Nuclear Matrix Elements from Lattice QCD

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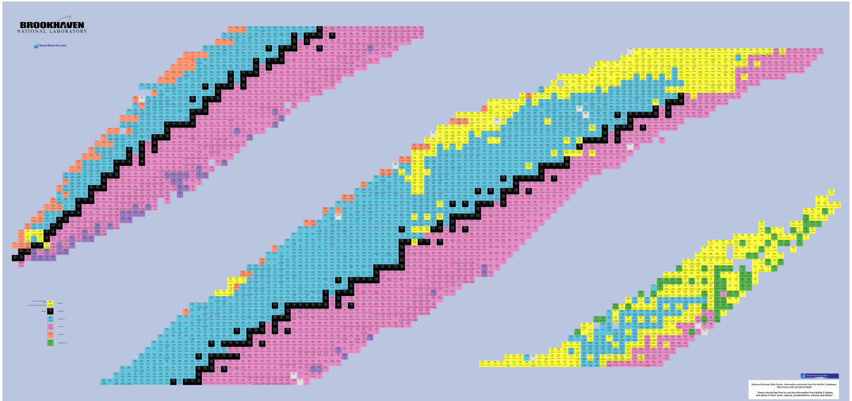
Nuclear Physics

- Nuclear structure and interactions in principle computable from lattice QCD (+ QED)
- In practice, costs are prohibitively high for large A
- Focus on few-nucleon systems ($A \leq 4$), match to EFT descriptions



Historical Overview

- Lattice QCD collaborations (NPLQCD, CalLat, HALQCD) started computing multi-nucleon systems about 15–20 years ago
- Calculations expensive – reduce cost with asymmetric correlation functions (different source/sink)
  - NPLQCD used local operator at source ("hexaquark"), bi-local operator at sink ("dibaryon")
- Correlation functions in LQCD equal to sum of exponentials

$$C(t) = \sum_n A_n e^{-E_n t} \to A_0 e^{-E_0 t}$$

- Effective mass ($-\ln C'(t)$) approaches E_0 from above for symmetric correlators ($A_n \geq 0$) but not for asymmetrics

Challenges

- Signal-to-noise problem: Degrades exponentially as $\exp\left[-A\left(m_N - \frac{3}{2}m_\pi\right)t\right]$
  - Milder at heavy pion masses
- Cost of contractions (naïvely) increases factorially in A
- EFT coefficients often sensitive to difference between nucleus and individual nucleons
  - Binding energies are $\lesssim 1\%$ of mass (0.1% for d)
  - Resolving $E_d - 2m_N$ from 0 requires permille precision on E_d
  - Matrix elements often need $\lesssim 5\%$ errors

Spectroscopy at $m_\pi \approx 800$ MeV (c. 2012)

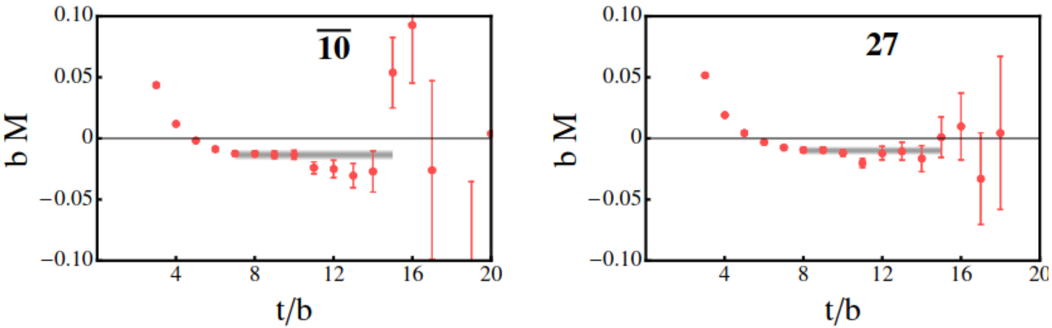
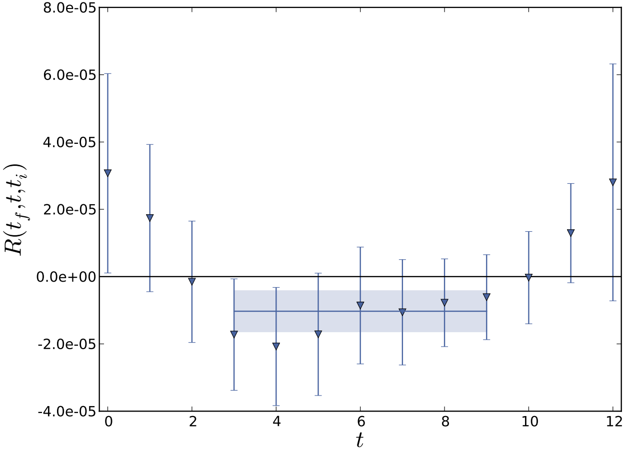


