Baryon Interactions from Lattice QCD with physical masses

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for HAL QCD Collaboration
Hadrons to Atomic nuclei from Lattice QCD
(HAL QCD Collaboration)

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H. Nemura, K. Sasaki (Univ. of Tsukuba)
The journey from Quarks to Universe

QCD vacuum → Baryons → Nuclei

QCD vacuum → 1st-principle Lattice QCD → Hadron Forces

Hadron Forces → 3N → APR

Hadron Forces → 2N → Y
dof

EoS of Dense Matter

Nuclear Forces / Hyperon Forces

QCD → Hadron Forces → Neutron Stars / Supernovae

Nucleosynthesis

J-PARC

Lattice QCD

ab-initio nuclear calc.

aLIGO/KAGRA

RIBF/FRIB

J1614-2230

PSR1913+16

Hitomi

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The journey from unphysical to physical quark masses

~2012

We were here

$M_\pi = 0.4 \text{ GeV}$
$L = 3 \text{ fm}$

$\rightarrow$ lighter $m_q$

K-computer

HPCI Strategic Program Field 5
“The origin of matter and the universe”
FY2010-15

Physical $M_\pi$
$L = 8 \text{ fm}$

Phys. point
• Outline
  – Introduction
  – (Theoretical framework) [↩ S. Aoki’s talk]
  – Challenges at physical quark masses
  – Results at physical quark masses
  – Summary / Prospects
[HAL QCD method]

- Nambu-Bethe-Salpeter (NBS) wave function

\[ \psi(\vec{r}) = \langle 0 | N(\vec{r}) N(\vec{0}) | N(\vec{k}) N(-\vec{k}); in \rangle \]

\[ (\nabla^2 + k^2)\psi(\vec{r}) = 0, \quad r > R \]

- phase shift at asymptotic region

\[ \psi(r) \approx A \frac{\sin(kr - l\pi/2 + \delta(k))}{kr} \]

**Extended to multi-particle systems**

- Consider the wave function at “interacting region”

\[ (\nabla^2 + k^2)\psi(r) = m \int dr' U(r, r') \psi(r'), \quad r < R \]

- \( U(r, r') \): faithful to the phase shift by construction
- \( U(r, r') \): E-independent, while non-local in general
  - Non-locality \( \Rightarrow \) derivative expansion

References:
- M. Luscher, NPB354(1991)531
- C.-J. Lin et al., NPB619(2001)467
- CP-PACS Coll., PRD71(2005)094504
- S. Aoki et al., PRD88(2013)014036
- Aoki-Hatsuda-Ishii PTP123(2010)89
HAL QCD method

\[ \psi_{NBS}(\vec{r}) = \langle 0 \mid N(\vec{r})N(\vec{0})\mid N(\vec{k})N(-\vec{k}), in \rangle \]
\[ R e^{i\delta(k)} \sin(kr - l\pi/2 + \delta_l(k))/(kr) \]
(at asymptotic region)

\[ (k^2/m_N - H_0) \psi(\vec{r}) = \int d\vec{r}' U(\vec{r}, \vec{r}') \psi(\vec{r}') \]

**E-indep \& non-local** Potential: Faithful to phase shifts

**Phase shifts**

**Phen. Potential**
Various Theoretical methods

**QCD**
- **quarks**
- **gluons**
  - #params = 4
  - quark masses & coupling

**Effective DoF**

**Chiral Sym.**
- (w/ Effective DoF)

**Lattice QCD**
- (HAL method)

**Lattice QCD**
- (Luscher’s method)

**Phen. potentials**
- #params(2NF) = O(40)
- #params(3NF) = several

**Pionfull/ Pionless EFT potentials**
- #params(2NF) = 24+…
- #params(3NF) = 2+…
- or
- #params(2NF) = 2+…
- #params(3NF) = 1+…

**LQCD potentials**
- #params(2NF) = 0
- #params(3NF) = 0
- #params(YN,YY,YNN) = 0

**Exp. Data**

(Comparison between 2 LQCD methods ➔ T. Iritani’s talk)
• **Outline**
  - Introduction
  - (Theoretical framework)
  - **Challenges at physical quark masses**
    - Signal/Noise Issue
    - Coupled Channel Systems
    - Computational Challenge
  - Results at physical quark masses
  - Summary / Prospects

