Lattice Methods for Hadron Spectroscopy: new (and old) ideas for making measurements

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Plan

- Something about homeworks
- Pros and cons of point propagators
- Smearing
- All-to-all propagators
- Distillation
  - Improving stochastically

Question 1

Wick contractions for flavour singlets

Question 2

At http://www.maths.tcd.ie/~ryan/INT2012/

you will find a data file called jpsi-correlator-16x128.dat

This is two-point correlator data for a J/Ψ meson generated with a sinlge interpolating operator: $\mathcal{O} = \bar{c}\gamma_i c$. The lattice is $16^3 \times 128$ and there are 20 configurations. The data are indexed by timeslice value for each configuration.

- Plot the correlator data to see the exponential (and time-symmetric) behaviour.
- Write a short program to determine the effective mass on each timeslice am_{eff} and plot the result.
- Hopefully you will see a plateau (no time dependence) at large times!
- Calculate the jackknifed errors for each point.

Question 3 Write a short program to implment the Metropolis algorithm (described on the full sheet) for the one-dimensional harmonic oscillator: $V(x) = x^2/2$ with $m = 1$. Calculate

$$G(t) = \frac{1}{N} \sum_j \langle x(t_j + t) x(t_j) \rangle \;\; \forall t = 0, 2a, \ldots (N-1)a$$

Try $N = 20$ sites with spacing $a = 0.5$ and $\epsilon = 1.4$. Use $N_{configs} = 25, 50, 100, 10000$ and see the effect.
Repeat for $V(x) = x^4/2$.

Point propagators

For better simulations of hadronic quantities look again at the building blocks: the quark propagators

Point propagator pros

- doesn't require vast computing resources

Point propagator cons

- restricts the accessible physics
  - flavour singlets and condenstates impossible: quark loops need props w sources everywhere in space
- restricts the interpolating basis used
  - a new inversion needed for every operator that is not restricted to a single lattice point
- entangles propagator calculation and operator construction
- throws away information encoded in configurations

Solutions?

- Improve the determination point props to access the physics of interest: smearing
- Compute all elements of the quark propagator: all-to-all propagators. Problem It's expensive - needs and unrealistic number of inversions.
- Work around: Use stochastic estimators (with variance reduction).
- Rethink the problem: combine smearing and propagation ie distillation

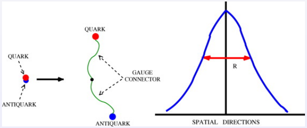
I am picking a few methods to focus on.
See references at the end of this lecture for full descriptions of these and other methods.

Smearing

Smearing techniques

- Hadrons are extended objects ($\mathcal{O}(1)fm$).
- So far the propagator and interpolating fields (operators) are point sources
  - they can have small overlap with the state of interest: quantified by $\mathcal{Z}_n$
  - optimise the projection onto the state we want to study
- Gauge-invariant smearing of quark fields:

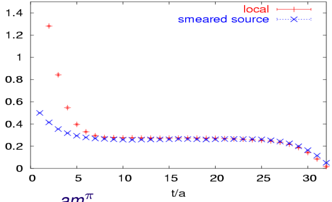
$$\Psi(\vec{x},t) = \sum_{\vec{y}} F(\vec{x},\vec{y},U(t))\Psi(\vec{y},t)$$



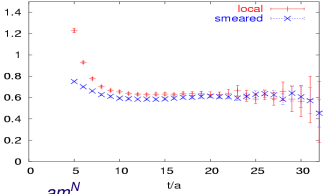
- Gaussian smearing: $F(\vec{x},\vec{y},U(t)) = (1+\kappa_s H)^{n_\sigma}$ and H is the lattice realisation of the covariant Laplacian in 3d
- Variations on a theme: Jacobi, Wuppertal ...
- More improvements to gauge noise by smearing the U fields in F: APE, HYP, Stout

Examples of effective mass plots

- Quenched at about 550 MeV pions:

