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Local multiboson factorization of the quark determinant

Marco Cè[a,b] Leonardo Giusti[c] Stefan Schaefer[d]

a. Scuola Normale Superiore and INFN, Pisa
b. Helmholtz-Institut Mainz, Johannes Gutenberg-Universität Mainz
c. Università di Milano-Bicocca and INFN, Milano-Bicocca
d. NIC, DESY, Zeuthen

based on M. Cè, L. Giusti and S. Schaefer
Phys. Rev. D **93** (2016) 094507 [arXiv:1601.04587]
Phys. Rev. D **95** (2017) 034503 [arXiv:1609.02419]

22nd June 2017

motivation: S/N problem

e.g. two-point function of the vector current

$$\langle C_{\gamma_i} \rangle = \sum_{\vec{x},\vec{y}} \langle \bar{u}(x)\gamma_i u(x) \cdot \bar{d}(y)\gamma_i d(y) \rangle \propto \mathrm{e}^{-M_\rho |x_0 - y_0|}$$

while its variance

$$\sigma^2_{C_{\gamma_i}} \propto \mathrm{e}^{-2M_\pi |x_0 - y_0|}$$

signal-to-noise ratio problem [Parisi 1984; Lepage 1989]

$$\frac{S}{N} \propto \frac{\langle C_{\gamma_i} \rangle}{\sqrt{\sigma^2/n}} = \sqrt{n}\mathrm{e}^{-(M_\rho - M_\pi)|x_0 - y_0|}$$

⇒ at large distance the noise dominates

standard Monte Carlo:

the noise scales with $n^{-1/2}$, where n is the number of samples

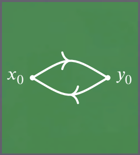
⇒ increasing $|x_0 - y_0|$ while keeping the same S/N, n scales exponentially

$$n \propto \mathrm{e}^{2(M_\rho - M_\pi)|x_0 - y_0|}$$

multilevel Monte Carlo

introduced for bosonic theories [Parisi, Petronzio, Rapuano 83; Lüscher, Weisz 2001; Meyer 2003]
update (thick) time slices of the lattice independently

$\langle C_{\gamma_i} \rangle =$



number of samples n_1 $= n_1$

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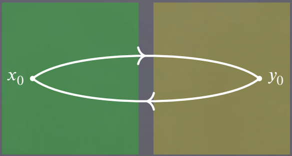

number of samples $n_1 \cdot n_1 \quad = n_1^2$

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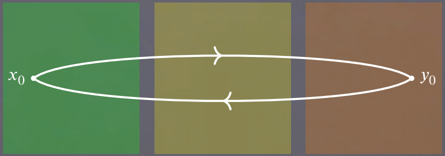
$\langle C_{\gamma_i} \rangle =$ 

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

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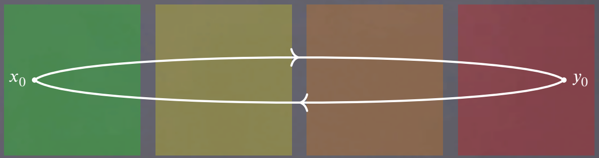


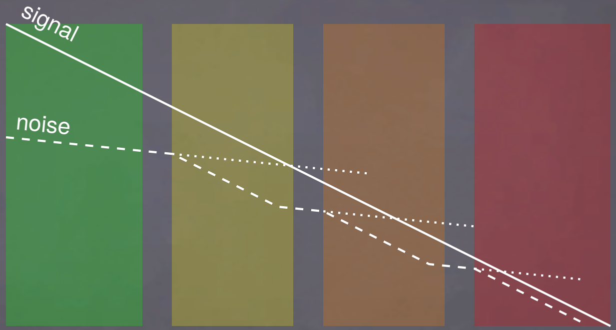
number of samples $n_1 \cdot n_1 \cdot n_1 \cdot n_1 = n_1^4$

$\Rightarrow$ the error is reduced with distance exponentially

$$\delta C_{\gamma_i} \propto \left(n_1^{-1/2}\right)^{\frac{|x_0-y_0|}{\Delta}} e^{-M_\pi |x_0-y_0|} = e^{-\left(M_\pi + \frac{\ln n_1}{2\Delta}\right)|x_0-y_0|}$$

