Hadron Structure using Distillation

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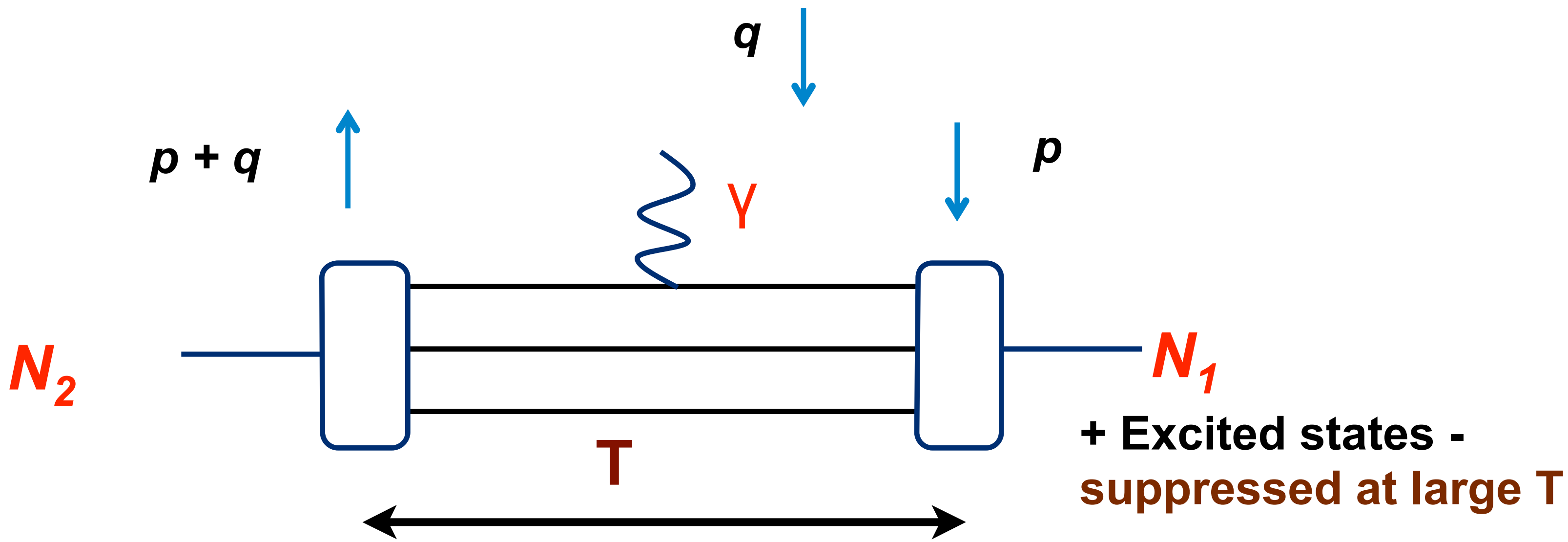
ABSTRACT

"A major challenge in precise calculations of the structure of the nucleon is performing calculations at reasonable cost in which the contribution of the ground state nucleon is sufficiently isolated. We propose to perform an exploratory study using ``distillation'' with an extensive basis of interpolating operators with the aim of greatly suppressing the contributions of excited states at relatively modest source-sink separations. We request a total of ***400K GPU-hours*** *on* ***K20 GPUs****, and* ***23M JPsi core-hours****. In addition, we require 36Tbyte of disk storage, equivalent to 720K JPsi-hours, and 7.5 TByte of tape storage, equivalent to 22.5K JPsi-hours."*

Hadron Structure



$$\Gamma_{N\mu N}(t_f, t; \vec{p}, \vec{q}) = \sum_{\vec{x},\vec{y}} \langle 0 \mid N(\vec{x}, t_f) V_\mu(\vec{y}, t) \bar{N}(\vec{0}, 0) \mid 0 \rangle e^{-i\vec{p}\cdot\vec{x}} e^{-i\vec{q}\cdot\vec{y}}$$