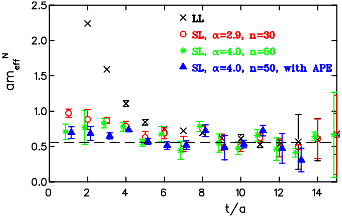


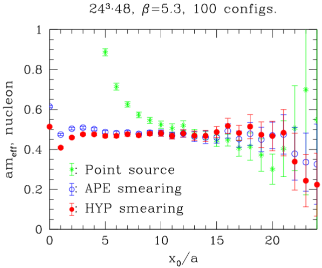
am^{π}_{eff}



am^{N}_{eff}

- Reduce gauge noise by using APE, hypercubic or stout smearing on the links U that enter the smearing function $F(\vec{x}, \vec{y}, U(t))$.
- $N_F = 2$





All-to-all propagators

About all-to-all propagators

- Computing all elements of the quark propagator would require full knowledge of the inverse - this is prohibitively expensive
- The lattice representation of the Dirac operator is a large, but very sparse matrix.
- If we are satisfied with an *unbiased estimator* of all elements then sparse matrix methods can be used. Stochastic estimation should be acceptable - we are already using it to generate gauge fields!
- Variance reduction will be crucial

All-to-all quark propagators

- Start with a spectral representation of $Q = \gamma_5 M$ (choose Q here because it is hermitian so eigenvalues are easier to compute).
- If we can compute all the eigenvectors and eigenvalues, $\{\lambda^{(i)}, v^{(i)}\}$ of

$$Q = \sum_{i=1}^{N} \lambda^{(i)} v^{(i)} \otimes v^{*(i)} \quad \text{and} \quad Q^{-1} = \sum_{i=1}^{N} \frac{1}{\lambda^{(i)}} v^{(i)} \otimes v^{*(i)}$$

- Unfortunately, finding even a small sub-set of eigenvectors is computationally expensive, so we are forced to truncate this representation at $N_{\mathrm{ev}} \ll N$
- Truncated sum violates reflection positivity. Must correct.

All-to-all (1)

Start again, this time find a stochastic representation of Q.

- Generate an ensemble of random, independent noise vectors $\left\{\eta_{[1]}, \eta_{[2]}, \ldots, \eta_{[N_r]}\right\}$, with property

$$\langle\langle \eta_{[r]}(x) \otimes \eta_{[r]}(y)^\dagger \rangle\rangle = \delta_{x,y}$$

  where $\langle\langle \cdots \rangle\rangle$ is the expectation value over the distribution of noise vectors. $Z_4 = \{1, i, -1, -i\}$ a good choice.
- Each component of the noise vectors has modulus 1

$$\eta^{i\alpha}(x)^* \eta^{i\alpha}(x) = 1 \quad \text{no summation}$$

- The solution vectors $\psi_{[r]}$ are obtained in the usual way

$$\psi_{[r]}(x) = Q^{-1} \eta_{[r]}(y)$$

  i, j are colour indices and α, β are spin.

all-to-all (2)

- The quark propagator from any point x to any point y is then

$$Q^{-1}(y,x)^{ij}_{\alpha\beta} = \langle\langle \psi_{[r]} \otimes \eta^{\dagger}_{[r]} \rangle\rangle^{ij}_{\alpha\beta} = \lim_{N_r\to\infty} \frac{1}{N_r} \sum_{r}^{N_r} \psi^{i\alpha}_{[r]}(y) \eta^{j\beta}_{[r]}(x)^{\dagger}$$

- Note that for N_r different sources the variance falls like $1/\sqrt{N_r}$. Can we do better?
- Recall, the exact propagator can be computed with a finite (but large!) amount of effort; use point-propagator methods with Kronecker delta sources put everywhere.
- Suggests a trick; break the vector space of the quark fields, V into d smaller sub-spaces $V = V_1 \oplus V_2 \oplus \ldots$ spanned by sub-sets of the basis vectors.
- This partitioning ("dilution") is arbitrary.