Figure credit: Beane et al. (NPLQCD), PRD 87, 034506 (1206.5219)

- Bound states for *np* and *nn*
- Corroborated by CalLat, conflicting results from HALQCD

Nuclear Parity Violation



$$\langle pp(^1S_0)|\mathcal{O}^{\Delta I=2}|pp(^3P_0)\rangle = -1.0(7)\times 10^{-5}$$

Figure credit: Kurth et al. (CalLat), hep-lat/1511.02260

Proton-Proton Fusion

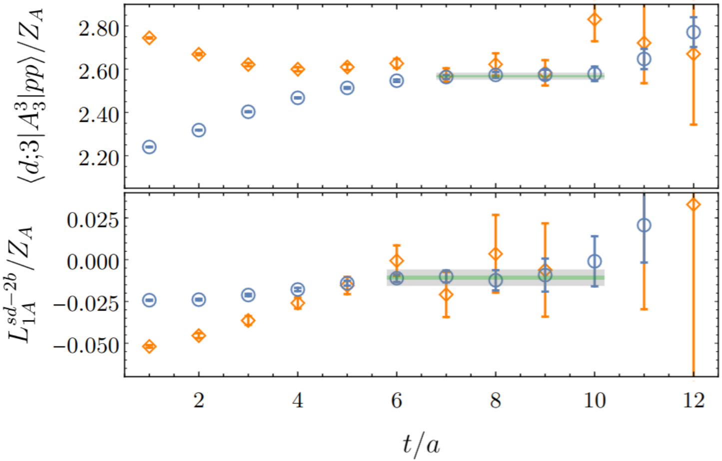
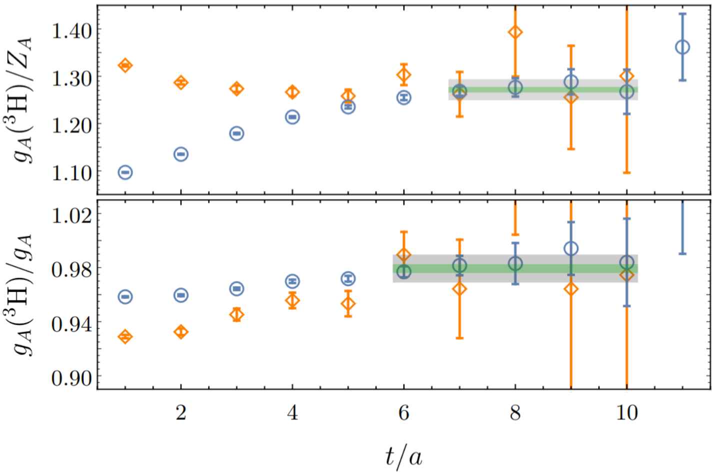


Figure credit: Savage et al. (NPLQCD), PRL 119, 062002 (1610.04545)

Tritium Beta Decay



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Neutrinoful Double-Beta Decay ($2\nu\beta\beta$)

- Rarest observed Standard Model process
- Experimental data used as inputs or tests of nuclear models of $0\nu\beta\beta$ (Engel, Menéndez, RPP 80, 046301 (1610.06548))

