition [Lüscher 2003, 2004]
- multiboson algorithm [Lüscher 1993; Boriçi, de Forcrand 1995; Jegerlehner 1995]

the original multiboson algorithm

lattice QCD realized as the limit of local bosonic theory [Lüscher 1993]

- define a polynomial approximation of $1/z$ in a suitable range

$$P_N(z) = \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^{N/2} (z - z_k)(z - z_k^*) \xrightarrow{N\to\infty} 1/z$$

- approximate $\det\left\{1/Q^2\right\}$ with the polynomial $(z_k^{1/2} = \mu_k + \mathrm{i}\nu_k)$

$$\det Q^2 \sim \prod_{k=1}^{N/2} \det\left\{(Q^2 - z_k)(Q^2 - z_k^*)\right\}^{-1} = \prod_{k=1}^{N} \det\left\{(Q - \mu_k)^2 + \nu_k^2\right\}^{-1}$$

- represents it with N bosonic field $\phi = \{\phi_1, \ldots, \phi_N\}$, i.e. multibosons

$$\det Q^2 \sim \int \mathcal{D}[\phi, \phi^\dagger] \exp\left\{-\textstyle\sum_{k=1}^N \int \mathrm{d}^4x \left|(Q - \mu_k)\phi_k\right|^2 + \nu_k^2 \left|\phi_k\right|^2\right\}$$

problem: N depends on the condition number of Q^2, $\simeq (8/am)^2$
with lighter quarks and finer lattices, the number of multiboson fields grows
$\Rightarrow$ the system becomes stiff and autocorrelation grows $\propto N$ [Jegerlehner 1995]
$\Rightarrow$ not currently in use

domain decomposition of fermion determinant

to obtain a theory that is local at the block level

[Phys. Rev. D **95** (2017) 034503, EPJ Web Conf. **175** (2018) 11005]

consider a decomposition in active (colored) and buffer (grey) thick time slices, the determinant of the hermitian Wilson–Dirac operator $Q = \gamma_5 D$

$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\prod_a \det\left\{P_a Q_{\bar{a}}^{-1} P_a\right\} \prod_b \det Q_b^{-1}}$$

where $Q_{\bar{a}}$ spans the two b regions next to a

domain decomposition of fermion determinant

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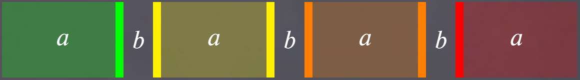

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where $Q_{\bar{a}}$ spans the two b regions next to a
and the operator w lives on the internal boundaries of the active regions

neglecting the small $\mathbb{1} - w$,
we can already update different thick time slices independently

domain decomposition, step by step

consider a decomposition in thick time slices

- active regions (colored, a)
- inactive buffers (grey, b)

LDU block-decompose the hermitian Dirac operator $Q = \gamma_5 D$

$$Q = \begin{pmatrix} Q_b & Q_{ba} \\ Q_{ab} & Q_a \end{pmatrix} = \begin{pmatrix} \mathbb{1} & \\ Q_{ab}Q_b^{-1} & \mathbb{1} \end{pmatrix} \begin{pmatrix} Q_b & \\ & S_a \end{pmatrix} \begin{pmatrix} \mathbb{1} & Q_b^{-1}Q_{ba} \\ & \mathbb{1} \end{pmatrix}$$

where $S_a = Q_a - Q_{ab}Q_b^{-1}Q_{ba}$ is the Schur complement of the block Q_b

$$\det Q = \det S_a \cdot \det Q_b$$

note: the inverse of S_a is in the block-inverse of Q, i.e. $S_a^{-1} = P_a Q^{-1} P_a$

$$Q^{-1} = \begin{pmatrix} Q_b^{-1} - Q_b^{-1}Q_{ba}S_a^{-1}Q_{ab}Q_b^{-1} & -Q_b^{-1}Q_{ba}S_a^{-1} \\ -S_a^{-1}Q_{ab}Q_b^{-1} & S_a^{-1} \end{pmatrix}$$

domain decomposition, step by step

$$\det Q = \frac{1}{\det S_a^{-1} \cdot \det Q_b^{-1}}$$

what does S_a look like?

