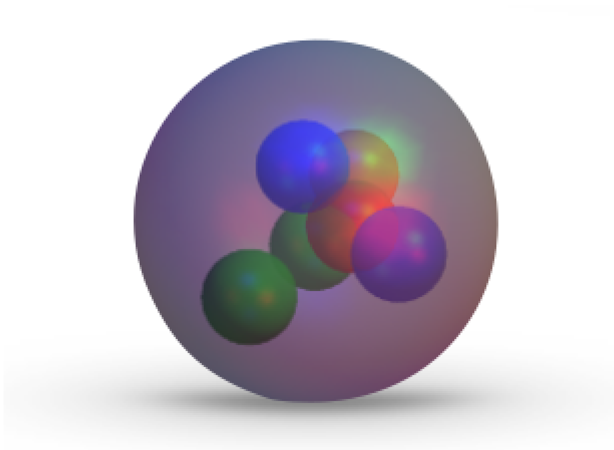
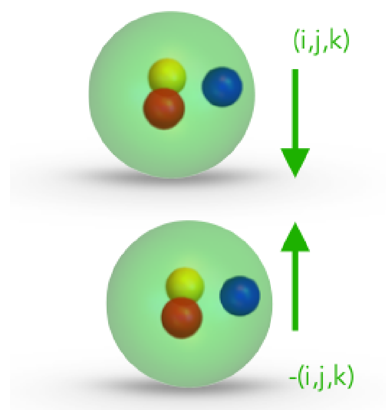
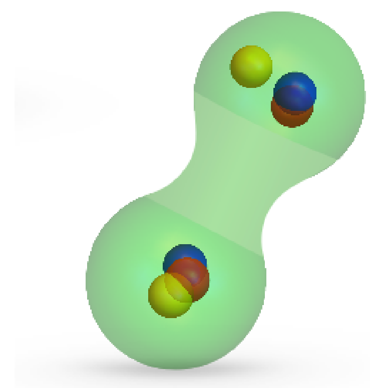
Studying Nuclear Physics with Lattice QCD







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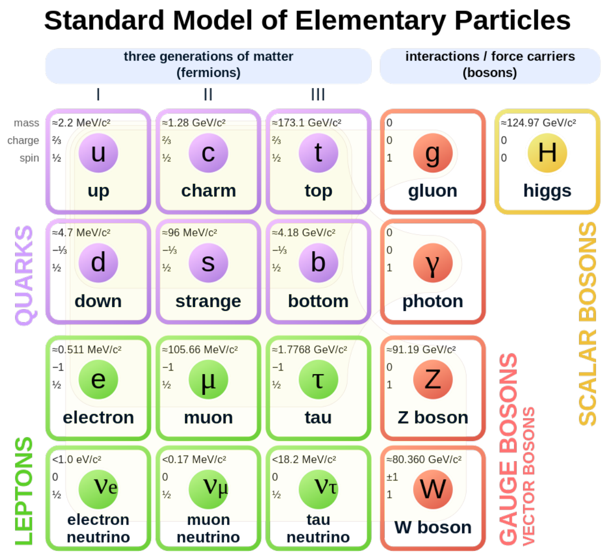
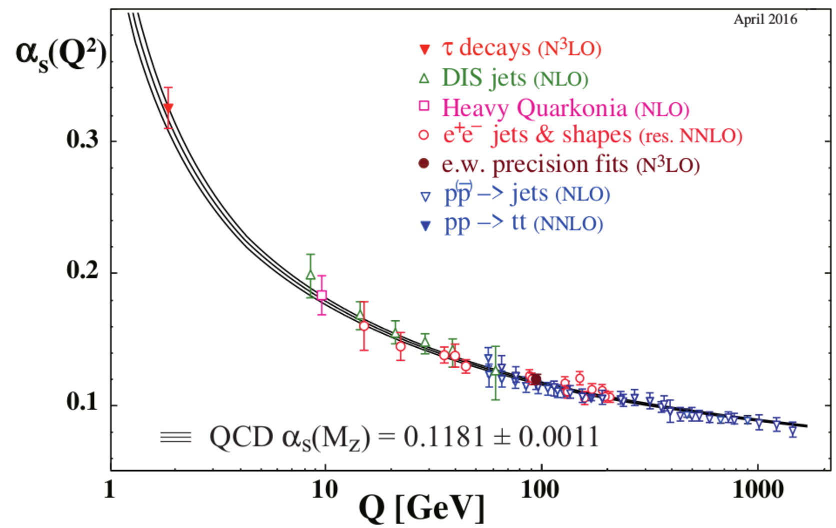
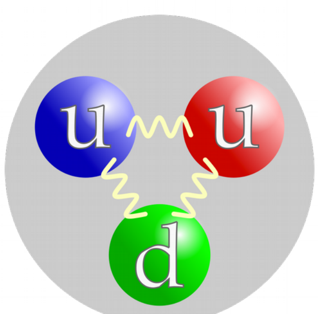
*University of Barcelona (current or alumni)

Nuclear Physics From QCD

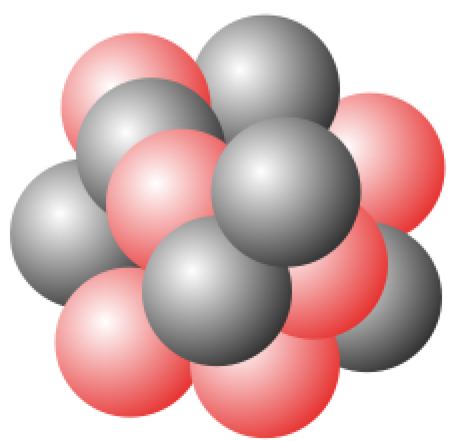






~1 fm = 10^{-15} m

https://en.wikipedia.org/wiki/File:Quark_structure_proton.svg



Residual meson exchange binds hadrons

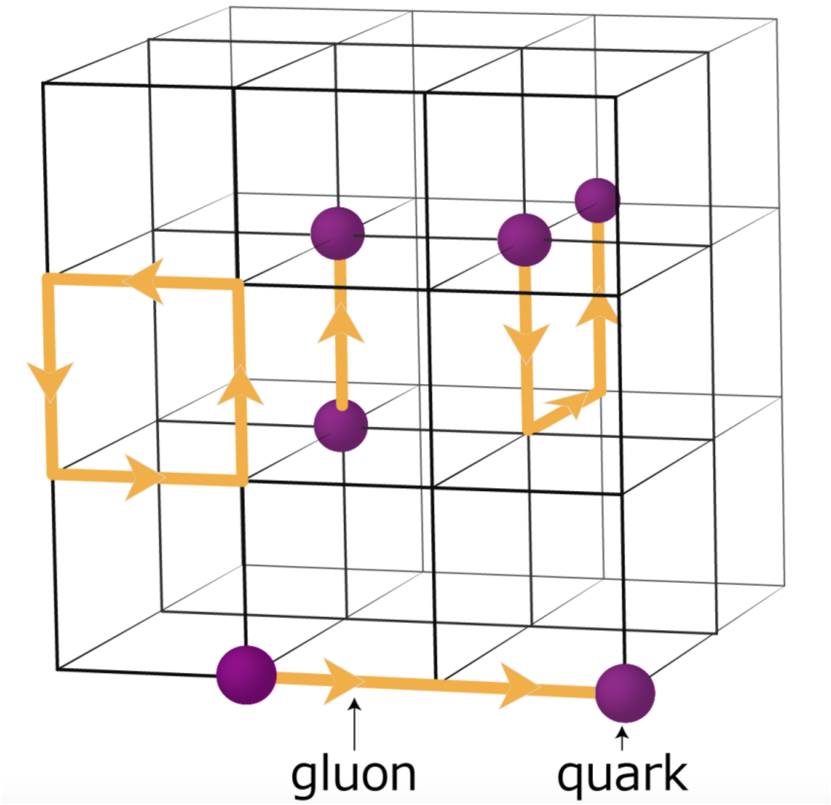
https://en.wikipedia.org/wiki/File:NuclearReaction.svg

https://en.wikipedia.org/wiki/File:PIA18848-PSRB1509-58-ChandraXRay-WiseIR-20141023.jpg

Motivation

- LQCD presents possibility of studying nuclear physics from first principles
- Precise experiments serach for new physics
  - Dark matter direct detection
  - Neutrino physics
  - Charged lepton flavour violation, ββ-decay,
  - proton decay, neutron-antineutron oscillations...
- **CHALLENGE**: understand the physics of nuclei used as targets
- Systems with strange quarks (hypernuclear physics)

Introduction to LQCD



$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int D\phi \, \mathcal{O}[\phi] \, e^{iS[\phi]}$$

- Provides a non-perturbative definition of field theory
- Discretize space-time.
- Place in finite volume
- Regulates IR and UV divergences → suitable for numerical evaluation

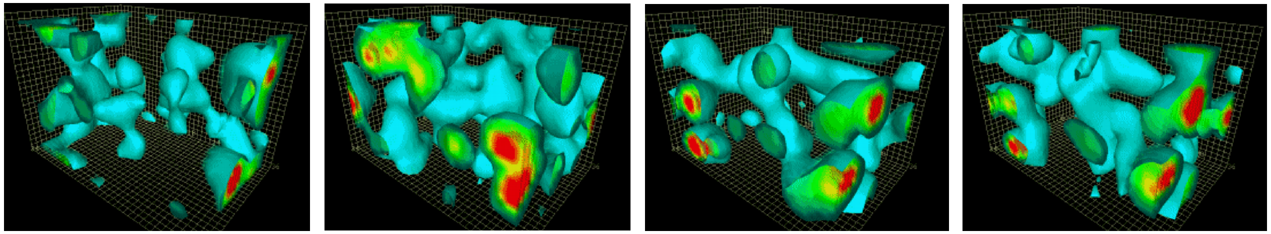
Monte Carlo Integration

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \prod_{i=1}^{N} \int d\phi(x_i) \mathcal{O}[\phi] e^{iS[\phi]}$$

$$N = N_L^3 \times N_T \sim 32^3 \times 64 = 2097152$$

- Approximate with Riemann sums? No! ~ $100^{2097152}$: completely impossible!
- Utilize importance sampling: only compute most important contributions:

$$P[\phi] = \frac{1}{Z} e^{-S[\phi]} \sim$$



http://www.physics.adelaide.edu.au/theory/staff/leinweber/VisualQCD/Nobel/index.html

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}[\phi_i]$$

Extrapolations

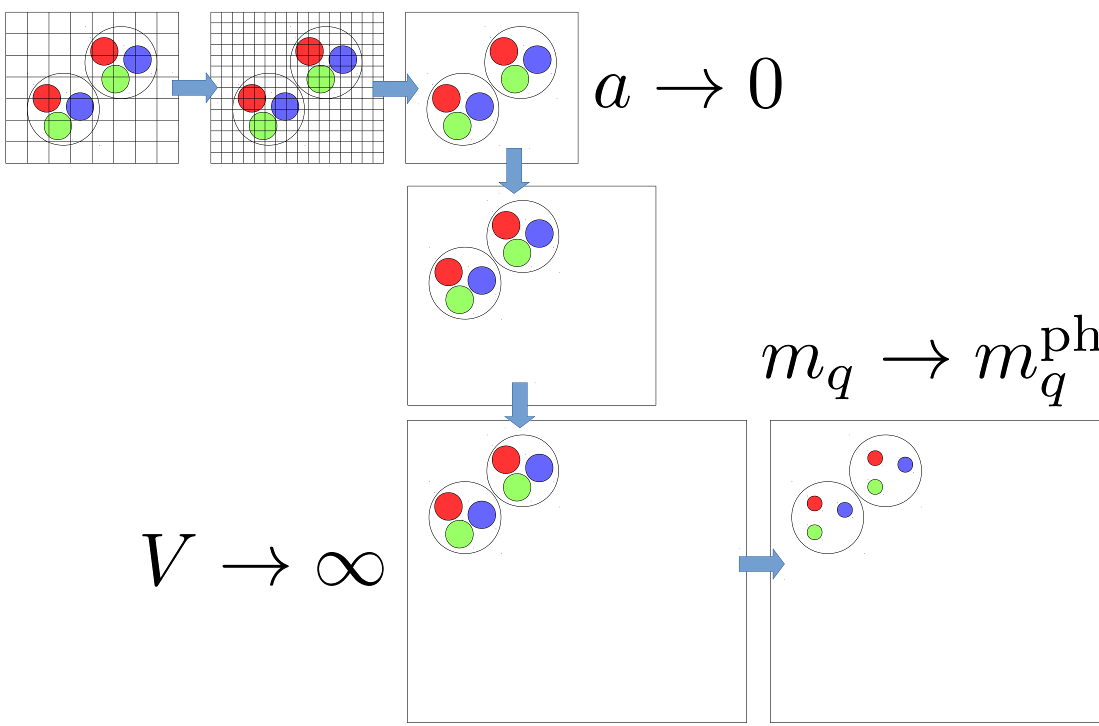
$$\text{cost} \sim \left[\frac{1}{m_q}\right]^x [N_L]^y \left[\frac{1}{a}\right]^z$$

