Nuclear Physics from Lattice QCD
Higher Partial Waves and Parity Violation

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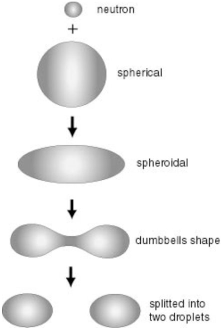
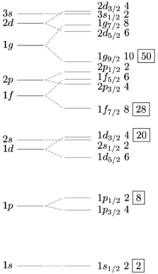
- Historically, Nuclear Physics **relied on Models**

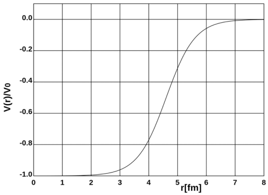
Liquid Drop



Shell



Mean Field

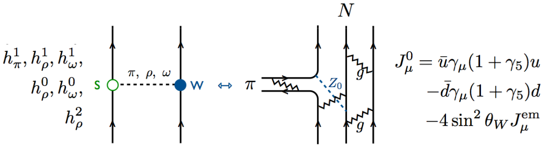


- However, we know that **QCD is the correct way to describe NP**

$$\mathcal{L}_{\text{QCD}} = \bar{\psi}(i\not{D} - m)\psi - \frac{1}{4}\text{Tr}(F^2)$$

Introduction II

- Using QCD as foundation for NP allows us to **relate nuclear ME to fundamental parameters of the SM Lagrangian**



- NP is int the (very) low energy regime of QCD $\Rightarrow$ **non-perturbative (difficult)**
- Lattice QCD: **numerical method for solving QCD non-perturbatively**
- **still extremely difficult**:
  - how do we project onto desired states?
  - disentangle signals from closely spaced energy levels (large V)
  - interpret FV results $\Rightarrow$ relate results to continuum physics
- Phenomenology: **nucleon scattering finely tuned** (Deuteron binding energy, di-neutron wave function)
- Provide input for EFT and models

Lattice QCD

- straightforward method to **solve QCD non-perturbatively with quantifiable uncertainties**
- based on stochastic sampling of (euclidian) QCD path integral

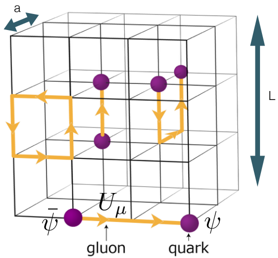
$$\langle\mathcal{O}\rangle_E = \int \mathrm{D}U\mathrm{D}\psi\mathrm{D}\bar{\psi}\,\mathcal{O}(U,\bar{\psi},\psi)\,e^{-S_g[U]-S_f[U,\bar{\psi},\psi]}$$

- solved by defining theory on a 4D lattice

$$\langle\mathcal{O}\rangle_E \approx \frac{1}{N}\sum_N \mathcal{O}(U,\bar{\psi},\psi)$$

- remove discretization and finite volume effects by performing **continuum- and infinite volume limit**

$$a \to 0, \quad L \to \infty$$



Correlation Functions

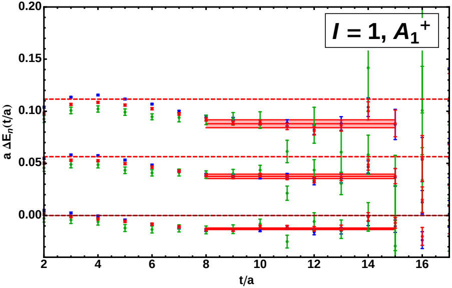
- correlation functions are **important observables**

$$C_N(t-t_0) \equiv \langle N_\mu(t)\bar{N}^\mu(t_0)\rangle \sim \sum_n |Z_n|^2 e^{-E_n^{(N)}(t-t_0)}$$

- Z_n: **overlap factors**, depending on the interpolating operator, e.g.

$$N^\mu(\mathbf{x},t) = \epsilon^{abc}\left(d_a^\mu u_b^\alpha \Gamma_{\alpha\beta} d_c^\beta\right)(\mathbf{x},t)$$

- $E_n^{(N)}$: **energy of state** n, extract from effective mass $-\partial_t \ln C(t-t_0)$



- correlation functions allow to compute masses, decay constants, **scattering observables**, etc..

