Numerical tools for manipulating quark propagators and correlation functions

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Asian School on LQCD, Mumbai, 14th March 2011

Overview - Lecture 1 - Monday 14th

- Introduction
- Fermionic correlation functions
  - Grassmann integration
  - Wick's theorem
- The lattice propagator
  - The "point-to-all" method
- Hadronic physics
  - Meson and baryon spectroscopy
  - Variational methods
  - Using other probes
  - Hadronic decay and mixing
- "All-to-all" methods
  - Stochastic estimation
  - Variance reduction
- Smearing

Introduction

- Lattice provides us with a **gauge-invariant, non-perturbative** regulator for QCD
- In a finite volume and at a non-zero lattice spacing, the path-integral is represented by a finite integration - solve numerically using **Monte Carlo**.
- Monte Carlo needs **importance sampling variance reduction** to give useful results in reasonable amounts of computer time
- Importance sampling means QCD must be defined in a **Euclidean** space-time.
- In Monte Carlo, **manipulating quark fields** is the dominant computational cost

Fermionic correlation functions

Fermions in the path integral

- In path integral, fermions are represented using **Grassmann** algebra.

$$\int d\eta = 0, \quad \int d\eta\, \eta = 1, \quad \eta^2 = 0$$

- Higher dimensions - anticommutation rule:

$$\eta_i \eta_j = -\eta_j \eta_i$$

- Expensive to manipulate directly by computer ...

Exercise 1

Find 3 4×4 matrices, α_1, α_2, μ such that for any f,

$$\int d\eta_1 d\eta_2 \;\; f(\eta_1, \eta_2) = \mathrm{Tr}\left\{\mu\, f(\alpha_1, \alpha_2)\right\}$$

Fermions in the path integral

- In QCD the action is (usually) bilinear.
- Consider computing a correlation function for the ρ-meson in 2-flavour QCD:

$$C_\rho(t_1, t_0) = \frac{\int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \ \bar{\psi}_u \gamma_i \psi_d(t_1)\ \bar{\psi}_d \gamma_i \psi_u(t_0)\ e^{-S_G[U] + \bar{\psi}_f M_f[U] \psi_f}}{\int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \ e^{-S_G[U] + \bar{\psi}_f M_f[U] \psi_f}}$$

- Integrate the grassmann fields analytically, giving:

$$C_\rho(t_1, t_0) = \frac{\int \mathcal{D}U \ \mathrm{Tr}\ \gamma_i M_d^{-1}(t_1, t_0) \gamma_i M_u^{-1}(t_0, t_1)\ \det M^2[U]\ e^{-S_G[U]}}{\int \mathcal{D}U\ \det M^2[U]\ e^{-S_G[U]}}$$

- Fermions in lagrangian → fermion determinant
- Fermions in measurement → propagators

Fermions in the path integral

- With more insertions, need **Wick's theorem**
- Example — four field insertions:

$$\langle \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \rangle$$

- and the pairwise contraction can be done in two ways:

$$\psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \quad \text{and} \quad \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l$$

- ...giving the propagator combination

$$M^{-1}_{ij} M^{-1}_{kl} - M^{-1}_{jk} M^{-1}_{il}$$

- the minus-sign comes from the anti-commutation needed in the second term.
- More fields means more combinations
- This is important in (eg.) isoscalar meson spectroscopy.

Exercise 2

For a system with six degrees of freedom, $\{\bar{\eta}_i, \eta_i\}, i = 1, 2, 3$, evaluate the grassmann integral

$$I_4 = \int \prod_{i=1}^{3} d\bar{\eta}_i d\eta_i \;\; \eta_1 \bar{\eta}_2 \eta_2 \bar{\eta}_1 \;\; e^{-\bar{\eta} M \eta}$$

and compare this answer to the prediction of Wick's theorem.

