Recent insights into baryon interactions with Lattice QCD

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Exploring the quantum chromodynamics phase diagram:
from hadrons and nuclei to matter under extreme conditions
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Exploring the quantum chromodynamics phase diagram:

from hadrons and nuclei to matter under extreme conditions

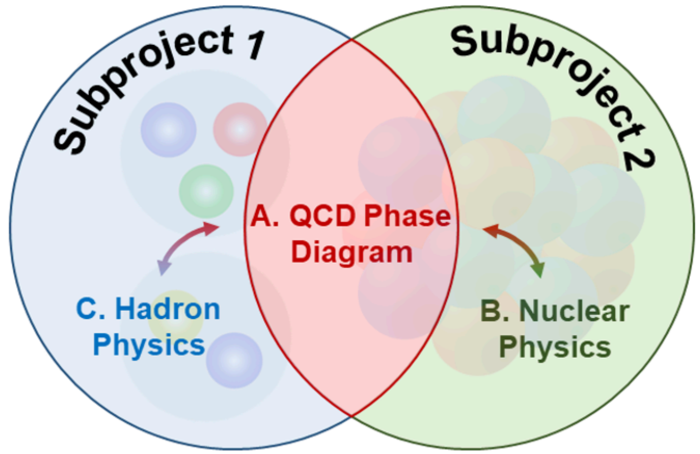

Fig 1: schematic representation of the three work packages that encompass our common interests and our subproject-specific research goals.

WP C. Hadron Physics

- WP C.3. Lattice QCD description of baryon-baryon interactions

  A. NN, YY close to physical light quark masses

  B. ΛN-ΣN: implications of hypertriton, femtoscopy and neutron star composition

Low-energy description of nuclear processes:

nonperturbative QCD information (LQCD) $\longleftrightarrow$ nuclear EFTs

+ many-body methods

$\downarrow$

predictions for properties of heavy nuclei

(beyond present-era LQCD calculations)

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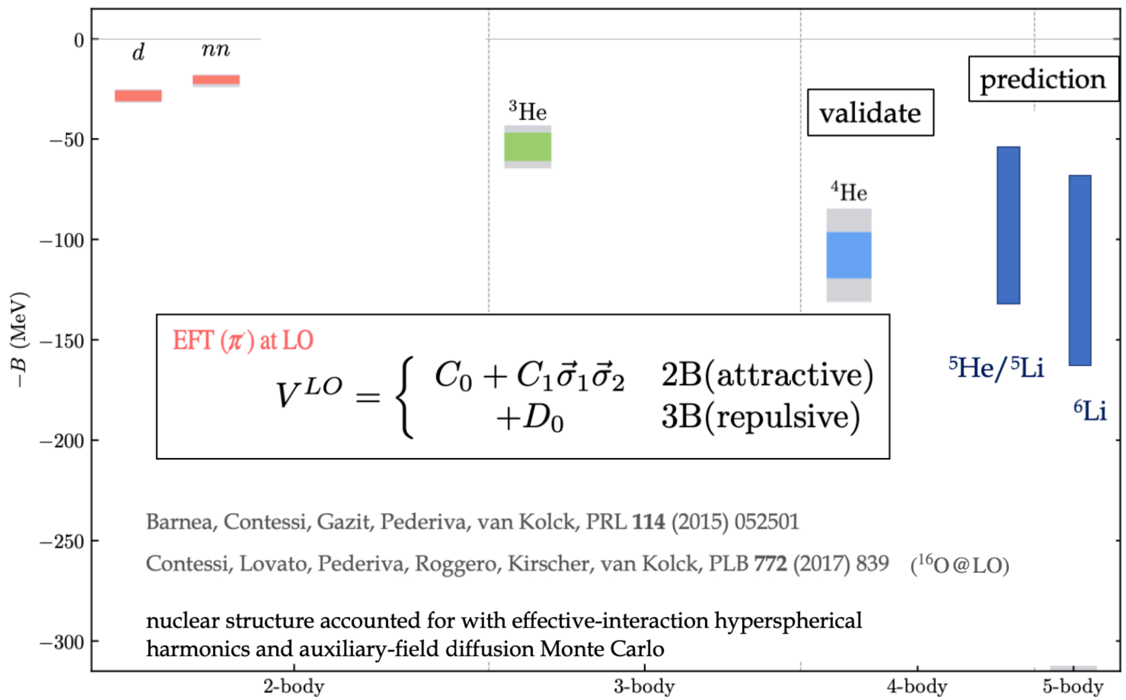
(beyond present-era LQCD calculations)

NPLQCD, Phys.Rev. D87 (2013) no.3, 034506;



no e.m. interactions

LQCD → FEW-BODY CALCS → NUCLEAR MANY-BODY CALCS

Long term expectation:

reduced systematic errors arising from nuclear-model uncertainty

increased sensitivity in experimental searches

LQCD calculations: Non-perturbative implementation of Field Theory using the Feynman Path Integral Formalism

Calculation of expectation values of operators:

$$\langle 0 \mid \hat{\mathcal{O}} \mid 0 \rangle = \frac{1}{Z} \int \mathcal{D}\psi \; \mathcal{D}\overline{\psi} \; \mathcal{D}A_\mu \; \hat{\mathcal{O}}[\psi, \overline{\psi}, A] \; e^{\mathrm{i}\, S_{\mathrm{QCD}}}$$

$$Z = \int \mathcal{D}\psi \; \mathcal{D}\overline{\psi} \; \mathcal{D}A_\mu \; e^{\mathrm{i}\, S_{\mathrm{QCD}}}$$

QCD partition function

For numerical calculations:

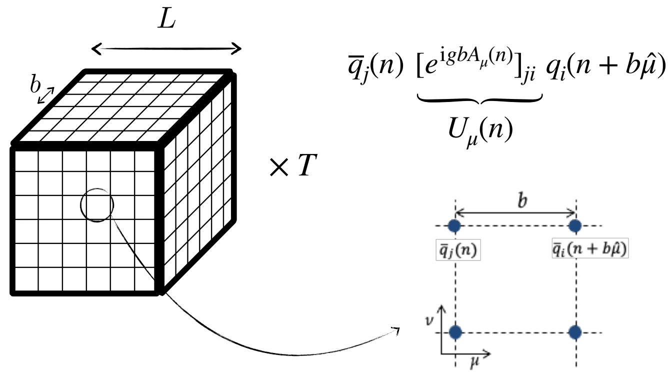
L >> relevant scales >> b

IR and UV cutoffs
(Euclidean spacetime)

Discretize spacetime $\quad b << \Lambda_{QCD}^{-1}$

Finite volume $\quad L^3 \times T$

Go to Euclidean time $\quad t \to -\mathrm{i}\,\tau$



$$\langle 0 \mid \hat{\mathcal{O}} \mid 0 \rangle = \frac{1}{Z} \int \mathcal{D}\psi \; \mathcal{D}\overline{\psi} \; \mathcal{D}U_\mu \; \hat{\mathcal{O}}[\psi, \overline{\psi}, U] \; e^{-S^E_{QCD}}$$

$$Z = \int \mathcal{D}U_\mu \; \underbrace{\det\, Q(U)\; e^{-S^E_g}}_{\sim P(U)}$$

$$\langle\, \hat{\mathcal{O}} \,\rangle \sim \frac{1}{N_{\mathrm{cnf}}} \sum_{k=1}^{N_{\mathrm{cnf}}} \hat{\mathcal{O}}\left(\{U\}_k\right)$$

important sampling methods

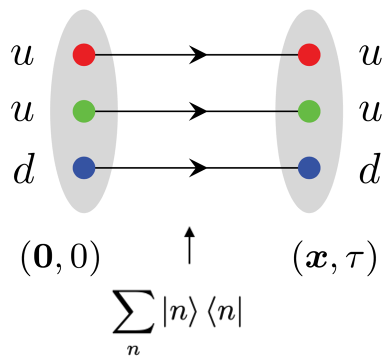
LQCD correlation function

Energy levels

$$C_{2pt}(\tau, \boldsymbol{p}) = \sum_{\boldsymbol{x}} e^{-\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p}}\, \Gamma_{\beta\alpha} \langle \mathcal{X}_\alpha(\boldsymbol{x}, \tau) \bar{\mathcal{X}}_\beta(\mathbf{0}, 0) \rangle$$

$$= \underbrace{Z_0^{snk} Z_0^{\dagger src} e^{-E^{(0)}t}}_{\text{dominates at large t}} + Z_1^{snk} Z_1^{\dagger src} e^{-E^{(1)}t} + \ldots$$

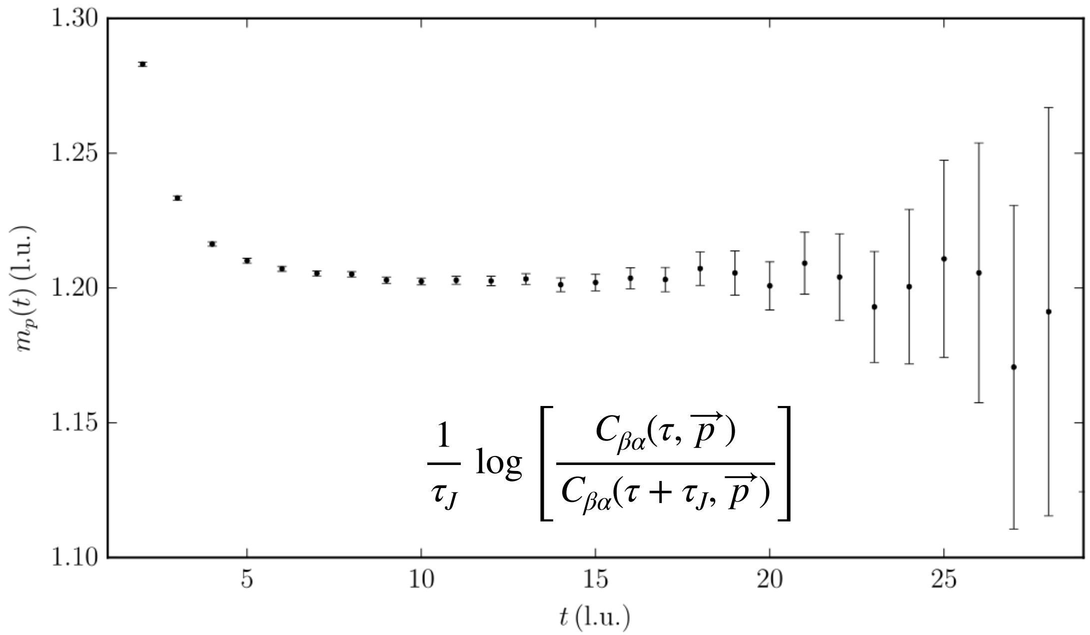
Tower of energy eigenstates
of the system
in the finite volume



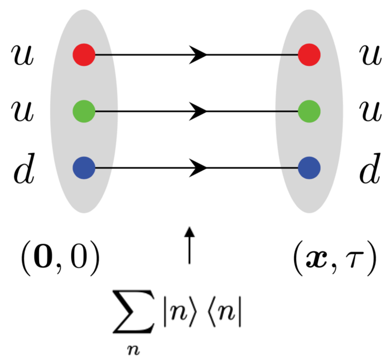
The lattice correlation function contains information on all the energy eigenstates of the system.