Extracting Scattering Information

- Maiani-Testa: **you cannot do scattering in Lattice QCD**!
- Reason: in an euclidian space-time and infinite volume, there are
  - no asymptotic in- and out-states $\Rightarrow$ **phase information is lost**

$$\langle \pi\pi | \mathcal{O}_{\mathsf{EW}} | K \rangle_E = \frac{1}{2} \left[\langle \pi\pi | \mathcal{O}_{\mathsf{EW}} | K \rangle + \langle K | \mathcal{O}_{\mathsf{EW}} | \pi\pi \rangle \right]$$

  - ground state domination for large $t \Rightarrow$ **non-physical amplitudes dominate over kinematically allowed**

$$\langle \pi(\mathbf{p})\pi(-\mathbf{p}) | \mathcal{O}_{\mathsf{EW}} | K(0) \rangle \stackrel{t\to\infty}{\longrightarrow} \langle \pi(0)\pi(0) | \mathcal{O}_{\mathsf{EW}} | K(0) \rangle$$

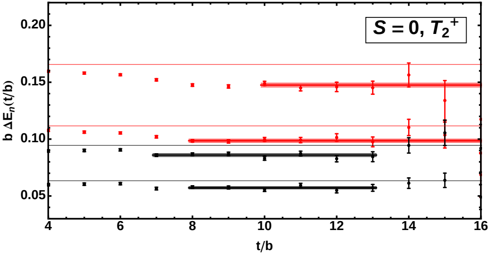
- Lüscher says: yep, you are right, **but why not keeping V finite**?
  (Lüscher [Commun.Math.Phys.105], [Nucl.Phys.B339])
  - energy levels are discrete in FV
  - energy shifts wrt. non-interacting system encode scattering information
- **Lüscher's formalism allows to relate FV spectra to scattering phase shifts**

Lüscher's Finite Volume Method Cookbook I

- **compute correlation functions** (interacting and non-interacting)

$$C_{NN}(t-t_0) \equiv \langle N(\mathbf{p})N(-\mathbf{p})\bar{N}(\mathbf{x}_0)\bar{N}(\mathbf{y}_0)\rangle$$
$$C_{N}(t-t_0) \equiv \langle N(\mathbf{p}=0)\bar{N}(\mathbf{x}_0)\rangle$$

- extract energy difference ΔE from effective mass plateau of C_{NN}/C_N^2



- evaluate **quantization condition** $\left(p^2 = (\Delta E/2 + m_N)^2 - m_N^2\right)$

$$p \cot\delta(p) = \frac{1}{\pi L} S\left(\left(\frac{pL}{2\pi}\right)^2\right), \; S(\eta) = \lim_{\Lambda\to\infty}\left[\sum_{\mathbf{j}<\Lambda}\frac{1}{|\mathbf{j}|^2-\eta^2} - 4\pi\Lambda\right]$$

Lüscher's Finite Volume Method Cookbook II

- But: **simple expression relies on absence of coupled channels**
- in real life **coupled channels exist**
  $\Rightarrow$ Deuteron most prominent example (mixing of ${}^3D_1$ with ${}^3S_1$)
- even worse: **unphysical PW mixing occurs due to breaking of RI**
  $\Rightarrow$ 1-to-1 correspondence between energy levels and phase-shifts lost
- irreps of discrete lattice symmetry group O_h cannot be mapped 1-to-1 to irreps of continuous $SO(3)$ continuum symmetry group
- what shall we do?
  - physical angular momentum $\Rightarrow$ **cubic irreducible representations**
  - compute energy levels of states in **new basis**
  - **disentangle PW mixing employing modified QC**
- scalar QC turns into determinant equation

$$\text{det}[\mathcal{M}^{-1} + \delta\mathcal{G}^V] = 0$$

- **very difficult to evaluate**

Cookbook Recipe

- create NN operator with orbital angular momentum and spin $\ell,\, m_\ell,\, s,\, m_s$
- use CG coefficients to translate them to total angular momentum "quantum numbers" $j,\, m_j$
- **subduce** obtained operators on to lattice irreducible representation
  Dudek et al. [1004.4930]

$$\mathcal{O}_{\Lambda,\mu} = \sum_{j,m_j} \mathrm{CG}(\Lambda,\mu; j, m_j)\, \mathcal{O}_{j,m_j}$$

  to **obtain interpolating operator with quantum numbers** Λ, μ
- extract relevant energy levels and solve e.g. (Briceno [1305.4903])

$$\det\left[\begin{pmatrix} \frac{\mathcal{M}_{1,D}}{\det \mathcal{M}_1} & -\frac{\mathcal{M}_{1,SD}}{\det \mathcal{M}_1} & 0 \\ -\frac{\mathcal{M}_{1,SD}}{\det \mathcal{M}_1} & \frac{\mathcal{M}_{1,S}}{\det \mathcal{M}_1} & 0 \\ 0 & 0 & \mathcal{M}_{3,D}^{-1} \end{pmatrix} + M_N c_{00}(p^2; L)\, \mathbf{1} \right.$$
$$\left. + \frac{M_N}{p^4} c_{40}(p^2; L) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \frac{2\sqrt{6}}{7} \\ 0 & \frac{2\sqrt{6}}{7} & \frac{2}{7} \end{pmatrix}\right] = 0$$

