WILL DETMOLD
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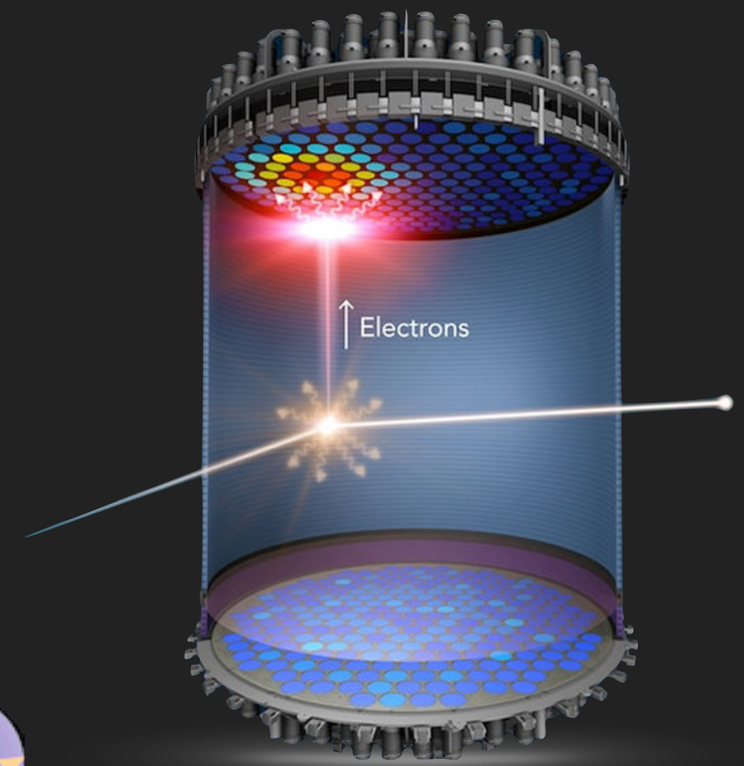
FINITE VOLUME EFFECTIVE FIELD THEORY FOR NUCLEI

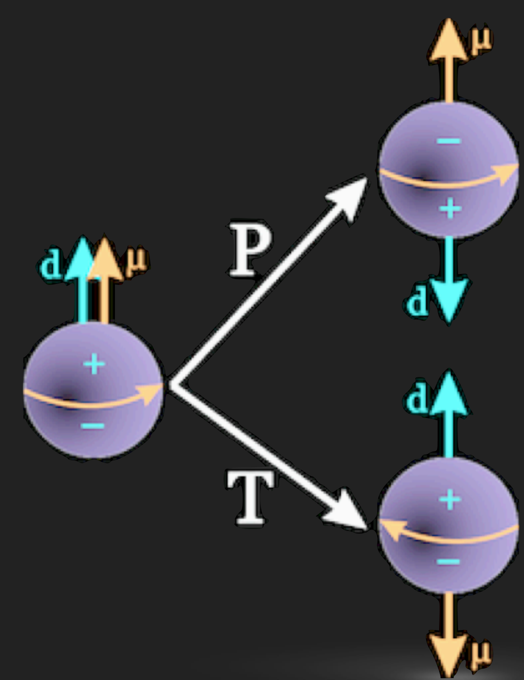
2202.03530 with X Sun, D Luo and P Shanahan
2102.04329 with P Shanahan

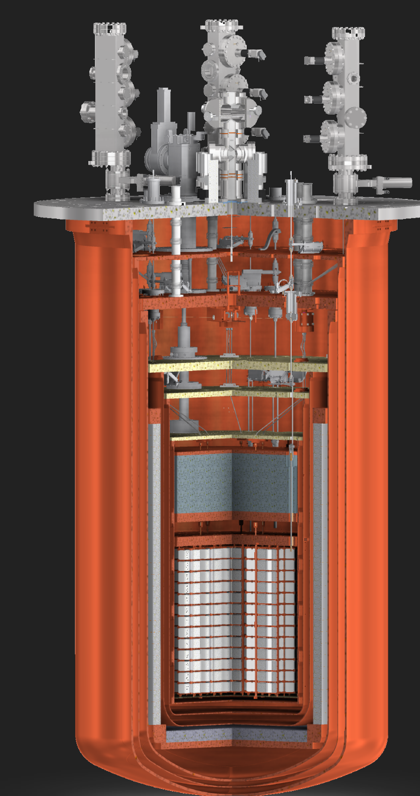
AIP Congress, Dec 13, 2022

NUCLEI AT THE INTENSITY FRONTIER

- Nuclei are vital to experiments
  - Dark matter direct detection
  - Long baseline neutrino experiments (DUNE)
  - Lepton flavour violation: μ2e
  - Precision spectroscopy
  - Electric dipole moments of neutrons and nuclei
  - Neutrinoless double beta decay

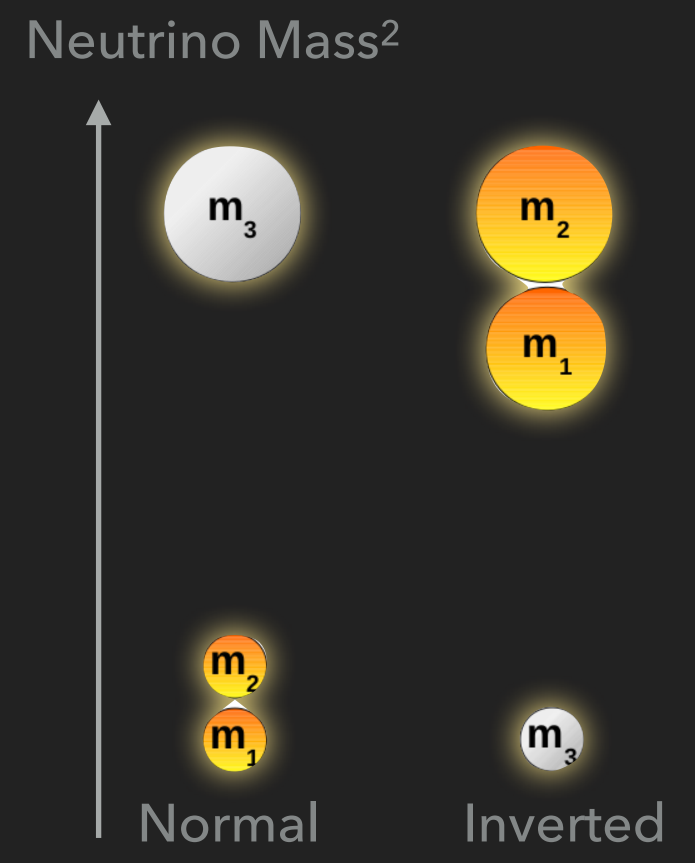




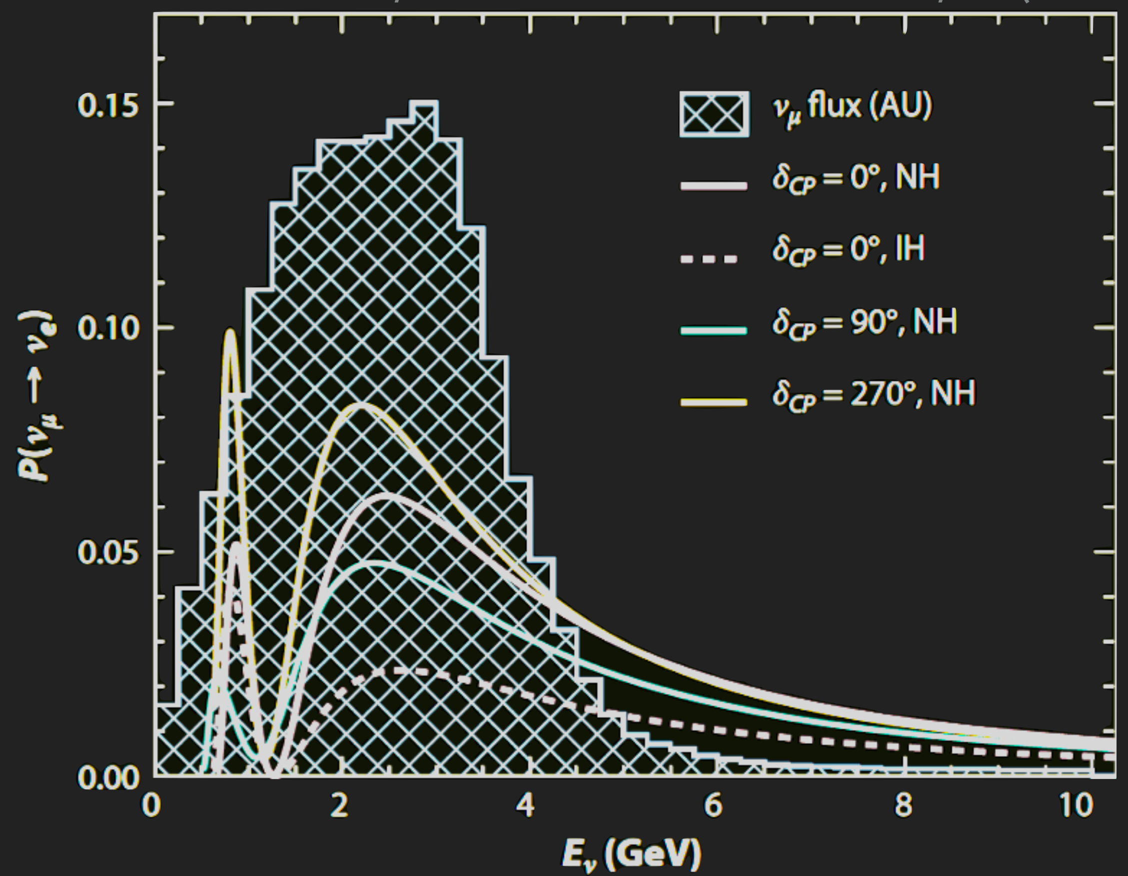


LONG BASELINE NEUTRINO EXPERIMENTS

- Deep Underground Neutrino Experiment
  - Flagship facility for US HEP for next decades
  - Determine neutrino mass hierarchy and extract mixing parameters
- Neutrino scattering on argon target
  - Need fluxes/energies to high accuracy
  - Need to know neutrino interactions with argon over a wide range of energies

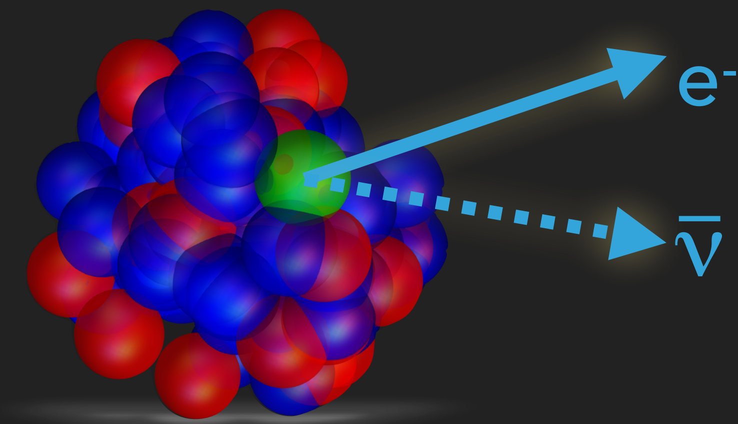


Diwan et al, Ann. Rev. Nucl. Part. Sci. 66, 47 (2016)

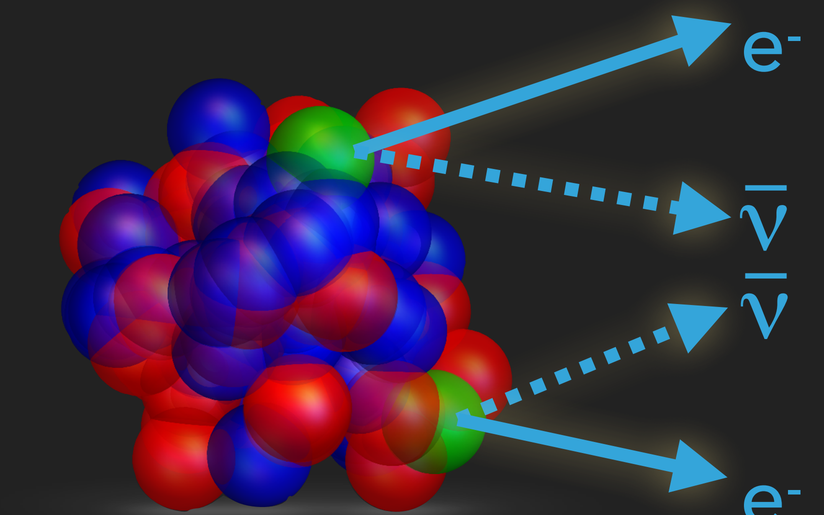


DOUBLE BETA DECAY

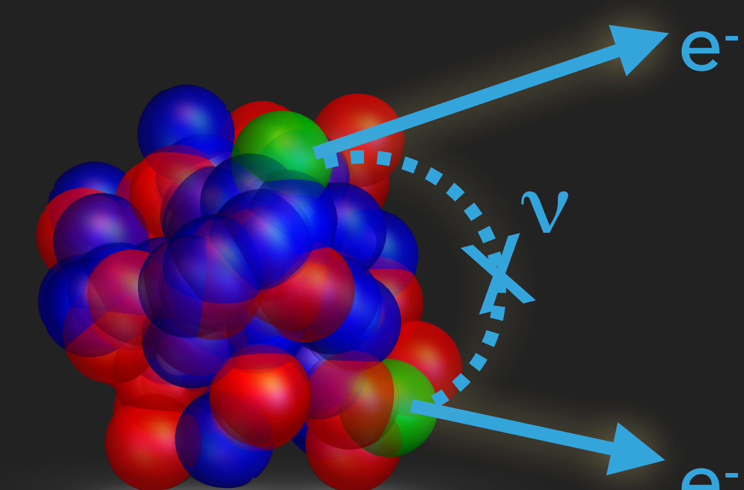
- Double β-decay
  - Neutrinoful case is rarest process observed
  - Neutrinoless case
    - Majorana particles? Lepton number violation? Baryon–antibaryon asymmtery?
  - Rates depend on nuclear matrix elements
    - Currently quite uncertain
    - Important for design of future DBD search experiments