$$S_a = Q_a - Q_{ab} Q_b^{-1} Q_{ba}$$

domain decomposition, step by step

$$\det Q = \frac{1}{\det S_a^{-1} \cdot \det Q_b^{-1}}$$

what does S_a look like?

$$S_a = \begin{pmatrix} \overbrace{Q_e - Q_{eb}Q_b^{-1}Q_{be}}^{S_e} & -Q_{eb}Q_b^{-1}Q_{bo} \\ -Q_{ob}Q_b^{-1}Q_{be} & \underbrace{Q_o - Q_{ob}Q_b^{-1}Q_{bo}}_{S_o} \end{pmatrix}$$

- partition active regions between even ones (e) and odd ones (o)

domain decomposition, step by step

$$\det Q = \frac{\det \tilde{W}}{\det S_e^{-1} \cdot \det S_o^{-1} \cdot \det Q_b^{-1}}$$

what does S_a look like?

$$S_a = \begin{pmatrix} S_e^{-1} & \\ & S_o^{-1} \end{pmatrix}^{-1} \underbrace{\begin{pmatrix} \mathbb{1} & -S_e^{-1} Q_{eb} Q_b^{-1} Q_{bo} \\ -S_o^{-1} Q_{ob} Q_b^{-1} Q_{be} & \mathbb{1} \end{pmatrix}}_{\tilde{W}}$$

- partition active regions between even ones (e) and odd ones (o)
- precondition with $\mathrm{diag}\left\{ S_e^{-1}, S_o^{-1} \right\}$

domain decomposition, step by step

$$\det Q = \frac{\det \tilde{W}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

what does S_a look like?

$$S_a = \begin{pmatrix} P_e Q_{\bar{e}}^{-1} P_e & \\ & P_o Q_{\bar{o}}^{-1} P_o \end{pmatrix}^{-1} \underbrace{\begin{pmatrix} \mathbb{1} & P_e Q_{\bar{e}}^{-1} Q_{bo} \\ P_o Q_{\bar{o}}^{-1} Q_{be} & \mathbb{1} \end{pmatrix}}_{\tilde{W}}$$

- partition active regions between even ones (e) and odd ones (o)
- precondition with $\operatorname{diag}\left\{S_e^{-1}, S_o^{-1}\right\}$
- use the property of the Schur complement

domain decomposition, step by step

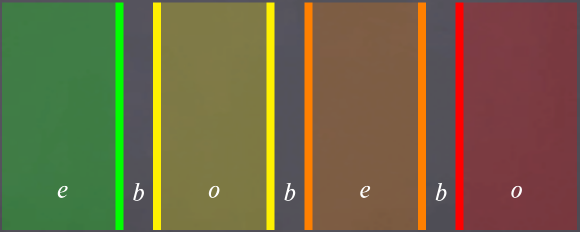
$$\det Q = \frac{\det\{1 - w\}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

what does S_a look like?

$$S_a = \begin{pmatrix} P_e Q_{\bar{e}}^{-1} P_e & \\ & P_o Q_{\bar{o}}^{-1} P_o \end{pmatrix}^{-1} \underbrace{\begin{pmatrix} \mathbb{1} & P_e Q_{\bar{e}}^{-1} Q_{bo} \\ P_o Q_{\bar{o}}^{-1} Q_{be} & \mathbb{1} \end{pmatrix}}_{\tilde{W}}$$

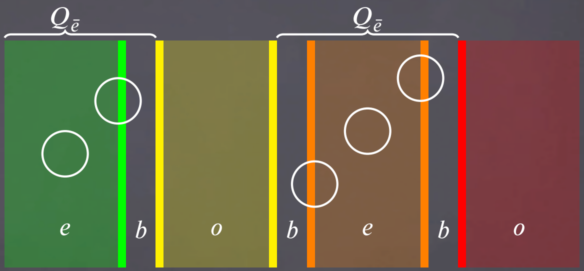
- partition active regions between even ones (e) and odd ones (o)
- precondition with $\mathrm{diag}\left\{S_e^{-1}, S_o^{-1}\right\}$
- use the property of the Schur complement
- $\det \tilde{W} = \det\left\{\mathbb{1} - P_{\partial e} Q_{\bar{e}}^{-1} Q_{bo} P_{\partial o} Q_{\bar{o}}^{-1} Q_{be}\right\} = \det\{\mathbb{1} - w\}$

domain decomposition, recap.



