# Quark-line disconnected diagrams 

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Talk was written in a haste. So there may be omissions and typos.

## Definitions

Lattice spacing: $a$. Sometimes (not considered here): $a_{s} \neq a_{t}$ (anisotropy). Lattice sites $x=n a, n=\left(n_{\mu}\right), \mu \in\{1,2,3,4\}, n_{\mu} \in\left\{0,1, \ldots, N_{\mu}-1\right\}$. Usually (zero temperature): $N_{s}:=N_{1}=N_{2}=N_{3} \leq N_{t}=N_{4}$. \# of 3-volume sites: $V_{3}=N_{s}^{3}$, \# of 4-volume sites: $V=V_{s} N_{t}$.
Gauge links $U_{x, \mu}=U_{x+a \hat{\mu},-\mu}^{\dagger} \in \mathrm{SU}(3)$ have toroidal boundary conditions: $U_{x+N_{\nu} \hat{\nu}, \mu}=U_{x, \mu}$.

Fermion fields $q_{x}$ are Grassmann variables and are antisymmetric in time: $q_{x+N_{t} a \hat{4}}=-q_{x}, q_{x+N_{s} a \hat{\imath}}=q_{x}$

Other boundaries are possible, e.g., open boundaries in time, Dirichlet in time (Schrödinger functional), twist in space etc.
Lattice momenta ( $N_{\mu}$ even): $p_{\mu}=\frac{2 \pi}{N_{\mu} a} \times\left\{-\frac{N_{\mu}}{2}+1,-\frac{N_{\mu}}{2}+2, \ldots, \frac{N_{\mu}}{2}\right\}$.
Largest momentum (in $3+1$ dimensions): $\left|p_{\max }\right|=\sqrt{\sum_{\mu} p_{\max , \mu}^{2}}=\frac{\sqrt{4} \pi}{a}$.

## Definitions II

- (Lattice)-Dirac matrix $M^{f}=\frac{1}{2 \kappa_{f}}\left(\mathbb{1}-\kappa_{f} D\right)$ : discretization of $a \emptyset+a m_{0}^{f} . D[U]$ depends on the gauge configuration $\left\{U_{x, \mu}\right\}$. Different $M^{f}=M\left(\kappa_{f}\right)$ for each (non-degenerate) flavour $f$.
- $M$ has position index $x$, colour index $a$ and spin index $\alpha$ at "source" and "sink" $\left(M_{X Y}=M(x \mid y)_{a b}^{\alpha \beta}, X=(x, a, \alpha), Y=(y, b, \beta)\right.$, $12 \mathrm{~V} \times 12 \mathrm{~V}$ sparse (!) matrix).
- lattice quark mass $m^{f}=\frac{1}{2 a}\left(\frac{1}{\kappa_{f}}-\frac{1}{\kappa_{\text {crit }}}\right)=\left(Z_{S} Z_{A} / Z_{P}\right) m_{\mathrm{AWI}}^{f}$. $m_{\overline{\mathrm{MS}}}^{f}(\mu)=Z_{S}^{-1}(\mu a) m^{f}(a)$ (all up to $\mathcal{O}(a)$-terms.)
- critical hopping parameter $\kappa_{\text {crit }}=\frac{1}{8}+\mathcal{O}\left(g^{2}\right), \quad m^{f} \rightarrow 0 \quad$ as $\quad \kappa_{f} \rightarrow \kappa_{\text {crit }}>\frac{1}{8}$.
- $\gamma_{5}$-symmetry:
$M^{\dagger}=\gamma_{5} M \gamma_{5}$, i.e. $M^{*}(y \mid x)_{b a}^{\alpha \beta}=\gamma_{5}^{\alpha \alpha^{\prime}} M(x \mid y)_{a b}^{\alpha^{\prime} \beta^{\prime}} \gamma_{5}^{\beta^{\prime} \beta}$
- Hermitian Dirac matrix $\mathrm{Q}=\gamma_{5} M=\mathrm{Q}^{\dagger}$.


## Interpolators

- Glueball: $\hat{O}_{G}^{\mathbf{p}}=\sum_{\mathbf{x}} e^{-i \mathbf{p x}} \sum_{n} v_{n} \cdot \operatorname{Tr}(\text { spatial loop } n)_{\mathbf{x}}$.
- Meson: $\hat{O}_{M}^{p}=a^{3} \sum_{\mathbf{x}} e^{-i \mathbf{p x}}\left(\bar{q}^{1} \Gamma_{A} D \Phi q^{2}\right)_{\mathbf{x}}$.
$\Gamma_{A}=\gamma_{1}^{n_{1}} \gamma_{2}^{n_{2}} \gamma_{3}^{n_{3}} \gamma_{4}^{n_{4}}$ acts on the Dirac spinor space. ( $n_{1}$ is the least significant bit of $A \in\{0, \cdots, 15\}: \Gamma_{0}=\mathbb{1}, \Gamma_{8}=\gamma_{4}, \Gamma_{15}=\gamma_{5}$ etc.)
$D$ contains derivatives and other gauge covariant transporters.
$\Phi$ is a smearing function. ( $D$ and $\Phi$ do not act on the spin index.)
- Baryon (example):
$\hat{O}_{N^{ \pm}, \alpha}^{\mathbf{p}}=a^{9 / 2} \sum_{\mathbf{x}} e^{-i \mathbf{p x}}\left[\epsilon_{a b c} P_{ \pm} \Phi_{1} u_{\alpha, a}\left(u_{b}^{T} C \gamma_{5} \Phi_{2} d_{c}\right)\right]_{\mathbf{x}}$
This Fermion contains an open Dirac spin index $\alpha$.
$P_{ \pm}=\frac{1}{2}\left(\mathbb{1} \pm \gamma_{4}\right)$ is a parity projector (for $\mathbf{p} \neq \mathbf{0}$ see $F$ Lee,
D Leinweber, NPPS 73 (99) 258).
$C=i \gamma_{2} \gamma_{4}=i \Gamma_{10}$ is the charge conjugation matrix.


## Two point functions

Two point Green (correlation) function:

$$
C(t)=\left\langle O\left(t+t_{0}\right) O^{\dagger}\left(t_{0}\right)\right\rangle
$$

We will often exploit the translational invariance of expectation values:

$$
\left\langle O_{x}\right\rangle_{u}=\left\langle O_{0}\right\rangle_{u}=\frac{1}{V} \sum_{x}\left\langle O_{x}\right\rangle_{u}
$$

From now on we choose $t_{0}=0$ and assume $L_{t}=N_{t} a=\infty$.
Spectral decomposition $\left(\sum_{n} \frac{1}{2 E_{n}}|n\rangle\langle n|=\mathbb{1}\right)$ :

$$
C(t)=\sum_{n}\langle\Omega| \hat{O}|n\rangle \frac{e^{-E_{n} t}}{2 E_{n}}\langle n| \hat{O}^{\dagger}|\Omega\rangle=\sum_{n} c_{n} e^{-E_{n} t},
$$

where $\left.c_{n}=|\langle n| \hat{O}| \Omega\right\rangle\left.\right|^{2} /\left(2 E_{n}\right) \geq 0$.
This holds for any $t$ for actions with point and link reflection positivity (e.g. Wilson) and for $t \geq t_{\text {min }}$ for less local actions ( $t / a \geq 1$ for clover). For different interpolators at source and sink $c_{n}$ can be negative.

