
WILL DETMOLD 

FINITE VOLUME PIONLESS EFFECTIVE FIELD THEORY FOR NUCLEAR SYSTEMS

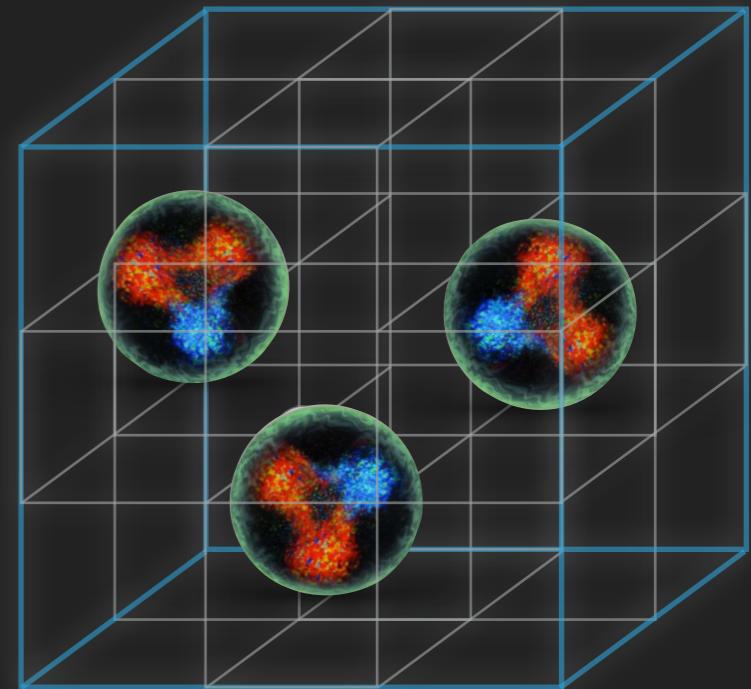
2102.04329 with P Shanahan

2202.03530 with X Sun, D Luo and P Shanahan

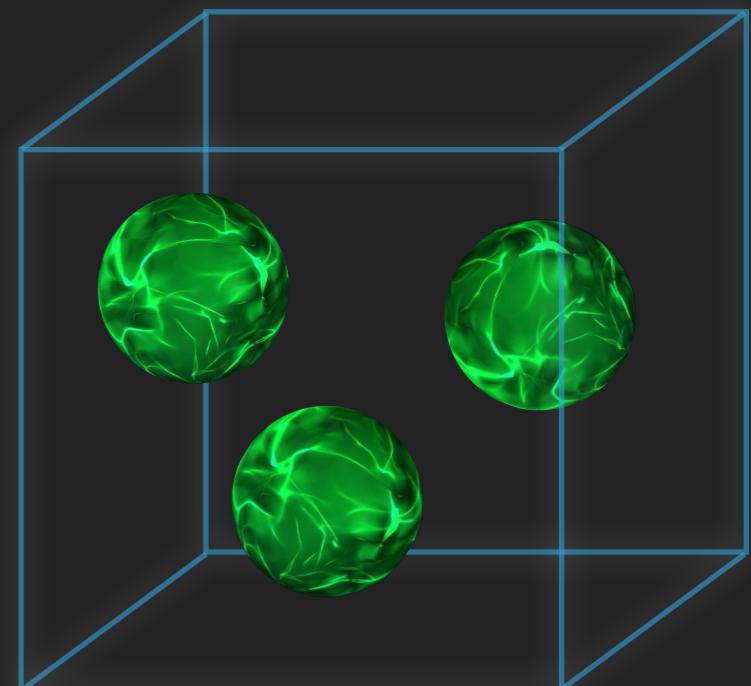
work in progress (D Luo, P Shanahan, F Romero-Lopez)

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



\approx



PIONLESS EFT

- ▶ Leading order pionless EFT Hamiltonian

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

- ▶ Two- and three-body interactions

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

Three body low energy constant

Two body low energy constants

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

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

VARIATIONAL METHOD

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

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

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

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

Vector
Wavefunction parameters

- ▶ Impose periodicity:

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

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

- ▶ Symmetrise spatial wavefunction under particle interchange

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

PIONLESS EFT

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

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

where eg

$$\begin{aligned} |\chi {}^3\text{H}, j_z = 1/2\rangle = & \frac{1}{\sqrt{6}} [|n^\uparrow p^\uparrow n^\downarrow\rangle - |n^\downarrow p^\uparrow n^\uparrow\rangle - |p^\uparrow n^\uparrow n^\downarrow\rangle \\ & + |p^\uparrow n^\downarrow n^\uparrow\rangle - |n^\uparrow n^\downarrow p^\uparrow\rangle + |n^\downarrow n^\uparrow p^\uparrow\rangle] \end{aligned}$$

- ▶ 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

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

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

- ▶ Integrals can be performed analytically

$$\begin{aligned} [\mathbb{N}]_{ij} &\equiv \int \Psi_L^{\text{sym}} (A_i, B_i, \mathbf{d}_i; \mathbf{x})^* \Psi_L^{\text{sym}} (A_j, B_j, \mathbf{d}_j; \mathbf{x}) d\mathbf{x} \\ &= \sum_{\mathcal{P}, \mathcal{P}'} \prod_{\alpha \in \{x, y, z\}} \sqrt{\frac{(2\pi)^n}{\text{Det} [C_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]}} \sum_{\mathbf{b}^{(\alpha)}}^{(\alpha)} | \leq \tilde{b} \exp \left[-\frac{1}{2} \Omega_{i\mathcal{P}; \mathcal{P}'}^{(\alpha)} \right] \end{aligned}$$

Objects built from the wavefunction parameters

STOCHASTIC VARIATIONAL METHOD

- ▶ Energy bound

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

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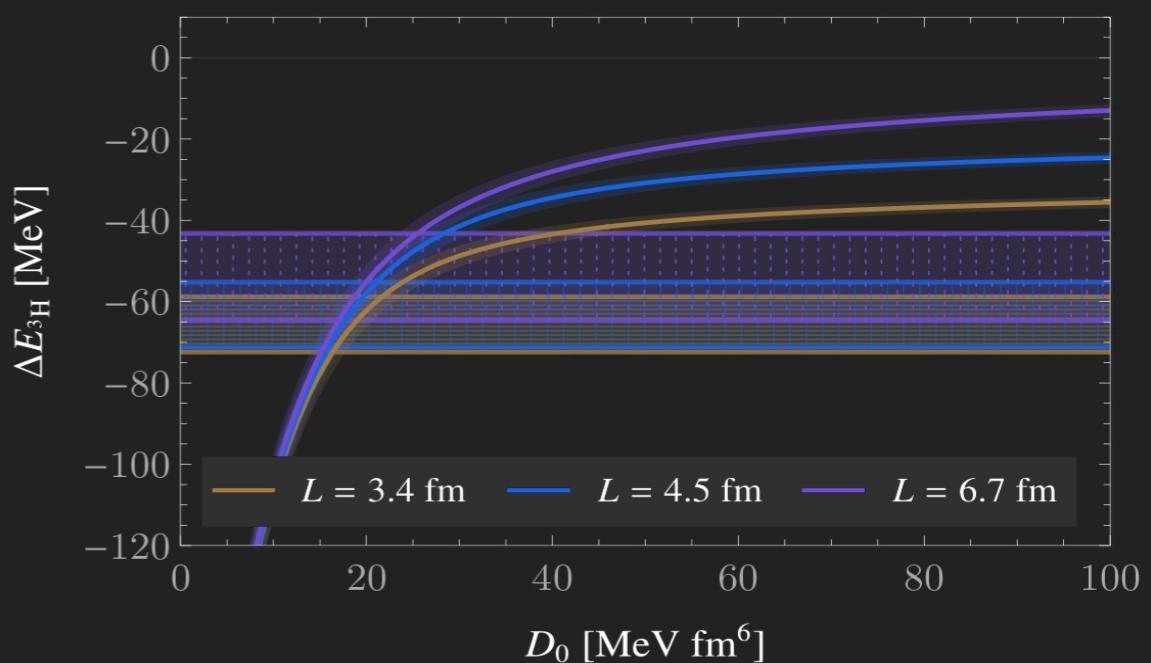
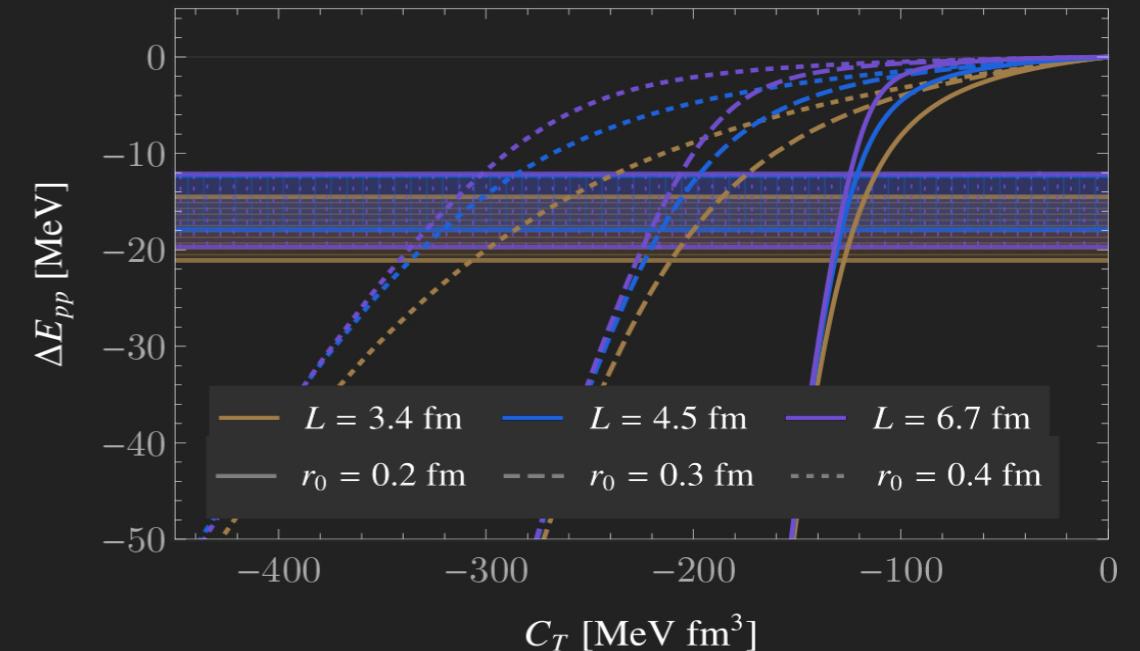
- ▶ Integrals can be performed analytically