Resolution of unity – insert states

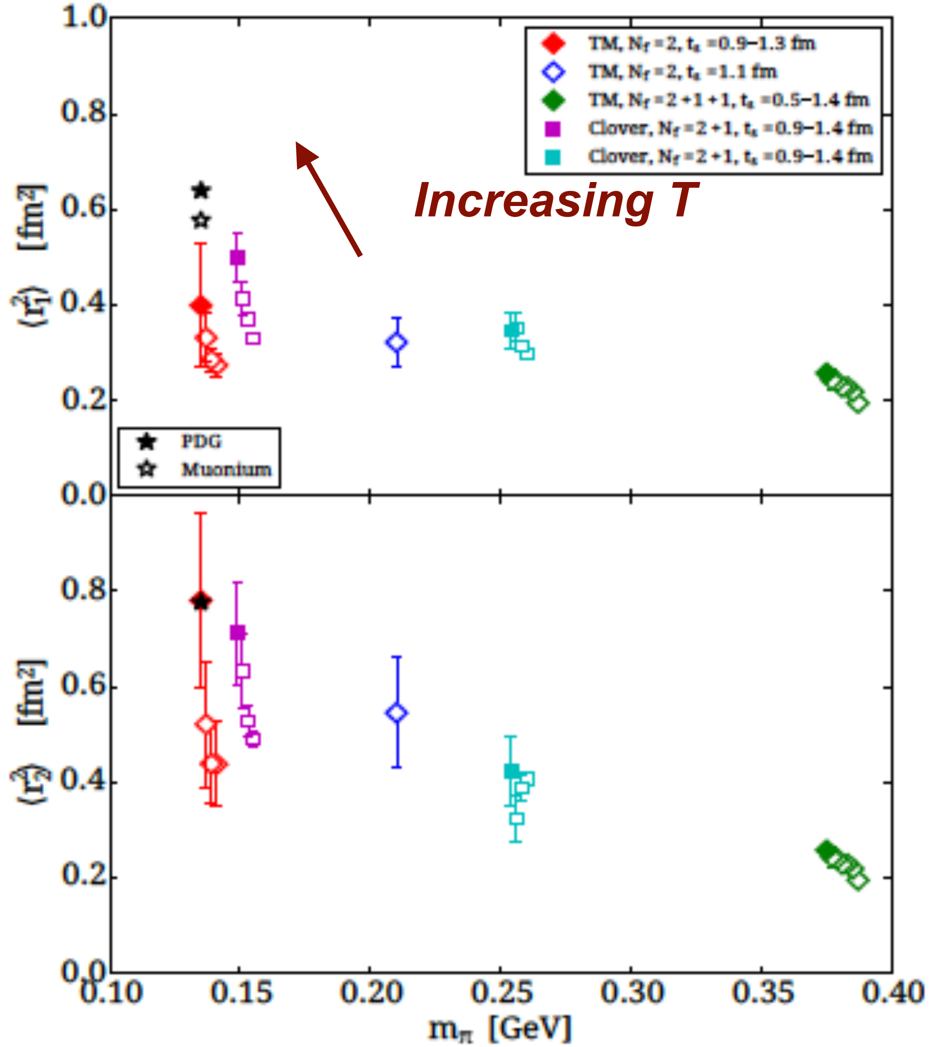
$$\longrightarrow \langle 0 \mid N \mid N, \vec{p}+\vec{q} \rangle \langle N, \vec{p}+\vec{q} \mid V_\mu \mid N \vec{p} \rangle \langle N, \vec{p} \mid \bar{N} \mid 0 \rangle e^{-E(\vec{p}+\vec{q})(t_f - t)} e^{-E(\vec{p})t}$$

Physics Goals

Excited-state contamination is a major systematic uncertainty in calculations of nucleon structure

Precision key if LQCD to impact discrepancy between charge radius determined in muonic hydrogen, and that from, e.g. electron scattering

M. Constantinou, plenary Lattice 2014, arXiv:1411.0078



Three approaches

- Work at sufficiently large T
- "Summation Method"

Exponential degradation of signal-to-noise with increasing T

LHPC, (Green et al) Phys. Rev. D 90, 074507 (2014)

$$R_q^\mu(\tau,T) = \frac{C_{3\mathrm{pt}}^{V_q^\mu}(\vec{p},\vec{p}\,',\tau,T)}{\sqrt{C_{2\mathrm{pt}}(\vec{p},T)C_{2\mathrm{pt}}(\vec{p}\,',T)}}\sqrt{\frac{C_{2\mathrm{pt}}(\vec{p},T-\tau)C_{2\mathrm{pt}}(\vec{p}\,',\tau)}{C_{2\mathrm{pt}}(\vec{p}\,',T-\tau)C_{2\mathrm{pt}}(\vec{p},\tau)}}$$

$$= \frac{\sum_{\lambda,\lambda'}\bar{u}(\vec{p},\lambda)\Gamma_{\mathrm{pol}}u(\vec{p}\,',\lambda')\langle p',\lambda'|V_q^\mu|p,\lambda\rangle}{\sqrt{2E(\vec{p})(E(\vec{p})+m_N)\cdot 2E(\vec{p}\,')(E(\vec{p}\,')+m_N)}} + O(e^{-\Delta E_{10}(\vec{p})\tau}) + O(e^{-\Delta E_{10}(\vec{p}\,')(T-\tau)}).$$

$$S(T) \equiv \sum_{\tau=\tau_0}^{T-\tau_0} R(\tau,T) = c + TM + O(Te^{-\Delta E_{\mathrm{min}}T}),$$