[T. Iritani’s talk]
Signal/Noise issue w/ ~continuum on Lat

- **Challenge in Luscher’s method**: ground state saturation

\[ S/N \sim \exp\left[ -A \times (m_N - 3/2m_\pi) \times t \right] \]

\[ 1/t \simeq \Delta E \simeq \frac{1}{m_N} \frac{(2\pi)^2}{L^2} \]

\[ S/N \propto \begin{cases} 10^{-4} & L = 3\text{fm} \\ 10^{-13} & L = 6\text{fm} \\ 10^{-25} & L = 8\text{fm} \end{cases} \]

\[ L = \infty \]

- **Time-dependent HAL method**
  - E-indep potential
  - \( \Rightarrow \) “Signal” from (elastic) excited states
  - G.S. saturation \( \Rightarrow \) Elastic states saturation

[Exponential Improvement]

Our solution:

- N.Ishii et al. PLB712(2012)437
Coupled Channel systems
(beyond inelastic threshold)

- Essential in many interesting physics
  - Hyperon Forces (e.g., H-dibaryon ($\Lambda\Lambda$-$\Xi\Sigma\Sigma$))
  - Exotic mesons, Resonances, etc. (e.g., $Zc(3900)$)

\[ \psi_{AB}(r, k) = \frac{1}{\sqrt{Z_A Z_B}} \langle 0 | \phi_A(x + r) \phi_B(x) | W \rangle \]
\[ \psi_{CD}(r, q) = \frac{1}{\sqrt{Z_C Z_D}} \langle 0 | \phi_C(x + r) \phi_D(x) | W \rangle \]

\[ W = \sqrt{m_A^2 + k^2} + \sqrt{m_B^2 + k^2} = \sqrt{m_C^2 + q^2} + \sqrt{m_D^2 + q^2} \]

S.Aoki et al. (HAL Coll.), PRD87(2013)034512
Computational Challenge

- Enormous comput. cost for multi-baryon correlators
  - Wick contraction (permutations)
    \[ \sim [(\frac{3}{2}A)!]^2 \quad (A: \text{mass number}) \]
  - color/spinor contractions
    \[ \sim 6^A \cdot 4^A \quad \text{or} \quad 6^A \cdot 2^A \]
  - Unified Contraction Algorithm (UCA)
    - A novel method which unifies two contractions

\[ \Pi^{2N} \approx \langle qqqqq(t)\bar{q}(\xi_1^{'})\bar{q}(\xi_2^{'})\bar{q}(\xi_3^{'})\bar{q}(\xi_4^{'})\bar{q}(\xi_5^{'})\bar{q}(\xi_6^{'})\rangle(t_0) \times \text{Coeff}^{2N}(\xi_1^{'}, \cdots, \xi_6^{'}) \]

Drastic Speedup

- $\times 192$ for $^3\text{H}/^3\text{He}$, $\times 20736$ for $^4\text{He}$, $\times 10^{11}$ for $^8\text{Be}$ (x add’l. speedup)

See also subsequent works: Detmold et al., PRD87(2013)114512
Gunther et al., PRD87(2013)094513
• **Outline**
  
  — Introduction
  
  – (Theoretical framework)
  
  – Challenges at physical quark masses
    
    • Signal/Noise Issue ➔ Time-dependent HAL method
    • Coupled Channel Systems ➔ Coupled channel HAL potential
    • Computational Challenge ➔ Unified Contraction Algorithm (UCA)
  
  – Results at physical quark masses
  
  – Summary / Prospects
Simulations w/ ~ physical masses

Gauge Config Generation

K-computer (RIKEN/ AICS)

10PFlops

FX100 (RIKEN/ Wako)

1PFlops

Baryon Forces

Calc of NBS

⇒ HAL QCD method

HA-PACS (Tsukuba U.)