- **requires parametrization of** $\mathcal{M}$ (e.g. ERE)

Scattering in Higher Partial Waves from Lattice QCD

Interpolating Operators I

- we want to assess parity even **and odd** PW $\Rightarrow$ anti-symmetric WF and thus involved operators needed (Luu, Savage [1101.3347])
- a) create **non-local operators** with ℓ, m_ℓ, s, m_s QN

$$\begin{aligned}\langle \mathbf{x}_0 | \ell, m_\ell; s, m_s \rangle \equiv & \left(\bar{N}\bar{N}\right)^{m_\ell, m_s}_{\ell, s}(\mathbf{x}_0) \\ = & \sum_{\{\Delta\mathbf{x}\},\alpha,\beta} Y_\ell^{m_\ell}\left(\widehat{\Delta\mathbf{x}}\right) \cdot \bar{N}_\alpha(\mathbf{x}_0 + \Delta\mathbf{x})\bar{N}_\beta(\mathbf{x}_0) \cdot \Gamma^{s,m_s}_{\alpha\beta}\end{aligned}$$

- b) **project onto total angular momentum** using CG coefficients

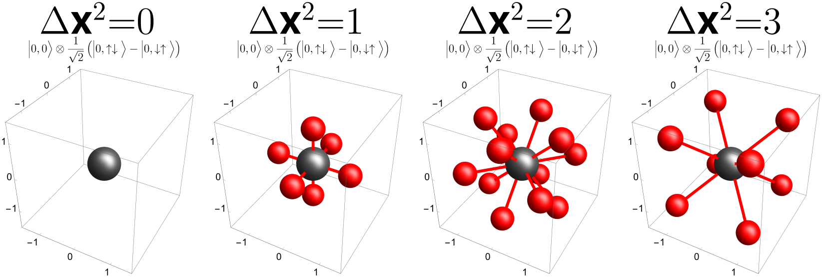
$$\langle \mathbf{x}_0 | j, m_j \rangle = \sum_{\ell, m_\ell, s, m_s} \mathrm{CG}(j, m_j; \ell, m_\ell; s, m_s) \left(\bar{N}\bar{N}\right)^{m_\ell, m_s}_{\ell, s}(\mathbf{x}_0)$$

- c) **subduce** result onto cubic irreps (Dudek et al. [1004.4930])

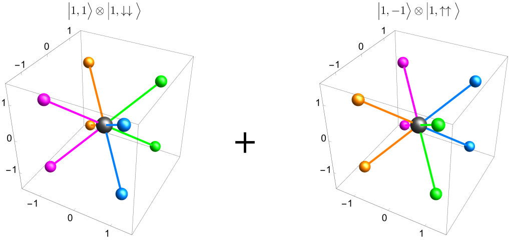
$$\langle \mathbf{x}_0 | \Lambda, \mu \rangle \equiv \left(\bar{N}\bar{N}\right)^{\mu}_{\Lambda}(\mathbf{x}_0) = \sum_{j, m_j} \mathrm{CG}(\Lambda, \mu; j, m_j) \langle \mathbf{x}_0 | j, m_j \rangle$$

Interpolating Operators II

- reasonable choices for $\Delta\mathbf{x}^2$ ($A_1^+ \sim {}^1S_0$)



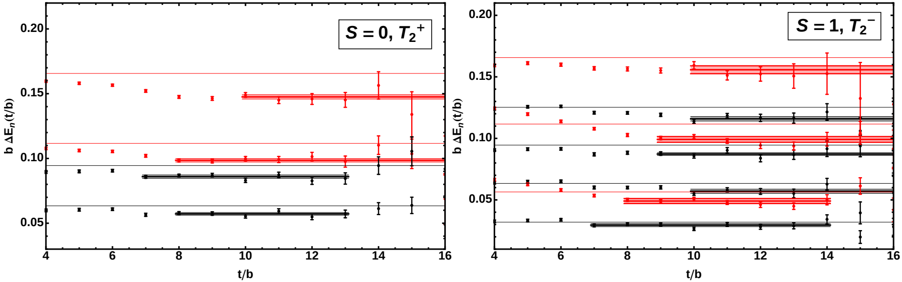
- example for $\Delta\mathbf{x}^3=3$ in T_1^- (${}^3P_1, {}^3F_3$)