$$\begin{aligned} [\mathbb{V}_3]_{ij} &\equiv D_0 \sum_{a \neq b \neq c}^{\text{cyc}} \int \Psi_L^{\text{sym}}(A_i, B_i, \mathbf{d}_i; \mathbf{x})^* g_\Lambda(\mathbf{x}_a - \mathbf{x}_b, L) g_\Lambda(\mathbf{x}_b - \mathbf{x}_c, L) \Psi_L^{\text{sym}}(A_j, B_j, \mathbf{d}_j; \mathbf{x}) d\mathbf{x} \\ &= D_0 \left(\frac{\Lambda^3}{8\pi^{3/2}} \right)^2 \sum_{\mathcal{P}, \mathcal{P}'} \sum_{a \neq b \neq c}^{\text{cyc}} \prod_{\alpha \in \{x, y, z\}} \sqrt{\frac{(2\pi)^n}{\text{Det}[\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}]}} \exp \left[-\frac{1}{2} \left(\mathbf{d}_{i\mathcal{P}}^{(\alpha)} \cdot B_{i\mathcal{P}}^{(\alpha)} \cdot \mathbf{d}_{i\mathcal{P}}^{(\alpha)} + \mathbf{d}_{j'}^{(\alpha)} \cdot B_{j'\mathcal{P}'}^{(\alpha)} \cdot \mathbf{d}_{j'}^{(\alpha)} \right) \right] \\ &\times \sum_{\mathbf{b}^{(\alpha)}}^{| \mathbf{b}^{(\alpha)} | \leq \tilde{b}} \exp \left[-\frac{1}{2} \left((L\mathbf{b}^{(\alpha)}) \cdot (A_{i\mathcal{P}}^{(\alpha)} + B_{i\mathcal{P}}^{(\alpha)}) \cdot (L\mathbf{b}^{(\alpha)}) + 2\mathbf{d}_{i\mathcal{P}}^{(\alpha)} \cdot B_{i\mathcal{P}}^{(\alpha)} \cdot (L\mathbf{b}^{(\alpha)}) - \Xi^{(\alpha)} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \right. \right. \\ &\times \sum_{q^{(\alpha)}=-\tilde{q}}^{\tilde{q}} \exp \left[-\frac{L^2}{r_0^2} q^{(\alpha)2} + \frac{q^{(\alpha)2} L^2}{2r_0^4} \mathfrak{P}_v^{[a,b]} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \mathfrak{P}_v^{[a,b]} + \frac{q^{(\alpha)} L}{r_0^2} \Xi^{(\alpha)} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \mathfrak{P}_v^{[a,b]} \right] \\ &\times \sum_{t^{(\alpha)}=-\tilde{q}}^{\tilde{q}} \exp \left[-\frac{L^2}{r_0^2} t^{(\alpha)2} + \frac{t^{(\alpha)2} L^2}{2r_0^4} \mathfrak{P}_v^{[b,c]} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \mathfrak{P}_v^{[b,c]} + \frac{t^{(\alpha)} L}{r_0^2} \Xi^{(\alpha)} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \mathfrak{P}_v^{[b,c]} \right] \\ &\times \exp \left[\frac{t^{(\alpha)} q^{(\alpha)} L^2}{r_0^4} \mathfrak{P}_v^{[b,c]} \cdot [\widehat{C}_{i\mathcal{P}; j\mathcal{P}'}^{(\alpha)}]^{-1} \cdot \mathfrak{P}_v^{[a,b]} \right] \end{aligned}$$

Objects built from the wf parameters

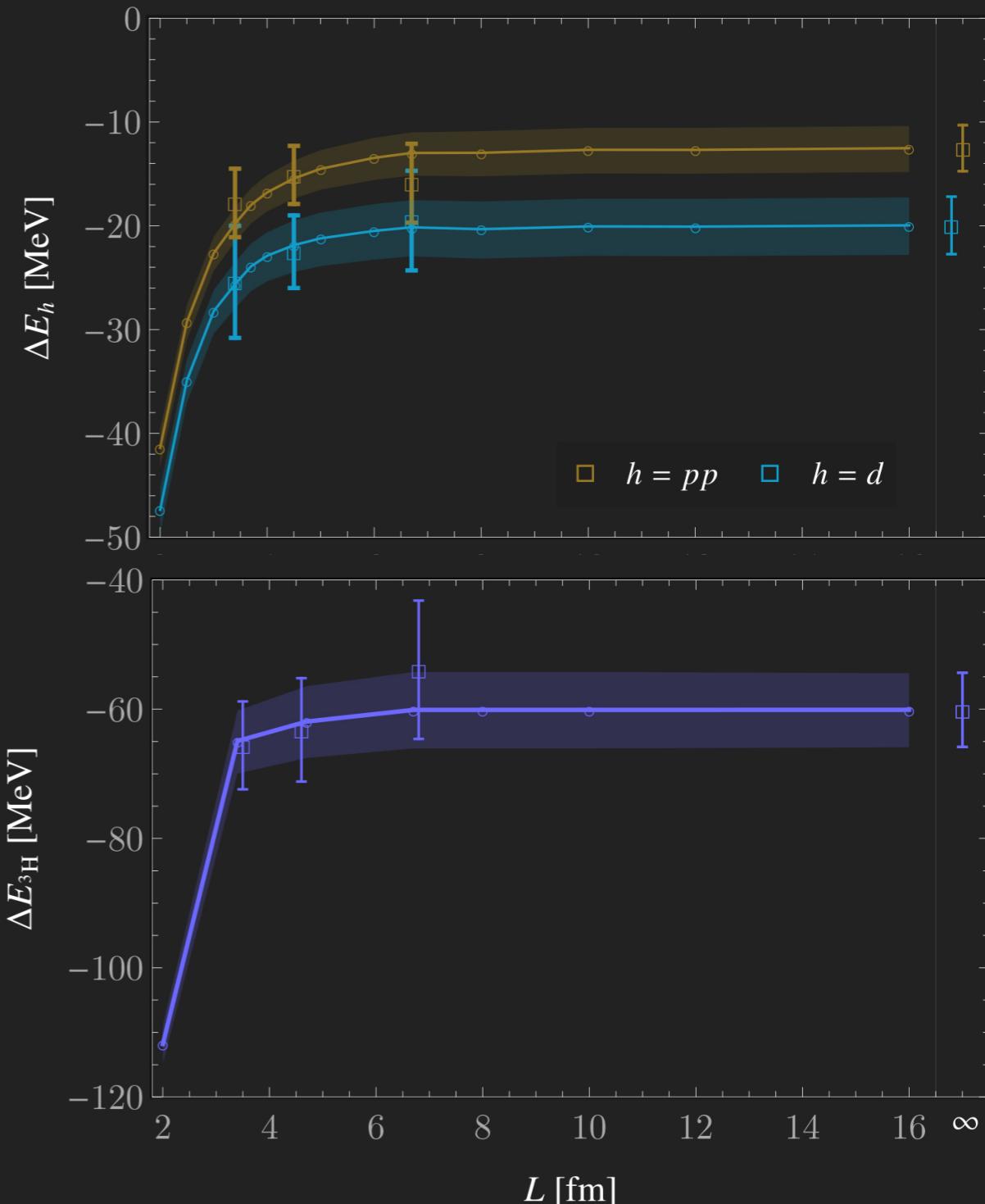
STOCHASTIC VARIATIONAL METHOD

- ▶ Match onto LQCD FV energies to determine nuclear wave functions
- ▶ NPLQCD 2012, 2017, $m_n=806$ MeV
- ▶ 2 and 3-body energies fix NN and NNN contact interactions
- ▶ ^4He has large uncertainties so does not improve constraints
- ▶ Determines infinite volume bindings
- ▶ NB: all LQCD calculations here at unphysically large quark masses



