



Exotic Nuclear Systems from Lattice QCD

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NPLQCD Collaboration

To The sufficient Trapel's of

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nye new

Generalitat de Catalunya Departament d'Economia i Coneixement



"strange" experimental program



updated from J. Pochodzalla, Int. Journal Modern Physics E, Vol 16, no. 3 (2007) 925-936



Former collaborators:

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Calculation of the properties and interactions of nuclear systems (A = 1, 2, 3, ...) including exotics (strange and hidden-charm)



For numerical calculations in QCD, the theory is formulated on a (Euclidean) space-time lattice ((anti) periodic (time) spatial boundary conditions) $N_s x N_s x N_s x N_t$



finite number of d.o.f (finite volume)

$$x = b(n_1, n_2, n_3, n_4) \qquad n_j \in \mathbb{Z}$$

nucleon-nucleon scattering

 $\Rightarrow m_{\pi} L >> 1$ (infrared cutoff)

$$b \ll \frac{1}{M_N}$$
 (ultraviolet cutoff)



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LQCD is a non-perturbative implementation of Field Theory, which uses the Feynman path-integral approach to evaluate transition matrix elements





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expectation values

When computing expectation values of any given operator *O*, the quark fields in *O* are re-expressed in terms of quark propagators using Wick's Theorem: **write all possible contractions for the fields** (removing the dependence of quarks as dynamical fields)

1. Generate an ensemble of N gauge-field configurations $\{U_i\}$ according to the probability distribution P(U)

$$Z = \int [dU] e^{-S_g[U]} \prod_f \det (D[U] + m_f) \sim P(U)$$

Boltzmann weight

2. Use the N gauge-field configurations previously generated to calculate the quark propagators on each configuration $Q^{-1}[U_i] \sim (D[U] + m_f)^{-1}$

3. Compute <u>correlation functions</u> (expectation values of local gauge-invariant operators):

$$\langle O(\boldsymbol{U}, \boldsymbol{q}, \boldsymbol{\bar{q}}) \rangle = \frac{1}{Z} \int [\boldsymbol{d}\boldsymbol{U}] \prod_{f} (D[\boldsymbol{U}] + m_{f})^{-1} \det (D[\boldsymbol{U}] + m_{f}) e^{-S_{g}[\boldsymbol{U}]}$$
propagators configurations (~P(U))

 $\left(D[{\color{black} {\it U}}]+m_f\right)^{-1}$

Repeated inversions are done using iterative solvers (CG) Computational cost ~ condition number ~ $1/m_f$ For light quark masses (u,d) this factor the cost is very large

→ Use large values of the light quark masses



USE UNPHYSICAL VALUES OF THESE PARAMETERS LATTICE ARTIFACTS

sources of systematic errors in the numerical calculation finite volume *L*, discretization (finite spacing) *b*, value of the light quark masses



Our method consists in a <u>direct extraction of the energy levels</u> from LQCD calculations of correlation functions for the one, two-, three- and 4 baryon systems in the non-strange and strange sectors.

One can use these energy extractions to obtain information about the binding energy of the system, on the scattering parameters, magnetic moments, polarizabilitites, etc.

We use different method analysis to ensure a robust extraction of the g.s.:

- ✓ Multiple exponential fits
- ✓ Matrix-Prony method
- ✓ Generalized-pencil-of-function method

Formalism: Direct Lattice QCD extraction \longleftrightarrow Compute correlation functions

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

$$t_{1} \leftarrow t$$

Effective mass plot → extract the g.s. energy (mass) from plateau

$$\frac{1}{t_J}\log\frac{C_A(t)}{C_A(t+t_J)} = E_{0A} \quad (m_A)$$

$$\Xi^{0}_{\alpha}(\vec{x},t) = \varepsilon^{ijk} s^{i}_{\alpha}(\vec{x},t) \Big(u^{j^{T}}_{\alpha}(\vec{x},t) C \gamma_{5} s^{k}(\vec{x},t) \Big)$$



noise-to-signal

Lepage, 1989

pions:

$$\frac{\sigma}{\langle C \rangle} \rightarrow \frac{1}{\sqrt{N}}$$

nucleons:

$$\frac{\sigma}{\langle C \rangle} \sim \frac{1}{\sqrt{N}} \times \exp\left(M_N - \frac{3m_{\pi}}{2}\right)t$$

for baryons, the noise grows exponentially with time





hadron-hadron scattering?

