Sparsening Algorithm for Multi-Hadron Lattice QCD Correlation Functions

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Motivation

- Traditionally: gauge cfgs. and propagators expensive, contractions cheap
- More recently, some nuclear physics calculations contraction-dominated
  - Multigrid solvers have accelerated HMC and propagators by $\mathcal{O}(10-100)$
  - Contraction costs grow exponentially in number of quarks
- Nuclear correlation functions typically computed from "baryon blocks":

$$\mathcal{B}_b^{a_1,a_2,a_3}(\vec{p},t;x_0)=\sum_{\vec{x}} e^{i\vec{p}\cdot\vec{x}} \sum_{k=1}^{N_{B(b)}} \widetilde{w}_b^{(c_1,c_2,c_3),k} \sum_{i_1,i_2,i_3} \epsilon^{i_1,i_2,i_3} S_{c_{i_1}}^{a_1}(x;x_0)\, S_{c_{i_2}}^{a_2}(x;x_0)\, S_{c_{i_3}}^{a_3}(x;x_0)$$

  - Usually many source locations, op. smearings, background fields, etc.
  - FFTs are dominant cost
  - Blocks can be stored and re-used between calculations
- **Idea:** explore multigrid-like "sparsening" targeting contractions
  - Sparsen at the propagator level and do contractions on coarsened lattice
  - Coarsening spatial directions by N reduces FFT and storage costs by $\sim N^3$

Sparsening

- Prescription: uniformly block spatial directions by a factor N, and take first site in each block to define sparsened propagators on coarse lattice
- Distinguish between **"full"** correlation functions

$$C_{\mathrm{full}}\left(\vec{p}, t; \vec{x}_0, t_0\right) = \left\langle 0 \middle| \sum_{\vec{x} \in \Lambda_3} e^{i\vec{p}\cdot\vec{x}} \mathscr{O}\left(\vec{x}, t\right) \mathscr{O}^{\dagger}\left(\vec{x}_0, t_0\right) \middle| 0 \right\rangle$$

$$\Lambda_3 = \left\{ \left(n_1, n_2, n_3\right) \middle| 0 \leq n_i < L \right\}$$

and **"sparse"** correlation functions

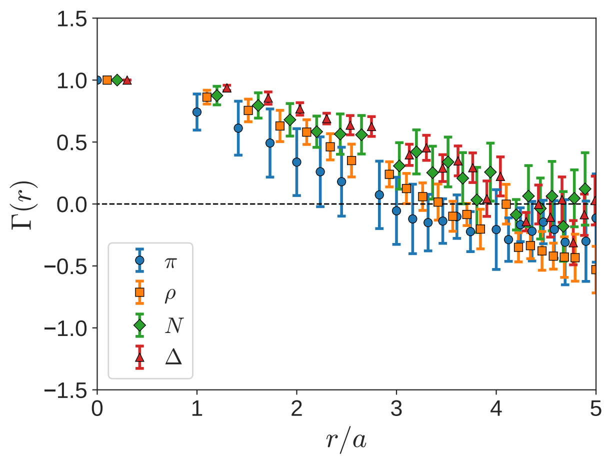
$$C_{\mathrm{sparse}}\left(\vec{p}, t; \vec{x}_0, t_0\right) = \left\langle 0 \middle| \sum_{\vec{x} \in \widetilde{\Lambda}_3(N)} e^{i\vec{p}\cdot\vec{x}} \mathscr{O}\left(\vec{x}, t\right) \mathscr{O}^{\dagger}\left(\vec{x}_0, t_0\right) \middle| 0 \right\rangle$$

$$\widetilde{\Lambda}_3(N) = \left\{ \left(n_1, n_2, n_3\right) \middle| 0 \leq n_i < L; n_i \equiv 0 \pmod{N} \right\}$$

- Simple interpretation as modified sink interpolator (partial mom. proj.)
  - Preserves FV spectrum and matrix elements (!)
  - Potentially modifies couplings to excited states, statistical noise, ... (?)
- Case study: examine two-point functions and ground state energy extractions on $32^3 \times 48$, $N_f = 3$, $m_\pi \approx 800$ MeV Wilson-clover ensemble