(in an ideal situation)

multilevel Monte Carlo



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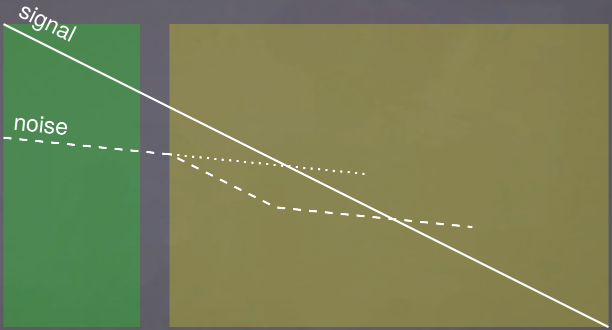
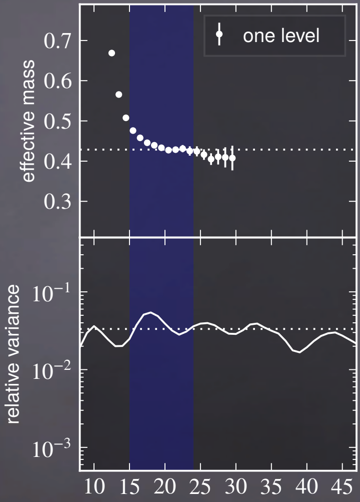


test the multilevel in the quenched theory
with 64×24^3, $a \approx 0.093\,\mathrm{fm}$, $aM_\pi \approx 0.216$ [Phys. Rev. D **93** (2016) 094507]
$n_0 = 50$ global updates and $n_1 = 30$ independent updates of two regions

$$\Lambda_0 = \{x : x_0 \in (0, 15)\} \qquad \Lambda_2 = \{x : x_0 \in (24, T)\}$$

while links in $\Lambda_1 = \{x : x_0 \in (16, 23)\}$ are frozen

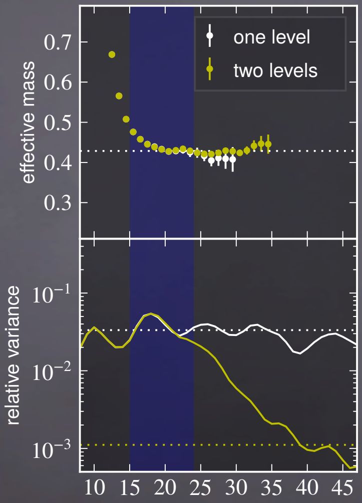
pseudoscalar correlator with $p^2 = 2$



new results:

- $n_0 = 50,\ n_1 = 30$
- stochastic $3d$-volume sources on time-slice $x_0 = 8a \in \Lambda_0$
- 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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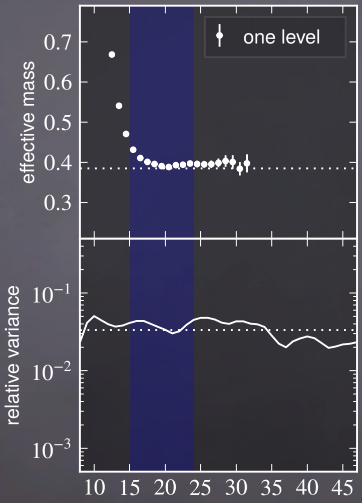
- two levels average
  $\Rightarrow$ improved variance reduction, $\propto 1/n_1^2$ for $y_0 \in \Lambda_2$

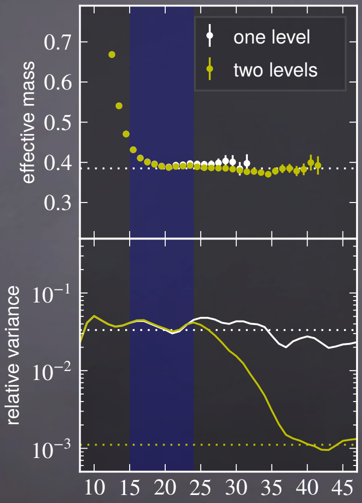
vector correlator



new results:

- $n_0 = 50$, $n_1 = 30$
- stochastic $3d$-volume sources on time-slice $x_0 = 8a \in \Lambda_0$
- 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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$\approx 1\,\mathrm{fm}$ gain, stopping at $n_1 = 30$

