Twelfth Workshop on Non-Perturbative QCD

Paris, June 10-14, 2013



NUCLEAR PHYSICS FROM LATTICE QCD Kostas Orginos





Hadron Interactions

Goals:

- * Challenge: Compute properties of nuclei from QCD
 - * Spectrum and structure
- * Confirm well known experimental observation for two nucleon systems
- * Explore the largely unknown territory of hyper-nuclear physics
- * Provide input for the equation of state for nuclear matter in neutron stars
- * Provide input for understanding the properties of multi-baryon systems



Scales of the problem

- Hadronic Scale: 1fm ~ 1x10⁻¹³ cm
- Lattice spacing << 1 fm</p>
 - take a=0.1fm
- Lattice size La >> 1fm
 - take La = 3 fm
- Lattice 32⁴
- Gauge degrees of freedom: $8x4x32^4 = 3.4x10^7$

imensions

colo



sites

The pion mass is an additional small scale



~ 6 fm boxes are needed

Two hadron bound state volume corrections $\sim e^{-\kappa L}$



 $\sim 1/m_{\pi} \sim 1.4 \text{fm}$

Binding momentum κ of the deuteron ~ 45MeV

Nuclear energy level splittings are a few MeV

Box sizes of about 10 fm will be needed

Bound States

Luscher Comm. Math. Phys 104, 177 '86

$$E_b = \sqrt{p^2 + m_1^2 + \sqrt{p^2 + m_2^2 - m_1 - m_2}}$$

$$E_b \approx \frac{p^2}{2\mu} = -\frac{\kappa^2}{2\mu}$$

$$\kappa = |p|$$

 $p^2 < 0$

κ is the "binding momentum" and μ the reduced mass

Finite volume corrections:

$$\Delta E_b = -3|A|^2 \frac{e^{-\kappa L}}{\mu L} + \mathcal{O}\left(e^{-\sqrt{2}\kappa L}\right)$$

cubic group irrep: A_1^+

Scattering on the Lattice

Luscher Comm. Math. Phys 105, 153 '86

Elastic scattering amplitude (s-wave):

$$A(p) = \frac{4\pi}{m} \frac{1}{p \cot \delta - i p}$$

At finite volume one can show:

Small p:

$$E_n = 2\sqrt{p_n^2 + m^2}$$

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S}\left(\frac{p^2 L^2}{4\pi^2}\right) \qquad \mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{|\mathbf{j}| < \Lambda} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda$$

$$p \cot \delta(p) = \frac{1}{a} + \frac{1}{2}rp^2 + \dots$$

a is the scattering length

Two Nucleon spectrum free nucleons



Signal to Noise ratio for correlation functions

$$C(t) = \langle N(t)\bar{N}(0)\rangle \sim Ee^{-M_N t}$$

$$var(C(t)) = \langle N\bar{N}(t)N\bar{N}(0)\rangle \sim Ae^{-2M_Nt} + Be^{-3m_\pi t}$$

$$StoN = \frac{C(t)}{\sqrt{var(C(t))}} = \sim Ae^{-(M_N - 3/2m_\pi)t}$$

- * The signal to noise ratio drops exponentially with time
- * The signal to noise ratio drops exponentially with decreasing pion mass
- * For two nucleons: $StoN(2N) = StoN(1N)^2$



Challenges for Nuclear physics

- * New scales that are much smaller than characteristic QCD scale appear
- * The spectrum is complex and more difficult to extract from euclidean correlators
- * Construction of multi-quark correlations functions may be computationally expensive
- * Monte-Carlo evaluation of correlation functions converges slowly

Challenges for Nuclear physics

- * New scales that are much smaller than characteristic QCD scale appear
- * The spectrum is complex and more difficult to extract from euclidean correlators
- * Construction of multi-quark correlations functions may be computationally expensive
- * Monte-Carlo evaluation of correlation functions converges slowly

We really need better algorithms to deal with an exponentially hard problem

Interpolating fields

Most general multi-baryon interpolating field

$$\bar{\mathcal{N}}^h = \sum_{\mathbf{a}} w_h^{a_1, a_2 \cdots a_{n_q}} \bar{q}(a_1) \bar{q}(a_2) \cdots \bar{q}(a_{n_q})$$

The indices α are composite including space, spin, color and flavor that can take N possible values

- * The goal is to calculate the tensors W
- * The tensors W are completely antisymmetric

* Number of terms in the sum are

 $\overline{(N-n_q)!}$

N!