Beta decay

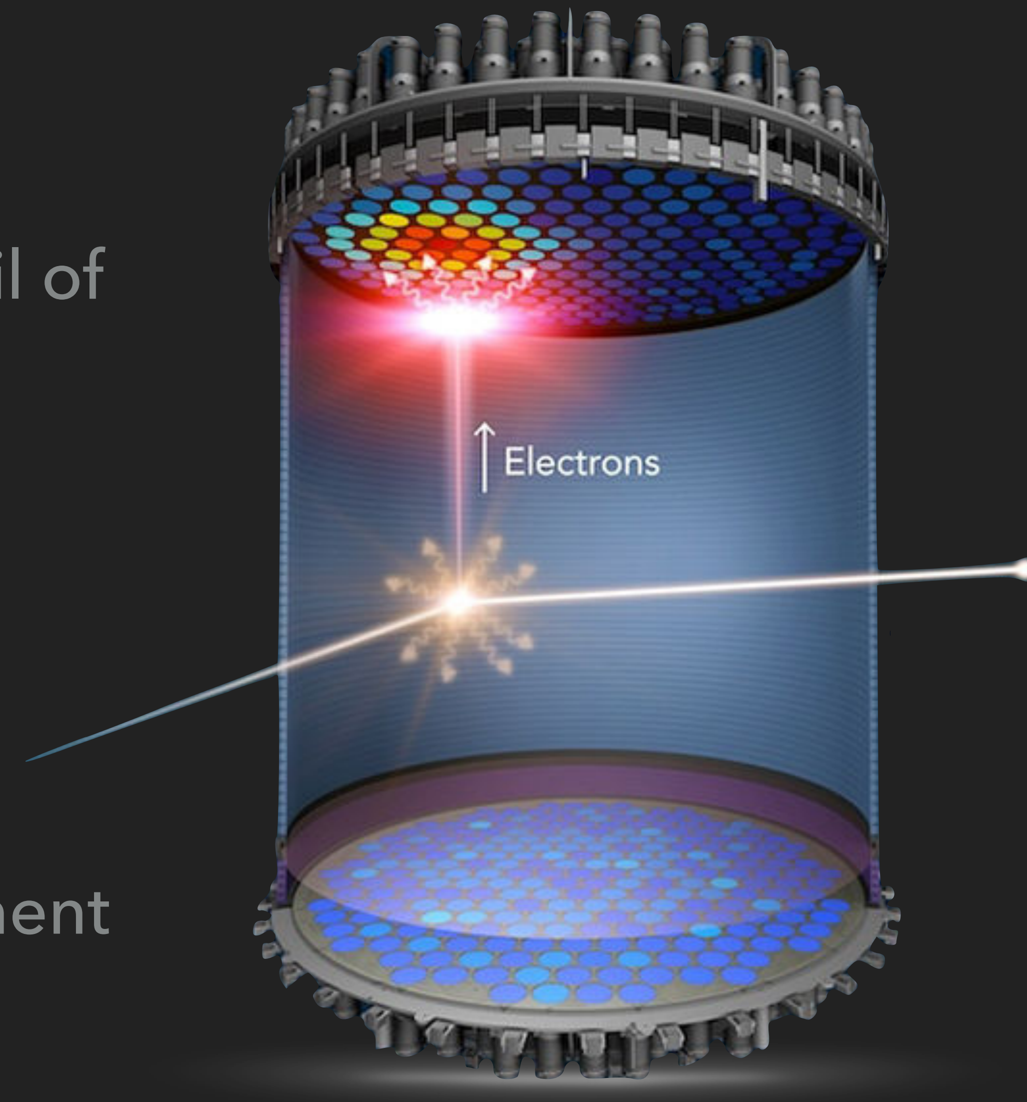


Two neutrino double β-decay



Neutrinoless double β-decay

DARK MATTER INTERACTIONS



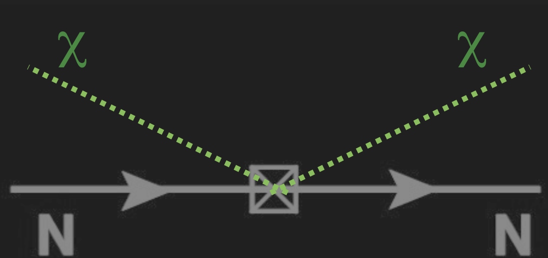
- DM direct detection experiments search for recoil of nucleus from DM scattering
- One popular class of DM interactions is through scalar exchange

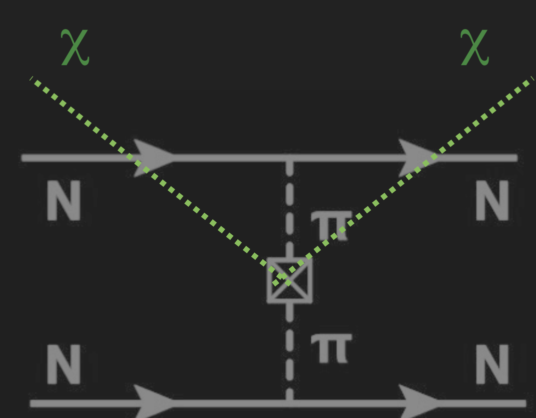
$$\mathcal{L} = \frac{G_F}{2} \sum_q \kappa_q (\overline{\chi}\chi)(\overline{q}q)$$

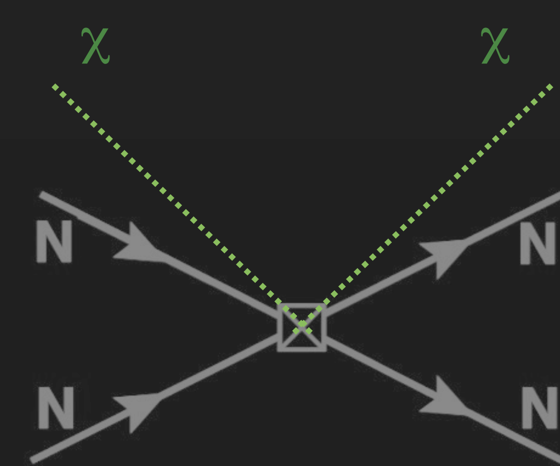
- Direct detection depends on nuclear matrix element

$$\overline{m}\langle Z, N|\overline{u}u + \overline{d}d|Z, N\rangle$$

- At hadronic/nuclear level

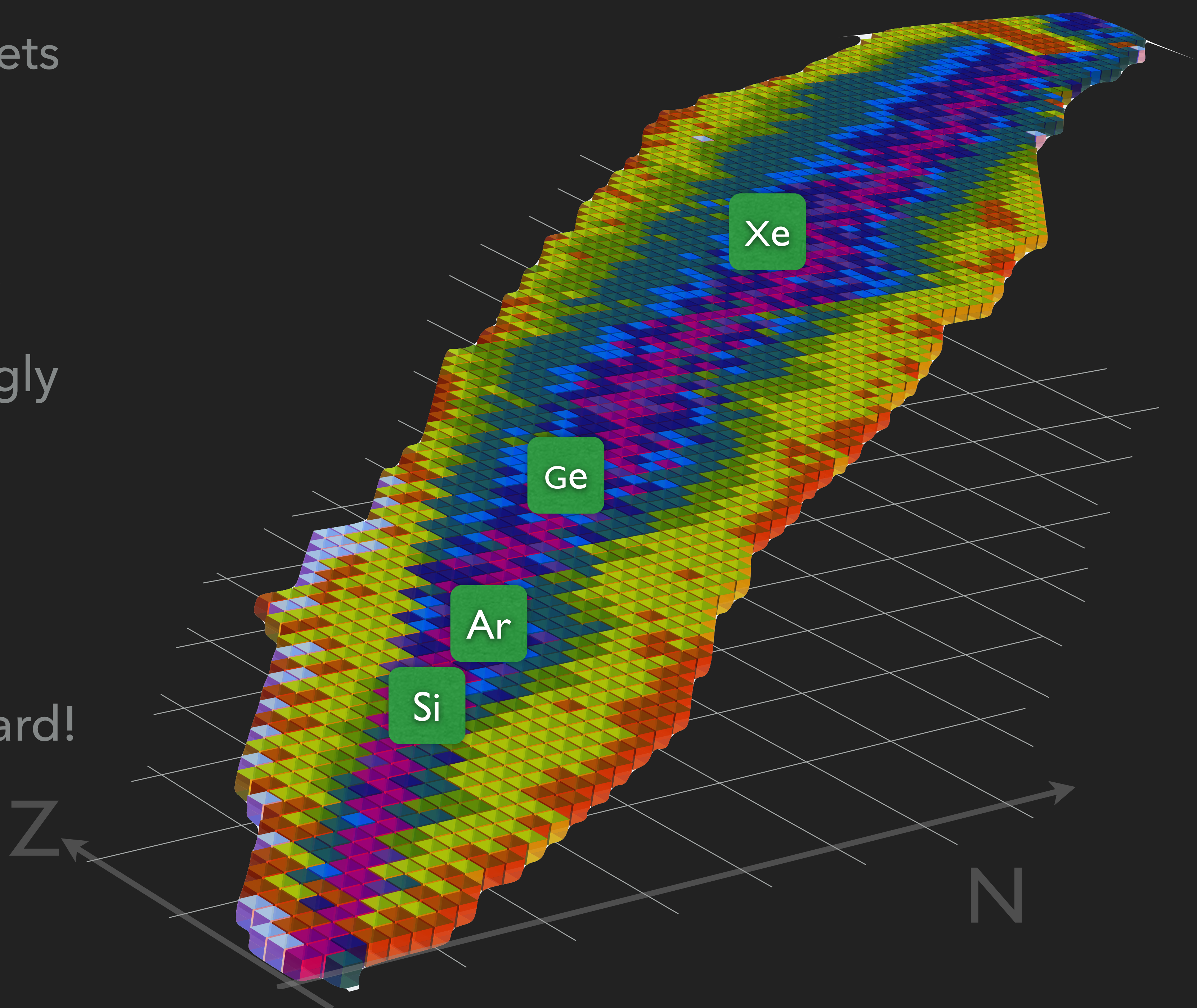






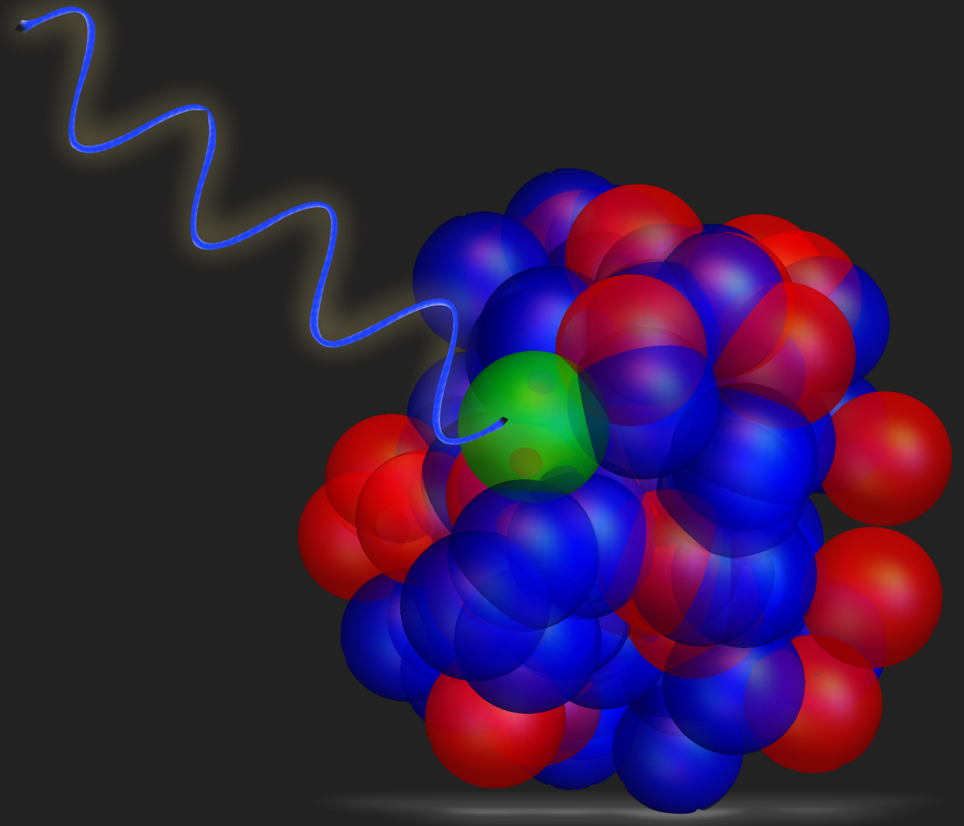
THE WEALTH OF NUCLEI

- Nuclei are often used as targets
  - High density
  - Can be assembled in bulk
- But nuclei are complex strongly interacting systems
- Theoretical understanding a challenge
  - Direct lattice QCD? Too hard!
  - Effective field theory

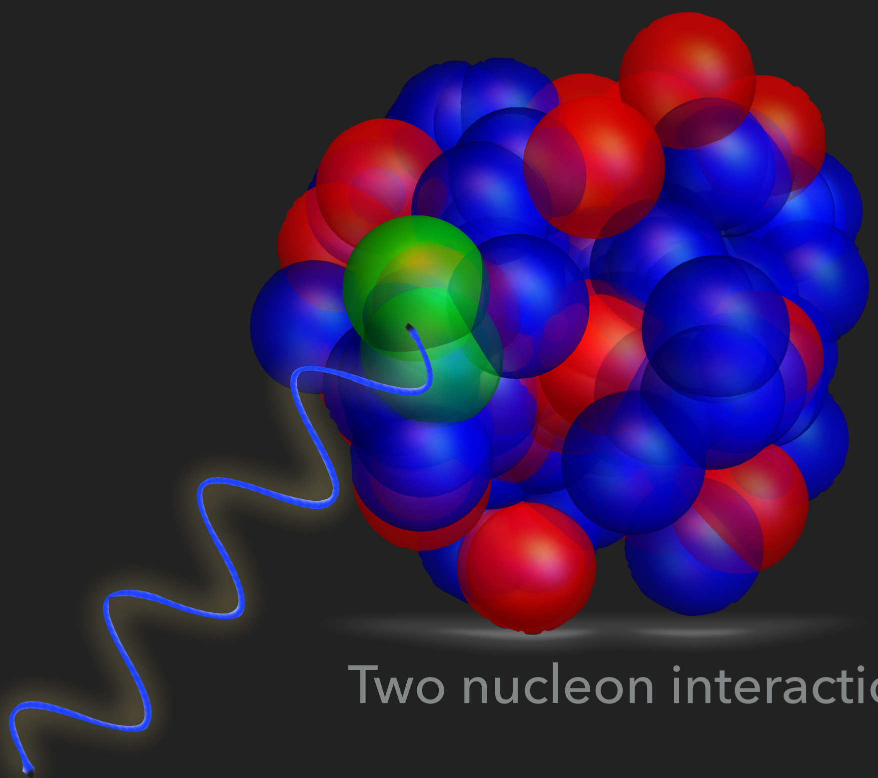


INTERACTIONS WITH NUCLEI

- Single nucleon coupling dominates
  - Determine from nucleon matrix element calculations
- Two nucleon contributions are sub-leading
  - Study A=2,3,4,.. systems
  - Match LQCD and EFT
  - Determine nuclear effects



