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Practical methods for estimating all elements of the lattice quark propagator

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A simple technique to estimate all elements of the lattice quark propagator will be presented. The hybrid method combines an exact spectral representation with a variance-reduced stochastic correction. The method makes the measurement of many currently difficult or inaccessible correlation functions feasible. Example applications will be described, including measuring correlation functions of light quarks bound to a static fundamental colour source.

Overview

- Motivation
- Theory - spectral representations and stochastic estimation
- The method in practise
- Results
- Conclusions and outlook

Method and some early results published in
"Practical all-to-all propagators for lattice QCD."
Justin Foley, K. Jimmy Juge, Alan O'Cais, Mike Peardon, Sinead M. Ryan, Jon-Ivar Skullerud
Comput.Phys.Commun.172:145-162,2005: **hep-lat/0505023**.

How to build an all-to-all propagator (1)

- Spectral representation
- Stochastic representation
- Variance reduction - dilution
- Hybrid method

Spectral representation:

Compute the eigenvalues and eigenvectors $\{v^{(i)}, \lambda_i\}$ of $Q = \gamma_5 D$, then

$$Q^{-1} = \sum_i^N \frac{1}{\lambda_i} v^{(i)} \otimes v^{(i)*}$$

Unfortunately, we can't compute all eigenvectors easily, so we must truncate this representation at $N_{\text{ev}} \ll N$.

This truncation is non-unitary and it is difficult to assign a systematic uncertainty in the error introduced by the truncation.

How to build an all-to-all propagator (2)

Stochastic representation:

Fill a vector, η with independent random numbers. We use $Z_4 = \{1, i, -1, -i\}$.

Since

$$\langle \eta_i \eta_j^* \rangle = \delta_{ij}$$

Z_N noise has the useful property that

$$\eta_i \eta_i^* = 1 \text{ (no sum)}$$

Apply the fermion solver $Q\psi = \eta$ and then

$$\langle \psi_i \eta_j^* \rangle = [Q^{-1}]_{ik} \delta_{kj} = [Q^{-1}]_{ij}$$

This gives an unbiased estimator of every entry in the quark propagator. Unfortunately, the variance of the estimator is large.

Variance reduction (1)

Variance reduction:

- We can reduce the variance of our estimator by gathering statistics, but the noise only falls like $1/\sqrt{m}$ for m noise vectors.
- The exact propagator can be computed using at most N inversions, by putting a single one in all entries of the source vector in turn (ie. using point propagators from all points!)
- This suggests a trick: break the vector space into d smaller pieces spanned by a sub-set of the basis vectors, eg.

$$V_1 = \{e^{(1)} = (1, 0, 0, \ldots), e^{(2)} = (0, 1, 0, \ldots)\}$$

- The "dilution" is defined by the user - eg. we could choose "time-dilution" where V_t is the N/N_t dimensional space of vectors with support on time-slice t.

Variance reduction (2)

Variance reduction:

- The basis is complete, so $V = V_1 \oplus V_2 \oplus \ldots V_d$ and $\eta = \eta^{(1)} + \eta_{(2)} + \eta_{(3)} \ldots + \eta_{(d)}$ where $\eta^{(2)} = \mathcal{S}_i \eta$ and S_i is the projector into vector space V_i.
- Since $\mathcal{S}_i^2 = \mathcal{S}_i$ and $\sum_i \mathcal{S}_i = I$ we can write

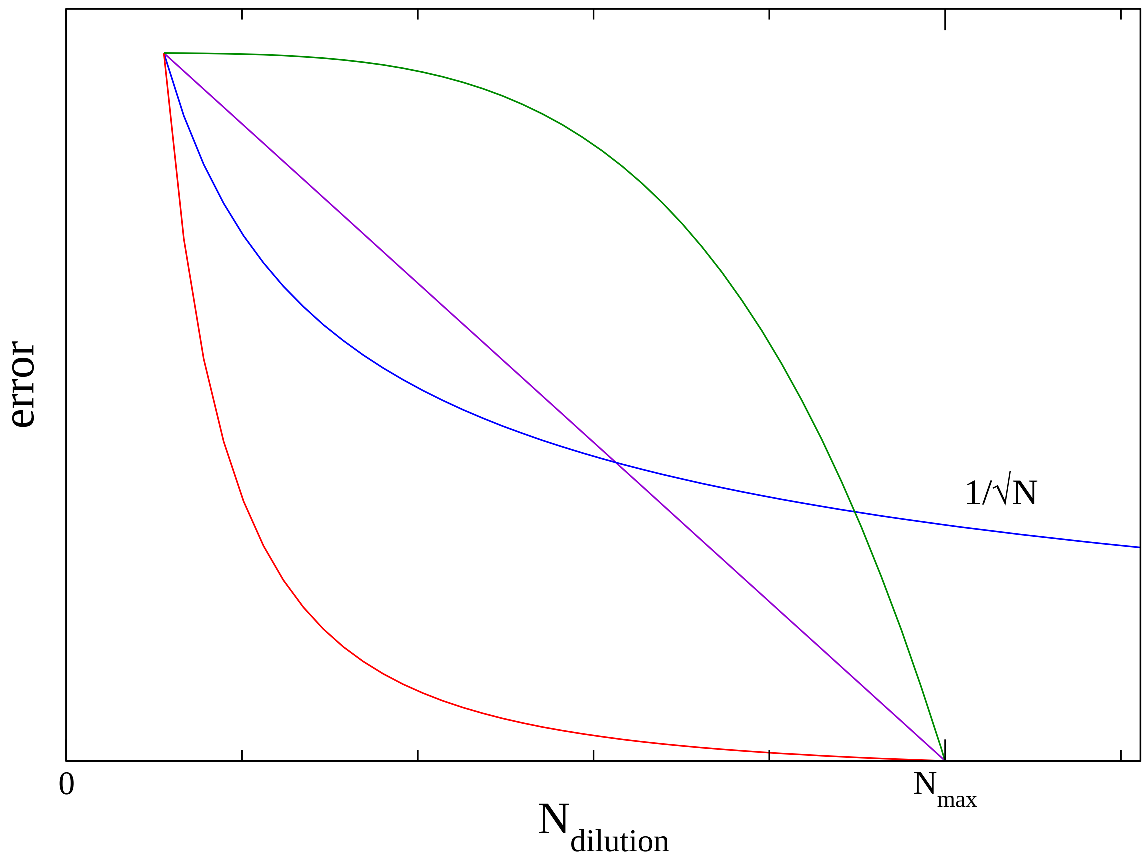
$$I = \sum_i \mathcal{S}_i = \sum_i \mathcal{S}_i^2 = \sum_i \mathcal{S}_i \langle \eta \otimes \eta^* \rangle \mathcal{S}_i$$

- Another representation of the propagator can be written

$$Q^{-1} = \sum_i Q^{-1} \mathcal{S}_i \langle \eta \otimes \eta^* \rangle \mathcal{S}_i = \sum_i \langle \psi^{(i)} \otimes \eta^{(i)*} \rangle$$

- The variance is reduced by explicit cancellation of terms whose expectation value is zero. In the "homeopathic limit" when $d = N$, the exact all-to-all propagator is recovered.