$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

domain decomposition, recap.



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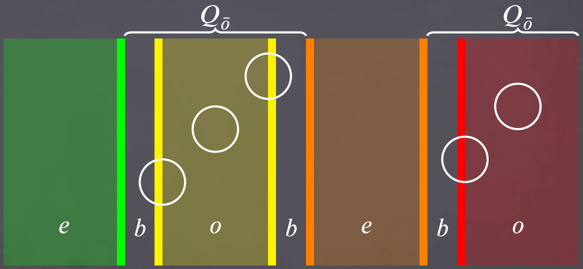
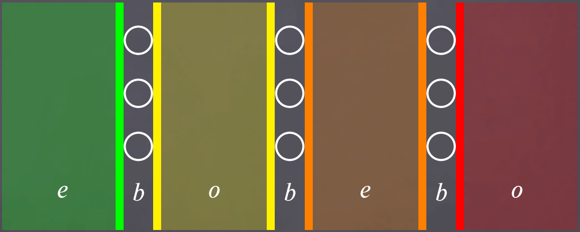
domain decomposition, recap.



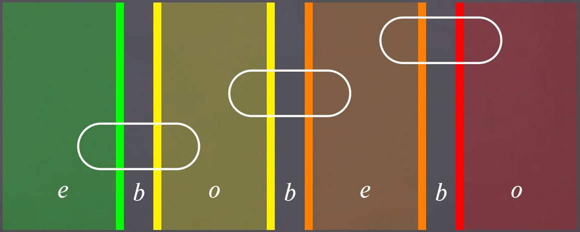
$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

domain decomposition, recap.



$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

domain decomposition, recap.



$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\det\left\{P_e Q_{\bar{e}}^{-1} P_e\right\} \cdot \det\left\{P_o Q_{\bar{o}}^{-1} P_o\right\} \cdot \det Q_b^{-1}}$$

note: if the contribution of $\det\{1 - w\}$ is small enough to be neglected
we could already update different active regions independently

domain decomposition, comparison

yet another equivalent rewriting

$$\det Q = \det S_e \det S_o \det Q_b \det\left\{ \mathbb{1} - P_{\partial e} Q_{\bar{e}}^{-1} Q_{bo} P_{\partial o} Q_{\bar{o}}^{-1} Q_{be} \right\}$$

cf. the original domain decomposition, e.g. in the DD-HMC algorithm

[Lüscher 2003, 2004]

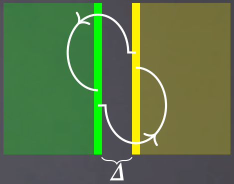
$$\det Q = \det Q_e \det Q_o \det\left\{ \mathbb{1} - P_{\partial e} Q_e^{-1} Q_{eo} P_{\partial o} Q_o^{-1} Q_{oe} \right\}$$

there is no inactive buffer region b

$\Rightarrow$ the last factor has no reason to be small

locality of w

$Q^{-1}(x,y)$ on every gauge configuration decays $\sim e^{-M_\pi |x-y|/2}$
$\Rightarrow$ the operator w is "small"

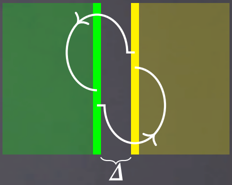


$$w = P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1} P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0}$$

(or $P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0} P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1}$)

locality of w

$Q^{-1}(x, y)$ on every gauge configuration decays $\sim \mathrm{e}^{-M_\pi |x-y|/2}$
$\Rightarrow$ the operator w is “small”

