Lattice QCD with the Stochastic LapH Method

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Overview

- Calculating temporal correlators in lattice QCD requires inverting the large but sparse Dirac matrix.

- We can exploit translation invariance for single hadron operators to fix the position of the source hadron in 2-point correlators (point-to-all method).

- But, isoscalar mesons and two-hadron operators present a serious challenge (require all-to-all or many-to-many quark propagators).

- The stochastic LapH method is an efficient method for approximating these quark propagators.

Temporal Correlators from Path Integrals

- stationary-state energies are extracted from $N \times N$ Hermitian correlation matrix

$$C_{ij}(t) = \langle 0|\, O_i(t+t_0)\, \overline{O}_j(t_0)\, |0\rangle$$

- correlators found from path integral over ψ, $\overline{\psi}$ and U fields

$$C_{ij}(t) = \frac{\int D[\overline{\psi},\psi,U]\; O_i(t+t_0)\, \overline{O}_j(t_0)\;\exp(-\overline{\psi}K[U]\psi - S_G[U])}{\int D[\overline{\psi},\psi,U]\;\exp(-\overline{\psi}K[U]\psi - S_G[U])}$$

- $K[U]$ is the fermion Dirac matrix
- integration over quarks can be done exactly

$$\int D[\overline{\psi},\psi] F[\overline{\psi},\psi] \exp(-\overline{\psi}K\psi) = W[K^{-1}(U)] \det K$$

Monte Carlo Estimate of Path Integrals

- correlators now have the following form

$$C_{ij}(t) = \frac{\int D[U]\ \det K\ W[K^{-1}(U)]\ \exp(-S_G[U])}{\int D[U]\ \det K\ \exp(-S_G[U])}$$

- use Monte Carlo methods to integrate over U
- generate set of gauge configurations $\{U_i\}$ according to

$$P[U] = \frac{\exp(-S_G[U]) \prod_{j=1}^{N_f} \det K_j[U]}{\mathcal{Z}}$$

- γ_5-Hermiticity of K guarantees $\det K$ is real, and $m_u = m_d$ makes $\det K_u = \det K_d$
- $\det K_s$ is not guaranteed to be positive, but it usually is
- inclusion of $\det K$ and evaluation of $K^{-1}[U]$ are computationally expensive

Quark Propagation

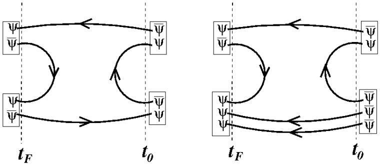
- quark propagator is inverse K^{-1} of Dirac matrix
  - rows/columns involve lattice site, spin, color
  - very large $N_{\text{tot}} \times N_{\text{tot}}$ matrix for each flavor

$$N_{\text{tot}} = N_{\text{site}} N_{\text{spin}} N_{\text{color}}$$

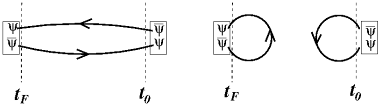
  - for $32^3 \times 256$ lattice, $N_{\text{tot}} \sim 101$ million
- not feasible to compute (or store) all elements of K^{-1}
- solve linear systems $Kx = y$ for source vectors y
- translation invariance can drastically reduce number of source vectors y needed
- multi-hadron operators and isoscalar mesons require large number of source vectors y

Quark Line Diagrams

- temporal correlations involving our two-hadron operators need
  - slice-to-slice quark lines (from all spatial sites on a time slice to all spatial sites on another time slice)
  - sink-to-sink quark lines



- isoscalar mesons also require sink-to-sink quark lines



- solution: the stochastic LapH method!