Dilution

- Dilute the noise vector η in some set of variables of that $\eta = \sum_j \eta^{(j)}$.
- For spectroscopy involving temporal correlations an important example is time dilution

$$\eta(\vec{x}, t) = \sum_{j=0}^{N_t-1} \eta^{(j)}(\vec{x}, t)$$

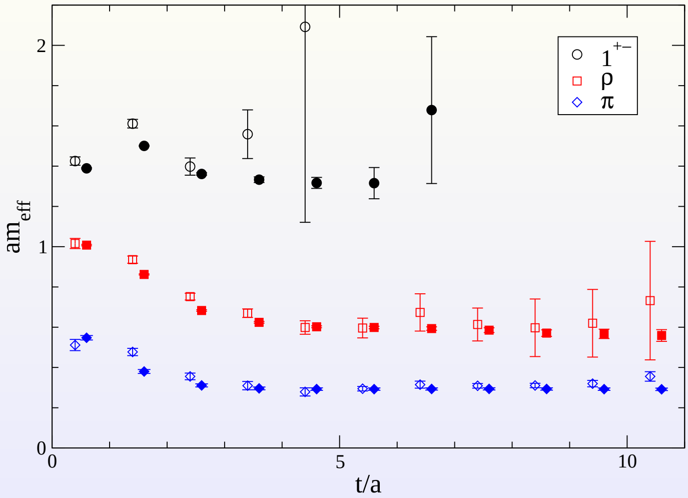
  and $\eta^{(j)}(\vec{x}, t) = 0$ unless $t = j$.
- Each diluted source is inverted, yielding N_d pairs of vectors $\{\psi^{(j)}, \eta^{(j)}\}$
- Get a an estimator of Q^{-1} with a single noise source

$$\sum_{i=0}^{N_d-1} \psi^{(i)}(\vec{x}, t) \otimes \eta^{(i)}(\vec{x}_0, t_0)^\dagger$$

A hybrid method

- In the homeopathic limit of dilution (one noise vector for each time,space,colour and spin) the *exact* propagator is recovered in a finited number of steps.
- Not practically in current simulations but the path of dilution may be optimised so gauge field noise dominates for manageable inversions.
- A hybrid method:
  - calculate N_{ev} eigenvalues and eigenvectors of Q exactly and determine $Q^{-1}_{N_{ev}}$
  - use the stochastic method with dilution to correct the truncation
  - there are some more nice tricks you can do to make this efficient and optimal but that needs more time ....

Comparing methods: point and all-to-all



$\beta = 5.7, 12^3 \times 24$ lattice Wilson fermions,
$\kappa = 0.1675 (m_\pi/m_\rho = 0.50)$ 75 configurations. 100 eigenvectors. Time/even-odd/spin dilution.

Distillation

Smearing

- **Smeared field:** $\tilde{\psi}$ from ψ, the “raw” quark field in the path-integral:

$$\tilde{\psi}(t) = \square[U(t)]\ \psi(t)$$

- Extract the essential degrees-of-freedom.
- Smearing should preserve symmetries of quarks.
- Now form creation operator (e.g. a meson):

$$O_M(t) = \bar{\tilde{\psi}}(t)\Gamma\tilde{\psi}(t)$$

- Γ: operator in $\{\underline{s}, \sigma, c\} \equiv \{\text{position,spin,colour}\}$
- Smearing: overlap $\langle n|O_M|0\rangle$ is large for low-lying eigenstate $|n\rangle$

Can redefining smearing help?

- Computing quark propagation in configuration generation and observable measurement is expensive.
- Objective: extract as much information from correlation functions as possible.

Two problems:

1. Most correlators: signal-to-noise falls exponentially
2. Making measurements can be costly:
   - Variational bases
   - Exotic states using more sophisticated creation operators
   - Isoscalar mesons
   - **Multi-hadron states**

- Good operators are **smeared**; helps with problem 1, can it help with problem 2?

