Factorization of fermions and multi-level integration

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Outline

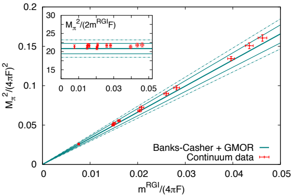
- Introduction to Signal/Noise problem:
  - Baryons
  - Vector correlators (HVP, HLbL)
  - Semileptonic form factors
  - . . .
- Multi-level integration
- Factorization of fermions:
  - Domain decomposition (overlapping blocks)
  - Multi-boson
- Multi-level integration with fermions. Numerical tests for:
  - Baryons
  - Vector correlators

- Conclusions & outlook

Numerical lattice QCD

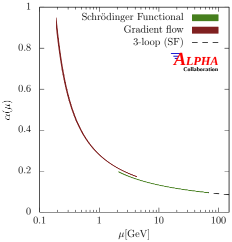
- Extraordinary conceptual, algorithmic and technical progress over the last 30 years:
  - ∗ Hybrid Monte Carlo (HMC) **[Duane et al. 87]**
  - ∗ Multiple time-step integration **[Sexton, Weingarten 92]**
  - ∗ Frequency splitting of determinant **[Hasenbusch 01]**
  - ∗ Domain Decomposition **[Lüscher 04; Del Debbio et al. 06]**
  - ∗ Mass preconditioning and rational HMC **[Urbach et al 05; Clark, Kennedy 06]**
  - ∗ Deflation of low quark modes **[Lüscher 07]**
  - ∗ Avoiding topology freezing **[Lüscher, Schaefer 12]**

[Engel, LG, Lottini, Sommer 15]



$$[\Sigma^{\mathrm{RGI}}]^{1/3}/F = 2.77(2)(4) \quad (N_f = 2)$$

[Bruno et al. 17]

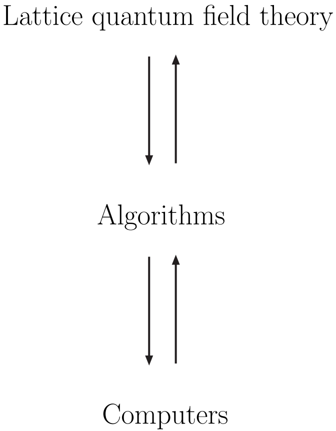


$$\alpha^{(5)}_{\overline{\mathrm{MS}}}(M_Z) = 0.11852(84)$$

- Light quarks at physical point can be simulated. Chiral regime of QCD is accessible
- Algorithms are designed to produce exact results up to statistical errors

Lattice QCD: a theoretical femtoscope

- Lattice QCD is the femtoscope for studying strong dynamics. Its lenses are made of quantum field theory, numerical techniques and computers
- It allows us to look also at quantities not accessible to experiments which may help understanding the underlying mechanisms
- Femtoscope still rather crude. Often we compute what we can and not what would like to
- A rather general strategy emerged: design special purpose algorithms which exploit known math. and phys. properties of the theory to be faster
- Results from first-principles when all syst. uncertainties quantified. This achieved without introducing extra free parameters or dynamical assumptions but just by improving the femtoscope



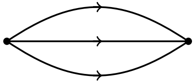
Signal/noise ratio: nucleon

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

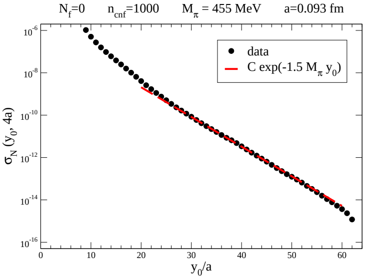
$$\sigma_N^2(y_0,x_0) \propto e^{-3M_\pi|y_0-x_0|}$$



- Signal/noise ratio decreases exponentially with time distance

$$\frac{n_{\rm cnf}\, C_N^2}{\sigma_N^2} \propto n_{\rm cnf}\, e^{-(2M_N-3M_\pi)|y_0-x_0|}$$

At the physical point $2M_N - 3M_\pi \simeq 7.4\,\mathrm{fm}^{-1}$



- Time distances of 1 fm or so are state of the art. For precise and accurate determinations of M_N, g_A,. . . , $\langle x\rangle_{u-d}$, . . . , ChPT suggests that ∼1.5 fm and ∼2.5 fm are needed for two- and three-point functions respectively **[Tiburzi 09, 15; Bär 15-17]**

Signal/noise ratio: HVP, HLbL,...