$\Rightarrow$ space for more gain

motivation: conclusions

multilevel integration results in an
exponential increase in S/N
w.r.t. standard techniques

- pseudoscalar correlator with non-zero momentum [new!]
  e.g. transition matrix elements, form factors, …
- vector correlator [new!]
  e.g. e.m. form factors, muon $g-2$ HVP contribution, …
- disconnected contributions [Phys. Rev. D **93** (2016) 094507; PoS(LATTICE2016)263]

studing correlator in the quenched approximation
is instrumental to the setup of the domain decomposition

factorization of QCD action

in Monte Carlo simulations the lattice Dirac action is integrated out exactly

$\Rightarrow$ non-local Dirac determinant

we can still update different time slices independently!

[Phys. Rev. D **95** (2017) 034503, Giusti's plenary talk]

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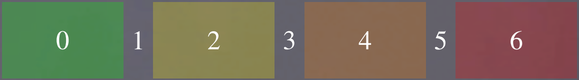

consider a decomposition in even (colored) and odd (grey) thick time slices, the determinant of the hermitian Wilson–Dirac operator $Q = \gamma_5(D + m)$

$$\det Q = \frac{\det\{\mathbb{1} - w\}}{\prod_{\text{even } i} \det\left\{ P_i Q_{i,3}^{-1} P_i \right\} \prod_{\text{odd } j} \det Q_j^{-1}}$$

where $Q_{i,3} = Q_{(i-1)\cup i \cup (i+1)}$

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the determinant of the hermitian Wilson–Dirac operator $Q = \gamma_5(D + m)$

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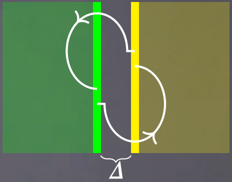
where $Q_{i,3} = Q_{(i-1)\cup i \cup (i+1)}$ and
the operator $\mathbb{1} - w$ lives on the internal boundaries of even domains

locality of the Dirac operator

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



$$w = P_{\partial 0} Q^{-1}_{0\cup 1} Q_{12} P_{\partial 2} Q^{-1}_{2\cup 1} Q_{10}$$

(or $P_{\partial 2} Q^{-1}_{2\cup 1} Q_{10} P_{\partial 0} Q^{-1}_{0\cup 1} Q_{12}$)

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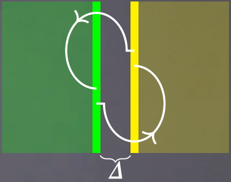

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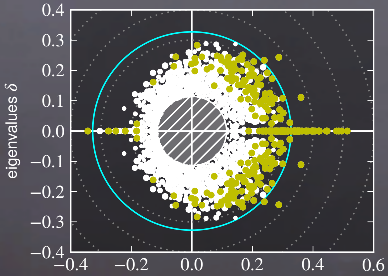
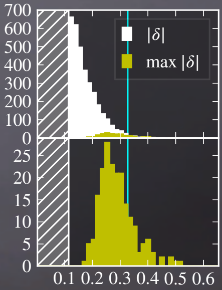
spectrum of w, with Λ_1 thickness $\Delta = 8a$

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





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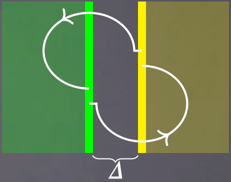

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spectrum of w, with Λ_1 thickness $\Delta = 12a$

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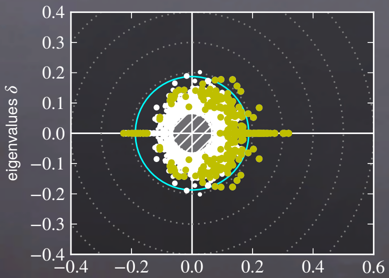

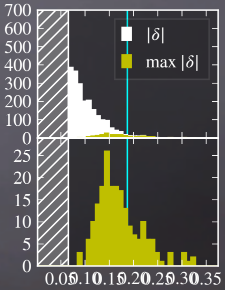

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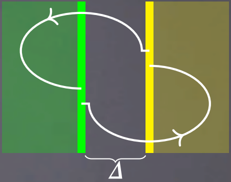