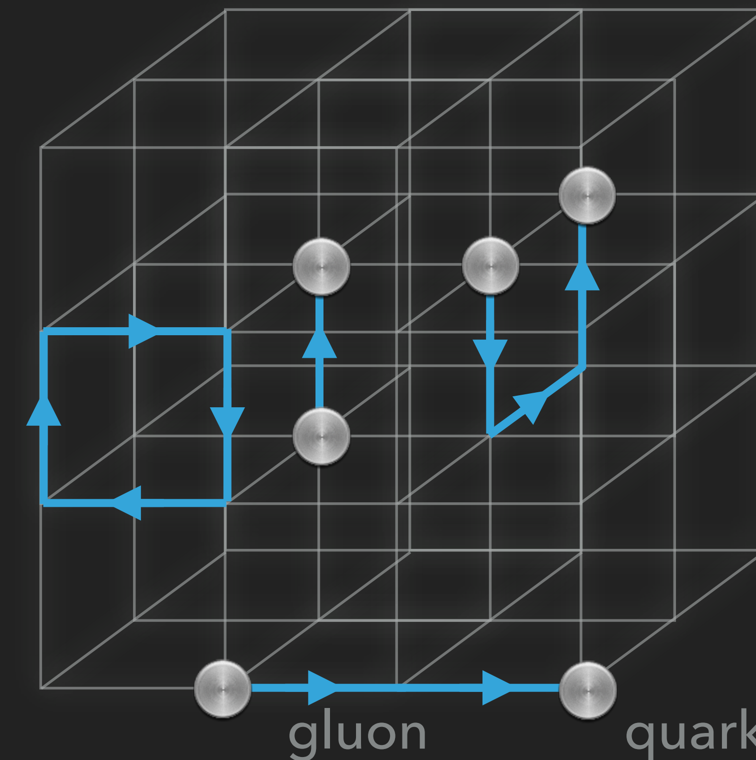
One nucleon interaction

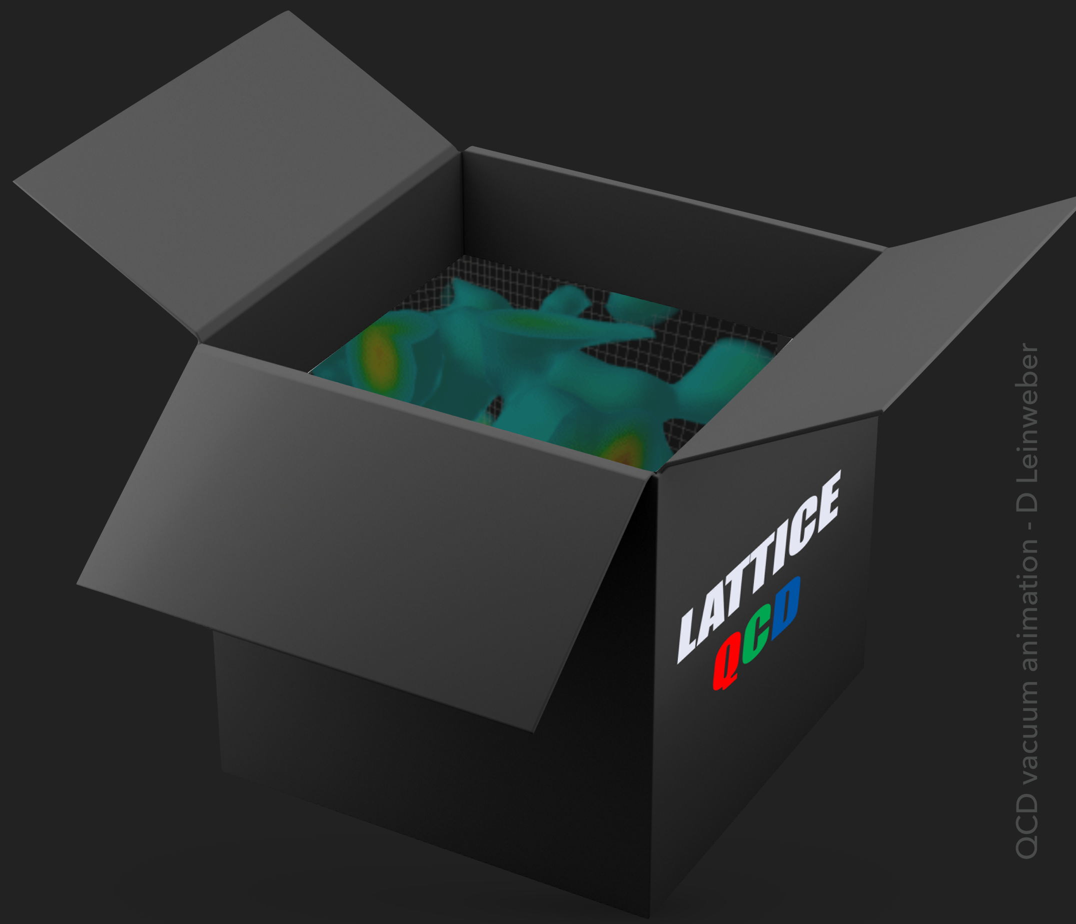


Two nucleon interaction

LATTICE QCD

- Strong coupling definition of QCD
- Numerical tool for nonperturbative QCD calculations
  - Discretise and compactify spacetime
  - Integration over 10^{12} degrees of freedom in current calculations using importance sampling Monte Carlo
  - Understand effects of discretisation and compactification and finite statistics

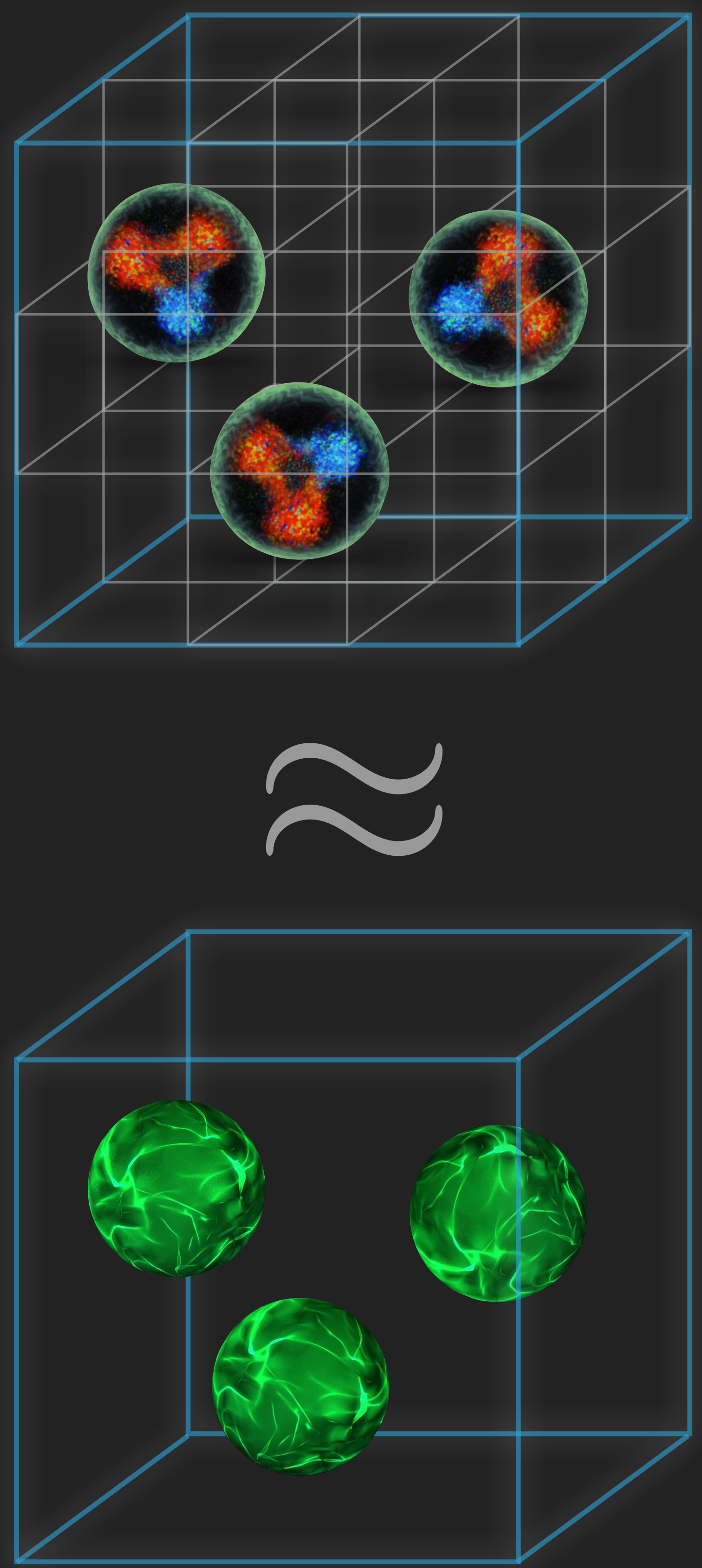




QCD vacuum animation - D Leinweber

FINITE VOLUME EFFECTS

- Major issue for LQCD calculations of nuclei is finite volume (FV) effects
- Well-known Lüscher method to understand FV effects in B=2 spectrum (and now B=3)
- Less well-developed technologies for effects on matrix elements
- Alternative: direct matching between LQCD and EFT in the same FV
  - Use EFT to extrapolate to infinite volume
  - Spectroscopy and matrix elements
  - Pionless EFT for simplicity



PIONLESS EFT

- Leading order pionless EFT Hamiltonian

$$H = -\frac{1}{2M_N}\sum_i \nabla_i^2 + \sum_{i<j} V_2\left(\mathbf{r}_{ij}\right) + \sum_{i<j<k} V_3\left(\mathbf{r}_{ij}, \mathbf{r}_{jk}\right)$$

- Two- and three-body interactions

Three body low energy constant

$$V_2\left(\mathbf{r}_{ij}\right) = \left(C_0 + C_1\sigma^{(i)}\cdot\sigma^{(j)}\right) g_\Lambda\left(\mathbf{r}_{ij}\right). \quad V_3\left(\mathbf{r}_{ij}, \mathbf{r}_{jk}\right) = D_0 \sum_{\text{cyc}} g_\Lambda\left(\mathbf{r}_{ij}\right) g_\Lambda\left(\mathbf{r}_{jk}\right)$$

Two body low energy constants

- Implement with Gaussian regulator with shifted copies to satisfy periodic boundary conditions

Regulator scale

$$g_\Lambda(\mathbf{r}, L) = \frac{\Lambda^3}{8\pi^{3/2}} \prod_{\alpha\in\{x,y,z\}} \sum_{q^{(\alpha)}=-\infty}^{\infty} \exp\left(-\Lambda^2\left(r^{(\alpha)} - Lq^{(\alpha)}\right)^2/4\right)$$

VARIATIONAL METHOD

- For any wavefunction, the variational method can bound energies of eigenstates

$$E_h \leq \mathcal{E}\left[\Psi_h\right] = \frac{\int \Psi_h(\mathbf{x})^* H \Psi_h(\mathbf{x}) d\mathbf{x}}{\int \Psi_h(\mathbf{x})^* \Psi_h(\mathbf{x}) d\mathbf{x}}$$

- Find wave functions that provide the most stringent bounds
    - Some increasingly large set of basis functions
    - Wavefunction as a neural network (ongoing)
- Correlated Gaussians in many-particle coordinate space
    - Computationally efficient (integrals analytic) and expressive

CORRELATED GAUSSIANS

- 3n spatial coordinates: $\mathbf{x} = (\mathbf{r}_1, \ldots, \mathbf{r}_n)$ with $\mathbf{x}^{(\alpha)} = (\mathbf{r}_{1,\alpha}, \ldots, \mathbf{r}_{n,\alpha})$
- Wavefunction built from correlated shifted Gaussians in each Cartesian direction $\alpha \in \{x, y, z\}$

$$\Psi_\infty^{(\alpha)}\left(A^{(\alpha)}, B^{(\alpha)}, \mathbf{d}^{(\alpha)}; \mathbf{x}^{(\alpha)}\right) = \exp\left[-\frac{1}{2}\mathbf{x}^{(\alpha)T} A^{(\alpha)} \mathbf{x}^{(\alpha)} - \frac{1}{2}\left(\mathbf{x}^{(\alpha)} - \mathbf{d}^{(\alpha)}\right)^T B^{(\alpha)} \left(\mathbf{x}^{(\alpha)} - \mathbf{d}^{(\alpha)}\right)\right]$$

Vector

Symmetric matrix

Wavefunction parameters

Diagonal matrix

- Impose periodicity:

$$\Psi_L^{(\alpha)}\left(A^{(\alpha)}, B^{(\alpha)}, \mathbf{d}^{(\alpha)}; \mathbf{x}^{(\alpha)}\right) = \sum_{\mathbf{b}^{(\alpha)}} \Psi_\infty^{(\alpha)}\left(A^{(\alpha)}, B^{(\alpha)}, \mathbf{d}^{(\alpha)}; \mathbf{x}^{(\alpha)} - \mathbf{b}^{(\alpha)} L\right)$$

$$\Psi_L(A, B, \mathbf{d}; \mathbf{x}) = \prod_{\alpha \in \{x,y,z\}} \Psi_L^{(\alpha)}\left(A^{(\alpha)}, B^{(\alpha)}, \mathbf{d}^{(\alpha)}; \mathbf{x}^{(\alpha)}\right)$$