HPCI Strategic Program Field 5
“The origin of matter and the universe”
FY2010-15
Simulation Setup

- $N_f = 2+1$ clover fermion + Iwasaki gauge action
  - APE-Stout smearing ($\alpha=0.1, n_{\text{stout}}=6$)
  - Non-perturbatively $O(a)$-improved
  - $1/a \sim 2.3$ GeV ($a \sim 0.085$ fm)
  - Volume: $96^4 \sim (8 \text{ fm})^4$
  - $m(\pi) \sim 145$ MeV, $m(K) \sim 525$ MeV
  - $\#_{\text{traj}} \sim 2000$ generated
  - DDHMC (ud) + UVPHMC (s) w/ preconditioning

\[ \frac{m_H/m_{\Omega}}{\text{lat}} / \frac{m_H/m_{\Omega}}{\text{exp}} - 1 \]

deviation from the Exp.:
\[ \delta m_\pi \sim +5\%, \quad \delta m_K \sim +2\%. \]
Simulation Setup

• **Measurements**
  – ud, s mass = sea mass (unitary point)
  – Wall source
    • Coulomb gauge fixing after smearing
    • Spacial PBC & Temporal DBC w/ forward/backward average
  – #stat = 200 configs x 4 rotation x 20-72 src in this talk
    • #stat $\rightarrow$ x1.3-4 in FY2015 (& add’l x2 in FY2016)
    • (Relativistic term omitted in this preliminary analyses)

• **Code development**
  – Efficient implementation of UCA
  – Many channels w/ $L^3$ dof in NBS
  – Block solver for multiple RHS
  – K-computer @ 2048 node (x 8core/node)
    • $\sim$25% efficiency ($\sim$65 TFlops sustained)
Strategy for phys point BB-forces calc

- Focus on the most important forces:
  - Central/tensor forces for all NN/YN/YY in P=(+) (S, D-waves)

\[
U(\vec{r}, \vec{r}') = V_c(r) + S_{12} V_T(r) + \vec{L} \cdot \vec{S} V_{LS}(r) + \mathcal{O}(\nabla^2)
\]

- Hyperon forces provide precious “predictions”

<table>
<thead>
<tr>
<th>S=0</th>
<th>S=-1</th>
<th>S=-2</th>
<th>S=-3</th>
<th>S=-4</th>
<th>S=-5, -6</th>
</tr>
</thead>
<tbody>
<tr>
<td>NN</td>
<td>ΔN, ΣN</td>
<td>ΔΛ, ΛΣ, ΣΣ, ΝΞ</td>
<td>ΔΞ, ΣΞ</td>
<td>ΞΞ</td>
<td>ΩΩ</td>
</tr>
</tbody>
</table>

“milestone-postdiction” Hypermixed phys @ J-PARC
H-dibaryon ?, Ξ-hypernuclei

Λ appearance in NS & EoS ?  New bound state(s) ?
ΩΩ system \((S=-6)\)

\(^1S_0\) : Pauli allowed channel, candidate for exotic bound state

Model varies from bound state to repulsive interactions

HAL study @ \(m(\pi)=0.7\text{GeV}\): nearly bound (Unitary Region)

M. Yamada et al., PTEP2015, 071B01

See also S. Aoki’s talk

c.f. Luscher’s method @ \(m(\pi)=0.39\text{GeV}\): weak repulsion
\(a = -0.16(22)\text{fm}\)

M. Buchoff et al, PRD85(2012)094511
ΩΩ system in $^1S_0$

Potential

m(eff) for single Ω

(200conf x 4rot x 72src)

t = 18 : ~0.2-0.3% sys error

[S. Gongyo / K. Sasaki]
ΩΩ system in $^1S_0$

Phase Shifts

Scatt. Length
$a = -3.53(18)(54) \text{ fm}$
(@ $t=18$ (&17))

The Most Strange Dibaryon

⇒ HIC experiments?