Imposing the anti-symmetry:

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{(a_{1},a_{2}\cdots a_{n_{q}}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},\cdots,i_{n_{q}}} \bar{q}(a_{i_{1}})\bar{q}(a_{i_{2}})\cdots\bar{q}(a_{i_{n_{q}}})$$

Reduced weights

Totally anti-symmetric tensor

$$\epsilon^{1,2,3,4,\cdots,n_q} = 1$$

* Total number of reduced weights:

 $\frac{N!}{n_q!(N-n_q)!}$

Hadronic Interpolating field

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{M_{w}} \underbrace{\tilde{W}_{h}^{(b_{1},b_{2}\cdots b_{A})}}_{i} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},\cdots,i_{A}} \bar{B}(b_{i_{1}}) \bar{B}(b_{i_{2}}) \cdots \bar{B}(b_{i_{A}})$$

hadronic reduced weights

baryon composite interpolating field

$$\bar{B}(b) = \sum_{k=1}^{N_{B(b)}} \tilde{w}_{b}^{(a_{1},a_{2},a_{3}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},i_{3}} \bar{q}(a_{i_{1}}) \bar{q}(a_{i_{2}}) \bar{q}(a_{i_{3}})$$

Basak et.al. PhysRevD.72.074501 (2005)

Calculation of weights

- * Compute the hadronic weights
- * Replace baryons by quark interpolating fields
- ***** Perform Grassmann reductions
- * Read off the reduced weights for the quark interpolating fields
- * Computations done in: algebra (C++)

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{M_{w}} \tilde{W}_{h}^{(b_{1},b_{2}\cdots b_{A})} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},\cdots,i_{A}} \bar{B}(b_{i_{1}}) \bar{B}(b_{i_{2}}) \cdots \bar{B}(b_{i_{A}})$$

$$\bar{\mathcal{N}}^{h} = \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{(a_{1},a_{2}\cdots a_{n_{q}}),k} \sum_{\mathbf{i}} \epsilon^{i_{1},i_{2},\cdots,i_{n_{q}}} \bar{q}(a_{i_{1}}) \bar{q}(a_{i_{2}}) \cdots \bar{q}(a_{i_{n_{q}}})$$

Interpolating fields

NPLQCD arXiv:1206.5219

Label	A	s	Ι	J^{π}	Local $SU(3)$ irreps	int. field size
N	1	0	1/2	$1/2^{+}$	8	9
Λ	1	-1	0	$1/2^{+}$	8	12
\sum	1	-1	1	$1/2^{+}$	8	9
Ξ	1	-2	1/2	$1/2^{+}$	8	9
d	2	0	0	1+	$\overline{10}$	21
nn	2	0	1	0^{+}	27	21
$n\Lambda$	2	-1	1/2	0^{+}	27	96
$n\Lambda$	2	-1	1/2	1^{+}	$8_A,\overline{10}$	48, 75
$n\Sigma$	2	-1	3/2	0^{+}	27	42
$n\Sigma$	2	-1	3/2	1^{+}	10	27
$n\Xi$	2	-2	0	1^{+}	8_A	96
$n\Xi$	2	-2	1	1^{+}	$8_A,10,\overline{10}$	$52,\!66,\!75$
Н	2	-2	0	0^+	1 , 27	$90,\!132$
³ H, ³ He	3	0	1/2	$1/2^{+}$	35	9
$^{3}_{\Lambda}{ m H}(1/2^{+})$	3	-1	0	$1/2^{+}$	$\overline{35}$	66
${}^{3}_{\Lambda}{\rm H}(3/2^{+})$	3	-1	0	$3/2^{+}$	$\overline{10}$	30
$^{3}_{\Lambda}\text{He},^{3}_{\Lambda}\tilde{\text{H}}, nn\Lambda$	3	-1	1	$1/2^{+}$	$27,\overline{35}$	30,45
$\frac{3}{\Sigma}$ He	3	-1	1	$3/2^+$	27	21
⁴ He	4	0	0	0+	$\overline{28}$	1
${}^4_{\Lambda}\text{He}, {}^4_{\Lambda}\text{H}$	4	-1	1/2	0^{+}	$\overline{28}$	6
$_{\Lambda\Lambda}^{4}$ He	4	-2	1	0+	$27,\overline{28}$	15, 18
$\Lambda \Xi^0 pnn$	5	-3	0	$3/2^{+}$	$\overline{10} +$	1