- Symmetrise spatial wavefunction under particle interchange

$$\Psi_L^{\mathrm{sym}}(A, B, \mathbf{d}; \mathbf{x}) = \sum_{\mathcal{P}} \Psi_L\left(A_{\mathcal{P}}, B_{\mathcal{P}}, \mathbf{d}_{\mathcal{P}}; \mathbf{x}\right)$$

X. Y. Yin and D. Blume, Phys. Rev. A 87, 063609 (2013)

PIONLESS EFT

- Focus on nuclei up to ^{4}He in s-wave
- Spatially symmetric, antisymmetric in spin-flavour

$$\Psi_h^{(N)}(\mathbf{x}) = \sum_{j=1}^{N} c_j \Psi_L^{\mathrm{sym}}\left(A_j, B_j, \mathbf{d}_j; \mathbf{x}\right) |\chi_h\rangle$$

where eg

$$\left|\chi^3\mathrm{H}, j_z = 1/2\right\rangle = \frac{1}{\sqrt{6}}\left[\left|n^\uparrow p^\uparrow n^\downarrow\right\rangle - \left|n^\downarrow p^\uparrow n^\uparrow\right\rangle - \left|p^\uparrow n^\uparrow n^\downarrow\right\rangle + \left|p^\uparrow n^\downarrow n^\uparrow\right\rangle - \left|n^\uparrow n^\downarrow p^\uparrow\right\rangle + \left|n^\downarrow n^\uparrow p^\uparrow\right\rangle\right]$$

- General ansatz with parameters: $\theta = \{\mathbf{c}, A, B, \mathbf{d}\}$

STOCHASTIC VARIATIONAL METHOD

- Wavefunction ansatz contains linear and nonlinear parameters
- Linear parameters can be optimised via an eigenvalue problem
- Nonlinear parameters optimised stochastically [Varga & Suzuki 1995]
  1. Propose a new Gaussian term with stochastically chosen parameters
  2. Calculate matrix elements of Hamiltonian between terms in set

$$[\mathbb{H}]_{ij} \equiv \int \Psi_i(\mathbf{x})^* \langle \chi_h | H | \chi_h \rangle \, \Psi_j(\mathbf{x}) d\mathbf{x} \quad [\mathbb{N}]_{ij} \equiv \int \Psi_i(\mathbf{x})^* \Psi_j(\mathbf{x}) d\mathbf{x}$$

  3. Solve generalised eigenvalue problem to determine coefficient

$$\mathbb{H}\mathbf{c} = \lambda \mathbb{N}\mathbf{c}$$

STOCHASTIC VARIATIONAL METHOD

- Energy bound

$$E_h \leq \mathcal{E}\left[\Psi_h\right] = \frac{\int \Psi_h(\mathbf{x})^* H \Psi_h(\mathbf{x}) d\mathbf{x}}{\int \Psi_h(\mathbf{x})^* \Psi_h(\mathbf{x}) d\mathbf{x}}$$

$$[\mathbb{H}]_{ij} \equiv \int \Psi_i(\mathbf{x})^* \left\langle \chi_h | H | \chi_h \right\rangle \Psi_j(\mathbf{x}) d\mathbf{x} \quad \mathbb{H} = \mathbb{K} + \mathbb{V}_2 + \mathbb{V}_3$$

- Integrals can be performed analytically

$$[\mathbb{N}]_{ij} \equiv \int \Psi_L^{\text{sym}}\left(A_i, B_i, \mathbf{d}_i; \mathbf{x}\right)^* \Psi_L^{\text{sym}}\left(A_j, B_j, \mathbf{d}_j; \mathbf{x}\right) d\mathbf{x}$$

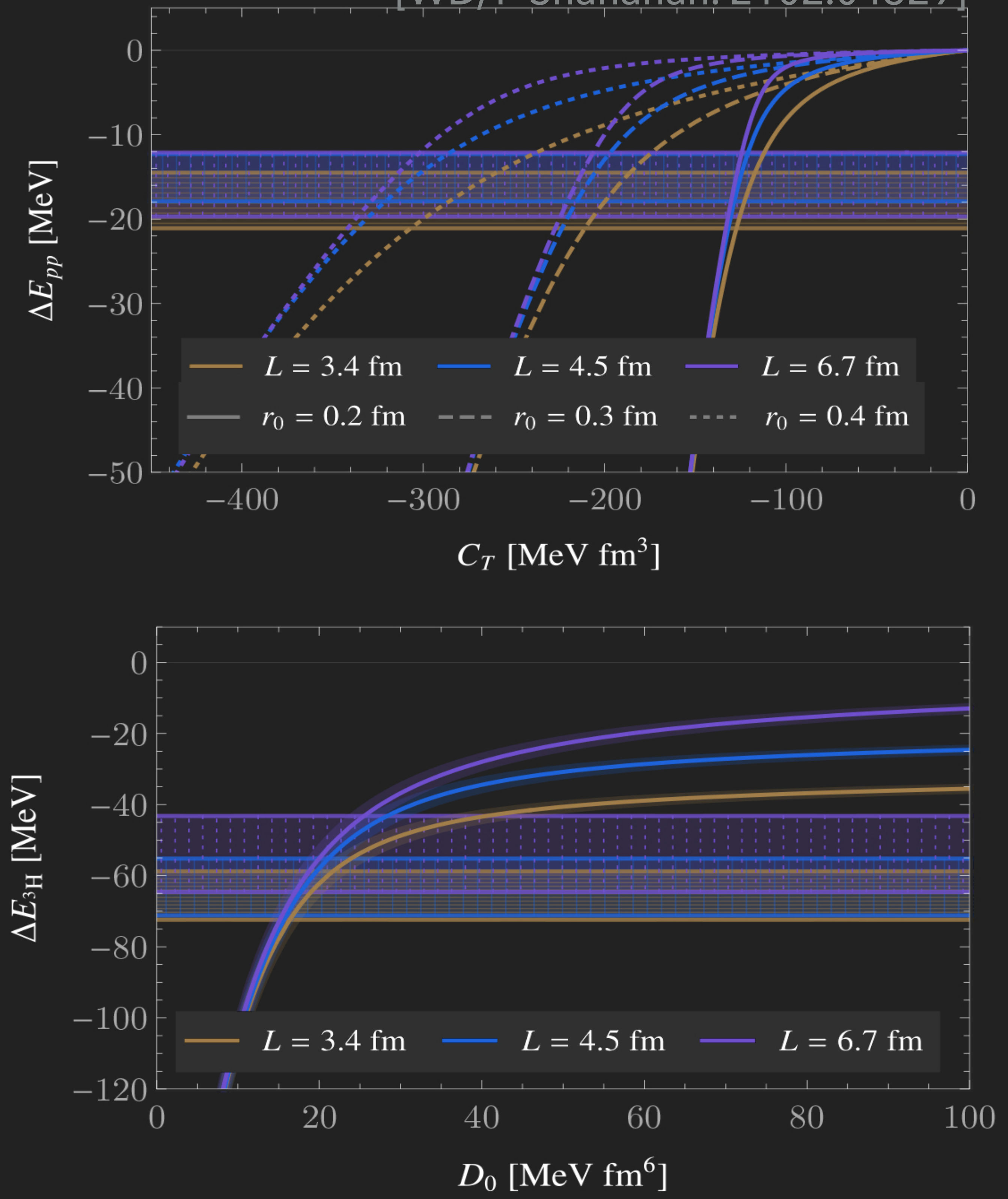
$$= \sum_{\mathcal{P},\mathcal{P}'} \prod_{\alpha \in \{x,y,z\}} \sqrt{\frac{(2\pi)^n}{\text{Det}\left[C^{(\alpha)}_{i\mathcal{P};j\mathcal{P}'}\right]} \sum_{\mathbf{b}^{(\alpha)}}^{(\alpha)} |\leq} \tilde{b} \exp\left[-\frac{1}{2}\Omega^{(\alpha)}_{i\mathcal{P};\mathcal{P}'}\right]$$

Objects built from the parameters

STOCHASTIC VARIATIONAL METHOD

[WD, P Shanahan. 2102.04329]

- Match onto LQCD FV energies to determine nuclear wave functions
  - 2 and 3-body energies fix NN and NNN contact interactions
- Determines infinite volume bindings
- NB: all LQCD calculations here at unphysically large quark masses



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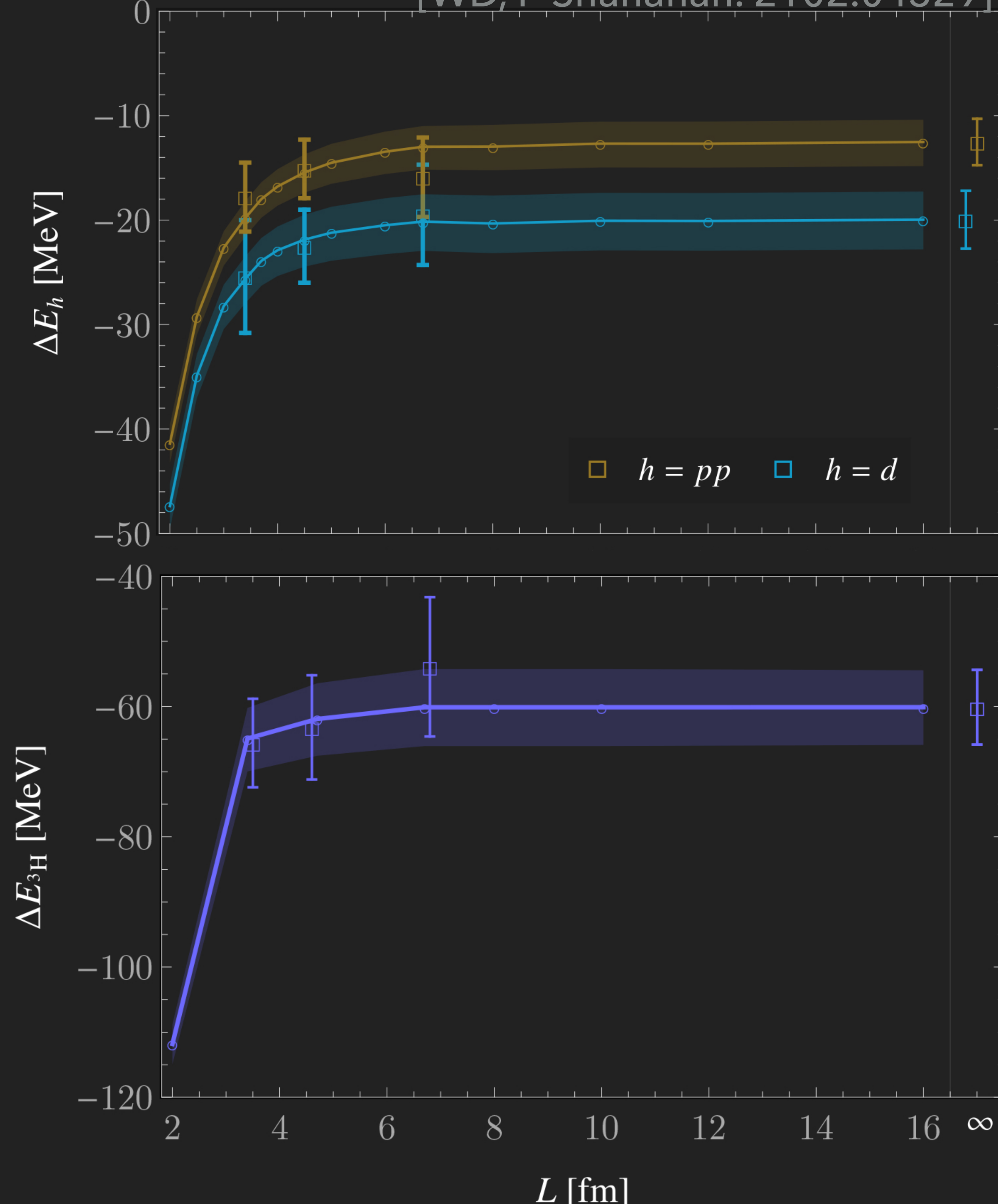


MATRIX ELEMENTS

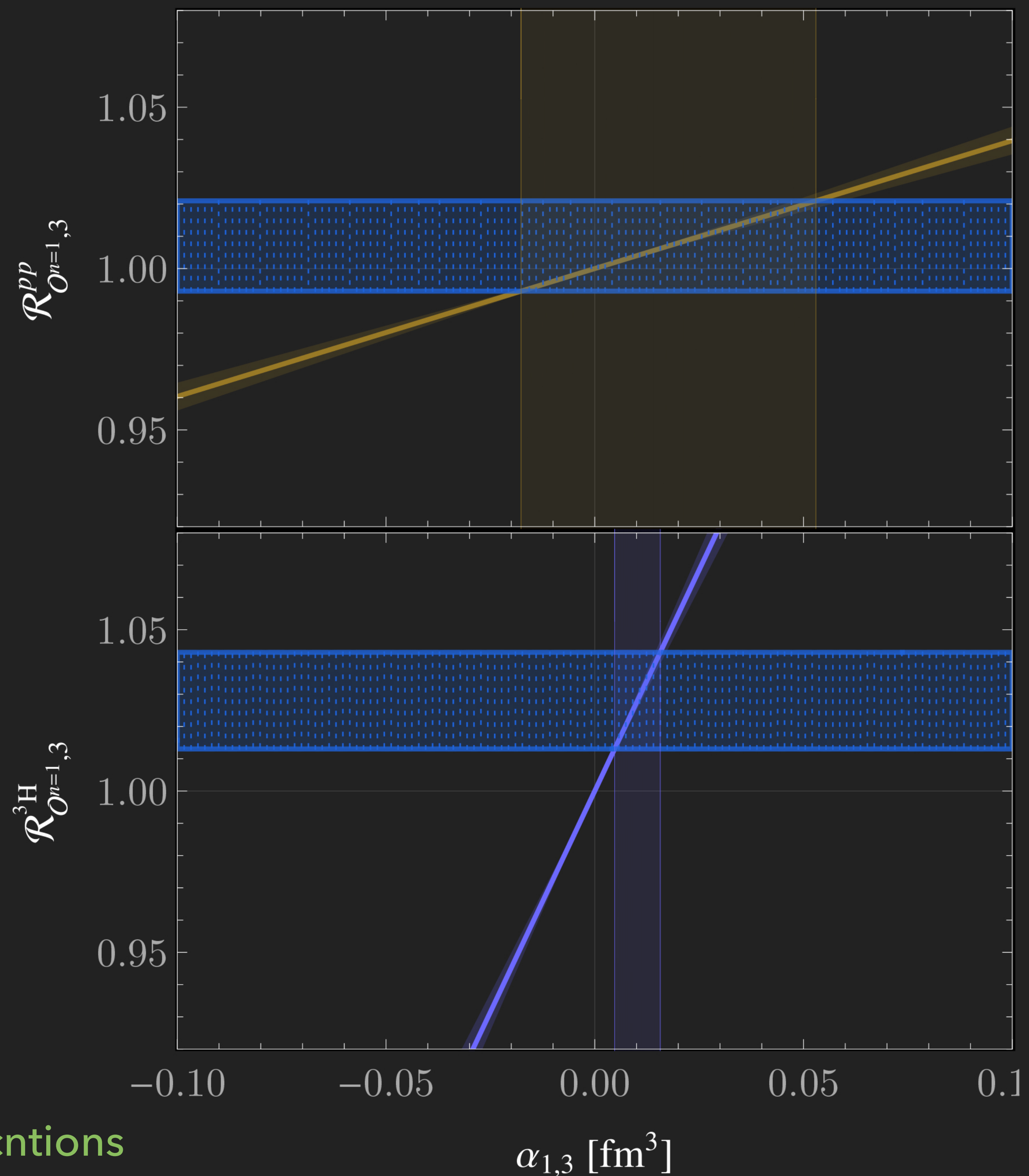
- Given EFT wavefunctions, matrix elements are easily computed
- LQCD matching determines EFT counterterms
  - Enables infinite volume prediction for matrix elements
  - Example: isovector momentum fraction