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- Computed for $nn \to pp$ transition from lattice QCD (Shanahan et al., PRL 119, 062003 (1701.03456); Tiburzi et al., PRD 96, 054505 (1702.02929))
  - Single lattice spacing and $m_\pi = 800$ MeV
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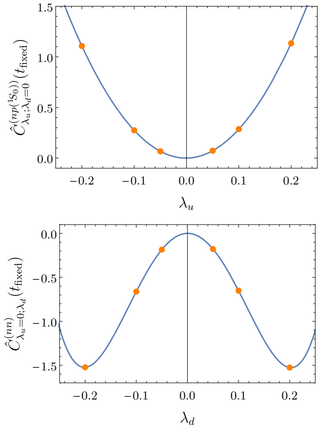
    - Single lattice spacing and $m_\pi = 800$ MeV
    - Computed matrix element to $\sim 2\%$ uncertainty (stat.) and extracted $2\nu\beta\beta$ counterterm
- No intermediate ν prop – weak currents decouple
    - Background field method – quark propagators computed in presence of uniform weak field (Fucito et al., PLB 115, 148; Martinelli et al., PLB 116, 434; Bernard et al., PRL 49, 1076)



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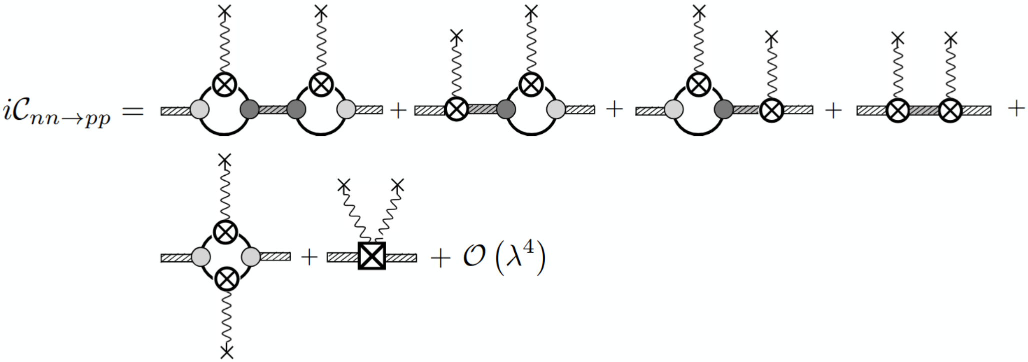

Two-current contact term: $\mathbb{H}_{2,S} = 4.7(1.3)(1.8)$ fm

(Tiburzi et al., PRD 96, 054505 (1702.02929))

Challenges for $0\nu\beta\beta$ in $nn \to pp$

$$C_{nn\to pp} = \sum_{\mathbf{x},\mathbf{y}} \int \frac{d^4q}{(2\pi)^4} \frac{e^{iq\cdot(x-y)}}{q^2} \langle \mathcal{O}_{pp}(t_+) J_\mu(x) J_\mu(y) \mathcal{O}^\dagger_{nn}(t_-)\rangle$$

- Current insertions coupled by ν propagator
  - Cannot use background field method

Davoudi, Detmold, Fu, **AVG**, Jay, Murphy, Oare, Shanahan, Wagman (NPLQCD), PRD 109, 114514 (2402.09362)

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- Signal-to-noise problem in nuclear systems
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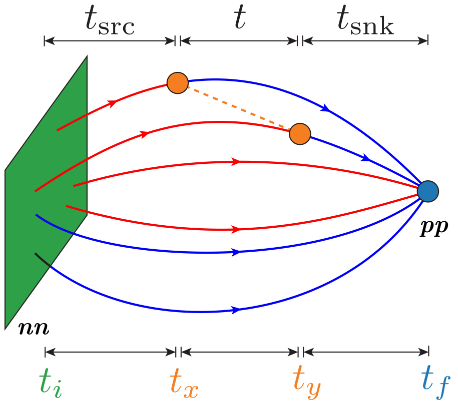
- Complexity of contractions $\propto N_q!$
  - $N_c!^4 N_u! N_d! = 6^4 24^2 \approx 10^6$ contractions needed

Davoudi, Detmold, Fu, **AVG**, Jay, Murphy, Oare, Shanahan, Wagman (NPLQCD), PRD 109, 114514 (2402.09362)