Spatial Correlations

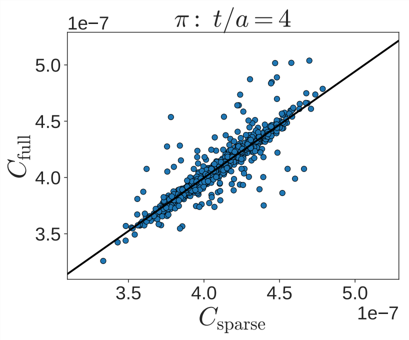
$$\Gamma(r) = \left\langle \left(C(\vec{p},t;\vec{x}_0,t_0) - \langle C(\vec{p},t;\vec{x}_0,t_0)\rangle\right)\left(C(\vec{p},t;\vec{x}_1,t_0) - \langle C(\vec{p},t;\vec{x}_1,t_0)\rangle\right)\right\rangle$$

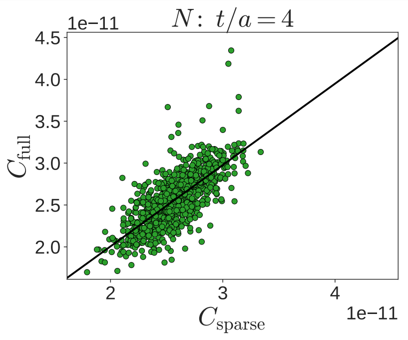


- Relevant scales: $(a\Lambda_{\mathrm{QCD}})^{-1} \approx 4.1$, $(am_\pi)^{-1} \approx 1.7$, $(a\Lambda_{\chi\mathrm{SB}})^{-1} \approx 1.4$, ...
- Block with $N = 4$ in remainder of talk

Consistency of Two-Point Functions: Early Time

- Sparsened vs. full two-point functions at fixed time separation
- Data has been averaged over source locations





$R^2 = 0.82$

$\mathrm{slope} = 0.95(2)$

$\mathrm{intercept} = 2.2(0.8) \times 10^{-8}$

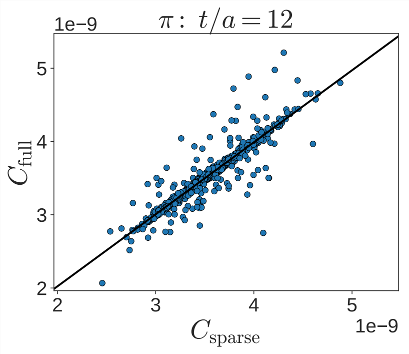
$R^2 = 0.52$

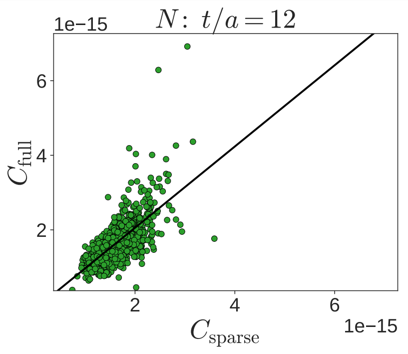
$\mathrm{slope} = 0.97(3)$

$\mathrm{intercept} = 6.3(8.6) \times 10^{-13}$

Consistency of Two-Point Functions: Late Time

- Sparsened vs. full two-point functions at fixed time separation
- Data has been averaged over source locations





$R^2 = 0.86$

$\text{slope} = 0.98(2)$

$\text{intercept} = 5.8(6.5) \times 10^{-11}$

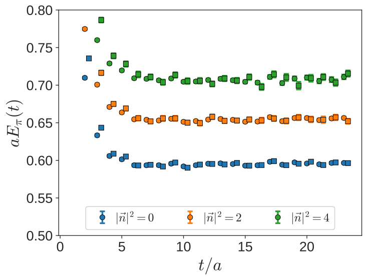
$R^2 = 0.41$

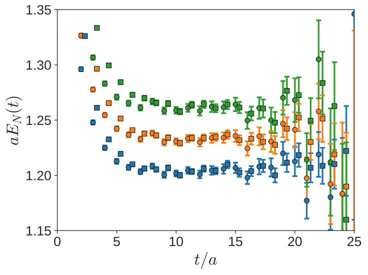
$\text{slope} = 1.09(8)$

$\text{intercept} = -1.2(1.3) \times 10^{-16}$

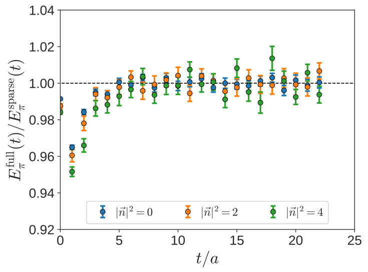
Single Hadron Spectrum: Effective Energy Signals