$$\mathcal{R}^h_{\mathcal{O}^n,3} \equiv \frac{A^h}{(Z^h - N^h)\langle x^n\rangle_3} \frac{\left\langle \Psi_h \middle| \mathcal{O}_3^{(n)} \middle| \Psi_h \right\rangle}{\langle \Psi_h \mid \Psi_h\rangle}$$

$$= \left(1 + \frac{\alpha_{n,3}}{(Z^h - N^h)\langle x^n\rangle_3} h_h(\Lambda, L)\right)$$

From wavefucntions

Two body counterterm



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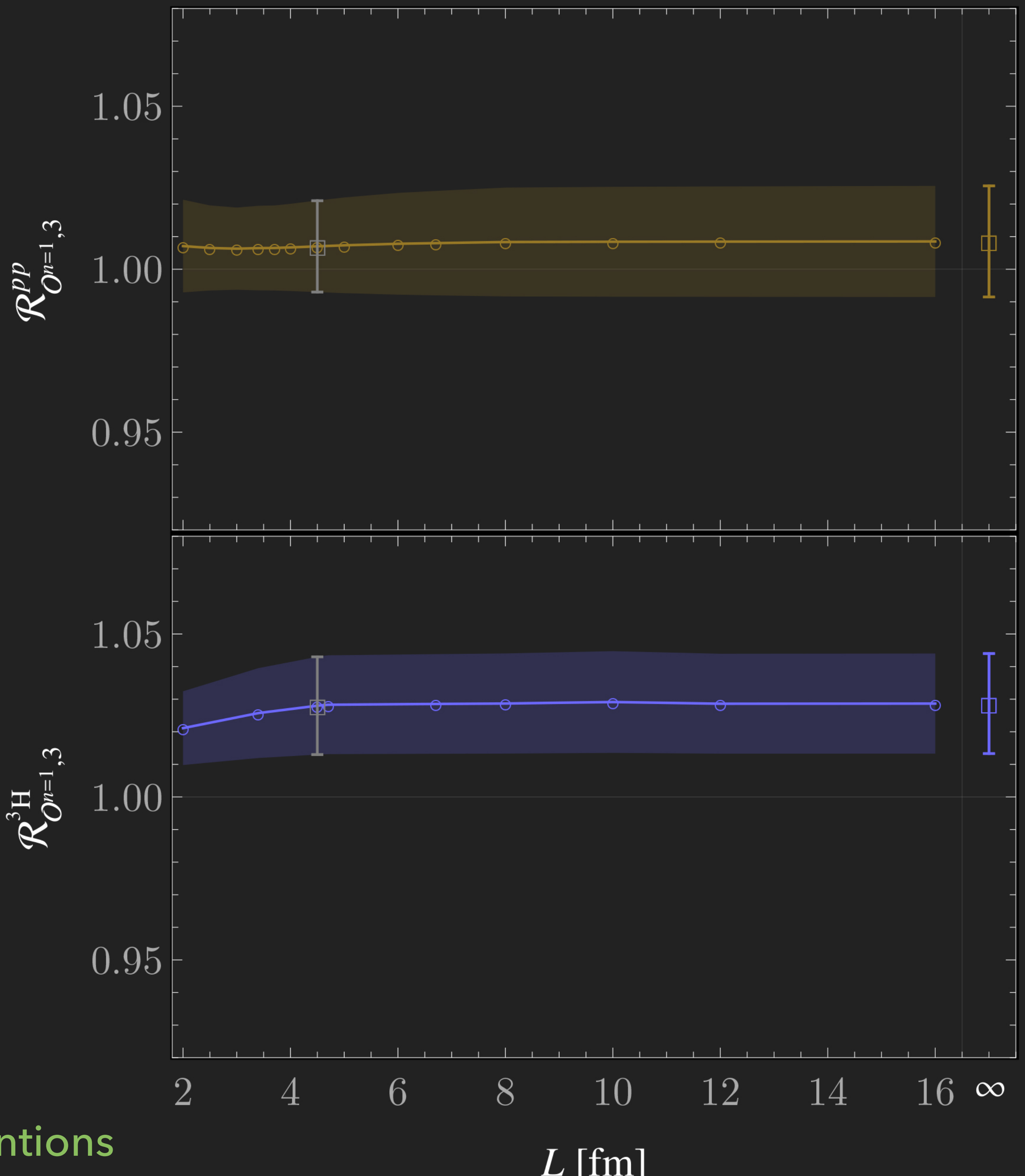

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From wavefucntions

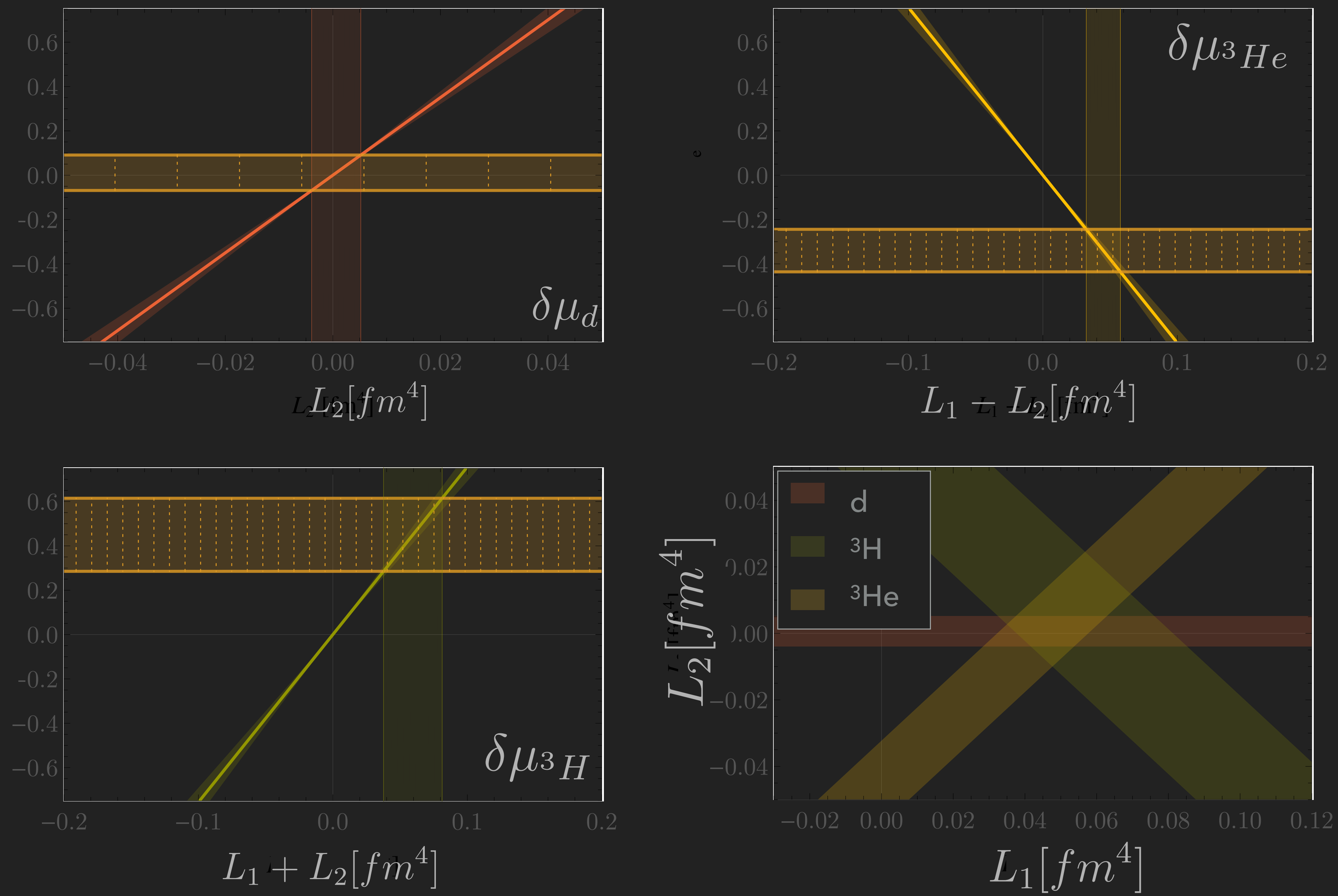
Two body counterterm

[WD, P Shanahan. 2102.04329]

MAGNETIC MOMENTS

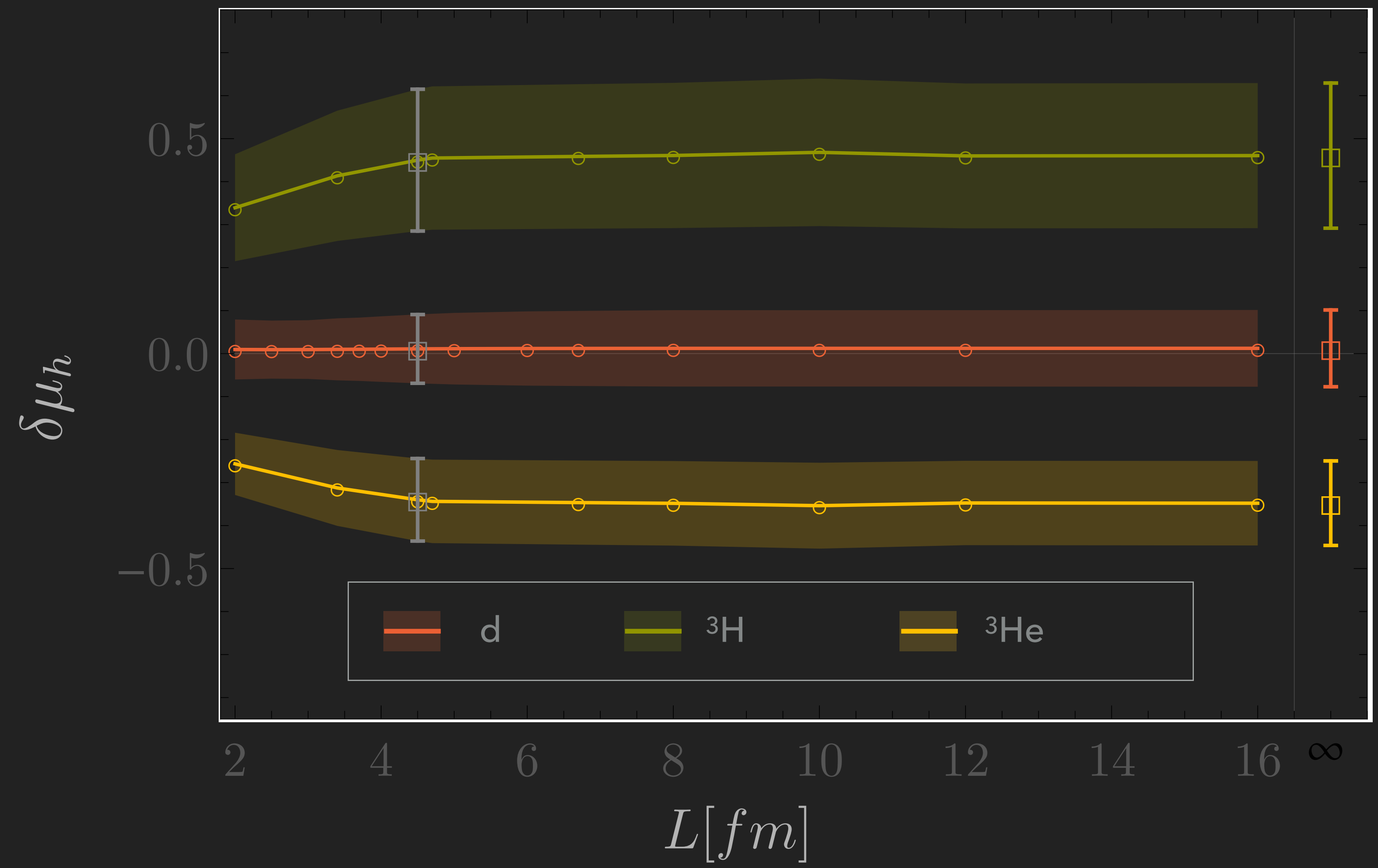
- Eg: magnetic moments

$$J_i^{EM} = \frac{e}{2M_N} N^\dagger \left(\kappa_0 + \tau_3 \kappa_1\right) \sigma_i N \quad - eL_2 i\epsilon_{ijk} \left(N^T P_k N\right)^\dagger \left(N^T P_j N\right) + eL_1 \left(N^T P_i N\right)^\dagger \left(N^T \bar{P}_3 N\right) + \text{ h.c.}$$