Interpolating fields

NPLQCD arXiv:1206.5219

Label	A	s	Ι	J^{π}	Local $SU(3)$ irreps	int. field size
N	1	0	1/2	$1/2^{+}$	8	9
Λ	1	-1	0	$1/2^{+}$	8	12
\sum	1	-1	1	$1/2^{+}$	8	9
Ξ	1	-2	1/2	$1/2^{+}$	8	9
d	2	0	0	1+	$\overline{10}$	21
nn	2	0	1	0^{+}	27	21
$n\Lambda$	2	-1	1/2	0^{+}	27	96
$n\Lambda$	2	-1	1/2	1^{+}	$8_{A},\overline{10}$	48, 75
$n\Sigma$	2	-1	3/2	0^{+}	27	42
$n\Sigma$	2	-1	3/2	1^{+}	10	27
$n\Xi$	2	-2	0	1^{+}	8_A	96
$n\Xi$	2	-2	1	1^{+}	$8_A,10,\overline{10}$	$52,\!66,\!75$
Н	2	-2	0	0^+	1 , 27	90,132
³ H, ³ He	3	0	1/2	$1/2^{+}$	$\overline{35}$	9
$^{3}_{\Lambda}{ m H}(1/2^{+})$	3	-1	0	$1/2^{+}$	$\overline{35}$	66
${}^{3}_{\Lambda}{\rm H}(3/2^{+})$	3	-1	0	$3/2^{+}$	$\overline{10}$	30
$^{3}_{\Lambda}\text{He},^{3}_{\Lambda}\tilde{\text{H}}, nn\Lambda$	3	-1	1	$1/2^{+}$	$27,\overline{35}$	30,45
$\frac{3}{\Sigma}$ He	3	-1	1	$3/2^+$	27	21
⁴ He	4	0	0	0^{+}	28	1
${}^4_{\Lambda}\text{He}, {}^4_{\Lambda}\text{H}$	4	-1	1/2	0^{+}	$\overline{28}$	6
$^{4}_{\Lambda\Lambda}$ He	4	-2	1	0^{+}	$27,\overline{28}$	15, 18
$\Lambda \Xi^0 pnn$	5	-3	0	$3/2^{+}$	$\overline{10} +$	1