- Work in **finite volume**
- Work with **finite lattice spacing**
- (often) work with **heavier than physical quark mass**

$$a = 0.1 \text{ fm}$$

$$V = L^3 \times T$$

$$m_q > m_q^{\text{phys}}$$



$$a \to 0$$

$$V \to \infty$$

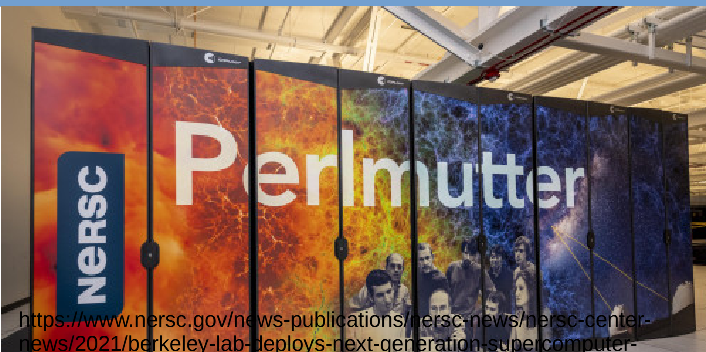
$$m_q \to m_q^{\text{phys}}$$

$$a = 0$$

$$V = \infty$$

$$m_q = m_q^{\text{phys}}$$

Computation



https://www.nersc.gov/news-publications/nersc-news/nersc-center-news/2021/berkeley-lab-deploys-next-generation-supercomputer-perlmutter-bolstering-u-s-scientific-research/

https://commons.wikimedia.org/wiki/File:Frontier_Supercomputer_(2).jpg

https://commons.wikimedia.org/wiki/File:Summit_(supercomputer).jpg

https://www.bsc.es/marenostrum/marenostrum

TOP 500 The List.

Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE DOE/SC/Oak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
2	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	4,742,808	585.34	1,059.33	24,687
3	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Microsoft Azure United States	1,123,200	561.20	846.84	
4	**Supercomputer Fugaku** - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
5	**LUMI** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,752,704	379.70	531.51	7,107
6	**Leonardo** - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, EVIDEN EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
7	**Summit** - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
8	**MareNostrum 5 ACC** - BullSequana XH3000, Xeon Platinum 8460Y+ 40C 2.3GHz, NVIDIA H100 64GB, Infiniband NDR200, EVIDEN EuroHPC/BSC Spain	680,960	138.20	265.57	2,560
9	**Eos NVIDIA DGX SuperPOD** - NVIDIA DGX H100, Xeon Platinum 8480C 56C 3.8GHz, NVIDIA H100, Infiniband NDR400, Nvidia NVIDIA Corporation United States	485,888	121.40	188.65	
10	**Sierra** - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL	1,572,480	94.64	125.71	7,438

https://www.top500.org/lists/top500/2023/11/

Successes of LQCD

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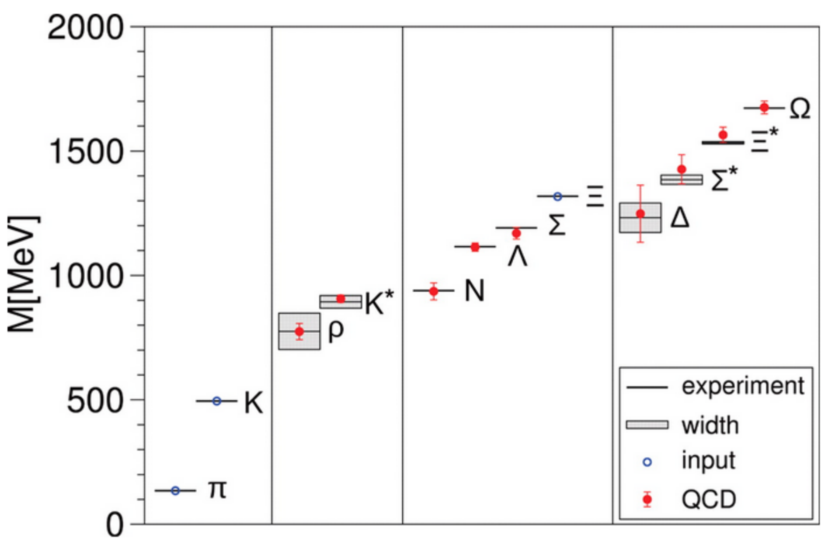
HOME > SCIENCE > VOL. 322, NO. 5905 > AB INITIO DETERMINATION OF LIGHT HADRON MASSES

REPORTS

Ab Initio Determination of Light Hadron Masses

S. DÜRR, Z. FODOR, J. FRISON, C. HOELBLING, R. HOFFMANN, S. D. KATZ, S. KRIEG, T. KURTH, L. LELLOUCH, [...], AND G. VULVERT +2 authors Authors Info & Affiliations

SCIENCE • 21 Nov 2008 • Vol 322, Issue 5905 • pp. 1224-1227 • DOI: 10.1126/science.1163233



S Durr et al., Science 322 (2008) 1224-1227

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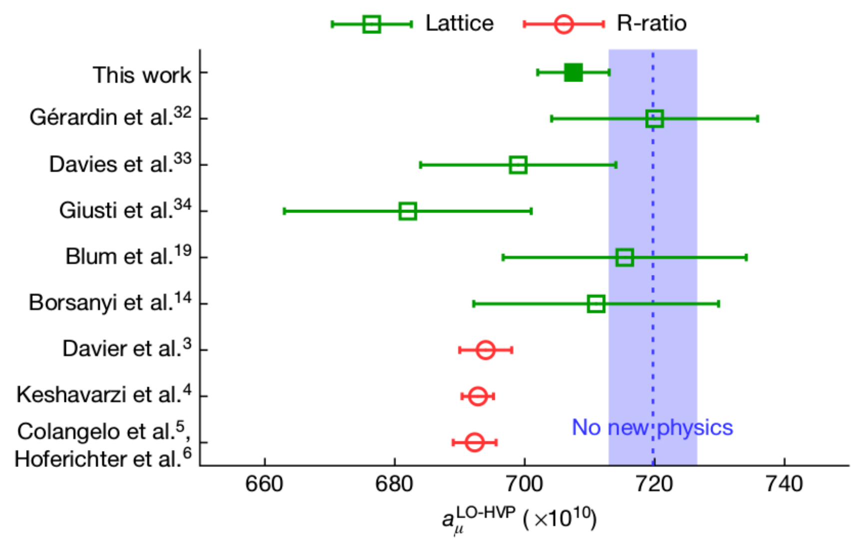
Article | Published: 07 April 2021

Leading hadronic contribution to the muon magnetic moment from lattice QCD

Sz. Borsanyi, Z. Fodor, J. N. Guenther, C. Hoelbling, S. D. Katz, L. Lellouch, T. Lippert, K. Miura, L. Parato, K. K. Szabo, F. Stokes, B. C. Toth, Cs. Torok & L. Varnhorst

Nature **593**, 51–55 (2021) | Cite this article



Borsanyi et al., Nature 593 (2021) 7857, 51-55

Hadron Spectroscopy in LQCD

$$C_{\chi\chi'}(t) = \langle 0|\hat{\mathcal{O}}_\chi(t)\hat{\mathcal{O}}^\dagger_{\chi'}(0)|0\rangle$$

- Insert a complete set of states:

$$\mathbb{I} = |0\rangle\langle 0| + \sum_n \int \frac{d^3p}{(2\pi)} \frac{1}{2E_n(\mathbf{p})} |n,\mathbf{p}\rangle\langle n,\mathbf{p}|$$

- Schrödinger picture: operators are time-independent:

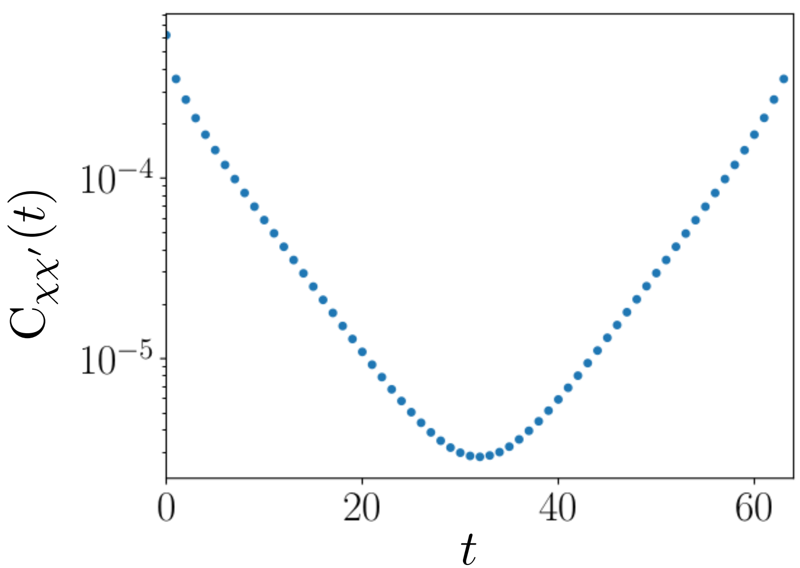
$$\hat{\mathcal{O}}(t) = e^{\hat{H}t}\hat{\mathcal{O}}e^{-\hat{H}t}$$

$$\hat{H}|n,\mathbf{p}\rangle = E_n(\mathbf{p})|n,\mathbf{p}\rangle$$

$$C_{\chi\chi'}(t) = \sum_{n=0}^{\infty} Z_{n\chi}Z^*_{n\chi'}\, e^{-tE_n}$$

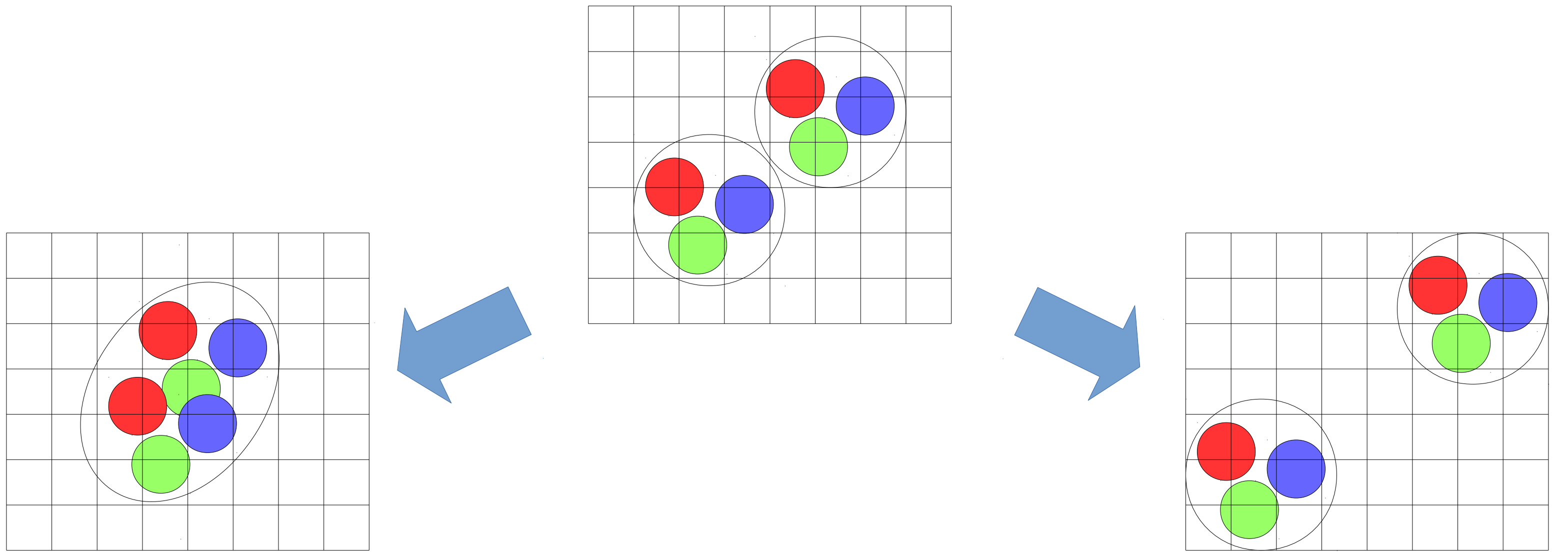
$$E_{\text{eff}} = \ln\frac{C_{\chi\chi'}(t)}{C_{\chi\chi'}(t+1)}$$

- Study time dependence of two-point correlators
- $\mathcal{O}_\chi$ is operator with quantum numbers of state of interest
- Admits spectral decomposition: time dependence determined by energy eigenstates.