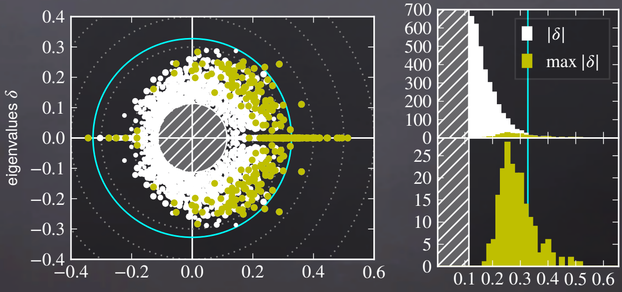


$$w = P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1} P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0}$$

$$\text{(or } P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0} P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1}\text{)}$$

spectrum of w, with b-region thickness $\Delta = 8a$

$(N_\mathrm{f} = 2,\ a = 0.0652(6)\,\mathrm{fm},\ M_\pi = 0.1454(5)/a = 440(5)\,\mathrm{MeV})$ $(\bar{\delta} = \mathrm{e}^{-M_\pi \Delta} \approx 0.327)$



locality of w

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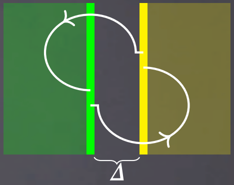


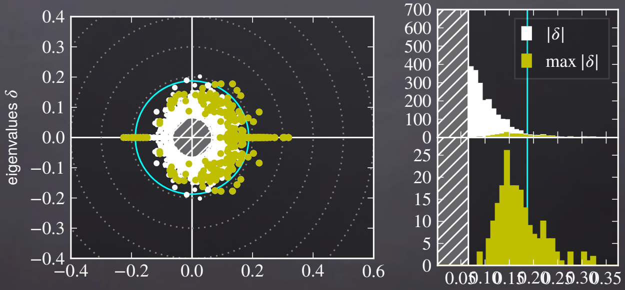
$$w = P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1} P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0}$$

$$(\text{or } P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0} P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1})$$

spectrum of w, with b-region thickness $\Delta = 12a$

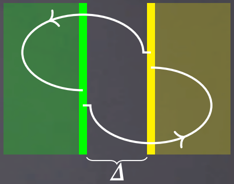
$(N_\mathrm{f} = 2,\ a = 0.0652(6)\,\mathrm{fm},\ M_\pi = 0.1454(5)/a = 440(5)\,\mathrm{MeV})$

$(\bar{\delta} = \mathrm{e}^{-M_\pi \Delta} \approx 0.187)$



locality of w

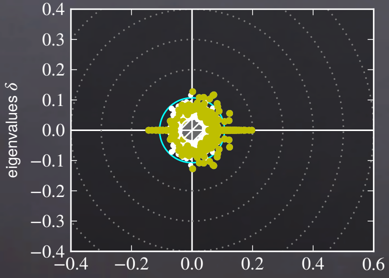
$Q^{-1}(x,y)$ on every gauge configuration decays $\sim \mathrm{e}^{-M_\pi|x-y|/2}$
$\Rightarrow$ the operator w is "small"

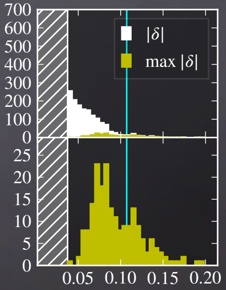


$$w = P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1} P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0}$$

$$\text{(or } P_{\partial 1} Q_{\bar{1}}^{-1} Q_{b0} P_{\partial 0} Q_{\bar{0}}^{-1} Q_{b1}\text{)}$$

spectrum of w, with b-region thickness $\Delta = 16a$
$(N_\mathrm{f} = 2,\ a = 0.0652(6)\,\mathrm{fm},\ M_\pi = 0.1454(5)/a = 440(5)\,\mathrm{MeV})$ $(\bar{\delta} = \mathrm{e}^{-M_\pi \Delta} \approx 0.107)$