MAGNETIC MOMENTS

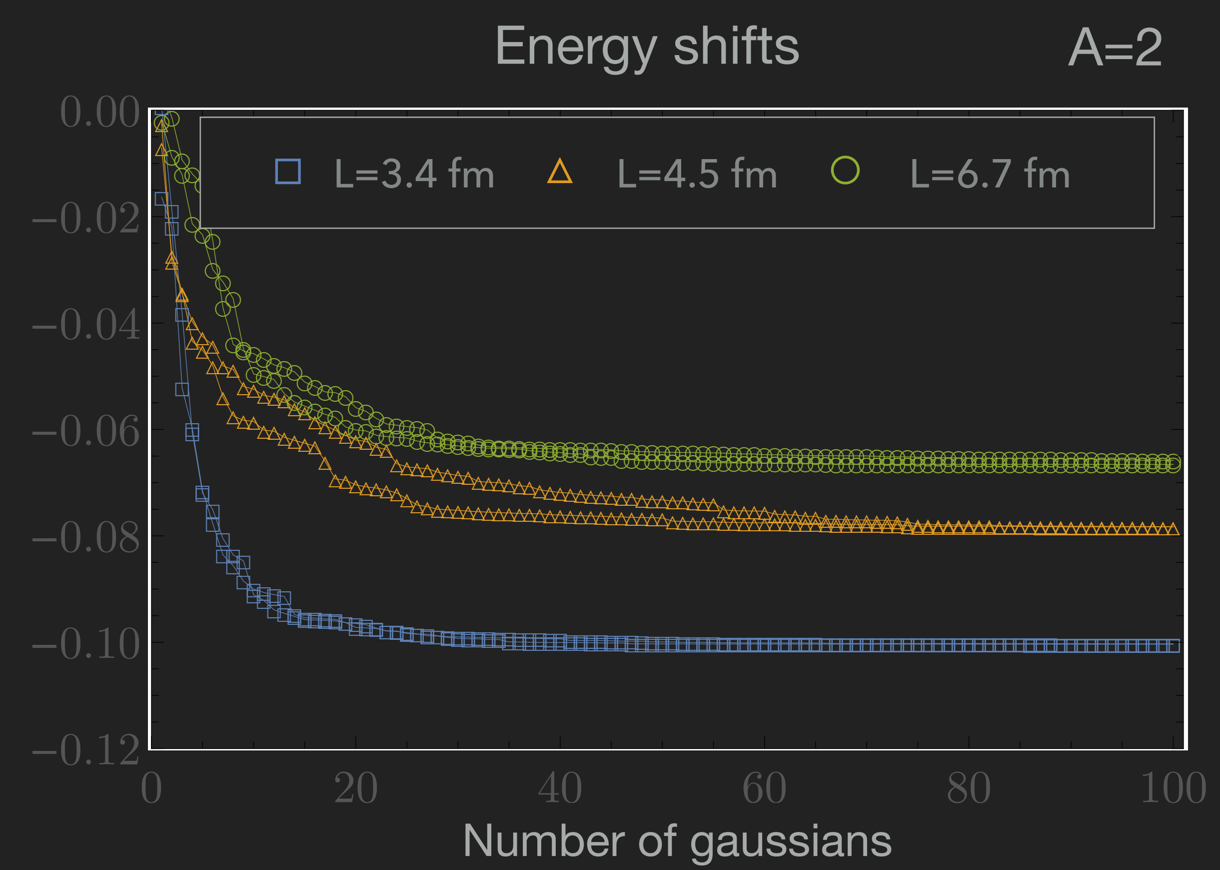
- LQCD-EFT matching can be extended to matrix elements
- Eg: magnetic moments

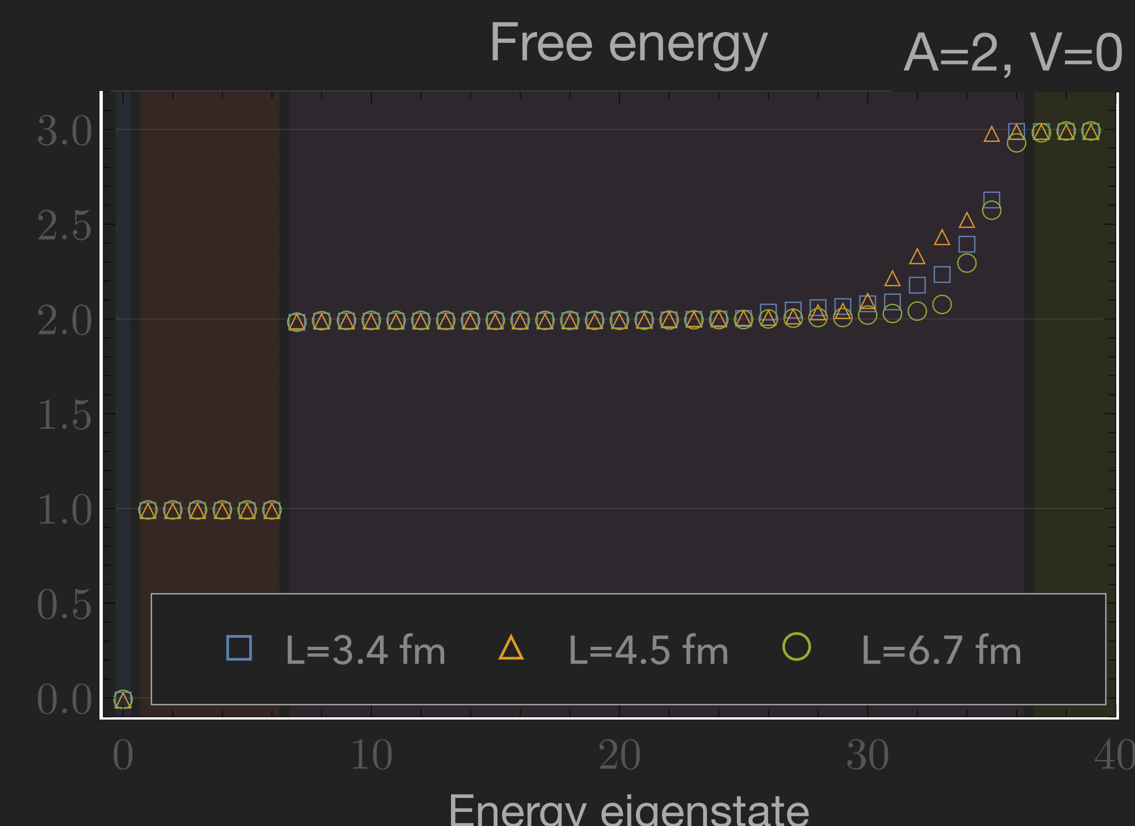


W. Detmold and P. E. Shanahan, Phys. Rev. D 103, 074503 (2021)

SVM

- SVM works but needs 100s of Gaussians to converge to FV ground state
  [M. Eliyahu, B. Bazak, and N. Barnea, PRC 2020]
  - Able to represent bound states
  - Also able to represent scattering states
- Cubic boundary conditions increase the cost significantly
- Going beyond A=3 is very challenging in FV





DIFFERENTIABLE PROGRAMMING

- Obviously better to optimise all parameters in wavefunction ansatz but how?
  - Need gradients of objective function (energy bound) w.r.t parameters

$$\mathcal{E}\left[\Psi_h^{(N)}(\theta)\right] = \frac{\mathbf{c}\cdot(\mathbb{K}+\mathbb{V}_2+\mathbb{V}_3)\cdot\mathbf{c}}{\mathbf{c}\cdot\mathbb{N}\cdot\mathbf{c}}$$

$$\nabla_\theta\mathcal{E} = -\frac{\mathbf{c}\cdot(\mathbb{K}+\mathbb{V}_2+\mathbb{V}_3)\cdot\mathbf{c}}{(\mathbf{c}\cdot\mathbb{N}\cdot\mathbf{c})^2}\nabla_\theta(\mathbf{c}\cdot\mathbb{N}\cdot\mathbf{c}) + \frac{1}{\mathbf{c}\cdot\mathbb{N}\cdot\mathbf{c}}\left(\nabla_\theta(\mathbf{c}\cdot\mathbb{K}\cdot\mathbf{c}) + \nabla_\theta\left(\mathbf{c}\cdot\mathbb{V}_2\cdot\mathbf{c}\right) + \nabla_\theta\left(\mathbf{c}\cdot\mathbb{V}_3\cdot\mathbf{c}\right)\right.$$

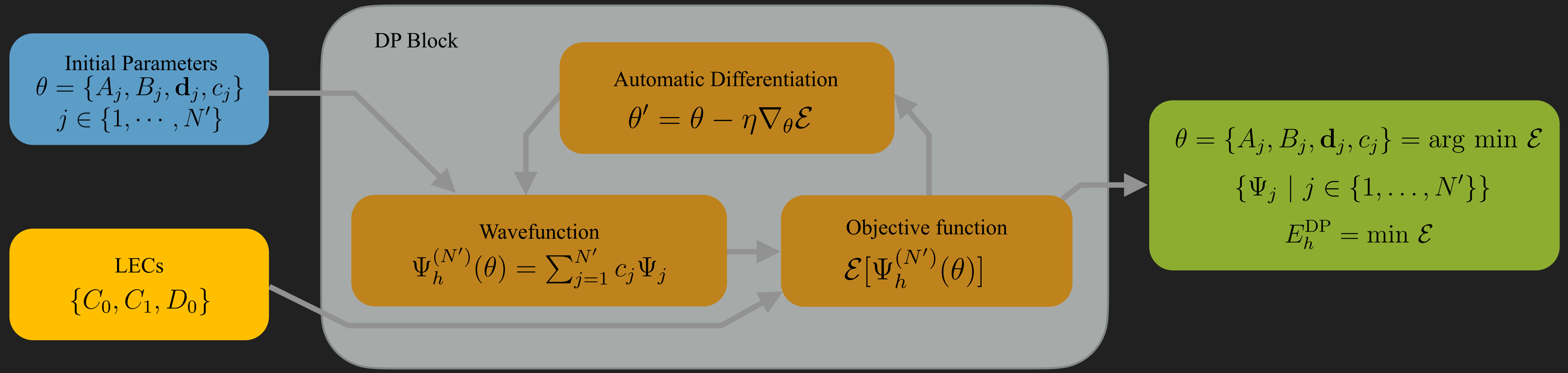
$$\nabla_\theta(\mathbf{c}\cdot\mathbb{X}\cdot\mathbf{c}) = \sum_{i,j}\left(\nabla_\theta\left(c_i c_j\right)[\mathbb{X}]_{ij} + c_i c_j\nabla_\theta[\mathbb{X}]_{ij}\right)$$

- Very large chain rule expressions can be computed using automatic differentiation
  - Automatic differentiation (AD) development driven by ML: at the heart of backpropagation for training of neural networks
  - Very efficient and easy too use implementations in ML frameworks

Sun et al., 2202.03530

DIFFERENTIABLE PROGRAMMING

- Implement in two stages
  - Stage 1: DP to optimise a set of N′ Gaussians given input LECs
  - Stage 2: combine sets of optimised Gaussians using GEVP