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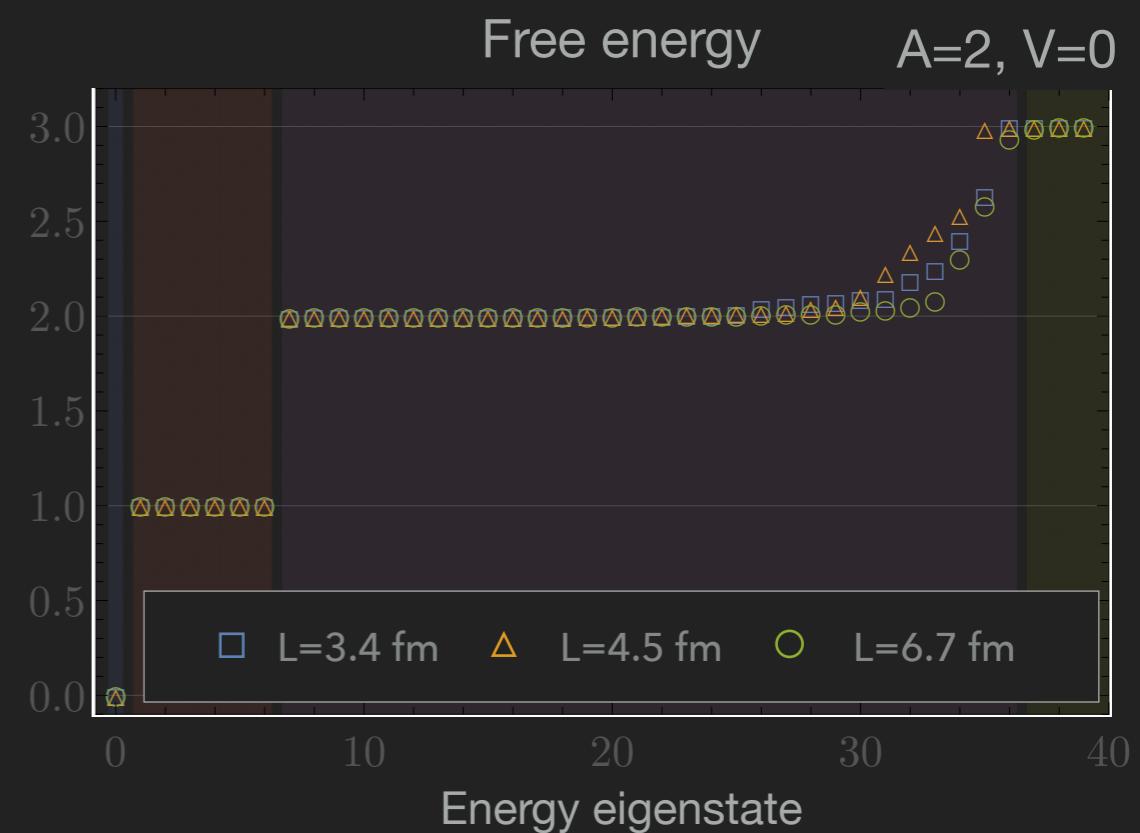
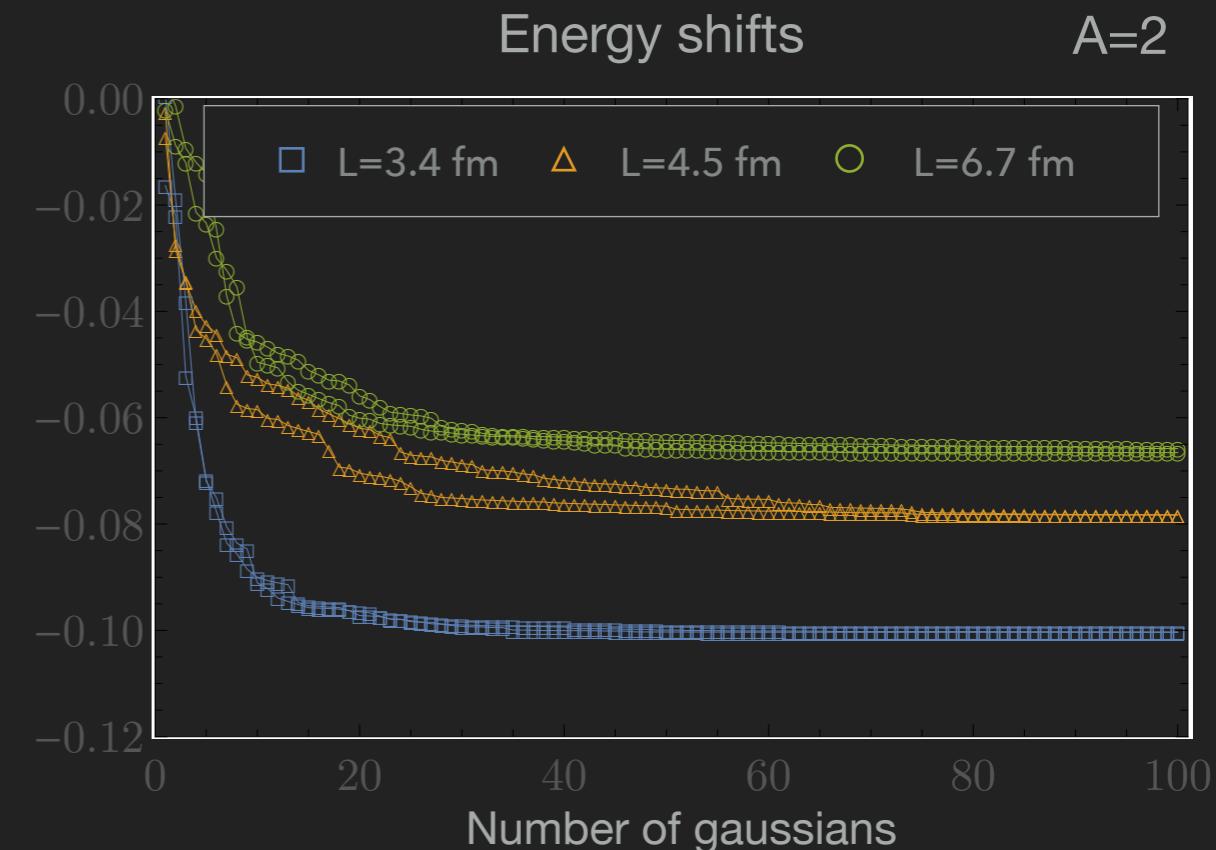


SVM

- ▶ 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

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

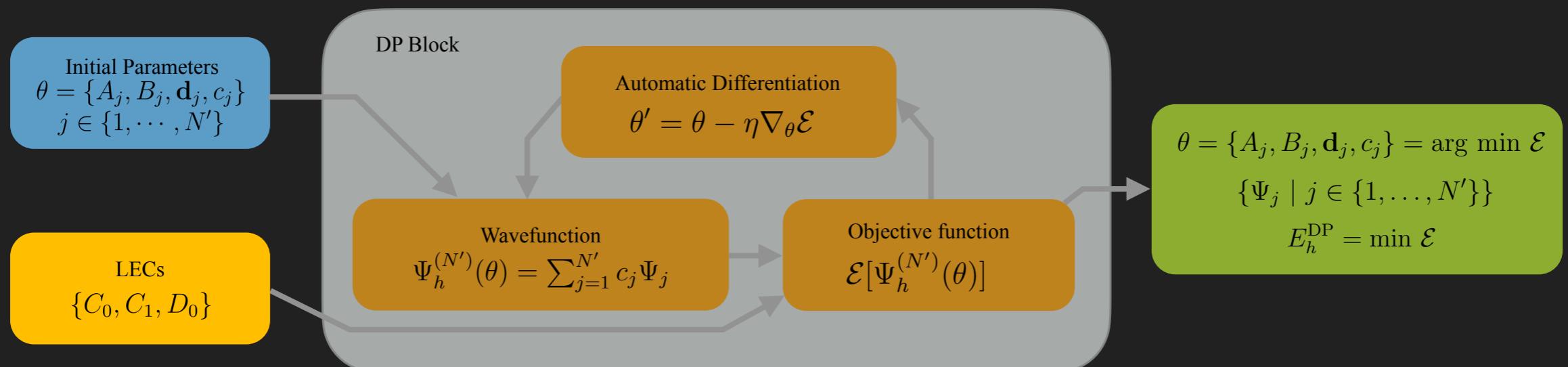
$$\nabla_{\theta} \mathcal{E} = - \frac{\mathbf{c} \cdot (\mathbb{K} + \mathbb{V}_2 + \mathbb{V}_3) \cdot \mathbf{c}}{(\mathbf{c} \cdot \mathbb{N} \cdot \mathbf{c})^2} \nabla_{\theta} (\mathbf{c} \cdot \mathbb{N} \cdot \mathbf{c}) + \frac{1}{\mathbf{c} \cdot \mathbb{N} \cdot \mathbf{c}} (\nabla_{\theta}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

