

Variational studies of (hyper)nuclear interactions from Lattice QCD

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Institut de Ciències del Cosmos UNIVERSITAT DE BARCELONA







EXCELENCIA MARÍA DE MAEZTU 3020-2023

 $\mathcal{L}_{QCD} = \overline{q}_{ij} \left(i \gamma^{u} \partial_{u} - m_{j} \right) q_{ij} + g(\overline{q}_{ij} \gamma^{u} \lambda_{a} q_{ij}) F_{u}^{a} - \frac{1}{\Delta} F_{uv}^{a} F_{a}^{uv}$ i = r, g, b j = u, d, c, s, t, b



Solving QCD



S. Bethke, G.Dissertori, G.P. Salam EPJ Web of Conferences 120 07005 (2016)

 $\mathcal{L}_{QCD} = \overline{q}_{ij} \left(i \gamma^{u} \partial_{u} - m_{j} \right) q_{ij} + g(\overline{q}_{ij} \gamma^{u} \lambda_{a} q_{ij}) F_{u}^{a} - \frac{1}{4} F_{uv}^{a} F_{a}^{uv}$ $i = r, g, b \quad j = u, d, c, s, t, b$



Solving QCD at low-energies. LQCD + EFT

Nuclear physics, the non-perturbative regime of QCD

The quantum propagation is expressed as a weighted sum over paths

PATH INTEGRAL Feynman, 1948

 $A = \int D(q) \, \exp\left(i\int_{i}^{f} dt \, L(q(t))\right)$

go to Euclidean space (numerical methods/important sampling)





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 $\mathcal{L}_{\mathrm{EFT}}\left[\pi, N, \ldots; m_{\pi}, m_{N}, \ldots; C_{i}\right]$ └→ LECs





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Lattice QCD calculations allow for:

Connection to QCD

Systematically improve the calculation

Control the uncertainties



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 $L_x \times L_v \times L_z \times T$

 $L > m_{\pi}^{-1}$ Finite volume

 $b < < \Lambda_{QCD}^{-1}$

discretize spacetime

Solving QCD at low-energies. LQCD + EFT

Nuclear physics, the non-perturbative regime of QCD

The quantum propagation is expressed as a weighted sum over paths

PATH INTEGRAL $A = \int D(q) \, \exp\left(i\int_{-1}^{f} dt \, L(q(t))\right)$ Feynman, 1948

go to Euclidean space (numerical methods/important sampling)

expectation values

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}q \, \mathcal{D}\overline{q} \, \mathcal{D}A_{\mu} \, \hat{\mathcal{O}}[q, \overline{q}, A] \, e^{\mathrm{i}S_{QCD}} \\ \downarrow t \to \mathrm{i}\tau$$

go to Euclidean space numerical methods/important sampling



 $\mathcal{L}_{QCD} = \overline{q}_{ij} \left(i \gamma^{u} \partial_{u} - m_{j} \right) q_{ij} + g(\overline{q}_{ij} \gamma^{u} \lambda_{a} q_{ij}) F_{u}^{a} - \frac{1}{\Delta} F_{uv}^{a} F_{a}^{uv}$ i = r, g, b j = u, d, c, s, t, b



 $L_x \times L_y \times L_z \times T$

 $L > m_{\pi}^{-1}$ Finite volume

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Solving QCD at low-energies. LQCD + EFT

expectation values

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 $L_x \times L_v \times L_z \times T$

 $L > m_{\pi}^{-1}$ Finite volume

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discretize spacetime

Solving QCD at low-energies. LQCD + EFT

expectation values

$$\langle \hat{\mathcal{O}} \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}q \, \mathcal{D}\overline{q} \, \mathcal{D}A_{\mu} \, \hat{\mathcal{O}}[q, \overline{q}, A] \, e^{\mathrm{i}A_{\mu}}$$