For two **non-interacting** particles of mass m in a volume L³ and zero CoM momentum :



spectral function

 $E_n = 2\sqrt{m^2 + |\vec{p}|^2} = 2\sqrt{m^2 + (\frac{2\pi}{L}|n|)^2}, n_i \in \mathbb{Z}$



energy spectrum



two **interacting** particles of mass m in a volume L³ and zero CoM momentum :





spectral function

E



shift in the energy spectrum

Lüscher, Hamber, Marinari, Parisi, Rebbi (QFT); Uhlenbeck 1930's; Bogoliubov 1940's; Lee, Huang, Yang 1950's

Two particles placed in finite volume suffer from energy shifts, $\Delta E,$ which depend on their interactions

We extract the energy of the interacting system of hadrons for a given $\{m_{\pi}, L, b\}$

$$G_{\Lambda\Lambda}(t) = \frac{C_{\Lambda\Lambda}(t)}{C_{\Lambda}(t)C_{\Lambda}(t)} \to A_0 e^{-\Delta E_{\Lambda\Lambda}t} \to \frac{1}{t_J} \log \frac{G(t)}{G(t+t_J)} \to \text{extract} \quad \Delta E$$



We can also extract the energy of the interacting system for a given $\{m_{\pi}, L, b\}$ set

$$G_{\Lambda\Lambda}(t) = \frac{C_{\Lambda\Lambda}(t)}{C_{\Lambda}(t)C_{\Lambda}(t)} \to A_0 e^{-\Delta E_{\Lambda\Lambda}t} \to \frac{1}{t_J} \log \frac{G(t)}{G(t+t_J)} \to \text{extract} \quad \Delta E$$



$$\Delta E_{0} = \frac{p^{2}}{M} = \frac{4\pi a}{ML^{3}} \left[1 - c_{1} \frac{a}{L} + c_{2} \left(\frac{a}{L} \right)^{2} + \dots \right] \quad \text{Ground state energy shift}$$
Recovering M. Lüscher, Commun. Math. Phys. 105, 153 (1986) (L>> a)
extract the scattering lentgh
Bound states?
$$\mathcal{M} \sim \mathcal{N} + \mathcal{N} + \dots = \frac{4\pi}{M} \frac{1}{p \cot \delta(p) - ip}$$
infinite volume
b.s. $p^{2} = -\gamma^{2}$
cot $\delta(i\gamma) = i$
finite volume:
b.s. $p^{2} = -\gamma^{2}$
cot $\delta(i\gamma) = i$
 $k^{2} < 0, \quad k = i\kappa$
 $\kappa = \gamma + \frac{g_{1}}{L} \left(e^{-\gamma L} + \sqrt{2} e^{-\sqrt{2}\gamma L} + \dots \right)$
 $B_{n} = \frac{\gamma^{2}}{M}$



PREDICTION (Bag model) m_H – 2 m_Λ ~ - 81 MeV

H-dibaryon

R.L. Jaffe, Phys. Rev. Lett. 38, 195 (1977); 38, 617 (1977) (E)

$$A = 2, s = -2, J = 0, I = 0$$

$$\boxed{\Lambda \Lambda - \Xi N - \Sigma \Sigma}$$

$$SU(3)_f \rightarrow \Psi_H = \frac{1}{\sqrt{8}} \left(\Lambda \Lambda + \sqrt{3}\Sigma\Sigma + 2\Xi N \right)$$

NAGARA EVENT, , KEK-E373, Takahashi et al. PRL 87 (2001) 212502



Experimental constraints

 $B_{\Lambda\Lambda}({}^{6}_{\Lambda\Lambda}\text{He}_{g.s.}) = 6.91 \pm 0.16 \text{ MeV}$ $\rightarrow \Delta B_{\Lambda\Lambda} - 2B_{\Lambda} = 1.01 \pm 0.20^{+0.18}_{-0.11} \text{MeV}$



NPLQCD, PRL 106, 162001 (2011) $n_f=2+1$, $b_s = 0.12 \text{ fm}$, L: 2, 2.5, 3, 3.9 fm, $m_{\pi} = 390 \text{ MeV}$ NPLQCD, Mod.Phys.Lett. A26 (2011) $n_f=2+1$, $b_s = 0.12 \text{ fm}$, L: 4fm, $m_{\pi} = 230 \text{ MeV}$ NPLQCD, PRD87 (2013) $n_f=3$, $b_s = 0.145 \text{ fm}$, L: 3.4, 4.5, 6.7 fm, $m_{\pi} = 807 \text{ MeV}$

HALQCD, PRL 106, 162002 (2011), NPA 881 (2012) $n_f=3$, $b_s = 0.12$ fm, L: 4 fm $m_{\pi} = 469, 670, 830, 1015, 1171$ MeV

Going beyond A=2

✓ Larger complexity as compared to calculations for single hadrons

 $\left((A+Z)!(2A-Z)!\right)$



- ✓ Demand larger lattice volumes
- ✓ Demand better accuracy



 $^{3}\text{H} \rightarrow 2880$ $^{4}\text{He} \rightarrow 518400$

Wick contractions ~ $N_u! N_d! N_s!$

Detmold & Savage, PRD82 (2010) 014511 Detmold & Orginos, PRD87 (2013) 11, 114512 Doi & Endres, Comput.Phys.Commun. 184 (2013) 117

$$\frac{\sigma}{\langle C \rangle} \sim \frac{1}{\sqrt{N}} \exp\left[\mathbf{A} \left(M_N - \frac{3m_\pi}{2} \right) t \right]$$