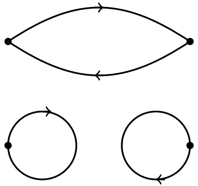
- The HVP contribution to muon $g-2$ reads

$$a_\mu^{\mathrm{HVP}} = \left(\frac{\alpha}{\pi}\right)^2 \int_0^\infty dx_0\, G(x_0)\tilde{K}(x_0, m_\mu)$$

where

$$G(x_0) = -\int d^3x \langle J_k^{\mathrm{em}}(x) J_k^{\mathrm{em}}(0)\rangle$$

with $\tilde{K}(x_0, m_\mu)$ being a known function

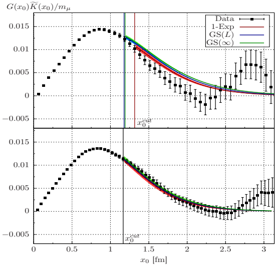


- For the connected contribution (largest and simplest to be computed)

$$\frac{n_{\mathrm{cnf}}\, G^2_{\mathrm{conn}}}{\sigma^2_{G_{\mathrm{conn}}}} \propto n_{\mathrm{cnf}}\, e^{-2(M_\rho - M_\pi)|y_0 - x_0|}$$

if m_ρ lighter than two-pion states. Signal lost at 1-1.5 fm due to exp. increase of stat error

[Della Morte et al. 17]



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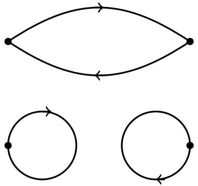
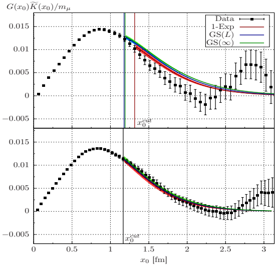


- The estimate from the Mainz group **[Della Morte et al. 17]**

$$a_\mu^{\mathrm{HVP}} = (654 \pm 32_{\mathrm{stat}} \pm 17_{\mathrm{syst}} \pm 10_{\mathrm{scale}} \pm 7_{\mathrm{FV}} {}^{+\ 0}_{-10}{}_{\mathrm{disc}}) \cdot 10^{-10}.$$

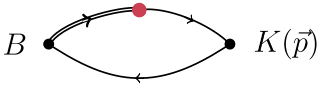
shows an error dominated by statistics and systematics due to the early cut. Reducible by one order of magnitude if good signal up to 2.5 fm or so.

[Della Morte et al. 17]



Signal/noise ratio: leptonic and semileptonic B decays

- Two (noisy) basic building blocks:
  - Mesons with (large) non-zero momentum
  - Static quark line



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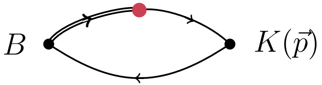
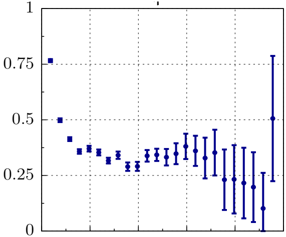


- Non-zero momentum correlators

$$\frac{n_{\rm cnf}\, C^2_{K,\vec{p}}}{\sigma^2_{K,\vec{p}}} \propto n_{\rm cnf}\; e^{-2(E_K(\vec{p})-M_K)|y_0-x_0|}$$