 $t \rightarrow i \tau$

go to Euclidean space numerical methods/important sampling













 $\{U^{[i]}\},$ (Markov process)

each configuration is created by the preceding one: $P(U^{[i-1]} \to U^{[i]}) P(U^{[i-1]}) = P(U^{[i]} \to U^{[i-1]}) P(U^{[i]})$

Basic Monte Carlo algorithm



LQCD algorithm

 $\left\{ U^{[i]} \right\},$ (Markov process)

each configuration is created by the preceding one:

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Basic Monte Carlo algorithm

For each gauge-field configuration, calculate the quark propagator (inverse of the fermion matrix)





LQCD algorithm



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Basic Monte Carlo algorithm

For each gauge-field configuration, calculate the quark propagator (inverse of the fermion matrix)





LQCD algorithm

In order to study hadrons, we need to contract propagators onto correlation functions $C_i(t)$

$$C(\Gamma^{\nu}, \vec{p}, t) = \sum_{\vec{x}_{1}} e^{-i\vec{p}\vec{x}_{1}} \Gamma^{\nu} \left\langle J(\vec{x}_{1}, t) \overline{J}(\vec{x}_{0}, 0) \right\rangle$$

for ex. $\overline{u}(x_{1})\gamma_{5}d(x_{1}) \quad \overline{d}(x_{0})\gamma_{5}u(x_{0})$
 $\pi^{+} = \overline{d}\gamma_{5}u$
 $\langle \pi^{\dagger}(x_{1}) \pi(x_{0}) \rangle = \langle \overline{u}(x_{1}) \gamma_{5} d(x_{1}) \overline{d}(x_{0}) \gamma_{5} u(x_{0}) \rangle$
 $OU \ \widehat{O} [Q(U)^{-1}] \det(Q(U)) e^{-S_{g}[U]}$

$$\widehat{O} = \frac{1}{Z} \int DU \ \widehat{O} \left[Q(U)^{-1} \right] \det \left(Q(U) \right) e^{-S_g[U]}$$
propagators configurations (~P(U))



$(x_0)\rangle$

 $\{U^{[i]}\},$ (Markov process)

each configuration is created by the preceding one:

 $\mathbf{P}\left(U^{[i-1]} \to U^{[i]}\right) P\left(U^{[i-1]}\right) = \mathbf{P}\left(U^{[i]} \to U^{[i-1]}\right) P\left(U^{[i]}\right)$

Basic Monte Carlo algorithm

For each gauge-field configuration, calculate the quark propagator (inverse of the fermion matrix)



$\left\langle \widehat{oldsymbol{O}} ight angle$:	$=\frac{1}{7}\int I$
	L°

REQUIRE MULTIPLE VOLUMES AND LATTICE SPACINGS to recover the continuum infinite limit

LQCD algorithm

In order to study hadrons, we need to contract propagators onto correlation functions $C_i(t)$

$$C(\Gamma^{\nu}, \vec{p}, t) = \sum_{\vec{x}_{1}} e^{-i\vec{p}\vec{x}_{1}} \Gamma^{\nu} \langle J(\vec{x}_{1}, t) \bar{J}(\vec{x}_{0}, 0) \rangle$$

for ex. $\vec{u}(x_{1})\gamma_{5}d(x_{1}) \quad \vec{d}(x_{0})\gamma_{5}u(x_{0})$
$$\pi^{+} = \vec{d}\gamma_{5}u$$

$$\langle \pi^{\dagger}(x_{1}) \pi(x_{0}) \rangle = \langle \overline{u}(x_{1}) \gamma_{5} d(x_{1}) \quad \vec{d}(x_{0}) \gamma_{5} u(x_{0}) \rangle$$

$$DU \quad \hat{O} [Q(U)^{-1}] \det(Q(U)) e^{-S_{g}[U]}$$

$$\underbrace{OU \quad \hat{O} [Q(U)^{-1}] \det(Q(U)) e^{-S_{g}[U]}}_{\text{propagators}} \quad \text{configurations } (\sim P(U))$$