Stochastic Estimation of Quark Propagator

- Need an approximation on the inverse of the Dirac matrix $K[U]$
- Use noise vectors η such that $E(\eta_i) = 0$ and $E(\eta_i \eta_j^*) = \delta_{ij}$
- $Z_4 = \{+1, -1, +i, -i\}$ noise
- Generate N_R noise vectors $\eta^{(r)}$ and solve $K[U]X^{(r)} = \eta^{(r)}$
- Then $E(X_i \eta_j^*) = E(K_{ik}^{-1} \eta_k \eta_j^*) = K_{ik}^{-1} E(\eta_k \eta_j^*) = K_{ij}^{-1}$

$$\implies K_{ij}^{-1} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} X_i^{(r)} \eta_j^{(r)*}$$

- Suppose $\eta_j = \sum_{s=1}^{N} \eta_j^{[s]}$, where $\eta_j^{[s]} = \eta_j \delta_{js}$ (no sum over j), then

$$\sum_{s=1}^{N} X_i^{[s]} \eta_j^{[s]*} = K_{ij}^{-1} \eta_j \eta_j^* = K_{ij}^{-1},$$

because $Var(\eta_i \eta_j^*) = 1 - \delta_{ij}$

Variance Reduction through Noise Dilution

- Introduce a complete set of projection operators $P^{(a)}$:

$$P^{(a)}P^{(b)} = \delta^{ab}P^{(a)}, \quad \sum_a P^{(a)} = 1, \quad P^{(a)\dagger} = P^{(a)}$$

$$\eta_k^{[a]} = P_{kk'}^{(a)}\eta_{k'}, \qquad \eta_j^{[a]*} = P_{jj'}^{(a)*}\eta_{j'}^*$$

- Define $X^{[a]}$ to be the solution of $K_{ik}X_k^{[a]} = \eta_i^{[a]}$, then

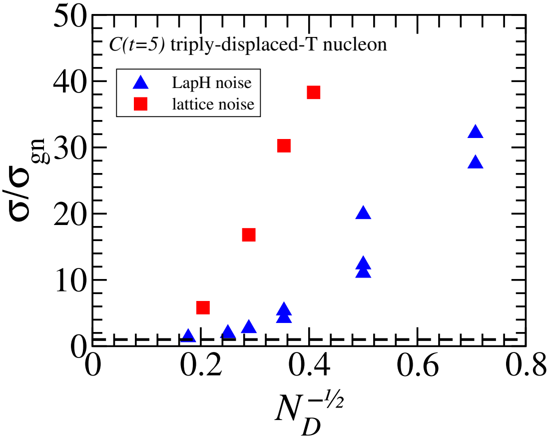
$$\sum_a E(X_i^{[a]}\eta_j^{[a]*}) = K_{ik}^{-1}\sum_a E(\eta_k^{[a]}\eta_j^{[a]*}) = K_{ik}^{-1}\sum_a P_{kj}^{(a)} = K_{ik}^{-1}$$

$$\implies K_{ij}^{-1} \approx \frac{1}{N_R}\sum_{r=1}^{N_R}\sum_a X^{(r)[a]}\ \eta_j^{(r)[a]*}$$

- An improvement because $Var(\sum_a \eta_k^{[a]}\eta_j^{[a]*}) < Var(\eta_k\eta_j^*)$

Laplacian Heaviside (LapH) Smearing

- why bother finding propagator to/from high energy modes?
- use the N_v lowest eigenvectors of the covariant Laplacian to define the LapH subspace



Excited States from Correlation Matrices

- in finite volume, energies are discrete

$$C_{ij}(t) = \sum_n Z_i^{(n)} Z_j^{(n)*} \; e^{-E_n t}, \qquad Z_j^{(n)} = \langle 0 | \, O_j \, | n \rangle$$

- not practical to do fits using above form
- define new correlation matrix $\widetilde{C}(t)$ using a single rotation

$$\widetilde{C}(t) = U^\dagger \; C(\tau_0)^{-1/2} \; C(t) \; C(\tau_0)^{-1/2} \; U$$

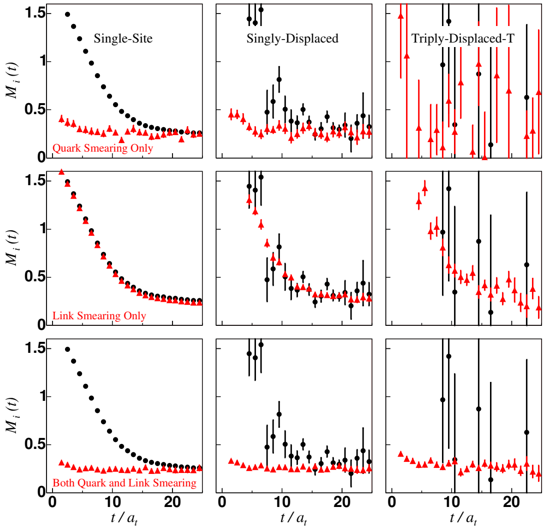
- columns of U are eigenvectors of $C(\tau_0)^{-1/2}\, C(\tau_D)\, C(\tau_0)^{-1/2}$
- choose τ_0 and τ_D large enough so $\widetilde{C}(t)$ diagonal for $t > \tau_D$
- effective energies