In principle, "smart" fitting would allow us to extract the lowest-energy state.

$$p_\alpha(\mathbf{x}, t) = \epsilon^{ijk} u^i_\alpha(\mathbf{x}, t) \left(u^{j\mathsf{T}}(\mathbf{x}, t) C\gamma_5 d^k(\mathbf{x}, t) \right)$$



Energy levels

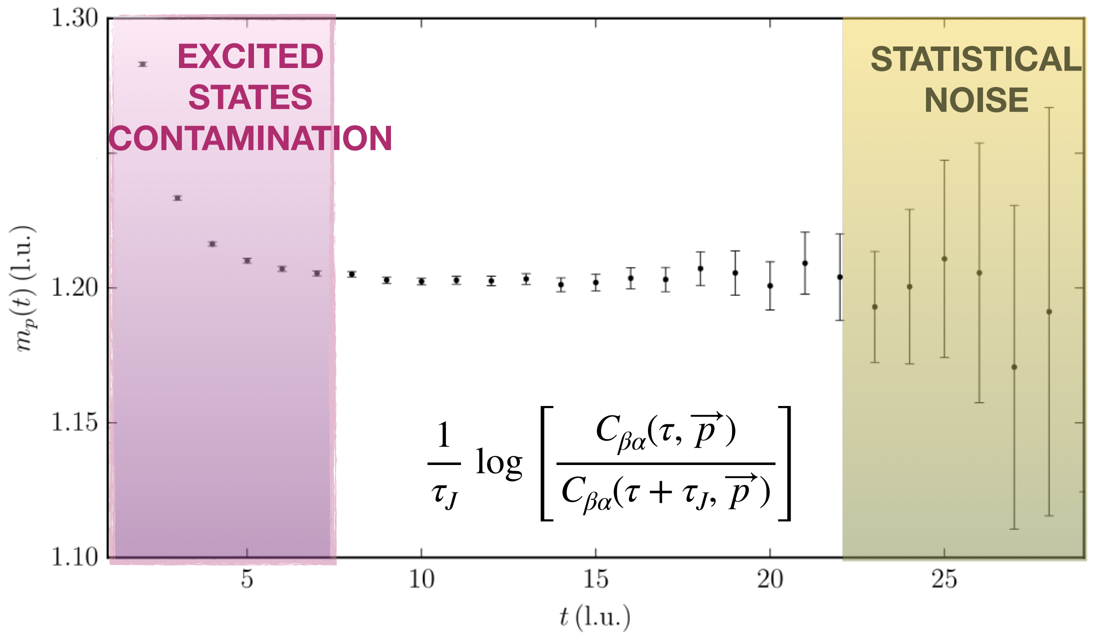


$$C_{2pt}(\tau, \boldsymbol{p}) = \sum_{\boldsymbol{x}} e^{-\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p}}\, \Gamma_{\beta\alpha} \langle \mathcal{X}_\alpha(\boldsymbol{x}, \tau) \bar{\mathcal{X}}_\beta(\mathbf{0}, 0) \rangle$$

$$= \underbrace{Z_0^{snk} Z_0^{\dagger src} e^{-E^{(0)}t}}_{\text{dominates at large t}} + Z_1^{snk} Z_1^{\dagger src} e^{-E^{(1)}t} + \ldots$$

signal-to-noise degradation

$$p_\alpha(\mathbf{x}, t) = \epsilon^{ijk} u^i_\alpha(\mathbf{x}, t) \left(u^{j\mathsf{T}}(\mathbf{x}, t) C\gamma_5 d^k(\mathbf{x}, t) \right)$$

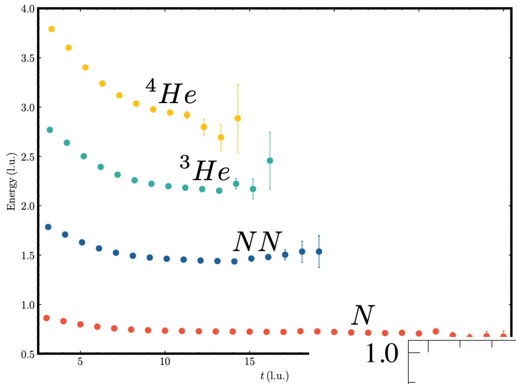


The lattice correlation function contains information on the tower of energy eigenstates of the system.

In principle, "smart" fitting would allow us to extract the ground state.

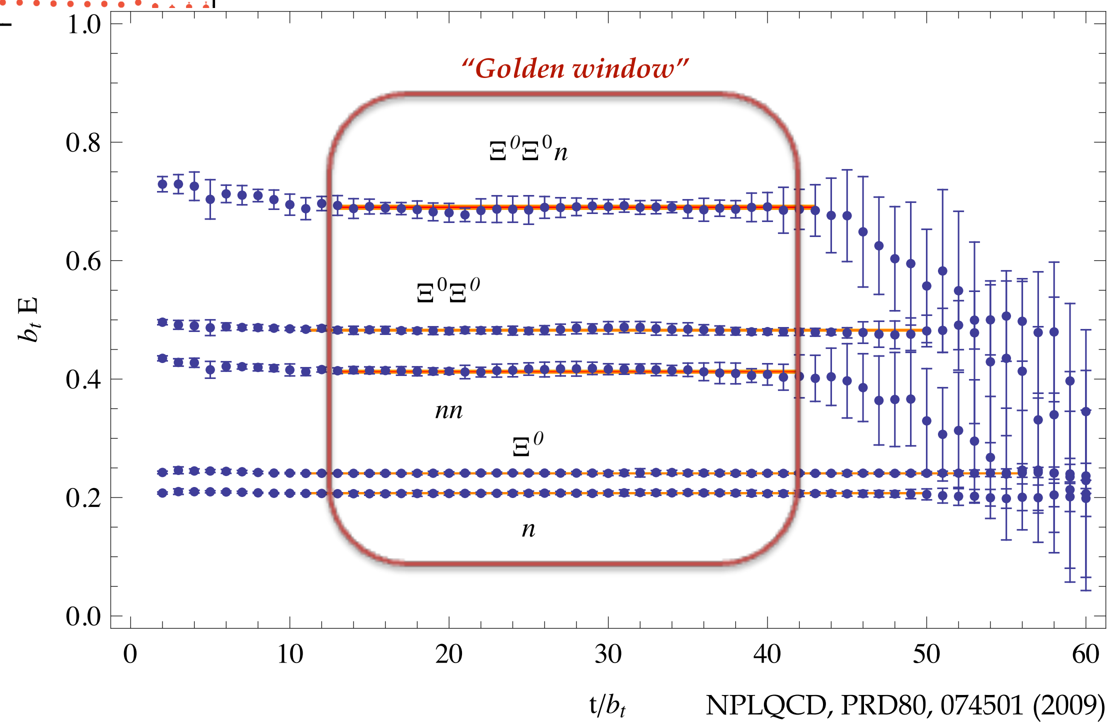
Expectation is that for A nucleons:

$$\frac{\sigma}{\langle C \rangle} \sim \frac{\exp\left[A\left(M_N - \frac{3m_\pi}{2}\right)t\right]}{\sqrt{N}}$$



G. Parisi, Phys.Rept. 103 (1984)
G.P. Lepage, Boulder TASI (1989)
M.L. Wagman, M.J. Savage, Phys.Rev.D 96 (2017)

signal-to-noise degradation



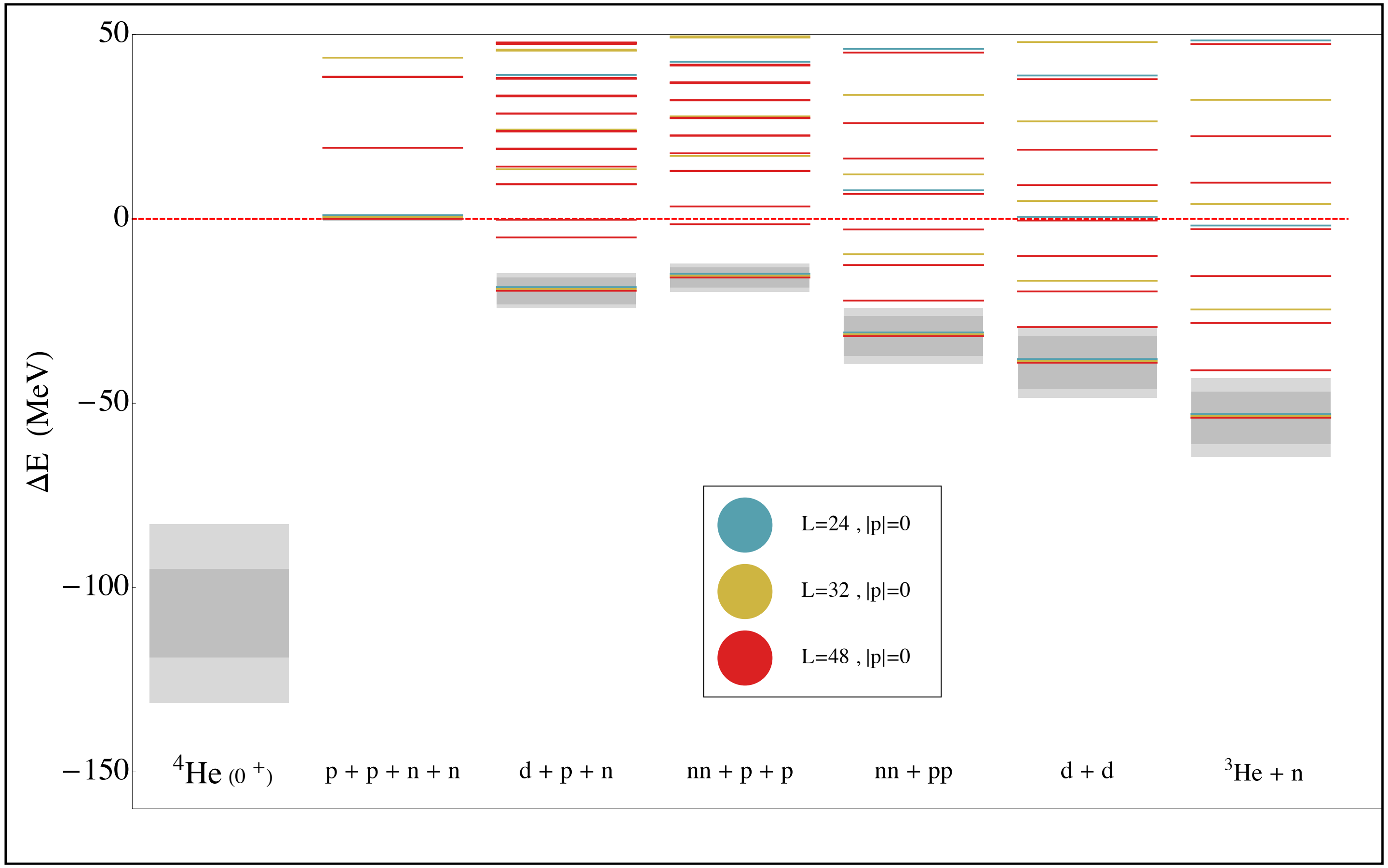
NPLQCD, PRD80, 074501 (2009)

Reduce the noise by

- increasing the statistics ($\sqrt{N}$ factor)
- increasing the pion (quark) mass

Perform calculations @ heavy quark masses:
$SU(3)_f$ symmetric point
($m_u = m_d = m_s^{phys}$)