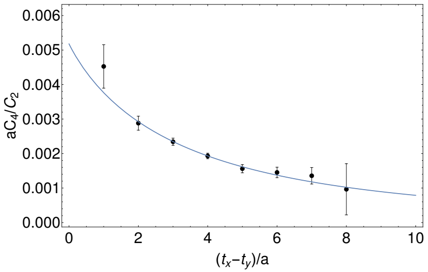
Dinucleon Interpolating Operators

- Dibaryon (bi-local) operators – good signal quality but computationally expensive
    - Require cost reduction techniques, e.g. sparsening (Detmold et al., PRD 104, 034502 (1908.07050), Amarasinghe et al., PRD 107, 094508 (2108.10835)), distillation (Peardon et al., PRD 80, 054506 (0905.2160); Hörz et al., PRC 103, 014003 (2009.11825))
- Hexaquark (point) operators – relatively cheap but significant contamination
- Wall operators – cheap and relatively little contamination but noisiest
- Variational analysis – expensive
- Compromise: Wall source, point sink
    - Improve signal with sparse (4^3) grid at sink



Neutrino Propagator

- Long-distance amplitude contains significant contribution from low-E_ν tail
  - Contribution from separation $t = t_y - t_x$ falls off as t^{-2}
  - Corresponds to large temporal separation between operators
  - Difficult to control (signal-to-noise problem)



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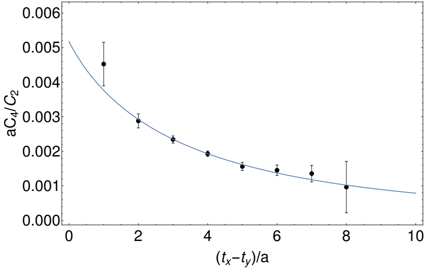


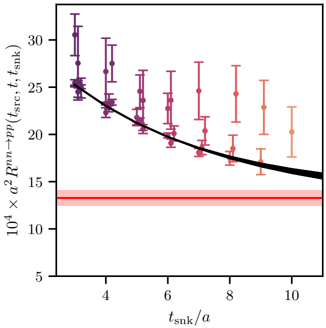
- Solution: Use zero-mode subtracted propagator (Davoudi and Kadam, PRL 126, 152003 (2012.02083))

$$S_\nu(\tau, \mathbf{z}) = \frac{m_{\beta\beta}}{2L^3} \sum_{\mathbf{q} \in \frac{2\pi}{L}\mathbb{Z}^3 \backslash \{\mathbf{0}\}} \frac{e^{i\mathbf{q}\cdot\mathbf{z}}}{|\mathbf{q}|} e^{-|\mathbf{q}||\tau|}$$

  - Contribution falls off exponentially in t
  - Match to zero-mode removed EFT amplitude

Fitting Procedure

- Asymmetric excited state contamination from source and sink
  - More severe from point sink than wall source
- Extrapolate $t_{\mathrm{src}}, t_{\mathrm{snk}} \to \infty$ at given operator separation t



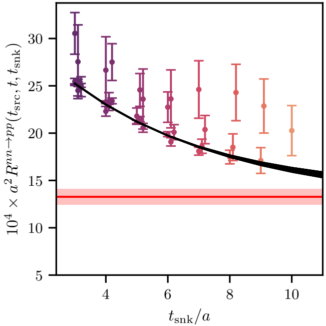
Fitting Procedure

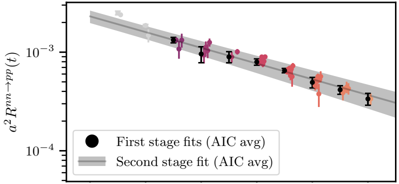
- Asymmetric excited state contamination from source and sink
  - More severe from point sink than wall source
- Extrapolate $t_{\text{src}}, t_{\text{snk}} \to \infty$ at given operator separation t
- Fit t dependence to exponential and integrate:

$$\langle pp|JJ|nn\rangle \propto 2m_{nn} \int_{-\infty}^{\infty} dt\, \frac{C_4(t,\tau)}{C_2(\tau)} = 0.14(3)\ \text{GeV}^2\ \text{(stat.)}$$