Gaussian smearing

- To build an operator that projects effectively onto a low-lying hadronic state need to use **smearing**
- Instead of the creation operator being a direct function applied to the fields in the lagrangian first smooth out the UV modes which contribute little to the IR dynamics directly.
- A popular gauge-covariant smearing algorithm — Gaussian smearing: Apply the linear operator

$$\Box_J = \exp(\sigma \nabla^2)$$

- ∇^2 is a lattice representation of the 3-dimensional gauge-covariant laplace operator on the source time-slice

$$\nabla^2_{x,y} = 6\delta_{x,y} - \sum_{i=1}^{3} U_i(x)\delta_{x+\hat{\imath},y} + U_i^\dagger(x-\hat{\imath})\delta_{x-\hat{\imath},y}$$

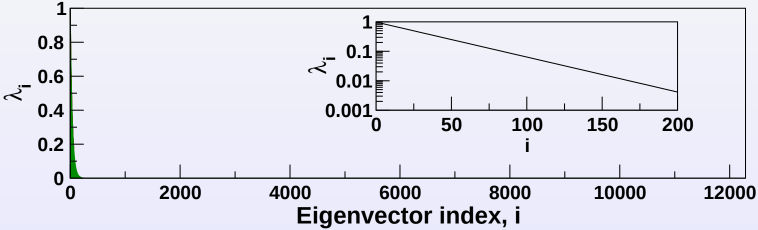
- Correlation functions look like $\mathrm{Tr}\ \Box_J M^{-1} \Box_J M^{-1} \Box_J \ldots$

Gaussian smearing

- **Gaussian** smearing:

$$\lim_{n\to\infty}\left(1+\frac{\sigma\nabla^2}{n}\right)^n = \exp(\sigma\nabla^2)$$

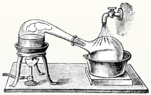
- This acts
  in the space of coloured scalar fields on a time-slice: $N_s \times N_c$



- Data from $a_s \approx 0.12\text{fm}\ 16^3$ lattice: $16^3 \times 3 = 12288$.

Distillation

"*distill*: to extract the quintessence of" [OED]



- Distillation: **define** smearing to be explicitly a very low-rank operator. Rank is $N_{\mathcal{D}}(\ll N_s \times N_c)$.

Distillation operator

$$\Box(t) = V(t)V^{\dagger}(t)$$

with $V^a_{\underline{x},c}(t)$ a $N_{\mathcal{D}} \times (N_s \times N_c)$ matrix

- Example (used to date): $\Box_{\triangle}$ the **projection operator into $\mathcal{D}_{\triangle}$, the space spanned by the lowest eigenmodes of the 3-D laplacian**
- Projection operator, so idempotent: $\Box_{\triangle}^2 = \Box_{\triangle}$
- $\lim_{N_{\mathcal{D}} \to (N_s \times N_c)} \Box_{\triangle} = I$
- Eigenvectors of ∇^2 not the only choice...

Distillation: preserve symmetries

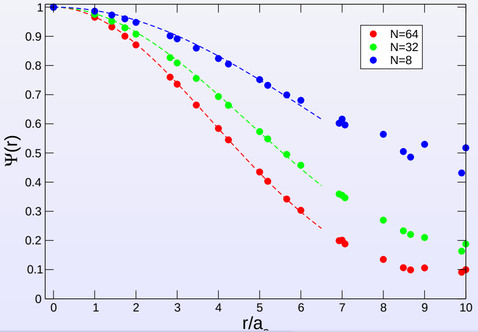
- Using eigenmodes of the gauge-covariant laplacian **preserves lattice symmetries**

$$U_i(\underline{x}) \xrightarrow{g} U_i^g(\underline{x}) = g(\underline{x})U_i(\underline{x})g^\dagger(\underline{x}+\hat{\underline{\imath}})$$

$$\Box_\nabla(\underline{x},\underline{y}) \xrightarrow{g} \Box_\nabla^g(\underline{x},\underline{y}) = g(\underline{x})\Box_\nabla(\underline{x},\underline{y})g^\dagger(\underline{y})$$