Dilution always wins (eventually)



A hybrid method (1)

A hybrid method:

- Most of the interesting physics is contained in the lowest few eigenvectors.
- Can we use the N_{ev} lowest eigenvectors and correct for the truncation using a stochastic estimator?
- Consider breaking V into the sub-spaces V_L, which is spanned by the lowest N_{ev} eigenvectors and V_H, spanned by the rest.
- Since Q leaves these vector spaces invariant, we can write the inverse

$$Q^{-1} = \bar{Q}_L + \bar{Q}_H = Q^{-1}\mathcal{P}_L + Q^{-1}\mathcal{P}_H$$

- $\bar{Q}_L$ is just the truncated eigenvector representation.
- Estimate $\bar{Q}_H$ stochastically with dilute noise. The action of $\bar{Q}_H$ can be computed from

$$\bar{Q}_H = Q^{-1}\mathcal{P}_H = Q^{-1}(1 - \mathcal{P}_L)$$

A hybrid method (2)

The recipe:

1. Compute N_{ev} eigenvectors and eigenvalues.
2. Generate a noise vector, η and dilute it: $\{\eta^{(1)}, \eta^{(2)}, \ldots\}$
3. For each noise vector, compute

$$\psi^{(i)} = Q^{-1}(1 - \mathcal{P}_L)\eta^{(i)}$$

   by first orthogonalising w.r.t the eigenvectors, and then applying the fermion inverse to the resulting vector.
4. Now, Q^{-1} can be estimated from

$$Q^{-1} = \sum_{i}^{N_{\text{ev}}} \frac{1}{\lambda_i} v^{(i)} \otimes v^{(i)*} + \sum_{d}^{N_d} \psi^{(d)} \otimes \eta^{(d)*}$$

This form suggests packing the two sets of vectors together into a "hybrid list".

Practical implementation (1)

$$Q^{-1} = \sum_i^{N_{\text{ev}}} \frac{1}{\lambda_i} v^{(i)} \otimes v^{(i)*} + \sum_d^{N_d} \psi^{(d)} \otimes \eta^{(d)*}$$

Write two "hybrid lists" of vectors:

$$w^{(i)} = \left\{ \gamma_5 \frac{v^{(1)}}{\lambda_1}, \cdots, \gamma_5 \frac{v^{(N)}}{\lambda_N}, \gamma_5 \eta^{(1)}, \cdots, \gamma_5 \eta^{(N_d)} \right\}$$

$$u^{(i)} = \left\{ v^{(1)}, \cdots, v^{(N)}, \psi^{(1)}, \cdots, \psi^{(N_d)} \right\}$$

and then

$$M^{-1} = \sum_i^{N_h} u^{(i)} \otimes w^{(i)*}$$

Practical implementation (2)

Computing physical correlation functions:

- We don't usually want to compute the quark propagator directly.
- Computing two-point functions

$$C_\pi(\Delta t) = \sum_t \langle \sum_y \bar{d}(y, t+\Delta t)\gamma_5 u(y, t+\Delta t) | \sum_x \bar{u}(x,t)\gamma_5 d(x,t)\rangle$$

becomes:

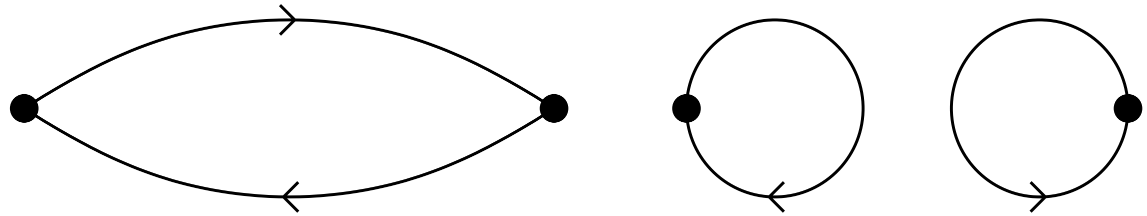
$$C_\pi(\Delta t) = \sum_t$$

$$\langle \sum_y w^*_{[1]}(y, t+\Delta t)\gamma_5 u_{[2]}(y, t+\Delta t) \sum_x w^*_{[2]}(x,t)\gamma_5 u_{[1]}(x,t)\rangle$$

- $\{u_{[1]}, w_{[1]}\}$ and $\{u_{[2]}, w_{[2]}\}$ are independent hybrid lists.

Practical implementation (3)

- Flavour singlet correlators can be computed



- Disconnected diagram for eg η' correlation function is

$$D(\Delta t) = \sum_t$$

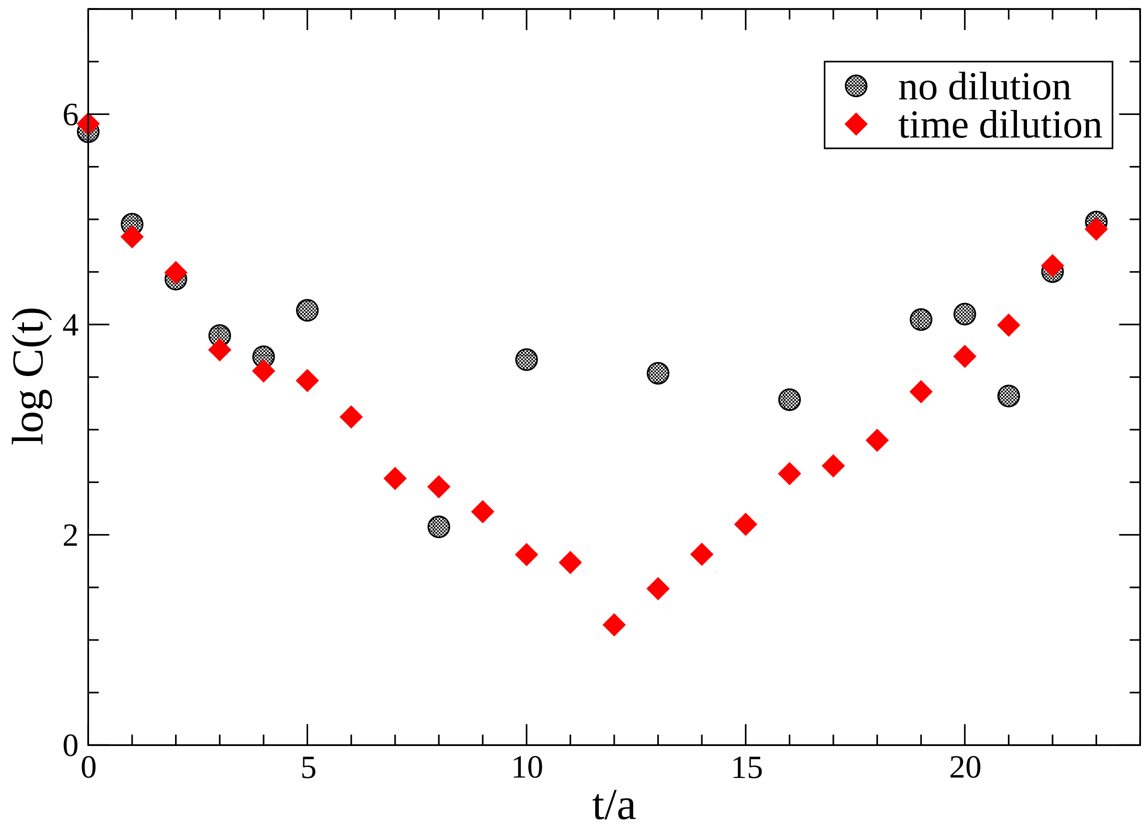
$$\langle \sum_y w^*_{[1]}(y, t + \Delta t)\gamma_5 u_{[1]}(y, t + \Delta t) \ \sum_x w^*_{[2]}(x, t)\gamma_5 u_{[2]}(x, t)\rangle$$

- Hybrid list indices are traced over individually for both the source and the sink.
- Correlations with gluonic operators can be measured.