Calculation Details

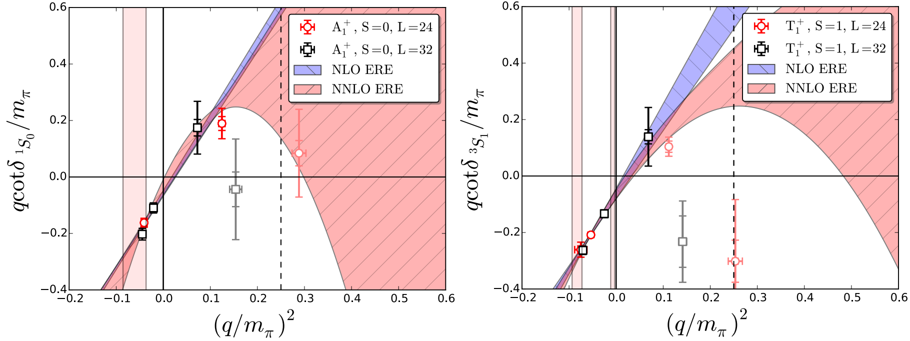
- calculations performed at ~ 800 MeV **pion mass**, to reduce noise in correlation functions
- ensemble overview: isotropic clover, $a \sim 0.145$ fm, 3900 configs for $24^3 \times 48$ and 1029 configs for $32^3 \times 48$ (HadSpec)
- 78K measurements each on $L = 24$ ($n_{\text{sources}} = 20$) and $L = 32$ ($n_{\text{sources}} = 75$)
- 8 displacements per source with on-axis distances 3 (24^3) and 5 (32^3) respectively ($\Delta\mathbf{x} \propto (\pm 5, \pm 5, \pm 5)$)
- choose cms $\mathbf{x}_0$ (quasi-)randomly $\Rightarrow$ approximate projection to cms-momentum $\mathbf{P} = 0$
- use momentum-space sinks with rel. momentum $\mathbf{p}^2 \in \{0, 1, 2, 3, 4, 5, 6\}$ (and $\mathbf{P} = 0$) $\Rightarrow$ **obtain multiple energy levels**
- unfortunately: have to **neglect PW mixing for now**
- all calculations were performed at LLNL (Surface/Edge, VULCAN) and NERSC (Edison)

Spectrum



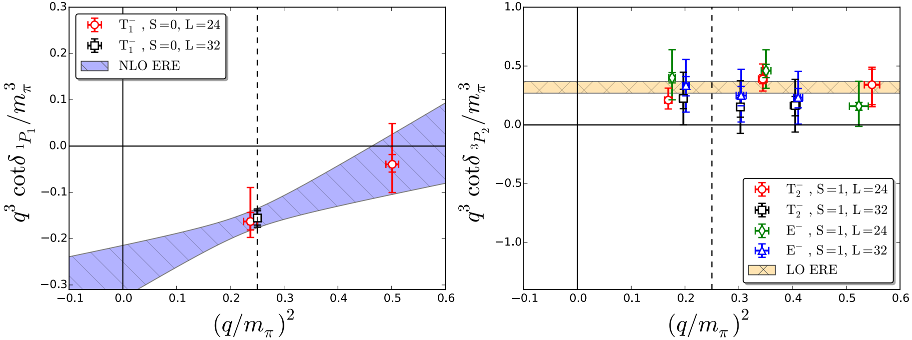
- clean separation between energy levels

S-Wave



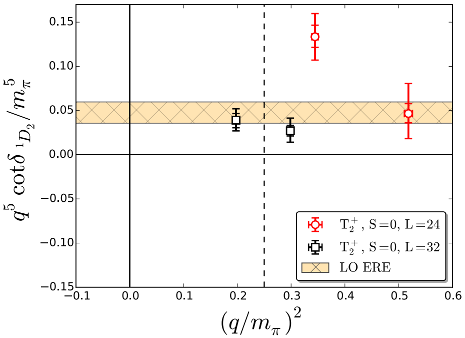
- fainted points show presumably **significant contributions from PW mixing** $\Rightarrow$ remove from fit
- agrees with previous results from NPLQCD (Beane et.al. [Phys.Rev. D87], [Phys.Rev. C88])