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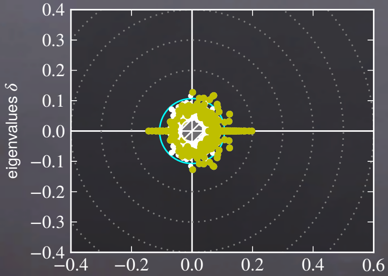
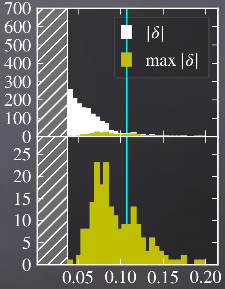
$$(\text{or } P_{\partial 2} Q^{-1}_{2\cup 1} Q_{10} P_{\partial 0} Q^{-1}_{0\cup 1} Q_{12})$$

spectrum of w, with Λ_1 thickness $\Delta = 16a$

($N_f = 2$, $a = 0.0652(6)\,\mathrm{fm}$, $M_\pi = 0.1454(5)/a = 440(5)\,\mathrm{MeV}$) ($\bar{\delta} = e^{-M_\pi \Delta} \approx 0.107$)





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

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complex “multiboson” representation [Lüscher 1993; Boriçi, de Forcrand 1995; Jegerlehner 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 $1/z$

$$P_N(z) = \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^{N} (z - z_k) \qquad (z_k\text{: roots of } P_N(z))$$

$$W_y = \begin{pmatrix} y\mathbb{1} & P_{\partial 0} Q^{-1}_{0\cup 1} Q_{12} \\ P_{\partial 2} Q^{-1}_{2\cup 1} Q_{10} & y\mathbb{1} \end{pmatrix}$$

multiboson representation

$N_\mathrm{f} = 2$ theory:

$$\frac{\det Q}{\det\left\{\mathbb{1} - R_{N+1}(\mathbb{1} - w)\right\}} \propto \frac{\overbrace{\prod_{k=1}^{N} \det\left\{ W^\dagger_{\sqrt{1-z_k}} W_{\sqrt{1-z_k}} \right\}^{-1}}^{N \text{ multiboson fields}}}{\underbrace{\det Q_1^{-2} \cdot \det\left\{ P_0 Q_{0\cup 1}^{-1} P_0 \right\}^2 \cdot \det\left\{ P_2 Q_{2\cup 1}^{-1} P_2 \right\}^2}_{\text{3 (or more) pseudofermion fields}}}$$

$$\propto \int \mathcal{D}[\phi_0, \phi_0^\dagger]\, \mathrm{e}^{-\left|P_0 Q_{0\cup 1}^{-1} \phi_0\right|^2} \cdot \int \mathcal{D}[\phi_2, \phi_2^\dagger]\, \mathrm{e}^{-\left|P_2 Q_{2\cup 1}^{-1} \phi_2\right|^2}$$

$$\int \mathcal{D}[\phi_1, \phi_1^\dagger]\, \mathrm{e}^{-\left|Q_1^{-1} \phi_0\right|^2} \cdot \prod_{k=1}^{N} \int \mathcal{D}[\xi_k, \xi_k^\dagger]\, \mathrm{e}^{-\left|W_{\sqrt{1-z_k}} \xi_k\right|^2}$$

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computation of HMC forces:

- gauge links $\in \Lambda_0$ dependence in $\left|P_0 Q_{0\cup 1}^{-1} \phi_0\right|$ and $\left|W_{\sqrt{1-z_k}} \xi_k\right|$
- gauge links $\in \Lambda_2$ dependence in $\left|P_2 Q_{2\cup 1}^{-1} \phi_2\right|$ and $\left|W_{\sqrt{1-z_k}} \xi_k\right|$
- multiboson forces do not mix $\in \Lambda_0$ and Λ_2 gauge links dependence

$\Rightarrow$ Λ_0 and Λ_2 can be updated independently

conclusions

spacetime domains can be updated independently in full QCD

we implemented the $N_\mathrm{f} = 2$, three thick time slices MB-DD-HMC algorithm

- active regions: Λ_0 and Λ_2
- thickness of Λ_1 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

different N_f, more domains is also possible

- active regions: even thick time slices

update also Λ_1 gauge field $\Rightarrow$ no multilevel

- multiboson algorithm for master fields simulation [Lüscher's plenary talk]

outlook

- smaller number of multiboson fields, thinner frozen region
  $\Rightarrow$ reweighting

$$\langle O \rangle = \frac{\langle O \mathcal{W}_N \rangle}{\langle \mathcal{W}_N \rangle} \qquad \mathcal{W}_N = \det\left\{ \mathbb{1} - R_{N+1}(\mathbb{1} - w) \right\}^2$$