Practical implementation (4)

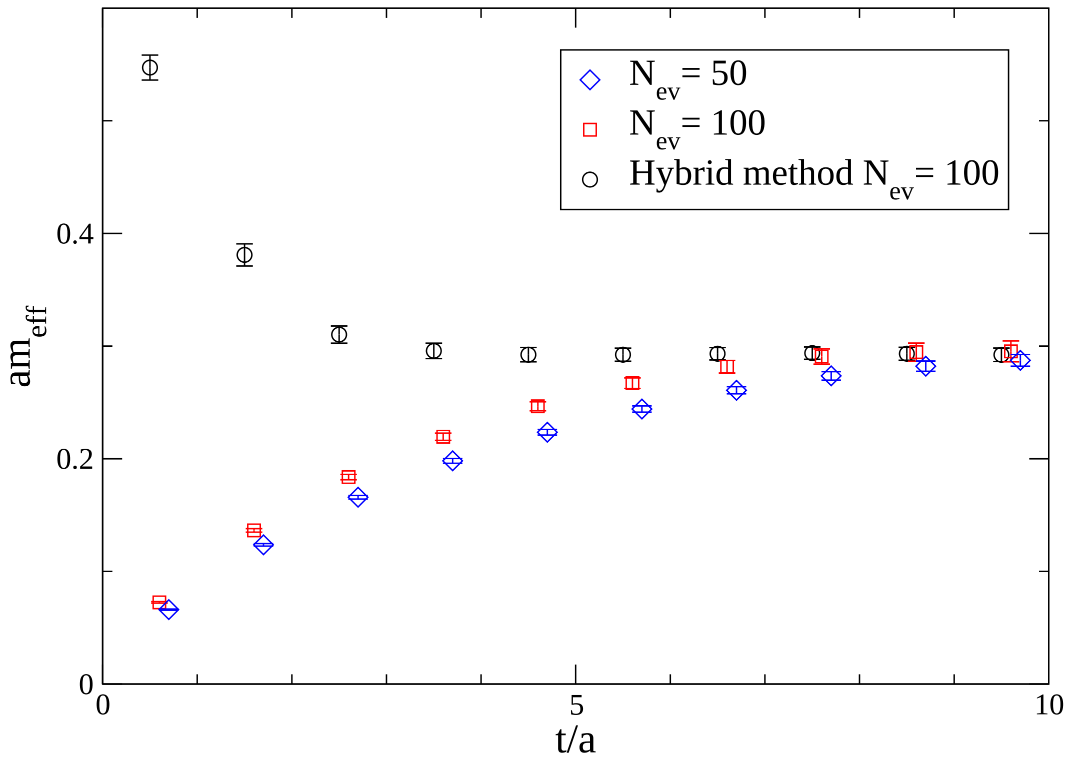
- ALL book-keeping can be hidden from end-user, who just writes a function to compute $a^*\gamma_5 b$ on a time-slice.
- The measurement and propagator calculations are decoupled (apart perhaps from consideration of which dilution is best).
- Operator construction is unrestricted - smearings, extended operators, etc. can be decided on at the final measurement phase.
- Large bases of operators can be built and cross-correlated to optimise ground-state (and excited-state) overlaps.
- More dilution can be applied post-hoc, making use of work done so far.
- More eigenvectors can be computed post-hoc, without the need to re-compute inversions.

Simple demonstration of dilution



$\beta = 5.7$, $12^3 \times 24$ lattice. Wilson fermions $\kappa = 0.1675$, $(m_\pi/m_\rho = 0.50)$

The hybrid method: correcting unitarity



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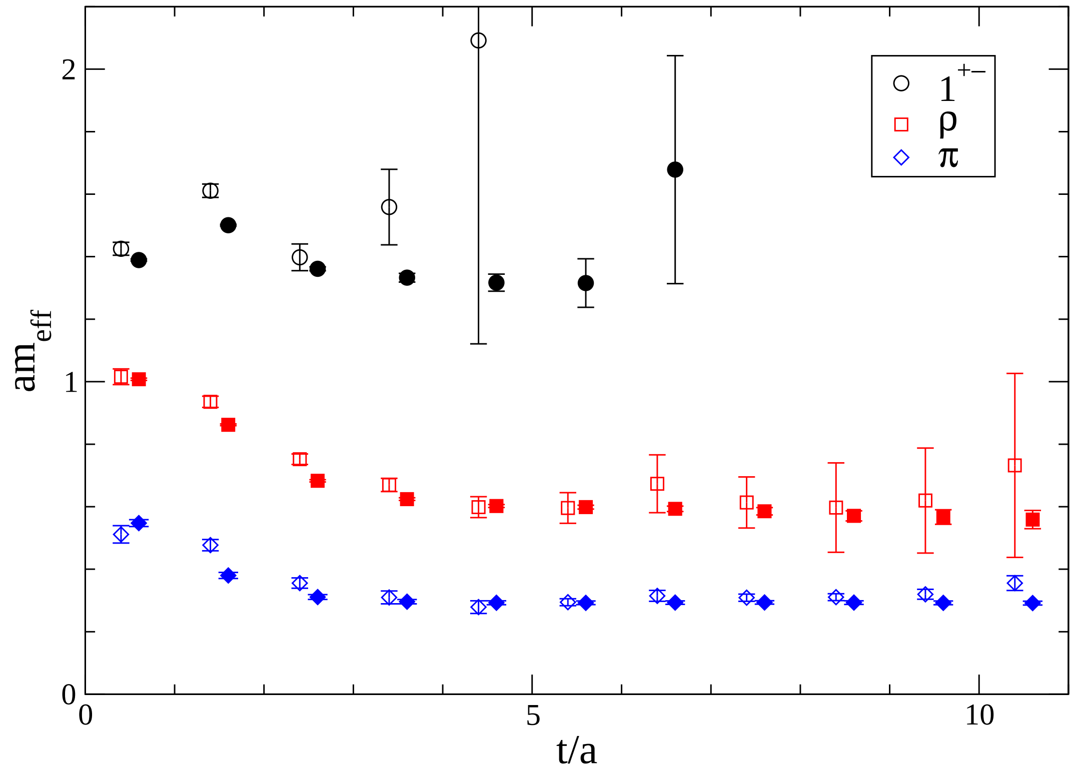
Comparing point propagators