[S. Gongyo / K. Sasaki]
$\Xi\Xi$ system ($S = -4$)

- $^1S_0 \sim 27$-plet
  $\Leftrightarrow$ $\text{NN}(^1S_0) + \text{SU}(3)$ breaking
  - Phen. model (Nijmegen) : possibly bound
  - EFT (Haidenbauer et al. ’14) : unbound favored

- $^3S_1 - ^3D_1 \sim 10$-plet
  $\Leftrightarrow$ unique w/ hyperon DoF
  $\Leftrightarrow$ $\Sigma^-$ in neutron star
\[ ^1S_0 \sim 27\text{-plet} \quad \Leftrightarrow \quad \text{attractive } V_c \]

\[ ^3S_1-^3D_1 \sim 10\text{-plet} \quad \Leftrightarrow \quad \text{repulsive } V_c, \text{weak } V_t \]

(200conf x 4rot x 44src)
$\Xi \Xi$ phase shifts ($^1S_0$)

$\Xi \Xi$ ($^1S_0$) is unbound

(t-dependence will be checked again w/ larger #stat)

(2-gauss + 2-OBEP fit)
(200conf x 4rot x 44src)

$\Xi \Xi$ (1S0) is unbound

Scatt. Length

$a = 1.35(047)$ fm (t=14)
$a = 1.97(113)$ fm (t=16)

m(\text{eff})$ for single $\Xi$

t = 14-18 : $\sim0.3$-1% sys error

$\Xi$ (CG05-CG05)

$\Xi$ (CG05-CG05)

$\Xi$ (CG05-CG05)

HIC experiments?
S=−3 systems

- \( \Xi\Sigma \) (I=3/2)
  - \(^1S_0 \sim 27\)-plet
    \( \leftrightarrow \) NN\(^1S_0\) + SU(3) breaking
  - \(^3S_1\)\(^-\)\(^3D_1 \sim 10^*\)-plet
    \( \leftrightarrow \) NN\(^3S_1\)\(^-\)\(^3D_1\) + SU(3) breaking

- \( \Xi\Lambda-\Xi\Sigma \) (I=1/2) : coupled channel
  - \(^1S_0 \sim 27\)-plet & 8s-plet
  - \(^3S_1\)\(^-\)\(^3D_1 \sim 10\)-plet & 8a-plet
ΞΣ(Ι=3/2, spin triplet)

V_C(r) [MeV] (ΞΣ spin-triplet)

Central

V_T(r) [MeV] (ΞΣ)

Tensor

(bar) phase shifts & mixing

ΞΣ spin triplet (δ_{0}^{\bar{R}})

unbound

ΞΣ spin triplet (δ_{2}^{\bar{R}})

ΞΣ spin triplet (ε_{1}^{\bar{R}})

Preliminary

N.B. t-dep should be checked; single m_B has ~0.3-3% sys @ t=10-14

(200conf x 4rot x 20src)

[N. Ishii]
H-dibaryon channel \((S=−2)\)

\({}^{1}S_{0}, \Lambda\Lambda−N\Xi−\Sigma\Sigma, \text{Coupled Channel}\)

R. Jaffe (1977), “Perhaps a Stable Dihyperon”

NAGARA-event (2001)

\[\Xi^- + {}^{12}\text{C} \rightarrow _{\Lambda\Lambda}{}^{6}\text{He} + {}^{4}\text{He} + t\]

- \(\Lambda\Lambda\) weak attraction
- No deeply bound H-dibaryon
H-dibaryon @ Nf=3, heavy masses

Inoue et al. (HAL QCD Coll.) PRL106(2011)162002
Beane et al. (NPLQCD Coll.) PRL106(2011)162001

c.f. B.E. = 74.6(3.3)(3.4) MeV @ $m_\pi=0.8\text{GeV}$ by NPL (’12)
H-dibaryon @ Nf=2+1, heavy masses

\[ \Lambda\Lambda \text{ and } N\Xi \text{ phase shifts} \]

- \( N_f = 2+1 \) full QCD with \( L = 2.9 \text{fm} \)
- Preliminary!