- Translation, parity, charge-conjugation symmetric

- O_h symmetric
- Close to $SO(3)$ symmetric
- "local" operator



- Consider an isovector meson two-point function:

$$C_M(t_1 - t_0) = \langle\langle \bar{u}(t_1)\Box_{t_1}\Gamma_{t_1}\Box_{t_1} d(t_1) \quad \bar{d}(t_0)\Box_{t_0}\Gamma_{t_0}\Box_{t_0} u(t_0)\rangle\rangle$$

- Integrating over quark fields yields

$$C_M(t_1 - t_0) = \langle \mathrm{Tr}_{\{\underline{s},\sigma,c\}} \left(\Box_{t_1}\Gamma_{t_1}\Box_{t_1} M^{-1}(t_1, t_0)\Box_{t_0}\Gamma_{t_0}\Box_{t_0} M^{-1}(t_0, t_1)\right)\rangle$$

- Substituting the low-rank distillation operator $\Box$ reduces this to a **much smaller** trace:

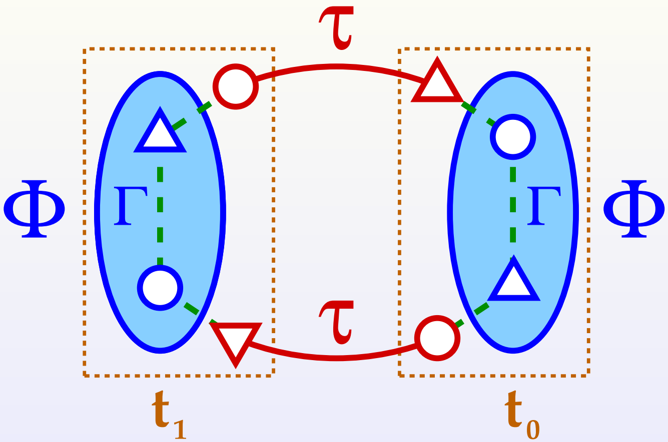
$$C_M(t_1 - t_0) = \langle \mathrm{Tr}_{\{\sigma,\mathcal{D}\}} \left[\Phi(t_1)\tau(t_1, t_0)\Phi(t_0)\tau(t_0, t_1)\right]\rangle$$

- $\Phi^{\alpha,a}_{\beta,b}$ and $\tau^{\alpha,a}_{\beta,b}$ are $(N_\sigma \times N_\mathcal{D}) \times (N_\sigma \times N_\mathcal{D})$ matrices.

$$\Phi(t) = V^\dagger(t)\Gamma_t V(t) \qquad \tau(t, t') = V^\dagger(t) M^{-1}(t, t') V(t')$$

The "perambulator"

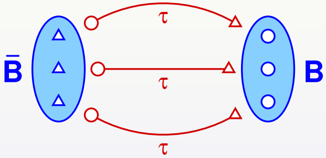
Meson two-point function



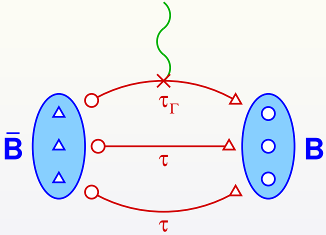
Distilled meson two-point correlation function

$$C_M(t_1 - t_0) = \mathrm{Tr}_{\{\sigma,D\}} \left[\Phi(t_1)\, \tau(t_1, t_0)\, \Phi(t_0)\, \tau(t_0, t_1) \right]$$

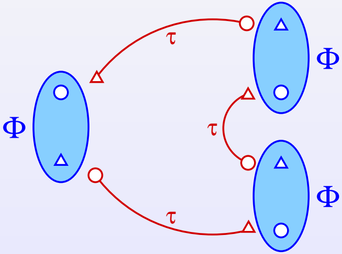
More diagrams



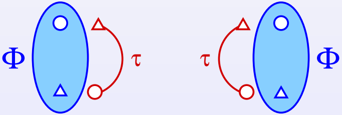
$\bar{B}_{abc}\tau_{aa'}\tau_{bb'}\tau_{cc'}B_{a'b'c'}$