Phase-Shifts from LQCD

Lüscher: Relate **volume dependence** to **phase shift**



Bound state

Scattering state

$$[E(L) - E(\infty)] \sim \frac{e^{-mL}}{L}$$

$$[E(L) - E(\infty)] \sim \frac{a}{ML^3}$$

k related to energies

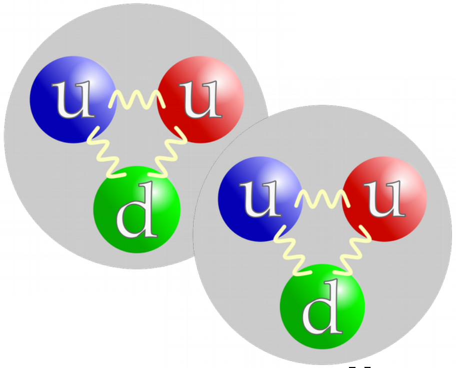
$$k \cot \delta(k) = \frac{2}{\sqrt{\pi}L} Z_{00}\left(1; \left(\frac{kL}{2\pi}\right)^2\right)$$

Z_{00} related to periodic box

UNIVERSITAT DE BARCELONA

Studying Nuclear Physics with Lattice QCD @ Universtiy of Barcelona

The NN Channel



- Before moving to more complicated observables, must demonstrate rigor of simple systems
- Smallest multi-nucleon system
- I=0 Deuteron: bound pn state (E_b~2 MeV)
- I=0, d*(2380) resonance
- I=1 dineutron (pp, nn, pn equivalent in isospin limit)
- Results for 800 MeV, currently calculating @ 170 MeV

To Bind or Not to Bind?

At m ~ 800 MeV,

- HALQCD: **unbound** deuteron and dineutron

  Aoki et al, Comput. Sci. Dis. 1 (2008)

  HAL QCD, Nucl. Phys. A881 (2012)

  Iritani et al, JHEP 1610 (2016)

  Iritani et al, PRD 96 (2017)

  HAL QCD, PRD 99 (2019)

  HAL QCD, JHEP 1903 (2019)

- PACS: **bound** deuteron and dineutron

  PACS-CS, PRD 81 (2010)

- NPLQCD: **bound** deuteron and dineutron

  NPLQCD, PRD 87 (2013)

  NPLQCD, PRD 87 (2017)

  NPLQCD PRD 107 (2023)

- CalLatt: **bound** deuteron and dineturon

  Berkowitz et al, Phys. Lett. B 285 (2017)

- Francis et al: **unbound** dineutron

  Francis, et al, PRD 99 (2019)

Why are Nuclear Systems Difficult?

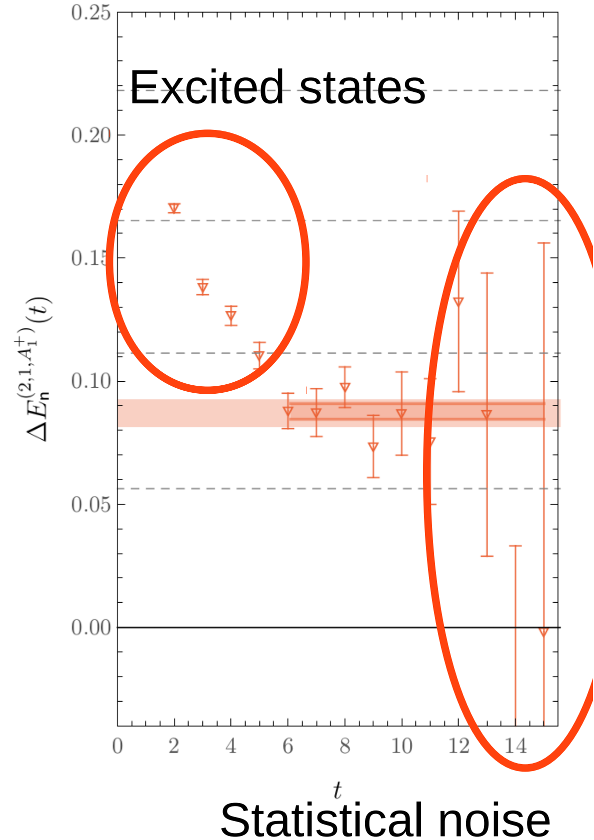
- Common to all lattice calculations:
  - Light quarks are expensive
  - Continuum limit requires multiple lattice ensembles
- BB: 6 quark system → large cost computing quark contractions
- StN problem at large Euclidean time
- Small energy gap:

$$C_{\chi\chi}(t) = |Z_{0\chi}|^2 e^{-tE_0} + |Z_{1\chi}|^2 e^{-tE_1} + \ldots$$

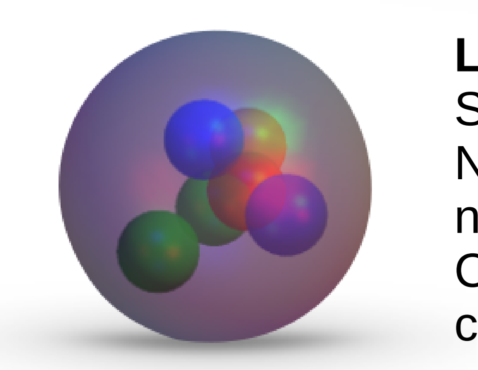
$$\Delta E = E_1 - E_0 \sim \frac{1}{L^2}$$

- Work @ 800 MeV to **validate**, move to 170 MeV to **post-dict**

$$E_{\text{eff}} = \ln \frac{C_{\chi\chi'}(t)}{C_{\chi\chi'}(t+1)}$$

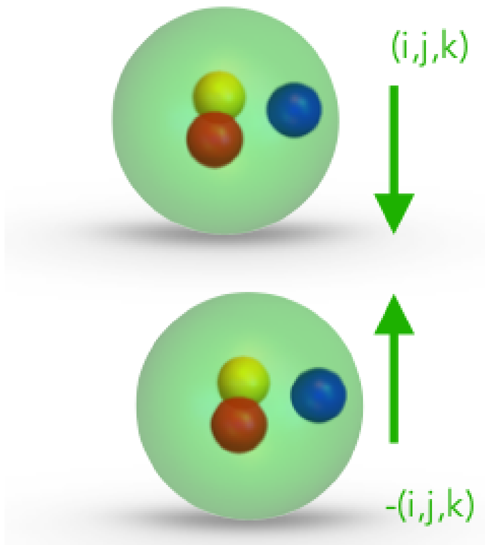


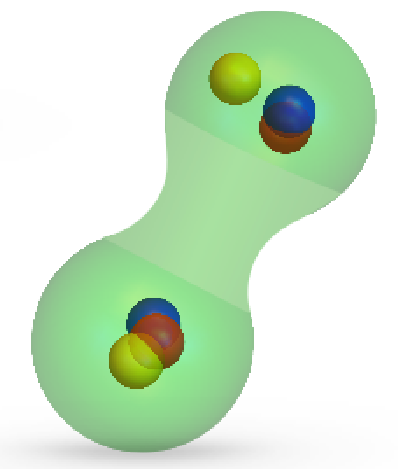
Types of Operators



Local hexaquark operators
Six Gaussian smeared quarks at a point
Novel basis of hexaquark operators which project onto two nucleons
Contains operators which cannot be factored into 3-quark color singlets

Dibaryon Operators
Two spatially-separated plane-wave baryons with relative momenta
Operators built products of positive and negative partity nucleon operators
Relative momentum: up to four units → 5 operators

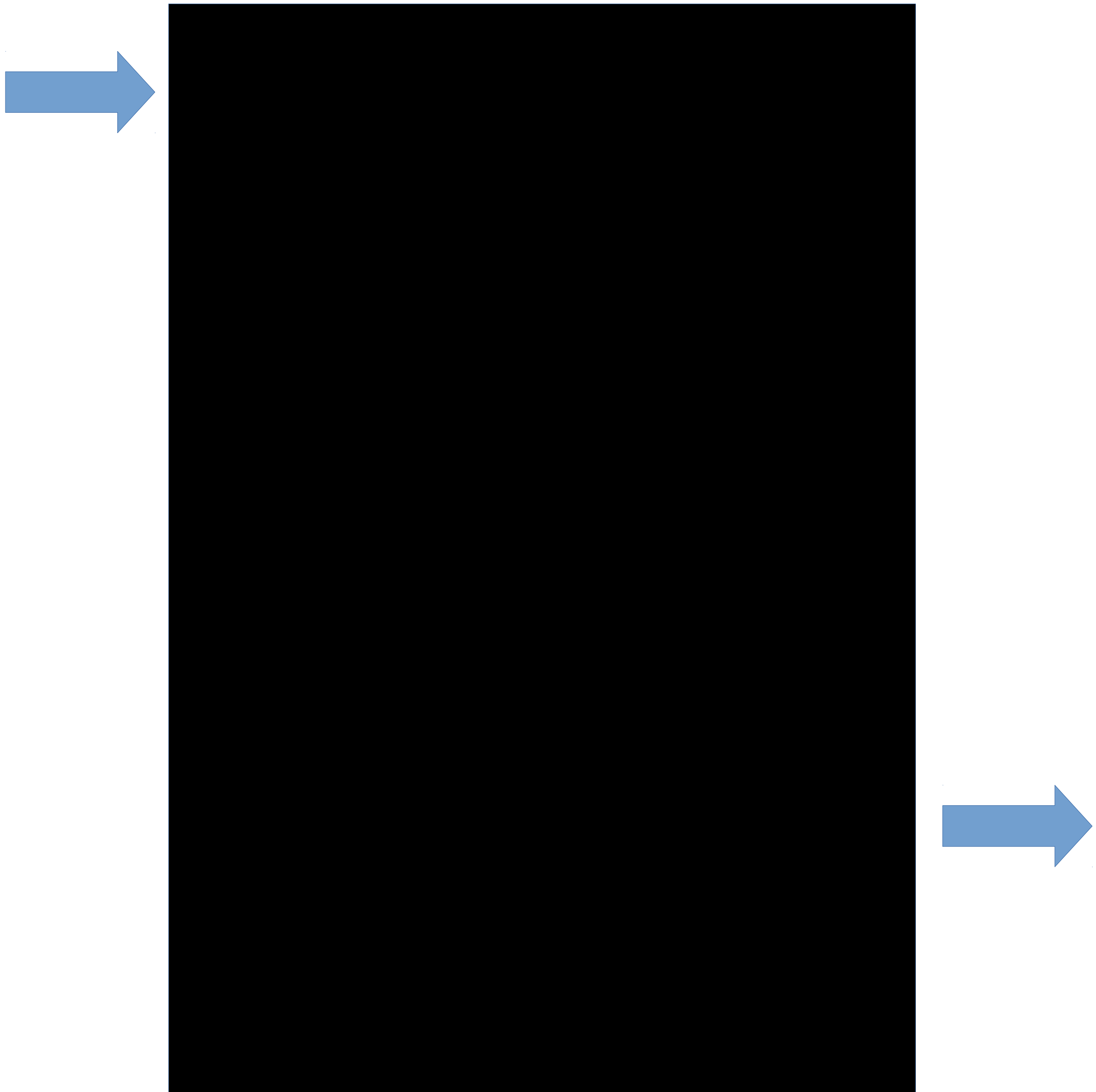




Quasi-local Operators
Two exponentially localized baryons
NN -EFT motivated deuteron-like structure

