Lattice Calculation of Proton-Proton Fusion Matrix Element

Zi –Yu Wang (王子毓) In collaboration: Xu Feng, Lu-chang Jin, Chuan Liu



Neutrinoless Double Beta Decay



2023 Long Range Plan For Nuclear Science

 \rightarrow LNV process

Significant progress in the pion sector

- @physical pion mass
- Include both LD and SD matrix elements

A. Nicholson et al., PRL121 (2018) 172501

- X. Feng, L. Jin, X. Tuo, S. Xia, PRL122 (2019) 022001
- X. Tuo, X. Feng, L. Jin, PRD100 (2019) 094511
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> But only NPLQCD collaboration has report their pioneering calculations

in nucleon sector $@m_{\pi}=806 \text{ MeV}$

M. Savage et al., PRL 119 (2017) 6, 062002P. E. Shanahan et al., PRL119 (2017)6, 062003Z. Davoudi et al., arXiv: 2402.09362

Anthony Grebe's plenary talk on 8.3

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> A simpler case of 1st order weak transiton: Proton-Proton Fusion

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Proton-Proton Fusion

The Proton-Proton Fusion Process

- Initiating the **proton-proton fusion chain reaction** that provides the dominant energy production mechanism in stars.
- It is related to **neutrino-induced deuteron-breakup reaction**, which is relevant to the measurement of **neutrino oscillations**.
- A first step towards understanding g_A quenching in nuclei.



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Lattice QCD Calculation of Proton-Proton Fusion

- P-P fusion process is hard to access in laboratory, but relatively easy to study by lattice calculation.
- All the techniques we developed here can be used for future double beta decay calculations.

Lattice Calculation

≻ Ensemble (RBC/UKQCD):

- 2+1 flavour **domain wall fermion + Iwasaki** gauge action,
- 162 cfgs, 128 meas./cfg.
- Field Sparsening: Computational cost reduced to 1/8 Y. Li et al., PRD 103 (2021) 1, 014514 W. Detmold, PRD 104 (2021) 3, 034502
- Based on the Qlattice package by Luchang Jin.

β	am _l	$L^3 \times T$	L(fm)	$a^{-1}(\text{GeV})$	$m_{\pi}(\text{MeV})$
2.13	0.01	$24^3 \times 64$	~ 2.65	1.7844(49)	432.2(1.4)

Two-nucleon Interpolators

To bind or not to bind: A question of various two-nucleon interpolators

Lattice 2023: FNAL 3rd August, 2023

NPLQCD, Yamazaki et al., CalLat (2015)



Compact, hexa-quark creation operator

HAL QCD Potential



diffuse - wall source

"Mainz" (Distillation) CoSMoN (stochastic LapH NPLQCD (sparsened momentum)



momentum-space creation & annihilation positive-definite correlation matrix

André Walker-Loud, Lattice 2023

Deep bound di-nucleons

no bound state

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This work: Utilizing in

matrix element calculation

no bound state

Interpolators Comparison

Hexa-quark Interpolators

- All six quarks are located on one site
- Significant excited-state contamination:

$$\sum_{x} N(x)N(x) = \sum_{p} \widetilde{N}(p)\widetilde{N}(-p)$$

Bi-local Interpolators

- Resemble the bi-local nature of NN system
- Suppressed excited-state contamination:

 $\sum_{x,y} N(x)N(y) = \widetilde{N}(0)\widetilde{N}(0)$



Ground-State Determination I: Variational Analysis

> Momentum space op. set $\{O_q | q = 000, 100, 110\}$





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The overlap between GEVP ground state and non-zero momentum state is weak, but it is crucial to the energy difference.

Ground-State Determination II: Multi-state Fit

> Multi-state Fit (t/a = 4 - 16)



Ground-State Determination II: Multi-state Fit



Ground-State Determination II: Multi-state Fit



The (elastic) excited-state contamination is effectively removed by GEVP at large time slices.