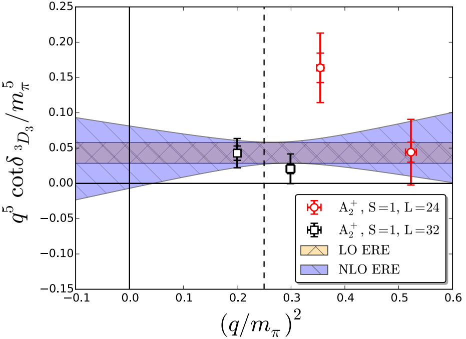
P-Wave



- clean signals

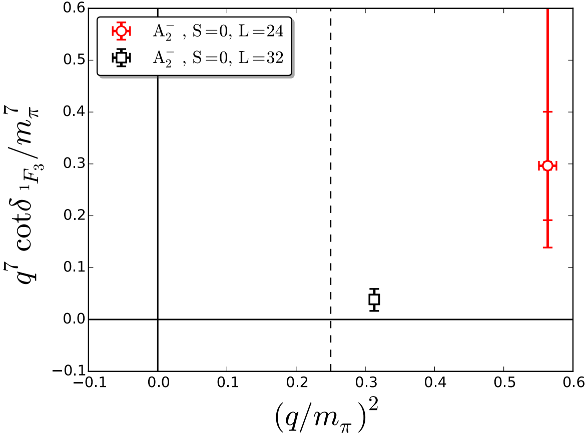
D-Wave





- clean signals, **but need more points for constraining ERE fit**
- potentially large PW mixing ⇒ **add more points for different source geometry** to obtain better contraints

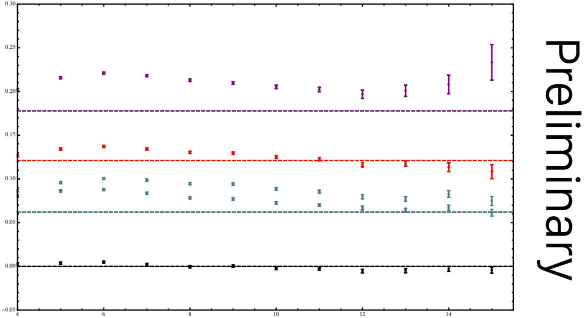
F-Wave



- extremely tough:
  - **only one state per volume** couples to this channel
  - **this state has p**$^2\!=\!3 \Rightarrow$ possible higher state contaminations and mixing
- ok, we should stop here
- **we got a signal however**

Summary Higher Partial Wave Calculation

- we **computed S-, P-, D- and F-wave contributions** to two-nucleon scattering
- sophisticated sources/sinks give **multiple, clearly separated energy levels** in most channels
- note: unclear how PW mixing (physical and unphysical) affects our results
- we will **investigate coupled channels in a forthcoming study**
- calculation for smaller pion mass is underway



- **match results to effective theories** (e.g. HOBET)

Nuclear Parity Violation from Lattice QCD

Motivation I

- GWS model of electroweak interaction is huge success
- **flavour changing charged current** is well understood from precision measurements in collider experiments:

$$J_\mu^+ = \cos\theta_C\, \bar{u}\gamma_\mu(1+\gamma_5)d + \sin\theta_C\, \bar{u}\gamma_\mu(1+\gamma_5)s$$

$$H_{\text{ew-eff}}^{CC,\Delta S=0} = \frac{G_F}{\sqrt{2}} J_\mu^{+\dagger} J^{+\mu} + \text{h.c.}$$

  - vector boson d.o.f. are integrated out
  - effective Hamiltonian has isospin changing $\Delta I{=}0,1,2$ interactions
  - $\boldsymbol{\Delta I{=}1}$ **component is suppressed** by $\tan^2\theta_C \approx \sin^2\theta_C \sim 0.04$
    $\Rightarrow \Delta I{=}0,2$ transitions strongly dominate EW CC interaction ($\Delta S{=}1$)
- $\Delta I{=}1$ **interaction is good probe for parity violating neutral current/hadronic neutral current (HNC)**

Motivation II

- **flavour conserving neutral current** is given by

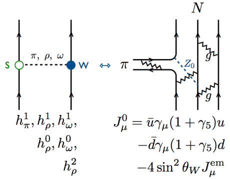
$$J_\mu^0 = \bar{u}\gamma_\mu(1+\gamma_5)u - \bar{d}\gamma_\mu(1+\gamma_5)d - 4\sin^2\theta_W J_\mu^{\text{em}}$$

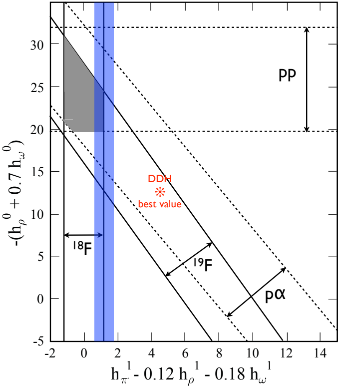
$$H_{\text{ew}-\text{eff}}^{NC} = \frac{G_F}{2\sqrt{2}} J_\mu^{0\dagger} J^{0\mu} + \text{h.c.}$$