The lattice propagator

Handling lattice propagators

- On a finite lattice, the propagator is the inverse of a very large matrix.
- It is **impractical to compute** all elements of the propagator directly using a standard elimination method.
- The action $Ma = b$ for vectors a, b in the space of quark fields is practical. Can store lattice quark fields but not matrices.
- Given χ, can **solve the linear system**

$$M\psi = \chi$$

Handling lattice propagators

- Krylov space solver: the Krylov space $\mathcal{K}_n(M, \chi)$ is defined by

$$\mathcal{K}_n(M, \chi) = \text{Span}\left\{\chi, M\chi, M^2\chi, \ldots M^n\chi\right\}$$

- Examples include CG, MinRes, BiCG, . . .
- As the physical quark mass is approached, so the convergence of these algorithm slows rapidly.
- Newer algorithms use **deflation**: simultaneously build an approximation to the low-modes of M
- Algebraic multi-grid is re-emerging too

Handling lattice propagators

- Most lattice fermions obey γ_5-hermiticity:

$$M^\dagger(x,y) = \gamma_5 M(y,x)\gamma_5$$

- QCD vacuum is translationally invariant. Solving $M\psi = \eta$ gives access to **one row** of M^{-1}

The point-to-all propagator

- Choose an origin y
- For all spin, colour combinations $\{\alpha, a\}$
  - construct a source, $\eta_{x,\beta,b} = \delta_{x,y}\delta_{\beta,\alpha}\delta_{b,a}$
  - solve $M\psi^{(y,\alpha,a)} = \eta$ with this rhs
- Now have a block-row (at y) of M^{-1}

- Simple isovector meson and baryon creation operators can be constructed from this data

Hadronic physics

Computing the spectrum (1)

- Energies of colourless QCD states extracted from **two-point functions** in Euclidean time

$$C(t) = \langle \Phi(t) | \Phi^\dagger(0) \rangle$$

- Euclidean time: $\Phi(t) = e^{Ht} \Phi e^{-Ht}$ so $C(t) = \langle \Phi | e^{-Ht} | \Phi \rangle$
- Insert a complete set of states then:

$$C(t) = \sum_{k=0}^{\infty} |\langle \Phi | k \rangle|^2 \ e^{-E_k t}$$

- Then $\lim_{t \to \infty} C(t) = Z e^{-E_0 t}$
- If the large-t exponential fall-off of $C(t)$ can be observed, the **energy** of a state can be measured

Computing the spectrum (2)

- **Excited-state** energies measured from matrix of correlators:

$$C_{ij}(t) = \langle \Phi_i(t) | \Phi_j^\dagger(0) \rangle$$

- Solve generalised eigenvalue problem:

$$C(t_1)\,\underline{v} = \lambda\, C(t_0)\,\underline{v}$$

  for different t_0 and t_1
  [M. Lüscher & U Wolff, C. Michael]
- Then $\lim_{(t_1 - t_0) \to \infty} \ \lambda_n = e^{-E_n(t_1 - t_0)}$
- Method constructs optimal ground-state creation operator, then orthogonal states

Isovector meson correlation functions

- To create a meson, we need to build functions that couple to quarks.
- Meson can be created by a quark bilinear. Appropriate gauge invariant creation operator (for isospin $I = 1$) would be

$$\Phi_{\text{meson}}(t) = \sum_{x} \bar{u}(\underline{x}, t)\Gamma U_{\mathcal{C}}(\underline{x}, \underline{y}; t) d(\underline{y}, t)$$

  where Γ is some appropriate Dirac structure, and $U_{\mathcal{C}}$ a product of (smeared) link variables.
- Operators that transform irreducibly under the lattice rotation group O_h are needed.

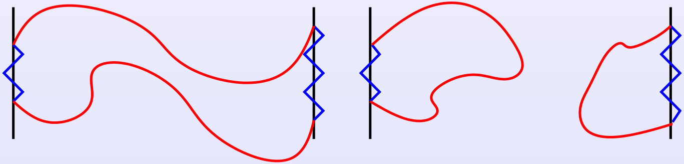
Isoscalar meson correlation functions

- If we are interested in measuring isoscalar meson masses, extra diagrams must be evaluated, since four-quark diagrams become relevant. The Wick contraction yields extra terms, since

$$\langle \psi_i \bar{\psi}_j \psi_k \bar{\psi}_l \rangle = M^{-1}_{ij} M^{-1}_{kl} - M^{-1}_{il} M^{-1}_{jk}$$

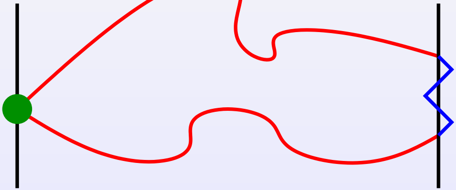
- Now

$$\langle 0 | \Phi_{I=0}(t) \Phi^{\dagger}_{I=0}(0) | 0 \rangle =$$
$$\langle 0 | \Phi_{I=1}(t) \Phi^{\dagger}_{I=1}(0) | 0 \rangle - \langle 0 | \mathrm{Tr}\, M^{-1} \Gamma U_{\mathcal{C}}(t) \mathrm{Tr}\, M^{-1} \Gamma U_{\mathcal{C}}(0) | 0 \rangle$$