- \( m_{\pi} = 700 \text{ MeV} \)
  - bound state
- \( m_{\pi} = 570 \text{ MeV} \)
  - resonance near \( \Lambda\Lambda \) threshold
- \( m_{\pi} = 410 \text{ MeV} \)
  - resonance near \( N\Xi \) threshold

H-dibaryon is unlikely bound state
H-dibaryon @ Nf=2+1, $m_\pi = 145$ MeV

**diagonal in SU(3)-irrep base**

- $m_{\Sigma\Sigma} = 2380$ MeV
- $m_{N\Xi} = 2260$ MeV
- $m_{\Lambda\Lambda} = 2230$ MeV

**Strong Attraction in flavor-singlet channel**

$(200 \text{conf} \times 4 \text{rot} \times 20 \text{src}, t=10)$
ΛΛ, \( \Lambda \Xi \) (effective) 2x2 coupled channel analysis

\( \Sigma \Sigma \) channel ↔ couples strongly to flavor octet channel ↔ noisy because they are quark-Pauli forbidden

→ Improve the S/N by considering only \( \Lambda \Lambda, \Lambda \Xi \) dof at low energies

\[ m_{\Sigma \Sigma} = 2380 \text{MeV} \]

\[ m_{\Lambda \Xi} = 2260 \text{MeV} \]

\[ m_{\Lambda \Lambda} = 2230 \text{MeV} \]

3x3 2x2
ΛΛ, NΞ (effective) 2x2 coupled channel analysis

ΛΛ, NΞ phase shifts

Preliminary

$m_{\Sigma\Sigma} = 2380\text{MeV}$

"Perhaps a Resonant Dihyperon"

$\Rightarrow$ J-PARC experiment (E42)

$m_{N\Xi} = 2260\text{MeV}$

H-resonance

$m_{\Lambda\Lambda} = 2230\text{MeV}$

N.B. t-dep should be checked; single $m_B$ has ~3% sys @ t=10

[K. Sasaki]
NΞ−-interactions (S=−2)

Ξ− could appear in the core of Neutron Star
  e.g., J. Schaffner-Bielich, NPA804(2008)309

KISO-event (2014)

\[ \Xi^- + ^{14}\text{N} \rightarrow \Lambda^{10}\text{Be} + \Lambda^5\text{He} \]

- First observation of Ξ-nuclei
- B.E. = 4.38(25) MeV
  (or 1.11(25) MeV)
Is interaction net attractive? Stay tuned!

(net attractive @ m(pi)=0.66-88GeV)
S=–1 systems

↔ strangeness nuclear physics (Λ-hypernuclei @ J-PARC)

Λ should (?) appear in the core of Neutron Star

↔ Huge impact on EoS of high dense matter

• $\Lambda N–\Sigma N$ ($I=1/2$) : coupled channel
  • $^1S_0 \sim 27$-plet & 8s-plet
  • $^3S_1$–$^3D_1 \sim 10^*$-plet & 8a-plet

• $\Sigma N$ ($I=3/2$)
  • $^1S_0 \sim 27$-plet
    ⇔ $NN(^1S_0)$ + SU(3) breaking
  • $^3S_1$–$^3D_1 \sim 10$-plet
ΛN–ΣN Vc potential in $^3S_1–^3D_1$ [H. Nemura]
ΛN–ΣN Vt potential in $^3S_1–^3D_1$

Very preliminary result of LN potential at the physical point

$$V_T(\ ^3S_1–^3D_1) = \frac{\sqrt{2}}{2\mu} \left( \frac{\nabla^2}{r} - \frac{\partial}{\partial t} \right) R(\vec{r}, t) = \int d^3r' U(\vec{r}, \vec{r}') R(\vec{r}', t) + O(k^4) = V_{LO}(\vec{r}) R(\vec{r}, t) + \cdots \ (8)$$

More in talk by H. Nemura
NN system \( (S = 0) \)
NN-Potentials

$^1S_0$  

$^3S_1 - ^3D_1$

- $V_c$: repulsive core + long-range attraction
- $V_t$: tensor force clearly visible

(200conf x 4rot x 44src)

Preliminary
NN-Potentials (tensor)

- Qualitatively similar tail as OPEP force
- Larger $t$ w/ larger #stat is desirable