  - Effective Hamiltonian generates $\Delta I{=}0,1,2$ interactions
  - no perturbative argument for enhancement/suppression of some components
  - **measure HNC in $\Delta I{=}1$, $\Delta S{=}0$ processes**
- hard to measure in collider experiments because it allows no FC
- **HNC least constrained observable in the Standard Model**
- nuclear systems perfect testbed for studying HNC
- challenge: EW effects suppressed by $G_F F_\pi^2 {\sim} \mathcal{O}(10^{-7})$ w/ respect to strong interaction

Motivation III

- some systems alleviate that constraint due to nearly-degenerate energy levels w/ opposite parity, but those have large A
  $\Rightarrow$ hard to control systematic uncertainties due to nuclear ME
- small nuclear systems have better controlled systematics
- ongoing experimental effort by NPDGamma at SNS (ORNL), measuring asymmetry in $np \to d\gamma$ with predicted sensitivity of $\mathcal{O}(10^{-8})$
  (Alarcon, Balascuta [Hyperfine Interact. 214, 149])
- **good understanding of QCD corrections is required**





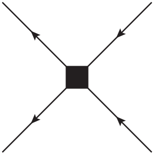
(Haxton, Holstein, Wasem)

Lattice Calculation of NPV

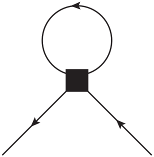
- focus on local isotensor operator

$$\mathcal{O}^{\Delta I=2}(\mathbf{p}{=}0) = \sum_{\mathbf{x},\mu} \left(\bar{q}\gamma_\mu\gamma_5\tau^+ q\right)(\mathbf{x}) \otimes \left(\bar{q}\gamma^\mu\tau^+ q\right)(\mathbf{x})$$

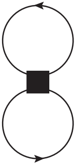
- ME can be related to coupling h_ρ^2
- why not $\Delta I{=}0, 1$?
  - **no disconnected** diagrams (isospin limit)



$\Delta I{=}0,\ 1,\ 2$



$\Delta I{=}0,\ 1$

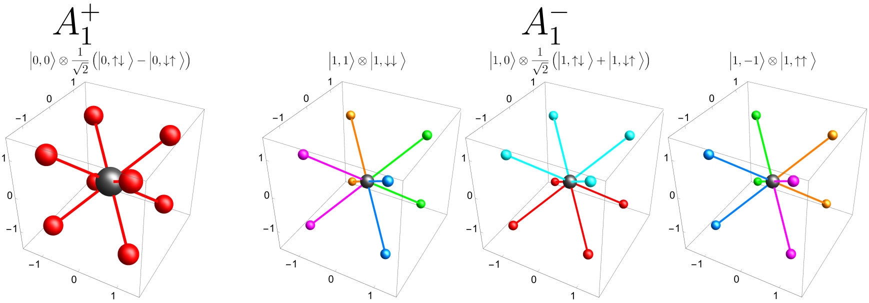


$\Delta I{=}0$

  - **no mixing** under renormalization (in absence of QED)

    (Tiburzi [1207.4996])
- evaluate this operator in $nn \to pp$ channel
  - reduces number of diagrams significantly

- use **local single-nucleon-interpolators** (Basak et al., [hep-lat/050801])
- **corner topology** ($\Delta \mathbf{x}^2 \propto 3$) for A_1^+ ($\sim {}^1S_0$) and A_1^- ($\sim {}^3P_0$)



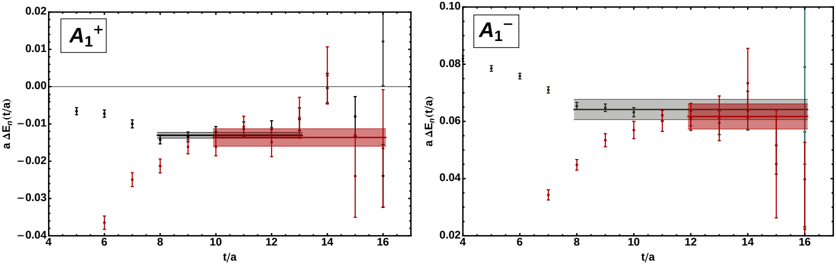
- successfully used in our higher PW nn-scattering calculation

Interpolating Operators II

- optimal sources/sink defined in **p**-space $\Rightarrow$ would **require all-to-all propagators (or stochastic $\mathcal{O}^{\Delta I}$ projection)** $\Rightarrow$ **x**-space sources/sinks
- stochastic projection to zero cms momentum

$$(\bar{N}\bar{N})^{\mu}_{\Lambda}(\mathbf{P}{=}0) \approx \sum_{\{\mathbf{x}_0\}\in\text{QMC(latt)}} (\bar{N}\bar{N})^{\mu}_{\Lambda}(\mathbf{x}_0)$$