## Example: meson

$$
\begin{aligned}
C_{M}^{\mathbf{p}}(t) & =\left\langle O_{M}^{\mathbf{p}}(t) O_{M}^{\mathrm{p}}(0)\right\rangle \\
& =a^{6} \sum_{\mathrm{x}, \mathrm{y}} e^{-\mathbf{p} \mathbf{p}(\mathrm{x}-\mathrm{y})}\left\langle\left(\bar{q}^{1}\left\ulcorner q^{2}\right)_{x}\left(\bar{q}^{1}\left\ulcorner q^{2}\right)_{y}^{\dagger}\right\rangle,\right.\right.
\end{aligned}
$$

where $x=(\mathbf{x}, t), y=(\mathbf{y}, 0)$. For simplicity, derivatives $D$ and smearing functions $\Phi$ are omitted.
We compute $\left(\bar{q}^{1} \Gamma q^{2}\right)^{\dagger}=-q^{2 \dagger} \Gamma^{\dagger} \gamma_{4} q^{1}= \pm \bar{q}^{2} \Gamma q^{1}\left(\gamma_{4} \Gamma=\mp \Gamma^{\dagger} \gamma_{4}\right)$, rename $\mathbf{x}_{\text {new }}=\mathbf{x}-\mathbf{y}$ and set $\mathbf{y}=\mathbf{0}$ (translational invariance):

$$
\begin{aligned}
C_{M}^{\mathbf{p}}(t) & = \pm V_{3} a^{6} \sum_{\mathbf{x}} e^{-i \mathbf{p x}}\left\langle\bar{q}_{x}^{1}\left\ulcorner q_{x}^{2} \bar{q}_{0}^{2} \Gamma q_{0}^{1}\right\rangle\right. \\
& =\mp V_{3} a^{6} \sum_{\mathbf{x}} e^{-i \mathbf{p x}}\left\langle\operatorname{Tr}\left[\Gamma\left(q_{x}^{2} \bar{q}_{0}^{2}\right) \Gamma\left(q_{0}^{1} \bar{q}_{x}^{1}\right)\right]\right\rangle,
\end{aligned}
$$

where the trace is over spin and colour (Wick contraction).

## Propagator

Fermionic contribution to Lagrangian: $a^{-1} \sum_{f} \bar{q}^{f} M^{f}[U] q^{f}$.
This means $a^{3}\left\langle q_{x}^{f} \bar{q}_{y}^{f}\right\rangle_{q}=M^{f-1}(x \mid y)$ where the subscript $q$ denotes the Fermionic expectation value.
$\gamma_{5}$-Hermiticity: $a^{3}\left\langle q_{0} \bar{q}_{x}\right\rangle_{q}=M^{-1}(0 \mid x)=\gamma_{5}\left[M^{-1}(x \mid 0)\right]^{\dagger} \gamma_{5}$. Then:

$$
C_{M}^{\mathbf{p}}(t)=\mp V_{3} \sum_{\mathbf{x}} e^{-i \mathbf{p x}}\left\langle\operatorname{Tr}\left[M^{2-1}(x \mid 0) \Gamma \gamma_{5}\left[M^{1-1}(x \mid 0)\right]^{\dagger} \gamma_{5} \Gamma\right]\right\rangle_{U}
$$

where the remaining expectation value is over gauge configurations.
The above expression is particularly simple for the $\pi\left(\Gamma=\gamma_{5}\right.$, i.e. $\left.\Gamma \gamma_{5}=\mathbb{1}\right)$.
For $q=q^{1}=q^{2}$ (flavour-/iso-singlet) an additional term appears in the Wick contraction and $M^{-1}(x \mid x)$ is needed.
Otherwise only the 12 columns of $M^{-1}$ starting from $y=0$ are required, the "point-to-all" propagator $S(x \mid 0)_{a b}^{\alpha \beta}=M^{-1}(x \mid 0)_{a b}^{\alpha \beta}$.

The point-to-all propagator $S(x \mid 0)(12 \times 12$ spin-colour matrices at all spacetime points $x$ ) is obtained by solving

$$
\sum_{x, \alpha, a} M(z \mid x)_{c a}^{\gamma \alpha} S(x \mid 0)_{a b}^{\alpha \beta}=\delta_{z 0} \delta_{c b} \delta^{\gamma \beta}
$$

for all $12 \beta \in\{1,2,3,4\}$ and $b \in\{1,2,3\} \delta$-sources.
It can be smeared at the sink with a smearing function $\Phi$ that only depends on the position and colour but commutes with 「-matrices.
Each source smearing requires 12 new solves of:

$$
\sum_{x, \alpha, a} M(z \mid x)_{c a}^{\gamma \alpha} S^{\Phi}(x \mid 0)_{a b}^{\alpha \beta}=\left(\Phi \delta_{\mathbf{0}, b}\right)(z \mid 0)_{c b} \delta^{\gamma \beta}
$$

where $\delta_{\mathbf{0}, b}$ denotes a colour vector with only one entry, at position 0 and colour $b$. Note that smearing does not need to be repeated for different spin.

## Symmetries

Action, measure and boundary conditions adhere global symmetries, e.g., (approximate) $\mathrm{H}(4)$ hypercubic symmetry, charge symmetry and translation symmetry.

We can decompose any observable $A=A_{\text {sing }}+A_{\text {nonsing }}$ where $\langle A\rangle_{U}=\left\langle A_{\text {sing }}\right\rangle_{U}$.
Above, due to translational invariance we got away with point-to-all propagators for non-flavour-singlet spectroscopy, replacing $\sum_{\mathbf{y}}(\bar{q} \Gamma q)_{\mathbf{y}}^{\dagger} e^{i \mathbf{p y}}$ by $V_{3}(\bar{q} \Gamma q)_{0}^{\dagger}$ at the source. However, doing this we loose statistics (self-averaging).
Likewise, with respect to local gauge transformations we can decompose any observable into $A_{\text {sing }}+A_{\text {nonsing }}$ where only $\left\langle A_{\text {sing }}\right\rangle U$ is non-vanishing. Again, $A_{\text {nonsing }}=0$ is desirable to reduce noise (and in this case can be achieved easily).

## Why all-to-all?

Often "all-to-all" is necessary:
nucleon structure:
$\left\langle N^{\dagger}(t)\right| J_{\mu}(t / 2)|N(0)\rangle:$
(Example: $J_{\mu}=\psi^{\dagger} \gamma_{\mu} \psi$ )
decays/scattering:



HW Hamber, E Marinari, G Parisi, C Rebbi, NPB225 (83) 475
(Appendix B)
GP Lepage, http://inspirehep.net/record/287173


Self-averaging over many source points increases statistics. Becomes increasingly important at small $m_{\pi}$.

## Low mode averaging

At light quark masses one may compute eigenvectors to deflate the solver.
Eigenvectors also offer the possibility of low mode averaging (LMA)
T DeGrand, S Schäfer CPC 159 (04) 185
L Giusti et al, JHEP 0404 (04) 013.

$$
C_{\mathrm{LMA}}(t)=C_{\mathrm{low}}(t)+\left[C^{\mathrm{pa}}(t)-C_{\mathrm{low}}^{\mathrm{pa}}(t)\right] .
$$

$C_{\text {low }}$ : contribution from low eigenmodes of $\mathrm{Q}=\gamma_{5} M\left(\mathrm{Q}=\mathrm{Q}^{\dagger}\right)$, all-to-all, averaged over the lattice volume.
$C^{\text {pa }}$ : standard point-to-all 2-point function.
$C_{\text {low }}^{\mathrm{pa}}$ : low mode contribution (point-to-all), needs to be subtracted since this is already included into $C^{\mathrm{pa}}$.