≻ Results

- We present the result of variational method as our final result. $(t_i/a = 9, t_f/a = 16)$ $m_p = 1.2649(42) \text{ GeV},$ $m_{1S_0} = 2.5104(90) \text{ GeV},$ $m_{3S_1} = 2.5045(89) \text{ GeV},$ $\Delta_{1S_0} \equiv m_{1S_0} - 2m_p = -19.4(7.9) \text{ MeV},$
 - $\Delta_{^{3}S_{1}} \equiv m_{^{3}S_{1}} 2m_{p} = -25.3(7.6) \,\mathrm{MeV},$

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- The ES contamination from single nucleon interpolator still need to improve in the future calculation.
- Since we already have a GEVP spectrum, let us take a look at their scattering properties.

Scattering Phase Shift of Dineutron/diproton (1S0)

➤ Lüscher's Method: FV spectrum → scattering phase shift

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Consistency check for a physical bound state:



T. Iritani, PRD(2017), 96(3), 034521

Scattering Phase Shift of Dineutron/diproton (1S0)

➤ Lüscher's Method: FV spectrum → scattering phase shift

Consistency check for a physical bound state:



- Current result of 1S0 channel:
 - No deep bound state
 - shallow bound state or scattering state



Scattering Phase Shift of Deuteron (3S1)

- ➤ Lüscher's Method: FV spectrum → scattering phase shift
- Consistency check for a physical bound state:



- Current result of 3S1 channel:
 - No deep bound state
 - Most likely to be a shallow bound state
 - Binding energy: E = 3(6) MeV



Summary of Two-nucleon Spectroscopy

➢ Results

- The **deuteron** is likely to be a **shallow bound state** at $m_{\pi} \sim 432$ MeV.
- The **dineutron/diproton** is a **scattering state** or a **shallow bound state**.
- A conclusive result still needs further improvement in accuracy and systematics.

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- We are confident for the cross-checked GEVP ground state energy.
- The excited state energy is above the inelastic threshold.

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- The excited state energy is above the inelastic threshold.
- As the pion mass continues to decrease, a larger spatial volume will be essential to ensure that the two-nucleon scattering is elastic. This is beyond the scope of this work.

Calculation of Matrix elements

> Methods

• Isospin rotation: Flavour changing process \rightarrow Flavour conserving process

$$\begin{split} \langle p | \mathcal{J}^{+} | n \rangle &= \sqrt{2} \langle p | \mathcal{J}_{3} | p \rangle, \\ \langle d | \mathcal{J}^{+} | p p(^{1} \mathbf{S}_{0}) \rangle &= - \langle d | \mathcal{J}_{3} | p n(^{1} \mathbf{S}_{0}) \rangle. \end{split}$$

- Sequential-source propagator technique: $3pt \rightarrow 2pt$
- Matrix elements extracted from the ratio: $R_3(t) = \frac{C_3(t)}{C_2(t)} = \left(\frac{\langle f | \mathcal{J} | i \rangle}{Z_A}\right)t + \cdots,$

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- Determination of nucleon axial charge

 $g_A = 1.190(10),$

Consistent with RBC/UKQCD (same ensamble): $g_A = 1.186(36)$ Yamazaki, et al., PRL, 100 (2008), 171602



- Applying the same techniques to two-nucleon interpolators: $R_3(t) = \frac{C_3(t)}{C_2(t)} = \left(\frac{\langle f | \mathcal{J} | i \rangle}{Z_A}\right)t + \cdots,$
 - \rightarrow Matrix elements of proton-proton fusion.

$$\frac{\langle d | \mathcal{J} | pp \rangle_{\rm PSPS}}{\sqrt{2}g_A} = 0.984(10),$$

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- A deviation of 3.4σ : The matrix element is less sensitive to excited states than effective mass.
- The excited-state contamination in numerator and denominator is partially cancelled.
- A "Pseudo plateau" may appear.
- Interpolator optimization is important for ME calculation at light pion mass.