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

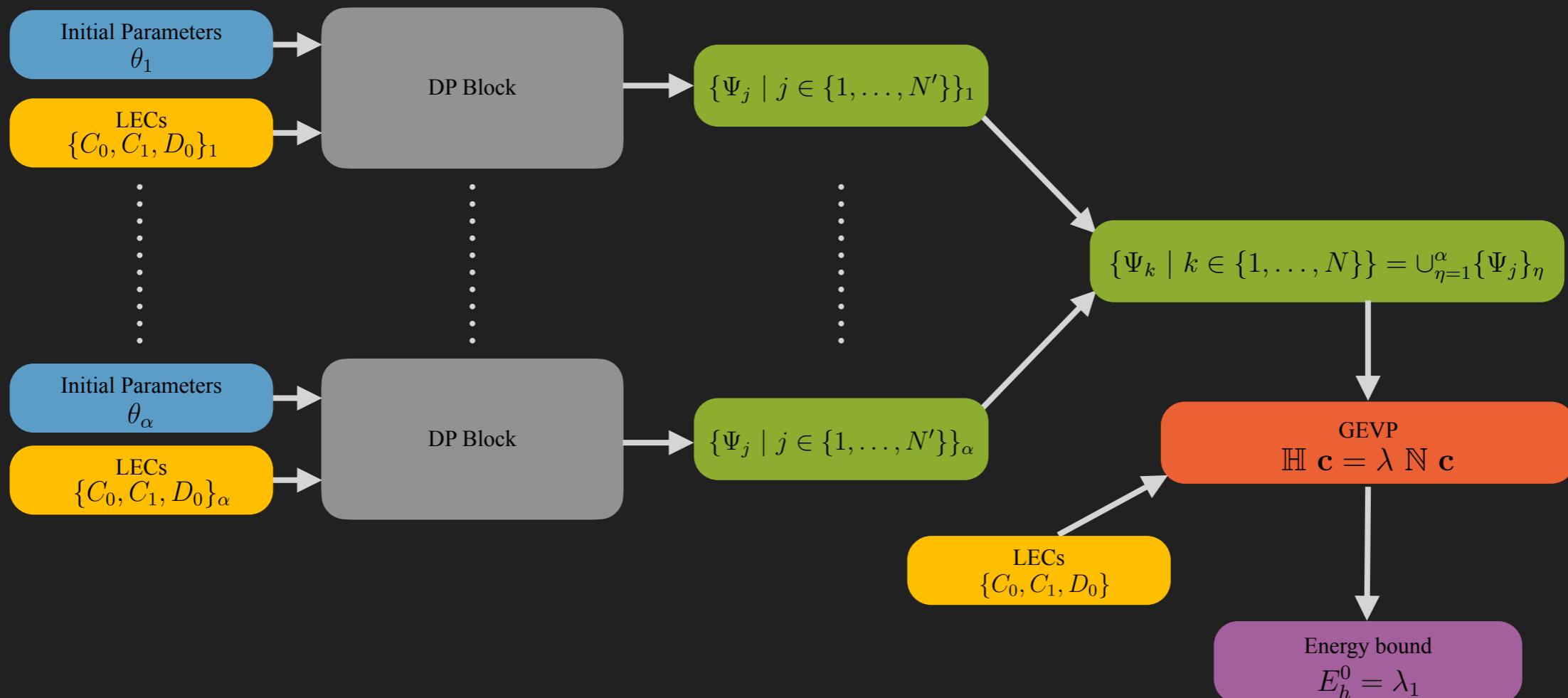
- ▶ Very large chain rule expressions can be computed using automatic differentiation
 - ▶ Automatic differentiation (AD) development driven by ML: at the heart of backpropagation for training of neural networks
 - ▶ Very efficient and easy too use implementations in ML frameworks

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



DIFFERENTIABLE PROGRAMMING

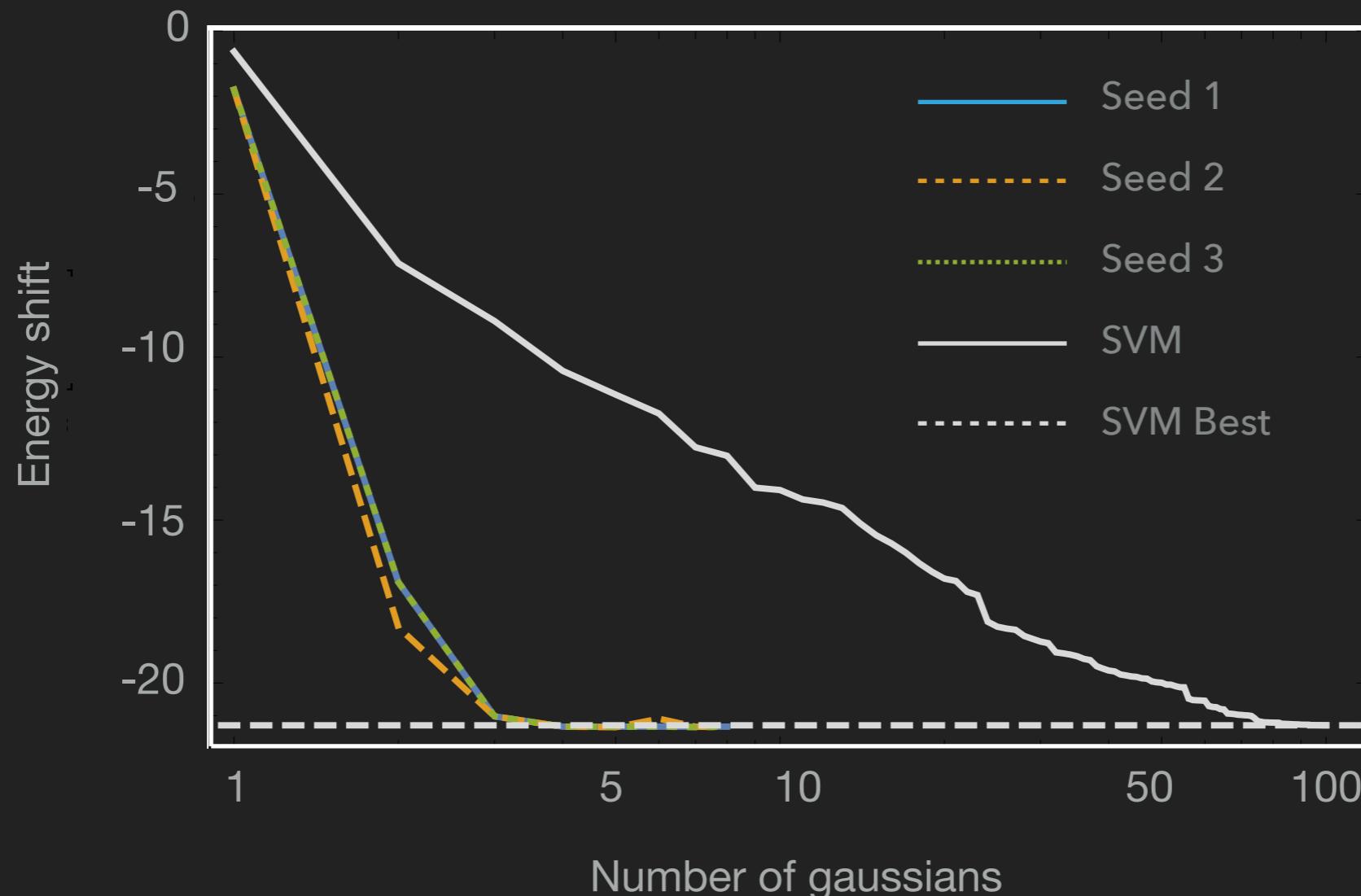


DIFFERENTIABLE PROGRAMMING

- ▶ 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: $O(N^2 n! n^3)$
- ▶ Sequential construction for $N = \alpha \times N'$ -term: $O(\alpha N'^2 n! n^3)$