[Della Morte et al. 12]



$$(\tfrac{a}{2\pi L})^2\vec{p}^2 = 2 \quad \Longrightarrow \quad Q^2 \simeq 18\ \mathrm{GeV}^2$$

$$m_{\rm eff}(x_0) = -\log\left\{\frac{C_{K,\vec{p}}(x_0+1)}{C_{K,\vec{p}}(x_0)}\right\}$$

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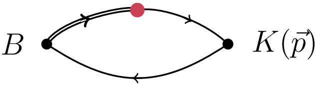

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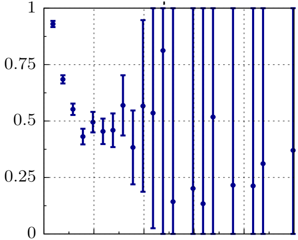

$$\left(\frac{a}{2\pi L}\right)^2 \vec{p}^2 = 4 \quad\Longrightarrow\quad Q^2 \simeq 15\ \mathrm{GeV}^2$$

$$m_{\rm eff}(x_0) = -\log\left\{\frac{C_{K,\vec{p}}(x_0+1)}{C_{K,\vec{p}}(x_0)}\right\}$$

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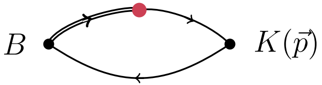
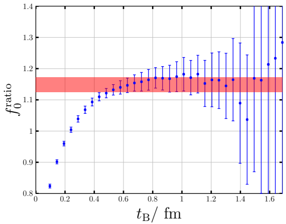


- Static and static-light correlators

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

relevant for $B \to l\nu, B \to \pi(K) l\nu, B \to K(K^*) ll, \ldots$

[Della Morte et al. 15]



$Q^2 \simeq 21\ {\rm GeV}^2$

- The interesting range $Q^2 = 5 - 15\ {\rm GeV}^2$ not reachable with standard MC integration
- Similar or worse problem for many other correlators, e.g. η', glueballs, disconnected, ...

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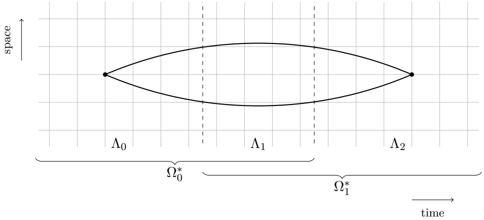
Multi-level integration

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

- If the action and the observable could be factorized

$$S[U] = S_0[U_{\Omega_0^*}] + S_2[U_{\Omega_1^*}] + \dots$$
$$O[U] = O_0[U_{\Omega_0^*}] \times O_2[U_{\Omega_1^*}]$$



then

$$\langle O[U] \rangle = \langle \langle\!\langle O_0[U_{\Omega_0^*}] \rangle\!\rangle_{\Lambda_0} \times \langle\!\langle O_2[U_{\Omega_1^*}] \rangle\!\rangle_{\Lambda_2} \rangle$$

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 $\langle\!\langle \cdot \rangle\!\rangle_{\Lambda_i}$ can be computed efficiently with a statistical error comparable to its central value, then the prefactor in the signal/noise ratio changes as

$$n_{\rm cnf} \to n_0\, n_1^2$$

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

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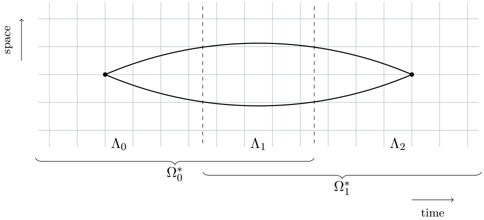

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- With more active blocks, at the cost of approximatively $n_0 n_1$ level-0 configurations,

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

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

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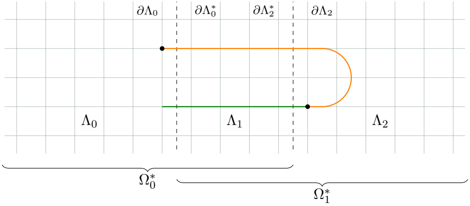
Factorization of the quark propagator