$$\widetilde{m}_\alpha^{\rm eff}(t) = \frac{1}{\Delta t} \ln \left(\frac{\widetilde{C}_{\alpha\alpha}(t)}{\widetilde{C}_{\alpha\alpha}(t+\Delta t)} \right)$$

  tend to N lowest-lying stationary state energies in a channel
- 2-exponential fits to $\widetilde{C}_{\alpha\alpha}(t)$ yield energies E_α and overlaps $Z_j^{(n)}$

Operator Smearing and Displacements

- Smearing quark fields reduces the excited state contamination
- Displacing quark fields captures extended structure of hadrons
- Smearing gauge-link fields reduces the error for displaced operators



Conclusion

- stochastic LapH method works very well
  - allows evaluation of all needed quark-line diagrams
  - does so efficiently and with low error

Questions?

Building Blocks for Single-hadron Operators

- building blocks: covariantly-displaced LapH-smeared quark fields
- stout links $\widetilde{U}_j(x)$
- Laplacian-Heaviside (LapH) smeared quark fields

$$\widetilde{\psi}_{a\alpha}(x) = \mathcal{S}_{ab}(x,y)\ \psi_{b\alpha}(y), \qquad \mathcal{S} = \Theta\left(\sigma_s^2 + \widetilde{\Delta}\right)$$

- 3d gauge-covariant Laplacian $\widetilde{\Delta}$ in terms of $\widetilde{U}$
- displaced quark fields:

$$q^A_{a\alpha j} = D^{(j)}\widetilde{\psi}^{(A)}_{a\alpha}, \qquad \overline{q}^A_{a\alpha j} = \widetilde{\overline{\psi}}^{(A)}_{a\alpha}\,\gamma_4\, D^{(j)\dagger}$$

- displacement $D^{(j)}$ is product of smeared links:

$$D^{(j)}(x,x') = \widetilde{U}_{j_1}(x)\ \widetilde{U}_{j_2}(x{+}d_2)\ \widetilde{U}_{j_3}(x{+}d_3)\dots\widetilde{U}_{j_p}(x{+}d_p)\delta_{x',\ x+d_{p+1}}$$

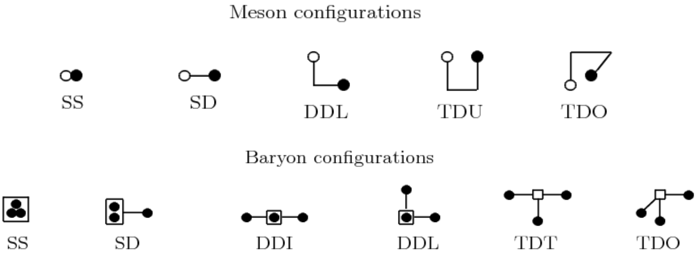
- to good approximation, LapH smearing operator is

$$\mathcal{S} = V_s V_s^\dagger$$

  - columns of matrix V_s are eigenvectors of $\widetilde{\Delta}$

Extended Operators for Single Hadrons

- quark displacements build up orbital, radial structure



$$\overline{\Phi}^{AB}_{\alpha\beta}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot(\mathbf{x}+\frac{1}{2}(\boldsymbol{d}_\alpha+\boldsymbol{d}_\beta))}\delta_{ab}\ \overline{q}^B_{b\beta}(\boldsymbol{x},t)\ q^A_{a\alpha}(\boldsymbol{x},t)$$

$$\overline{\Phi}^{ABC}_{\alpha\beta\gamma}(\boldsymbol{p},t) = \sum_{\boldsymbol{x}} e^{i\boldsymbol{p}\cdot\mathbf{x}}\varepsilon_{abc}\ \overline{q}^C_{c\gamma}(\boldsymbol{x},t)\ \overline{q}^B_{b\beta}(\boldsymbol{x},t)\ \overline{q}^A_{a\alpha}(\boldsymbol{x},t)$$