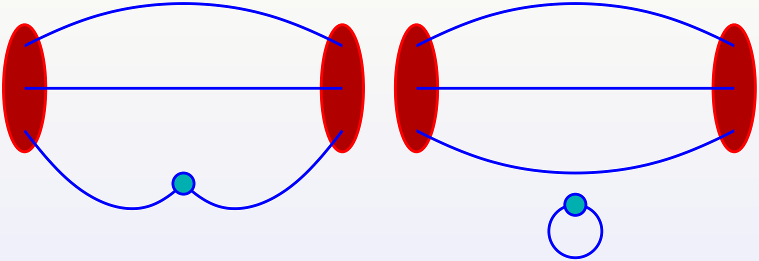
Isovector meson correlation functions (3)

The most general operator.



A restricted correlation function accessible to one point-to-all computation.

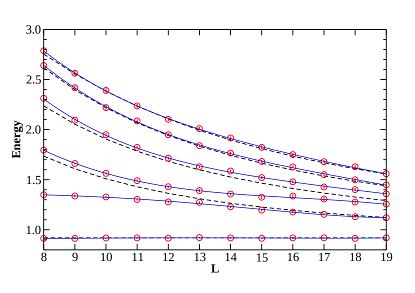
Current insertions



- All-to-all important for (eg) current insertion in a baryon where we want to sum over many insertion points

Studying scattering with Monte Carlo data

Data from $O(4)$ sigma-model [Giudice, MP and McManus].



- Maiani-Testa no-go: scattering data can not be computed in Euclidean field theory
- Lüscher: can infer scattering phase shifts from studying changes in spectrum

Computing scattering and decay needs:

- Multiple volumes
- Precision data on the spectrum, including excitations
- Variational basis including multi-hadron operators

All-to-all quark propagator methods

Stochastic estimators

- Since we are doing **Monte Carlo** over gauge fields in any case, it should be sufficient to **estimate** diagrams involving quark lines.
- Consider $\{\chi_1, \chi_2, \ldots\}$ a set of complex **stochastic variables** with the properties

$$E[\chi_i] = 0, \quad E[\chi_i \chi_j^*] = \delta_{ij}$$

- Now solve the linear system

$$M\phi = \chi$$

  (NB: only access have to M^{-1} numerically)
- Then clearly,

$$E[\phi_i \chi_j^*] = M^{-1}_{ij}$$

- and we have an estimator of **all elements** of the quark propagator

Stochastic estimators (2)

- **Variance too high**
- Reduced by recalculating estimator for m different random sources. Errors fall like $1/\sqrt{m}$. Do better?
- The exact propagator can be computed with finite (but large) effort (point-propagator methods with sources put everywhere).
- This suggests a trick; break up vector space of quark fields, V into d smaller sub-spaces $V = V_1 \oplus V_2 \oplus \dots$ spanned by sub-sets of basis vectors. E.g. even-odd partitioning:

$$V_1 = \left\{ e^{(1)} = (1, 0, 0, 0, \dots), e^{(3)} = (0, 0, 1, 0 \dots) \right\}$$

$$V_2 = \left\{ e^{(2)} = (0, 1, 0, 0, \dots), e^{(4)} = (0, 0, 0, 1, \dots) \right\}$$

This partitioning ("dilution") is arbitrary. A useful example is "time dilution", where N_T sub-spaces are defined, with support on one time-slice only.

Stochastic estimators (3)

- The basis is complete, so if $\mathcal{S}_i$ is a projector into space V_i and $\eta^{(i)} = \mathcal{S}_i \eta$ then $\eta = \sum_{i=1}^{d} \eta^{(i)}$. Since $\mathcal{S}_i^2 = \mathcal{S}_i$, we can write an identity

$$1 = \sum_{i=1}^{d} \mathcal{S}_i = \sum_{i=1}^{d} \mathcal{S}_i^2 = \sum_{i=1}^{d} \mathcal{S}_i E[\eta \otimes \eta^*] \mathcal{S}_i = \sum_{i=1}^{d} E[\eta^{(i)} \otimes \eta^{*(i)}]$$

  and another representation of the propagator can be written as

$$Q^{-1} = \sum_{i=1}^{d} E[\psi^{(i)} \otimes \eta^{*(i)}] \quad \text{where} \quad \psi^{(i)} = Q^{-1} \eta^{(i)}$$

- The variance in this estimator is reduced by explicit cancellation of terms that vanished before only as $m \to \infty$. If $d = N$, the **exact** propagator is recoved.
- A good choice of dilution should beat statistics.