Small excited-state gaps may lead to incorrect identification of ground-state energy



$$Z_0 e^{-E_0 t}\left(1 + \frac{Z_1}{Z_0} e^{-\delta t} + \ldots\right)$$

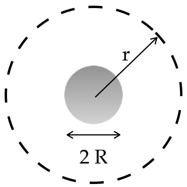
with

$$\delta \equiv E_1 - E_0 \sim \frac{4\pi^2}{ML^2}$$

S.R. Beane et al. [NPLQCD], Phys.Rev.D 87 (2013)

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

Infinite volume



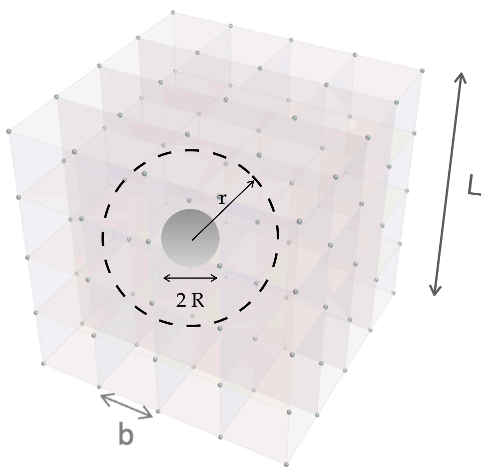
$$u_l(r;k) = \alpha_l(k) j_l(kr) + \beta_l(k) n_l(kr)$$

$$e^{2i\delta_l(k)} = \frac{\alpha_l(k) + i\beta_l(k)}{\alpha_l(k) - i\beta_l(k)}$$

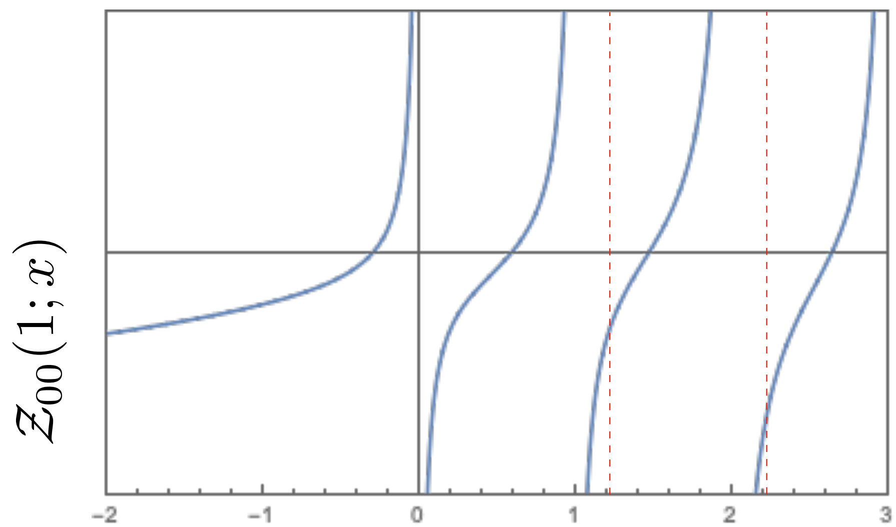
Scattering information in Euclidean space-time and FV

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

Finite volume



$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1;(\tfrac{k^*L}{2\pi})^2)$$



$$x = \left(\frac{k^* L}{2\pi}\right)^2$$

$$\det\left[(\mathscr{M}^{\infty})^{-1} + \delta\mathscr{G}^{V}\right] = 0$$

$\cot\delta(k_n)$

Infinite volume
scattering information

Generalized $\mathcal{Z}$ function

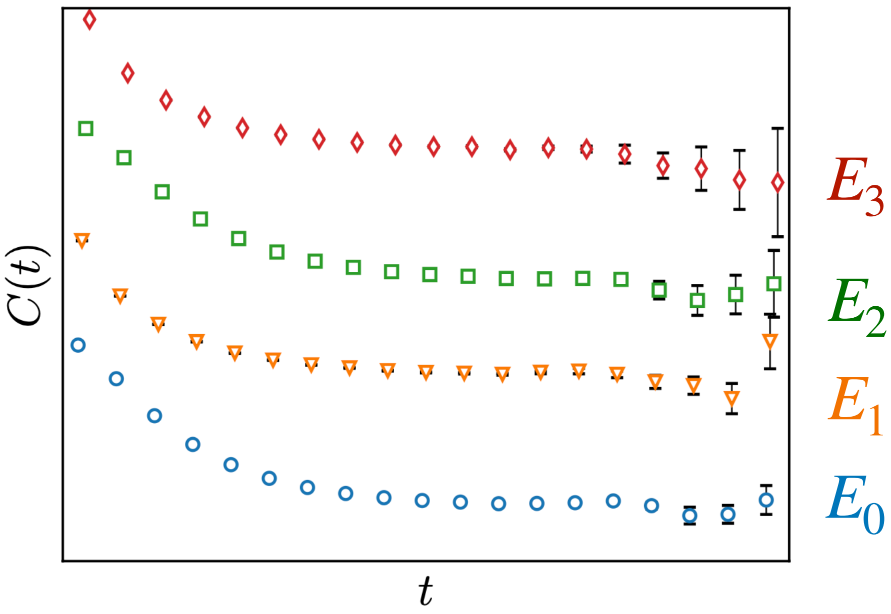
$$\mathcal{Z}^{\boldsymbol{d}}_{lm}(s;q^2) = \sum_{\boldsymbol{r}} \frac{r^l Y_{lm}(\hat{\boldsymbol{r}})}{(|\boldsymbol{r}|^2 - q^2)^s}$$

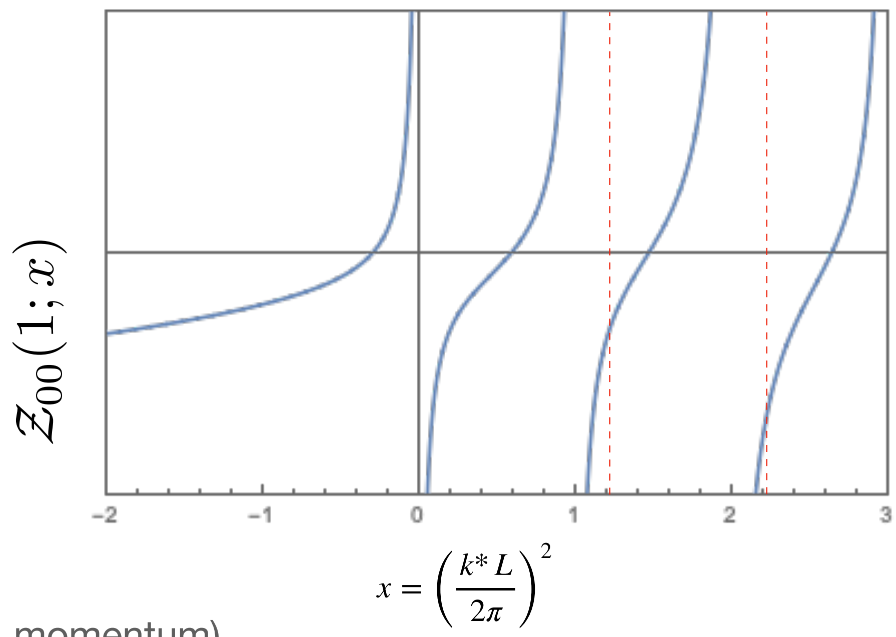
M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

1.- Determine finite-volume energies

(LQCD output)

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}(1;(\frac{k^*L}{2\pi})^2)$$





$\Delta E = E_{N_1N_2} - E_{N_1} - E_{N2} \to k^*$ (CM momentum)

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

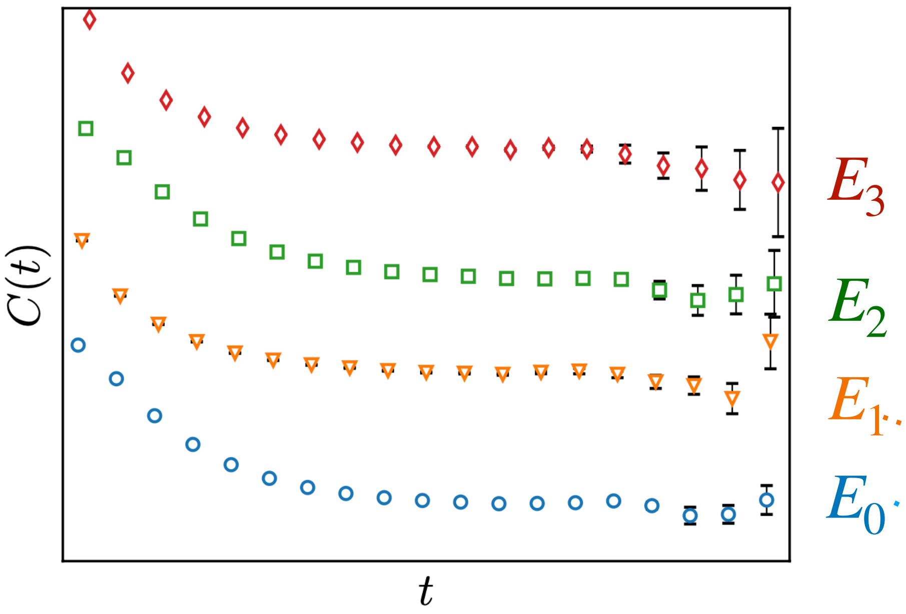
1.- Determine finite-volume energies

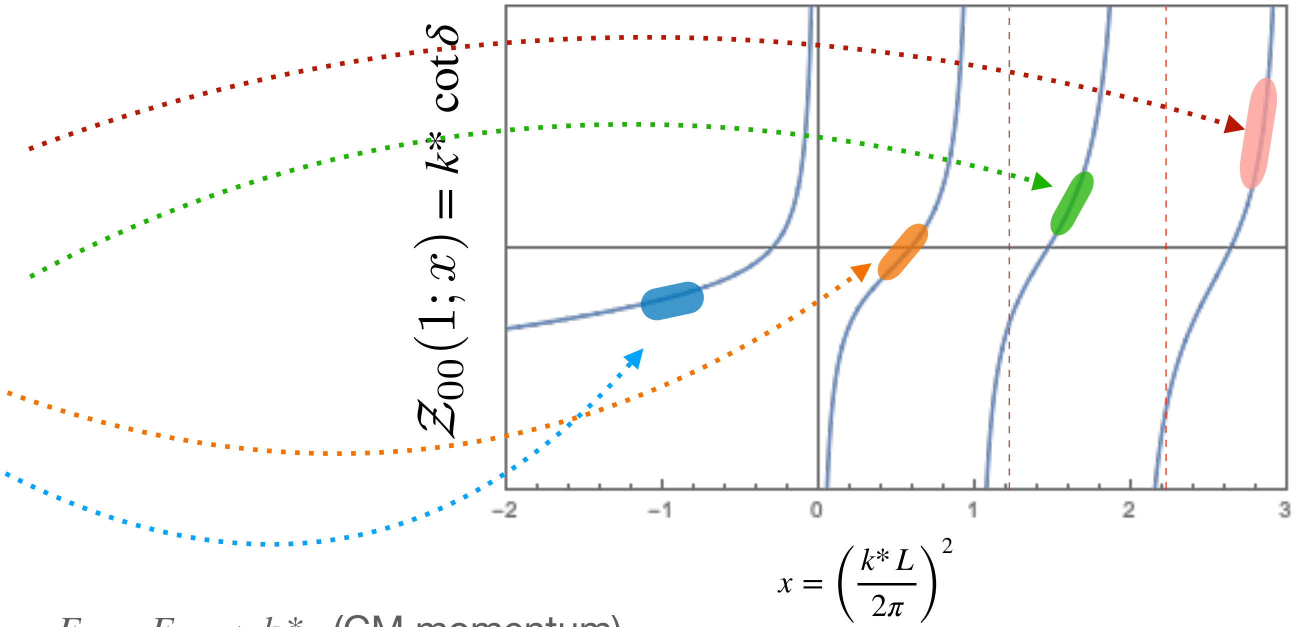
(LQCD output)