$(x_0)\rangle$

Energy levels





LQCD DIRECT METHOD: FV Energy levels from two-point correlation functions





Energy levels



 $C_{2pt}(\tau, \boldsymbol{p}) = \sum e^{-\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p}} \Gamma_{\beta}$

 $= Z_0^{snk} Z_0^{\dagger^{src}} e^{-E^{(0)}t} + Z_1^{snk} Z_1^{\dagger^{src}} e^{-E^{(1)}t} + \dots$

LQCD DIRECT METHOD: FV Energy levels from two-point correlation functions

$$_{\beta\alpha}\langle \mathcal{X}_{\alpha}(\boldsymbol{x},\tau)\bar{\mathcal{X}}_{\beta}(\boldsymbol{0},0)\rangle$$

Tower of energy eigenstates of the system in the finite volume





Energy levels





LQCD DIRECT METHOD: FV Energy levels from two-point correlation functions





$$C_{2pt}(\tau, \boldsymbol{p}) = \sum_{\boldsymbol{x}} e^{-i\boldsymbol{x}\cdot\boldsymbol{p}} \Gamma_{\boldsymbol{\beta}}$$
$$= Z_0^{snk} Z_0^{\dagger^{src}} e^{-i\boldsymbol{k}\cdot\boldsymbol{p}}$$

dominates at large t

Challenges with LQCD studies of nuclear systems











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











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



Challenges with LQCD studies of nuclear systems

Increase the statistics / Increase the pion mass

Construct operators with a better overlap with the ground state

signal-to-noise degradation













"Challenges" with LQCD studies of nuclear systems

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

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



LQCD DIRECT METHOD: FV Energy levels from two-point correlation functions

Increase the statistics / Increase the pion mass

Construct operators with a better overlap with the ground state

signal-to-noise degradation

Direct method

Misidentification of the plateau

E. Berkowitz et al. [CalLat], Phys.Lett.B 765 (2017) S.R. Beane et al. [NPLQCD], arXiv:1705.09239 [hep-lat] T. Yamazaki et al. [PACS], EPJ Web Conf. 175 (2018)

pre-variational \rightarrow bound variational $\rightarrow ???$

Nuclear physics with LQCD - Methods

Potential method

Only applicable at the energy of the calculation/system

Test convergence expansion

Ground-state saturation requirement Short-distance operator dependence

T. Iritani et al. [HAL QCD], Phys.Rev.D 99 (2019)

 $R(\tau, \boldsymbol{r}) = \frac{C_{B_1 B_2}(\tau, \boldsymbol{r})}{C_{B_1}(\tau, \boldsymbol{r})C_{B_2}(\tau, \boldsymbol{r})}$ $\left(\frac{\partial_{\tau}^2}{4m_{R}} - \partial_{\tau} - H_0\right) R(\tau, \boldsymbol{r}) = \int d^3 \boldsymbol{r}' U(\boldsymbol{r}, \boldsymbol{r}') R(\tau, \boldsymbol{r}')$ $U(\boldsymbol{r}, \boldsymbol{r}') = V(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}') + \mathcal{O}(\nabla_{\boldsymbol{r}}^2 / \Lambda^2)$ $k^* \cot \delta$ B

not bound

NN systems at unphysical m_{π}

$8 \otimes 8 = 27 \oplus 8_S \oplus 1 \oplus 1\overline{0} \oplus 10 \oplus 8_A$

Finite Volume LQCD energy eigenstates can be classified by:

- their baryon number B,
- total isospin I,
- strangeness and

For ex, for I=1 NN,

• cubic irrep Γ_{I} , which plays the role of the continuum, infinite-volume total angular momentum, J.