Sum over different temporal separations

- Variational Method
- Variational Method + Distillation

Exponential improvement in signal-to-noise by working at small T

Complementary to proposal of Syritsyn, Gupta et al

Efficient Correlation fns: Distillation

Eigenvectors of Laplacian

- Observe $$L^{(J)} \equiv (q - \frac{\kappa}{n}\Delta)^n = \sum_i f(\lambda_i)\xi^i \otimes \xi^{i*}$$
- Truncate sum at sufficient i to capture relevant physics modes
- *Baryon* correlation function

$$C_{ij}(t) = \Phi^{i,(p,q,r)}_{\alpha\beta\gamma}(t)\Phi^{j,(\bar{p},\bar{q},\bar{r})\dagger}_{\bar{\alpha}\bar{\beta}\bar{\gamma}}(0) \times \Big[\tau^{p\bar{p}}_{\alpha\bar{\alpha}}(t,0)\tau^{q\bar{q}}_{\beta\bar{\beta}}(t,0)\tau^{r\bar{r}}_{\gamma\bar{\gamma}}(t,0) - \tau^{p\bar{p}}_{\alpha\bar{\alpha}}(t,0)\tau^{q\bar{r}}_{\beta\bar{\gamma}}(t,0)\tau^{r\bar{q}}_{\gamma\bar{\beta}}(t,0)\Big]$$

M. Peardon *et al.*, PRD80,054506 (2009)

where

$$\Phi^{i,(p,q,r)}_{\alpha\beta\gamma} = \epsilon^{abc} S^i_{\alpha\beta\gamma} (\mathbf{\Gamma}_1 \xi^{(p)})^a (\mathbf{\Gamma}_2 \xi^{(q)})^b (\mathbf{\Gamma}_3 \xi^{(r)})^c$$

Perambulators →

$$\tau^{p\bar{p}}_{\alpha\bar{\alpha}}(t,0) = \xi^{\dagger(p)}(t) M^{-1}_{\alpha\bar{\alpha}}(t,0)\xi^{(\bar{p})}(0)$$

Brown and Orginos, arXiv:1210.1953

Color-wave formalism

$$\xi^{(i)}(\vec{x}) \equiv \xi_p(\vec{x}) = e^{-i\vec{p}\cdot\vec{x}}\delta_{s,s'}\delta_{c,c'}; \quad \vec{p}^2 \leq 4$$

Baryon Operators

Aim: interpolating operators of *definite* (continuum) JM: O^{JM}

$$\langle 0 \mid O^{JM} \mid J', M' \rangle = Z^J \delta_{J,J'} \delta_{M,M'}$$

Starting point $\quad B = \left(\mathcal{F}_{\Sigma_F} \otimes \mathcal{S}_{\Sigma_S} \otimes \mathcal{D}_{\Sigma_D}\right)\{\psi_1 \psi_2 \psi_3\}$

Introduce circular basis:

$$\overleftrightarrow{D}_{m=-1} = \frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x - i\overleftrightarrow{D}_y\right)$$

R.G.Edwards et al., arXiv:1104.5152

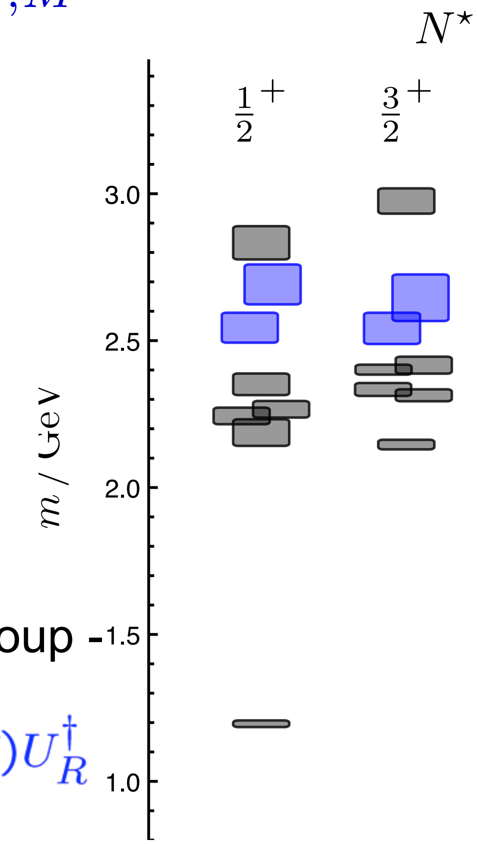
$$\overleftrightarrow{D}_{m=0} = i\overleftrightarrow{D}_z$$