$\bar{B}_{abc}\tau_{aa'}\tau^{\Gamma}_{bb'}\tau_{cc'}B_{a'b'c'}$



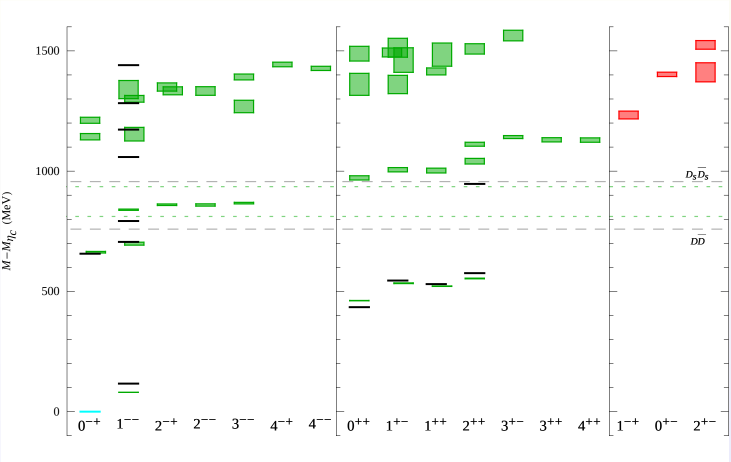
$\mathrm{Tr}\left[\Phi\tau\Phi\tau\Phi\tau\right]$



$\mathrm{Tr}\left[\Phi\tau\right]\ \mathrm{Tr}\left[\Phi\tau\right]$

Good news: precision spectroscopy

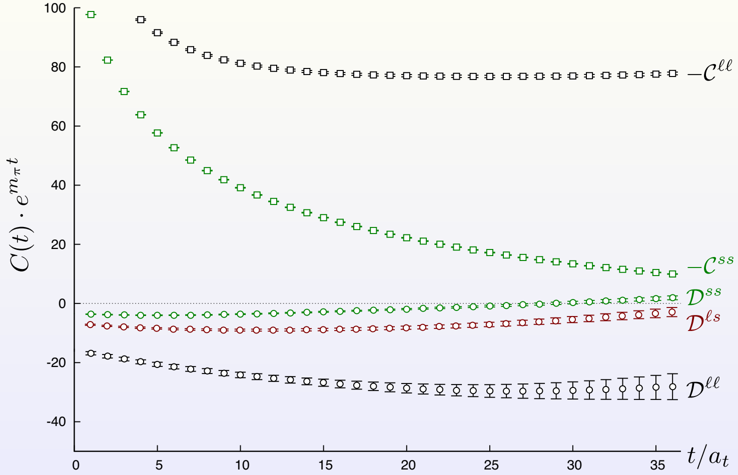
Charmonium



- Quark model: $1S, 1P, 2S, 1D, 2P, 1F, 2D, \ldots$ all seen.
- Not all fit quark model: spin-exotic (and non-exotic) hybrids seen [Liu et.al. arXiv:1204.5425]

Good news: precision spectroscopy (2)

Isoscalar mesons



- Correlation functions for $\bar{\psi}\gamma_5\psi$ operator, with different flavour content (s, l).
- 16^3 lattice (about 2 fm). [arXiv:1102.4299]

Limitation

- Distillation does not give direct access to all modes of the Dirac operator, only those low-modes relevant for spectroscopy
- Cannot use the method to calculate eg the strangeness content of the nucleon.

$$\langle N(t_f, \vec{q}| \sum_x e^{-i\vec{q}\cdot\vec{x}} \bar{s}(t', \vec{x} \Gamma s(t', \vec{x})|N(0, \vec{0})\rangle$$

- Use standard all to all instead.

Bad news: the bill!