- By introducing the matrix

$$\omega = P_{\partial\Lambda_0}\, Q^{-1}_{\Omega^*_0}\, Q_{\Lambda_{1,2}}\, Q^{-1}_{\Omega^*_1}\, Q_{\Lambda_{1,0}}$$



which :

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

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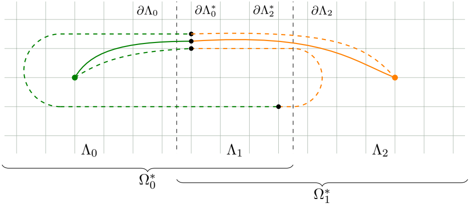

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- The exact propagator for $x \in \Lambda_0$ and $y \in \Lambda_2$ is given by

$$Q^{-1}(y,x) = -Q^{-1}_{\Omega^*_1}(y,\cdot)\, Q_{\Lambda_{1,0}}\, \frac{1}{1-\omega}\, Q^{-1}_{\Omega^*_0}(\cdot,x)$$

and analogously for the other components

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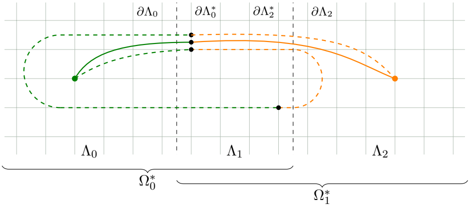

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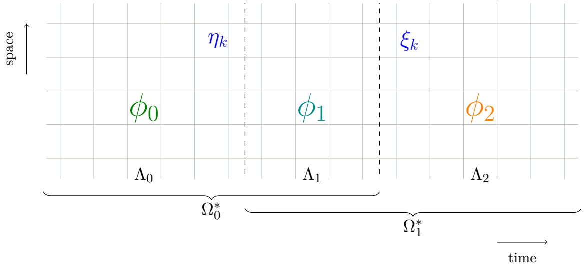
and analogously for the other components

- Propagator is a sum of terms whose full gauge-field dependence is factorized. Built by quarks looping around the boundaries, each loop bringing a suppression factor $\propto e^{-M_\pi \Delta}$. Merit of SAP **[Schwarz 1870]** with overlapping domains

Multi-boson block factorization



- Factorization of gauge-field dependence of the determinant accomplished ($N_f = 2$) :

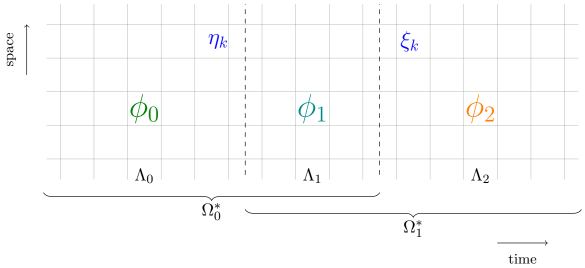
$$\frac{\det Q^2}{\det\{1-w^{N+1}\}^2} = \int \mathcal{D}\phi \ldots \exp\left\{ -|P_{\Lambda_0} Q^{-1}_{\Omega_0^*}\phi_0|^2 - |Q^{-1}_{\Lambda_{1,1}}\phi_1|^2 - |P_{\Lambda_2} Q^{-1}_{\Omega_1^*}\phi_2|^2 - \sum_{k=1}^{N} |W_{\sqrt{u_k}}\chi_k|^2 \right\}$$

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

$$|W_z\chi_k|^2 = |P_{\partial\Lambda_0} Q^{-1}_{\Omega_0^*} Q_{\Lambda_{1,2}}\xi_k|^2 + |P_{\partial\Lambda_2} Q^{-1}_{\Omega_1^*} Q_{\Lambda_{1,0}}\eta_k|^2 + z(\xi_k, Q_{\Lambda_{2,1}} Q^{-1}_{\Omega_0^*}\eta_k) + \ldots$$