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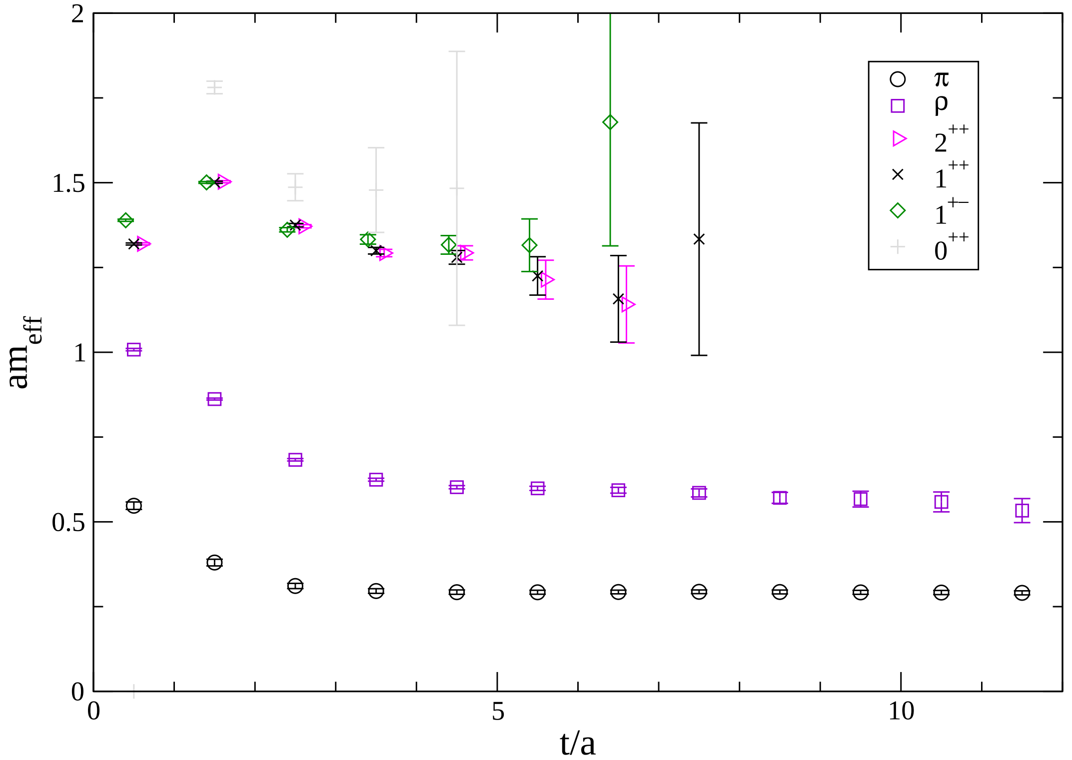
75 configurations.T+S+C+G+E dilution + 100 ev

Isovector mesons



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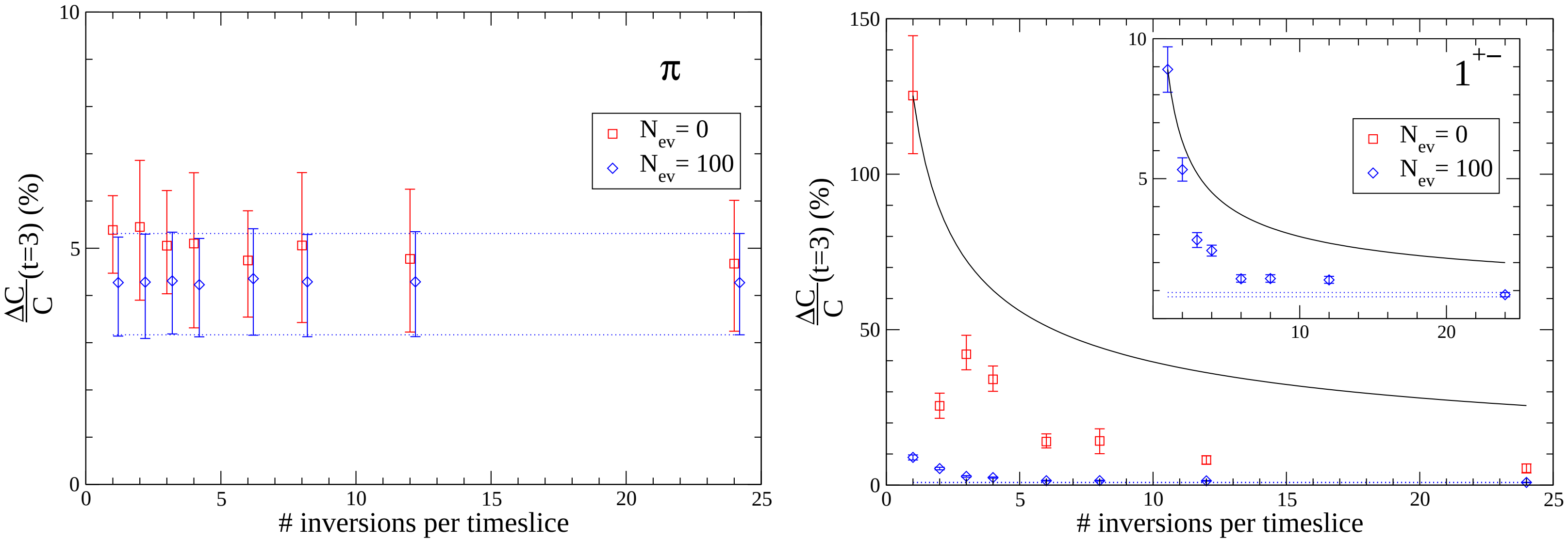
75 configurations.T+S+C+G+E dilution + 100 ev

Paths of dilution

Comparing different dilution methods and the use of eigenvectors.