This does not affect the expectation value but may reduce the error, due to the self-averaging of the low-mode contribution.
This works well for positive parity baryons and negative parity mesons GB, L Castagnini, S Collins, PoS (LATTICE2010) 096

## Effective masses




## Example: meson

$$
\mathrm{Q}\left|u^{i}\right\rangle=q_{i}\left|u^{i}\right\rangle, \quad\left\langle u^{i} \mid u^{j}\right\rangle=\delta_{i j}, \quad q_{i} \in \mathbb{R}, \quad \mathrm{Q}=\gamma_{5} M .
$$

This means that,

$$
\mathrm{Q}=\sum_{i=1}^{12 V} \frac{1}{q_{i}}\left|u^{i}\right\rangle\left\langle u^{i}\right| .
$$

We need to truncate: $i \in\{1,2, \ldots, m\}$ where $m \propto V$. So the number of operations increases $\propto V^{2}$.
The eigenvectors have position, spin and colour components:
$u^{i}(x)_{\alpha}^{a}=\left\langle x, a, \alpha \mid u^{i}\right\rangle$.

$$
\left.C_{\text {low }}(t)= \pm \sum_{i, j}\left\langle\left.\frac{1}{q_{i} q_{j}} t\left\langle u^{j}\right| \gamma_{5} \Gamma \right\rvert\, u^{i}\right\rangle_{t 0}\left\langle u^{i}\right| \gamma_{5} \Gamma\left|u^{j}\right\rangle_{0}\right\rangle_{U},
$$

where the subscript $t$ denotes a projection of the vector onto timeslice $t$.

The point-to-all low mode contribution can be obtained using (Note that $u^{i}(x)=\left\langle x \mid u^{i}\right\rangle$ is a spin-colour vector),

$$
C_{\text {low }}^{\mathrm{pa}}(t)= \pm \sum_{i, j}\left\langle\left.\frac{1}{q_{i} q_{j}} t\left\langle u^{j}\right| \gamma_{5} \Gamma \right\rvert\, u^{i}\right\rangle_{t} u^{i}(0)^{\dagger} \gamma_{5}\left\lceil u^{j}(0)\right\rangle_{u}
$$

It is straight-forward to add momenta and smearing functions. The latter cannot be factorized out of the inner product; the eigenvectors have a colour component.

What about eigenmodes of $M$ ?
Left $\left\langle\ell^{i}\right|$ and right $\left|r^{i}\right\rangle$ eigenvectors of an eigenvalue $\lambda_{i} \in \mathbb{C}$ need to be distinguished. These fulfill the biorthonormality relations $\left\langle\ell^{i} \mid r^{i}\right\rangle=\delta_{i j}$ and $M^{-1}=\sum_{i} \frac{1}{\lambda_{i}}\left|r^{i}\right\rangle\left\langle\ell^{i}\right|$. Moreover, $\left\langle r_{i}\right| \gamma_{5}$ and $\gamma_{5}\left|\ell_{i}\right\rangle$ are left and right eigenvectors, respectively, with eigenvalue $\lambda_{i}^{*}$. It turns out that this converges badly L Castagnini et al, PoS (LATTICE2010) 096: the dynamics appears to be driven by eigenmodes of the Hermitian Dirac operator Q.

## The singular value decomposition (SVD)

$m \times n$ Matrix (here $m=n=12 \mathrm{~V}$ ) can be decomposed:

$$
M=U \Sigma V^{\dagger}
$$

where $U$ and $V$ are $m \times m$ and $n \times n$ unitary matrices, respectively, and $\Sigma$ is an $m \times n$ matrix with non-negative real entries on its diagonal.
Singular values are uniquely determined, $U$ and $V$ are not.
Eigenvectors of $\mathrm{Q}=\gamma_{5} M$ are $E V$ s of $\mathrm{Q}^{2}=M^{\dagger} M$. Right singular vectors of $M$ (i.e. columns of $V$ ) are EVs of $M^{\dagger} M$ :

$$
\gamma_{5} M\left|u^{i}\right\rangle=\left|u^{i}\right\rangle q_{i}
$$

$M \underbrace{\left(\left|u_{1}\right\rangle, \ldots,\left|u_{12 v}\right\rangle\right)}_{V}=\underbrace{\gamma_{5}\left(\operatorname{sign}\left(q_{1}\right)\left|u_{1}\right\rangle, \ldots, \operatorname{sign}\left(q_{12 v}\right)\left|u_{12 v}\right\rangle\right)}_{U} \underbrace{\operatorname{diag}\left(\left|q_{1}\right|, \ldots,\left|q_{12 v}\right|\right)}_{\Sigma}$
Note that eigenvectors of $M$ do not depend on $\kappa$ while its singular vectors (eigenvectors of Q ) do.

Stochastic methods K Bitar et al, NPB 313 (89) 348:
Generate a set of random noise vectors $\left|\eta^{\ell}\right\rangle, \ell=1, \ldots, n$ where

$$
\begin{aligned}
\frac{1}{n} \sum_{\ell}\left|\eta^{\ell}\right\rangle\left\langle\eta^{\ell}\right|=\overline{|\eta\rangle\left\langle\left.\eta\right|_{n}\right.} & =\overline{|\eta\rangle\langle\eta|}=\mathbb{1}+\mathcal{O}(1 / \sqrt{n}) \\
\overline{\langle\eta|} & =\mathcal{O}(1 / \sqrt{n})
\end{aligned}
$$

Often: $\eta^{\ell}(x)_{a}^{\alpha} \in Z=\mathbb{Z}_{2} \otimes i \mathbb{Z}_{2} / \sqrt{2}$ S Dong, K-F Liu, PLB 328 (94) 130. Other choices: $Z=\mathbb{Z}_{2}, \mathbb{Z}_{3}, \mathrm{U}(1), \mathrm{SU}(3)$.
By solving

$$
M\left|s^{\ell}\right\rangle=\left|\eta^{\ell}\right\rangle
$$

for the $\left|s^{\ell}\right\rangle$ one can construct an unbiased estimate:

$$
\begin{aligned}
M_{E}^{-1} & =\overline{|s\rangle\langle\eta|} \\
& =M^{-1}+M^{-1} \underbrace{(|\eta\rangle\langle\eta|}_{\mathcal{O}(1 / \sqrt{n})}-\mathbb{1})
\end{aligned}
$$

$\Rightarrow n \ll 12 V$ solver applications only !

On each configuration an estimate $A_{E}$ of $A$ has a stochastic error $\Delta_{\text {stoch }} A=\mathcal{O}(1 / \sqrt{n})$. We define:

$$
\sigma_{A, \text { stoch }}^{2}:=\frac{\left\langle\left(\Delta_{\text {stoch }} A\right)^{2}\right\rangle_{U}}{N} \propto \frac{1}{N n} \text { for } n, N \text { large }
$$

where $N$ is the number of gauge configurations. The configuration average $\left\langle A_{E}\right\rangle_{U}$ carries the statistical error $\sigma_{A, \text { gauge }}$ :

$$
\sigma_{A, \text { gauge }}^{2} \geq \sigma_{A, \text { stoch }}^{2}
$$

Both sides scale $\propto 1 / N$.
$\sigma_{A, \text { gauge }} \simeq \sigma_{A, \text { stoch }} \Rightarrow$ increase $n$.
$\sigma_{A, \text { gauge }} \gg \sigma_{A, \text { stoch }} \Rightarrow$ reduce $n$ and increase $N$ (or the source positions).
The optimal choice depends on the observable $A$.
Increasing $n$ is usually not the smartest thing to do.
It is better to reduce the coefficient of the $1 / \sqrt{n}$ term.

