Towards Lattice QCD Calculations of Pion Production

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Image credit: Fermilab
Deep Underground Neutrino Experiment

- Beam from Fermilab to South Dakota to study $\nu$ oscillations
- Oscillation parameters depend on $P(\nu_\mu \rightarrow \nu_e)$ as function of $L/E$
- Experimental $\nu$ beams inherently broadband
- Will require reconstruction of $E_\nu$
- Need energy-dependent cross-sections for $\nu$-nucleus interactions

Image credit: B. Abi et al. (DUNE Collaboration), 2006.16043
Several varieties of nuclear many-body methods (A. Lovato, Tues. 9:00)
- GFMC (J. Carlson et al., 1412.3081), AFDMC (A. Lovato et al., 2206.10021), spectral functions (N. Steinburg, Tues. 11:10)

All require nuclear Hamiltonian + couplings to external currents

$\nu$-A cross-sections $\leftrightarrow$ $\nu$-$N$ cross-sections
**ν-Δ Cross-Sections**

- Quasi-elastic regime – based on nucleon elastic form factor
- DIS regime – perturbative
  - Factorization theorems, nucleon PDFs
- Resonant regime – dominated by $N \rightarrow \Delta$
  - Peak of DUNE beam
  - Need $\sim 3\%$ uncertainty for DUNE (D. Simons et al., 2210.02455)

Image credit: Adapted from J. A. Formaggio, G. P. Zeller (1305.7513)
Neutrinoproduction

\[ \nu_\mu N \rightarrow \mu \Delta \]

- Mediated through electroweak current
  \[ \bar{N}(\gamma_\mu - \gamma_\mu \gamma_5)\Delta \]
- Vector component known from \( eN \rightarrow e\Delta \)
- Axial component difficult to measure experimentally
- \( \Delta \) resonance above \( N\pi\pi \) threshold
  \[ \Delta \rightarrow N\pi, N\pi\pi \]
- Goal: Understand \( N\pi, N\pi\pi \) spectrum up to \( m_\Delta \)
$N \rightarrow \Delta$ Form Factors

- $N \rightarrow \Delta$ transition factorizes as

$$
\langle \Delta(p', s')|A^3_\mu|N(p, s)\rangle = i \sqrt{\frac{2}{3}} \left( \frac{m_\Delta m_N}{E_\Delta(p')E_N(p)} \right)^{1/2} \bar{u}_\Delta \left[ \left( \frac{C^A_3(q^2)}{m_N} \gamma^\nu + \frac{C^A_4(q^2)}{m^2_N} p'^\nu \right) (g_{\lambda\mu}g_{\rho\nu} - g_{\lambda\rho}g_{\mu\nu}) q^\rho + C^A_5(q^2) g_{\lambda\mu} + \frac{C^A_6(q^2)}{m^2_N} q_\lambda q_\mu \right] u_N
$$

- Need to extract $C^A_3$, $C^A_4$, $C^A_5$, $C^A_6$ as functions of $q^2$
Bubble Chamber Fits

\[ \nu_\mu d \rightarrow \mu^- p \pi^+ n \]

\[ \frac{d\sigma}{dq^2} \left(10^{-38} \text{ cm}^2 \text{ GeV}^{-2}\right) \]

Figure credit: E. Hernandez et al., 1001.4416
Extracting Form Factors

- Target: Know all $C_i^A(q^2)$ with few-percent uncertainty
- Experimental data have large ($\gtrsim 15\%$) statistical uncertainties
- Additional systematic uncertainties from deuteron binding
- 4 form factors – need to measure various kinematics, polarizations
- Models of QCD $\rightarrow$ relations among $C_i^A$
- Uncontrolled systematics from model assumptions

$$C_5^A \propto Q^2 C_6^A$$

$$C_3^A \sim 0$$

$$C_4^A \sim -\frac{C_5^A}{4}$$
Lattice QCD

- Discretize equations of QCD on 4-dimensional space-time lattice
- Finite box required (extrapolate $L \to \infty$ at end)
- Non-perturbative (works for large coupling constants)
- First-principles, model-independent solution to hadronic physics
- Only input = Lagrangian of QCD ($\{m_q\}, \alpha_s$)
- Systematically controllable errors (A. Kronfeld, Mon. 1:30 pm)

Image credit: JICFuS, Tsukuba
Brute Force Is The Last Resort of the Incompetent

Image credit: Oak Ridge National Laboratory
Finite Volume Spectrum

\[ E_{N\pi} = \sqrt{m_N^2 + p^2} + \sqrt{m_\pi^2 + p^2} \]

\[ p \in 2\pi\mathbb{Z}^3/L \]

- Parities: \( P(N) = P(\Delta) = 1 \), \( P(\pi) = -1 \)
- \( P(N\pi) = -1 \), needs momentum to match \( P(\Delta) \)
- \( P(N\pi\pi) = 1 = P(\Delta) \) even at \( p = 0 \)
Matching to Many-Body

Two main options to match to nuclear EFT:

1. Lellouch-Lüscher formalism (Lellouch and Lüscher, hep-lat/0003023; Briceño et al., 1706.06223)
   - Extrapolate lattice results to infinite volume
   - Relies on extracting phase shifts from FV spectrum
   - Worked out in 2-particle case, progress in 3-particle case but not completely resolved (Hansen and Sharpe, 1901.00483)