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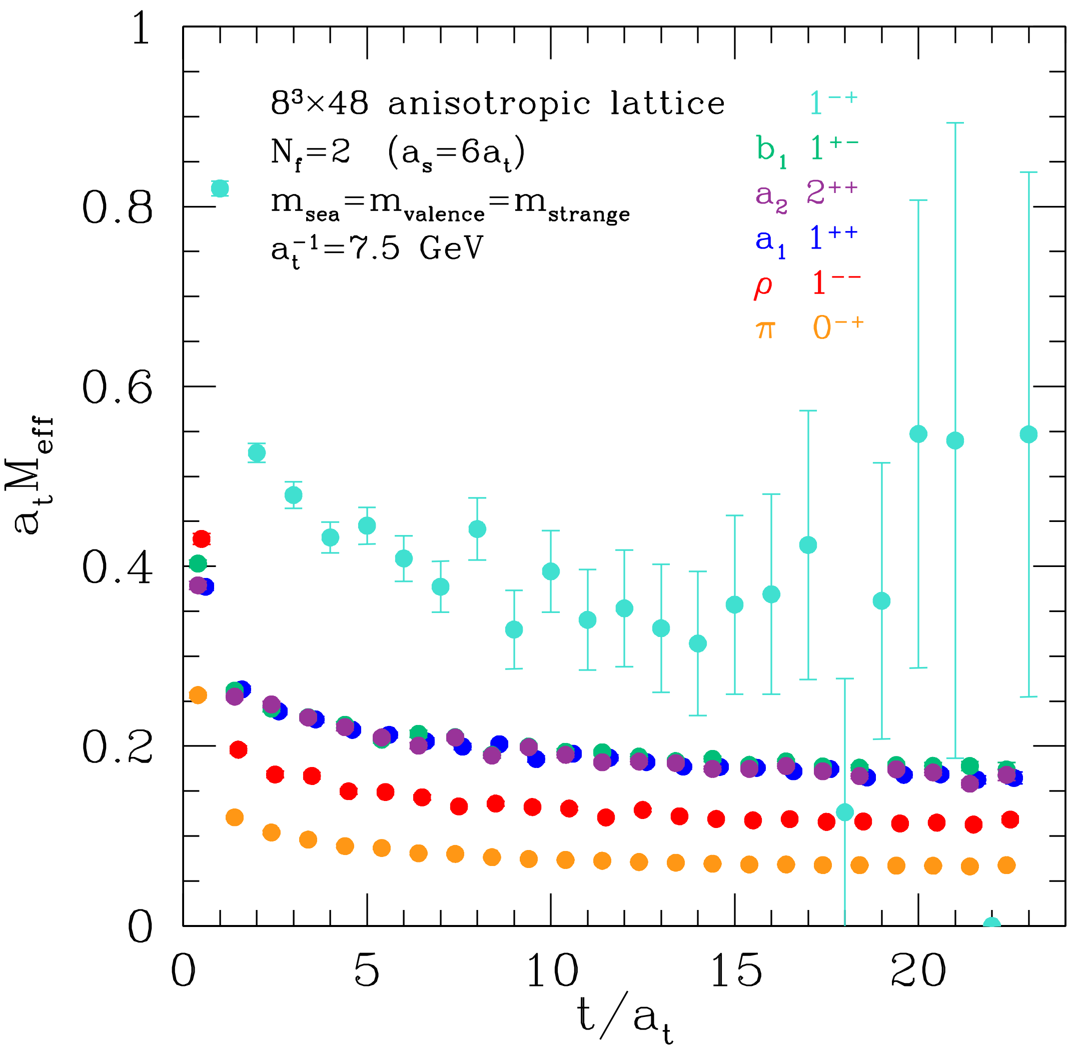
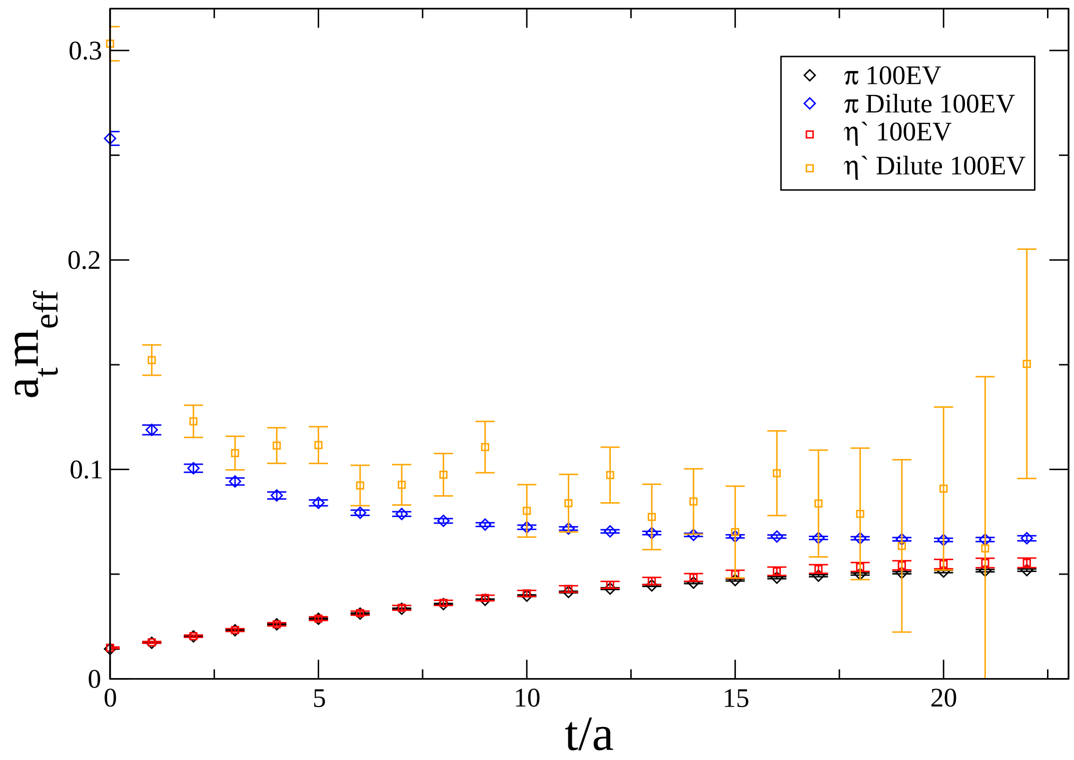
Light spectroscopy



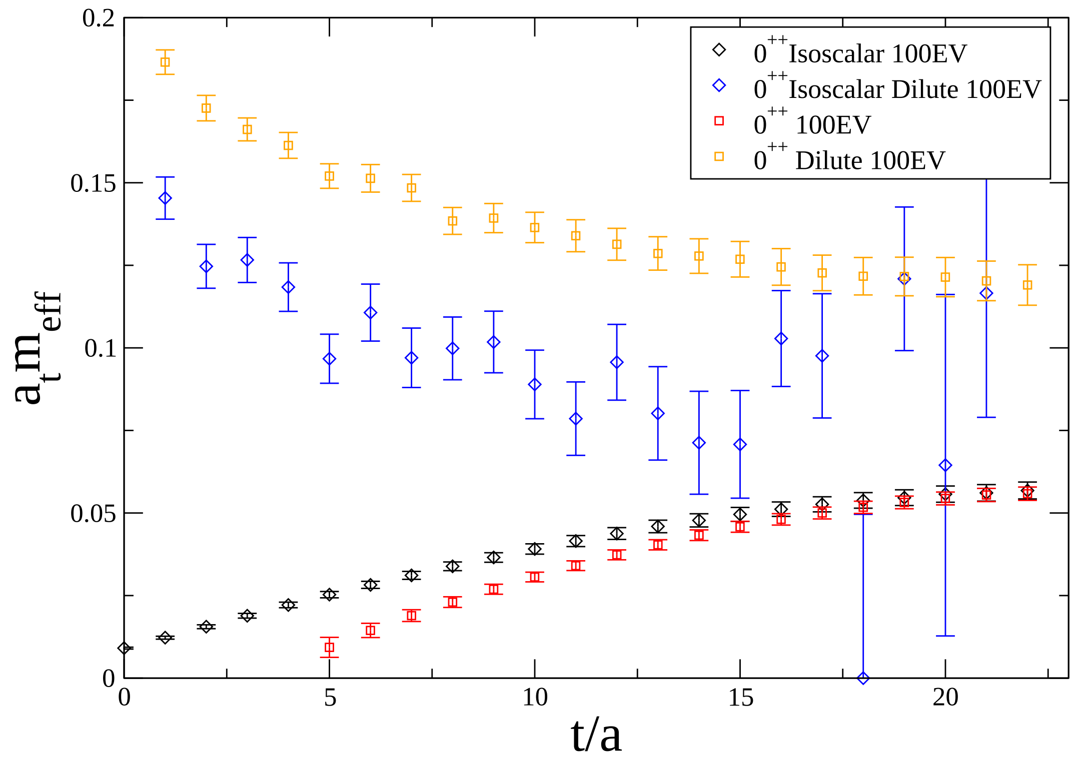
(Exploratory) dynamical anisotropic lattice, $N_f = 2$.

Disconnected diagrams: the π and η'