## The stochastic error

$$
\begin{aligned}
& {\left[\Delta M_{X Z}^{-1}\right]^{2}:=\left[\Delta_{\text {stoch }} M_{X Z}^{-1}\right]^{2}=\sum_{Y}\left[M^{-1}-M_{E}^{-1}\right]_{X Y}\left[M^{-1}-M_{E}^{-1}\right]_{Y Z}^{\dagger},} \\
& {\left[\Delta M^{-1}\right]^{2}=M^{-1} \mathbb{O}\left[M^{-1} \mathbb{O}\right]^{\dagger},}
\end{aligned}
$$

where

$$
\mathbb{O}=\mathbb{1}-\overline{|\eta\rangle\langle\eta|}=\mathcal{O}\left(\frac{1}{\sqrt{n}}\right)
$$

is an off-diagonal $12 \mathrm{~V} \times 12 \mathrm{~V}$ matrix. $[X=(x, a, \alpha)]$. This means that,

$$
\begin{aligned}
{\left[\Delta M_{X Z}^{-1}\right]^{2} } & \propto \frac{1}{n} \sum_{Y \neq X, Z} M_{X Y}^{-1} M_{Y Z}^{-1 \dagger} \\
{\left[\Delta\left(\operatorname{Tr}\left\lceil M^{-1}\right)\right]^{2}\right.} & \propto \frac{1}{n} \sum_{x, y} \bar{q}_{y} \Gamma \gamma_{5} q_{y} \bar{q}_{x} \Gamma \gamma_{5} q_{x} \quad \text { minus diagonal terms }
\end{aligned}
$$

This is a sum over a mesonic two point function $c_{M}(y-x)$ !

Hence

$$
\Delta \operatorname{Tr} \Gamma M^{-1} \propto\left[(V / n) \sum_{y \neq 0} c(y)+\frac{1}{n}(\text { non-diagonal terms at } y=0)\right]^{1 / 2}
$$

$c(y)$ is the point-point correlation function of $\hat{O}_{M}=\bar{q} \Gamma \gamma_{5} q$.
Biggest contributions are from the "neighbourhood", where $c(y)$ is large. Intuitively this was already clear from $M_{E}^{-1}-M^{-1}=M^{-1}(\overline{|\eta\rangle\langle\eta|}-\mathbb{1})$ but above derivation sketch is gauge invariant.

Exercise: repeat derivation for a mesonic two-point-function with and without one-end-trick (see below).

## Hopping parameter expansion (HPE)

C Thron et al, PRD 57 (98) 1642;
C Michael et al, NPPS 83 (00) 185.
For static-light mesons: SESAM: GB et al, PRD 71 (05) 114513.

$$
\begin{aligned}
M^{-1} & =2 \kappa(\mathbb{1}-\kappa D)^{-1}=2 \kappa \sum_{j}(\kappa D)^{j} \\
& =2 \kappa \sum_{j=0}^{n-1}(\kappa D)^{j}+(\kappa D)^{n} M^{-1}
\end{aligned}
$$

Convenient generalization for clover:
V Gülpers, G von Hippel, H Wittig, 1309.2104

$$
\begin{aligned}
& D=D_{\mathrm{W}}+c_{\mathrm{SW}} \frac{i}{2} \sigma_{\mu \nu} F_{\mu \nu}, \quad A:=\mathbb{1}-\kappa c_{\mathrm{SW}} \frac{i}{2} \sigma_{\mu \nu} F_{\mu \nu} \\
& M=\frac{1}{2 \kappa}\left(A-\kappa D_{\mathrm{W}}\right)=\frac{A}{2 \kappa}\left(\mathbb{1}-A^{-1} \kappa D_{\mathrm{W}}\right) \\
& \text { (Regensburg) }
\end{aligned}
$$

Then ( $A$ is local in spacetime but a matrix in spin and color)

$$
M^{-1}=2 \kappa \sum_{j=0}^{n-1}\left(A^{-1} \kappa D_{\mathrm{W}}\right)^{j} A^{-1}+\left(A^{-1} \kappa D_{\mathrm{W}}\right)^{n} M^{-1}
$$

The first terms of the HPE contribute most to the noise.

- These may vanish identically:
example 1: for the Wilson action, $\operatorname{Tr}\left(\Gamma M^{-1}\right)=\operatorname{Tr}\left(\Gamma \kappa^{n} D^{n} M^{-1}\right)$, $n=4,8$, depending on $\Gamma \neq \mathbb{1}$.
example 2: 2-point function at distances $t>n a$.
- These may be calculated explicitly. Trivial for first order of $\operatorname{Tr}\left(\mathbb{1} M^{-1}\right)$. Usually contains plaquettes and more complicated loops. See M Deka et al, PRD 79 (09) 094502. (coined "unbiased subtraction method").
- First few terms are cheap to compute numerically and may be estimated with a larger number of estimates (see TSM below). HPE only works for ultra-local actions. No Neuberger Fermions!

Heavy quarks (charm) C Ehmann, GB, PoS (LATTICE2008) 114


Obviously works best for heavy quarks.

## Truncated solver method (TSM)

Obtain approximate solutions $\left|s_{n_{t}}^{\ell}\right\rangle$ after $n_{t}$ solver iterations (before convergence), and estimate the difference stochastically to obtain an unbiased estimate of $M^{-1}$ S Collins et al, PoS (LAT2007) 141:

$$
M_{E}^{-1}={\left.\overline{\left|s_{n_{t}}\right\rangle}\right\rangle\left\langle\left.\eta\right|_{n_{1}}+{\left.\overline{(|s\rangle}-\left|s_{n_{t}}\right\rangle\right)\langle\eta|}_{n_{2}} \quad \text { with } \quad n_{2} \ll n_{1} . . . .\right.}
$$

$n_{2} / n_{1}$ can be optimized to minimize the cost for a given error.


Also studied in C Alexandrou et al,
CPC 183 (12) 1215, 1309.2256;
GB, S Collins, A Schäfer, CPC 181
(10) 1570.

Do $\exists$ other factorizations of $M^{-1}$ into an expensive part with a small error and a cheap part with a larger error?
Iterative schemes to fight $\sqrt{V / n}$ problem?

## "All mode averaging" (AMA)

"Covariant approximation averaging". T Blum, T Izubuchi, E Shintani, PRD 88(13) 094503; E Shintani et al 1402.0244
New words for combining

$$
\left\langle\frac{1}{V} \sum_{x} A_{x}\right\rangle=\left\langle A_{0}\right\rangle
$$

with other well-known methods like TSM or LMA. The idea again is to decompose

$$
C(t)=C_{\text {approx }}(t)+\left[C_{\text {exact }}^{\mathrm{pa}}(t)-C_{\mathrm{approx}}^{\mathrm{pa}}(t)\right]
$$

$C_{\text {approx }}(t)$ may be computed for many source points. Using the CG solver was found to reduce computational effort by factors $5-16$, relative to point-to-all method for hadron spectroscopy with domain wall fermions. Problem (also with TSM): more efficient solver $\Rightarrow$ less gain. Attention has to be paid not to introduce a bias in non-linear applications of such tricks.