for I=0 NN $\otimes \Gamma_S$ $, T_1^+ \}$ S=1

$L\left[\texttt{fm} ight]$	$T\left[\texttt{fm}\right]$	
3.4	6.7	
4.5	6.7	
6.7	9	

b[fm] = 0.1453(16)

 $m_{\pi} \sim 800 \text{ MeV}$

no e.m. interactions

LQCD - Binding energies - $SU(3)_f$

away from the SU(3)_f limit

Baryon-baryon interaction @ $m_{\pi} \sim 450 \text{ MeV}$

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

away from the SU(3)_f limit

BB systems @ $m_{\pi} \sim 450 \text{ MeV}$

BB systems, quark mass extrapolations

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

* EXP

Nuclear physics with LQCD - Controversy

Misidentification of the plateau?

E. Berkowitz et al. [CalLat], Phys.Lett.B 765 (2017) S.R. Beane et al. [NPLQCD], arXiv:1705.09239 [hep-lat] T. Yamazaki et al. [PACS], EPJ Web Conf. 175 (2018)

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

- Is the fitting interval correctly identified?
- Are we missing excited state contributions?
- Is there an operator dependence on the energy levels extracted?

Reduce uncertainty at small time: GPoF, matrix Prony, variational

Nuclear physics with LQCD - Controversy

like operators

Nuclear physics with LQCD - Variational calculations

Stochastic Laplacian Heaviside method

CalLat B. Hörz et al., Phys.Rev.C 103 (2021)

Hermitian 2x2 matrix with dibaryon-like operators

Nuclear physics with LQCD - Variational calculation

 $m_{\pi} \sim 714 \text{ MeV}$

UNBOUND NN I=1

 $b \sim 0.086 \; {\rm fm}$ $L = 48 b \sim 4.1 \text{ fm}$

Variational calculation - Types of operators

Local hexaquark operators

• Six Gaussian smeared quarks at a point

Dibaryon Operators

- Two spatially-separated plane-wave baryons with relative momenta
- Relative momentum: up to four units \rightarrow 5 operators

Quasi-local Operators

- Two exponentially localized baryons
- NN -EFT motivated deuteron-like structure

Nuclear physics with LQCD - Variational calculation

NPLQCD, PRD 107 (2023) 9, 094508: Largest set of operators to date b=0.145 fm , L/b=32 (4.7 fm aprox)

of correlators:

Solve Generalized Eigenvalue Problem (GEVP):

GEVP Eigenvalues provide rigorous (stochastic) variational upper bounds on energy levels Variational methods lead to correlation functions with positive definite spectral representations $C(t) = \Sigma$

For ex., the effective mass provides a genuine upper bound on the g.s. energy:

$$E(t) = -\ln\left[\frac{C(t+1)}{C(t)}\right] = -\ln\left[\frac{\sum_{n} e^{-E_{n}} e^{-E_{n}t}}{\sum_{n} e^{-E_{n}t}}\right] \ge -\ln\left[\frac{e^{-E_{0}} \sum_{n} e^{-E_{n}t}}{\sum_{n} e^{-E_{n}t}}\right] = E_{0} \qquad \text{where } E_{n}$$

Nuclear physics with LQCD - Variational calculation

Our first variational results added dibaryon operators at the source and sink through the (Hermitian) matrix

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

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

$$\sum_{n} |Z_n|^2 e^{-E_n t}$$

Cauchy Interlacing theorem

true energy-eigenvalues of the LQCD system

It tell us the minimum number of energy eigenvalues below a particular effective mass extracted from the GEVP

Nuclear physics with LQCD - Variational calculation

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

- S₀ contains all operators except the quasi-locals
- (hexaquark and dibaryons ops with different relative momentum)
- Set without a particular dibaryon operator
- (taking out a dibaryon op with a given value of the relative momentum)
- Set with only the whole set of dibaryon operators (NO hexaquark)

Interpolating-operator set

Similarly with what happens in the meson sector, removing the operator structure with maximum overlap on to a given energy level leads to missing energy levels

Importance of using an interpolating-operator set with significant overlap onto all energy levels of interest.