2.- Solve a (multi-hadron) quantization condition

$$k^* \cot \delta = \frac{2}{\sqrt{\pi} L} \mathcal{Z}_{00}(1; (\tfrac{k^* L}{2\pi})^2)$$

constrain a parameterized scattering amplitude





$\Delta E = E_{N_1 N_2} - E_{N_1} - E_{N2} \rightarrow k^*$ (CM momentum)

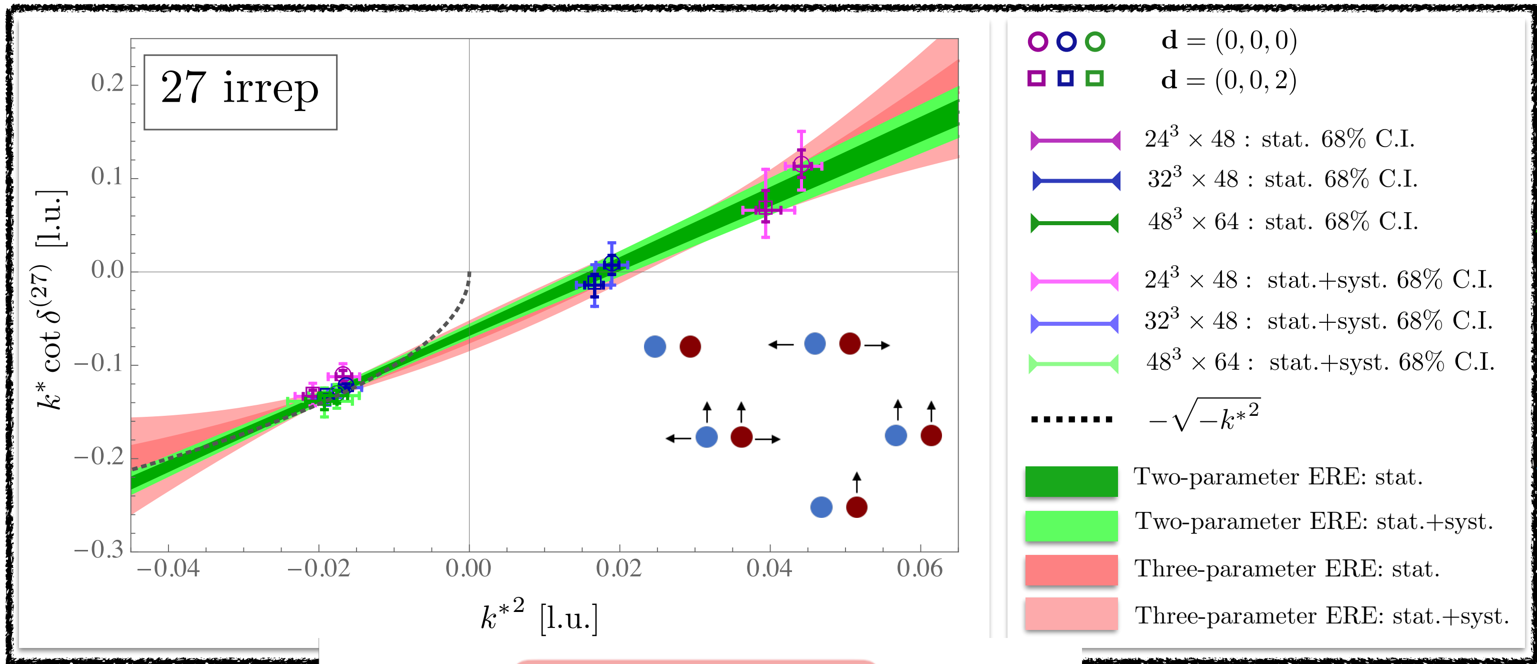
Scattering information in Euclidean space-time and FV

M. Lüscher, Comm. Math. Phys. 105 (1986), Nuc. Phys. B 354 (1991)

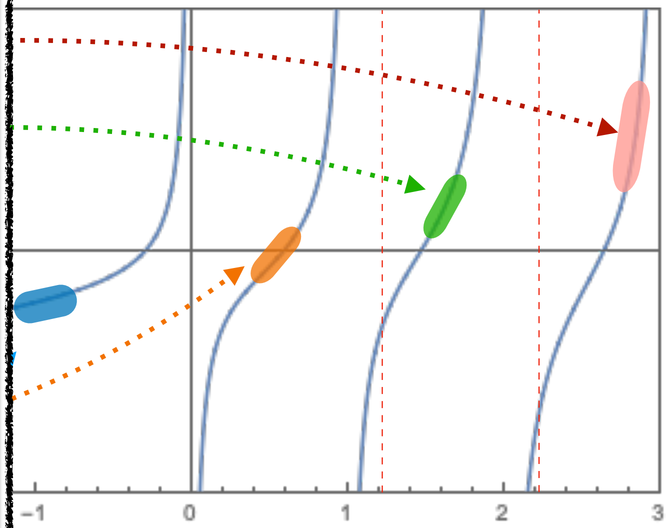
2.- Solve a (multi-hadron) quantization condition

$$k^* \cot\delta = \frac{2}{\sqrt{\pi}L}\mathcal{Z}_{00}\left(1; \left(\frac{k^* L}{2\pi}\right)^2\right)$$

a parameterized scattering amplitude

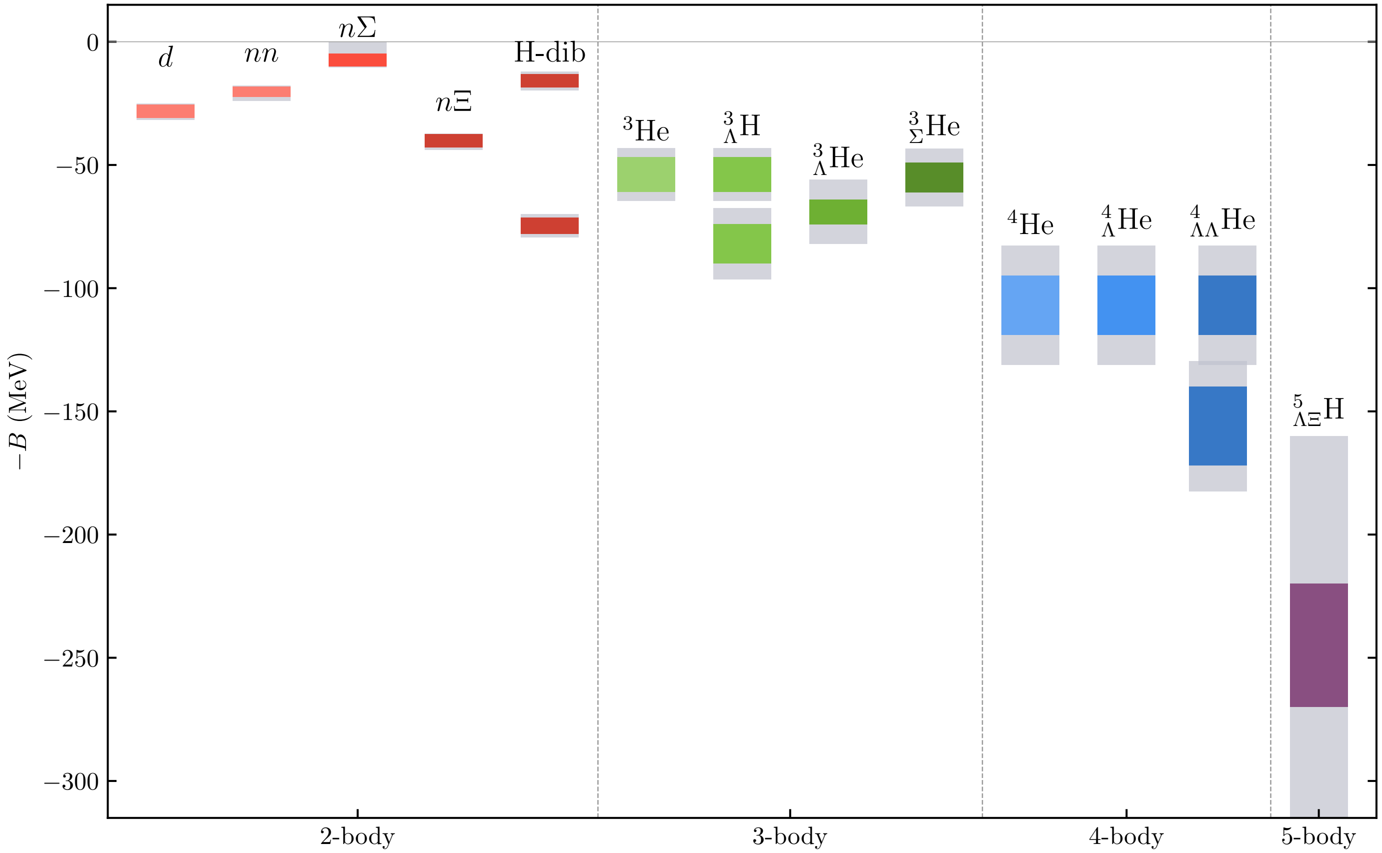


$$k^* \cot\delta = -\frac{1}{a} + \frac{1}{2}rk^{*2} + Pk^{*4} + \mathcal{O}(k^{*6})$$

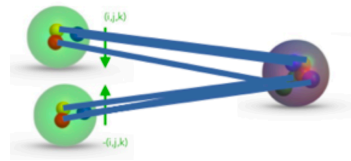


$$x = \left(\frac{k^* L}{2\pi}\right)^2$$

The use of heavier than physical pion masses reduces the exponentially bad StN problem (at a reduced computational cost) of multi-nucleon LQCD calculations ⟶ benchmark for nuclear spectrum calculations using LQCD



