Lattice QCD calculations of Nuclear Physics at unphysical quark masses

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Hirschegg 2023 Effective field theories for nuclei and nuclear matter January 16-20, 2023





Institut de Ciències del Cosmos UNIVERSITAT DE BARCELONA EXCELENCIA MARÍA DE MAEZTU 3020-2023

Nonstrange sector (u, d) V=126 Seconds 10+15 10-01 10-02 0+10 1=82 10-03 0+07 10-04 10+05 10-05 10+04 10-06 10+03 10+02 10-07 10+01 10-15 < 10-15 10+00 unknown =20 www.nndc.bnl.gov



Connection to QCD

Systematically improve the calculation

Control the uncertainties



LATTICE QCD CALCULATIONS FOR NUCLEAR PHYSICS. MOTIVATION

T_{lab} (MeV)

LATTICE QCD CALCULATIONS FOR NUCLEAR PHYSICS. MOTIVATION





Connection to QCD

Systematically improve the calculation

Control the uncertainties



LATTICE QCD CALCULATIONS FOR NUCLEAR PHYSICS. MOTIVATION



First collected in Dover and Feschback, Ann. Phys. 198 (1990)

UPDATED BY MARC ILLA, UW e-Print: 2109.10068 [hep-lat]

Femtoscopy: correlation function C(k) as a function of relative momentum k



STAR, HADES and ALICE Collaborations

Some physical implications

@ Marc Illa thesis, e-Print: 2109.10068 [hep-lat]





Solving QCD at low-energies. LQCD + EFT

Nuclear physics, the non-perturbative regime of QCD

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

$$i = r, g, b \quad j = u, d, c, s, t, b$$

$$\mathcal{L}_{EFT} \left[\pi, N, \dots; m_{\pi}, m_{N}, \dots; C_{i} \right]$$

$$\mathcal{L}_{ECS}$$

$$\mathcal{L}_{Ci}$$

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go to **Euclidean space** (numerical methods/important sampling)

LQCD calculations

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

Nonperturbative (numerical) solution

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

$$\downarrow t \to \mathrm{i} \, t$$

go to **Euclidean space** numerical methods/important sampling



 $L >> m_{\pi}^{-1} \qquad b << \Lambda_{QCD}^{-1}$

 $\boldsymbol{U}_{u}(x)$

ν

 $U_{\mu}^{b}(x) \equiv e^{ig \int_{x}^{x+b\mu} A_{\mu} dx^{\mu}}$

(SU(3)_c matrices, "links")

 $a^{igbA_{\mu}^{\ b}(x)}$

LQCD calculations landscape

800

 $SU(3)_f$

800

1000

1000

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





M. Illa, e-Print: 2109.10068 [hep-lat]

 $b < < \Lambda_{QCD}^{-1}$ $L > > m_{\pi}^{-1}$



Energy levels

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



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

Energy levels

$$C_{2pt}(\tau, \boldsymbol{p}) = \sum_{\boldsymbol{x}} e^{-\mathrm{i}\boldsymbol{x}\cdot\boldsymbol{p}} \Gamma_{\beta\alpha} \langle \mathcal{X}_{\alpha}(\boldsymbol{x}, \tau) \bar{\mathcal{X}}_{\beta}(\boldsymbol{0}, 0) \rangle$$
$$= Z_{0}^{snk} Z_{0}^{\dagger src} e^{-E^{(0)}t} + Z_{1}^{snk} Z_{1}^{\dagger src} e^{-E^{(1)}t} + \dots$$

Tower of energy eigenstates of the system in the finite volume



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

Energy levels

 $\sum \ket{n}ra{n}$

u

u

d

(0, 0)





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









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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





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

Infinite volume



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

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

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



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

 $(L \gg R)$

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



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



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



LQCD DIRECT METHOD: FV Energy levels



LQCD DIRECT METHOD: FV Energy levels





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



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

no e.m. interactions



no e.m. interactions

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

away from the SU(3)_f limit

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



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

away from the SU(3)_f limit

 $n_f = 2 + 1$ $m_{\pi} = 450(5) \text{MeV}$ b = 0.117(2) fm L = 2.8, 3.7, 5.6 fm T = 7.5, 11.2, 11.2 fmBoosted and back-to-back momenta

no e.m. interactions





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

BB systems, quark mass extrapolations

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





$$B_{\rm lin}(m_{\pi}) = B_{\rm lin}^{(0)} + B_{\rm lin}^{(1)}m_{\pi}$$

$$B_{\text{quad}}(m_{\pi}) = B_{\text{quad}}^{(0)} + B_{\text{quad}}^{(1)} m_{\pi}^2$$



NPLQCD, PRD 96, 114510 (2017)

29

Extracting scattering information

NPLQCD, PRD 103, 054508 (2021)

 $m_{\pi} = 450 \text{ MeV}$



most constrained values show unnaturalness (r/a ~0.2 - 0.3)