✓ Small energy splittings in nuclear physics
 ↓
 Need of high statistics calculations

Going beyond A=2

Perform calculations at heavier light-quark masses:

- ✓ signal-to-noise ratio improves
- ✓ reduced computational resources to generate LQCD configurations, *i.e.*, larger statistics



n	o continuum extrapolation							-			
L/b	T/b	β	$b m_q$	<i>b</i> (fm)	<i>L</i> (fm)	T (fm)	<i>m</i> _π (MeV)	$m_{\pi}L$	$m_{\pi}T$	$N_{\rm cfg}$	N _{src}
24	48	6.1	-0.2450	0.145	3.4	6.7	806.5(0.3)(0)(8.9)	14.3	28.5	3822	96
32	48	6.1	-0.2450	0.145	4.5	6.7	806.9(0.3)(0.5)(8.9)	19.0	28.5	3050	72
48	64	6.1	-0.2450	0.145	6.7	9.0	806.7(0.3)(0)(8.9)	28.5	38.0	1905	54

infinite volume extrapolation









many body: EFT + EIHH/AFDMC



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Reusing the nuclear correlation functions Quarkonium-nucleus

PRD 91, 114503 (2015)

Brodsky, Schmidt, de Téramond, PRL 64, 1011 (1990) (spin-spin correlations in pp scattering)

> no Pauli blocking no quark-exchange

Q̄ΓQ A A

$$\label{eq:m_m} \begin{split} m_{\pi} &= m_{K} \sim 807 \, MeV \\ b &= 0.145 \, fm \\ L &\sim 3.4, 4.5 \, and \, 6.7 \, fm \end{split}$$

EXPERIMENTAL SEARCH PROGRAM ATHENNA (Jlab), PANDA@FAIR, JPAC

For the compound system:

$$C_{\mathcal{AB}}(t) = \left\langle 0 \left| \chi_{\mathcal{A}}(t) \chi_{\mathcal{B}}^{\dagger}(0) \right| 0 \right\rangle$$
$$\chi_{\mathcal{A}} = \chi_{A} \chi_{\bar{Q} \Gamma Q}$$

(Rel. Heavy Quark action for the charmonium)

Combination of analysis methods (included in the systematics)

one-state, two-states and
$$\mathcal{R}(t) = \frac{C_{\mathcal{AB}}(t)}{C_{AB}(t)C_{\overline{Q}\Gamma Q}(t)}$$



Reusing the nuclear correlation functions Magnetic moments of nuclei

> Background field method: Uniform, timeindependent background magnetic field

$$e\left|B\right| = \frac{6\pi}{L^2}\tilde{n}, \quad \vec{B} = \hat{z} \cdot B$$





$$U_{\mu}^{b}(x) \to U_{\mu}^{b}(x)U_{\mu}^{ext}(x)$$

$$U_{0}^{ext}(x) = U_{3}^{ext}(x) = 1 \qquad U_{1}^{ext}(x) = \begin{cases} 1 & x_{1} \neq L - b \\ e^{-i\beta x_{2}} & x_{1} = L - b \end{cases} \qquad U_{2}^{ext}(x) = e^{i\beta x_{1}}$$

$$\beta \sim q_{q} Bb^{2}$$

NPLQCD, Phys. Rev .Lett. 113 (2014) 25, 252001

Reusing the nuclear correlation functions Magnetic moments of nuclei

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NPLQCD, Phys. Rev .Lett. 113 (2014) 25, 252001





$$E(B) = M + \frac{|QeB|}{2M} - \mu \cdot B - 2\pi\beta |B|^2 + \dots$$

Landau levels (*charged particles*)

$$\delta E^{B} = E^{B}_{+j} - E^{B}_{-j}$$
$$\delta E^{B} = -2\mu |B| + \gamma_{3} |B|^{3}$$

Use background magnetic fields

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

.

$$e |B| = \frac{6\pi}{L^2} \tilde{n}, \quad \overline{B} = \hat{z} \cdot B \quad (e|B| \sim 0.046 \ \overline{n} \ \text{GeV}^2)$$

From our calculated correlation functions:

$$R(B) = \frac{C_{j_{z}}^{B}(t) C_{-j_{z}}^{0}(t)}{C_{-j_{z}}^{B}(t) C_{j_{z}}^{0}(t)} \xrightarrow{t \to \infty} Ze^{-\delta E^{\theta}t} \\ \delta E^{\theta} = E_{+j}^{\theta} - E_{-j}^{\theta}$$

$$E(B) = M + \frac{|QeB|}{2M} - \mu \cdot B - 2\pi\beta |B|^2 + \dots \\ \delta E^{\theta} = -2\mu |B| + \gamma_3 |B|^3$$