NPLQCD, Phys.Rev. D87 (2013) no.3, 034506; Phys.Rev. D96 (2017) no.11, 114510



$\boxed{SU(3)_f}$

$m_\pi \sim 800$ MeV

$b[fm] = 0.1453(16)$

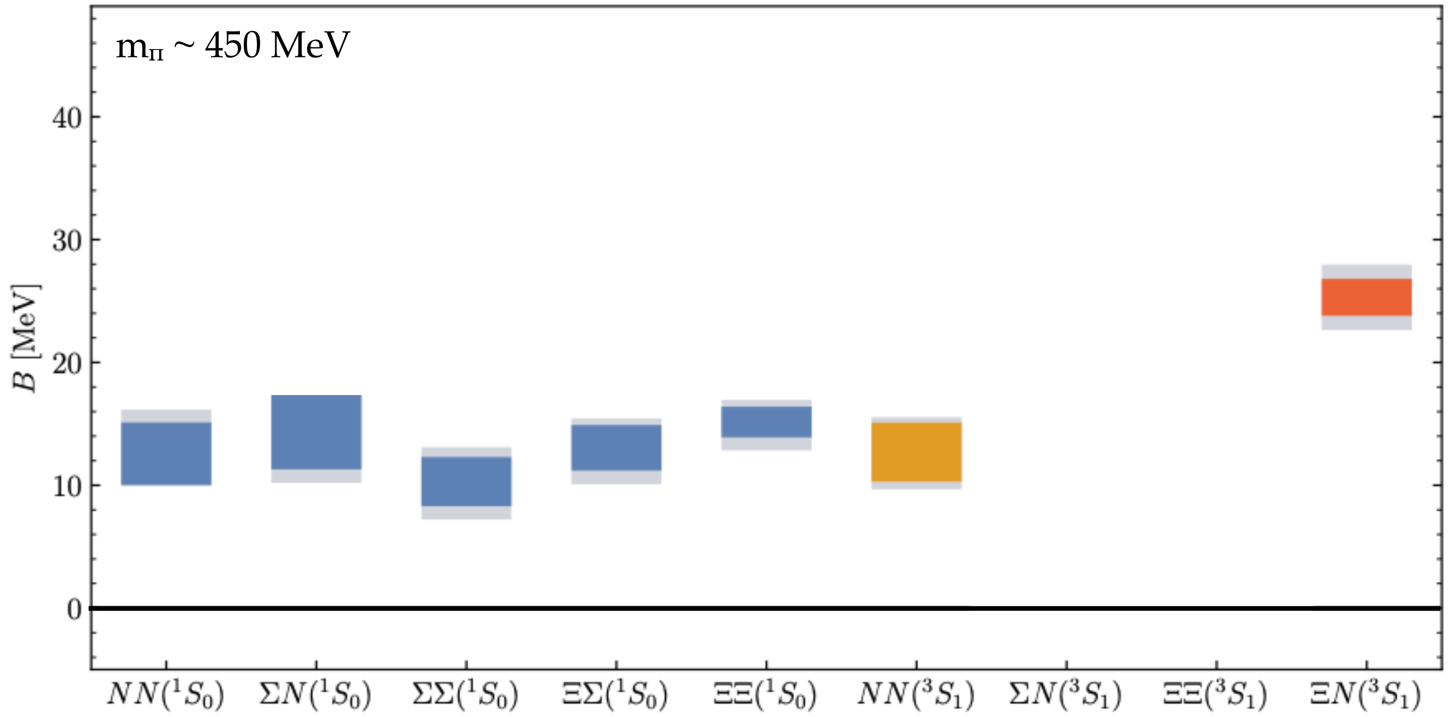
$L = 3.4, 4.5, 6.7$ fm

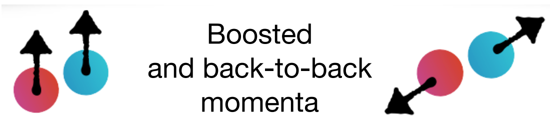
$T = 6.7, 6.7, 9.0$ fm

O(10^5) measurements:
Different quark smearings

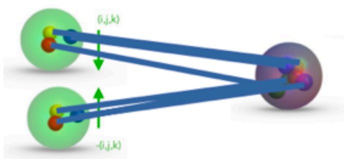
no e.m. interactions

Marc Illa et al (NPLQCD) PRD 103 (2021) 5, 054508

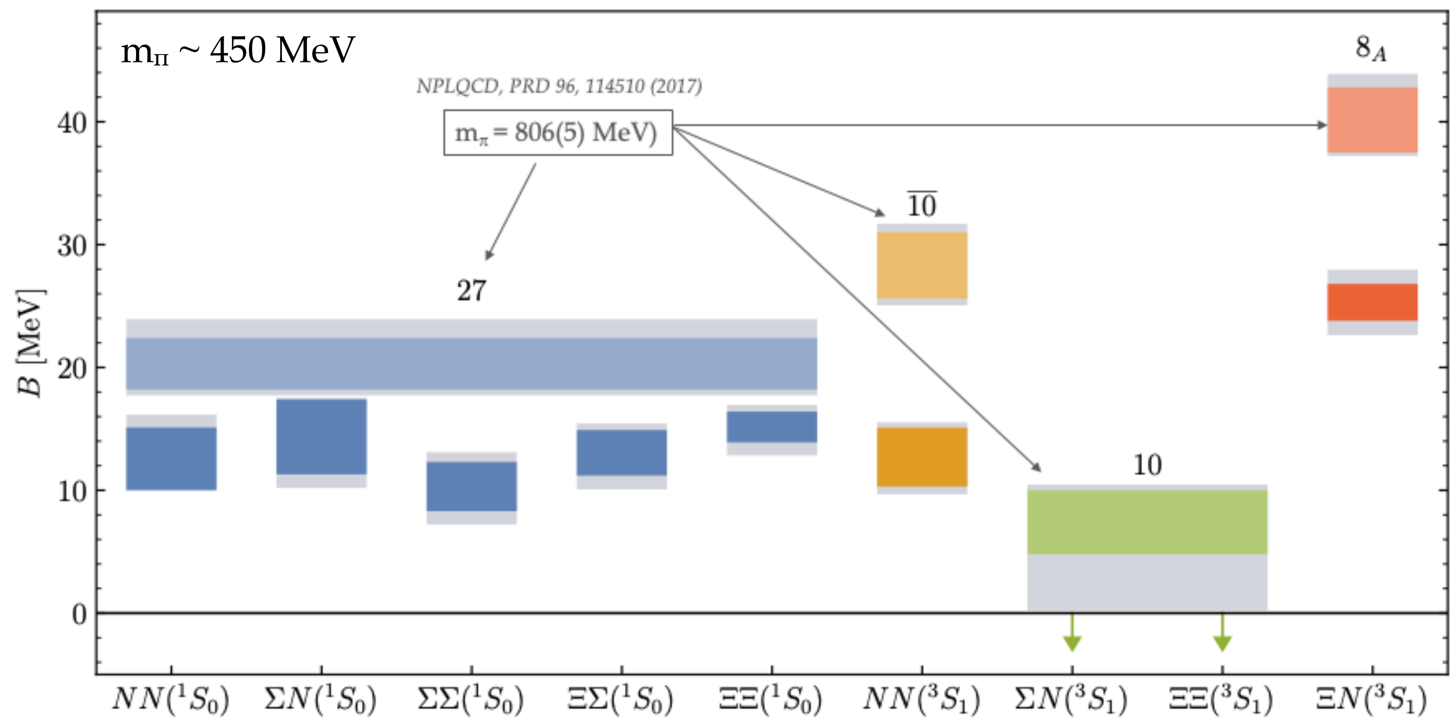


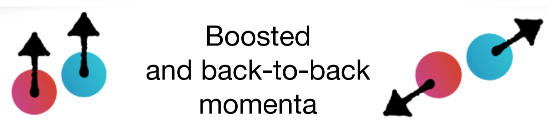


no e.m. interactions

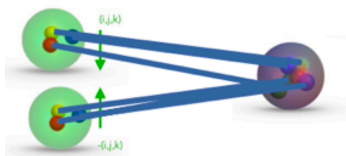


Marc Illa et al (NPLQCD) PRD 103 (2021) 5, 054508

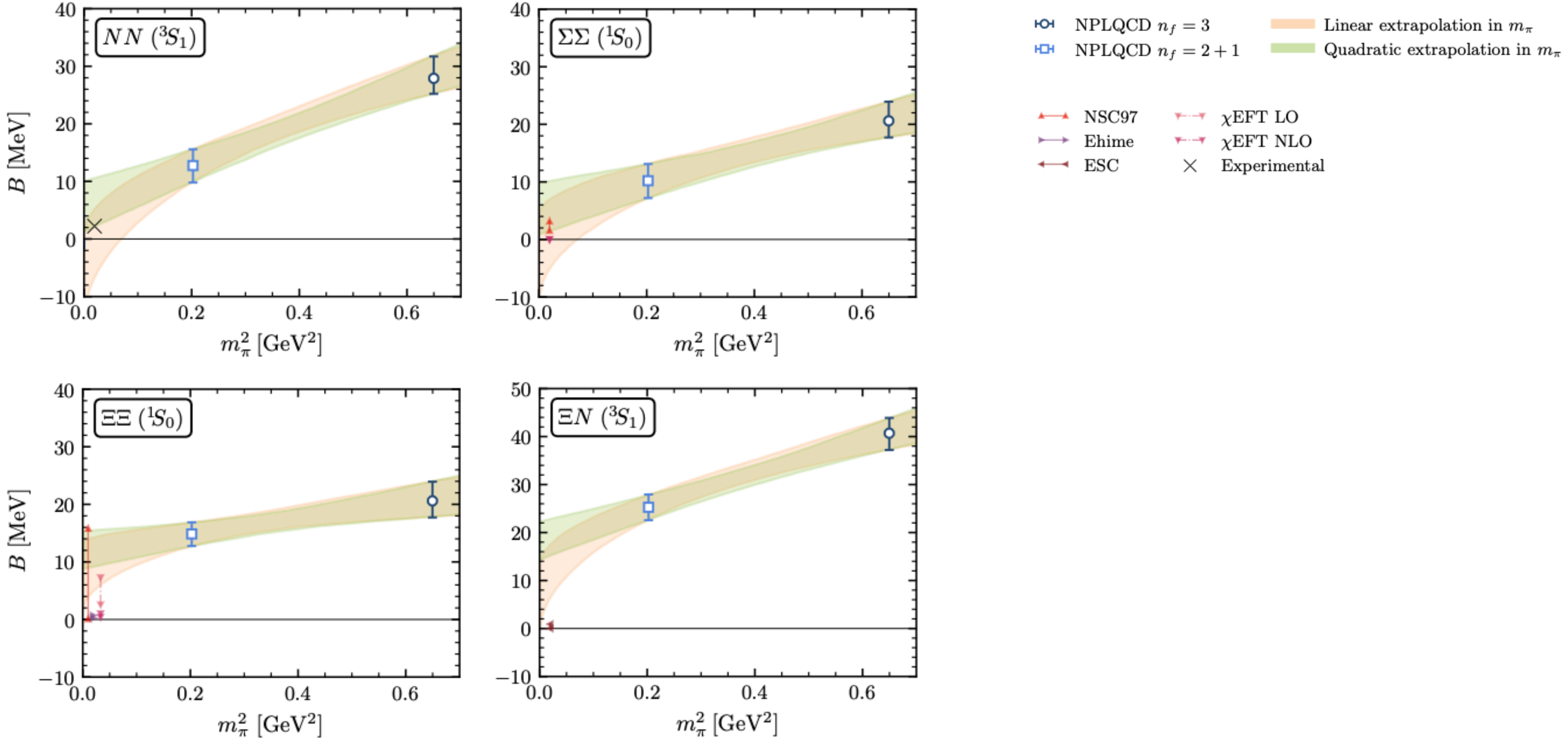




no e.m. interactions



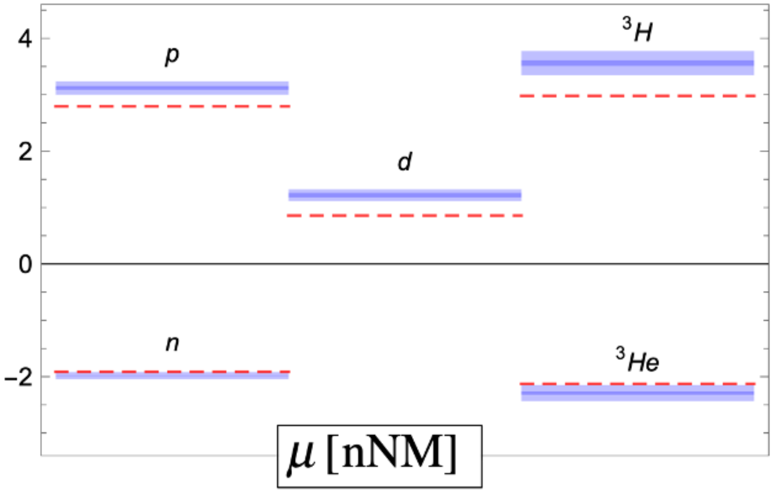
Marc Illa et al (NPLQCD) PRD 103 (2021) 5, 054508