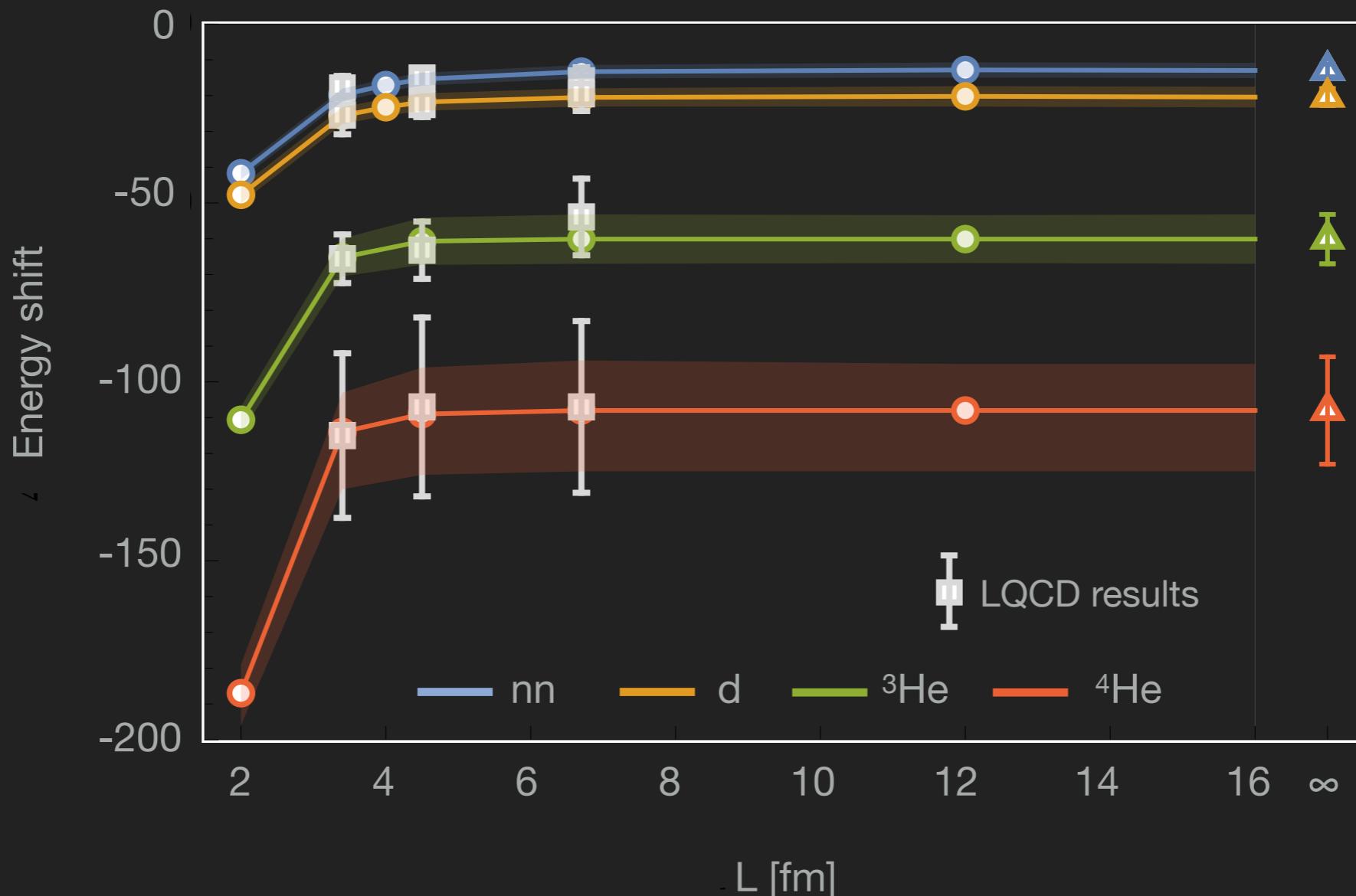
DIFFERENTIABLE PROGRAMMING

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



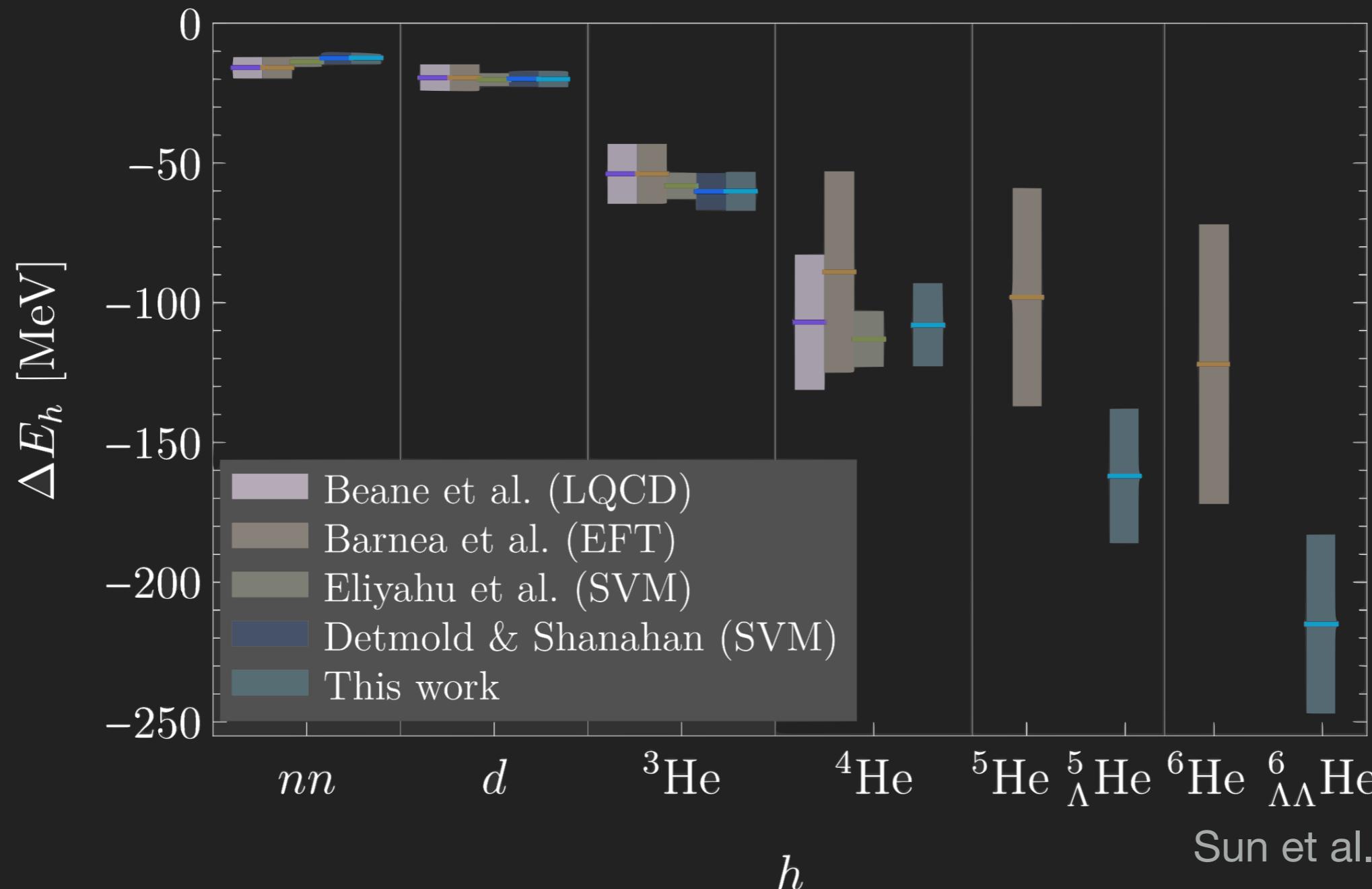
FVEFT SPECTRA USING DIFFERENTIABLE PROGRAMMING

- Once LECs determined can study volume dependence



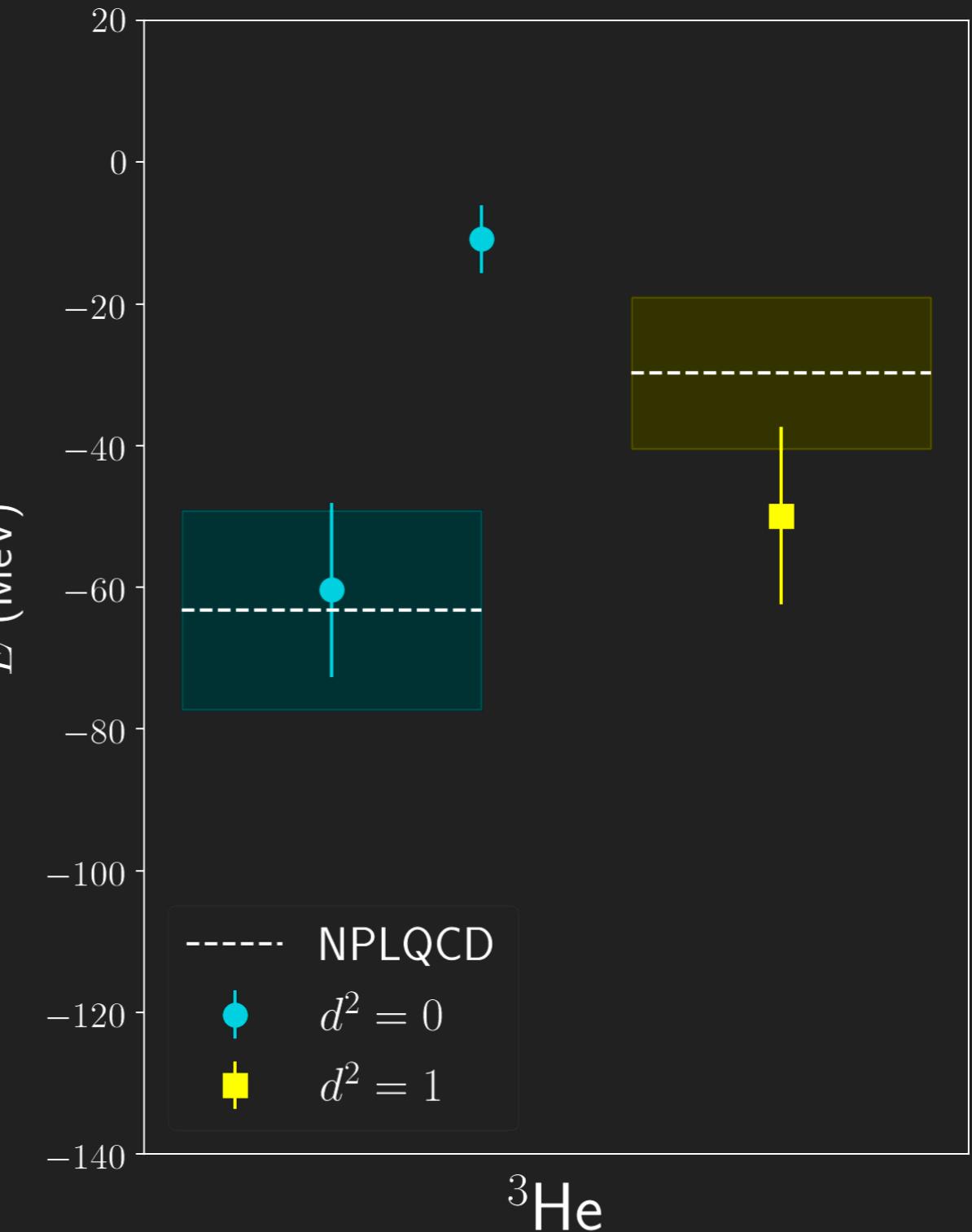
INFINITE VOLUME SPECTRA USING DIFFERENTIABLE PROGRAMMING

- ▶ Diff programming offers better way to optimise wavefunction



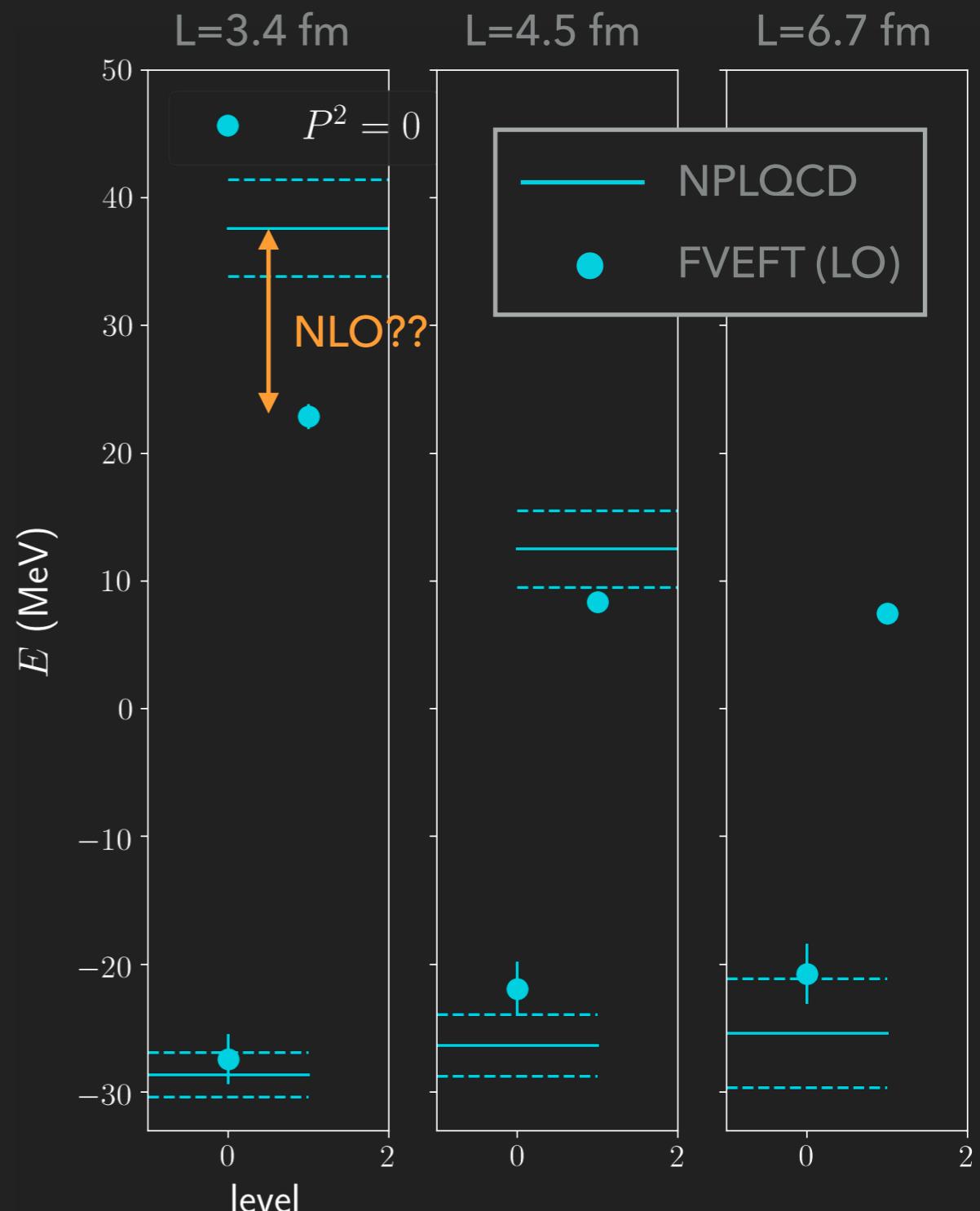
BOOSTED SYSTEMS

- ▶ Gaussian WFs do not have definite total momentum P but FV eigenstates do
- ▶ Can measure P^2 on optimised states
 - ▶ Find values very close to integers up to $P^2=3$
 - ▶ Better optimisation required to go higher