## Partitioning

S Bernardson et al, CPC 78 (93) 256; J Viehoff et al, NPPS 63
(98) 269; W Wilcox, arXiv:hep-lat/9911013
(also known as the spin-explicit-method (SEM) or dilution)
Decompose $\mathcal{R}=$ volume $\otimes$ colour $\otimes$ spin into $n_{\mathrm{p}}$ subspaces:

$$
\mathcal{R}=\oplus_{j=1}^{n_{\mathrm{p}}} \mathcal{R}_{j}
$$

Set $\left|\eta_{\mid j}^{\ell}\right\rangle$ to zero outside of the domain $\mathcal{R}_{j}$.
Calculate restricted solutions (setting $\eta(x)_{a}^{\alpha}=0$ outside of domain),

$$
M\left|s_{\mid j}^{\ell}\right\rangle=\left|\eta_{\mid j}^{\ell}\right\rangle
$$

Now: $M_{E}^{-1}=\sum_{j} \overline{\left|s_{\mid j}\right\rangle\left\langle\eta_{\mid j}\right|}$
This can be used to black out large off-diagonal error terms.
It is sensible to choose the same random vector components within each subspace (if they have the same dimension). This allows for hand-coding of, e.g., the spin structure (SEM).

Partitioning does not do any obvious harm but it may unnecessarily increase the number of estimates per configuration:


Comparison of partitioning patterns in mesonic three point functions R Evans, S Collins, GB, PRD 82 (10) 094501.

Often not all columns of $M^{-1}$ are required (e.g. time partitioning for 3 -point functions). Then the gain is obvious.

Spin partitioning often leads to an error reduction larger than the additional cost (factor four, i.e. error has to be reduced by a factor bigger than two).

The partitioning pattern can be adapted to the problem: staggered spin dilution (SSD).
C Ehmann, GB, PoS (LATTICE2008) 114.
There is also the possibility of "recursive noise subtraction".

## Truncated eigenmode approach (TEA)

H Neff et al, PRD 64 (01) 114509; GB et al, NPPS 140 (05) 609; PRD 71 (05) 114513; A O’Cais et al, NPPS 140 (05) 844; CPC 172 (05) 145.

Calculate the $m$ lowest eigenvalues and eigenvectors of $Q=\gamma_{5} M, q_{i}$ and $\left|v_{i}\right\rangle$. Projection operator:

$$
\mathbb{P}=\sum_{i=1}^{m}\left|v_{i}\right\rangle\left\langle v_{i}\right| .
$$

With

$$
M\left|s_{\perp}^{\ell}\right\rangle=\left|\eta_{\perp}^{\ell}\right\rangle=\gamma_{5}(\mathbb{1}-\mathbb{P}) \gamma_{5}\left|\eta^{\ell}\right\rangle
$$

one obtains

$$
M_{E}^{-1}=\overline{\left|s_{\perp}\right\rangle\left\langle\eta_{\perp}\right|}+\sum_{i=1}^{m}\left|v_{i}\right\rangle q_{i}^{-1}\left\langle v_{i}\right| \gamma_{5}
$$

Deflation is included for free and with the CG algorithm, the solution does not need to be projected back.

## Reduction of the stochastic error at fixed cost

Same cost result for $\operatorname{Tr}\left(\Gamma \mathrm{M}^{-1}\right)$ (per configuration) S Collins, $\mathrm{GB}, \mathrm{A}$ Schäfer, PoS (LATTICE2008) 161; CPC 181 (10) 1570:

(a) Partitioning, HPE, TSM

- Significant gain for all Гs.
- Using different combinations of methods allows one to obtain similar gains at different quark masses.


## Some one-end literature

- One-end-trick

R Sommer, NPPS 42 (95) 186;
M Foster, C Michael, PRD 59 (99) 074503

- Spin-explicit OET

C McNeile, C Michael, PRD 73 (06) 074506

- Sequential use in 3-point functions

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ETMC: S Simula et al, PoS (LAT2007) 371;
UKQCD: P Boyle et al, JHEP 0807 (08) 112;
R Evans et al, PRD 82 (10) 094501
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- Sequential use in 4 -point functions

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CP-PACS: S Aoki et al, PRD 76 (07) 094506
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- Twice applied in mesonic 4-point functions

C Alexandrou, G Koutsou, PRD 78 (08) 094506

- OET in baryons
$\chi$ QCD: A Li et al, PRD 82 (10) 114501;
L Castagnini et al, forgotten to write up

Define noise $\eta^{\ell}(x)_{a}^{\alpha} \in Z$ that is zero for any $t \neq t_{0}$.

$$
\frac{1}{n} \sum_{\ell=1}^{n}\left|\eta^{\ell}\right\rangle\left\langle\eta^{\ell}\right|=\mathbb{1}_{t_{0}}+\mathcal{O}\left(\frac{1}{\sqrt{n}}\right) \approx \sum_{\mathbf{x}, \alpha, a}|x, a, \alpha\rangle\langle x, a, \alpha|,
$$

where $x_{4}=t_{0}$. Consider the (not gauge averaged) pion two-point function $\left(t_{0}=0, y=(\mathbf{y}, t)\right)$,

$$
\begin{aligned}
c(t) & =\sum_{\mathbf{x y}} \operatorname{Tr} M^{-1}(y \mid x)\left[M^{-1}(x \mid y)\right]^{\dagger} \approx c_{E}(t) \\
& =\sum_{\mathbf{y}} \frac{1}{n} \sum_{\ell=1}^{n} \operatorname{Tr}\langle y| M^{-1}\left|\eta^{\ell}\right\rangle\left\langle\eta^{\ell}\right| M^{-1 \dagger}|y\rangle \\
& =\sum_{\mathbf{y}} \frac{1}{n} \sum_{\ell=1}^{n} \operatorname{Tr}\left\langle y \mid s^{\ell}\right\rangle\left\langle s^{\ell} \mid y\right\rangle=\sum_{\mathbf{y}, b, \beta} \frac{1}{n} \sum_{\ell=1}^{n}\left|s^{\ell}(y)_{b}^{\beta}\right|^{2},
\end{aligned}
$$

where $M\left|s^{\ell}\right\rangle=\left|\eta^{\ell}\right\rangle$. $c_{E}(t)$ differs from $c(t)$ by terms of $\mathcal{O}(1 / \sqrt{n})$. Since the noise is unbiased, $C(t)=\langle c(t)\rangle_{U}=\left\langle c_{E}(t)\right\rangle_{U}$.