Dudek, Edwards, arXiv:1201.2349

$$\overleftrightarrow{D}_{m=+1} = -\frac{i}{\sqrt{2}}\left(\overleftrightarrow{D}_x + i\overleftrightarrow{D}_y\right).$$

Straight forward to project to definite spin: $J = 1/2, 3/2, 5/2$

$$\big|[J,M]\big\rangle = \sum_{m_1,m_2} \big|[J_1,m_1]\big\rangle \otimes \big|[J_2,m_2]\big\rangle \langle J_1 m_1; J_2 m_2 | JM\rangle$$



Use projection formula to find subduction under irrep. of cubic group - operators are closed under rotation!

$$O^{[J]}_{\Lambda\lambda}(t,\vec{x}) = \frac{d_\Lambda}{g_{O_h^D}} \sum_{R \in O_h^D} D^{(\Lambda)*}_{\lambda\lambda}(R) U_R O^{J,M}(t,\vec{x}) U_R^\dagger$$

$$= \sum_M S^{J,M}_{\Lambda,\lambda} O^{J,M}$$

Irrep, Row

Irrep of R in Λ

Action of R

Distillation and Matrix Elements

- Simple to implement by replacing one of the perambulators by a so-called generalized perambulator with current inserted.

$$S^{ij}(t_f, t, t_i) = \xi^{(i)\dagger}(t_f) M^{-1}(t_f, t) \Gamma(t) M^{-1}(t, t_i) \xi^{(j)}(t_i)$$

Variational Method

$$C(t) v^{(N)}(t, t_0) = \lambda_N(t, t_0) C(t_0) v^{(N)}(t, t_0).$$

$$\lambda_N(t, t_0) \longrightarrow e^{-E_N(t-t_0)},$$

Eigenvectors enable us to define an *"ideal operator"* for each which we can use in our three-point function