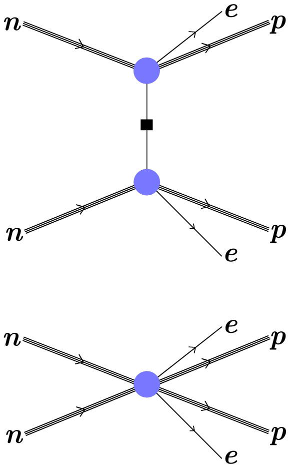
- Need high stats (5M total sources) to resolve dependence on $t, t_{\text{src}}, t_{\text{snk}}$

Thanks to XSEDE/ACCESS, TACC, and RCAC for compute time!





Nuclear EFT for $0\nu\beta\beta$



- Neutrino energy can be hard or soft
- Low-energy contribution factorises into two SM weak currents
  - Can be computed from existing experimental data
- High-energy intermediate ν outside of EFT validity
- Need contact term g_{NN}^{ν} to absorb high-energy behavior (Cirigliano et al., PRC 97, 065501 (1710.01729), PRL 120, 202001 (1802.10097))
- Contact term promoted to leading order in EFT

Extracting g_{NN}

$$\frac{\langle pp|JJ|nn\rangle}{2m_{nn}}\frac{1}{\mathcal{R}(E)\mathcal{M}(E)^2} = (1+3g_A^2)(J^\infty + \delta J^V) - \frac{m_n^2}{8\pi^2}\tilde{g}_\nu^{NN}$$

- $\langle pp|JJ|nn\rangle = 0\nu\beta\beta$ amplitude from LQCD
- $\tilde{g}_\nu^{NN} \propto g_\nu^{NN} =$ EFT counterterm of interest
- Known functions of NN interactions:
  - $\mathcal{M} = NN$ scattering (from effective-range expansion)
  - $\mathcal{R} =$ Lellouch-Lüscher residue
  - $J^\infty =$ contribution from soft ν exchange
  - $\delta J^V =$ FV correction
- Effective range parameters well-determined at physical point but not at $m_\pi \approx 800$ MeV

Kaplan et al., PLB 424, 390 (nucl-th/9801034); Lellouch and Lüscher, CMP 219, 31 (hep-lat/0003023); Davoudi and Kadam, PRD 102, 114521 (2007.15542), PRL 126, 152003 (2012.02083), PRD 105, 094502 (2111.11599)

Generalized Eigenvalue Problem

$$C(t) = \sum_n |Z_n|^2 e^{-E_n t} \to |Z_0|^2 e^{-E_0 t}$$

- With same source and sink, guaranteed to approach from above
  - Harder (but not impossible) to plateau to wrong value
- Can have set of operators $\{\mathcal{O}_i\}$, form matrix of correlators between all combinations at source/sink
- Eigendecomposition of matrix $\to$ lowest-energy state (and higher excitations)
- Operators are typically formed from either nucleon plane waves (NPLQCD) or different eigenmodes of smearing operator (CalLat/CoSMoN)

Deuteron Spectrum ($m_\pi \approx 800$ MeV)

- Deuteron (and dineutron) are attractive ($\Delta E < 0$ in FV)
- Consistent with scattering state ($\Delta E \to 0$ as $V \to \infty$)
- Possible to reconstruct old asymmetric plateau from linear combination of symmetric eigenvalues
  - Also possible to reconstruct these levels from spectrum that includes a bound state
- Calls into question old spectroscopy calculations, possibly also nuclear matrix elements
- Push to redo former calculations with symmetric correlators

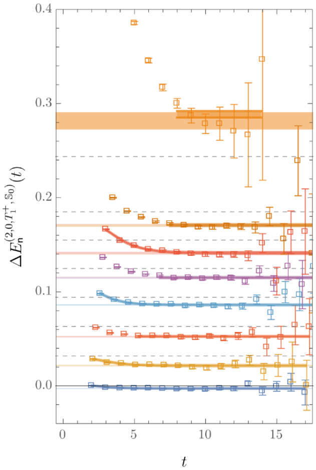


Figure credit: Amarasinghe et al. (NPLQCD), PRD 107, 094508, (2108.10835)