- 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 exact scheme for multi-level integration is:

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

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

- Given the large spectral gap of $(1-\omega)$, and depending on the target statistical error, $\mathcal{W}_N$ 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

A crucial test on the spectrum of ω

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

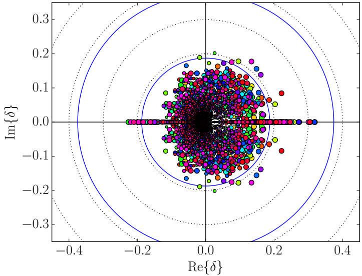
$$a = 0.065 \text{ fm} \quad T \times L^3 = 4 \times 2^3 \text{ fm}^4$$

$$M_\pi = 440 \text{ MeV} \qquad n_{\rm cnf} = 200$$

- Computed 60 eigenvalues with largest norm

$$\omega \, \mathbf{v_i} = \delta_i \, \mathbf{v_i}$$

$\Delta = 12a$



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

Δ/a	$\bar{\delta}$	$\langle \max_i \lvert\delta_i\rvert \rangle$	$\sigma(\max_i \lvert\delta_i\rvert)$	$\max\max_i \lvert\delta_i\rvert$
8	0.3273	0.2886	0.0616	0.5130
12	0.1710	0.1692	0.0453	0.3193
16	0.1072	0.0951	0.0284	0.1977

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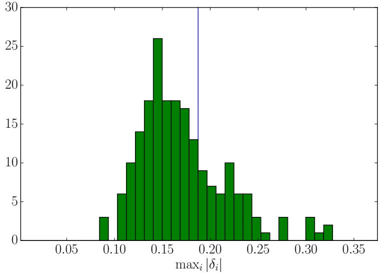

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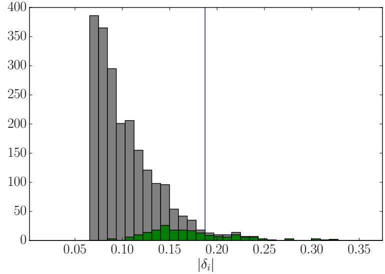

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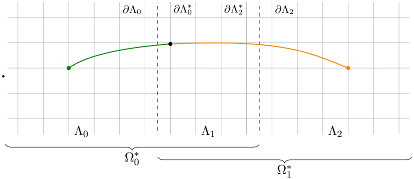
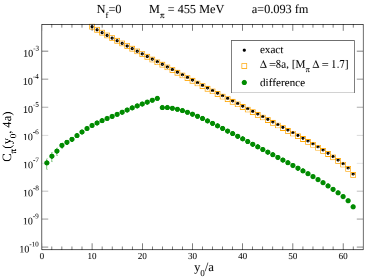
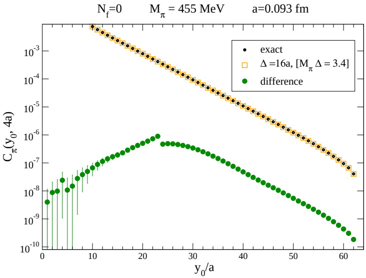
Simplest factorized approximation of propagator

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







- Factorized gauge-field dependence in Wick contractions of hadron correlators too

Outline

- Introduction to Signal/Noise problem:

  - Baryons
  - Vector correlators (HVP, HLbL)
  - Semileptonic form factors
  - . . .