Finite Volume Analysis

Two kinds of contributions

- The two-body contribution:
 - Related to the low energy constant $L_{1,A}$
 - The FV correction for $2 \to 1 \to 2$ process: $L^6 \left| \left\langle E_f, L \left| \mathcal{J}^{2B} \left| E_i, L \right\rangle \right|^2 = \mathcal{R}(E_f) W^{2B}(E_i, E_f) \mathcal{R}(E_i),$

Where $R(E_i)$ and $R(E_f)$ are the Lellouch-Lüscher factors



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- The one-body contribution "triangle diagram":
 - Related to nucleon axial charge g_A
 - FV formalism has present by:

- PRD 94 (2016) 1, 013008
- Relativistic: R.A. Briceño & M. T. Hansen
- Non-relativistic: Z. Davoudi & S. V. Kadam

PRD 102 (2020) 11, 114521



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A nice example of charge conservation in FV analysis
 R.A. Briceño et al., PRD 100 (2019) 11, 114505

• If applying the FV formalism of $2 + J \rightarrow 2$ process to charge operator: $\widehat{Q} \equiv \int d^3 \mathbf{x} \mathcal{J}^0(x)$,

$$\begin{split} L^{3} \langle P_{n,f}, L | \mathcal{J}^{\mu} | P_{n,i}, L \rangle &= \mathcal{W}_{L,df}^{\mu}(P_{n,f}, P_{n,i}, L) \sqrt{\mathcal{R}(P_{n,f}, L)\mathcal{R}(P_{n,i}, L)}, \\ \to \langle P_{n}, L | \widehat{Q} | P_{n}, L \rangle &= \frac{\mathcal{F}^{0}(P) + f(0) \left[2EG(P, L) - 2G^{0}(P, L) \right]}{-\partial_{E}\mathcal{M}^{-1}(s) + 2EG(P, L) - 2G^{0}(P, L)} \Big|_{P=P_{n}(L)}, \\ \to \langle P_{n}, L | \widehat{Q} | P_{n}, L \rangle &= Q_{0}, \end{split}$$

• The charge conservation is non-trivially recovered in $2 + J \rightarrow 2$ FV formalism.

 $\rightarrow \langle P_n, L | \widehat{\mathbf{Q}} | P_n, L \rangle = \mathbf{Q}_0,$

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Two key ingredient

- Relation between Lellouch-Lüscher factor and the kinematic function G(P,L)
 - Relation from Ward-Takahashi identity: $\mathcal{F}^{0}(P) = \frac{Q_{0}}{\mathcal{M}^{2}(s)} \frac{\partial}{\partial E} \mathcal{M}(s) = -Q_{0} \frac{\partial}{\partial E} \mathcal{M}^{-1}(s)$
- The charge conservation is non-trivially recovered in $2 + J \rightarrow 2$ FV formalism.

> The one-body contribution of axial current



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• The NR finite volume formalism of proton-proton fusion
$$\begin{split} & L^{6} \left| \left\langle E_{f}, L \left| \left. \mathcal{J}^{1\mathrm{B}} \right| E_{i}, L \right\rangle \right|^{2} & Z. \text{ Davoudi, S. V. Kadam, PRD 102 (2020) 11, 114521} \\ &= g_{A}^{2} \mathcal{R}(E_{f}) \mathcal{R}(E_{i}) \left(\mathcal{M}(E_{f}) \mathcal{M}(E_{i}) F_{1}(E_{i}, E_{f}) + \frac{\mathcal{M}(E_{i}) - \mathcal{M}(E_{f})}{E_{i} - E_{f}} \right)^{2}, \end{split}$$