Spectral representations

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

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

- Unfortunately, finding even a small sub-set of eigenvectors is computationally expensive, so we are forced to truncate this representation at $N_{\text{ev}} \ll N$

Hybrid method (1)

- Most physics contained in the lowest few eigenvectors of Q.
- Hybrid method: use an exact representation of the lowest few eigenvectors and corrects for truncation using stochastic estimator.
- Break V into two subspaces, V_L and V_H, with V_L the space spanned by the lowest N_{ev} eigenvectors.

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

- $\bar{Q}_L$ is the truncated eigenvector representation, and $\bar{Q}_H$ can be estimated with the dilution method. The action of $\bar{Q}_H$ is

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

  which is a Gram-schmidt orthogonalisation against known eigenvectors followed by application of M^{-1}.

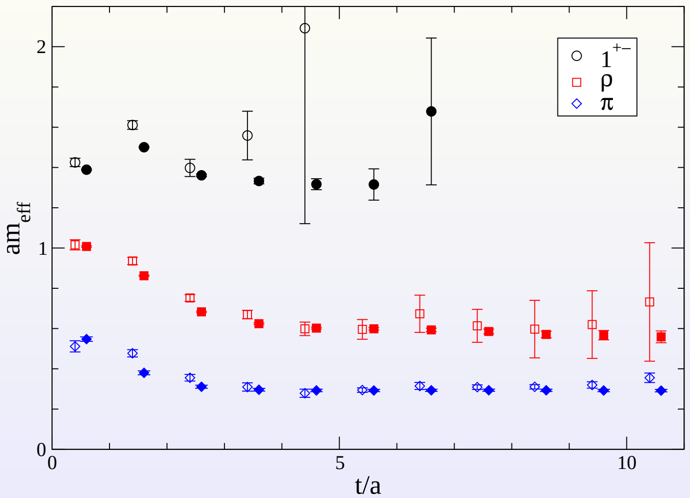
The Hybrid all-to-all method

- Compute N_{ev} eigenvectors and eigenvalues, $\{\lambda^{(i)}, v^{(i)}\}$
- Generate **one** noise vector, and dilute $\{\eta^{(1)}, \eta^{(2)}, \dots\}$
- For each dilute vector, compute $\psi^{(i)} = Q^{-1}(1 - \mathcal{P}_L)\eta^{(i)}$
- Now Q^{-1} is estimated as

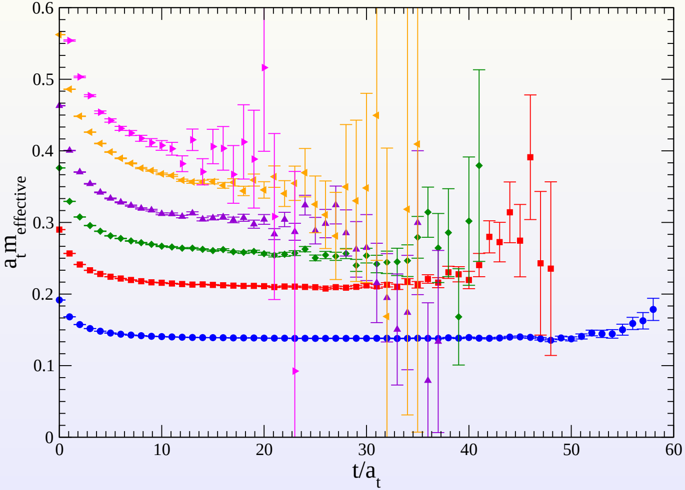
$$Q^{-1} = \sum_{i=1}^{N_{ev}} \frac{1}{\lambda^{(i)}} v^{(i)} \otimes v^{*(i)} + \sum_{j=1}^{N_d} \psi^{(j)} \otimes \eta^{*(j)}$$

- Since both terms are sums of outer products, they can be packed into a single sum over $j = 1 \dots N_{ev} + N_d$. The “hybrid list” representation becomes $Q^{-1} = \sum_{j=1}^{N_{ev}+N_d} u^{(j)} \otimes w^{*(j)}$

Isovector mesons - comparing methods



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



$12^3 \times 80$ anisotropic lattice Wilson fermions

Uses variational method to get excitations

Exercise 3

Using a toy model for a propagator in one dimension $M^{-1}(x, y) = \exp\{-\lambda|x - y|\}$ (using a periodic distance), investigate numerically the variance in an estimator of this propagator using different dilution schemes for a small 1-d lattice.