Contraction methods





* quark to hadronic interpolating fields* quark to quark interpolating fields

Quarks to Quarks

$$\begin{split} [\mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)] &= \int \mathcal{D}q\mathcal{D}\bar{q} \; e^{-\mathcal{S}_{QCD}} \; \sum_{k'=1}^{N'_{w}} \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{\prime(a_{1}',a_{2}'\cdots a_{n_{q}}'),k'} \; \tilde{w}_{h}^{(a_{1},a_{2}\cdots a_{n_{q}}),k} \times \\ &\times \sum_{\mathbf{j}} \sum_{\mathbf{i}} \epsilon^{j_{1},j_{2},\cdots,j_{n_{q}}} \epsilon^{i_{1},i_{2},\cdots,i_{n_{q}}} q(a_{j_{n_{q}}}') \cdots q(a_{j_{2}}') q(a_{j_{1}}') \times \bar{q}(a_{i_{1}}) \bar{q}(a_{i_{2}}) \cdots \bar{q}(a_{i_{n_{q}}}) \\ &= \; e^{-\mathcal{S}_{eff}} \; \sum_{k'=1}^{N'_{w}} \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{\prime(a_{1}',a_{2}'\cdots a_{n_{q}}'),k'} \; \tilde{w}_{h}^{(a_{1},a_{2}\cdots a_{n_{q}}),k} \times \\ &\times \sum_{\mathbf{j}} \sum_{\mathbf{i}} \epsilon^{j_{1},j_{2},\cdots,j_{n_{q}}} \epsilon^{i_{1},i_{2},\cdots,i_{n_{q}}} S(a_{j_{1}}';a_{i_{1}}) S(a_{j_{2}}';a_{i_{2}}) \cdots S(a_{j_{n_{q}}}';a_{i_{n_{q}}}) \end{split}$$

Define the matrix:

$$G(j,i)^{(a'_1,a'_2\cdots a'_{n_q});(a_1,a_2\cdots a_{n_q})} = S(a'_j;a_i)$$

Quarks to Quarks

The matrix:

$$G(j,i)^{(a'_1,a'_2\cdots a'_{n_q});(a_1,a_2\cdots a_{n_q})} = S(a'_j;a_i)$$

The Correlation function:

$$\left[\mathcal{N}_{1}^{h}(t)\bar{\mathcal{N}}_{2}^{h}(0)\right] = \sum_{k'=1}^{N'_{w}} \sum_{k=1}^{N_{w}} \tilde{w}_{h}^{\prime(a'_{1},a'_{2}\cdots a'_{n_{q}}),k'} \tilde{w}_{h}^{(a_{1},a_{2}\cdots a_{n_{q}}),k} \times \left|G^{(a'_{1},a'_{2}\cdots a'_{n_{q}});(a_{1},a_{2}\cdots a_{n_{q}})}\right|$$

Total momentum projection is implicit in the above



Quarks to Quarks

Naive Cost: $n_u!n_d!n_s! \times NM$ Actual Cost: $n_u^3 n_d^3 n_s^3 \times MN$

* Loop over all source and sink terms

* Compute the determinant for each flavor

single point source

* Cost is polynomial in quark number



H-dibaryon



S=-2, B=2, J^p=0⁺

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

- * Proposed by R. Jaffe 1977
 - * Perturbative color-spin interactions are attractive for (uuddss)
 - * Diquark picture of scalar diquarks (ud)(ds)(su)
- * Experimental searches of the H have not found it
 - * BNL RHIC (+model): Excludes the region [-95, 0] MeV
 - A. L. Trattner, PhD Thesis, LBL, UMI-32-54109 (2006).

* KEK: Resonance near threshold

C. J. Yoon et al., Phys. Rev. C 75, 022201 (2007).

Several Lattice QCD calculations have been addressing the existence of a bound H

NPLQCD: lattice set up

* Anisotropic 2+1 clover fermion lattices
* a ~ 0.125 fm (anisotropy of ~ 3.5)
* pion mass ~ 390 MeV
* Volumes 16³ x 128, 20³ x 128, 24³ x 128, 32³ x 256 largest box 4fm
* Smeared source - 3 sink interpolating fields

* Interpolating fields have the structure of s-wave Λ - Λ system * I=0, S=-2, A₁, positive parity

H-dibaryon: Towards the physical point

H-dibaryon: Is bound at heavy quark masses. May be unbound at the physical point S. Beane et.al. arXiv:1103.2821 Mod. Phys. Lett. A26: 2587, 2011]

0.2

0.4

 m_{π}^2 (GeV²)

HALQCD:Phys.Rev.Lett.106:162002,2011

0.6

HALQCD $n_f=3$

0.8

ChiPT studies indicate the same trend: P. Shanahan et.al. arXiv:1106.2851 J. Haidenbauer, Ulf-G. Meisner arXiv:1109.3590

-10

-20∟ 0.0

H-dibaryon: Towards the physical point



HALQCD:Phys.Rev.Lett.106:162002,2011

NP.