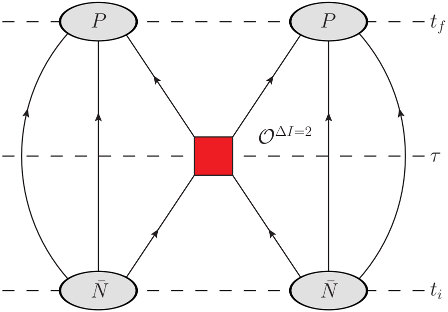
- **x**-space sources/sinks have overlaps with A_1^+ and A_1^- ground states



- **x**-space setup **reduces cost for contractions**

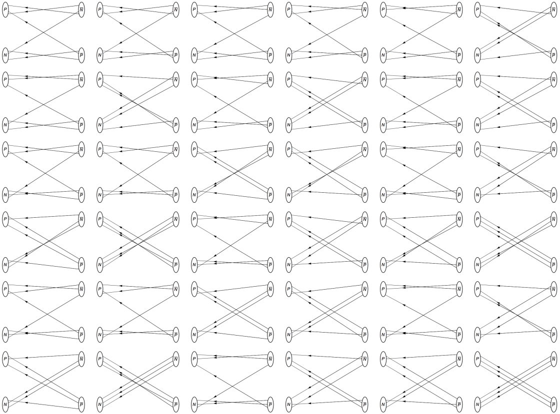
Contractions I

- setup:
  - A_1^+ source at t_i
  - A_1^- sink at t_f
  - τ varies between t_i, t_f
- use unified contraction method at source and sink (Doi, Endres [1205.0585], Detmold, Orginos [1207.1452])
- factor out 4-quark-object and propagators connecting blocks and EW insertion $\Rightarrow$ **complete factorization**
- perform $s=1$ projection at sink and $s=0$ projection at source
- also compute reversed process



Contractions II

- isospin limit: **576 diagrams**
  ⇒ generate contractions and optimized code automatically
- code generator written in Mathematica: converts products of quark bilinears into product of propagators
- convert this expression into code or human readable diagrammatic representation



Calculation Details I

- calculations performed at $\sim$800 MeV **pion mass**, to reduce noise in correlation functions
- ensemble overview: $a\sim 0.145$ fm, 4800 measurements on $24^3\times 48$ lattice and 8×8 displacements per measurement with distance 6, i.e. $\Delta\mathbf{x} = (\pm 6, \pm 6, \pm 6)$
- no renormalization performed yet, but **can be done pertubatively at our requested level of preicsion** (Tiburzi [1207.4996])
- Lellouch-Luscher matching functions for relating finite volume ME to infinite volume counterpart has to be computed

$$\left\langle pp(^3P_1)\mathcal{O}^{\Delta I=2}pp(^1S_0)\right\rangle_{V=\infty} \equiv LL\left(\delta_{^1S_0}, \frac{\partial\delta_{^1S_0}}{\partial E}, \delta_{^3P_0}, \frac{\partial\delta_{^3P_0}}{\partial E}\right)\left\langle pp(^3P_1)\mathcal{O}^{\Delta I=2}pp(^1S_0)\right\rangle_V$$

- we computed phase shifts for nn-scattering in P and S-wave
- all results are **preliminary**

Calculation Details II

- The bare PV amplitude is time-dependent and contains vacuum overlaps (Z-factors) which depend on the interpolating operators
- for removing all of these, compute

$$\begin{aligned} C_{++}(t) &\sim \langle A_1^+(t)|A_1^+(0)\rangle, \\ C_{--}(t) &\sim \langle A_1^-(t)|A_1^-(0)\rangle, \\ C_{-+}(t_f, t, t_i) &\sim \langle A_1^-(t_f)|\mathcal{O}^{\Delta I=2}(t)|A_1^+(t_i)\rangle, \\ C_{+-}(t_f, t, t_i) &\sim \langle A_1^+(t_f)|\mathcal{O}^{\Delta I=2}(t)|A_1^-(t_i)\rangle \end{aligned}$$