polynomial approximation

the condition number of $\mathbb{1} - w$ is $\epsilon \sim (1 + \mathrm{e}^{-M_\pi \Delta})/(1 - \mathrm{e}^{-M_\pi \Delta})$
$\Rightarrow \mathcal{O}(1)$, can be made arbitrarily close to 1 increasing Δ

polynomial approximation

the condition number of $\mathbb{1} - w$ is $\epsilon \sim (1 + \mathrm{e}^{-M_\pi \Delta})/(1 - \mathrm{e}^{-M_\pi \Delta})$
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complex multiboson representation [Lüscher 1993; Boriçi, de Forcrand 1995]

$$\frac{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}}{\det\{\mathbb{1} - w\}} = \det\left\{P_N(\mathbb{1} - w)\right\} = c_N \prod_{k=1}^{N/2} \det\left\{ W^\dagger_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}$$

where N is an even integer and $P_N(z)$ is a polynomial approximation of $1/z$

$$P_N(z) = \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^{N} (z - z_k) \xrightarrow{N\to\infty} 1/z$$

and (note: $\det \tilde{W} = \det W_1$)

$$W_y = \begin{pmatrix} y\mathbb{1} & P_{\partial e} Q_{\bar{e}}^{-1} Q_{bo} \\ P_{\partial o} Q_{\bar{o}}^{-1} Q_{be} & y\mathbb{1} \end{pmatrix}$$

multiboson representation

two active regions, $N_\mathrm{f} = 2$ theory:

$$\frac{\det Q^2}{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1}-w)\right\}^2} \sim \frac{\overbrace{\prod_{k=1}^{N} \det\left\{ W^\dagger_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}^{-1}}^{N \text{ multiboson fields}}}{\underbrace{\det Q_b^{-2} \cdot \det\left\{ P_0 Q_{\bar{0}}^{-1} P_0 \right\}^2 \cdot \det\left\{ P_1 Q_{\bar{1}}^{-1} P_1 \right\}^2}_{\text{pseudofermion fields (at least one per active region)}}}$$

$$\sim \int \mathcal{D}[\phi_0, \phi_0^\dagger]\, \mathrm{e}^{-\left|P_0 Q_{\bar{0}}^{-1} \phi_0\right|^2} \cdot \int \mathcal{D}[\phi_1, \phi_1^\dagger]\, \mathrm{e}^{-\left|P_1 Q_{\bar{1}}^{-1} \phi_1\right|^2}$$
$$\int \mathcal{D}[\phi_b, \phi_b^\dagger]\, \mathrm{e}^{-\left|Q_b^{-1} \phi_b\right|^2} \cdot \prod_{k=1}^{N} \int \mathcal{D}[\chi_k, \chi_k^\dagger]\, \mathrm{e}^{-\left|W_{\sqrt{1-z_k}} \chi_k\right|^2}$$

multiboson representation

two active regions, $N_\mathrm{f} = 2$ theory:

$$\frac{\det Q^2}{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}^2} \sim \frac{\overbrace{\prod_{k=1}^{N} \det\left\{ W^\dagger_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}^{-1}}^{N \text{ multiboson fields}}}{\underbrace{\det Q_b^{-2} \cdot \det\left\{ P_0 Q_{\bar{0}}^{-1} P_0 \right\}^2 \cdot \det\left\{ P_1 Q_{\bar{1}}^{-1} P_1 \right\}^2}_{\text{pseudofermion fields (at least one per active region)}}}$$

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$$\int \mathcal{D}[\phi_b, \phi_b^\dagger]\, \mathrm{e}^{-\left|Q_b^{-1} \phi_b\right|^2} \cdot \prod_{k=1}^{N} \int \mathcal{D}[\chi_k, \chi_k^\dagger]\, \mathrm{e}^{-\left|W_{\sqrt{1-z_k}} \chi_k\right|^2}$$

computation of HMC forces:

- $|P_0 Q_{\bar{0}}^{-1} \phi_0|$ and $|W_{\sqrt{1-z_k}} \chi_k|$ depend on gauge links in region 0 (and b)
- $|P_1 Q_{\bar{1}}^{-1} \phi_1|$ and $|W_{\sqrt{1-z_k}} \chi_k|$ depend on gauge links in region 1 (and b)
- $|W_{\sqrt{1-z_k}} \chi_k|$ forces do not mix the gauge-link dependence of active regions