Proof-of-principles calculations @ unphysical quark masses

Nuclear magnetic moments

NPLQCD, Phys. Rev .Lett. 113 (2014)



$$\mathrm{nNM} = \frac{e}{2M_N^{\mathrm{latt}}} = \frac{e}{2M_N(m_\pi^{\mathrm{latt}})}$$

LQCD @ $m_\pi \sim 800$ MeV

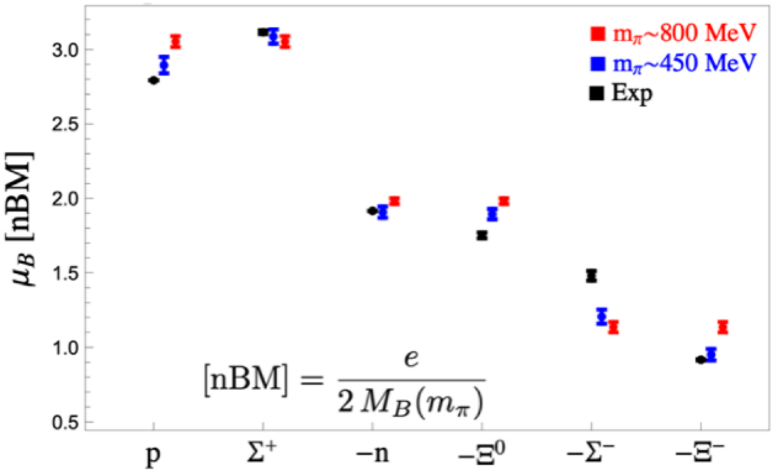
experiment

Shell-model predictions

$$\mu(^3H) = \mu_p$$
$$\mu(^3He) = \mu_n$$
$$\mu_d = \mu_n + \mu_p$$

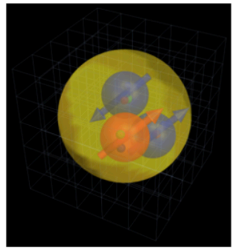
Octet baryon magnetic moments

NPLQCD, PRD95, 114513 (2017)



$(\mu_{-B} \equiv -\mu_B)$

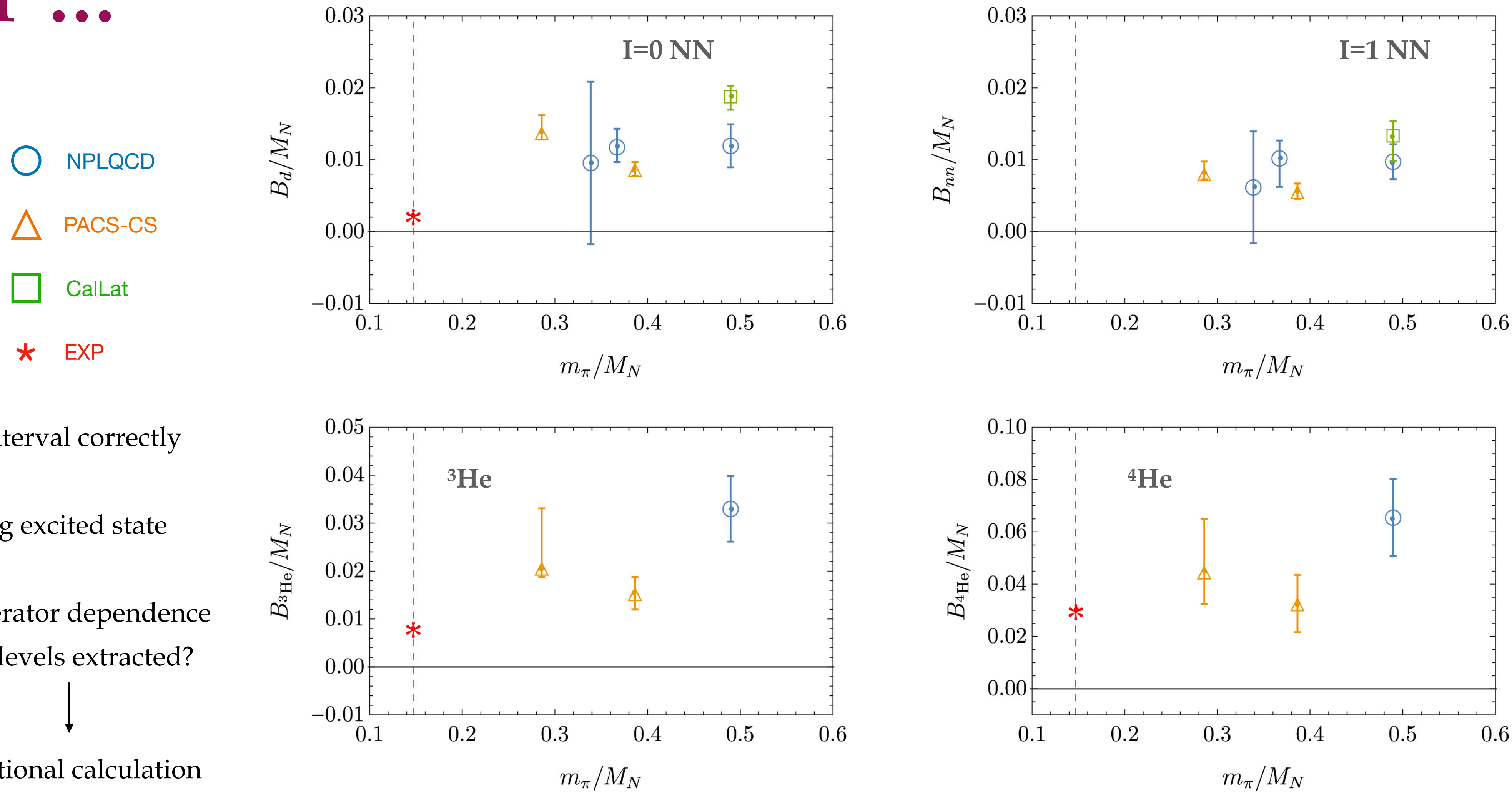
Magnetic Moments



PRD **95**, 114513 (2017)
PRL **116**, 112301 (2016)
PRD **92**, 114502 (2015)
PRL **113**, 252001 (2014)

Davoudi, Detmold, Shanahan, Orginos, Parreño, Savage, Wagman, Physics Reports 900 (2021) 1–74

BUT ...



Is the fitting interval correctly identified?

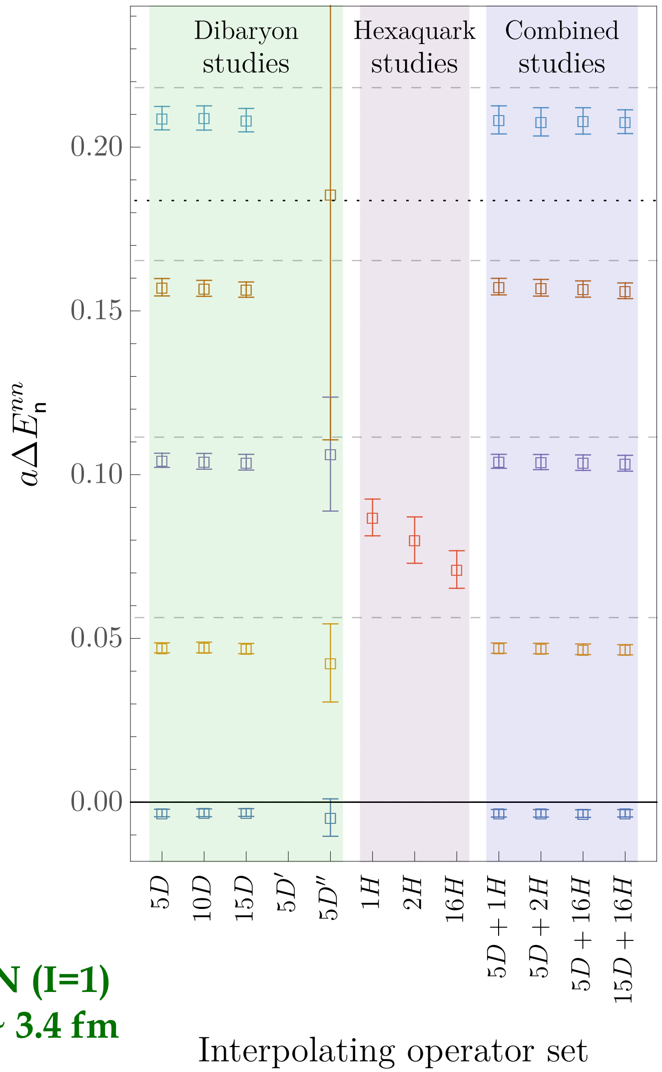
Are we missing excited state contributions?

Is there an operator dependence on the energy levels extracted?

↓

variational calculation

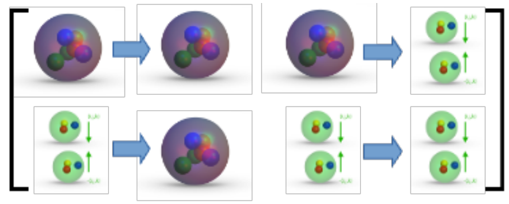
NN spectroscopy @ 800 MeV - Variational calculation



NN (I=1)
L ~ 3.4 fm

Large set of operators
b=0.145 fm
m$_\pi$ ~ 806 MeV
L ~ 4.5 fm and 3.4 fm

$$\mathbf{C}(t) =$$

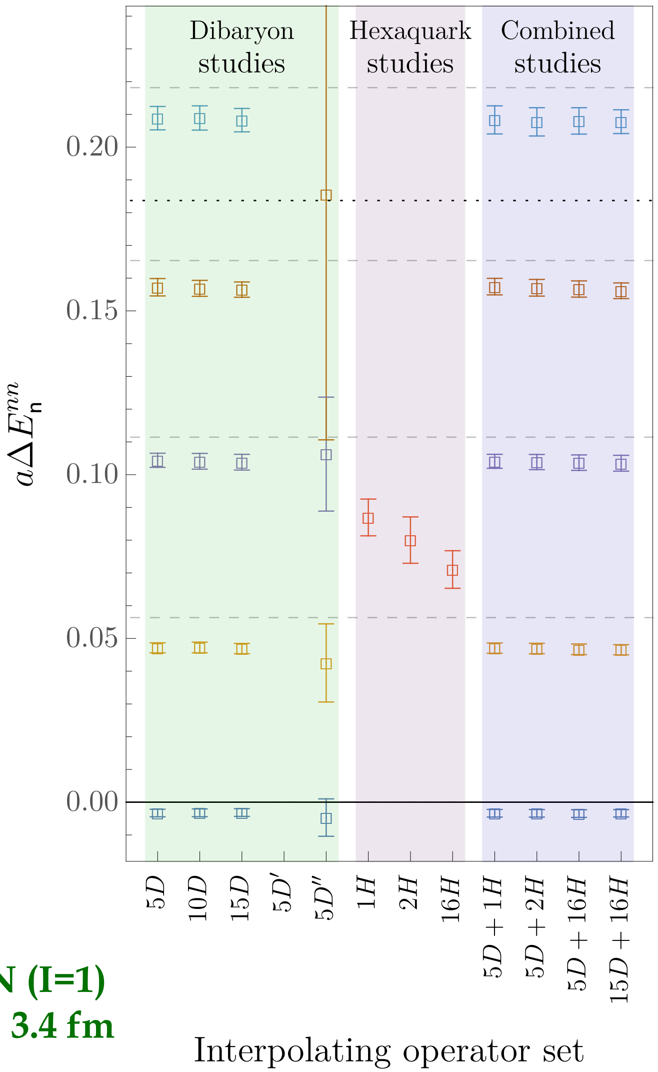


Solve **Generalized Eigenvalue Problem** (GEVP):