Analysis

$\hat{C}_n(t, t_0, t_{\text{ref}})$

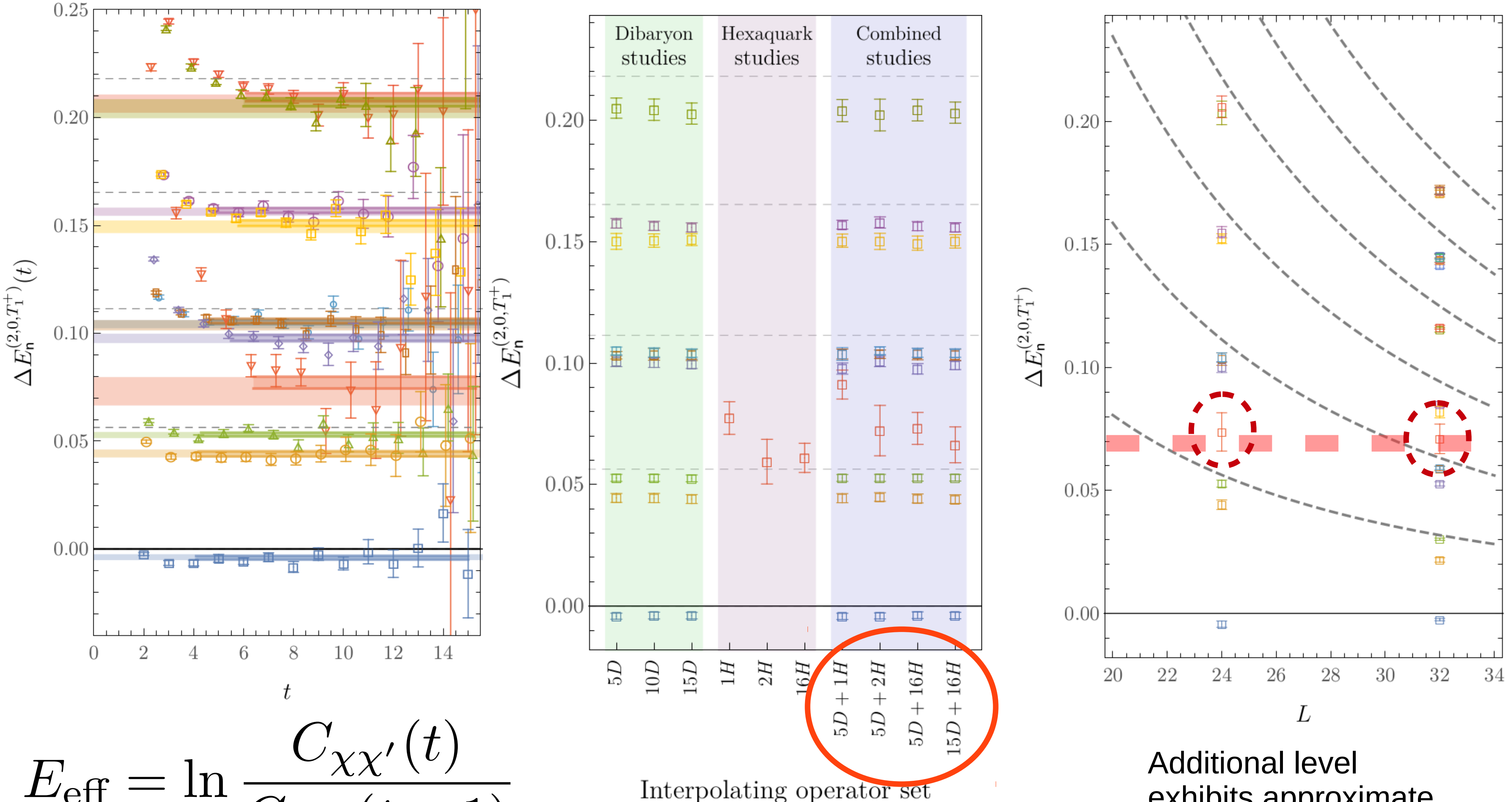


$E_0 \leq e_0$

$E_1 \leq e_1$

$\vdots$

Deuteron (I=0)

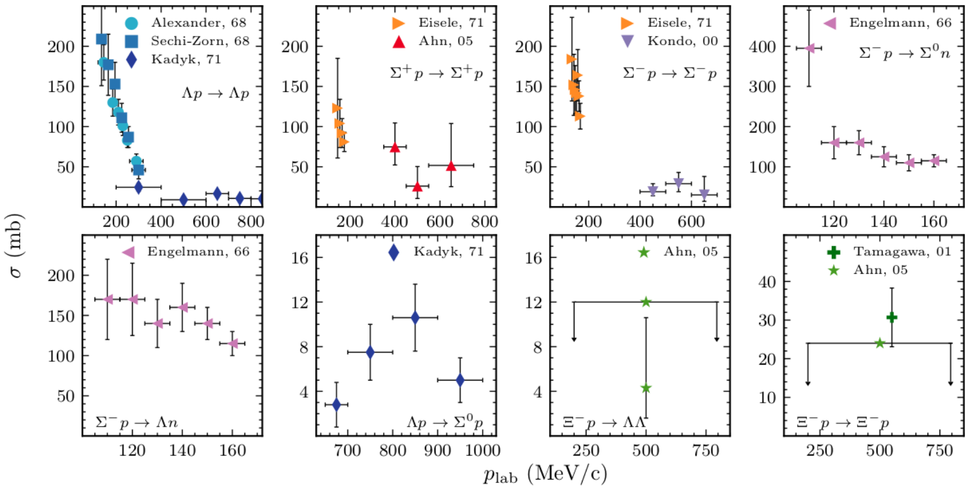


$$E_{\text{eff}} = \ln \frac{C_{\chi\chi'}(t)}{C_{\chi\chi'}(t+1)}$$

Additional level exhibits approximate volume independence!

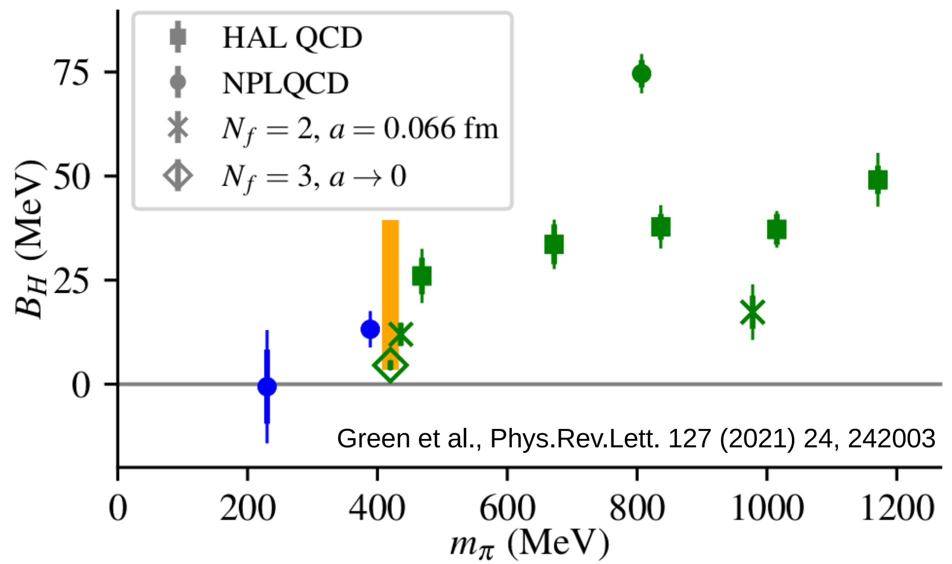
H-Dibaryon

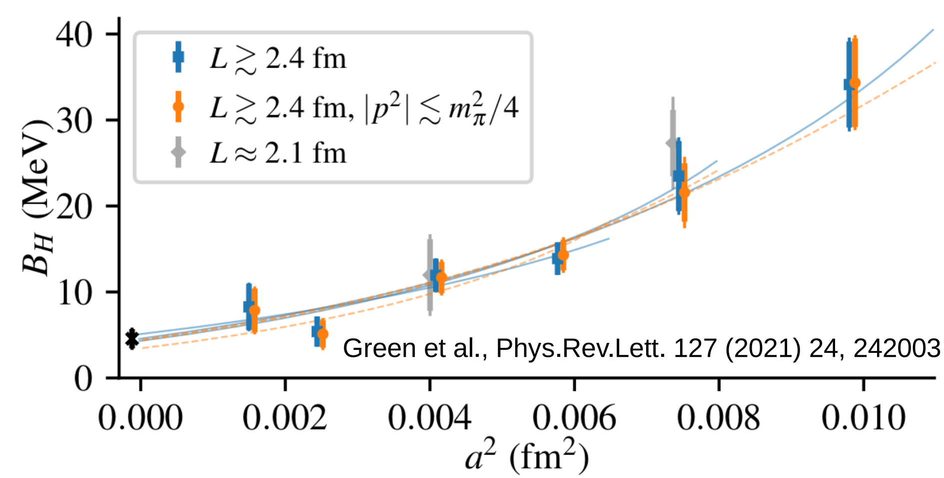
- Are there other dibaryon bound states?
- Jaffe (1976): Yes – Lambda-Lambda
- S=-2 hexaquark
- Experimentally challenging:



M. Illa, 2021 “Approaching nuclear interactions with lattice QCD”

- Lattice can contribute… provided we understand systematics





Status

- Two lattice volumes: consistent negative shift on ground-state
- Must convert to physical units to determine binding energy

$V = 24^3 \times 48$

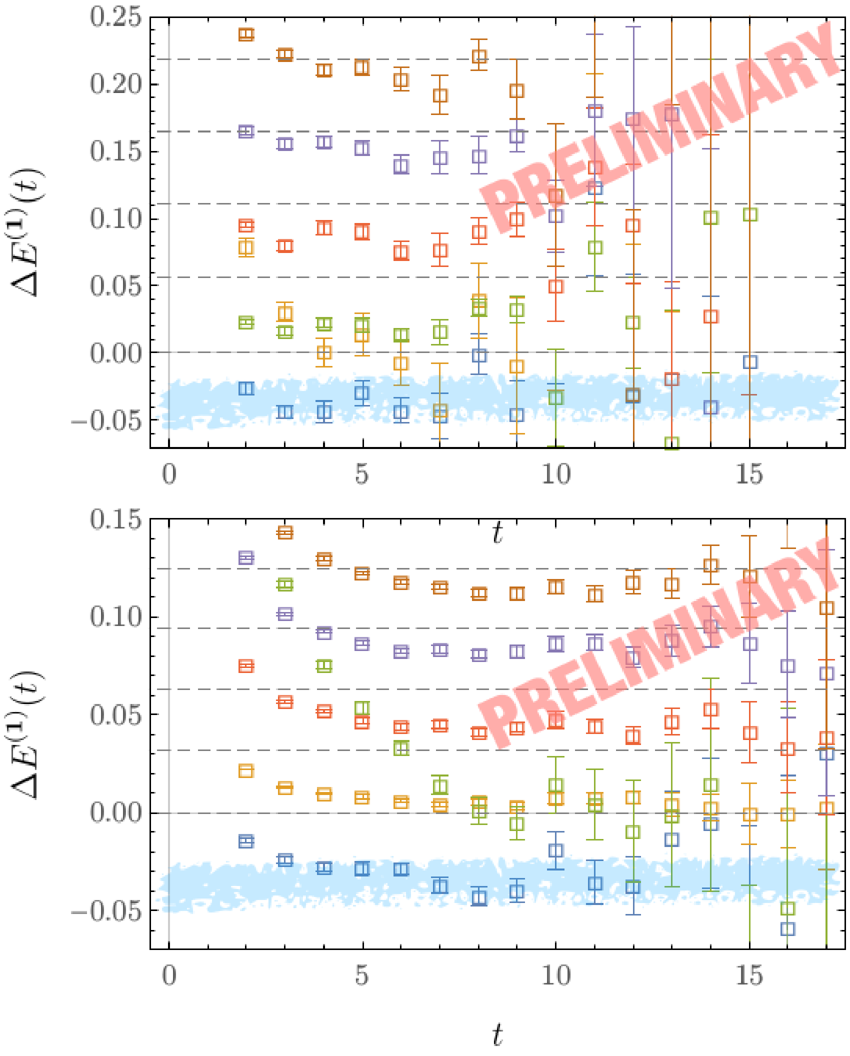
$L = 3.4\,\text{fm}$

$N_{\text{cfgs}} = 40$

$V = 32^3 \times 48$

$L = 4.5\,\text{fm}$

$N_{\text{cfgs}} = 101$



Conclusions

- LQCD presents possibility of studying nuclear physics from first principles
- Relevant for experimental program
- In principle rigorous predictions of nuclear systems
- Theoretically & technically challenging
- Current questions about control of systematic uncertainties
- Currently studying NN, YN systems with LQCD at UB

Additional State

- Lattice artifact?
- Symmetric spectra for dineutron and deuteron predicted in heavy quark limit. Natural to see approx. degenerate spectra at these quark masses.
- Lack of volume dependence consistent with resonance
- Difficult to interpret at heavy pion mass.