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

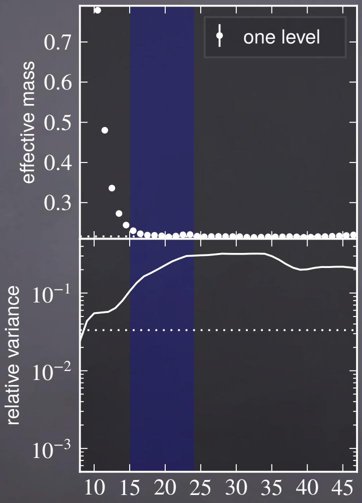
update also Λ_1 gauge field $\Rightarrow$ no multilevel

- multiboson algorithm for master fields simulation [Lüscher's plenary talk]

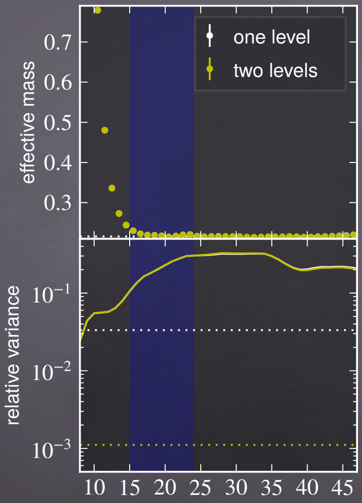
thanks
for your attention!