- group-theory projections onto irreps of lattice symmetry group

$$\overline{M}_l(t) = c^{(l)*}_{\alpha\beta}\ \overline{\Phi}^{AB}_{\alpha\beta}(t) \qquad \overline{B}_l(t) = c^{(l)*}_{\alpha\beta\gamma}\ \overline{\Phi}^{ABC}_{\alpha\beta\gamma}(t)$$

- definite momentum $\boldsymbol{p}$, irreps of little group of $\boldsymbol{p}$

Two-hadron Operators

- our approach: superposition of products of single-hadron operators of definite momenta

$$c^{I_{3a} I_{3b}}_{\boldsymbol{p}_a \lambda_a;\ \boldsymbol{p}_b \lambda_b} \ B^{I_a I_{3a} S_a}_{\boldsymbol{p}_a \Lambda_a \lambda_a i_a} \ B^{I_b I_{3b} S_b}_{\boldsymbol{p}_b \Lambda_b \lambda_b i_b}$$

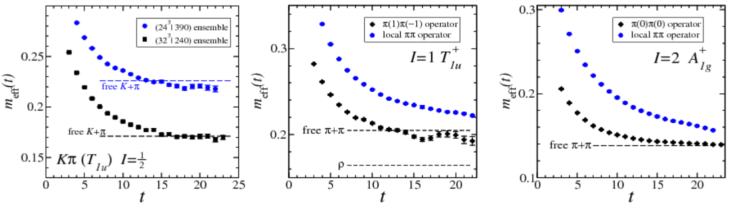
- fixed total momentum $\boldsymbol{p} = \boldsymbol{p}_a + \boldsymbol{p}_b$, fixed $\Lambda_a, i_a, \Lambda_b, i_b$
- group-theory projections onto little group of $\boldsymbol{p}$ and isospin irreps
- restrict attention to certain classes of momentum directions
  - on axis $\pm\widehat{\boldsymbol{x}},\ \pm\widehat{\boldsymbol{y}},\ \pm\widehat{\boldsymbol{z}}$
  - planar diagonal $\pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{y}},\ \pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{z}},\ \pm\widehat{\boldsymbol{y}} \pm \widehat{\boldsymbol{z}}$
  - cubic diagonal $\pm\widehat{\boldsymbol{x}} \pm \widehat{\boldsymbol{y}} \pm \widehat{\boldsymbol{z}}$
- efficient creating large numbers of two-hadron operators
- generalizes to three, four, ... hadron operators

Testing our Two-meson Operators

- (left) $K\pi$ operator in T_{1u} $I=\frac{1}{2}$ channels
- (center and right) comparison with localized $\pi\pi$ operators

$$(\pi\pi)^{A_{1g}^{+}}(t) = \sum_{\boldsymbol{x}} \pi^{+}(\boldsymbol{x},t)\ \pi^{+}(\boldsymbol{x},t),$$

$$(\pi\pi)^{T_{1u}^{+}}(t) = \sum_{\boldsymbol{x},k=1,2,3}\Big\{\pi^{+}(\boldsymbol{x},t)\ \Delta_k\pi^{0}(\boldsymbol{x},t) - \pi^{0}(\boldsymbol{x},t)\ \Delta_k\pi^{+}(\boldsymbol{x},t)\Big\}$$



- less contamination from higher states in our $\pi\pi$ operators

Quark Line Estimates in Stochastic LapH

- Only need noise vectors in the LapH subspace

  $$\rho_{\alpha k}(t), \qquad t = \text{time}, \alpha = \text{spin}, \ k = \text{eigenvector number}$$

- dilutions projectors
  - time indices (full for fixed src, interlace-16 for relative src)
  - spin indices (full)
  - LapH eigenvector indices (interlace-8 mesons, interlace-4 baryons)