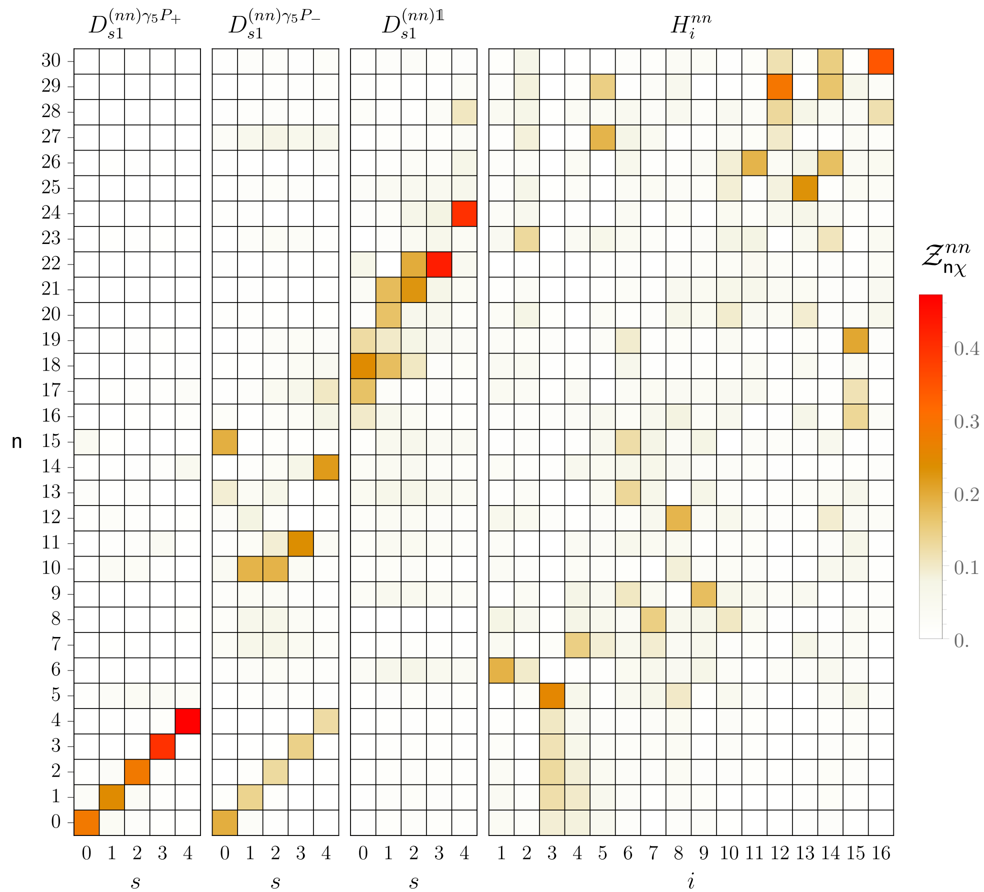
$$C(t)\,\vec{v}_n(t,t_0) = \lambda_n(t,t_0)\,C(t_0)\,\vec{v}_n(t,t_0)$$

GEVP Eigenvalues provide **rigorous (stochastic) variational upper bounds on energy levels**

NN spectroscopy @ 800 MeV - Variational calculation

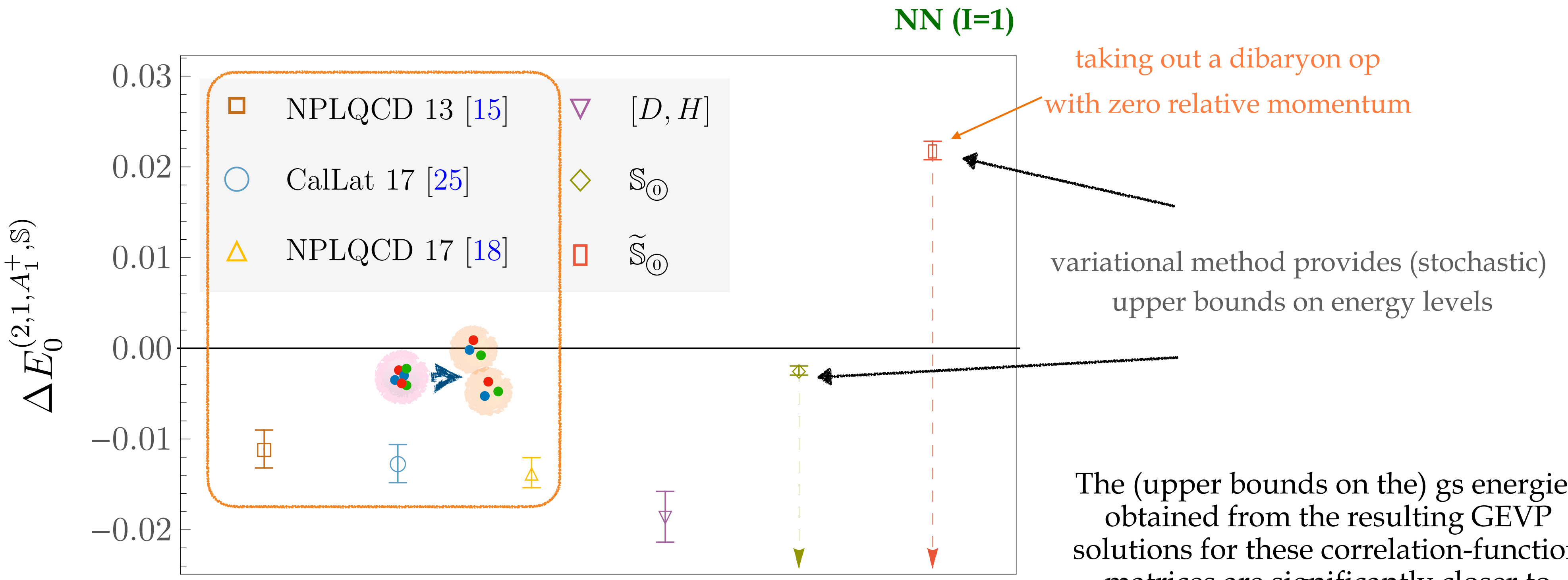


NN (I=1)
L ~ 3.4 fm



relative overlap factors

Results consistent if viewed as variational bounds



calculations made on the same set of configurations

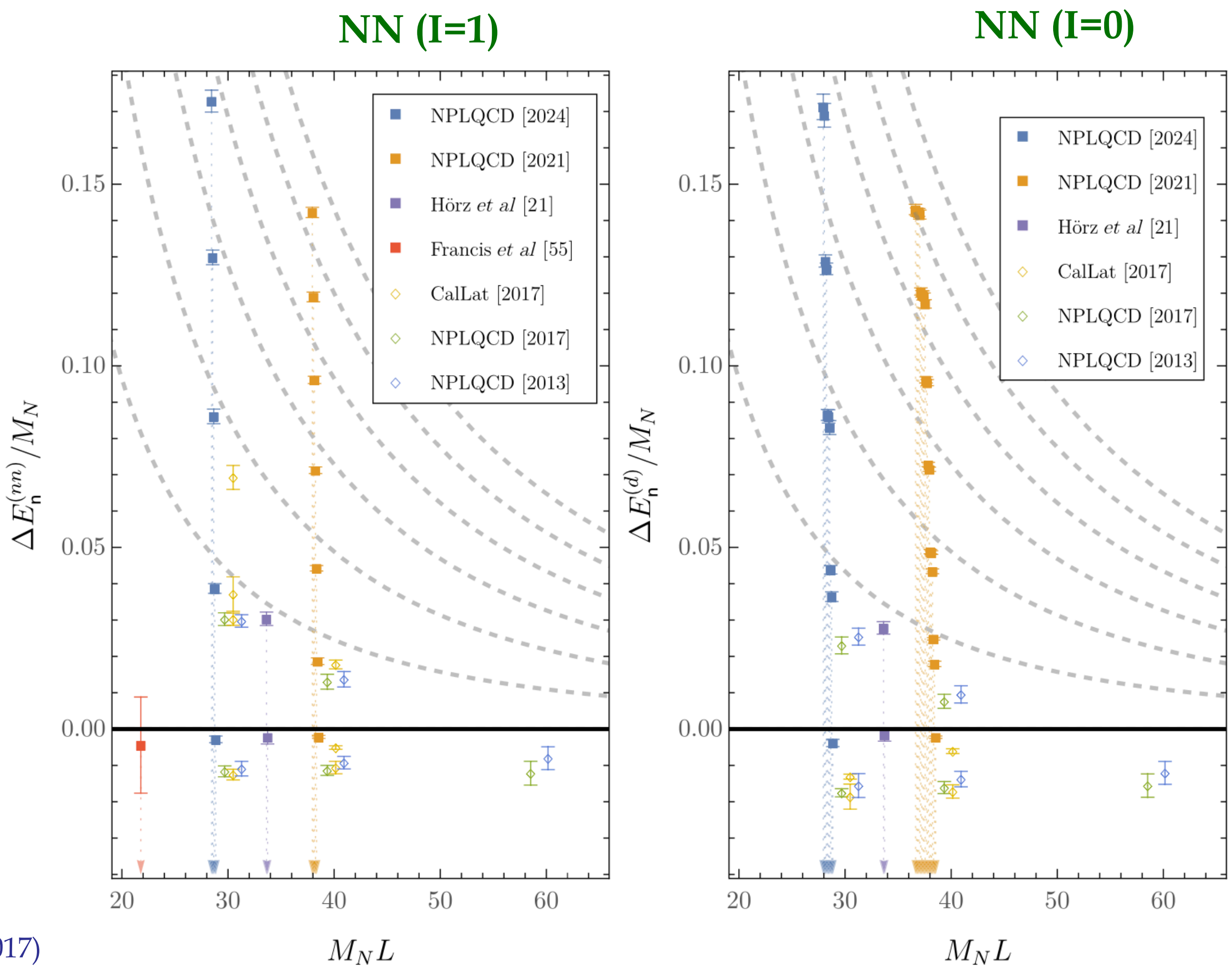
S. Amarasinghe et al (NPLQCD) PRD 107 (2023) 9, 094508

The (upper bounds on the) gs energies obtained from the resulting GEVP solutions for these correlation-function matrices are significantly closer to threshold than those obtained using hexaquark sources and dibaryon sinks (in all previous studies using the same gauge-field ensemble)