ChiPT studies indicate the same trend: P. Shanahan et.al. arXiv:1106.2851 J. Haidenbauer, Ulf-G. Meisner arXiv:1109.3590

Monday, June 10, 13

H-dibaryon:

Two baryon bound states



Avoiding the noise

Work with heavy quarks

$$StoN = \frac{C(t)}{\sqrt{var(C(t))}} = \sim Ae^{-(M_N - 3/2m_\pi)t}$$

Lattice Setup

* Isotropic Clover Wilson with LW gauge action

- * Stout smeared (1-level)
- * Tadpole improved
- ***** SU(3) symmetric point
 - * Defined using m_{π}/m_{Ω}
- * Lattice spacing 0.145fm
 - * Set using Y spectroscopy
- * Large volumes

* 24³ x 48 32³ x 48 48³ x 64

* 3.5fm 4.5fm 7.0fm

NPLQCD arXiv:1206.5219

6000 configurations,

200 correlation functions per configuration

computer time: XSEDE/NERSC

Nuclear spectrum

NPLQCD

0 1^{+} $\overline{S} = -1$ S = 0S = -2 0^{+} 0^{+} -20 1^{+} 1^{+} -40 $\frac{3}{2}^{+}$ -60 $\frac{1}{2}^{+}$ $\frac{1}{2}^{+}$ $\frac{1}{2}^{+}$ 0^{+} -80 B [MeV] $\frac{3}{2}^+$ -100 0^{+} 0^{+} 0^{+} -120 -140 0^{+} -1602-body 3-body -180 4-body -200^l $^{3}_{\Lambda}$ H ³ He $^{3}_{\Lambda}$ He $^{3}_{\Sigma}$ He $^{4}_{\Lambda}$ He H-dib n Ξ 2 H $n\Sigma$ 4 He $^{4}_{\Lambda\Lambda}$ He nn

Nucleon Phase shifts

Luscher Comm. Math. Phys 105, 153 '86

Elastic scattering amplitude (s-wave):

$$A(p) = \frac{4\pi}{m} \frac{1}{p \cot \delta - i p}$$

At finite volume one can show:

Small p:

$$E_n = 2\sqrt{p_n^2 + m^2}$$

$$p \cot \delta(p) = \frac{1}{\pi L} \mathbf{S}\left(\frac{p^2 L^2}{4\pi^2}\right) \qquad \mathbf{S}(\eta) \equiv \sum_{\mathbf{j}}^{|\mathbf{j}| < \Lambda} \frac{1}{|\mathbf{j}|^2 - \eta} - 4\pi\Lambda$$

$$p \cot \delta(p) = \frac{1}{a} + \frac{1}{2}rp^2 + \dots$$

a is the scattering length

$$E(p) = 2\sqrt{p^2 + m^2 - 2m}$$

Two Body spectrum in a box

$$p \cot \delta(p) = S(\frac{p^2 L^2}{4\pi^2})$$

$$p \cot \delta(p) = \frac{1}{a} + r^2 p^2 + \cdots$$



nucleon-nucleon phase shifts







t/a









Expected Carbon spectrum in the 32³ box



Expected Carbon spectrum in the 32³ box



Conclusions

- * We have a systematic way of constructing all possible interpolating fields
- * Using heavy quarks noise is reduced
- * Special care needs to be given to the selection of interpolating fields
 - * Minimize number of terms in the interpolating field and optimize the signal
- * NPLQCD: Presented results for the spectrum of nuclei with A<5 and S>-3
 NPLQCD arXiv:
 * ... and nucleon-nucleon phase shifts
 NPLQCD 1206.5219,1301.5790
- * We have an algorithm for quark contractions in polynomial time for A>5
- * Future work must focus on the improved sampling methods to reduce statistical errors at light quark masses