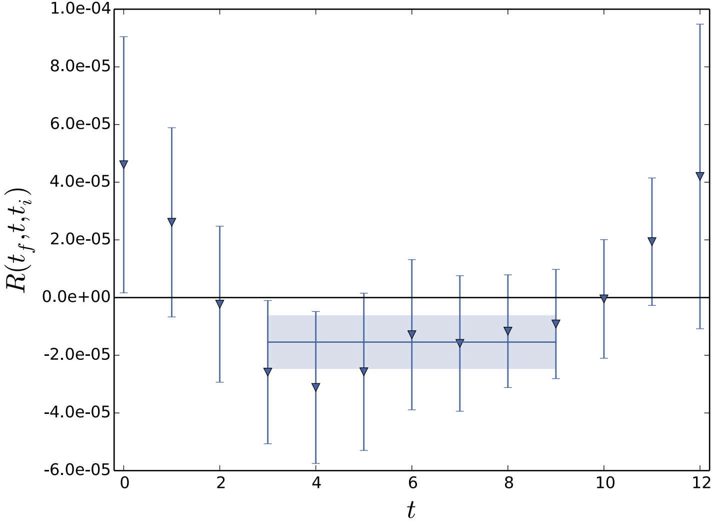
- compute ratio to **cancel overlap factors and energy dependence**

$$R_{-+}(t_f, t, t_i) = \frac{C_{-+}(t_f, t, t_i)}{\sqrt{C_{--}(t_f - t_i)C_{++}(t_f - t_i)}} \sqrt{\frac{C_{--}(t_f - t)C_{++}(t - t_i)}{C_{++}(t_f - t)C_{--}(t - t_i)}}$$

- use asymmetric subtraction to **remove energy injection by** $\mathcal{O}^{\Delta I=2}$

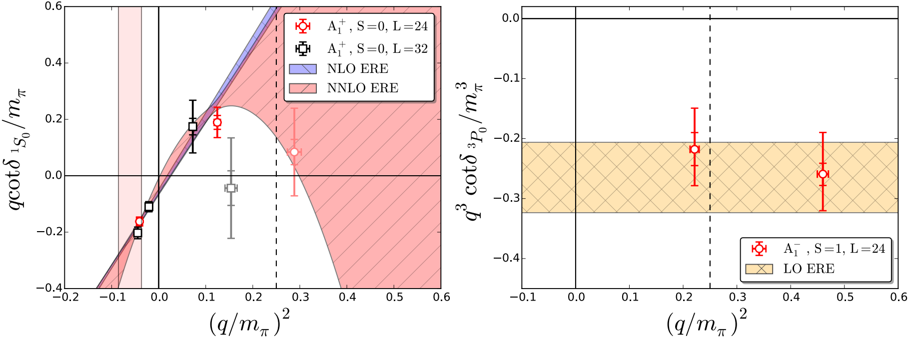
$$R(t_f, t, t_i) \equiv \frac{1}{2}\big(R_{-+}(t_f, t, t_i) - R_{+-}(t_f, t, t_i)\big)$$

Bare Matrix Element



- looks promising and **more statistics on it's way**

Phase Shifts



- **needed for LL factor**
- energy dependence of $\delta_{^1S_0}$ determined
- need to
  - augment statistics for $\delta_{^3P_0}$
  - estimate PW mixing in A_1^-

Summary Nuclear Parity Violation

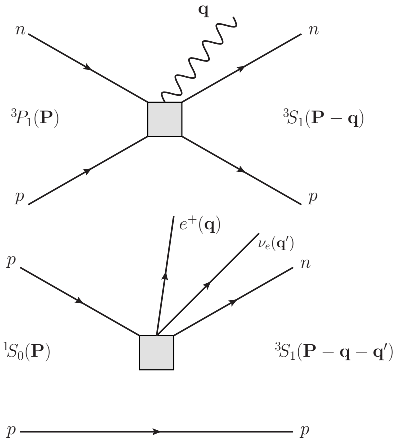
- hadronic neutral current least constrained observable of the SM
- NPDGamma is trying to improve that constraint
  $\Rightarrow$ Lattice QCD can help to improve systematic uncertainties
- we **built framework for and started calculation** of nuclear parity violation in Lattice QCD
- use of non-local interpolating operators necessary
  $\Rightarrow$ **calculation is 160 times more expensive**
- **S- and P-wave strong scattering needs to be fully understood** before serious attempts for computing NPV can be made $\Rightarrow$ we are almost there
- developed automatic code generator to generate optimized code

Outlook Nuclear Parity Violation

- increase statistics and finish calculation of h_ρ^2 at $m_\pi \sim 800$ MeV
- compute LL factor
- investigate possibilities to compute ME for $\Delta I = 1$ (difficult) and $\Delta I = 0$ (very difficult)
- stochastic estimation of disconnected diagrams fits into our decompositionial approach $\Rightarrow$ only minor changes necessary
- use point-split instead of local current (removes divergencies for $a \to 0$)
- exploratory calculations at lighter pion mass are underway

Further Outlook

- **direct calculation** of $np \to d\gamma$ amplitude
- proton-proton-fusion
- double beta decay



- **match lattice results to effective theory**
- exciting times for nuclear physics on the lattice

Thank You