- Multi-level integration

- Factorization of fermions:

  - Domain decomposition (overlapping blocks)
  - Multi-boson

- Multi-level integration with fermions. Numerical tests for:

  - Baryons
  - Vector correlators

- Conclusions & outlook

Correlation functions of gluonic operators

- We have computed the gluonic fields

$$\bar{e}(x_0) = \frac{1}{4} \sum_{\vec{x}} F^a_{\mu\nu}(x) F^a_{\mu\nu}(x)$$

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

and the expectation values

$$C_e(x_0) = \frac{1}{L^3} \langle \bar{e}(x_0) \rangle$$

$$C_{qq}(y_0, x_0) = \frac{1}{L^3} \langle \bar{q}(y_0)\, \bar{q}(x_0) \rangle$$

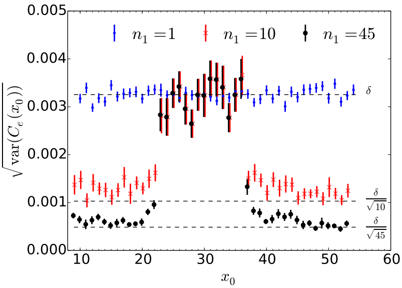
- Blocking with two level integration in Λ_0 and Λ_2

$\Lambda_0 : x_0 \in [0, 23a]$, $\Lambda_1 : x_0 \in [24a, 35a]$

$\Lambda_2 : x_0 \in [36a, 63a]$, $a = 0.065$ fm , $N = 12$

the gain turns out to be the best possible one

$N_f = 2$ $n_{\rm cnf} = 200$ $n_0 = 32$



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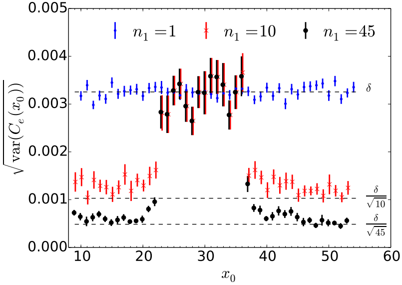

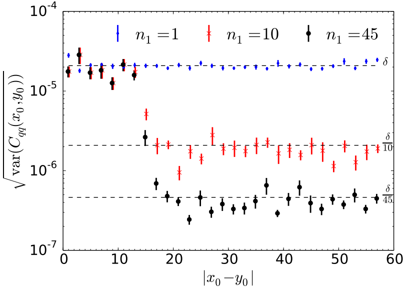

Connected vector two-point correlation function

- Wilson glue with quenched Wilson quarks

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

$$a = 0.093\ \mathrm{fm}\,, \quad M_\pi = 455\ \mathrm{MeV}$$

$$n_0 = 50\,, \qquad n_1 = 30$$

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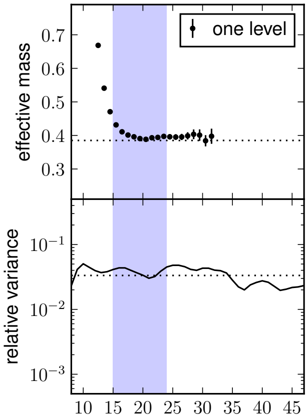
- 1 fm gain in plateau at $n_1 = 30$. Larger n_1 in progress. Expected space for more gain.



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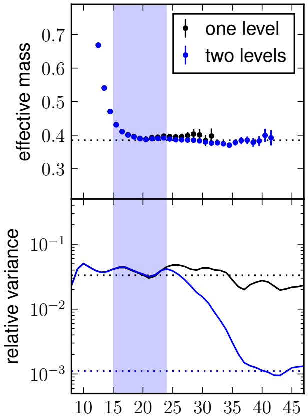

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Multi-level for nucleon two-point function

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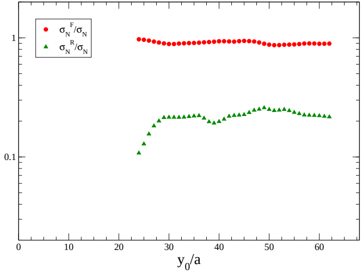
$$W_N(y_0,x_0) = W_N^{\mathrm{fact}}(y_0,x_0) + W_N^{r}(y_0,x_0)$$

where W_N^{fact} is an approximation built from the factorized quark propagator



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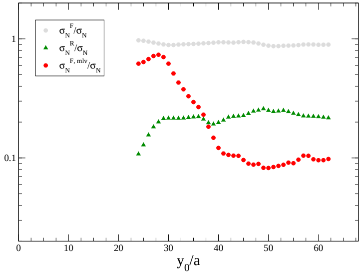