- ▶ NPLQCD 2012 results for $A=2$ for $P^2=0,1,2$ and $A=3$ for $P^2=0,1$
 - ▶ EFT matched only to $P^2=0$
 - ▶ In principle can also project to given total momentum by adding constraint term to Hamiltonian



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



PIONLESS EFT

- ▶ LQCD-EFT matching is a powerful tool to extrapolate to infinite volume
 - ▶ 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 pionless EFT, Pionful EFT

FIN

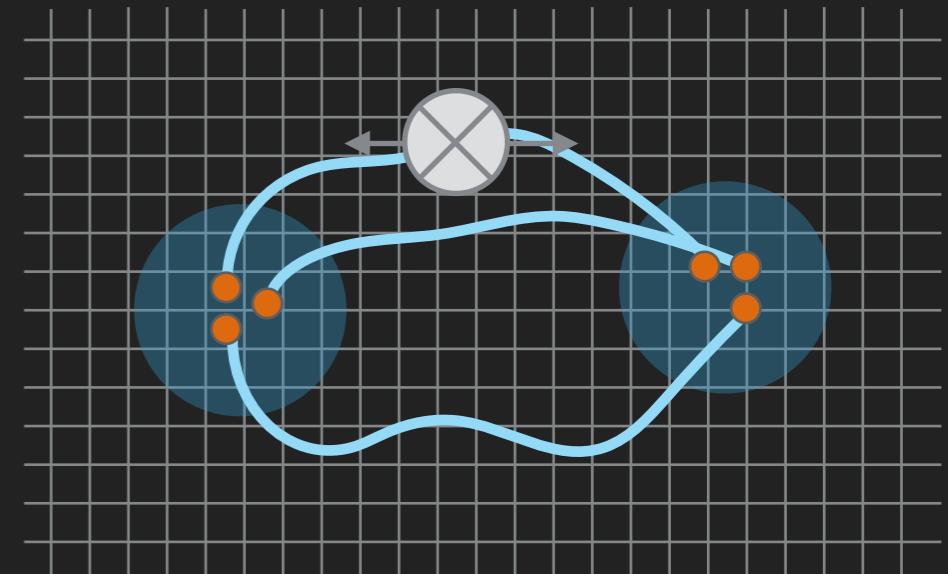
LQCD MOMENTUM FRACTIONS

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

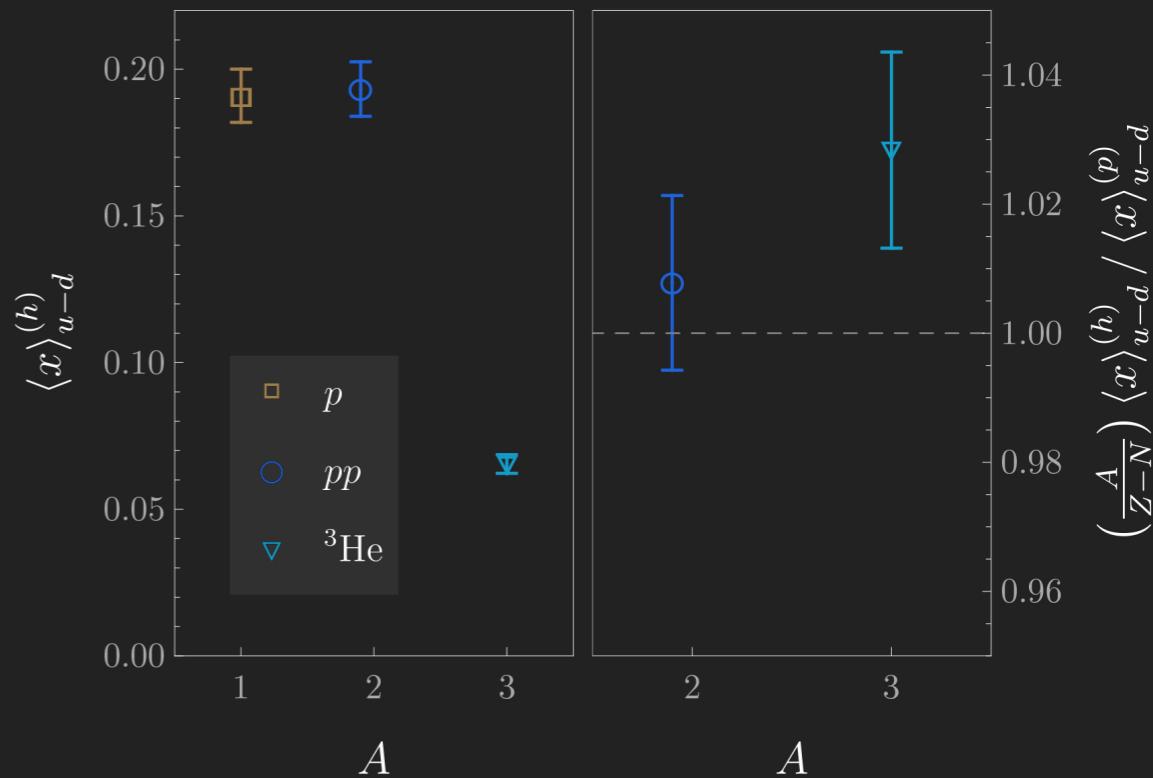
$$\bar{q} \gamma^{\{\mu_1} D^{\mu_2} \dots D^{\mu_n\}} q$$