backup

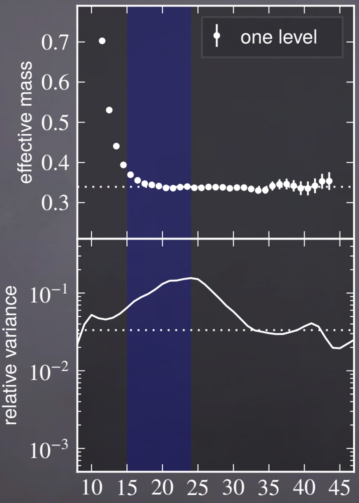
pseudoscalar correlator, $p^2 = 0$



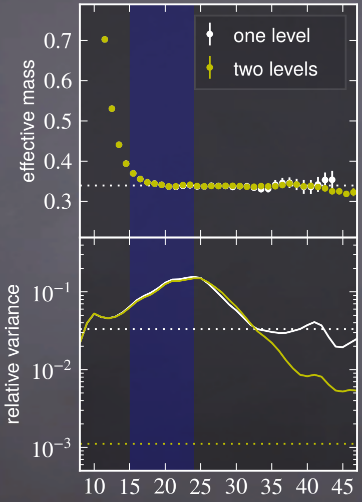
pseudoscalar correlator, $p^2 = 0$



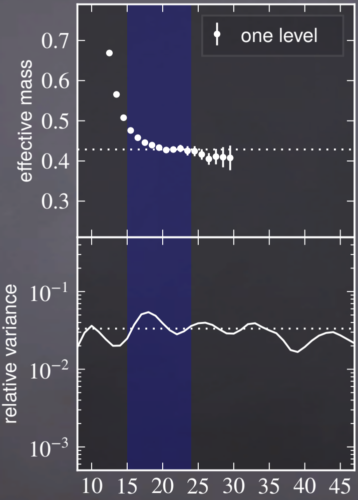
pseudoscalar correlator, $p^2 = 1$



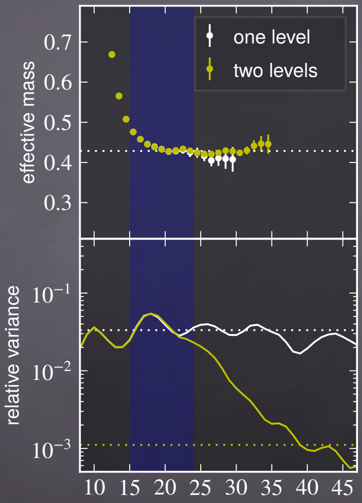
pseudoscalar correlator, $p^2 = 1$



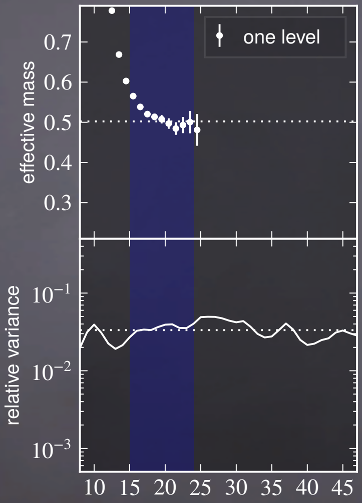
pseudoscalar correlator, $p^2 = 2$



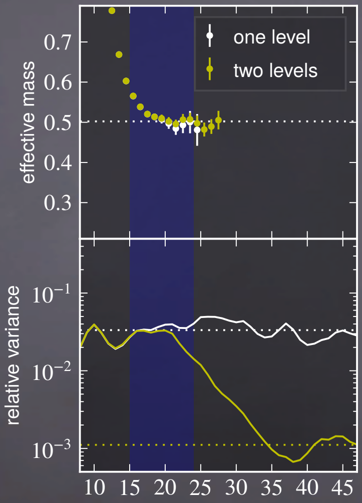
pseudoscalar correlator, $p^2 = 2$



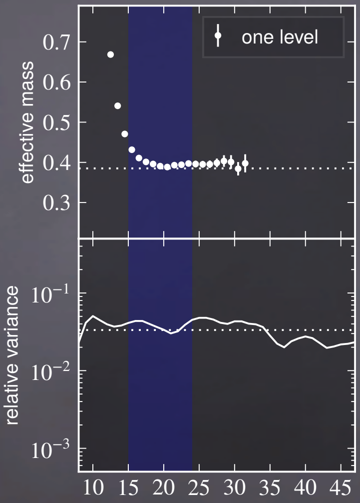
pseudoscalar correlator, $p^2 = 3$



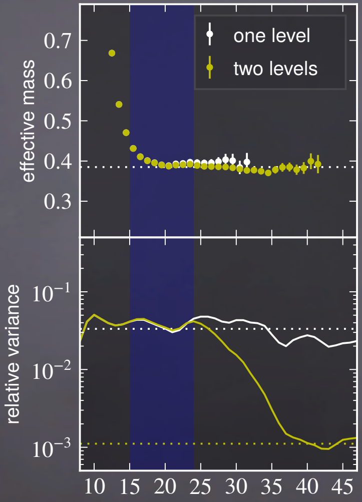
pseudoscalar correlator, $p^2 = 3$



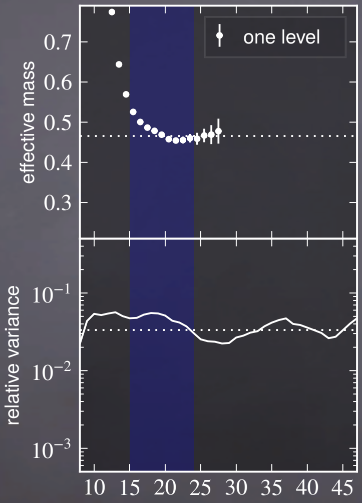
vector correlator, $p^2 = 0$



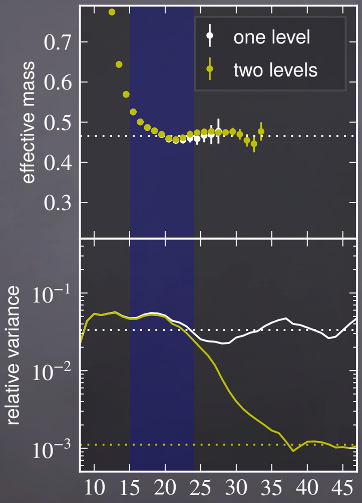
vector correlator, $p^2 = 0$



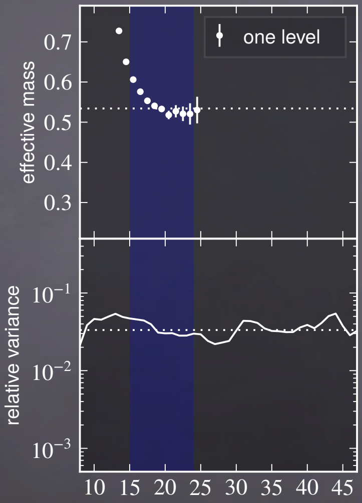
vector correlator, $p^2 = 1$



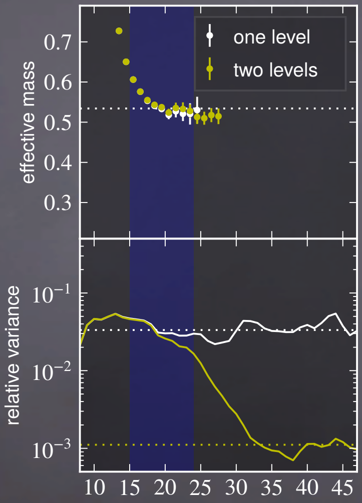
vector correlator, $p^2 = 1$



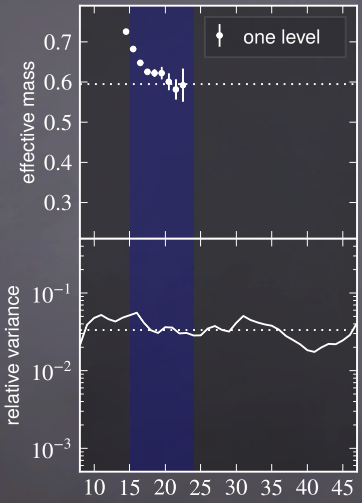
vector correlator, $p^2 = 2$



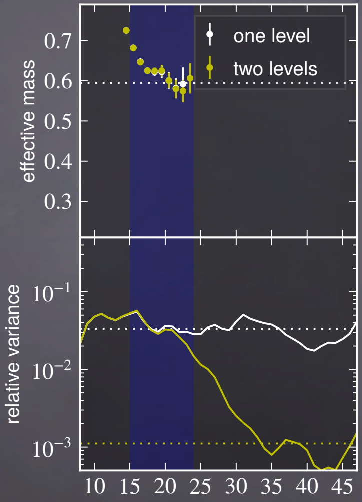
vector correlator, $p^2 = 2$



vector correlator, $p^2 = 3$



vector correlator, $p^2 = 3$



factorization of QCD action

in Monte Carlo simulations the lattice Dirac action is integrated out exactly
$\Rightarrow$ non-local Dirac determinant