Variational Method

- Solve the generalized eigenvalue problem (GEVP):

$$\sum_{\chi'} C_{\chi\chi'}(t) v_{n\chi'}(t, t_0) = \lambda_n(t, t_0) \sum_{\chi'} C_{\chi\chi'}(t_0) v_{n\chi'}(t, t_0)$$

- $\lambda_n(t, t_0) = e^{-(t-t_0)E_n(t,t_0)}$ are eigenvalues, $v_{n\chi}(t, t_0)$ are eigenvevtors

- Construct optimized interpolating operators

$$\mathcal{O}_n(t_{\mathrm{ref}}, t_0, t) = \sum_{\chi} v_{n\chi}(t_{\mathrm{ref}}, t_0) \mathcal{O}_\chi(t)$$

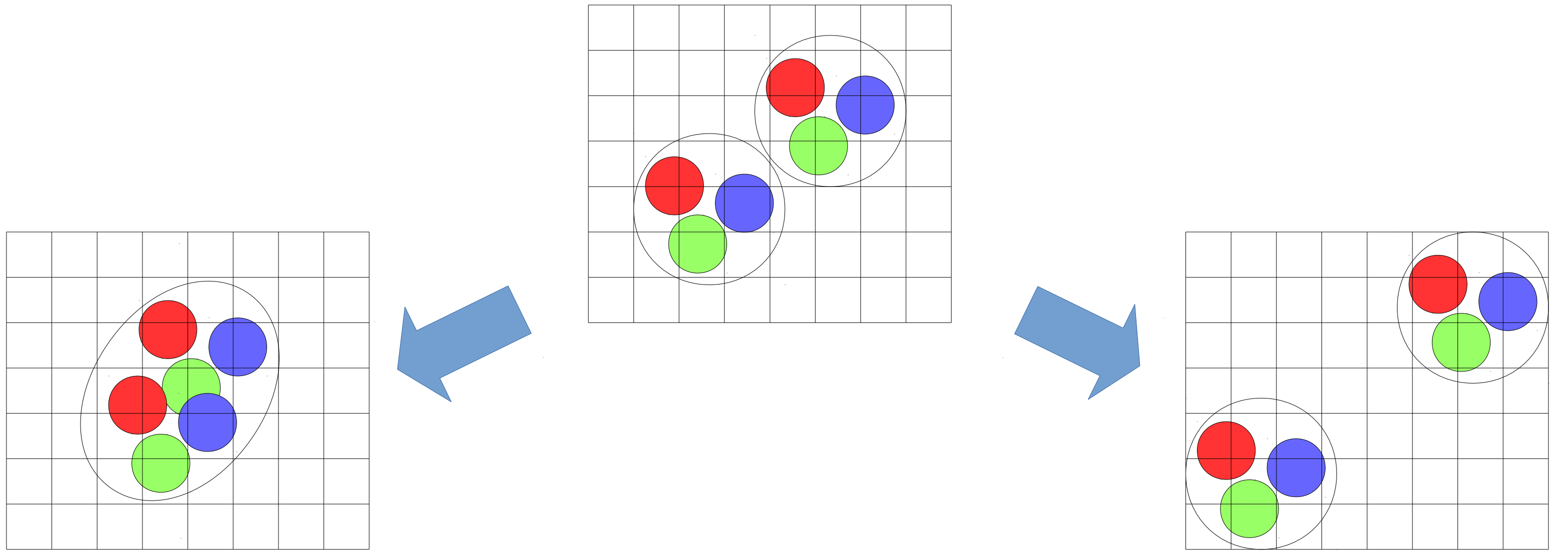
- Compute resulting two-point correlators

$$\hat{C}_n(t, t_0, t_{\mathrm{ref}}) = \sum_{n=0}^{\infty} |Z_n(t_0, t_{\mathrm{ref}})|^2 \, e^{-tE_n} > 0$$

Rigorous upper bounds!

Volume Dependence

$$C_{\chi\chi'}(t) = \langle 0|\hat{\mathcal{O}}_{\chi}(t)\hat{\mathcal{O}}^{\dagger}_{\chi'}(0)|0\rangle$$



Bound state

Scattering state

$$[E(L) - E(\infty)] \sim \frac{e^{-mL}}{L}$$

$$[E(L) - E(\infty)] \sim \frac{a}{ML^3}$$

Lüscher: Relate volume dependence to phase shift

No-Go Theorem

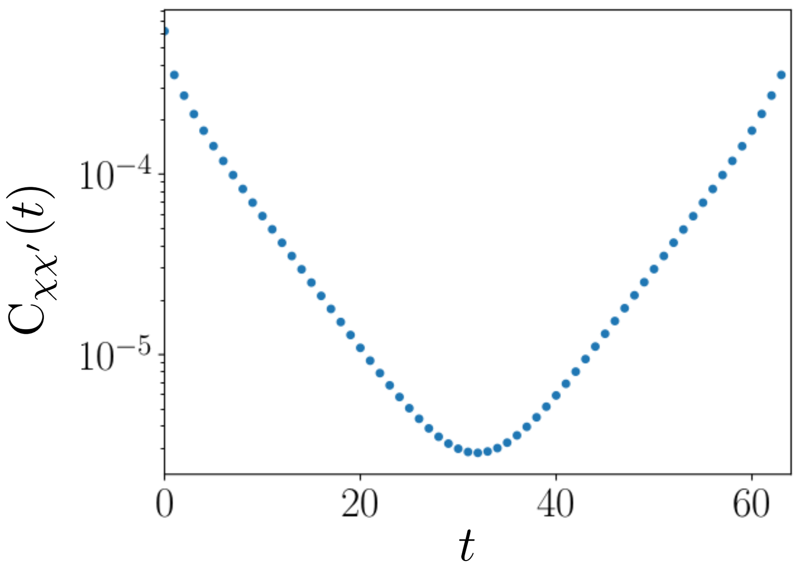
- LSZ: Scattering amplitudes are residues of poles of n-point correlation function
- LQCD: Formulated with Euclidean time
- Maiani-Testa:

  S-matrix elements cannot be extracted from infinite-volume Euclidean-space Green functions except at kinematic thresholds
- Cannot isolate single particle states.

Hadron Spectroscopy in LQCD

$$C_{\chi\chi'}(t) = \langle 0 | \mathcal{O}_\chi(t) \mathcal{O}^\dagger_{\chi'}(0) | 0 \rangle$$

- Study time dependence of two-point correlators
- $\mathcal{O}_\chi$ is operator with quantum numbers of state of interest
- Admits spectral decomposition: time dependence determined by energy eigenstates.



$$C_{\chi\chi'}(t) = \sum_{n=0}^{\infty} Z_{n\chi} Z^*_{n\chi'} \, e^{-tE_n}$$

Operator Sets

Consider operator sets with

- Dibaryon only:
  - 5D: positive parity, 5 different momenta
  - 10D: positive & negative parity, 5 different momenta
  - 15D: positive & negative parity, lower spin components, 5 different momenta
- Hexaquark only:
  - 1H: Most important hexaquark
  - 2H: Most important hexaquarks
  - 16H: Full basis
- Union of these two sets:
  - 5D+1H, 5D+2H, 5D+16H, 15D+16H

Interlacing Theorem

Provides **rigorous bounds** on number of energy levels at or below effective mass*

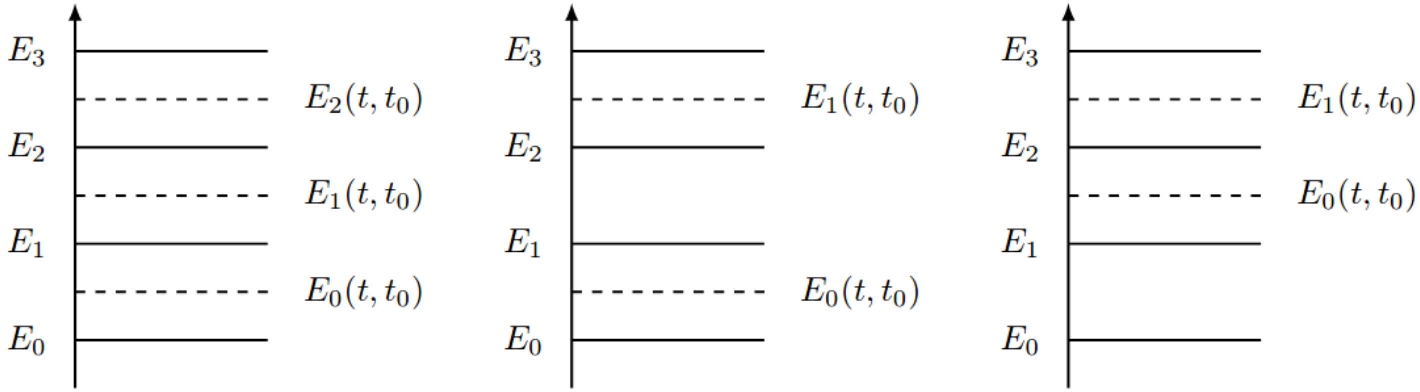
Theorem (Eigenvalue Interlacing Theorem) *Suppose* $A \in \mathbb{R}^{n\times n}$ *is symmetric. Let* $B \in R^{m\times m}$ *with* $m < n$ *be a principal submatrix (obtained by deleting both* i*-th row and* i*-th column for some values of* i*). Suppose* A *has eigenvalues* $\lambda_1 \leq \cdots \leq \lambda_n$ *and* B *has eigenvalues* $\beta_1 \leq \cdots \leq \beta_m$*. Then*

$$\lambda_k \leq \beta_k \leq \lambda_{k+n-m} \text{ for } k = 1, \ldots, m$$

And if $m = n - 1$,

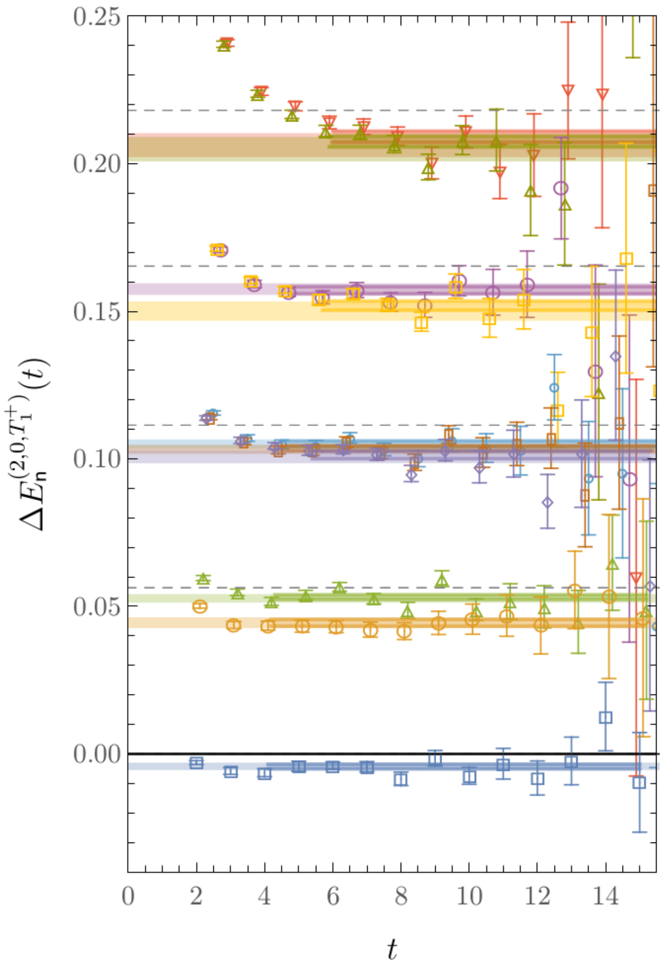
$$\lambda_1 \leq \beta_1 \leq \lambda_2 \leq \beta_2 \leq \cdots \leq \beta_{n-1} \leq \lambda_n$$

$$\lambda_n = e^{-E_n(t-t_0)} \qquad \beta_n = e^{-E_n(t,t_0)(t-t_0)}$$

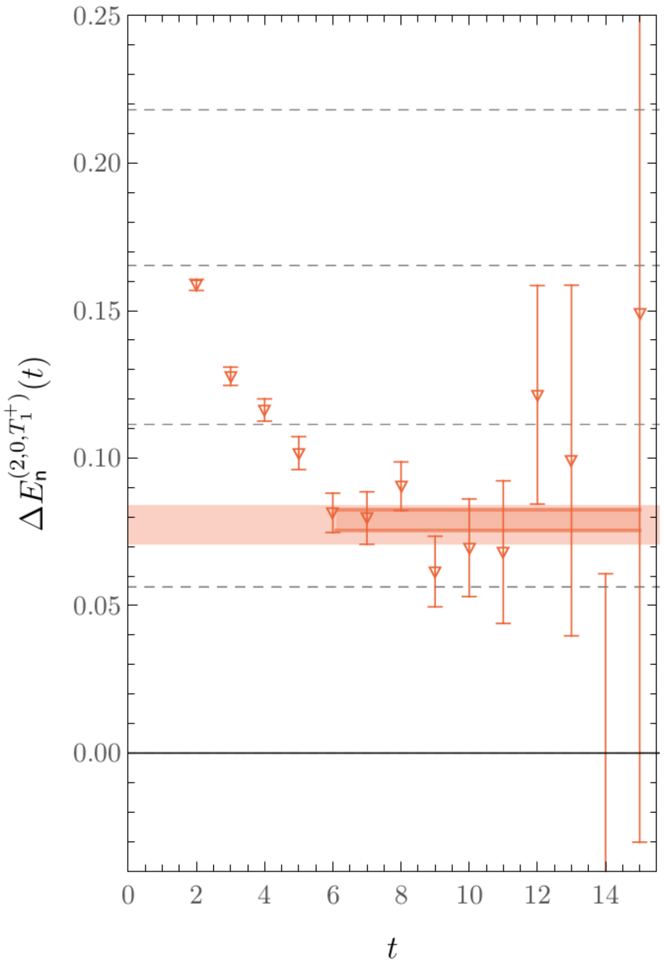


*Fleming, Lattice 2023 (2023)