$\Rightarrow$ the two active regions can be updated independently

determinant factorization, conclusions

separate spacetime regions can be updated independently in full QCD

we tested the algorithm in a two active regions, $N_\mathrm{f} = 2$ setup

- $a = 0.0652(6)\,\mathrm{fm}$, $M_\pi = 0.1454(5)/a = 440(5)\,\mathrm{MeV}$, OBC in time
- thickness of the buffer region: $\Delta = 12a \;\Rightarrow\; \mathrm{e}^{-M_\pi \Delta} \approx 0.187$
- 5 pseudofermion forces with mass preconditioning
- 12 multiboson fields for $N = 12$
- negligible $R_{N+1}(\mathbb{1} - w)$
  $\Rightarrow$ very good approximation with a small number of multiboson fields

the algorithm presented here

- naturally represents a single quark flavour
- an arbitrary number of active thick time slice regions is possible

determinant factorization, outlook

- smaller number of multiboson fields, thinner frozen region
  ⇒ correct with a reweighting factor

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle_N}{\langle \mathcal{W}_N \rangle_N} \qquad \mathcal{W}_N = \det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}^{N_\mathrm{f}}$$

- study the multiboson forces, tune the integration steps
- compute observables, study autocorrelations
  ⇒ experience from quenched study is valuable

other ideas can profit from the locality properties

- multiboson algorithm for master fields simulation [Lüscher 2017]

polynomial approximation, step by step

[Phys. Rev. D **95** (2017) 034503]

$$\frac{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}}{\det\{\mathbb{1} - w\}} = \det\left\{P_N(\mathbb{1} - w)\right\} = c_N \prod_{k=1}^{N} (\mathbb{1} - z_k - w)$$

the condition number of $\mathbb{1} - w$ is $\epsilon \sim (1 + \mathrm{e}^{-M_\pi \Delta})/(1 - \mathrm{e}^{-M_\pi \Delta})$
$\Rightarrow \mathcal{O}(1)$, can be made arbitrarily close to 1 increasing Δ

polynomial approximation, step by step

[Phys. Rev. D **95** (2017) 034503]

$$\frac{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}}{\det\{\mathbb{1} - w\}} = \det\left\{P_N(\mathbb{1} - w)\right\} = c_N \prod_{k=1}^{N/2} (\mathbb{1} - \bar{z}_k - w^\dagger)(\mathbb{1} - z_k - w)$$

the condition number of $\mathbb{1} - w$ is $\epsilon \sim (1 + \mathrm{e}^{-M_\pi \Delta})/(1 - \mathrm{e}^{-M_\pi \Delta})$
$\Rightarrow \mathcal{O}(1)$, can be made arbitrarily close to 1 increasing Δ
choosing N even, with a bit of algebra

polynomial approximation, step by step

[Phys. Rev. D **95** (2017) 034503]

$$\frac{\det\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\}}{\det \tilde{W}} = \det\{P_N(\mathbb{1} - w)\} = c_N \prod_{k=1}^{N/2} \det\left\{ W^\dagger_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}$$

the condition number of $\mathbb{1} - w$ is $\epsilon \sim (1 + \mathrm{e}^{-M_\pi \Delta})/(1 - \mathrm{e}^{-M_\pi \Delta})$
$\Rightarrow \mathcal{O}(1)$, can be made arbitrarily close to 1 increasing Δ
choosing N even, with a bit of algebra, and introducing

$$W_y = \begin{pmatrix} y\mathbb{1} & P_{\partial e} Q_{\bar{e}}^{-1} Q_{bo} \\ P_{\partial o} Q_{\bar{o}}^{-1} Q_{be} & y\mathbb{1} \end{pmatrix}$$

polynomial approximation, step by step

[Phys. Rev. D **95** (2017) 034503]

$$\frac{\det\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\}}{\det \tilde{W}} = \det\{P_N(\mathbb{1} - w)\} = c_N \prod_{k=1}^{N/2} \det\left\{ W^{\dagger}_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}$$