$L_S^3 \times L_T = 32^3 \times 48$ and $24^3 \times 48$

W. Detmold et al. (NPLQCD) *Phys.Rev.D* 111 (2025) 11, 114501

Comparison of two-nucleon variational bounds with other calculations at similar quark masses employing variational methods or asymmetric correlators in the total momentum $|\vec{P}| = 0$ sector



B. Hörz et al., Phys. Rev. C 103, 014003 (2021)
A. Francis et al., Phys. Rev. D 99, 074505 (2019)
CalLat 17: E. Berkowitz et al., Phys. Lett. B 765, 285 (2017)
NPLQCD 17: M.L. Wagman et al., Phys. Rev. D 96, 114510 (2017)

Excited-state uncertainties in lattice-QCD calculations of multi-hadron systems

William Detmold,[1] Anthony Grebe,[2,3] Daniel C. Hackett,[3] Marc Illa,[4,5]
Robert J. Perry,[1] Phiala E. Shanahan,[1] and Michael L. Wagman[3]
(NPLQCD Collaboration)

coming out of the oven…

Courtesy of Robert J. Perry

Two-point correlator

$$\widetilde{C}_{ab}(t) = \frac{1}{Z}\mathrm{Tr}[T^{(L_t-t)}\mathcal{O}_a T^t \mathcal{O}_b^\dagger],$$

Transfer matrix:

$$T\,|n\rangle = \lambda_n\,|n\rangle\,,$$

Eigenvalues related to finite-volume energy eigenvalues

$$E_n = -\ln\lambda_n.$$

Lanczos allows for access to transfer-matrix eigenvalues. Importantly: **two-sided bounds**, B computable from correlator data

$$E_n \in \left[-\ln\left(\lambda_k^{(m)} + \sqrt{B_k^{R/L(m)}}\right),\right. \\ \left. -\ln\left(\lambda_k^{(m)} - \sqrt{B_k^{R/L(m)}}\right)\right].$$

Residual bounds

Valid for **all Euclidean separations** (independent of size of energy gaps)

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Two sided bounds are phenomenologically useful!

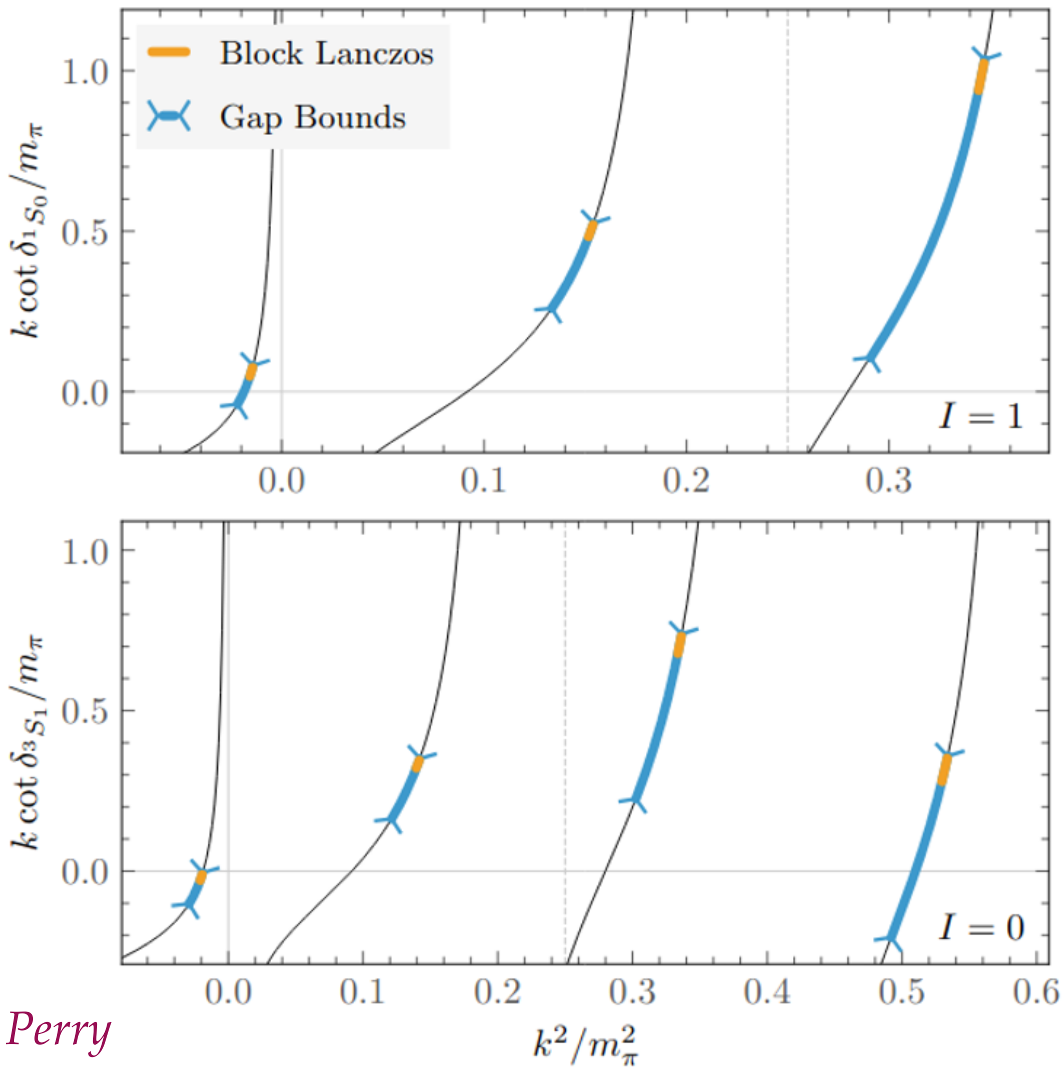
Two versions of bounds:

1. Residual bounds: assume Hermiticity of Transfer matrix
2. **Gap bounds:** Assume spectrum is qualitatively known

Gap + variational bounds lead to phenomenologically interesting constraints on scattering phase-shift.

No need to assume N-state saturation in correlation function

Residual & Gap bounds provide **two-sided bounds** which constitute a paradigmatic improvement.



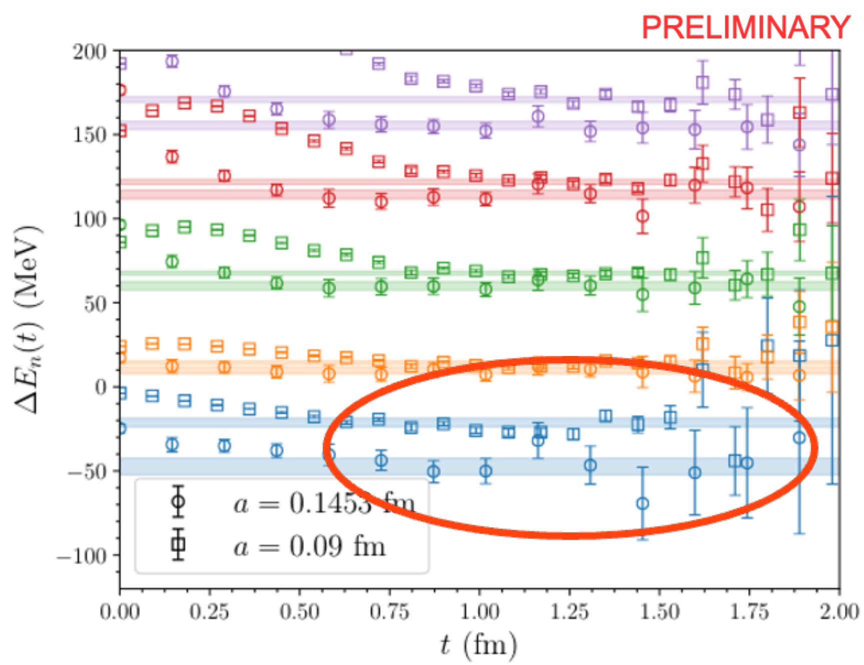
Courtesy of Robert J. Perry

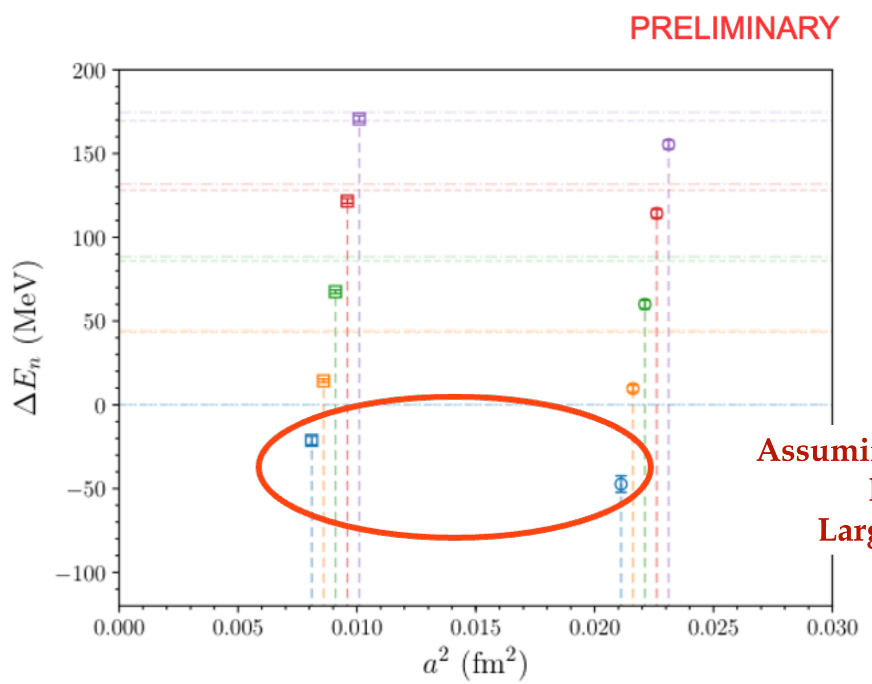
In 2023 we started a study of all SU(3) irreps at two different lattice spacings

Previous calculations by other groups:
Green, Hanlon, Junnarkar, Wittig, PRL 127 (2021)

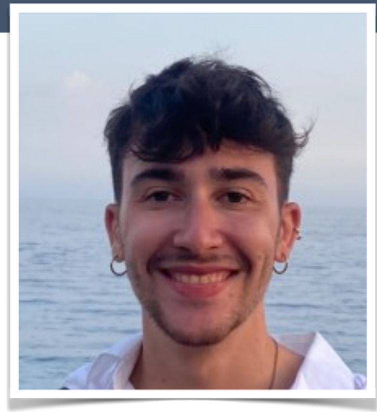
L/a	T/a	L (fm)	T (fm)	a (fm)
48	64	4.13	5.50	0.086
32	48	4.64	6.96	0.145

flavor singlet channel
(H-dibaryon)





Assuming variational bounds
have saturated
Large lattice artifacts!



Other theoretical techniques to obtain the energy eigenvalues of the QCD Hamiltonian

Neural-network-based variational methods

Martí has been applying the variational method to study simple quantum mechanical systems and interacting scalar field theories.

His thesis goal is to compute the energy eigenvalues of the lattice-regularized Hamiltonian for QCD, using a trial wave function based on a neural network —> to explore the spectrum of single- and few-hadron systems in QCD

with Robert J. Perry (MIT) and Assumpta Parreño (UB)