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L⁶ | \lap{E_f, L | J^{1B} | E_i, L \rangle|^2 Z. Davoudi, S. V. Kadam, PRD 102 (2020) 11, 114521
= g_A^2 \mathcal{R}(E_f) \mathcal{R}(E_i) \left(\mathcal{M}(E_f) \mathcal{M}(E_i) F_1(E_i, E_f) + \frac{\mathcal{M}(E_i) - \mathcal{M}(E_f)}{E_i - E_f} \right)^2,
The F_1(E_i, E_f) can be rewritten in the following way when E_i = E_f:



Definition of NR kinematic functions

$$F_{1}(E_{i}, E_{f})\big|_{E_{i}, E_{f} = E_{n}} = -\frac{\mathrm{d}}{\mathrm{d}E}F_{0}(E_{n}),$$

$$F_{0}(E) = \left(\frac{1}{L^{3}}\sum_{p} -\int \frac{\mathrm{d}^{3}p}{(2\pi)^{3}}\right)\frac{1}{E - p^{2}/m + i\epsilon},$$

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= g²_A 𝔅(E_f)𝔅(E_i) (𝔅(E_f)𝔅(E_i)F₁(E_i, E_f) + (𝔅(E_i) − 𝔅(E_f))/(E_i − E_f))²,
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Definition of NR kinematic functions

$$\begin{split} F_1(E_i, E_f) \Big|_{E_i, E_f = E_n} &= -\frac{\mathrm{d}}{\mathrm{d}E} F_0(E_n), \end{split} \\ F_0(E) = \left(\frac{1}{L^3} \sum_{\mathbf{p}} -\int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3}\right) \frac{1}{E - \mathbf{p}^2/m + i\epsilon}, \\ The second term can also be rewritten when $E_i = E_f: \\ \frac{\mathcal{M}(E_i) - \mathcal{M}(E_f)}{E_i - E_f} \Big|_{E_i, E_f = E_n} &= \frac{\mathrm{d}}{\mathrm{d}E} \mathcal{M}(E) \Big|_{E = E_n} = -\mathcal{M}^2(E_n) \frac{\mathrm{d}}{\mathrm{d}E} \mathcal{M}^{-1}(E_n). \end{split} \\ F_0(E) = \left(\frac{1}{L^3} \sum_{\mathbf{p}} -\int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3}\right) \frac{1}{E_i - \mathbf{p}^2/m + i\epsilon} \frac{1}{E_f - \mathbf{p}^2/$$$

The one-body contribution of axial current

- The NR finite volume formalism of proton-proton fusion
 L⁶ | (E_f, L | J^{1B} | E_i, L)|² Z. Davoudi, S. V. Kadam, PRD 102 (2020) 11, 114521
 = g_A² R(E_f) R(E_i) (M(E_f) M(E_i)F₁(E_i, E_f) + M(E_i) M(E_f)/(E_i E_f))²,
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- The F₁(E_i, E_f) can be rewritten in the following way when E_i = E_f: F₁(E_i, E_f)|_{E_i, E_f = E_n} = -^d/_{dE}F₀(E_n), F₁(E_i, E_f)|_{E_i, E_f = E_n} = -^d/_{dE}F₀(E_n), F₀(E) = (¹/_{L³} ∑_p - ∫ (^{d³p}/_{(2\pi)³})) 1/_{E - p²/m + i\epsilon}, F₁(E_i, E_f) = (¹/_{L³} ∑_p - ∫ (^{d³p}/_{(2\pi)³})) 1/<sub>E_i - p²/m + i\epsilon} 1/<sub>E_f - p²/m + i\epsilon}, M(E_i) - M(E_f)|_{E_i, E_f = E_f} = -^d/_{dE}M(E)|_{E=E_n} = -M²(E_n) d/_{dE}M⁻¹(E_n).
 </sub></sub>
- Now, we have all the key ingredients:

$$\begin{split} L^6 \left| \left\langle E_n, L \left| \left. \mathcal{J}^{1\mathrm{B}} \left| \left. E_n, L \right\rangle \right|^2 &= g_A^2 \left(\frac{-\mathcal{M}^2(E_n) \frac{\mathrm{d}}{\mathrm{d}E} F_0(E_n) - \mathcal{M}^2(E_n) \frac{\mathrm{d}}{\mathrm{d}E} \mathcal{M}^{-1}(E_n)}{-\mathcal{M}^2(E_n) \frac{\mathrm{d}}{\mathrm{d}E} \left[F_0(E_n) + \mathcal{M}^{-1}(E_n) \right]} \right)^2 \\ &= g_A^2. \end{split}$$