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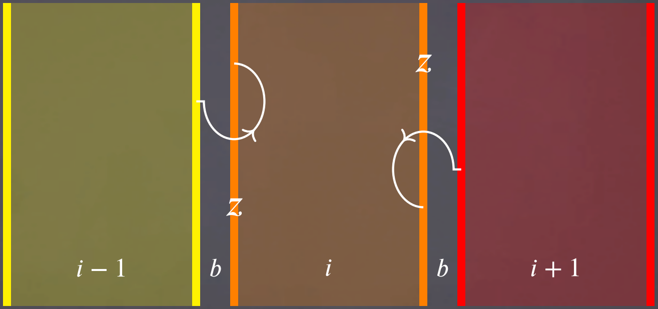
choosing N even, with a bit of algebra, and introducing

$$W_y = \begin{pmatrix} y\mathbb{1} & P_{\partial e} Q_{\bar{e}}^{-1} Q_{bo} \\ P_{\partial o} Q_{\bar{o}}^{-1} Q_{be} & y\mathbb{1} \end{pmatrix}$$

approximation for a disk centred in $z = 1$: geometric series

$$P_N(z) = \sum_{p=1}^{N} (1 - z)^p \quad \Rightarrow \quad \begin{array}{c} R_{N+1}(z) = (1 - z)^{N+1} \\ z_k = 1 - e^{\mathrm{i}\frac{2\pi k}{N+1}} \end{array}$$

multiboson HMC forces

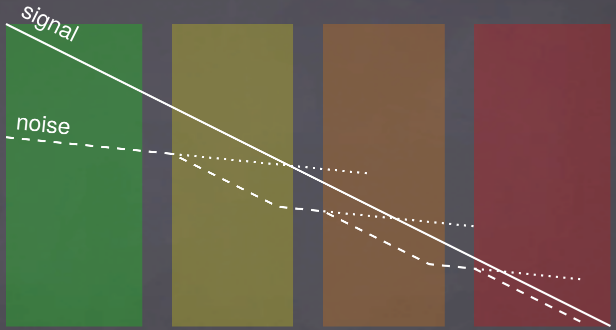


the multiboson action is ($\chi_{i,k} = P_{\partial i}\chi_i$)

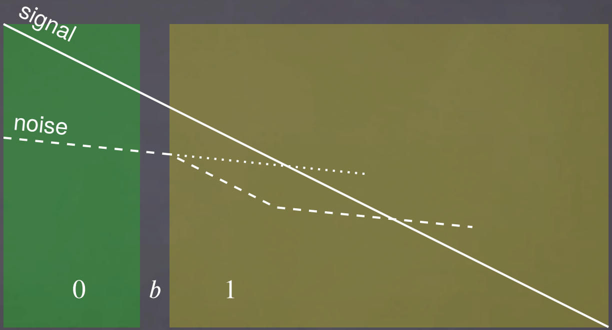
$$\left|W_z\chi_k\right|^2 = \sum_{i\in a}\left|z\chi_{i,k} + P_{\partial i}Q_{\bar{i}}^{-1}\left[Q_{b,i-1}\chi_{i-1,k} + Q_{b,i+1}\chi_{i+1,k}\right]\right|^2$$

$\Rightarrow$ each term in the sum depends only on gauge links in region i (and b)

multi-level Monte Carlo with fermions



multi-level Monte Carlo with fermions



test the multi-level in the quenched theory
with 64×24^3, $a \approx 0.093\,\mathrm{fm}$, $aM_\pi \approx 0.216$ [Phys. Rev. D **93** (2016) 094507]
$n_0 = 50$ global updates and $n_1 = 30$ independent updates of two regions

region $0 = \{x : x_0 \in (0, 15)\}$ region $1 = \{x : x_0 \in (24, T)\}$

while links in region $b = \{x : x_0 \in (16, 23)\}$ are frozen