2. Finite-volume EFT matching
   - Perform nuclear EFT calculations within finite box
   - Can then match directly to lattice QCD calculation
Excited State Contamination

- Determine particle energies from correlation functions
  \[ C_2(t) = \langle \mathcal{O}(t)\mathcal{O}^\dagger(0) \rangle = \sum_n \frac{Z_n^2}{2E_n} e^{-E_n t} \]
  - Sum runs over all states with same quantum numbers as \( \mathcal{O} \)
  - At large Euclidean time, dominated by ground state
  \[ C_2(t) \rightarrow \frac{Z_0^2}{2E_0} e^{-E_0 t} \]
  - Cannot take \( t \rightarrow \infty \) due to noisy data
  - At moderate \( t \), can have contamination from higher-energy states
Importance of $N\pi$ State

- Need to compute $N \rightarrow N$ matrix elements for form factors
- $N\pi$ only separated from $N$ by $m_\pi$ (if $L = \infty$)
- $N\pi$ final state suppressed by $e^{-m_\pi t}$
  - $e^{-m_\pi t} \approx 0.25$ if $t = 2$ fm
  - Overlap factors $Z_n$ can be large for $N\pi$ states
- Form factors can be wrong due to contamination unless $N\pi$ state accounted for (R. Gupta, Mon. 2:40 pm)

Figure credit: C. Alexandrou et al., 2011.13342
Variational Methods

- Interpolating operator $\mathcal{O}$ for state not unique
- Can take many operators $\{\mathcal{O}_i\}$ with same quantum numbers
- $\mathcal{O}_i$ will have different overlaps to ground, excited states $\rightarrow$ different contamination
- Optimal linear combination of $\mathcal{O}_i$ has minimal contamination
  - Found via generalized eigenvalue problem (GEVP)

Figure credit: G. Silvi et al., 2101.00689
Motivation

Lattice QCD

Methodology

Results

△ Resonance on Lattice

Figure credit: G. Silvi et al., 2101.00689
Importance of $N\pi\pi$ State

- Useful to remove states above energy level of interest
- Essential to understand those below level of interest
- $m_N + 2m_\pi < m_\Delta$ (1.21 GeV < 1.23 GeV)

Figure credit: C. Alexandrou et al., 2307.12846
Methodology

- Want to compute
  \[ \langle N(\tau)\pi(\tau)\pi(\tau)\bar{N}(0)\bar{\pi}(0)\bar{\pi}(0) \rangle \]

- Naïvely requires all-to-all propagators (timeslice-to-self $\pi$ loops)

- Cost: $O(V^2)$ for inversions, $O(V^6)$ for contractions

- Contraction cost reduced to $O(V^3)$ by computing sequential propagators through $\pi$

- Contraction cost further reduced by eightfold by parity projecting all quarks
Propagator Sparsening

- Nearby sites on lattices highly correlated
- Can compute propagators on coarse grid without much loss of information (W. Detmold et al., 1908.07050; Y. Li, 2009.01029; S. Amarasinghe et al., 2108.10835)
  - In momentum space, corresponds to incomplete Fourier projection
- Loss of information further reduced by Gaussian smearing
- Sparsening by factor of $f$ in each direction reduces inversion costs by $f^3$ and seqprop construction cost in contractions by $f^9$
Ensemble Details

- $a = 0.15$ fm, $L = 4.8$ fm, $m_{\pi,p} = 135$ MeV HISQ ensemble from FNAL/MILC
- Clover fermions used for valence quarks ($m_{\pi,\text{val}} \approx 170$ MeV)
- Gradient flow smearing used to reduce mixed-action artifacts
- Propagators computed using QUDA multigrid inverter (M. Clark et al., 0911.3191, 1612.07873) on $8^3$ grid on each timeslice
- Gaussian smearing applied at source and sink
Contraction Code

- Standalone code to read in propagators from QUDA and compute $N\pi$, $N\pi\pi$ contractions
- Designed to support CPU and GPU targets
- Leverages MKL BLAS or cuBLAS for sequential propagator construction
- Performs all Wick contractions from these sequential propagators
$N\pi$, $p = 0$
$N\pi\pi, \ p = 0$

![Graph showing the effective mass squared as a function of the reduced time $t/a$.](image)

- **$N\pi\pi$, $I = 1/2$**
- **$N\pi\pi$, $I = 3/2$**
- **$N\pi\pi$, $I = 5/2$**

The graph displays data for different channel quantum numbers, with error bars indicating the uncertainty in the measurements.
$N_\pi$, $l = 1/2$, $|p| = 1$
Conclusions

- $N \rightarrow \Delta$ and therefore $N \rightarrow N\pi$, $N\pi\pi$ axial transitions needed for DUNE
- Spectroscopy calculations – first step in producing good $N\pi(\pi)$ interpolators
- Future plans:
  - Increased statistics
  - GEVP to study states in same parity/isospin sectors
  - Finite-volume phase shifts to study $\Delta$ resonance
  - 3-point functions for axial/vector form factors
Isospin Splitting in $N\pi$

\begin{align*}
I = \frac{3}{2} & \quad am_{eff} \\
I = \frac{1}{2} & \quad am_{eff}
\end{align*}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{isospin_splitting}
\caption{Isospin splitting in $N\pi$.}
\end{figure}
Resonance on Lattice

Figure credit: G. Silvi et al., 2101.00689