$m_{\text{eff}}$ for single N

$t = 8-10 : \sim 2-4\% \text{ sys error}$
Summary

The 1st LQCD for Baryon Interactions at ~ phys. point

- $m(\pi) \approx 145$ MeV, $L \approx 8$ fm, $1/a \approx 2.3$ GeV
- Central & Tensor forces calculated for all $NN/YN/YY$ in $P=(+)$ channel
- Key formula / algorithm
  - t-dep HAL QCD method
  - Coupled channel formalism
  - Unified contraction algorithm (UCA)
- Various exciting results
  - $\Omega\Omega (^1S_0)$: a new exotic dibaryon state
  - $\Xi\Xi (^1S_0)$: most likely an unbound state
  - H-dibaryon: indication of a resonance
  - $NN$: tensor force is clearly visible

Prospects

- #stat will be $\sim x3 - x8$ from today’s figs
- New techniques to improve S/N are under R&D
- [Exascale-Era] LS-forces, $P=(-)$ channel, 3-baryon forces, etc., & EoS
3N-forces (3NF)

**Nf=2+1, m_\pi=0.51\ GeV**

**Nf=2, m_\pi=0.76-1.1\ GeV**

Kernel: \(\sim 50\%\) efficiency achieved!

T.D. et al. (HAL Coll.) PTP127(2012)723
+ t-dep method updates etc.
Backup Slides
Reliability Test of LQCD methods

- High-stat study for BB-system (@m(pi)=0.5GeV)
  - Benchmark w/ two LQCD setup (wall & smeared src)

  ➞ Physical outputs should NOT depend on these setup

**Luscher’s method (traditional)**

\[ \Delta E = m \Xi - 2m \Xi \]

- \( t \) vs \( \Delta E \) (phase shift)
- Inconsistent “signal” (red (wall) vs blue (smeared))
- cannot judge which (or neither) is reliable

**HAL method (new !)**

- \( V_{\text{eff}}(r) \) from wall & \( V^{\text{LO}}(r) \) from wall+smeared
- are consistent

\[ \text{S/N} \approx \exp(-\alpha t) \]

\[ V_{\text{wall}}(r, 11) \quad V_{\text{LO}}(r) \text{ at } t = 11 \]
Understand the origin of “fake plateaux”

Potential

Solve Schrodinger eq. in Finite V

Eigen-wave functions

Decompose NBS correlator to each eigenstates

NBS correlator $\Psi(r,t)$

Smeared wall

Eigen-energies

<table>
<thead>
<tr>
<th>$n$-th A1</th>
<th>$\Delta E_n$ [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-2.58(1)</td>
</tr>
<tr>
<td>1</td>
<td>52.49(2)</td>
</tr>
<tr>
<td>2</td>
<td>112.08(2)</td>
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<tr>
<td>3</td>
<td>169.78(2)</td>
</tr>
<tr>
<td>4</td>
<td>224.73(1)</td>
</tr>
</tbody>
</table>
NBS correlator $\Psi(r,t)$

Contribution from each (excited) states (@ $t=0$)

R-correlator
$R(t) = \sum_r \Psi(r,t)$

(R(t) w/ smeared has been used in Luscher’s method)

Contribution from each (excited) states (@ $t=0$)

Decompose NBS correlator to each eigenstates

excited states NOT suppressed  excited states suppressed

Blue: smeared  Red: wall

G.S. Excited States

G.S.

Excited States

$\Delta E_n$ [MeV]

$\Delta E_n$ [MeV]
Understand the origin of “fake plateaux”

We are now ready to “predict” the behavior of $m(\text{eff})$ of $\Delta E$ at any “$t$”

“prediction” reproduce the real data well

To obtain a “real plateau”, $t/a > 100 \ (t > 10\text{fm})$ is necessary

Extreme care is necessary for the results from the Luscher’s method
Understand the origin of "fake plateaux"

We are now ready to “predict” the behavior of m(eff) of $\Delta E$ at any “t”.

To obtain a “real plateau”, $t/a > 100$ ($t > 10$ fm) is necessary.

Extreme care is necessary for the results from the Luscher’s method.

"prediction" reproduce the real data well.