- each of our quark lines is the product of matrices

  $$Q_{ij} = D_i \mathcal{S} K^{-1} \gamma_4 \mathcal{S} D_j^{\dagger}$$

- displaced-smeared-diluted quark source and quark sink vectors:

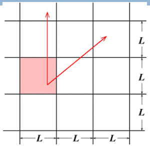
  $$\varrho^a(\rho) = D_j V_s P^a \rho, \qquad \varphi^a(\rho) = D_j \mathcal{S} K^{-1} \gamma_4 \ V_s P^a \rho$$

- estimate in stochastic LapH by

  $$Q_{ij} \approx \frac{1}{N_R} \sum_{r=1}^{N_R} \sum_a \varphi_i^{(r)[a]} \varrho_j{}^{(r)[a]\dagger}$$

Quantum Numbers in Toroidal Box

- periodic boundary conditions in cubic box
  - not all directions equivalent $\Rightarrow$ using J^{PC} is wrong!!



- label stationary states of QCD in a periodic box using irreps of cubic space group even in continuum limit
  - zero momentum states: little group O_h

$$A_{1a}, A_{2ga}, E_a, T_{1a}, T_{2a}, \quad G_{1a}, G_{2a}, H_a, \qquad a = g, u$$

  - on-axis momenta: little group C_{4v}

$$A_1, A_2, B_1, B_2, E, \quad G_1, G_2$$

  - planar-diagonal momenta: little group C_{2v}

$$A_1, A_2, B_1, B_2, \quad G_1, G_2$$

  - cubic-diagonal momenta: little group C_{3v}

$$A_1, A_2, E, \quad F_1, F_2, G$$

- include G parity in some meson sectors (superscript $+$ or $-$)

Spin Content of Cubic Box Irreps

- numbers of occurrences of Λ irreps in subduced reps of $SO(3)$ restricted to O

J	A_1	A_2	E	T_1	T_2	J	G_1	G_2	H
0	1	0	0	0	0	$\frac{1}{2}$	1	0	0
1	0	0	0	1	0	$\frac{3}{2}$	0	0	1
2	0	0	1	0	1	$\frac{5}{2}$	0	1	1
3	0	1	0	1	1	$\frac{7}{2}$	1	1	1
4	1	0	1	1	1	$\frac{9}{2}$	1	0	2
5	0	0	1	2	1	$\frac{11}{2}$	1	1	2
6	1	1	1	1	2	$\frac{13}{2}$	1	2	2
7	0	1	1	2	2	$\frac{15}{2}$	1	1	3

Common Hadrons

- What hadrons will appear in the different irreps at rest?

Hadron	Irrep	Hadron	Irrep
π	A_{1u}^-	K_1	T_{1g}
ρ	T_{1u}^+	Λ, Ξ	G_{1g}
a_0	A_{1g}^+	η, η'	A_{1u}^+
b_1	T_{1g}^+	K^*	T_{1u}
N, Σ	G_{1g}	h_1	T_{1g}^-
K	A_{1u}	π_1	T_{1u}^-
ω, ϕ	T_{1u}^-	Δ, Ω	H_g
f_0	A_{1g}^+		

Ensembles and Run Parameters

- plan to use three Monte Carlo ensembles
  - $(32^3|240)$: 412 configs $32^3 \times 256$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 4.4$
  - $(24^3|240)$: 584 configs $24^3 \times 128$, $m_\pi \approx 240$ MeV, $m_\pi L \sim 3.3$
  - $(24^3|390)$: 551 configs $24^3 \times 128$, $m_\pi \approx 390$ MeV, $m_\pi L \sim 5.7$
- anisotropic improved gluon action, clover quarks (stout links)
- QCD coupling $\beta = 1.5$ such that $a_s \sim 0.12$ fm, $a_t \sim 0.035$ fm
- strange quark mass $m_s = -0.0743$ nearly physical (using kaon)
- work in $m_u = m_d$ limit so $SU(2)$ isospin exact
- generated using RHMC, configs separated by 20 trajectories
- stout-link smearing in operators $\xi = 0.10$ and $n_\xi = 10$
- LapH smearing cutoff $\sigma_s^2 = 0.33$ such that
  - $N_v = 112$ for 24^3 lattices
  - $N_v = 264$ for 32^3 lattices