Extracting scattering information

Assuming *SU*(3)_f, at leading order we have M.J. Savage, M. Wise, Phys.Rev.D 53 (1996) $\mathcal{L}_{BB}^{(0), SU(3)} = -c_1 \operatorname{Tr}(B_i^{\dagger} B_i B_j^{\dagger} B_j) - c_2 \operatorname{Tr}(B_i^{\dagger} B_j B_j^{\dagger} B_i) - c_3 \operatorname{Tr}(B_i^{\dagger} B_j^{\dagger} B_i B_j)$ $- c_4 \operatorname{Tr}(B_i^{\dagger} B_j^{\dagger} B_j B_i) - c_5 \operatorname{Tr}(B_i^{\dagger} B_i) \operatorname{Tr}(B_j^{\dagger} B_j) - c_6 \operatorname{Tr}(B_i^{\dagger} B_j) \operatorname{Tr}(B_j^{\dagger} B_i)$

$$c_1, \ldots, c_6 \longrightarrow c^{(27)}, \ldots, c^{(8_a)}$$



Assuming *SU*(3)_f, at leading order we have M.J. Savage, M. Wise, Phys.Rev.D 53 (1996) $\mathcal{L}_{BB}^{(0), SU(3)} = -c_1 \operatorname{Tr}(B_i^{\dagger} B_i B_j^{\dagger} B_j) - c_2 \operatorname{Tr}(B_i^{\dagger} B_j B_j^{\dagger} B_i) - c_3 \operatorname{Tr}(B_i^{\dagger} B_j^{\dagger} B_i B_j)$ $- c_4 \operatorname{Tr}(B_i^{\dagger} B_j^{\dagger} B_j B_i) - c_5 \operatorname{Tr}(B_i^{\dagger} B_i) \operatorname{Tr}(B_j^{\dagger} B_j) - c_6 \operatorname{Tr}(B_i^{\dagger} B_j) \operatorname{Tr}(B_j^{\dagger} B_i)$

$$c_1, \ldots, c_6 \longrightarrow c^{(27)}, \ldots, c^{(8_a)}$$

$$V^{LO} = \begin{cases} C_0 + C_1 \vec{\sigma}_1 \vec{\sigma}_2 & 2B(\text{attractive}) \\ + D_0 & 3B(\text{repulsive}) \end{cases}$$

Barnea, Contessi, Gazit, Pederiva, van Kolck, PRL **114** (2015) 052501 Contessi, Lovato, Pederiva, Roggero, Kirscher, van Kolck, PLB **772** (2017) 839

nuclear structure accounted for with effective-interaction hyperspherical harmonics and auxiliary-field diffusion Monte Carlo

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



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



no e.m. interactions

extension to larger systems $(SU(3)_f)$

PHYSICAL REVIEW C 98, 054301 (2018)

Pion-less effective field theory for atomic nuclei and lattice nuclei

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(Received 29 December 2017; revised manuscript received 29 June 2018; published 1 November 2018)

We compute the medium-mass nuclei ¹⁶O and ⁴⁰Ca using pion-less effective field theory (EFT) at next-toleading order (NLO). The low-energy coefficients of the EFT Hamiltonian are adjusted to experimental data for nuclei with mass numbers A = 2 and 3, or alternatively to results from lattice quantum chromodynamics at an unphysical pion mass of 806 MeV. The EFT is implemented through a discrete variable representation in the harmonic oscillator basis. This approach ensures rapid convergence with respect to the size of the model space and facilitates the computation of medium-mass nuclei. At NLO the nuclei ¹⁶O and ⁴⁰Ca are bound with respect to decay into alpha particles. Binding energies per nucleon are 9–10 MeV and 21–40 MeV at pion masses of 140 and 806 MeV, respectively.

DOI: 10.1103/PhysRevC.98.054301

$$V_{NN}^{\text{LO}}({}^{1}S_{0}) = \tilde{C}_{{}^{1}S_{0}} = C_{S} - 3C_{T}, \quad V_{NN}^{\text{NLO}}({}^{1}S_{0}) = C_{{}^{1}S_{0}}(p^{2} + {p'}^{2}),$$

$$V_{NN}^{\text{LO}}({}^{3}S_{1}) = \tilde{C}_{{}^{3}S_{1}} = C_{S} + C_{T}, \quad V_{NN}^{\text{NLO}}({}^{3}S_{1}) = C_{{}^{3}S_{1}}(p^{2} + {p'}^{2}).$$

Extension to ¹⁶O and ⁴⁰Ca

Our results also suggest that medium-mass nuclei can be connected to lattice QCD input. Further progress in this direction, however, requires a resolution of the controversy between the different lattice QCD approaches to light nuclei, increasing the precision of the lattice QCD results that are input to EFTs, and finally, moving towards the physical pion mass.

Nuclear physics with LQCD - Controversy

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



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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?

Deep bound states

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







S. Amarasinghe et al (NPLQCD), arXiv:2108.10835



Largest set of operators to date (ongoing work)

b=0.145 fm , L/b=32 (4.7 fm aprox)



NN (I=1)

S. Amarasinghe et al (NPLQCD), arXiv:2108.10835



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)

S. Amarasinghe et al (NPLQCD), arXiv:2108.10835

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

NEEDS MORE WORK

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







strong overlap with a particular operator





S. Amarasinghe et al (NPLQCD), arXiv:2108.10835



NN (I=1)

calculations made on the same set of configurations

S. Amarasinghe et al (NPLQCD), arXiv:2108.10835



calculations made on the same set of configurations

Potentially important



Marc Illa @ HYP22

Potentially important



Detmold @ Bethe Forum 2022, Bonn, Aug 18th, 2022

Are we really missing a deep bound state?

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





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

- During the last 2 decades we have witnessed great advances in the calculation of nuclear interactions with Lattice QCD, partly thanks to the technological development but also thanks to the development of algorithms and communication between different communities (computing science, theoretical physics, nuclear).
- Calculations near the physical pion mass (coarse extrapolations at the moment) are under way
- Are lattice artefacts important? Probably more statistics is needed to answer this question
- Excited state contamination
- Operator dependence: Variational studies have revealed significant interpolating-operator dependence in LQCD calculations of NN energy spectrum with unphysical quark masses
- Variational bounds don't provide conclusive evidence for (or against) bound states.
- Ongoing and future work: include a larger operator set (complete basis of local 6 quark operators), additional volumes, multi-exponential fits vs GEVP
- The analysis of analogous calculations in the strange sector are underway ($\Lambda\Lambda$)