Having a large interpolating-operator set is not sufficient to guarantee that a set will have good overlap onto the ground state or a particular excited state

Variational upper bounds. No evidence for (or against) bound states

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

Operator dependence on variational bounds

"Additional bound": large overlap to Hex

calculations made on the same set of configurations

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

matrices are significantly closer to threshold than the those obtained using hexaquark sources and dibaryon sinks (in this work and in previous studies using the same gauge-field ensemble)

NPLQCD, e-Print: **2404**.**12039** [*hep-lat*]

NN spectroscopy @ 800 MeV - Variational calculation

NN (I=1)

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

NPLQCD, e-Print: **2404.12039** [*hep-lat*]

NN spectroscopy @ 800 MeV - Variational calculation

 $L_S^3 \times L_T = 24^3 \times 48$ NN (I=0)

Summary of variational bounds $L_S^3 \times L_T = 24^3 \times 48$

NPLQCD, e-Print: **2404.12039** [*hep-lat*]

NN spectroscopy @ 800 MeV - Variational calculation

NN (I=0)

NN (I=1)

0.20

0.10

0.05

 $a\Delta E_{\rm n}^{nn}$

Updated variational calculation:

A complete basis of local NN hexaquark operators is included

No evidence for (or against) bound states

Operator dependence on variational bounds

The additional bound is observed at two lattice volumes

0.00The additional state exhibits weak volume dependence compared with the states that fall near the non-interacting levels and overlap strongly with the dibaryon operators.

M. Lüscher, Nucl. Phys. B 364, 237 (1991) resonance?

NN spectroscopy @ 800 MeV - Variational calculation

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

Experimental evidence supports the existence of a resonance :

$$I = 0, J^P = 3^+ \rightarrow d^*(2380)$$

Bashkanov et al., PRL 102, 052301 (2009) *Adlarson et al. (WASA-at-COSY), PRL 106, 242302 (2011)* Adlarson et al. (WASA-at-COSY), PLB 743, 325 (2015) *Bashkanov et al., Eur. Phys. J. A51, 87 (2015)* Adlarson et al., Eur. Phys. J. A52, 147 (2016)

 $\Gamma_J = \Gamma_\ell \otimes \Gamma_S$, where $\Gamma_S \in \{A_1^+, T_1^+\}$ S=0 / S=1

NN spectroscopy @ 800 MeV - Variational calculation

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

Lattice artifacts?

Potentially important

Marc Illa @ HYP22

large statistical uncertainties in the region where single-state dominates the nucleon correlator

Green, Hanlon, Junnarkar, Wittig, PRL 127 (2021)

We have started a study of all SU(3) irreps at two different lattice spacings

L/a	T/a	$L~({\rm fm})$	$T ~({\rm fm})$	$a~({ m fm})$
48	64	4.13	5.50	0.086
32	48	4.64	6.96	0.145
				and a man and a property of the second second

Ex: flavor singlet channel (H-dibaryon)

- energy spectrum with unphysical quark masses
- Variational bounds don't provide conclusive evidence for (or against) bound states
- The combination of dibaryon and hexaquark operators provides strong evidence for the presence of an additional energy level below in both the deuteron and dineutron channels
- Similar analysis in the strange sector are underway
- Are lattice artefacts important? Very preliminary results seem to indicate that this is the case, but more statistics is needed to answer this question

We have started a study of all SU(3) irreps at two different lattice spacings

In order to make physical statements and predictions, quantities determined from LQCD calculations must be extrapolated to the continuum limit.

Calculations near the physical pion mass (coarse extrapolations at the moment) are under way We have started studies of Octet Baryon - Octet Baryon @ m_{π} = 170 MeV

Variational studies have revealed significant interpolating-operator dependence in LQCD calculations of NN