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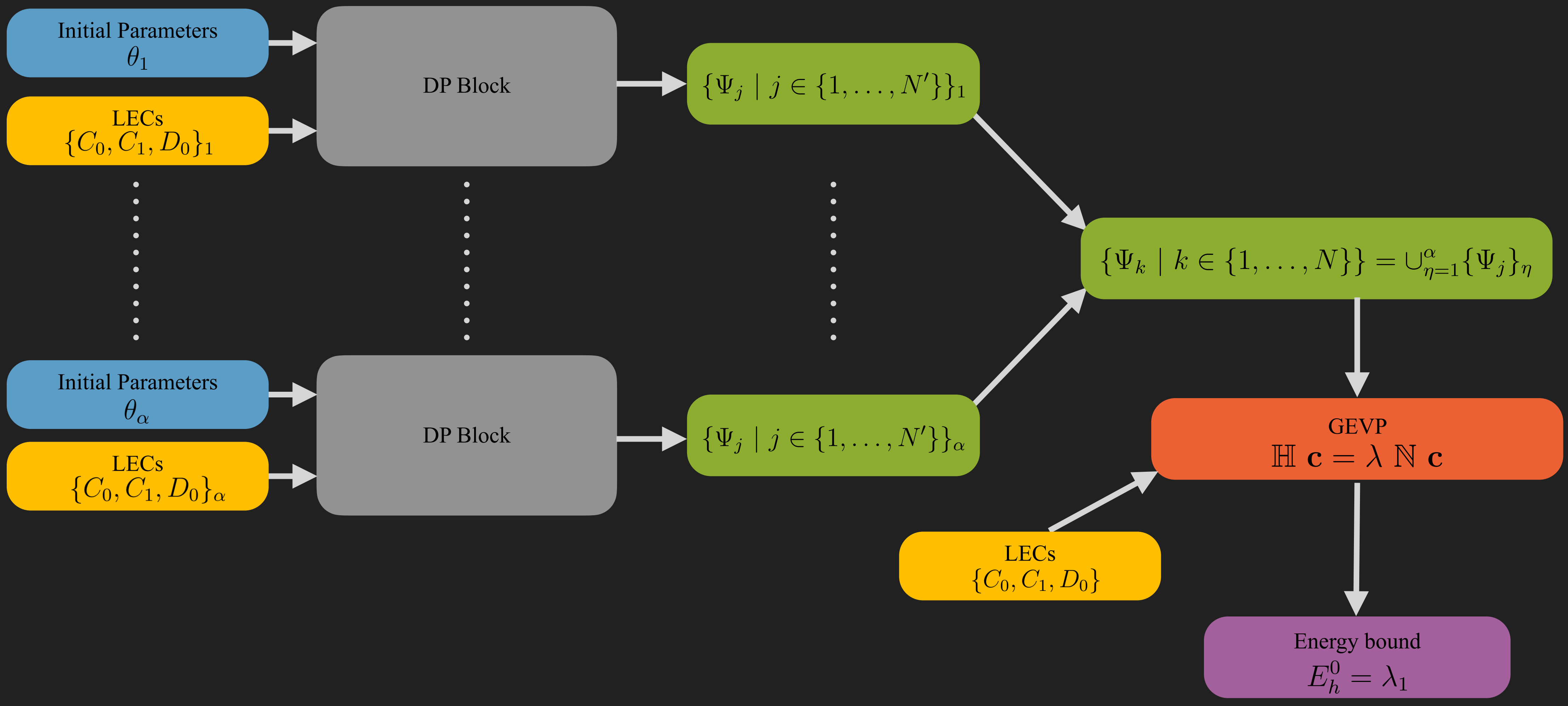
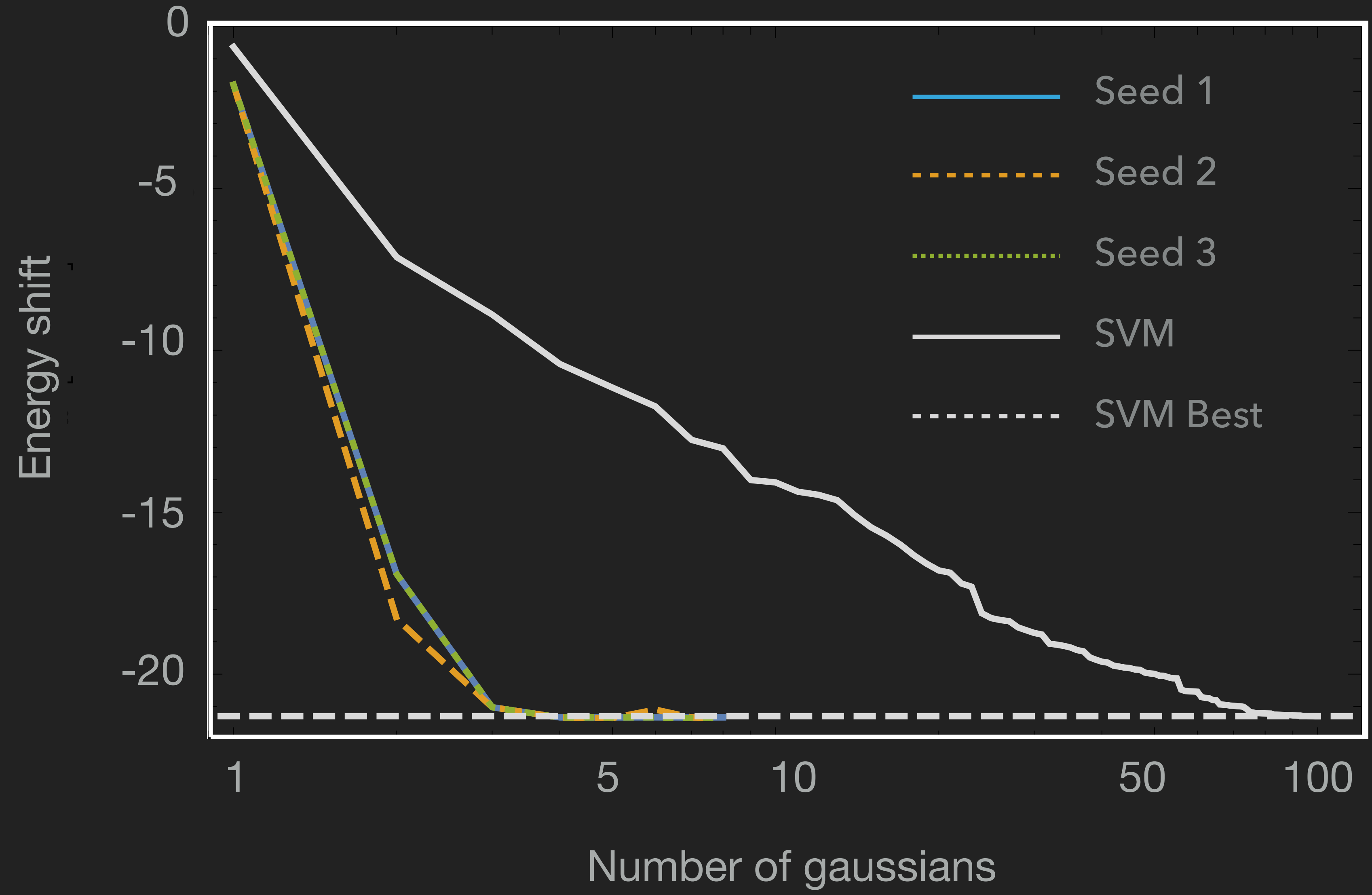


DIFFERENTIABLE PROGRAMMING

- Batched AD controls memory use (necessary for GPU)
    - Computational graph of the program computed in chunks and discarded after gradient computed
- First order gradient descent based on AD gradients
    - Self-adaptive step sizes
    - Step clipping
- Optimisation cost for n-body N-term wavefunction: $O\left(N^2 n! n^3\right)$
    - Sequential construction for N=α×N'-term: $O\left(\alpha N'^2 n! n^3\right)$

DIFFERENTIABLE PROGRAMMING

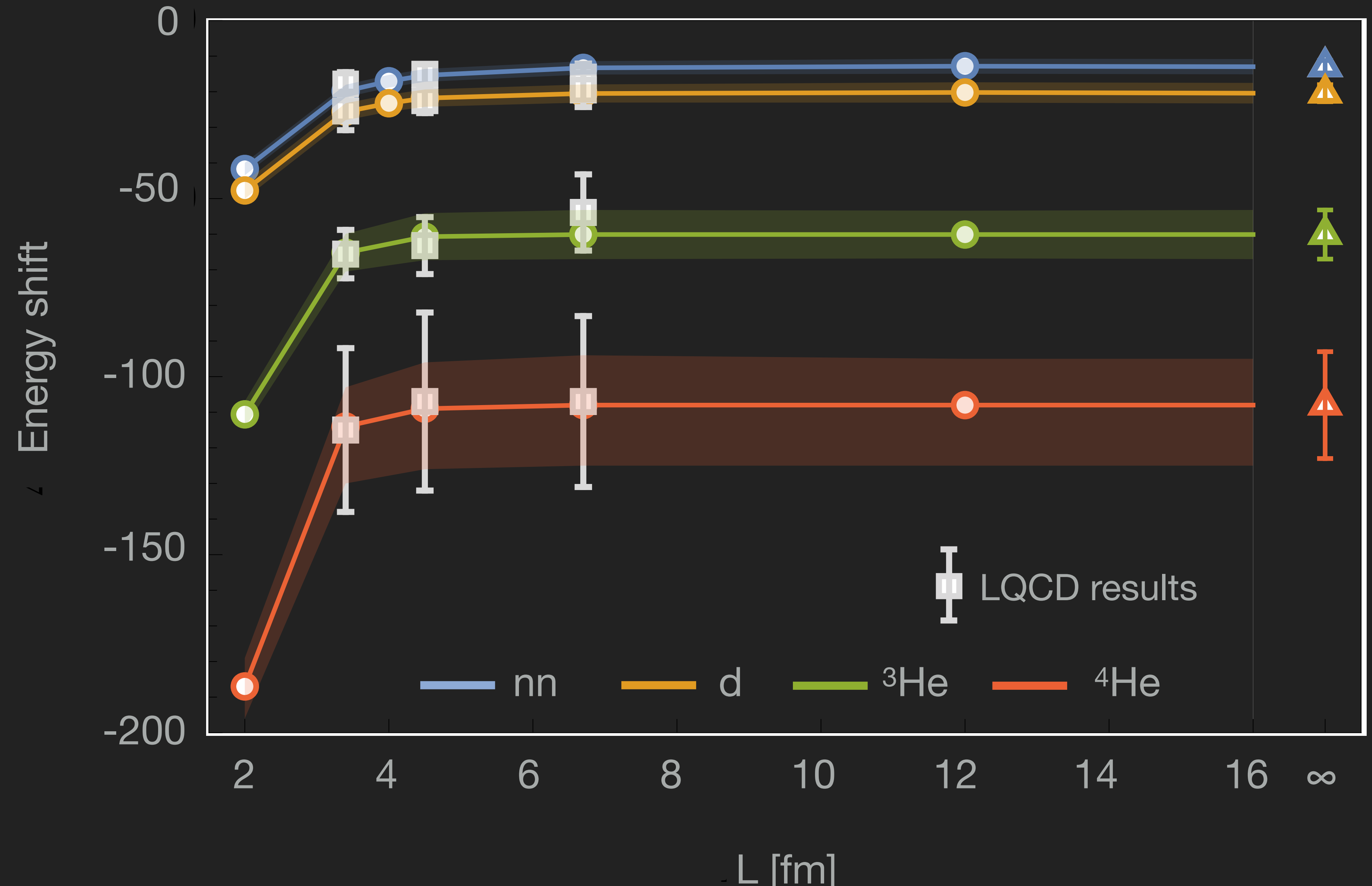
- DP-GEVP converges MUCH faster than SVM and finds slightly lower minimum



Sun et al., 2202.03530

FVEFT SPECTRA USING DIFFERENTIABLE PROGRAMMING

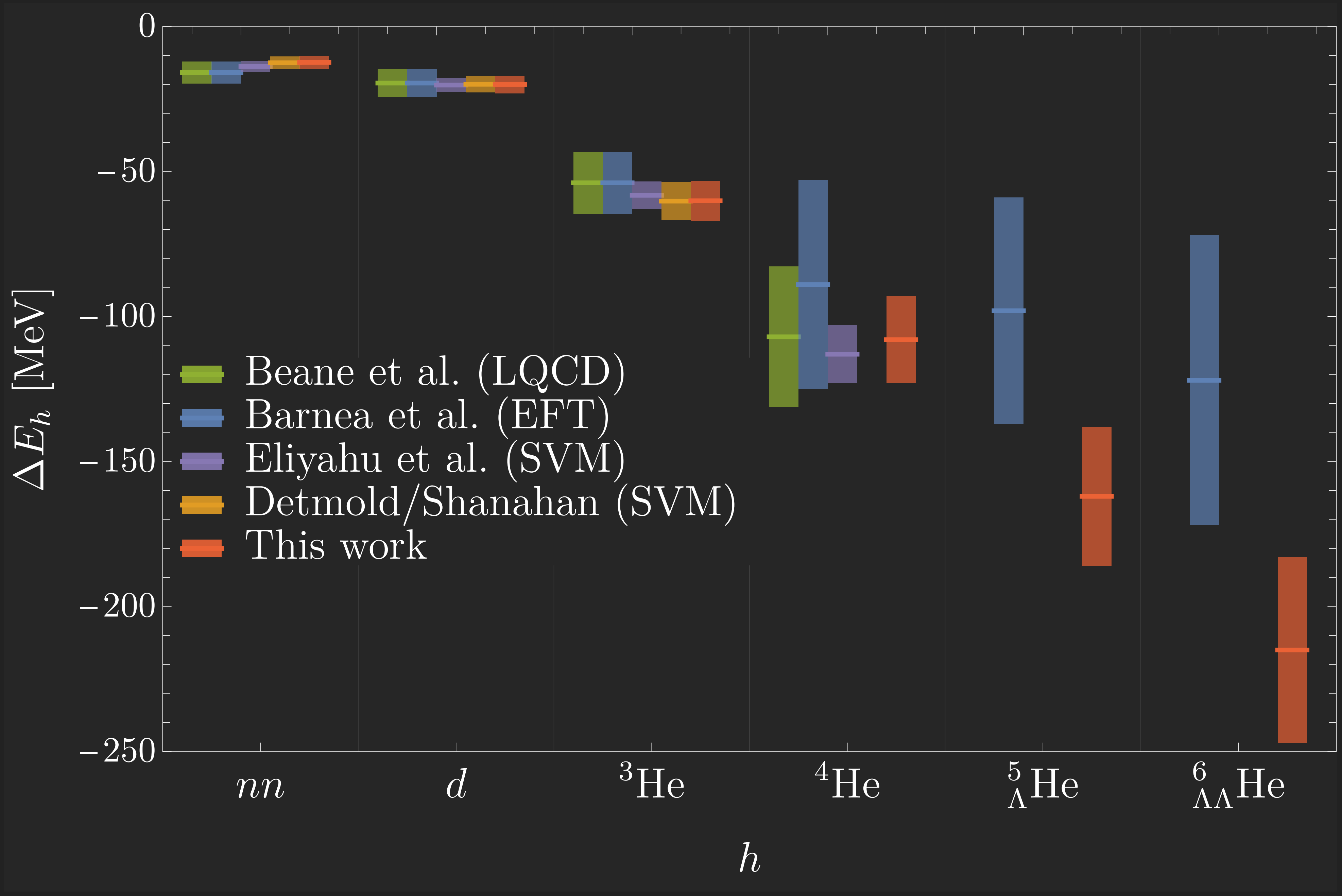
- Once LECs determined can study volume dependence