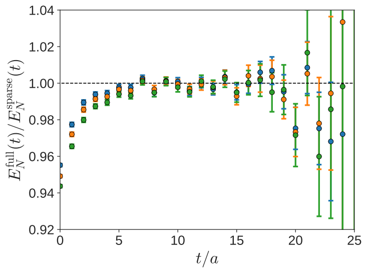
- Full (circles) and sparsened (squares) effective energy signals:





- Correlated ratios:

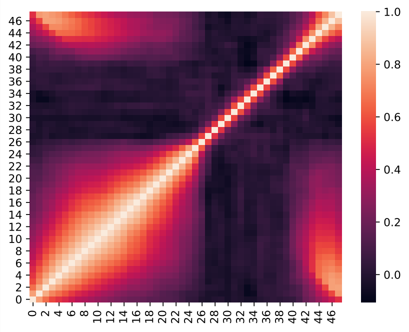




Single Hadron Spectrum: Nucleon Covariance Matrix

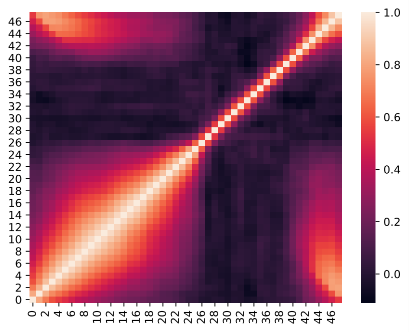
$$\Sigma_{ij} = \left\langle \left(C_\alpha(\vec{p}, t_i) - C(\vec{p}, t_i) \right) \left(C_\alpha(\vec{p}, t_j) - C(\vec{p}, t_j) \right) \right\rangle_\alpha$$

Full



$\kappa(\Sigma) = 5.1 \times 10^7$

Sparse



$\kappa(\Sigma) = 3.2 \times 10^7$

- Plots show correlation matrix: $\rho_{ij} = \Sigma_{ij}/\sigma_i\sigma_j$
- No significant modification to correlations in time direction

Single Hadron Spectrum: Ground State Energy Extraction

State	$\|\vec{n}\|^2$	Full			Sparse		
		aE	χ^2/dof	$\kappa(\Sigma)$	aE	χ^2/dof	$\kappa(\Sigma)$
π	0	0.5948(3)	1.3(7)	3.8×10^6	0.5947(3)	1.4(7)	2.6×10^6
	2	0.6537(4)	1.3(7)	4.9×10^8	0.6537(4)	1.9(8)	8.8×10^7
	4	0.7065(4)	1.2(7)	7.9×10^8	0.7065(4)	1.4(7)	1.7×10^8
N	0	1.204(2)	0.7(7)	5.1×10^7	1.205(1)	0.7(7)	3.2×10^7
	2	1.233(2)	0.6(6)	5.8×10^7	1.234(1)	0.2(4)	3.5×10^7
	4	1.260(2)	0.6(6)	6.1×10^7	1.263(2)	0.4(5)	3.8×10^7

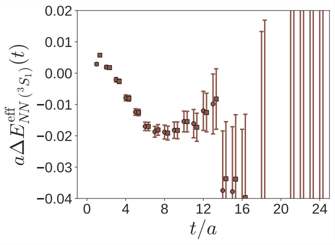
- Ground-state energies extracted from correlated, single-exponential fits

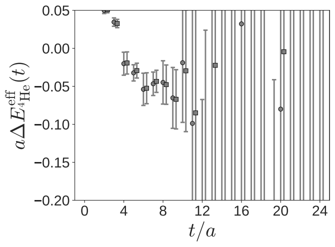
$$f(t; Z_{\mathrm{src}}, Z_{\mathrm{snk}}, E) = \begin{cases} \dfrac{Z_{\mathrm{src}} Z^*_{\mathrm{snk}}}{2E}\left(e^{-Et} + e^{-E(T-t)}\right), & \text{mesons} \\ \dfrac{Z_{\mathrm{src}} Z^*_{\mathrm{snk}}}{2E} e^{-Et}, & \text{baryons} \end{cases}$$