How to update different time slices independently? [Phys. Rev. D **95** (2017) 034503, Giusti's plenary talk]

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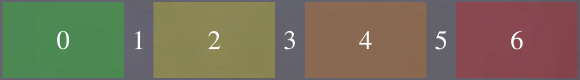

consider a decomposition in even (colored) and odd (grey) thick time slices, the hermitian massive Dirac operator $Q = \gamma_5(D+m)$

$$Q = \begin{pmatrix} Q_o & Q_{oe} \\ Q_{eo} & Q_e \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ Q_{eo}Q_o^{-1} & \mathbb{1} \end{pmatrix} \begin{pmatrix} Q_o & Q_{oe} \\ 0 & S_e \end{pmatrix}$$

where $S_e = Q_e - Q_{eo}Q_o^{-1}Q_{oe}$
⇒

$$\det Q = \det S_e \cdot \det Q_o$$

factorization of QCD action

$$\det Q = \frac{1}{\det S_e^{-1} \cdot \det Q_o^{-1}}$$

what does S_e look like?

$$S_e = Q_e - Q_{eo} Q_o^{-1} Q_{oe}$$

factorization of QCD action

$$\det Q = \frac{1}{\det S_{0\cup 2}^{-1} \cdot \det Q_1^{-1}}$$

what does S_e look like?

$$S_{0\cup 2} = \begin{pmatrix} Q_0 - Q_{01} Q_1^{-1} Q_{10} & -Q_{01} Q_1^{-1} Q_{12} \\ -Q_{21} Q_1^{-1} Q_{10} & Q_2 - Q_{21} Q_1^{-1} Q_{12} \end{pmatrix}$$

- consider a simplified setup: 3 thick time slices Λ_0, Λ_1, Λ_2

factorization of QCD action

$$\det Q = \frac{\det \tilde{W}}{\det S_0^{-1} \cdot \det S_2^{-1} \cdot \det Q_1^{-1}}$$

what does S_e look like?