- ▶ Unphysical quark masses for which pion mass is 806 MeV
- ▶ Single fixed volume $L \sim 4.5$ fm
- ▶ pp and ${}^3\text{He}$ systems

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



[WD et al. PRL 2021]



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:

$$\bar{q}\gamma^{\{\mu_1} D^{\mu_2} \dots D^{\mu_n\}} q \longrightarrow + c_n N^\dagger \mathcal{V}^{\mu_1\dots\mu_n} N + c'_n N^\dagger S^{\{\mu_1} A^{\mu_2} \mathcal{V}^{\mu_3\dots\mu_n\}} N + \dots$$

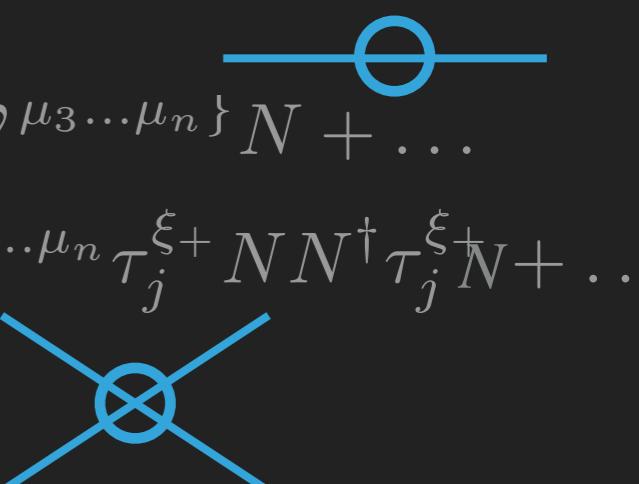
$$+ \alpha_n N^\dagger \mathcal{V}^{\mu_1\dots\mu_n} N N^\dagger N + \beta_n N^\dagger \mathcal{V}^{\mu_1\dots\mu_n} \tau_j^{\xi+} N N^\dagger \tau_j^{\xi+} N + \dots$$

Two body counterterms

▶ where

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

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



[J W Chen, WD PLB 2005]

NUCLEAR PDF MOMENTS

- ▶ Nucleon matrix elements (includes pion loop effects)

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

- ▶ Nuclear matrix elements

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

Dominant term

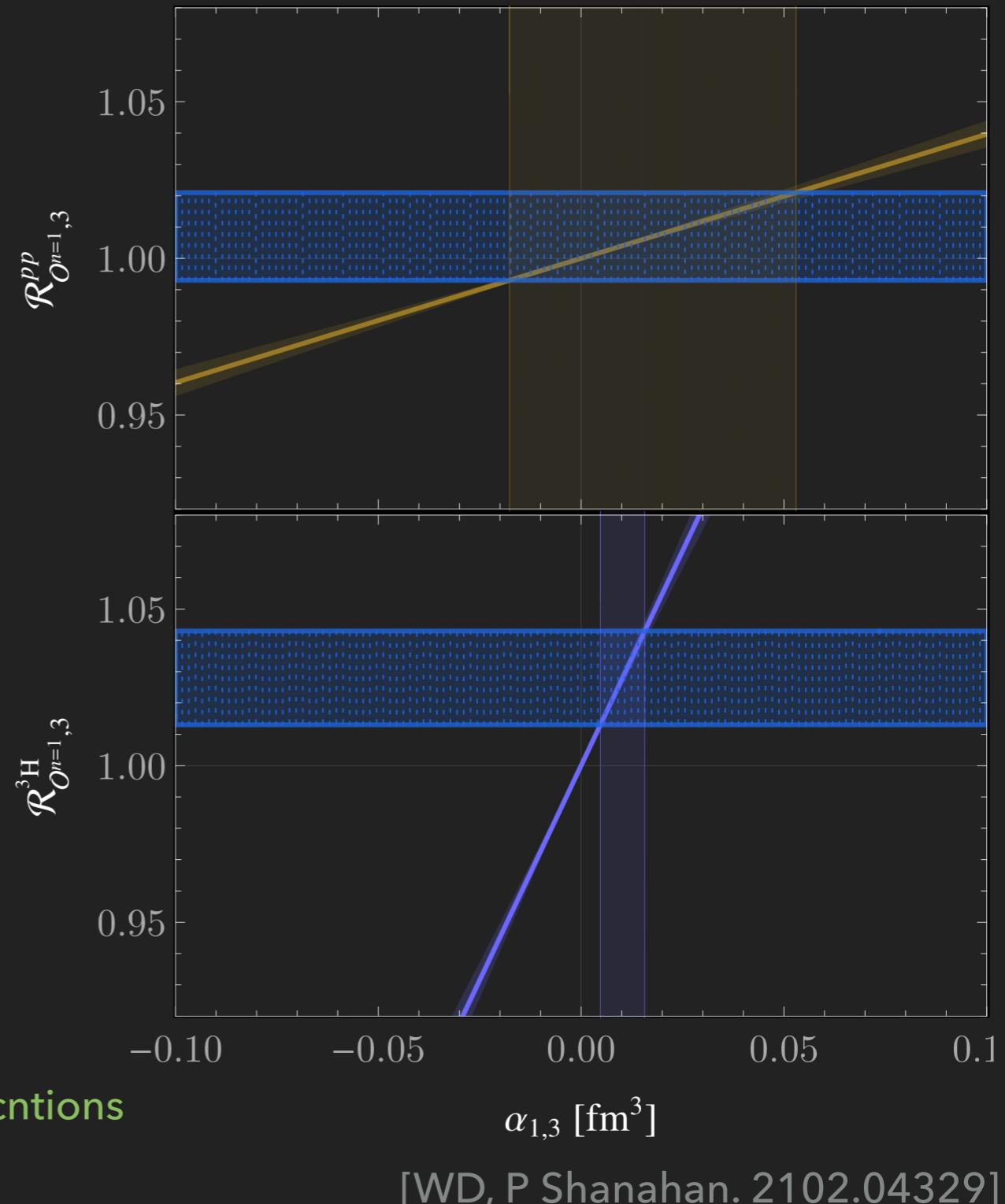
- ▶ β_n term suppressed by N_c^2 [Kaplan & Savage 96; K & Manohar 97]
- ▶ Ellipsis includes higher-body operators, terms with derivatives: higher-order in power-counting

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

$$\begin{aligned} \mathcal{R}_{\mathcal{O}^n,3}^h &\equiv \frac{A^h}{(Z^h - N^h) \langle x^n \rangle_3} \frac{\left\langle \Psi_h \left| \mathcal{O}_3^{(n)} \right| \Psi_h \right\rangle}{\langle \Psi_h | \Psi_h \rangle} \\ &= \left(1 + \frac{\alpha_{n,3}}{(Z^h - N^h) \langle x^n \rangle_3} h_h(\Lambda, L) \right) \end{aligned}$$