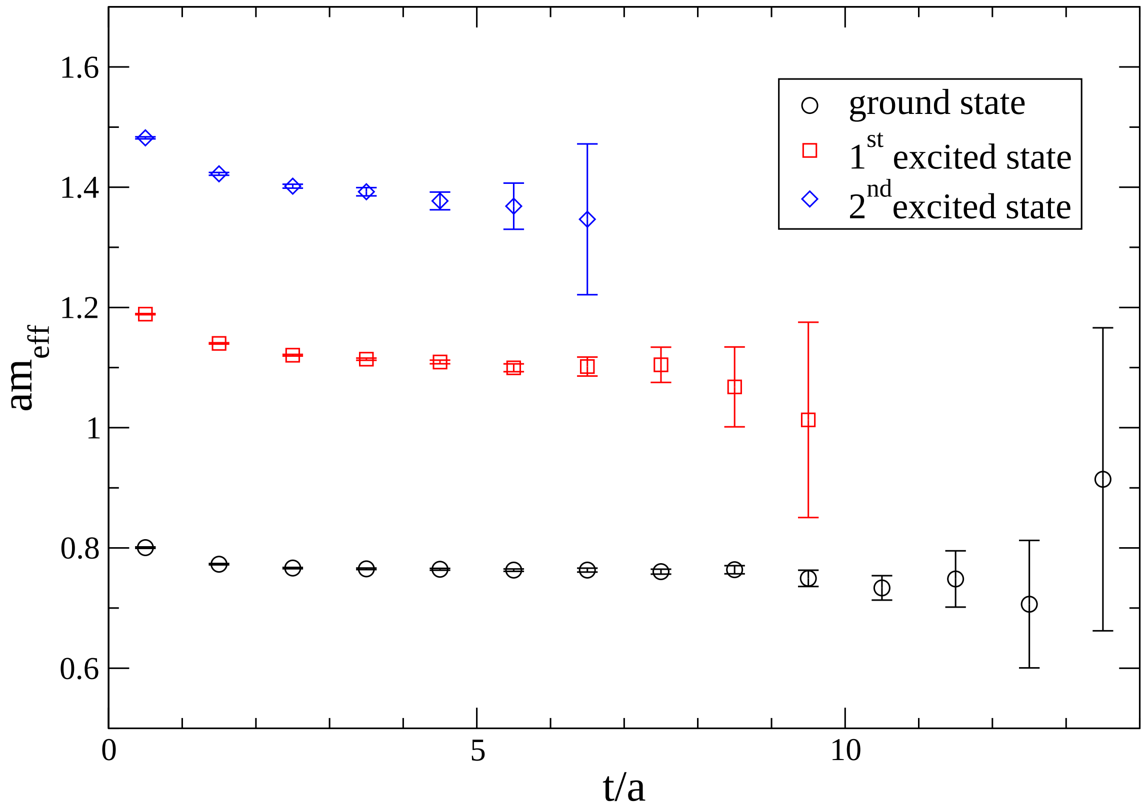
(Exploratory) dynamical anisotropic lattice, $N_f = 2$.

Disconnected diagrams: the f_0 and a_0



(Exploratory) dynamical anisotropic lattice, $N_f = 2$.

The static-light meson and radial excitations



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75 configurations.

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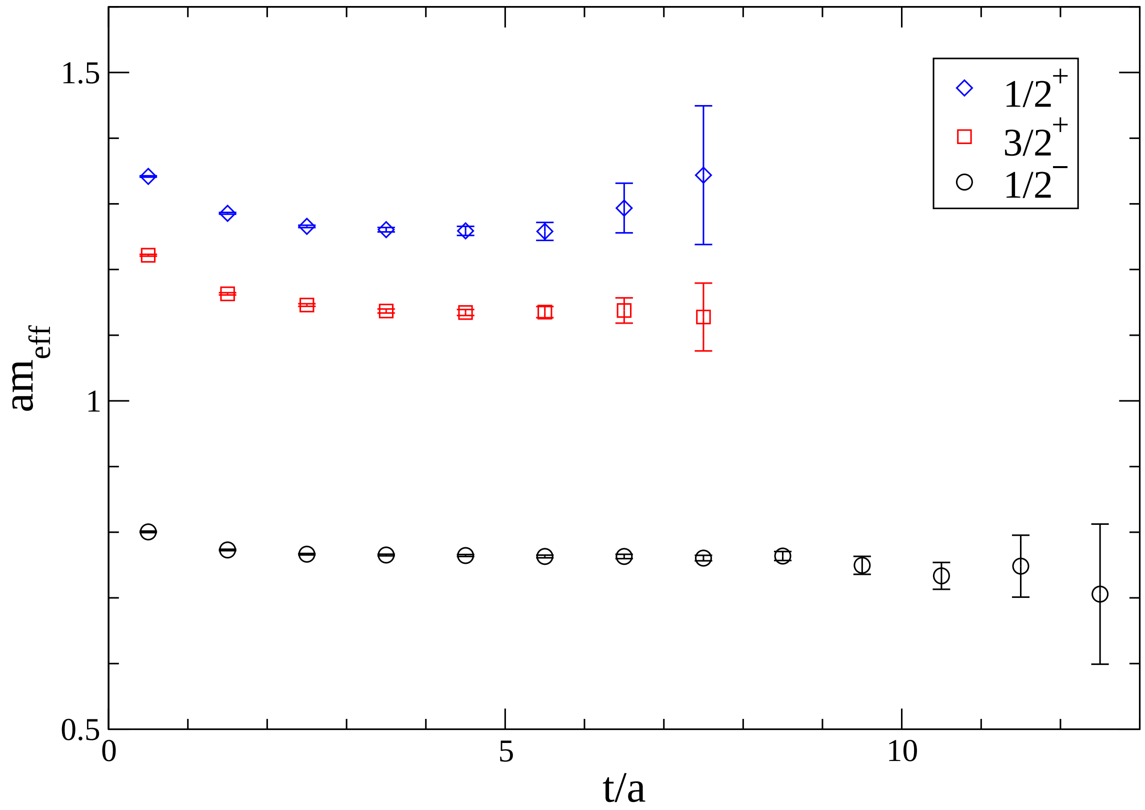
Orbitally excited static-light mesons



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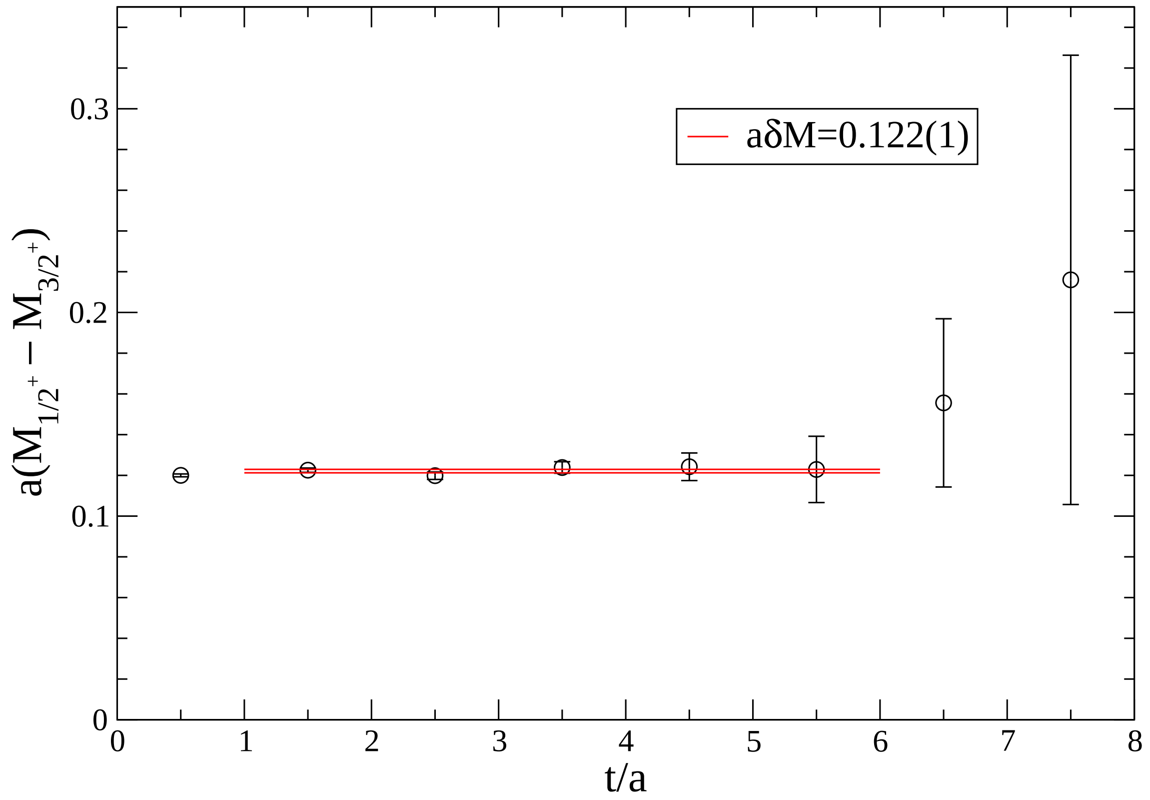
75 configurations.