- No significant effect on extracted ground state energies

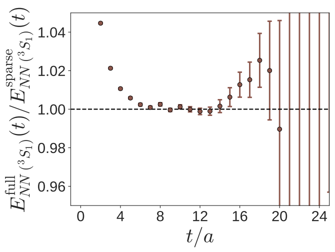
Multi-Hadron Spectrum: Effective Energy Signals

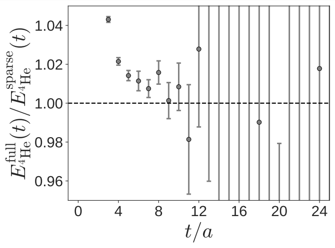
- $R_A(t) = C_A(t) / [C_N(t)]^A \overset{t/a \gg 1}{\propto} \exp(-\Delta E \cdot t)$, $\Delta E \equiv E_A - A \cdot E_N$
- Full (circles) and sparsened (squares) effective binding energy signals:





- Correlated ratios:





Multi-Hadron Spectrum: Ground State Energy Extraction

State	aE	χ^2/dof	aE	χ^2/dof
$NN\ (^1S_0)$	2.3961(25)	0.41(52)	2.3961(25)	0.35(48)
$NN\ (^3S_1)$	2.3919(25)	0.61(65)	2.3918(25)	0.53(60)
^3He	3.5726(83)	0.55(74)	3.5726(84)	0.55(72)
^4He	4.769(29)	0.37(57)	4.766(27)	0.57(72)

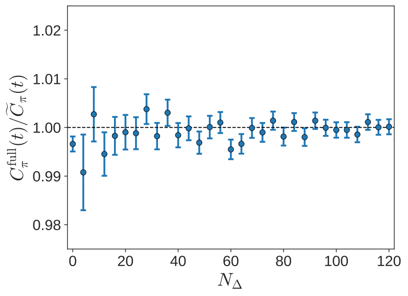
State	$a\Delta E$	χ^2/dof	$a\Delta E$	χ^2/dof
$NN\ (^1S_0)$	−0.0140(18)	0.46(67)	−0.0138(18)	0.53(72)
$NN\ (^3S_1)$	−0.0180(17)	0.26(50)	−0.0180(17)	0.29(53)
^3He	−0.0434(72)	0.37(67)	−0.0431(75)	0.44(74)
^4He	−0.055(13)	0.36(49)	−0.054(13)	0.55(67)

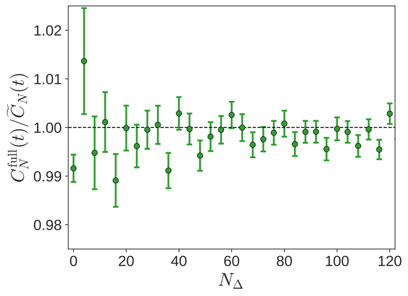
Controlling Excited State Effects

- Can modify sparsened estimator to control coupling to excited states:

$$\widetilde{C}(\vec{p},t) = \frac{1}{N_{\rm sparse}} \sum_{x_0 \in \Lambda_{\rm sparse}} C_{\rm sparse}(\vec{p},t;x_0) + \frac{1}{N_\Delta} \sum_{x_0' \in \Lambda_\Delta} \left(C_{\rm full}(\vec{p},t;x_0') - C_{\rm sparse}(\vec{p},t;x_0') \right)$$

- Similar to all-mode averaging (AMA) technique [Blum et. al., PRD 88, 094503]
- $\Lambda_\Delta \subset \Lambda_{\rm sparse}$, ideally $N_\Delta \ll N_{\rm sparse}$





- Note: in this study sources are densely packed and highly correlated!

Conclusions

- We have explored a cost-reduction algorithm for multi-hadron correlation functions based on sparsening at the propagator level
- Ground state energies extracted from sparsened and full correlation functions are consistent
- Excited state effects are modified, but this can be controlled with an AMA-like technique
- We are now using these ideas in production calculations:
  1. NPLQCD light nuclear spectrum and MEs @ $m_\pi = 170$ MeV: $N = 6 \Rightarrow$ $\sim$ **100× speed-up!**
  2. Coarse all-to-all propagators for spectrum of $SU(2)$ Adjoint theory with one Dirac flavor [**A. Grebe, Friday @ 16:10**]
- Paper to appear on the arXiv soon....

Thank you!