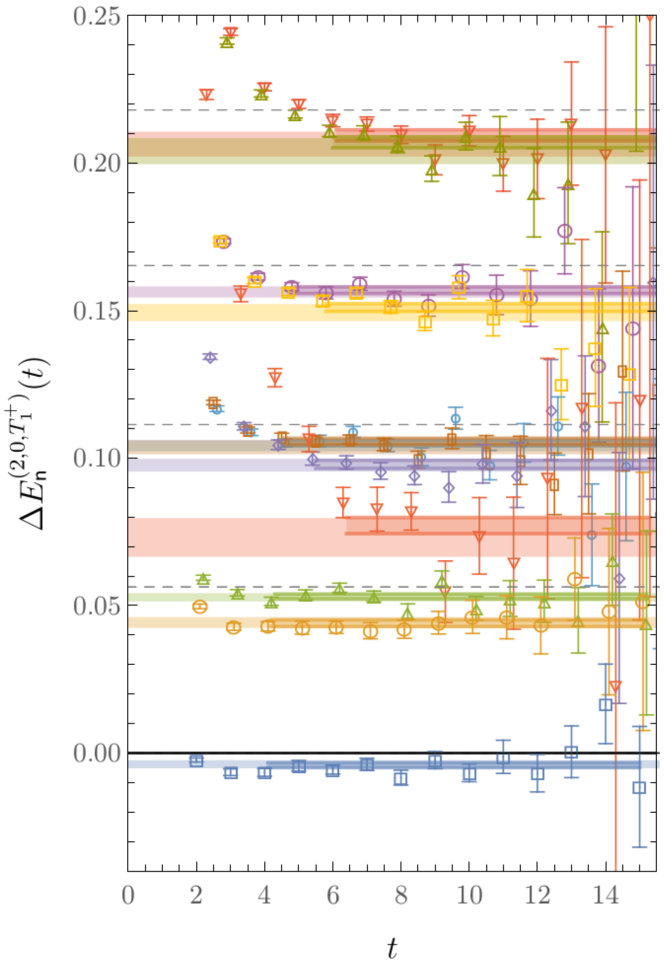
Deuteron (I=0)



5D

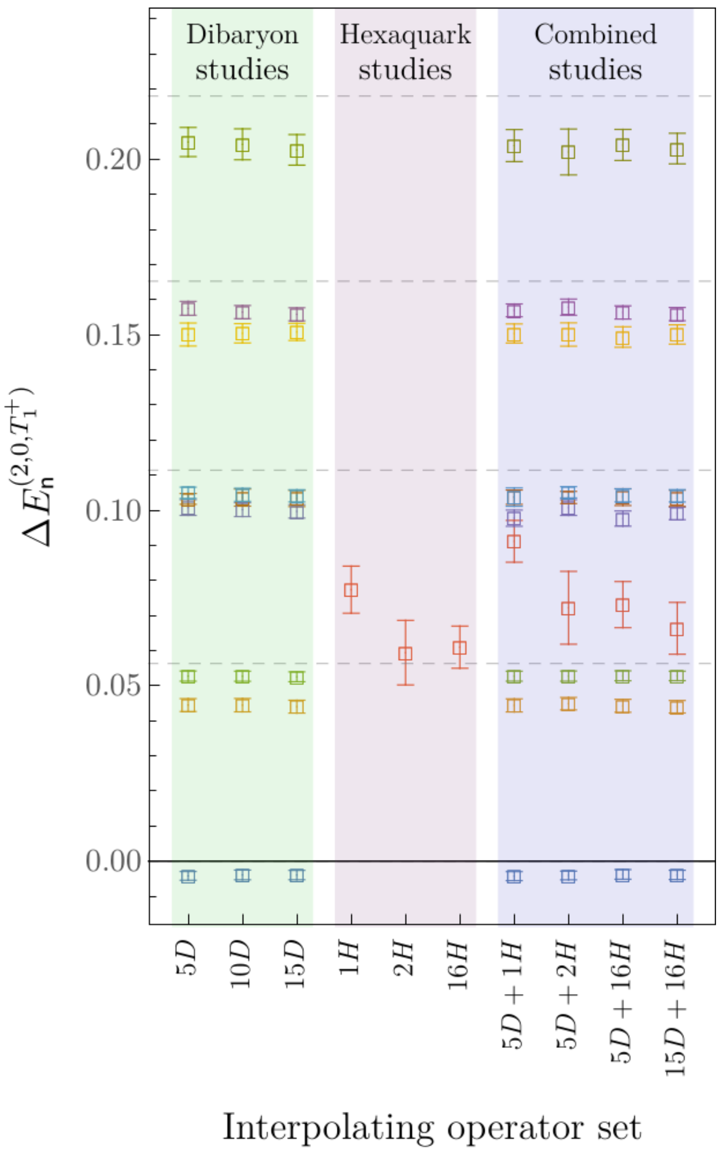


1H



5D+1H

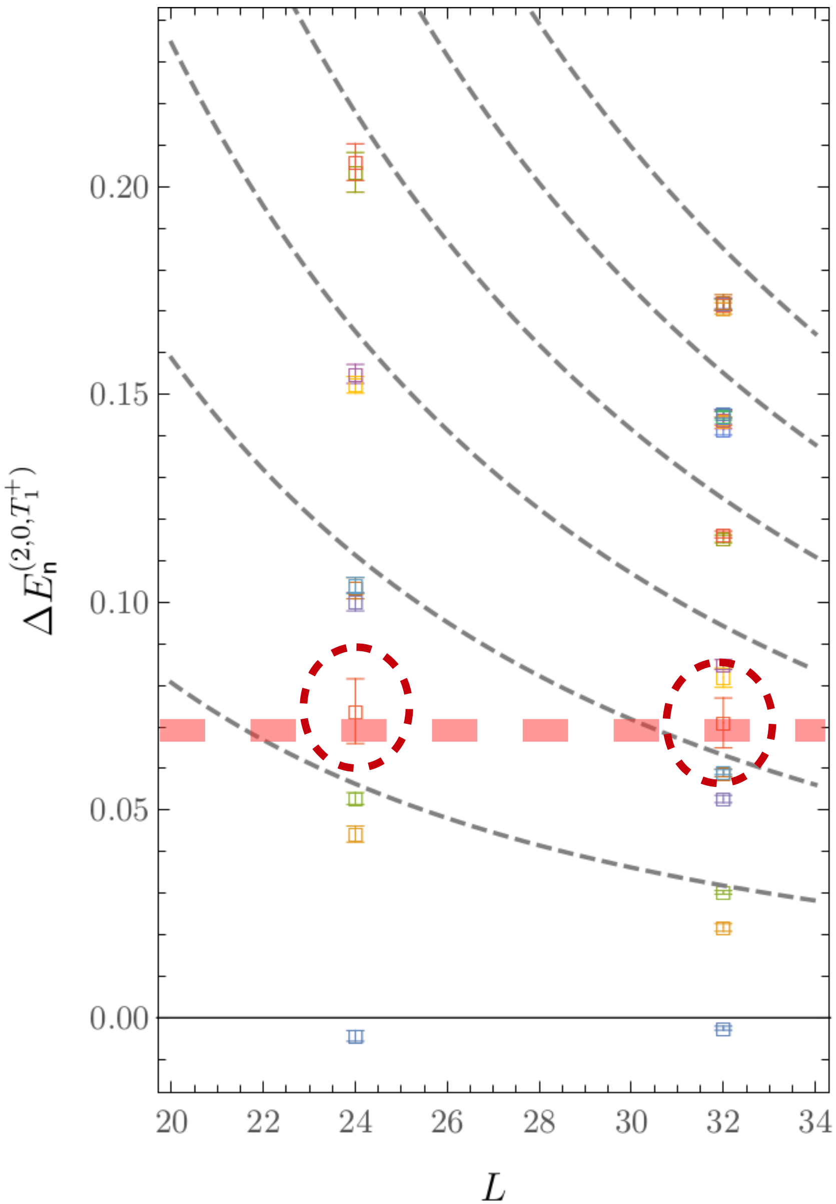
Deuteron (I=0)



- 5D, 10D and 15D agree within 1 sigma
- 1H, 2H and 16H poor variational bounds
- 5D+1H etc lead to union of two sets of variational bounds!
- Additional state not present in non-interacting theory

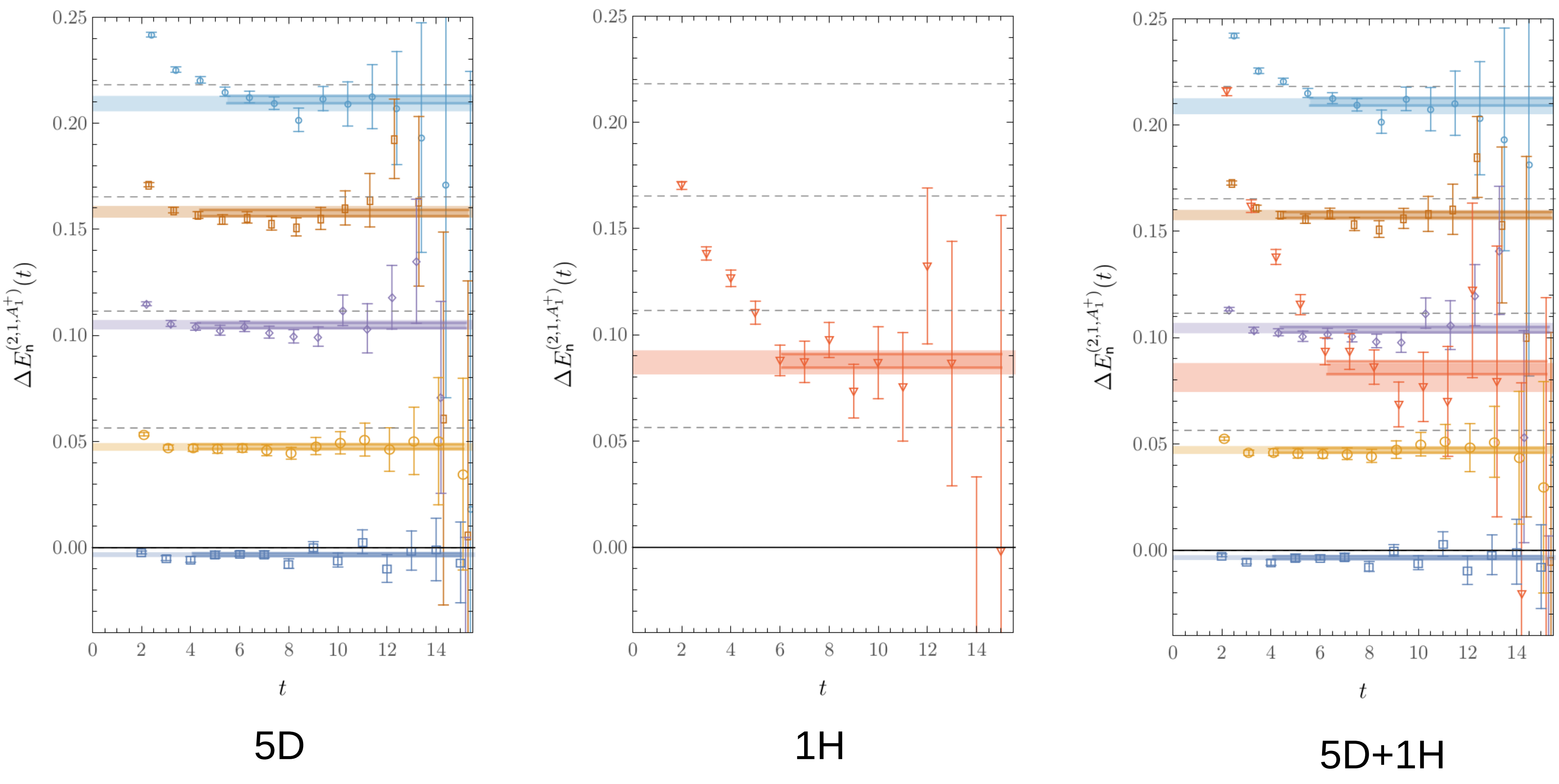
Volume Dependence

Additional level exhibits approximate volume independence! Suggestive of resonance.