- For constant resolution distillation space scales with N_s
- The cost of a calculation scales with V^2

The problem:

- To maintain constant resolution, need $N_{\mathcal{D}} \propto N_s$
- **Budget:**

Fermion solutions	construct τ	$\mathcal{O}(N_s^2)$
Operator constructions	construct Φ	$\mathcal{O}(N_s^2)$
Meson contractions	$\mathrm{Tr}[\Phi\tau\Phi\tau]$	$\mathcal{O}(N_s^3)$
Baryon contractions	$\bar{B}\tau\tau\tau B$	$\mathcal{O}(N_s^4)$

- Ok for reasonable lattices (eg with $N_s = 16^3, N_D = 64$) but scaling this to a 32^3 volume requires $N_D = 512$. Expensive.
- Distillation does not preclude stochastic estimation - use both for large V.

Stochastic estimation and distillation

[arXiv:1104.3870]

- Construct a **stochastic identity matrix** in $\mathcal{D}$: introduce a vector η with $N_{\mathcal{D}}$ elements and with

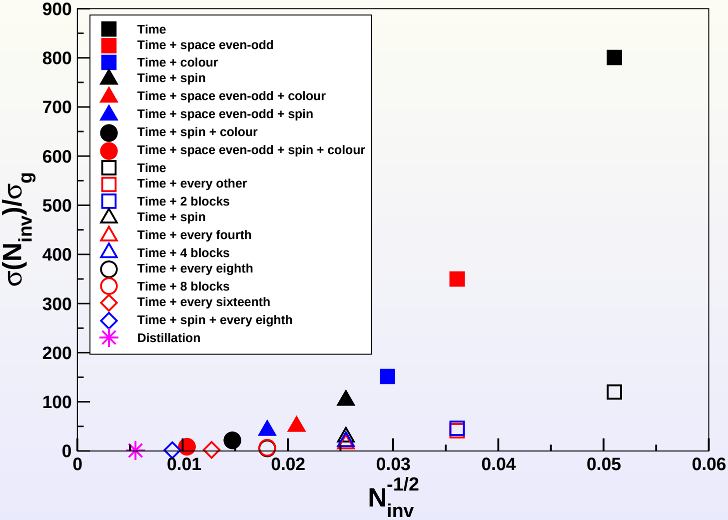
$$E[\eta_i] = 0 \text{ and } E[\eta_i \eta_j^*] = \delta_{ij}$$

- Now the distillation operator is written

$$\square = E[V\eta\eta^\dagger V^\dagger] = E[WW^\dagger]$$

- Introduces noise into computations
- **Dilution:** "thin out" the stochastic noise with N_η orthogonal projectors to make a variance-reduced estimator of $I_{\mathcal{D}} = E[WW^\dagger] = \sum_{k=1}^{N_\eta} E[V\mathcal{P}_k\eta\eta^\dagger\mathcal{P}_k V^\dagger]$, with $W_k = V\mathcal{P}_k\eta$, a $N_\eta \times (N_s \times N_c)$ matrix

Stochastic estimation: baryon correlator



- Convergence faster for noise in distillation space

[arXiv:1011.0481]

Summary

- Need good algorithms and new ideas for **both** effects
- Quark propagator is expensive to calculate and too large to store: either **compute one column of it, or estimate it stochastically**
- Don't need all entries to make hadrons - redefine smearing
- Distillation is a promising method for making hadrons
- Works well, but it is expensive and scales poorly
- Stochastic estimators rescue us again
- Know the limitations and pitfalls in each and choose to suit your budget and taste!

References

- APE smearing APE collaboration, M. Albanese et al., *Glueball masses and string tension in lattice QCD*, Phys. Lett. B192 (1987) 163.
- Hyper-cubic (HYP) smearing A. Hasenfratz and F. Knechtli, *Flavor symmetry and the static potential with hypercubic blocking*, Phys. Rev. D64 (2001) 034504.
- Stout-link smearing C. Morningstar and M.J. Peardon, *Analytic smearing of SU(3) link variables in lattice QCD*, Phys. Rev. D69 (2004) 054501.
- All-to-all propagators Foley et al, hep-lat/0505023 and references 1-13 therein.
- Distillation Peardon et al, arXiV:0905.2160
- Stochastic distillation: LaPH, Morningstar et al, arXiv:1104.3870