Without the OET we would have needed two sets of sources $\left|\eta_{1}^{\ell}\right\rangle$ and $\left|\eta_{2}^{\ell}\right\rangle$ :

$$
\begin{aligned}
c_{E}^{\operatorname{trad}}(t) & =\sum_{\mathbf{y}} \frac{1}{n^{2}} \sum_{\ell, k=1}^{n} \operatorname{Tr}\left\langle y \mid s_{1}^{\ell}\right\rangle\left\langle\eta_{1}^{\ell} \mid \eta_{2}^{k}\right\rangle\left\langle s_{2}^{k} \mid y\right\rangle \\
& =\sum_{\mathbf{y}} \frac{1}{n^{2}} \sum_{\ell, k=1}^{n} \operatorname{Tr}\langle y| M^{-1} \overline{\left|\eta_{1}\right\rangle\left\langle\eta_{1}\right|} \overline{\left|\eta_{2}\right\rangle\left\langle\eta_{2}\right|} M^{-1 \dagger}|y\rangle .
\end{aligned}
$$

Each product with $\overline{|\eta\rangle\langle\eta|}$ involves a sum over $12 V_{3}$ randomly oscillating components of moduli $\mathcal{O}(1 / \sqrt{n})$.
This means that the OET error scales $\propto \sqrt{V_{3} / n}$ while the traditional error is $\propto \sqrt{V_{3}^{2} / n}$. Source self-averaging yields a factor $\propto 1 / \sqrt{V_{3}}$.
For baryons the OET error is $\propto \sqrt{V_{3}^{2} / n}$ while without the OET (LHPC: R Edwards et al, PoS (LAT2007) 108) it will scale $\propto \sqrt{V_{3}^{3} / n}$. This error can be reduced by a constant factor by recycling random sources: $\frac{1}{n^{2}} \sum_{\ell, k}^{n}\left\langle\eta_{1}^{\ell} \mid \eta_{2}^{k}\right\rangle \mapsto \frac{1}{n(n-1)} \sum_{\ell \neq k}^{2 n}\left\langle\eta^{\ell} \mid \eta^{k}\right\rangle,\{|\eta\rangle\}=\left\{\left|\eta_{1}\right\rangle\right\} \cup\left\{\left|\eta_{2}\right\rangle\right\}$. J Foley et al, CPC 172 (05)145

The OET can be made spin-explicit, defining,

$$
\eta^{\ell, \alpha}(x)_{a}^{\beta}=\delta^{\alpha \beta} \tilde{\eta}^{\ell}(x)_{a}
$$

where $|\tilde{\eta}\rangle$ is a (spin-independent) noise colour vector in the timeslice $t_{0}=x_{4}$. With solutions,

$$
M\left|s_{\Phi}^{\ell \alpha}\right\rangle=\Phi\left|\eta^{\ell \alpha}\right\rangle \quad \text { and } \quad M\left|s_{\Phi, \mathbf{p}}^{\ell \alpha}\right\rangle=e^{i \mathbf{p x}} \Phi\left|\eta^{\ell \alpha}\right\rangle
$$

we can contract,

$$
\begin{aligned}
c_{\Gamma, \Phi}^{\mathbf{p}}(y) & =\sum_{\mathbf{x}}\left[M^{-1} \Phi\right](y \mid x) e^{i \mathbf{p x}} \Gamma\left[\left[\Phi M^{-1}\right](x \mid y)\right]^{\dagger} \\
& \approx \frac{1}{n} \sum_{\ell, \alpha, \beta}\left\langle y \mid s_{\Phi, \mathbf{p}}^{\ell \alpha}\right\rangle \Gamma_{\alpha \beta}\left\langle s_{\Phi}^{\ell \beta} \mid y\right\rangle .
\end{aligned}
$$

This can now be contracted with $e^{-i \mathbf{p y}}$, smearing and a $\Gamma$ at the sink and averaged over gauge configurations.
For each momentum $\mathbf{p} \neq \mathbf{0}$ and each smearing function $\Phi$ four solves are required.

Remarks

- The non-gauge invariant wall source method of A Billoire, E Marinari, G Parisi, PL 162B (85) 160 is actually equivalent to the spin-explicit (gauge invariant) OET with $n=1 \mathrm{SU}(3)$ noise sources per configuration.
- OET can be combined with the sequential source technique (L Maiani et al, PLB 176 (86) 445; NPB 293 (87) 420) for threeand four-point functions as long as $n$ can be kept small (for each $n 12$ sequential solves are necessary).


## The "thinning"/ grid noise idea

The OET error scaling (ignoring the benefit of self-averaging) is $\propto \sqrt{V_{3} / n}$ for mesons and $\propto \sqrt{V_{3}^{2} / n}$ for baryons. The $V_{3}$ factors are due to the number of non-zero entries of the stochastic noise vectors.

Reducing the number of non-zero entries to $M$ points yields $\sqrt{M / n}$ and $\sqrt{M^{2} / n}$ behaviour, respectively, while self-averaging (for $M$ not taken overly small) largely remains unaffected, in particular at light quark masses. R Sommer, NPPS 42 (95) 186; L Castagnini et al, in preparation.

This looks like partitioning, however only the number of points matters. Their positions are only relevant with respect to self-averaging (and autocorrelations in the time series).

Grid noise was combined with low mode substitution (rather than averaging) in $\chi$ QCD: A Li et al, PRD 82 (10) 114501.

## Nucleon effective masses on $V=32^{3} 64$ at equal cost



## Error ratios for the nucleon effective mass



## Connected 3-point functions

Stochastic methods have also successfully been applied to connected 3-point functions, replacing the sequential propagator.

- More flexibility and cheaper, in particular if interested in different sinks (e.g. baryons, smearing, momenta).
- More statistics, due to averaging over polarizations and equivalent momenta.
- Can average over forward and backward propagation.
- Can move source in space (statistics) and time (check ground state saturation) with only 12 additional solves (1 propagator) per quark mass.

See R Evans, GB, S Collins, PRD 82 (10) 094501; ETM: C Alexandrou et al, 1302.2608; J Najjar et al, 1311.1718.

## Point-point propagator for (disconnected) spectroscopy?

Point-point correlation function of $J=0$ meson $\left(N_{s} a=N_{t} a=\infty\right)$ :

$$
C(x)=\int_{-\pi}^{\pi} \frac{d^{4} k}{(2 \pi)^{4}} e^{i k \cdot x}\left(\sum_{j} \frac{c_{j}}{\hat{k}^{2}+m_{j}^{2}}\right),
$$

where $\hat{k}_{\mu} \approx \frac{2}{a} \sin \frac{a k_{\mu}}{2}$ (This is the simplest latticized and not necessarily correct ansatz.), $\hat{k}^{2}=\sum_{\mu} \hat{k}_{\mu}^{2}$.
Masses were extracted from fits to $C(x)$ in
M Chu, J Grandy, S Huang, PRD 48 (93) 3340;
D Leinweber, PRD 51 (95) 6369;
C Allton, S. Capitani, NPB 526 (98) 463;
L Levkova, C DeTar, PRD 83 (11) 074504.

The momentum projected correlation function reads,

$$
\begin{aligned}
C^{\mathbf{p}}(t) & =\int \frac{d^{3} x d^{4} k}{(2 \pi)^{4}} \frac{c_{1} e^{i k t} e^{i \mathbf{x}(\mathbf{k}-\mathbf{p})}}{\hat{k}^{2}+m_{1}^{2}}+\cdots=\int \frac{d k_{4}}{2 \pi} \frac{c_{1} e^{i k_{4} t}}{\hat{k}_{4}^{2}+\hat{\mathbf{p}}^{2}+m_{1}^{2}}+\cdots \\
& =\sum_{j} \frac{c_{j}}{2 E_{j}} e^{-E_{j} t} \quad \text { where } \quad \sinh \frac{a E_{j}}{2}=\frac{a}{2} \sqrt{\hat{\mathbf{p}}^{2}+m_{j}^{2}} \quad\left(E=-i k_{4}\right) .
\end{aligned}
$$

This dispersion relation agrees with the continuum relation up to $\mathcal{O}\left(a^{2}\right)$ terms.