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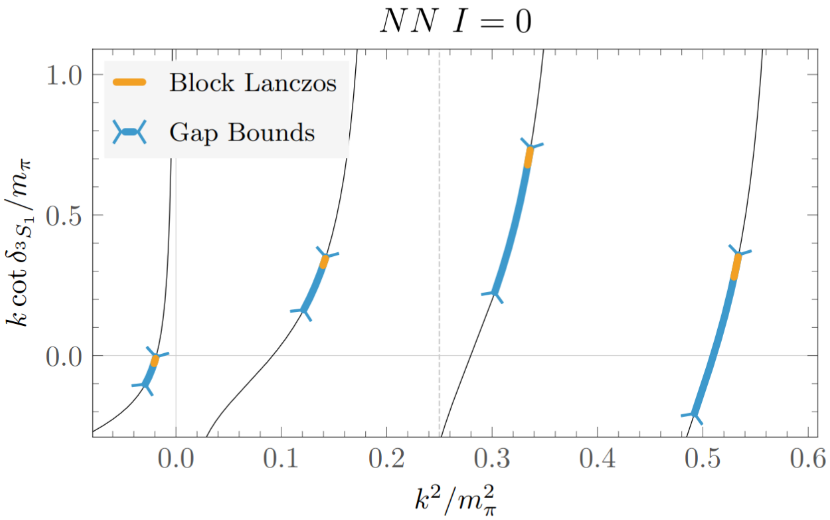
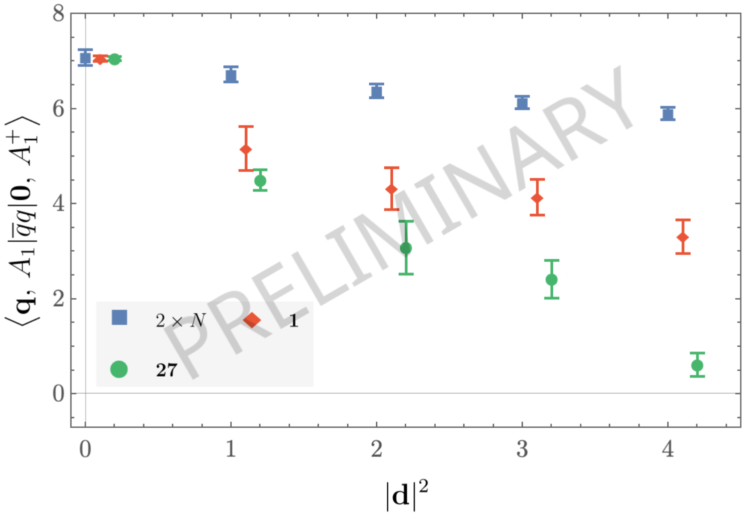
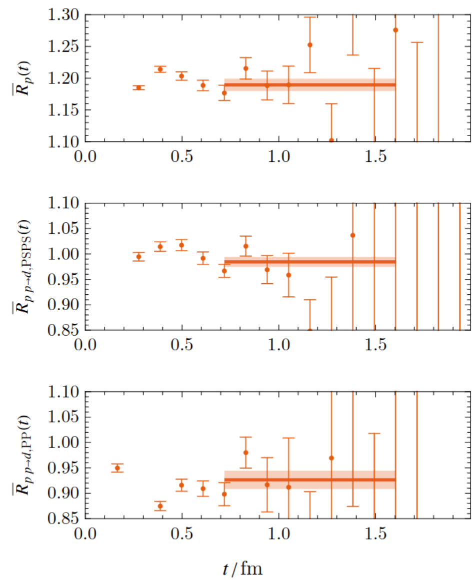


Detmold, **AVG**, et al. (NPLQCD), hep-lat/2601.22272

Scalar Hyperon Form Factors ($m_\pi = m_K \approx 800$ MeV)