ME of one-body contribution exactly reproduced g_A when $E_i = E_f$



Numerical Results of FV Correction

FV Correction of one-body contribution

• If $E_i \neq E_f$, The one-body contribution will receive a non-zero correction:

$$\begin{split} L^3 \left| \left\langle E_f, L \left| \left. \mathcal{J}^{1\mathrm{B}} \left| \left. E_i, L \right\rangle \right| = g_A \sqrt{\mathcal{R}(E_f) \mathcal{R}(E_i)} \left(\mathcal{M}(E_f) \mathcal{M}(E_i) F_1(E_i, E_f) + \frac{\mathcal{M}(E_i) - \mathcal{M}(E_f)}{E_i - E_f} \right), \right. \right| \\ &= g_A (1 - \delta_{1\mathrm{B}}). \end{split}$$

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FV Correction of two-body contribution

• LL-factors for both initial and final states.

$$\begin{split} L^6 \left| \left\langle E_f, L \left| \left| \mathcal{J}^{2\mathrm{B}} \right| E_i, L \right\rangle \right|^2 &= \mathcal{R}(E_f) W_{2\mathrm{B}}^2(E_i, E_f) \mathcal{R}(E_i) \\ L^3 \left| \left\langle E_f, L \left| \left| \mathcal{J}^{2\mathrm{B}} \right| E_i, L \right\rangle \right| &\equiv L_{1,A}^{sd-2b} (1 - \delta_{2\mathrm{B}}) \end{split}$$



short-distance two-body contribution

• The numerical result is $\delta_{2B} = 0.19(45)$.

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- $L_{1,A}^{sd-2b}$ comes from LQCD while the experimental value of all other quantities are used.
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- The LEC constrained by our work ($m_{\pi} \sim 432$ MeV) is

 $L_{1,A} = 3.5(1.3) \text{ fm}^3$ (Ignoring both δ_{1B} and δ_{2B})

 $L_{1,A} = 3.4(1.5) \text{ fm}^3 (\delta_{2B} \text{ included})$

 $L_{1,A} = 21(84) \text{ fm}^3$ (Both δ_{1B} and δ_{2B} included)

NPLQCD's result at $m_{\pi} \sim 806$ MeV : $L_{1,A} = 3.9(0.2)(1.4)$ fm³ (Ignoring both δ_{1B} and δ_{2B})

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The major FV correction comes from **one-body** contribution. Because the **two-body** contribution accounts for only about 2% of the matrix elements.

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Neutrinoless Double Beta Decay (Preliminary)

- Massive neutrino scheme is used to remove the divergence of neutrino propagator.
- This scheme can also simplify finite volume analysis. Xu Feng et al., PRD 103 (2021) 3, 034508
- We noticed that the loop momentum can easily exceed the pion production threshold,

so the match requires chiral EFT, which is currently not available.



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Conclusion

Lattice Calculation of Proton-Proton Fusion Matrix Element

- **Bi-local interpolators** can effectively reduce the excited-state contamination.
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- **Diproton/dineutron** is likely to be **a shallow bound state** or **scattering state**.
- We obtained the **p-p fusion matrix element** and constrained corresponding **LEC** *L*_{1,A}.
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Outlooks

- We will use ensembles with larger spatial volume to control FV effects and other systematics.
- Improving the accuracy of two-nucleon FV spectrum is essential to the FV corrections.
- With these techniques, we are able to move on to more physical pion mass.

Thanks.