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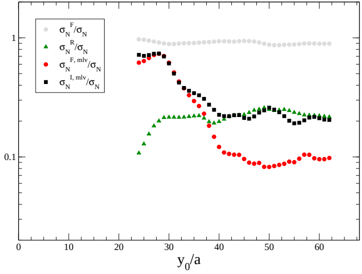

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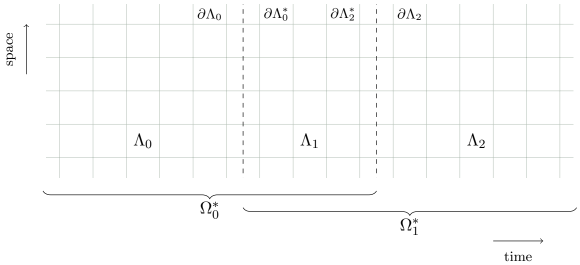
- At large time distances the multi-level works at its best. The (signal/noise)^2 is proportional to n_1^2 (as opposed to n_1) until it hits the green curve

- Refined definitions of $W_N^{\mathrm{fact}}(y_0, x_0)$ are desirable to make computation even cheaper ...

Conclusions & Outlook

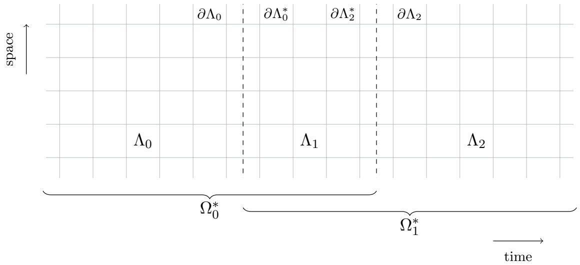


- The effective quark interaction among the gauge field at distant points can be factorized out in (L)QCD by exploiting a decomposition of the space-time in overlapping domains
- By introducing (a small number of) multi-boson auxiliary fields, the resulting action is local in the block scalar and gauge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

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

- 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



- A breakthrough for the computations of many interesting quantities sensitive to SM and hopefully to BSM physics: baryons (g_A, . . . , $< x >_{u-d}$), $g-2$, leptonic, semileptonic and hadronic decays, ρ ,η', ...

- For instance they are within reach (with hard work):

  - subpercent precision in the hadronic vacuum polarization within QCD
  - $Q^2 = 10 - 15$ GeV^2 for semileptonic B decays

- Domains need neither to have a particular shape nor to be connected. 4D decomposition opens the window to large volumes ($10 - 20$ fm with present computers), and therefore to a new class of problems

Pseudoscalar correlators at non-zero momentum

$$a^2\vec{p}^2 = 2$$

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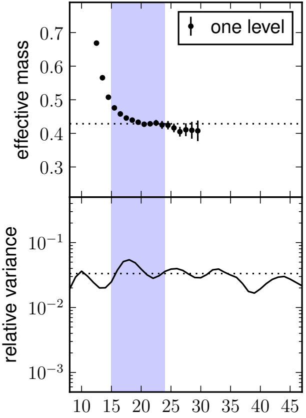

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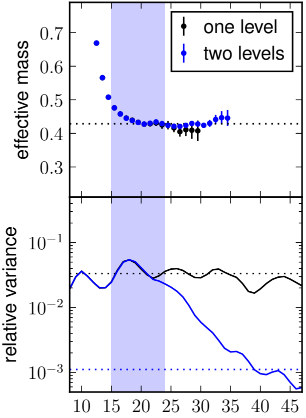

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