Hopping parameter expansion

- The hopping parameter expansion of the inverse of the Wilson fermion matrix starts with $M = I - \kappa D$.
- Taylor series expansion (for small κ) about $M = I$ is

$$
\begin{aligned}
M^{-1} &= I + \kappa D + \kappa^2 D^2 + \kappa^3 D^3 + \ldots \\
&= \sum_{h=0}^{\infty} \kappa^h D^h
\end{aligned}
$$

- Splitting at H terms gives

$$
\begin{aligned}
M^{-1} &= \sum_{h=0}^{H} \kappa^h D^h + \sum_{h=H+1}^{\infty} \kappa^h D^h \\
&= \sum_{h=0}^{H} \kappa^h D^h + \kappa^{H+1} D^{H+1} \sum_{h=0}^{\infty} \kappa^h D^h \\
&= \sum_{h=0}^{H} \kappa^h D^h + \kappa^{H+1} D^{H+1} M^{-1}
\end{aligned}
$$

Hopping parameter expansion (2)

- Splitting at H terms gives

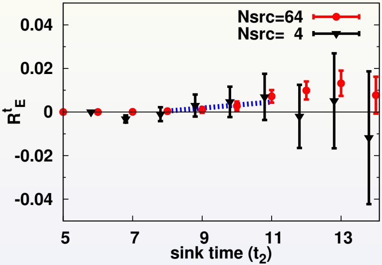
$$M^{-1} = \sum_{h=0}^{H} \kappa^h D^h + \kappa^{H+1} D^{H+1} M^{-1}$$

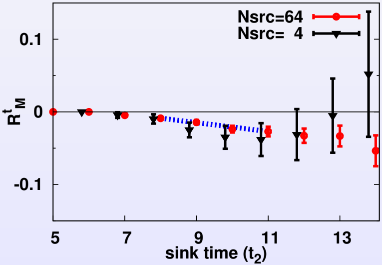
- For a number of local insertions (like $\bar{\psi}(x)\psi(x)$) the **first term** can be computed analytically for small H (depends on small Wilson loops).
- The second term is handled stochastically or by hybrid methods.
- It is usually smaller and so has smaller variance.
- Works for any approximation to the inverse, $\bar{M}$:

$$M^{-1} = \bar{M} + M^{-1} - \bar{M} = \bar{M} + (1 - \bar{M}M)M^{-1}$$

Example - nucleon strangeness

- Example - strangeness content of the nucleon
- **Doi** *et. al* **Phys.Rev.D80:094503,2009.**
- Requires stochastic computation of the disconnected diagram with a strange quark loop





Quark-field smearing

Smearing - an essential ingredient for precision

- 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; Jacobi/Wuppertal smearing: Apply the linear operator

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

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

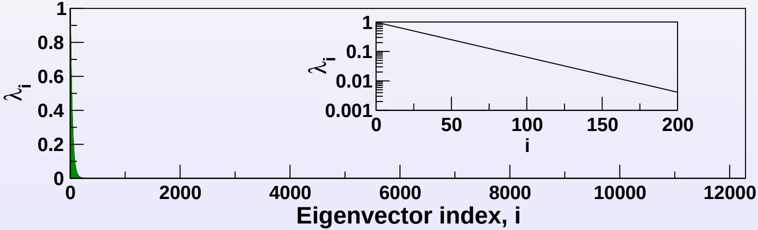
$$\Delta^2_{x,y} = 6\delta_{x,y} - \sum_{i=1}^{3} U_i(x)\delta_{x+\hat{\imath},y} + U_i^\dagger(x-\hat{\imath})\delta_{x-\hat{\imath},y}$$

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

- **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: $16^3 \times 3 = 12288$.

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?

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 $|n\rangle$