Sun et al., 2202.03530

INFINITE VOLUME SPECTRA USING DIFFERENTIABLE PROGRAMMING

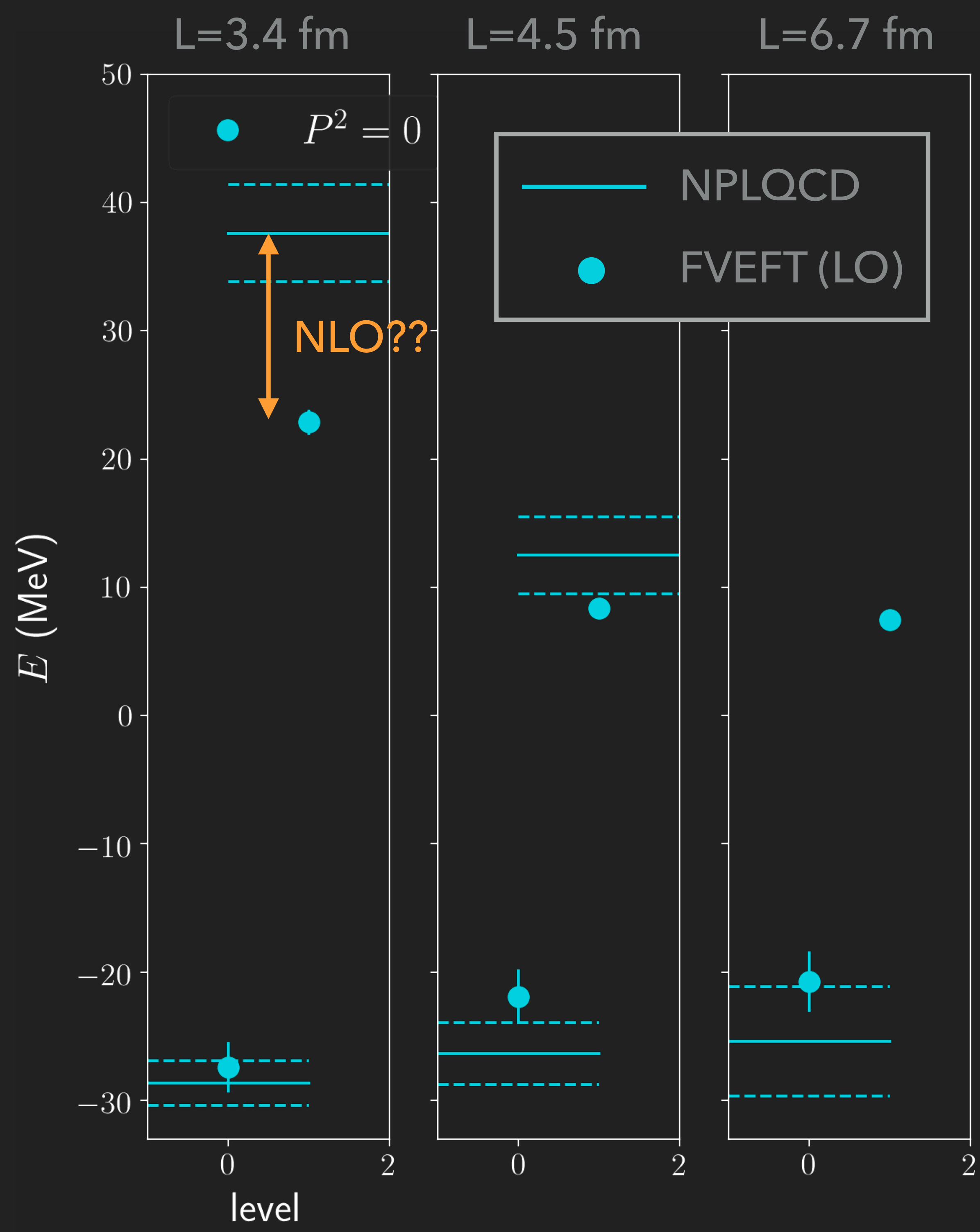
- Diff programming offers better way to optimise wavefunction



Sun et al., 2202.03530

BEYOND LEADING ORDER – EXCITED STATES

- Variational method produces more than ground state
- LQCD not restricted to ground states
  - Excited FV NN scattering states from NPLQCD 2012 (A_1^+ cubic rep)
  - Many more NN states from recent variational study
- Figure shows FVEFT with only LO
- Currently implementing terms from NLO Lagrangian
  - Will match to excited states to determine NLO counterterms (including S-D mixing)



PIONLESS EFT

- LQCD-EFT matching is a powerful tool to connect LQCD to phenomenology
  - Spectroscopy and matrix elements
- Differential programming approach vastly improves on SVM
  - More efficient representation of states
  - Able to go to larger nuclei
- Extensions
  - Hypernuclei and excited states
  - NLO EFT (+ pions)

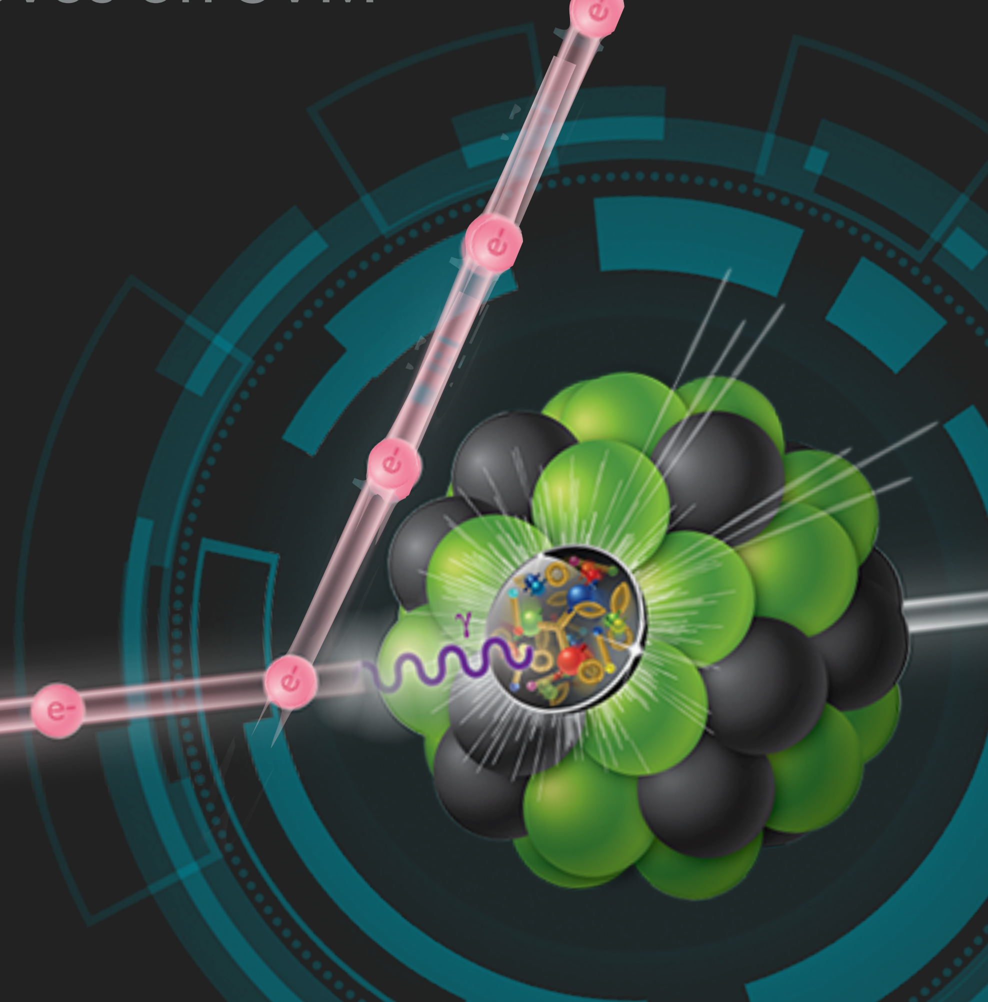
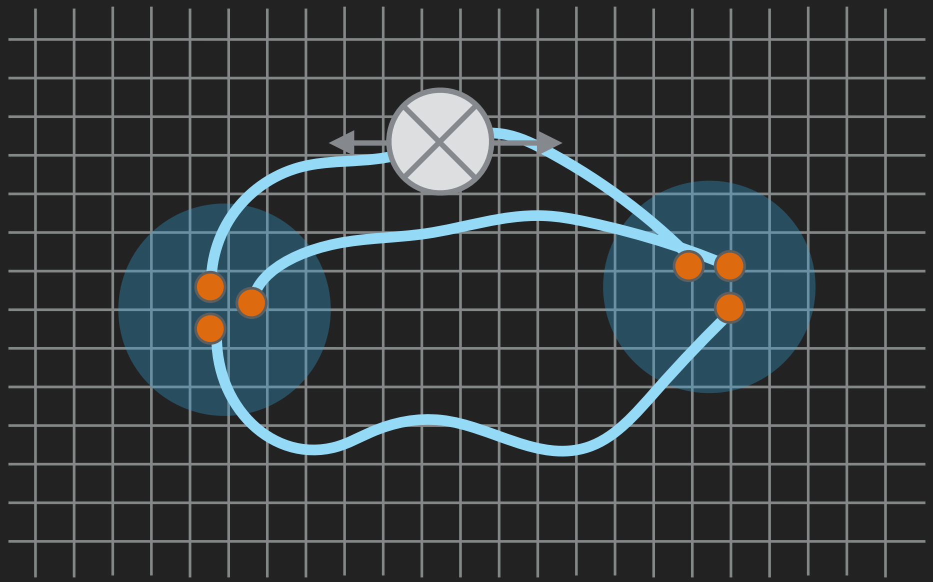


image credit: Brookhaven National Lab

FIN

LQCD MOMENTUM FRACTIONS

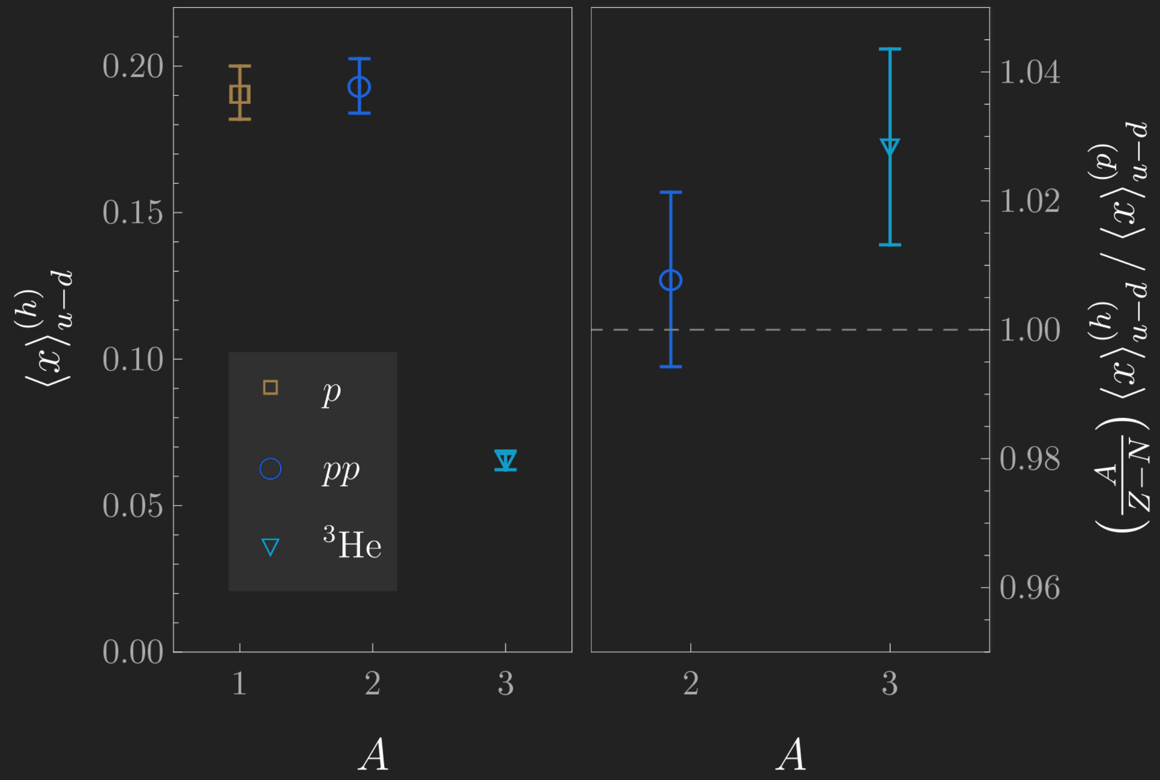


- NPLQCD calculation of various matrix elements in nuclei: focus on momentum fraction
  - Local twist-2 operator matrix element

$$\bar{q}\gamma^{\{\mu_1} D^{\mu_2} \ldots D^{\mu_n\}} q$$

  - Unphysical quark masses for which pion mass is 806 MeV
  - Single fixed volume L~4.5 fm
  - *pp* and ^{3}*He* systems

[WD et al. PRL 2021]



	p	pp	^{3}He
$\langle x \rangle^{(h)}_{u-d}$	0.191(1)(9)	0.194(2)(9)	0.066(1)(3)
$\left(\frac{A}{Z-N}\right) \frac{\langle x \rangle^{(h)}_{u-d}}{\langle x \rangle^{(p)}_{u-d}}$	–	1.007(14)	1.028(15)

See Phiala Shanahan's talk EG.00002 @ 11:57 today

TWIST-2 OPERATORS

- EFT: match QCD operators to all possible hadronic operators with same symmetries
- Used in pion and N sectors to connect lattice PDF moments to experiment [Arndt & Savage; Chen & Ji; Detmold et al.,…]
- Isoscalar, spin independent operator matching:

$$\bar{q}\gamma^{\{\mu_1} D^{\mu_2} \ldots D^{\mu_n\}} q \longrightarrow + c_n N^\dagger \mathcal{V}^{\mu_1 \cdots \mu_n} N + c_n' N^\dagger S^{\{\mu_1} A^{\mu_2} \mathcal{V}^{\mu_3 \cdots \mu_n\}} N + \ldots$$
$$+ \alpha_n N^\dagger \mathcal{V}^{\mu_1 \cdots \mu_n} N N^\dagger N + \beta_n N^\dagger \mathcal{V}^{\mu_1 \cdots \mu_n} \tau_j^{\xi+} N N^\dagger \tau_j^{\xi+} N + \ldots$$

Two body counterterms

- where

$$\mathcal{V}^{\mu_1 \cdots \mu_n} = \left(v + i\frac{D}{M}\right)^{\mu_1} \ldots \left(v + i\frac{D}{M}\right)^{\mu_n}$$

$$\tau_j^{\xi\pm} = \frac{1}{2}\left(\xi^\dagger \tau_j \xi \pm \xi \tau_j \xi^\dagger\right)$$

[J W Chen, WD PLB 2005]

NUCLEAR PDF MOMENTS

- Nucleon matrix elements (includes pion loop effects)

$$v_{\mu_1} \ldots v_{\mu_n} \langle N | \mathcal{O}^{\mu_1 \cdots \mu_n} | N \rangle = \langle x^n \rangle_q$$

- Nuclear matrix elements

$$\begin{aligned} \langle x^n \rangle_{q|A} &\equiv v_{\mu_1} \ldots v_{\mu_n} \langle A | \mathcal{O}^{\mu_1 \cdots \mu_n} | A \rangle \\ &= \langle x^n \rangle_q \left[A + \alpha_n \left\langle A \middle| \left(N^\dagger N\right)^2 \middle| A \right\rangle + \beta_n \left\langle A \middle| \left(N^\dagger \tau N\right)^2 \middle| A \right\rangle \right] + \ldots \end{aligned}$$

Dominant term

- β_n term suppressed by N_c^2 [Kaplan & Savage 96; K & Manohar 97]
- Ellipsis includes higher-body operators, terms with derivatives: higher-order in power-counting

[J W Chen, WD PLB 2005]