Orbitally excited static-light mesons



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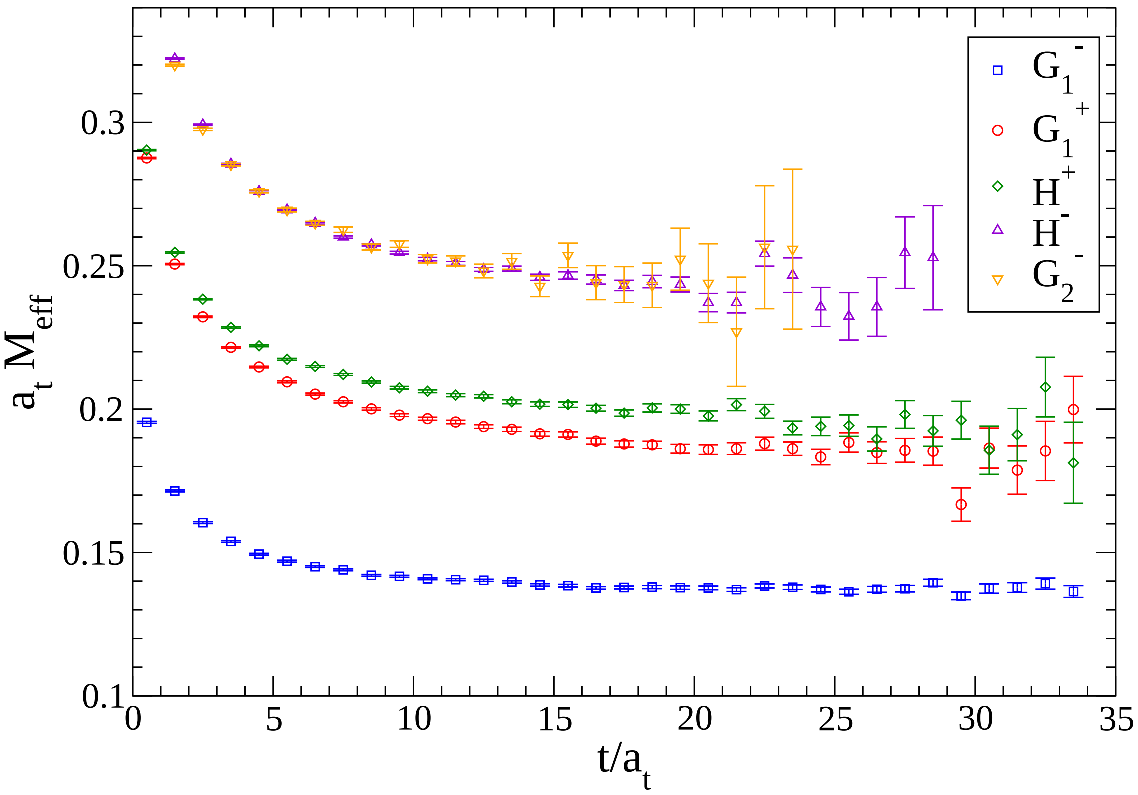
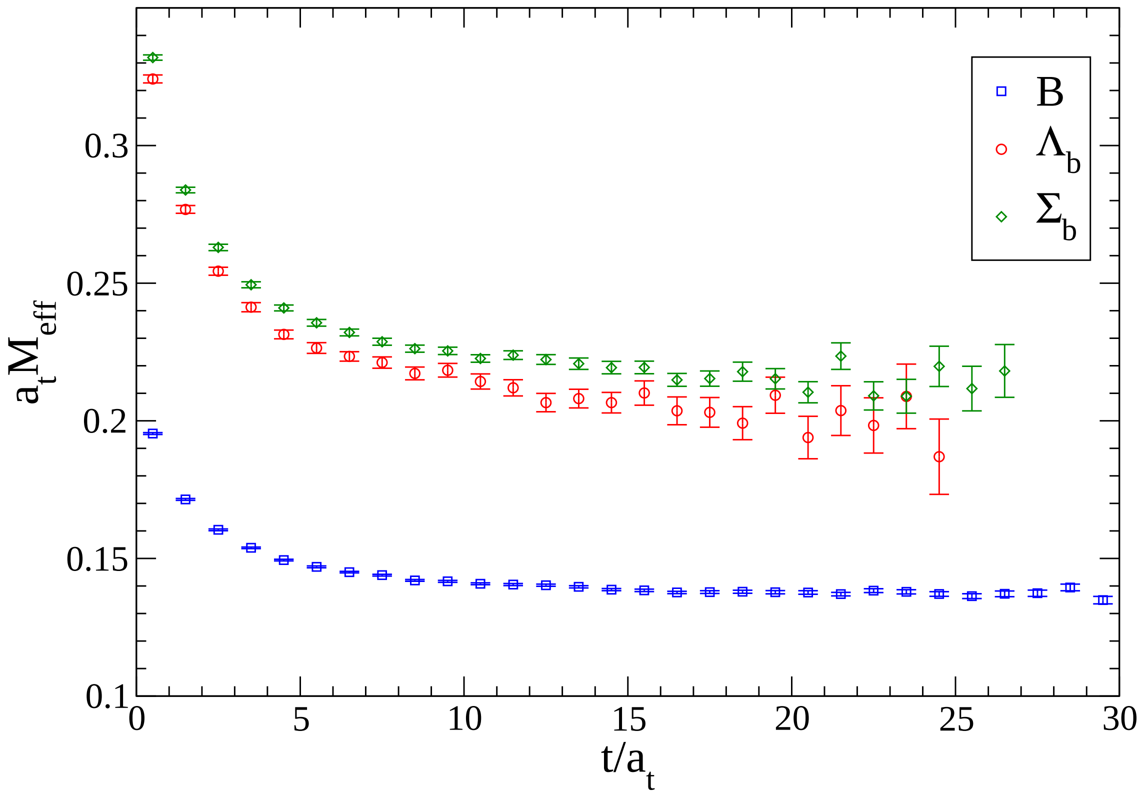
75 configurations.

Static-light mesons on anisotropic lattices



(Exploratory) dynamical anisotropic lattice, $N_f = 2$.

Static-light baryons



(Exploratory) dynamical anisotropic lattice, $N_f = 2$.