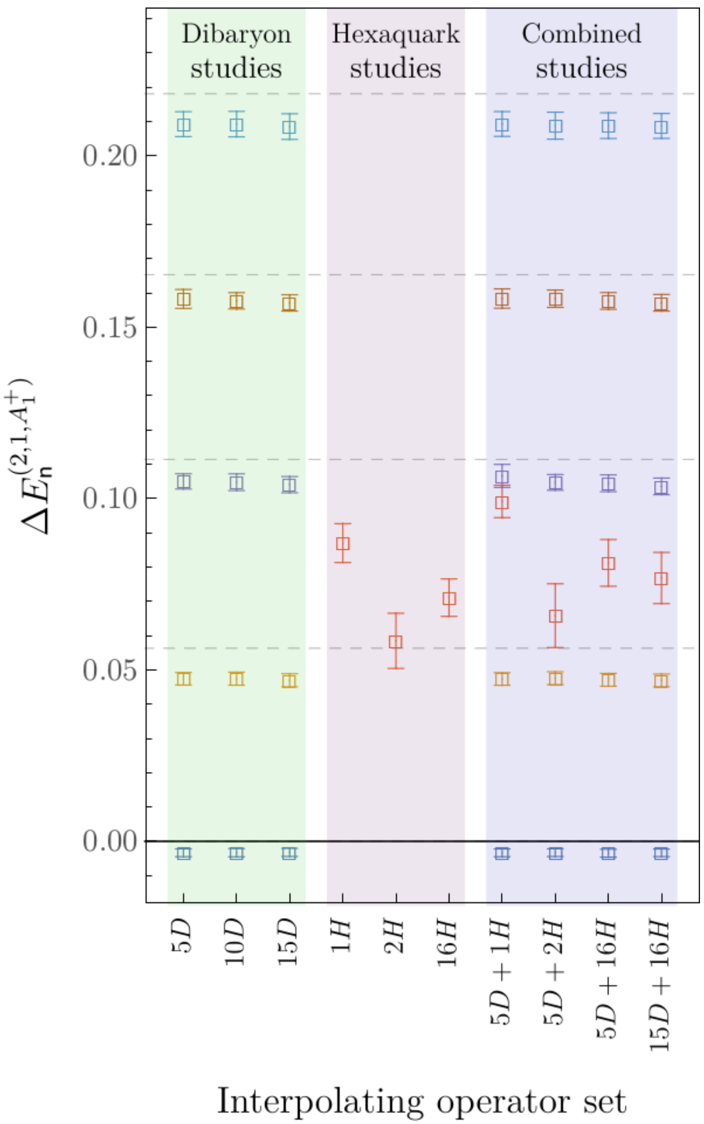


L=32 data from NPLQCD: Phys.Rev.D 107 (2023) 9, 094508

Dineutron (I=1)



Dineutron (I=1)



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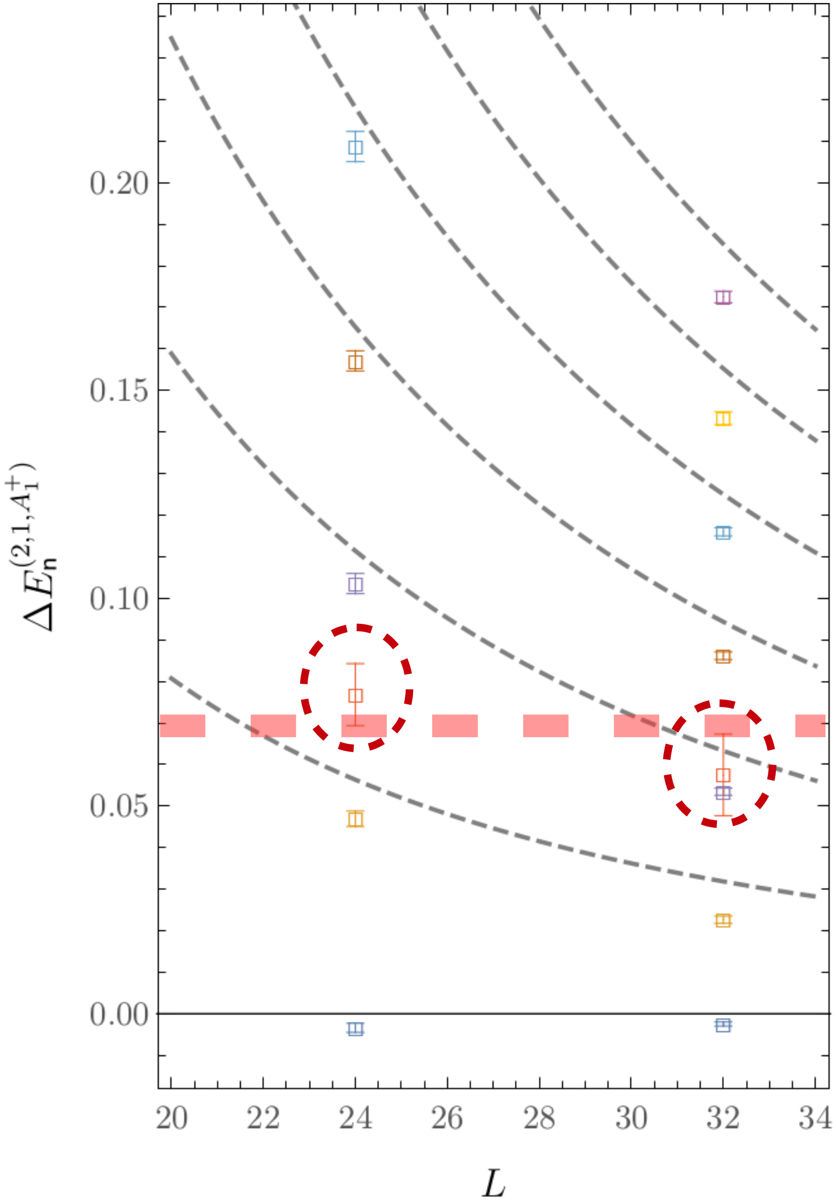
Volume Dependence



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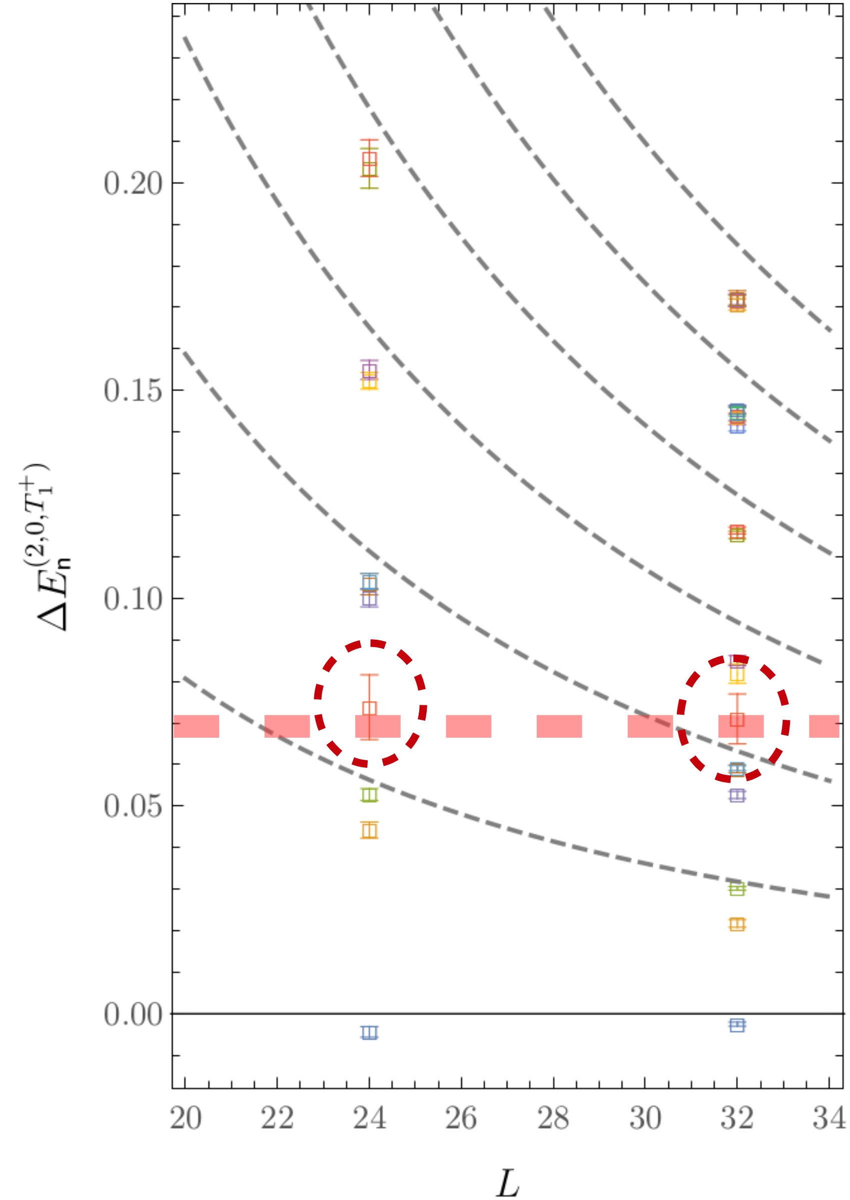
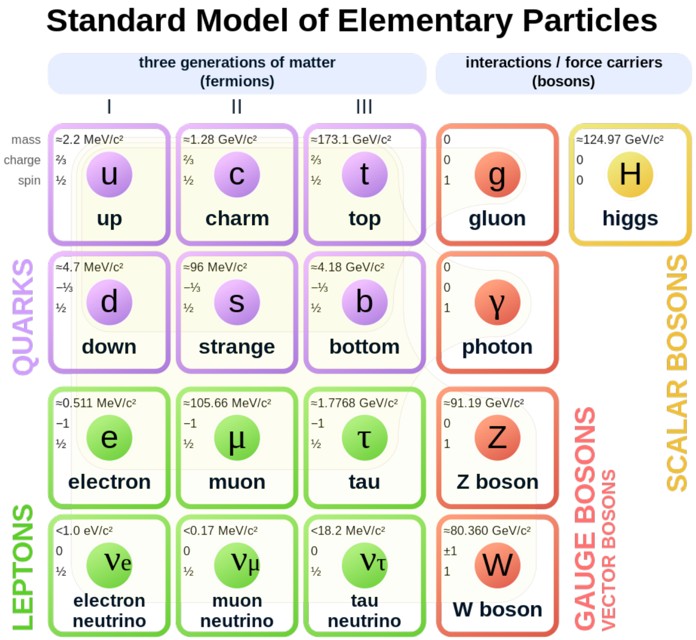


L=32 data from NPLQCD: Phys.Rev.D 107 (2023) 9, 094508

Outline

- Motivation
- Scattering Amplitudes from Lattice QCD
- Variational Analysis of NN
  - Observation of resonant-like state at de ~ 0.07.
- Conclusions

Motivation



LQCD can provide important input for both understanding the SM and constraining BSM physics.