Proton-Proton Fusion



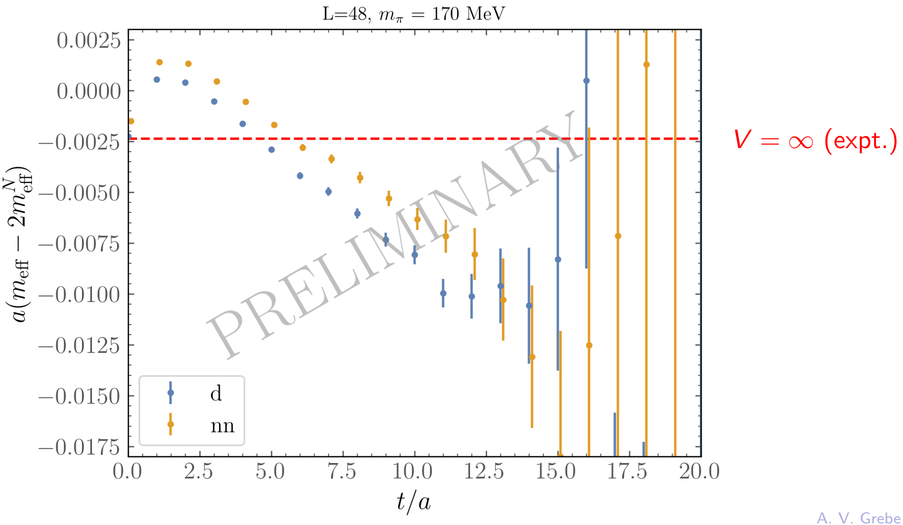
- Performed at $m_\pi \approx 432$ MeV
- Computed with both local (P) and bi-local (PS) operators
  - Consistent at $\sim 2\sigma$ level
- Find $\langle d|\mathcal{J}|pp\rangle/g_A = 0.984(10)$
  - Deviation from 1 $\rightarrow$ measurable effect of 2-body currents

Figure credit: Wang et al., hep-lat/2603.09554

Physical Point Calculations

- − More expensive inversions
- − Exponentially worse signal-to-noise problem
- + Results directly relevant to experiment
- + Scattering parameters/binding energies can be validated experimentally

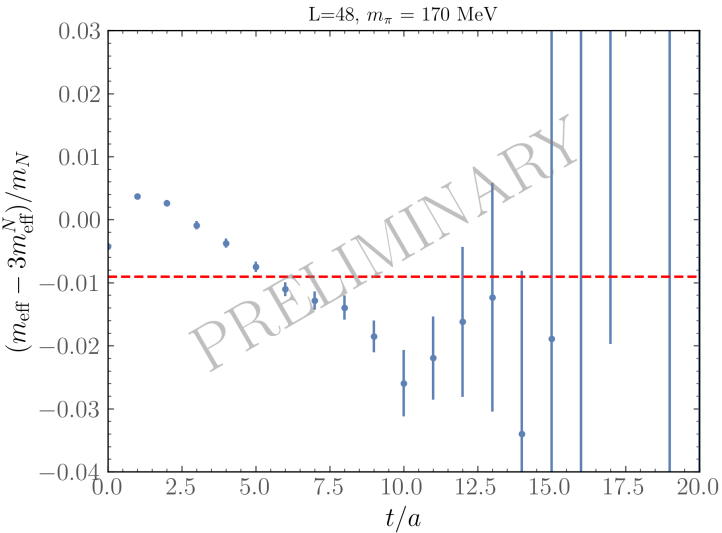
Deuteron Binding Energy



Form Factor Calculation

- Ongoing work to measure vector and axial form factors of deuteron
- Can compute deuteron charge radius, $\sigma(np \to d\gamma)$ as validation
- Can also compute *pp* fusion cross section
- Axial form factor can improve on precision of deuterium bubble chamber experiments
  - Needed for predictions of neutrino-nuclear interactions for DUNE

Triton Binding Energy



$V = \infty$ (expt.)