Problems with these point-to-point correlators: no smearing possible, no exponential suppression of excitations. But: better signal over noise. The usual position sum includes contributions from large Euclidean distances (little signal but noise).

## ... is related to smearing

Ground state wavefunctions have no nodes and are smooth. $\rightarrow$ employ extended operators $\bar{q}_{x}^{1} \Gamma \Phi_{x, z} q_{z}^{2}$ where the smearing function $\Phi$ mimics a wavefunction to maximize $c_{1}$.

This was done
(1) Using Coulomb gauge fixing, e.g.: T DeGrand, RD Loft, CPC 65 (91) 84; T DeGrand, M Hecht, PLB 275 (92) 435; T Draper, C McNeile, NPPS 34 (94) 453.
(2) Employing gauge covariant iterative procedures. Wuppertal=Gauss smearing: S Güsken et al, PLB 227 (89) 266; S Güsken, NPPS 17 (90) 361. Jacobi smearing: UKQCD: C Allton et al, PRD 47 (93) 5128.
(3) Using more general gauge covariant basis vectors. "free form smearing": G von Hippel et al, JHEP 1309 (13) 014. Distillation: HSP: M Peardon et al, PRD 80 (09) 054506.

## Wuppertal smearing

Define a covariant lattice Laplacian in $d=3$ spatial dimensions, acting on a scalar or vector field $\psi_{\mathbf{y}}$ :

$$
a^{2}\left(\nabla^{2} \psi\right)_{\mathbf{x}}=-2 d \psi_{\mathbf{x}}+\sum_{j= \pm 1}^{ \pm 3} \bar{U}_{\mathbf{x}, j} \psi_{\mathbf{x}+a \hat{\jmath}} .
$$

It is advisable (SESAM: GB et al, NPPS 140 (05) 609; S Güsken, NPPS 17 (90) 361) to use a smeared covariant transporter $\bar{U}$ instead of $U$. Wuppertal smearing amounts to iteratively replacing:

$$
\psi^{(n+1)}=\psi^{(n)}+\frac{\delta}{1+2 d \delta} a^{2} \nabla^{2} \psi^{(n)} .
$$

$\delta=0.3$ is a reasonable value for the free parameter. The (arbitrary) normalization convention is chosen to avoid numerical overflows for large iteration counts $n$. This can be employed checkerboard or "all-at-once".

We introduce a fictitious time $t=n \Delta t$. Now (ignoring $U_{x, \mu} \neq \mathbb{1}$ ):

$$
\frac{\partial \psi(t)}{\partial t} \approx \frac{\psi(t+\Delta t)-\psi(t)}{\Delta t}=\kappa \nabla^{2} \psi(t) \quad \text { with } \quad \kappa=\frac{a^{2}}{\Delta t} \frac{\delta}{1+2 d \delta} .
$$

This diffusion equation is formally solved by,

$$
\psi(t) \approx e^{\kappa t \nabla^{2}} \psi(0)
$$

Starting from $\psi_{\mathbf{x}}(0)=\delta_{\mathbf{x} 0}$ this gives a Gauss packet with the rms width of $\psi^{\dagger} \psi$ :

$$
\Delta r=d \sqrt{\kappa t}=d a \sqrt{\frac{\delta}{1+2 d \delta} n} .
$$

The diffusion speed is maximal for $\delta \rightarrow \infty\left(\kappa \rightarrow a^{2} /(2 d \Delta t)\right)$ while the resulting wavefunction is more continuum-like for $\delta \rightarrow 0(\kappa \rightarrow 0)$.

The Wuppertal (and Jacobi) smearing operators
(1) are gauge covariant and singlets under $\mathrm{O}_{h}$, charge and parity transformations,
(2) are translationally invariant in space,
(3) are Hermitian and commute with $\Gamma \mathrm{s}$,
(4) Wuppertal has the property: $\Phi^{\left(n_{1}\right)} \Phi^{\left(n_{2}\right)}=\Phi^{\left(n_{1}+n_{2}\right)}$.

Properties 1-2 mean that smearing can be added, without affecting the irrep, gauge invariance or momentum projection.
Property 3 means that Wick-contractions remain the same.
Properties 3-4 mean that within mesons (not containing derivatives) smearing can freely be distributed between the quarks: in the equal mass case evenly, to minimize the computer time. Source smearing can be performed on the heavier quark, whose propagator is cheaper to generate. This is also statistically favourable. (At the (non-momentum-projected) source things are not symmetric with respect to the quarks).

The Gauss-Wuppertal smearing operator can be written as,

$$
\Phi^{(n)} \approx\left(e^{\kappa \Delta t \nabla^{2}}\right)^{n}
$$

$\nabla^{2}$ is a scalar, Hermitian, translationally invariant, gauge covariant operator. It contains smeared transporters $\bar{U}$. Define eigenvectors of $\nabla^{2}$ at a fixed timeslice, $\left|v_{i}\right\rangle \in \mathbb{C}^{V_{3} N_{c}}$ :

$$
\nabla^{2}\left|v_{i}\right\rangle=\omega_{i}^{2}\left|v_{i}\right\rangle, \quad\left\langle v_{i} \mid v_{j}\right\rangle=\delta_{i j}, \quad v_{i, \mathbf{x}, a}=\left\langle\mathbf{x}, a \mid v_{i}\right\rangle .
$$

From this we can define a projector onto the "LapH" subspace HSP: M Peardon et al, PRD 80 (09) 054506 of the timeslice,

$$
\triangle=\sum_{i}\left|v_{i}\right\rangle\left\langle v_{i}\right| \theta\left(\sigma^{2}-\omega_{i}^{2}\right), \quad \triangle_{a b}^{\mathrm{xy}}=\sum_{i} v_{i, \mathrm{x}, a}^{\dagger} v_{i, \mathrm{y}, b} \theta\left(\sigma^{2}-\omega_{i}^{2}\right)
$$

where (obviously) $\triangle^{2}=\triangle . \sigma$ cuts out all eigenvectors with eigenvalues $\omega_{i}>\sigma$. The number of remaining eigenvalues $M(\sigma) \ll V_{3} N_{c}$ scales at fixed $\sigma^{2} \approx 1 / 3$ with $V_{3}=N_{s}^{3}$.

The "wavefunction"

$$
\Psi(\mathbf{r})=\sqrt{\operatorname{Tr}\left(\triangle_{\mathbf{0}} \triangle_{\mathbf{r} \mathbf{0}}\right)}
$$

(averaging the zero point over all lattice points) approaches the $\delta$-function for $M \rightarrow N_{s}^{3} N_{c}$ (Distillation becomes a basis transformation).