$$S_{0\cup 2} = \begin{pmatrix} S_0^{-1} & \\ & S_2^{-1} \end{pmatrix}^{-1} \underbrace{\begin{pmatrix} \mathbb{1} & -S_0^{-1} Q_{01} Q_1^{-1} Q_{12} \\ -S_2^{-1} Q_{21} Q_1^{-1} Q_{10} & \mathbb{1} \end{pmatrix}}_{\tilde{W}}$$

- consider a simplified setup: 3 thick time slices Λ_0, Λ_1, Λ_2
- precondition with $\mathrm{diag}\left\{S_0^{-1}, S_2^{-1}\right\}$

factorization of QCD action

$$\det Q = \frac{\det \tilde{W}}{\det\left\{P_0 Q_{0\cup1}^{-1} P_0\right\} \cdot \det\left\{P_2 Q_{2\cup1}^{-1} P_2\right\} \cdot \det Q_1^{-1}}$$

what does S_e look like?

$$S_{0\cup2} = \begin{pmatrix} P_0 Q_{0\cup1}^{-1} P_0 & \\ & P_2 Q_{2\cup1}^{-1} P_2 \end{pmatrix}^{-1} \underbrace{\begin{pmatrix} \mathbb{1} & P_0 Q_{0\cup1}^{-1} Q_{12} \\ P_2 Q_{2\cup1}^{-1} Q_{10} & \mathbb{1} \end{pmatrix}}_{\tilde{W}}$$

- consider a simplified setup: 3 thick time slices Λ_0, Λ_1, Λ_2
- precondition with $\mathrm{diag}\left\{S_0^{-1}, S_2^{-1}\right\}$
- use the property of the Schur complement, i.e. $S_i^{-1} = P_i Q^{-1} P_i$

original multiboson algorithm

rewrite the inverse of Q^2 as [Lüscher 1993; Boriçi, de Forcrand 1995; Jegerlehner 1995]

$$\frac{1}{\det Q^2} = \lim_{N\to\infty} \det\left\{ P_N(Q^2) \right\}$$

where $P_N(z)$ is a polynomial approximation of $1/z$

$$P_N(z) = \frac{1 - R_{N+1}(z)}{z} = c_N \prod_{k=1}^{N} (z - z_k) \qquad (z_k\text{: roots of } P_N(z))$$

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problem: the condition number of Q^2 is $\simeq (8/am)^2$

$\Rightarrow$ large number of roots needed to have a decent approximation

$\Rightarrow$ large number of multiboson fields, large autocorrelation

polynomial approximation

our work: [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

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

$$W_y = \begin{pmatrix} y\mathbb{1} & P_{\partial 0} Q^{-1}_{0\cup 1} Q_{12} \\ P_{\partial 2} Q^{-1}_{2\cup 1} Q_{10} & y\mathbb{1} \end{pmatrix}$$

polynomial approximation

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

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

multiboson HMC forces

$$W_y \xi_k = \begin{pmatrix} y\mathbb{1} & P_{\partial 0} Q_{0\cup 1}^{-1} Q_{12} \\ P_{\partial 2} Q_{2\cup 1}^{-1} Q_{10} & y\mathbb{1} \end{pmatrix} \begin{pmatrix} \xi_{\partial 0,k} \\ \xi_{\partial 2,k} \end{pmatrix}$$

splitting $\xi_k = \xi_{\partial 0,k} + \xi_{\partial 2,k}$, where $\xi_{\partial i,k} = P_{\partial i} \xi_k$

$$\begin{aligned} \left| W_y \xi_k \right|^2 = |y|^2 \left| \xi_{\partial 0,k} \right|^2 + |y|^2 \left| \xi_{\partial 2,k} \right|^2 \\ + \left| P_{\partial 2} Q_{2\cup 1}^{-1} Q_{10} \xi_{\partial 0,k} \right|^2 + \left| P_{\partial 0} Q_{0\cup 1}^{-1} Q_{12} \xi_{\partial 2,k} \right|^2 \\ + \left[y \xi_{\partial 2,k}^{\dagger} Q_{21} Q_{0\cup 1}^{-1} \xi_{\partial 0,k} + \bar{y} \xi_{\partial 0,k}^{\dagger} Q_{01} Q_{2\cup 1}^{-1} \xi_{\partial 2,k} + \text{c.c.} \right] \end{aligned}$$

- derivatives with respect to Λ_0 gauge links do not depend on Λ_2 links
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