Double-Beta Decay

- Want to repeat double-beta decay calculation with symmetric interpolating operators (and physical m_π)
- Difficulty: Bi-local interpolators expensive, even with sparsening
- Must integrate operator insertions over full volume (not V_s) or use stochastic estimator (noisy)
- Naïve cost: $O(V_s^4 V^2)$
- Can reduce this to $\tilde{O}(V_s^3 V)$ with sequential blocks and FFTs
    - Expensive but feasible in next couple years

Major Questions

Lattice QCD provides a first-principles, nonperturbative method to obtain EFT coefficients

- If you could get one number from LQCD, what would it be?
  - Pion mass dependence
  - Deuteron form factors
  - Double-beta decay ($2\nu\beta\beta$ and $0\nu\beta\beta$)
  - $3N$ systems (^{3}H and nnn)
  - Nucleon-hyperon interactions
- What is the best way to match EFTs/LECs to matrix elements in finite volume?
  - How easy is it to perform EFT calculations in FV?
  - What box sizes are needed? (Contraction costs scale as L^9)

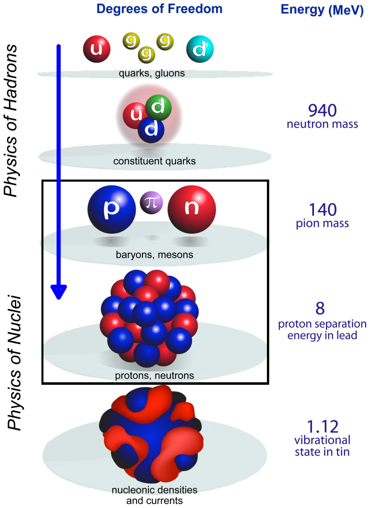
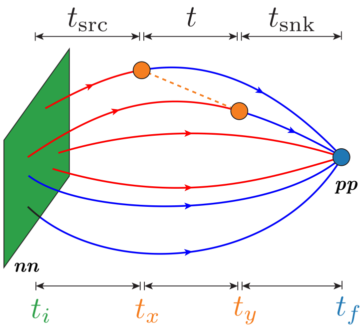


Figure credit: DOE/NSF NSAC (0809.3137)

Reducing Computational Cost

- 4-point function requires nuclear contractions ($O(10^6)$) and convolution over operator positions ($O(V^2)$): $10^6 V^2 \sim 10^{15}$



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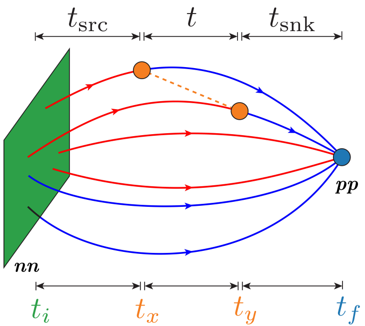

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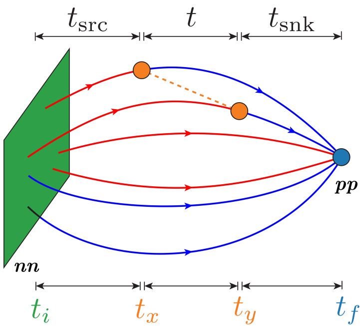

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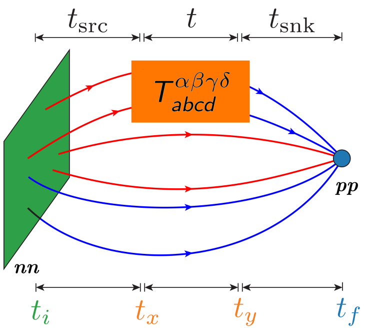
- Decouple operator position sum from nuclear contractions
  - Sum 4-quark tensor $T^{\alpha\beta\gamma\delta}_{abcd}$ over x, y
  - Reduces work to

$$(N_c N_s)^4 V \log V + 10^6 \sim 10^{10}$$



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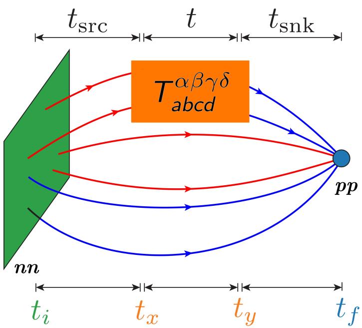

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- Total cost of $O(10^9)$ prop multiplications/sink location/(t_x, t_y, T)
  - ~ 200 CPU core-hours/config