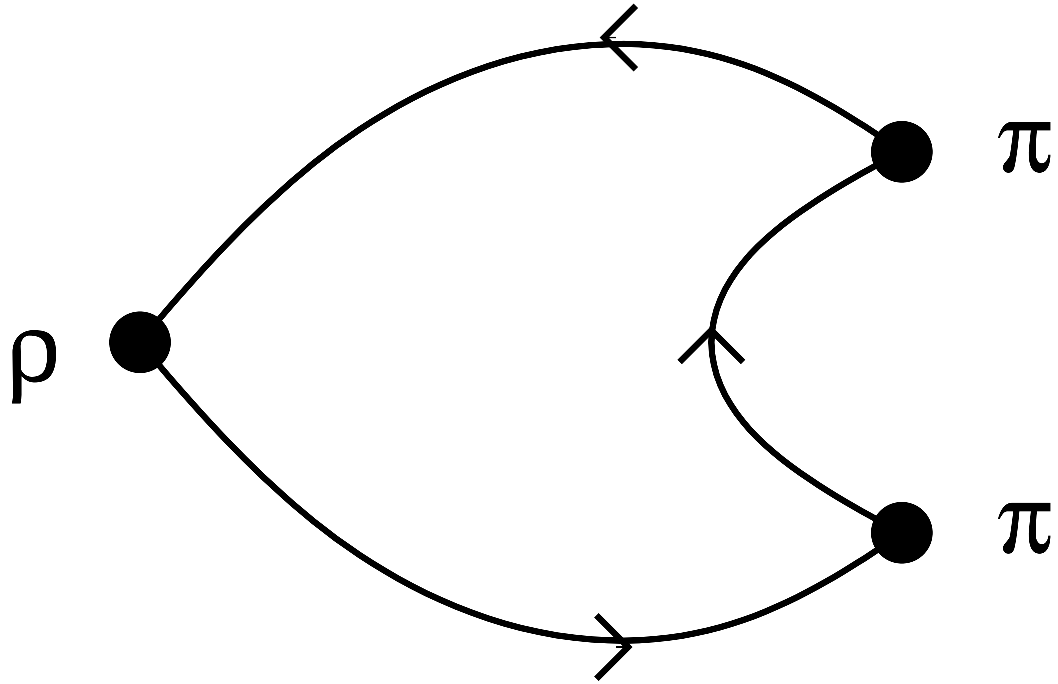
Future directions (1)

$\boxed{\boxed{\text{Exploit the freedom to build correlation functions easily}}}$

- Example (1): the diagrams needed to compute the width of the ρ meson
- Example (2): the diagrams needed to compute the width of the glueball
- Example (3): the diagrams needed to compute QCD contribution to $B \longrightarrow \pi \ell \nu$

Future directions (2)

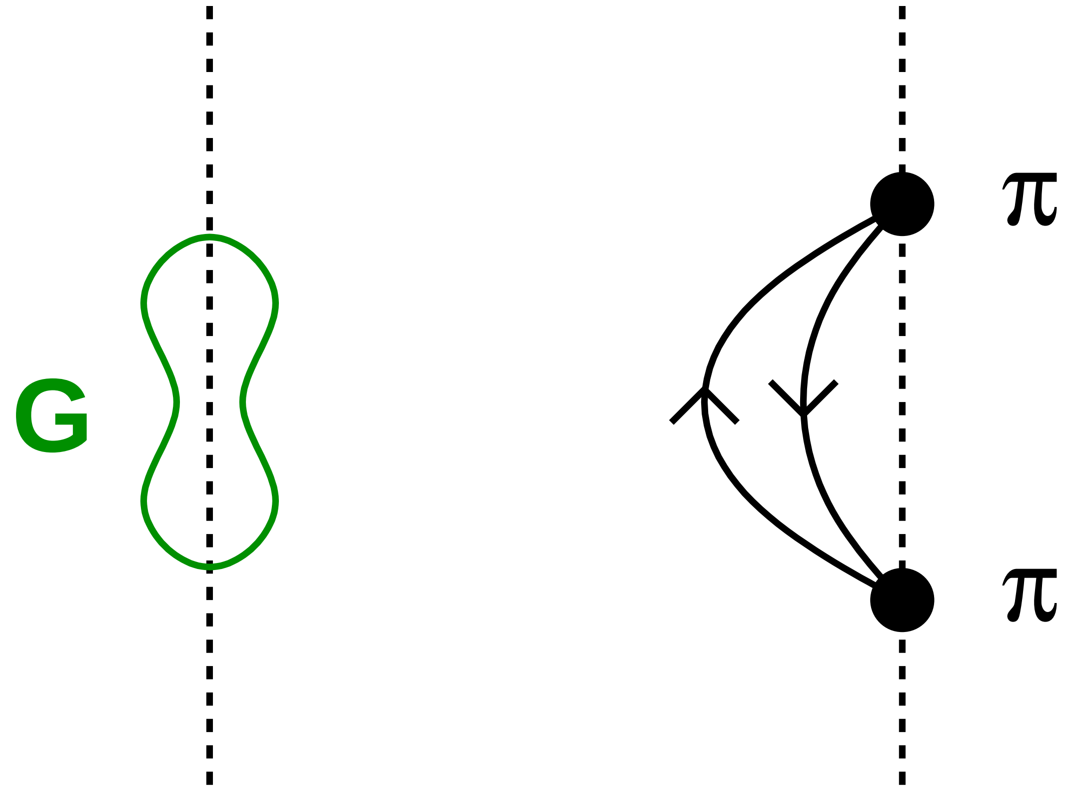
A diagram of the form



Becomes the evaluation of $\mathrm{Tr}\ (\mathcal{O}_\pi(t') \times \mathcal{O}_\pi(t') \times \mathcal{O}_\rho(t))$.

Future directions (3)

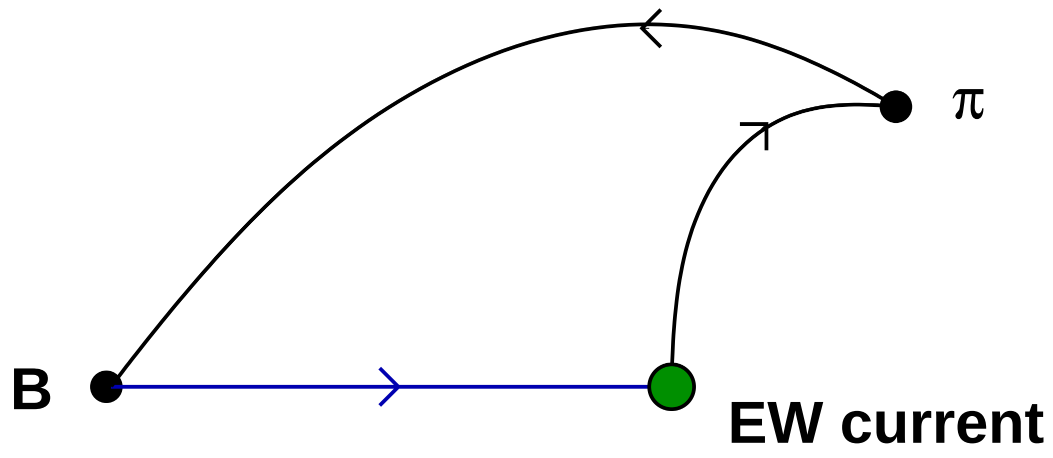
A diagram of the form



Becomes the evaluation of $G(t')\times$ Tr $(\mathcal{O}_\pi(t) \times \mathcal{O}_\pi(t))$.

Future directions (4)

A diagram of the form



becomes the evaluation of Tr $w^*(t)\Gamma U(t,t')u(t') \otimes C_\pi(t'')$

Conclusions

- We have developed and tested a **simple** hybrid scheme to compute all elements of the quark propagator.
- Extra precision can be computed post-hoc, if needed
- Because our representation of the inverse is a sum of outer-products of vectors, we can write a "hybrid list", and make easy-to-use black box codes.
- The end-user needs to only write code to compute the operator acting on fields.
- Results are promising - some more work to understand the details is needed.
- Stop using point propagators!