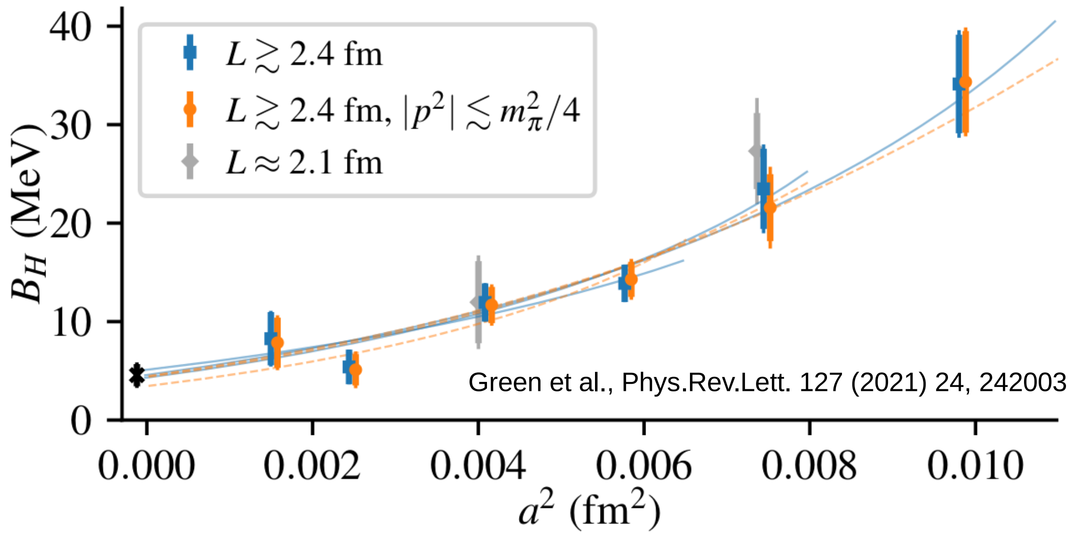
Nuclear matrix elements required for:

- double-beta decay,
- dark matter direct detection,
- neutrino-nucleus scattering
- Constrain nuclear EFTs

Conclusions

- LQCD can connect QCD to nuclear physics
- Challenge to control systematic uncertainties
- Variational Analysis of NN
  - Resonant-like state at dE~0.07.
  - Need to move towards physical point to interpret
  - Currently underway!

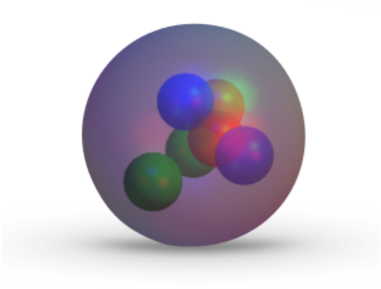
H-Dibaryon



B_H (MeV)
0
10
20
30
40
$L \gtrsim 2.4$ fm
$L \gtrsim 2.4$ fm, $|p^2| \lesssim m_\pi^2/4$
$L \approx 2.1$ fm
Green et al., Phys.Rev.Lett. 127 (2021) 24, 242003
0.000
0.002
0.004
0.006
0.008
0.010
a^2 (fm^2)

Two Volumes

Hexaquark Operators



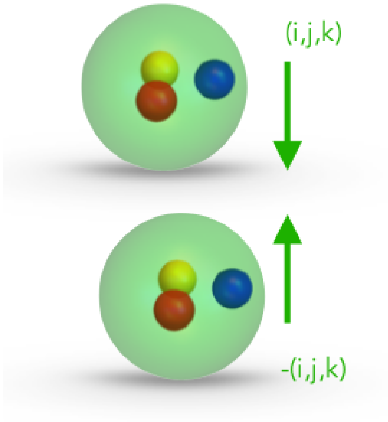
$$\mathcal{H}^K(x) = \mathcal{H}^{C_1C_2C_3}_{\Gamma_1,F_1;\Gamma_2,F_2;\Gamma_3,F_3}(x) = T^{C_1C_2C_3}_{abcdef}\mathcal{D}^{ab}_{\Gamma_1,F_1}(x)\mathcal{D}^{cd}_{\Gamma_2,F_2}(x)\mathcal{D}^{ef}_{\Gamma_3,F_3}(x)$$

Many ways to construct color singlet operator.

$$\mathbf{3} \otimes \mathbf{3} = \mathbf{6} \oplus \overline{\mathbf{3}}$$

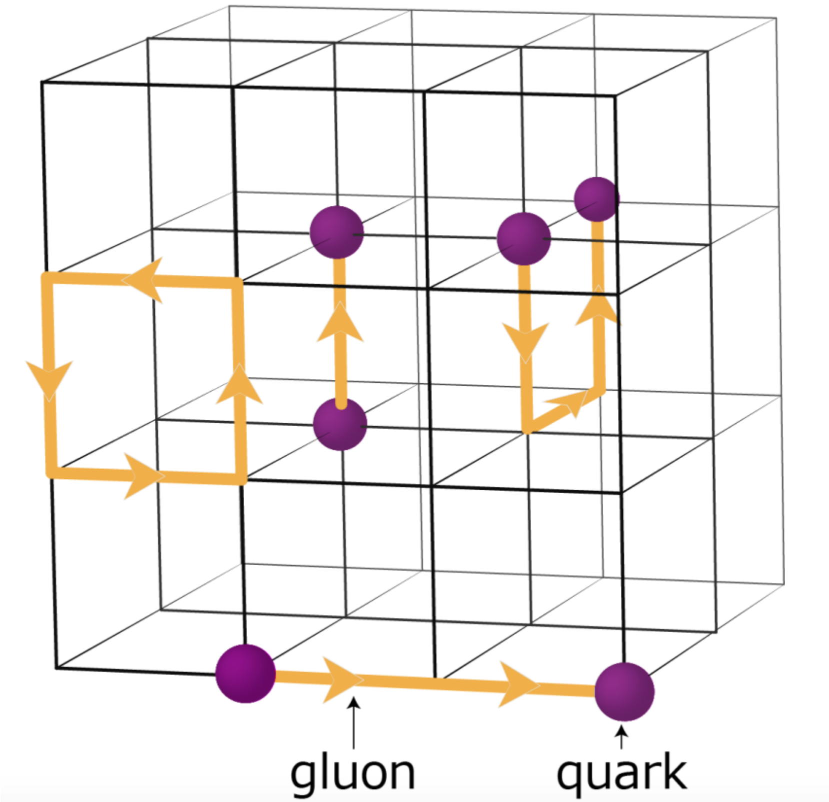
$$(\mathbf{3} \otimes \mathbf{3}) \otimes (\mathbf{3} \otimes \mathbf{3}) \otimes (\mathbf{3} \otimes \mathbf{3}) = (\mathbf{6} \oplus \overline{\mathbf{3}}) \otimes (\mathbf{6} \oplus \overline{\mathbf{3}}) \otimes (\mathbf{6} \oplus \overline{\mathbf{3}})$$

Dibaryon Operators

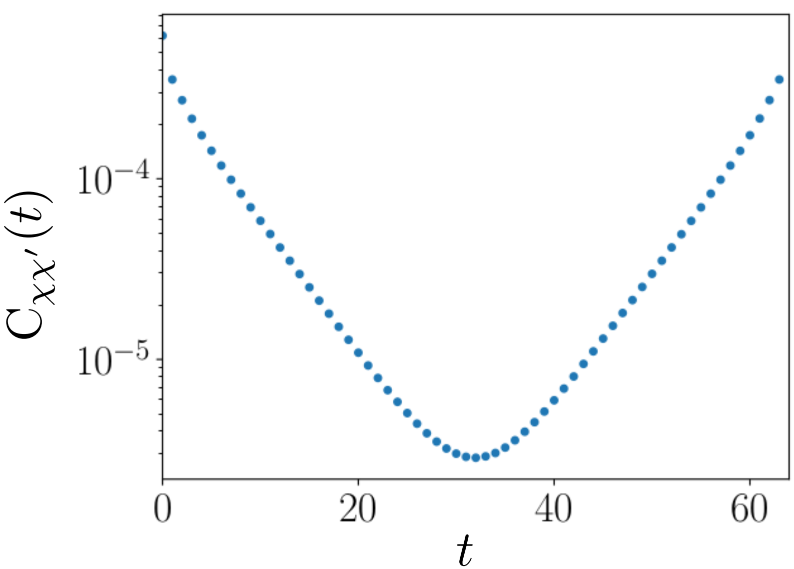


$L^3 \times T$	β	m_q	a [fm]	L [fm]	T [fm]	$m_\pi L$	$m_\pi T$	$N_{\rm cfg}$	$N_{\rm src}$
$24^3 \times 48$	6.1	-0.2450	0.1453(16)	3.4	6.7	14.3	28.5	469	216

Hadron Spectroscopy in LQCD



$$C_{\chi\chi'}(t) = \langle 0|\mathcal{O}_\chi(t)\mathcal{O}^\dagger_{\chi'}(0)|0\rangle$$

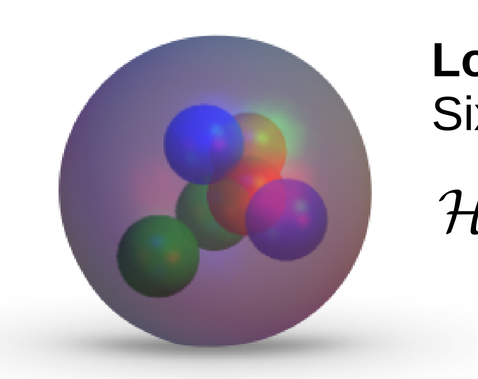


$$\langle \mathcal{O}\rangle = \frac{1}{Z}\int D\phi\,\mathcal{O}[\phi]\,e^{-S[\phi]}$$

$$= \frac{1}{N}\sum_{i=1}^{N}\mathcal{O}[\phi_i], \qquad \phi \sim \frac{1}{Z}e^{-S[\phi]}$$

$$C_{\chi\chi'}(t) = \sum_{n=0}^{\infty} Z_{n\chi}Z^*_{n\chi'}\,e^{-tE_n}$$

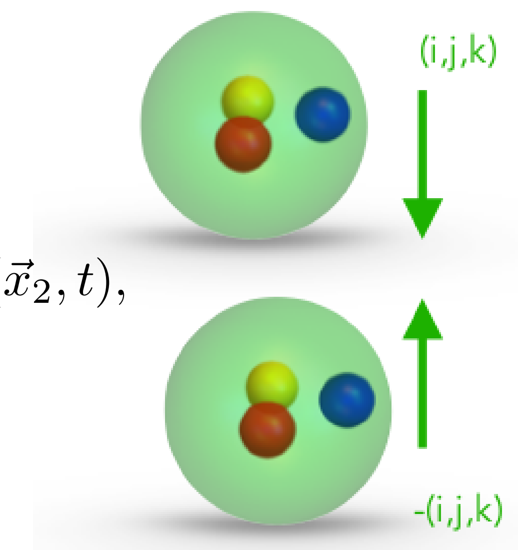
Types of Operators



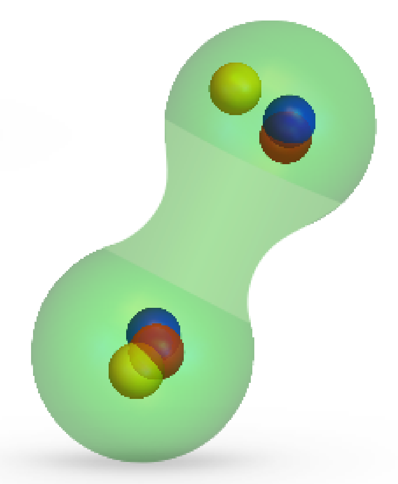
Local hexaquark operators
Six Gaussian smeared quarks at a point

$$\mathcal{H}^K(x) = T^{C_1 C_2 C_3}_{abcdef} \mathcal{D}^{ab}_{\Gamma_1, F_1}(x) \mathcal{D}^{cd}_{\Gamma_2, F_2}(x) \mathcal{D}^{ef}_{\Gamma_3, F_3}(x)$$

Dibaryon Operators
Two spatially-separated plane-wave baryons
with relative momenta



$$D^{\Gamma}_{\rho}(\vec{n}, t) = \sum_{\vec{x}_1, \vec{x}_2} e^{i2\pi\vec{n}/L\cdot(\vec{x}_1 - \vec{x}_2)} \sum_{\sigma, \sigma'} v^{\sigma\sigma'}_{\rho} N^{\Gamma}_{\sigma}(\vec{x}_1, t) N^{\Gamma}_{\sigma'}(\vec{x}_2, t),$$



Quasi-local Operators
Two exponentially localized baryons
NN -EFT motivated deuteron-like structure

$$Q^{\Gamma}_{\rho}(\kappa, t) = \sum_{\vec{R}} \sum_{\vec{x}_1, \vec{x}_2} e^{-\kappa|\vec{x}_1 - \vec{R}|} e^{-\kappa|\vec{x}_2 - \vec{R}|} \sum_{\sigma, \sigma'} v^{\sigma\sigma'}_{\rho} N^{\Gamma}_{\sigma}(\vec{x}_2, t) N^{\Gamma}_{\sigma'}(\vec{x}_1, t),$$