## Mesonic two point functions

Destruction operator:

$$
\hat{O}^{\mathbf{p}}=\sum_{\mathbf{x}, \mathbf{y}, \mathrm{z}, \mathbf{w}} e^{-i \mathbf{p x}} \bar{q}_{\mathrm{x}}^{1} \triangle_{\mathrm{xy}} \underbrace{e^{-i \mathbf{p y}} \Gamma D_{\mathrm{yz}}}_{A_{\mathrm{yz}}} \triangle_{z w} q_{w}^{2}
$$

where we have suppressed colour and spin indices and $A$ depends on $\mathbf{p}, \Gamma$ and $D . \triangle$ depends on $M$. Correlation function (We allow for $\hat{\tilde{O}} \neq \hat{O}$ ):

$$
\begin{aligned}
C(t)= & \left\langle\tilde{O}(t) O^{\dagger}(0)\right\rangle \\
= & \pm\left\langle\bar{q}^{2}(t) \triangle(t) \tilde{A}(t) \triangle(t) q^{1}(t) \bar{q}^{1}(0) \triangle(0) A^{\dagger}(0) \triangle(0) q^{2}(0)\right\rangle \\
= & \pm \sum_{i, j, k, \ell}\left\langle\left\langle\bar{q}^{2}(t) \mid v_{i}(t)\right\rangle \tilde{A}_{i j}(t)\left\langle v_{j}(t) \mid q^{1}(t)\right\rangle\right. \\
& \left.\quad \times\left\langle\bar{q}^{1}(0) \mid v_{k}(0)\right\rangle \tilde{A}_{k \ell}^{\dagger}(0)\left\langle v_{\ell}(0) \mid q^{2}(t)\right\rangle\right\rangle
\end{aligned}
$$

where $\tilde{A}_{i j}(t)=\left\langle v_{i}(t)\right| \tilde{A}(t)\left|v_{j}(t)\right\rangle$ and $A_{k \ell}^{\dagger}(0)=\left\langle v_{k}(0)\right| A^{\dagger}(0)\left|v_{\ell}(0)\right\rangle$ also depend on (not displayed) spinor indices.

This can now be factorized,

$$
\begin{aligned}
C(t) & \left.=\mp\left\langle\tilde{A}_{i j}^{\alpha \gamma}(t) A_{k \ell}^{\dagger \beta \delta}(0)\left\langle v_{j}(t)\right| S^{1}(t \mid 0)^{\alpha \beta} \mid v_{k}(0)\right\rangle\left\langle v_{\ell}(0)\right| S^{2}(0 \mid t)^{\gamma \delta}\left|v_{i}(t)\right\rangle\right\rangle_{u} \\
& =\mp\left\langle\tilde{A}_{i j}^{\alpha \gamma}(t) A_{k \ell}^{\dagger \beta \delta}(0) \tau^{(1)}(t \mid 0)_{j k}^{\alpha \beta} \tau^{(2)}(0 \mid t)_{\ell i}^{\gamma \delta}\right\rangle_{u},
\end{aligned}
$$

where the generalized propagators for flavour $f$ ("perambulators"),

$$
\tau^{(f)}(t \mid 0)_{i j}^{\alpha \beta}=\left\langle v_{i}(t)\right| S^{f}(t \mid 0)^{\alpha \beta}\left|v_{j}(0)\right\rangle,
$$

are $\mathrm{LapH} \otimes \operatorname{spin}(4 M \times 4 M)$ matrices that can be obtained by inverting the Dirac operator on all $\left|v_{j}(0)\right\rangle$ (times the four different source spin- $\delta \mathrm{s}$ ), and contracting the resulting propagators at the sink with $\left\langle v_{i}(t)\right|$ : the colour times position indices are replaced by LapH indices $i$ and $j$. Note that the computation of the antiquark pram,

$$
\tau(0 \mid t)_{i j}=\left\langle v_{i}(t)\right| \gamma_{5} S(t \mid 0) \gamma_{5}\left|v_{j}(0)\right\rangle=\gamma_{5}\left\langle v_{i}(t)\right| S(t \mid 0)\left|v_{j}(0)\right\rangle \gamma_{5}
$$

does not require any additional solves, due to the $\gamma_{5}$-Hermiticity.

## Summary of Distillation

- This has been generalized to baryons etc. (straight-forward).
- This timesliceLapH-to-allLapH method is much more expensive than the standard point-to-all method. The price for the inversions scales like $V V_{3}$ (rather than $V$ ), and for mesonic contractions even like $\left(V V_{3}\right)^{2}$.
- The $A_{i j}$ can be exchanged a posteriori. This turns the method competitive when many operators are involved, in particular with derivatives at the source. Also some source "self-averaging" is built in.
- All components within the $\sum_{i j k \ell}$ have the quantum numbers of $A$ and are gauge invariant. So different truncations can be chosen for ij and $k \ell$ (corresponding to different sink/source smearings). See also C Lang et al, PRD 84 (11) 054503.
- The smearing profiles can in principle be varied by introducing weight functions $f\left(\omega_{i}\right)$ in the contraction of a LapH index $i$, a possibility that could be worth exploring.


## Stochastic estimates in the LapH basis

It seems possible to reduce the computational overhead of the distillation method by stochastically estimating the perambulators within the LapH space HSC: C Morningstar et al, PRD 83 (11) 114505. Introduce spin-explicit noise vectors in LapH space:

$$
\left|\eta^{\ell \alpha}\right\rangle=\sum_{i=1}^{M} \eta_{i}^{\ell} e^{\alpha}\left|v_{i}(0)\right\rangle
$$

where $\eta_{i}^{\ell} \in Z, \ell \in\{1, \ldots, n\}, e^{\alpha}$ is a unit spin vector in direction $\alpha$ and $\left|v_{i}(0)\right\rangle$ are LapH basis vectors on timeslice 0 .
Now solve,

$$
M\left|s^{\ell \alpha}\right\rangle=\left|\eta^{\ell \alpha}\right\rangle .
$$

Estimates of the prams are now given by,

$$
\tau_{E}(t \mid 0)_{i k}^{\alpha \beta}=\frac{1}{n} \sum_{\ell=1}^{n}\left\langle v_{i}(t) \mid s^{\ell \alpha}\right\rangle\left\langle\eta^{\ell \beta} \mid v_{k}(0)\right\rangle
$$

In C Jost, B Knippschild, C Urbach, F Zimmermann, 1311.5469 it was reported that LapH did a bad job regarding the ground state overlap of pseudoscalar mesons.

Moreover, the stochastic LapH method was found to be by a factor 20 more expensive for computations of the $\eta$-mass than standard stochastic methods.

However, perambulators, once obtained, allow for a lot of flexibility: the hadrons of interest ( $D, \Gamma$ and $\mathbf{p}$ ) can be specified subsequently.

## Warnings

- Best method depends on quark mass, volume, observable, solver and ease of implementation.
- As there are no one-size-fits-all solutions, and in the end all of us are primarily interested in physics-output, there exist few systematic and realistic cost comparisons.
- Re-inventing and re-naming old methods can be confusing.
- Honest assessments of pros and cons and real cost comparison would be more beneficial to the field than pure advertizing.
- For details on the particular methods please consult the references I cited (and those that I may have forgotten).


## Summary \& Questions

- All-to-all methods are needed in particular at small $m_{\pi}$ where many hadrons become unstable. Also isosinglet contributions to hadronic structure should become more important.
- Note that OET is a timeslice-to-all, distillation a timesliceLapH-to-allLapH method.
- Combinations of (new?) methods can easily save large factors of computer time.
- Efficient method of obtaining first few SVD vectors of $M$ (exact or inexact) would be very welcome!
- Scaling $n \propto V$ or $n \propto V_{3}$ : can this be overcome?
- The number of low eigenmodes of Q scales like $V$ but $4 / m_{\pi}^{\text {phys }}$ is almost 6 fm . Similarly the LapH space can become large for such volumes. Is there any "inexact" eigen/domain method?