LQCD calculations of magnetic moments of light nuclei

NPLQCD, Phys. Rev .Lett. 113 (2014) 25, 252001





$j_{nn} = 0$

© www.nersc.gov Artist's impression of a triton. Neutrons in blue and protons in red, with quarks inside; the arrows indicate the alignments of the spins. Image: William Detmold, MIT

 $\mu(^{3}H) = \mu_{p}$ $\mu(^{3}He) = \mu_{n}$ $\mu_{d} \sim \mu_{n} + \mu_{p}$

Nowadays we have calculations of :

- ✓ nucleon-nucleon interactions
- \checkmark hyperon-nucleon interactions
- ✓ hyperon-hyperon interactions
- ✓ first exploration of s-shell (hyper) nuclei at the SU(3) symmetric point (m_{π} ~ 800 MeV)
- ✓ magnetic properties of light nuclei have been addressed at unphysical values of m_{π}
- \checkmark the $np \rightarrow d\gamma$ cross section has been studied (not shown here)

We continue our program including:

- analysis of $m_{\pi} \sim 450$ MeV lattice data
- present run at $m_{\rm II} \sim 300 \,{\rm MeV}$

Agenda: light nuclear matrix elements of the axial current, $vd \rightarrow npe$...





Summary & Prospects

Major challenge in LQCD calculations for Nuclear Physics:

recover the experimentally known properties of the two-nucleon systems







 $np \rightarrow d\gamma$

Illustration of how the long-distance and short-distance contributions can be isolated with lattice OCD.



with



isovector nucleon magnetic moment

 $Z_{d} = \frac{1}{\sqrt{1 - \gamma_{0} r_{2}}} \qquad \text{EFT}(\pi) \qquad Kaplan (1997); Kaplan, Savage, Wise (1998, 1999)$ van Kolck (1999): Reave Savage (2007)

$np \rightarrow d\gamma$ cross section

Detmold, Savage, NPA743 (2004) 170-193

Illustration of how the long-distance and short-distance contributions can be isolated with lattice QCD.

$$\begin{bmatrix} p \cot \delta_1 - \frac{S_+ + S_-}{2\pi L} \end{bmatrix} \begin{bmatrix} p \cot \delta_3 - \frac{S_+ + S_-}{2\pi L} \end{bmatrix} = \begin{bmatrix} \frac{|eB|l_1}{2} + \frac{S_+ - S_-}{2\pi L} \end{bmatrix}^2$$

with $S_{\pm} \equiv S \left(\frac{L^2}{4\pi^2} \left(p^2 \pm |eB|\kappa_1 \right) \right)$

$$\Delta E_{{}^{3}S_{1},{}^{1}S_{0}}\left(\vec{B}\right) = 2\left(\kappa_{1} + \gamma_{0} Z_{d}^{2} \tilde{l}_{1}\right) \frac{e}{M} \left|\vec{B}\right| + O\left(\left|\vec{B}\right|^{2}\right)$$

$$\delta E_{{}^{3}S_{1},{}^{1}S_{0}}\left(\vec{B}\right) \equiv \Delta E_{{}^{3}S_{1},{}^{1}S_{0}}\left(\vec{B}\right) - \left[E_{p,\uparrow} - E_{p,\downarrow}\right] + \left[E_{n,\uparrow} - E_{n,\downarrow}\right] \rightarrow 2\bar{L}_{1} \frac{\left|e\vec{B}\right|}{M} + O\left(\left|\vec{B}\right|^{2}\right)$$

 $np \rightarrow d\gamma$ cross section



$$\Delta E_{{}^{3}S_{1},{}^{1}S_{0}}(\vec{B}) = 2\left(\kappa_{1} + \gamma_{0} Z_{d}^{2} \tilde{l}_{1}\right) \frac{e}{M} |\vec{B}| + O\left(|\vec{B}|^{2}\right) \qquad \text{A magnetic field mixes the } \mathbf{I}_{z} = j_{z} = 0 \text{ np states}$$

in the ${}^{1}S_{0}$ and ${}^{3}S_{1} - {}^{3}D_{1}$ channels
$$\delta E_{{}^{3}S_{1},{}^{1}S_{0}}(\vec{B}) \equiv \Delta E_{{}^{3}S_{1},{}^{1}S_{0}}(\vec{B}) - \left[E_{p,\uparrow} - E_{p,\downarrow}\right] + \left[E_{n,\uparrow} - E_{n,\downarrow}\right] \rightarrow 2\overline{L}_{1} \frac{|e\vec{B}|}{M} + O\left(|\vec{B}|^{2}\right)$$