$$\Omega_N = \sqrt{2 m_N} e^{-m_N t_0/2} v_i^{(N)} \mathcal{O}_i$$

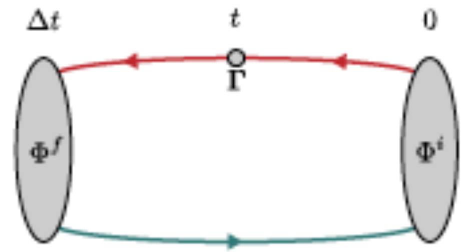
Operators NON-LOCAL

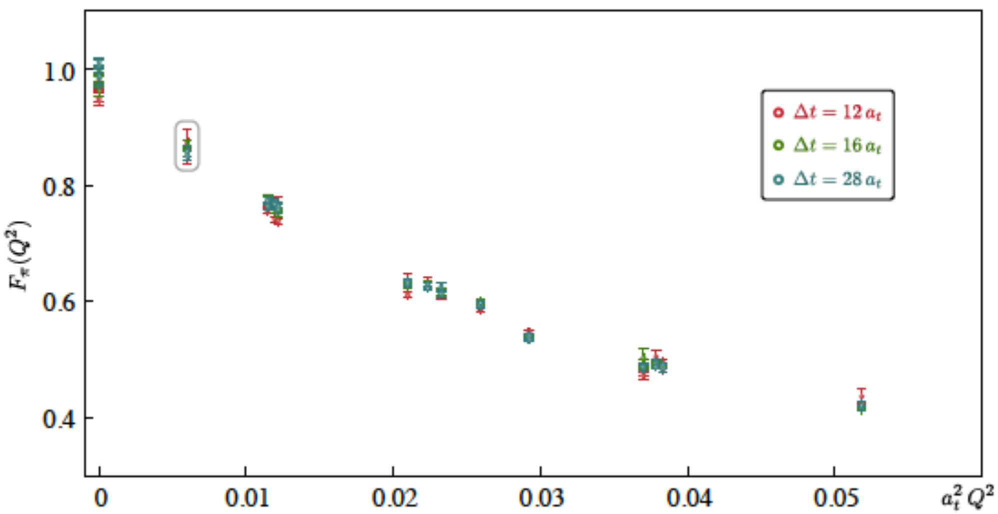
Radiative Transitions for Mesons

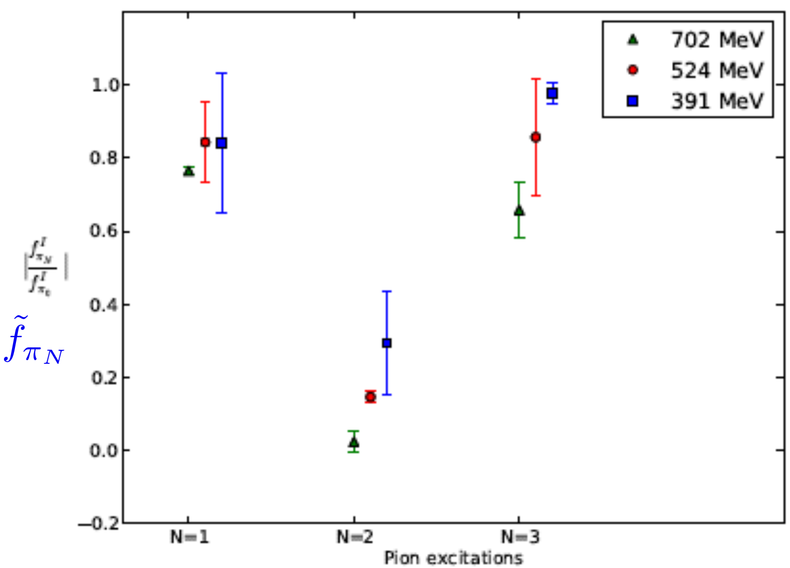
- Formalism for EM matrix elements already demonstrated for mesons by HadSpec collaboration.

$$F(Q^2;t) = F(Q^2) + f_f e^{-\delta E_f(\Delta t - t)} + f_i e^{-\delta E_i t}$$

Shultz, Dudek and Edwards, arXiv:1501.07457







$$C_{A_4,N}(t) = \frac{1}{V_3} \sum_{\vec{x},\vec{y}} \langle 0 \mid A_4(\vec{x},t)\Omega_N^\dagger(\vec{y},0) \mid 0 \rangle \longrightarrow e^{-m_N t} m_N \tilde{f}_{\pi_N}$$

E. Mastropas, DGR, PRD(2014)

Proposal: isotropic clover

Thanks to Baiint

V	m_π (MeV)	a (fm)	Flavors	$m_\pi L$	#traj	Comments
32^3x64	~410	0.085	2+1	5.6	5138	Suspended to push to lighter mass
32^3x64	~300	0.081	2+1	4.0	2638	Suspended to push to lighter mass
48^3x96	~200	0.079	2+1	3.8	674	Suspended to go to bigger volume
64^3x128	~200	0.078	2+1	~5	~2000	1110 traj in original stream 3 other streams (310,270,324 traj respectively) — about 1000 usable, τ_{MD}=0.5
64^3x128	~150	~0.078	2+1	~3.8	40	Barely started. Masses, lattice spacings etc are expectations based on extrapolation and need to be verified

Proposal

- Use isotropic clover lattices generated under the proposals of Edwards et al and Orginos et al
- Demonstration: perform calculations at pion masses of 300 and 400 MeV. *Excited-state contamination increases as quark mass decreases.*
- For this proof-of-principle proposal, focus on the local currents and $\bar{\psi}\gamma_\mu D_\nu \psi$ giving rise to momentum fraction
- Generator soln. vectors on GPUs

Quark	m_π (MeV)	Volume	Time/propagator	N_{vec}	N_{src}	N_{cfg}	Total
u/d	305	$32^3 \times 64$	0.4	33	64	300	254K
u/d	400	$32^3 \times 64$	0.24	33	64	300	152K
TOTAL							400K

- Construction of Generalized Perambulators and of correlation functions require 23M core-hours on the CPUs

Summary

- Reducing the contribution from excited states in study of hadron structure is a crucial for precision calculations
- The approach of the variational method + distillation is a powerful way of addressing this issue compared to other approaches:
  - Efficient implementation of large variation basis should enable elements to be extracted at far smaller source-sink separations: *exponential reduction in noise.*
  - Distillation allow momentum projections to be made at both the source and sink points, and at the operator insertion: *increase in statistics.*
  - Efficient computational framework in which solution vectors are computed on the GPUs
- If effective, expectation is that it will be adopted by isoclover (and other?) matrix element projects.