From wavefunctions
Two body counterterm

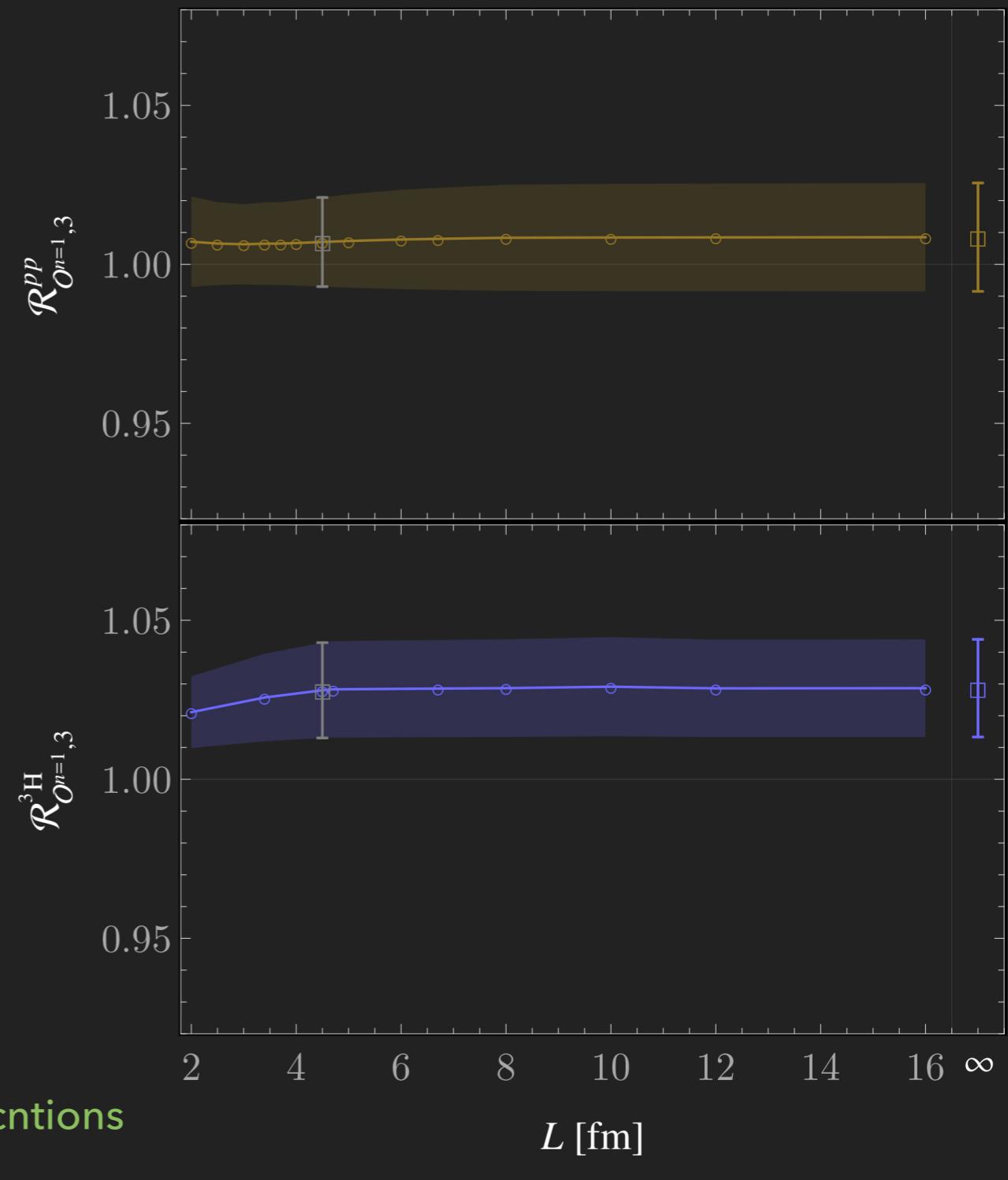


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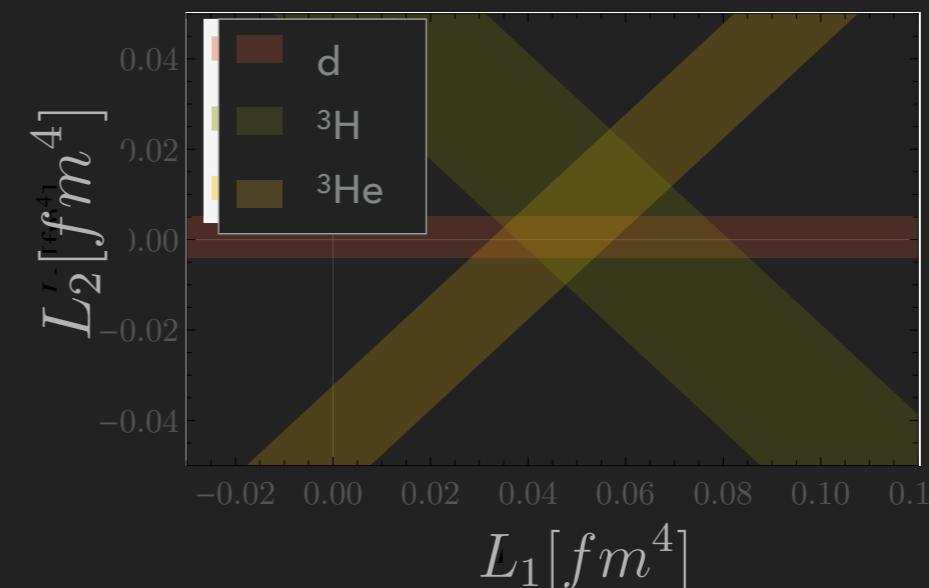
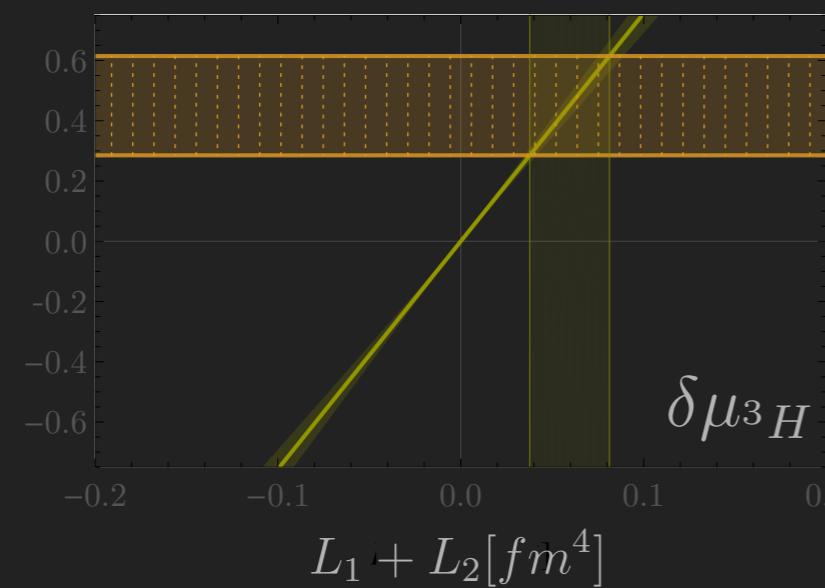
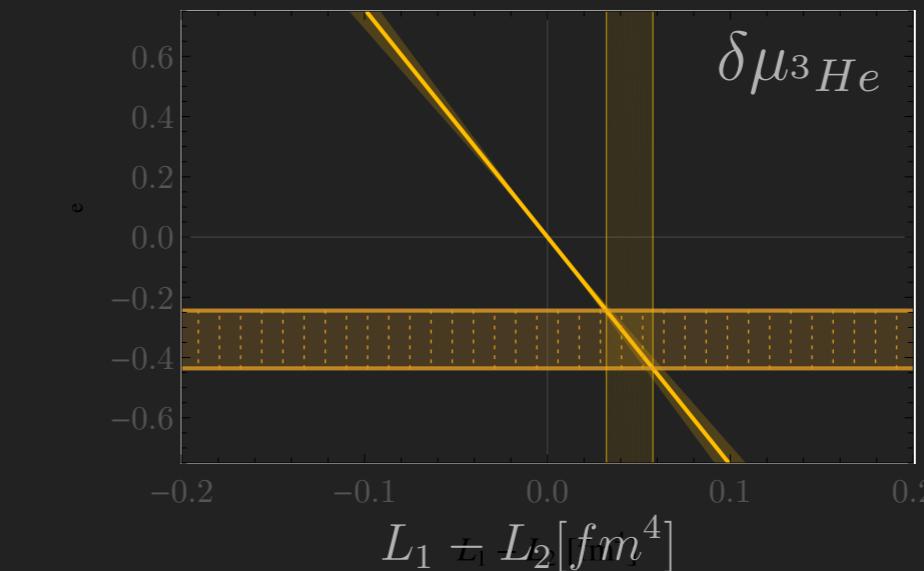
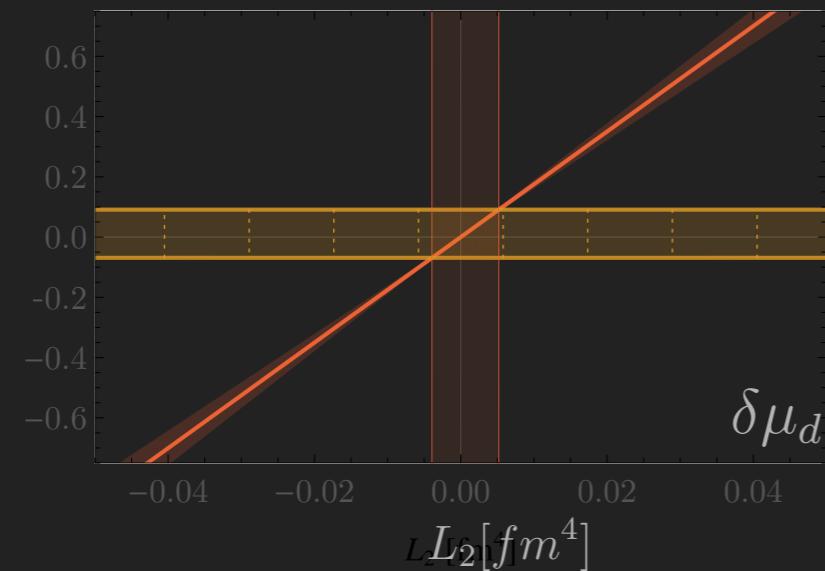
From wavefunctions
Two body counterterm



MAGNETIC MOMENTS

- Eg: magnetic moments

$$J_i^{EM} = \frac{e}{2M_N} N^\dagger (\kappa_0 + \tau_3 \kappa_1) \sigma_i N - e L_2 i \epsilon_{ijk} (N^T P_k N)^\dagger (N^T P_j N) + e L_1 (N^T P_i N)^\dagger (N^T \bar{P}_3 N) + \text{h.c.}$$



MAGNETIC MOMENTS

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

