Lattice QCD and Baryon Spectroscopy

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Outline

- Lattice QCD
  - Background, actions, observables, …

- Methodology
  - Group theory and operator design
  - Variational method
  - Ensembles, parameter and analysis

- Numerical Results
  - Octet and decuplet
  - Other ±-parity, spin-1/2 and 3/2 states
  - Roper from full QCD

- Conclusions and Outlook
Lattice QCD is a discrete version of continuum QCD theory.
Lattice QCD is a discrete version of continuum QCD theory

\[ \psi(x+\mu) \]

\[ U_\mu(x) \]

\[ \psi(x) \]

Physical observables are calculated from the path integral

\[ \langle 0| O(\bar{\psi}, \psi, A) |0 \rangle = \frac{1}{Z} \int [dA][d\bar{\psi}][d\psi] \ O(\bar{\psi}, \psi, A) e^{i \int d^4 x \mathcal{L}_{\text{QCD}}(\bar{\psi}, \psi, A)} \]

Use Monte Carlo integration combined with the “importance sampling” technique to calculate the path integral.

Take \( a \to 0 \) and \( V \to \infty \) in the continuum limit
Lattice QCD

A wide variety of first-principles QCD calculations can be done:

- In 1970, Wilson wrote down the original lattice action
- Progress is limited by computational resources...
  but assisted by advances in algorithms.
T.D. Lee uses an “analog computer” to calculate stellar radiative transfer equations.
Lattice QCD

2007: The 13 Tflops cluster at Jefferson Lab

Other joint lattice resources within the US: Fermilab, BNL. Non-lattice resources open to USQCD: ORNL, LLNL, ANL.
Lattice QCD

Lattice QCD is computationally intensive

\[
\text{Cost} \approx \left( \frac{L}{\text{fm}} \right)^5 L_s \left( \frac{\text{MeV}}{M_\pi} \right) \left( \frac{\text{fm}}{a} \right)^6 \left( C_0 + C_1 \left( \frac{\text{fm}}{a} \right) \left( \frac{\text{MeV}}{M_K} \right)^2 + C_2 \left( \frac{a}{\text{fm}} \right)^2 \left( \frac{\text{MeV}}{M_\pi} \right)^2 \right)
\]

Norman Christ, LAT2007

Current major US 2+1-flavor gauge ensemble generation:
- MILC: staggered, \( a \sim 0.06 \text{ fm} \), \( L \sim 3 \text{ fm} \), \( M_\pi \sim 250 \text{ MeV} \)
- RBC+UKQCD: DWF, \( a \sim 0.09 \text{ fm} \), \( L \sim 3 \text{ fm} \), \( M_\pi \sim 330 \text{ MeV} \)

Chiral domain-wall fermions (DWF) at large volume (6 fm) at physical pion mass may be expected in 2011

But for now…

need a pion mass extrapolation \( M_\pi \rightarrow (M_\pi)_{\text{phys}} \)

(use chiral perturbation theory, if available)
Lattice Fermion Actions

**Chiral fermions (e.g., Domain-Wall/Overlap):**
- Automatically $O(a)$ improved,
  - good for spin physics and weak matrix elements
- Expensive
  \[
  D_{x,s;x',s'} = \delta_{x,x'}D_{s,s'}^\perp + \delta_{s,s'}D_{x,x'}^\parallel
  \]
  \[
  D_{s,s'}^\perp = \frac{1}{2}[(1 - \gamma_5)\delta_{s+1,s'} + (1 + \gamma_5)\delta_{s-1,s'} - 2\delta_{s,s'}]
  \]
  \[
  - \frac{m_f}{2}[(1 - \gamma_5)\delta_{s,L_s-1}\delta_{0,s'} + (1 + \gamma_5)\delta_{s,0}\delta_{L_s-1,s'}],
  \]

**(Improved) Staggered fermions (asqtad):**
- Relatively cheap for dynamical fermions (good)
- Mixing among parities and flavors or “tastes”
- Baryonic operators a nightmare — not suitable

**Wilson/Clover action:**
- Moderate cost; explicit chiral symmetry breaking

**Twisted Wilson action:**
- Moderate cost; isospin mixing
Mixed Action Parameters

**Mixed action:**
- Staggered sea (cheap) with domain-wall valence (chiral)
- Match the sea Goldstone pion mass to the DWF pion
- Only mixes with the “scalar” taste of sea pion
- Free light quark propagators (LHPC & NPLQCD)

In this calculation:
- Pion mass ranges 300–750 MeV
- Volume fixed at 2.6 fm, box size of $20^3 \times 32$
- $a \approx 0.125$ fm, $L_s = 16$, $M_5 = 1.7$
- HYP-smeared gauge fields
Lattice QCD: Observables

- Two-point Green function
  e.g. spectroscopy

- Three-point Green function
  e.g. form factors, structure functions, …

\[
\sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{\text{snk}}) J(X_{\text{src}}) \rangle_{\alpha, \beta}
\]

\[
\sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{\text{snk}}) O(X_{\text{int}}) J(X_{\text{src}}) \rangle_{\alpha, \beta}
\]
Lattice QCD: Observables

Two-point Green function

\[ \sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{snk}) J(X_{src}) \rangle_{\alpha, \beta} \]

Three-point Green function

\[ \sum_{\alpha, \beta} \Gamma^{\alpha, \beta} \langle J(X_{snk}) O(X_{int}) J(X_{src}) \rangle_{\alpha, \beta} \]

After taking spin and momentum projection
(ignoring the variety of boundary condition choices)

Two-point correlator

\[ \sum_n Z_{n, B} e^{-E_n(\mathbf{P})t} \]

Three-point correlator

\[ \sum_n \sum_{n'} Z_{n', B}(p_f) Z_{n, A}(p_i) \times \text{FF's} \times e^{-(t_f - t)E_{n'}(\mathbf{p}_f)} e^{-(t-t_i)E_n(\mathbf{p}_i)} \]

At large enough \( t \), the ground-state signal dominates.
Motivations and Methodology
Why Baryons?

Lattice QCD spectrum

- Successfully calculates many ground states (Nature, …)
- Nucleon spectrum, on the other hand… not quite

Example: $N$, $P_{11}$, $S_{11}$ spectrum
Strange Baryons

Strange baryons are of particular interest; challenging even to experiment

Example from PDG Live:

\[ \Xi BARYONS \ (S = -2, \ I = 1/2) \]

\[ \Xi^0 \quad 1/2(1/2^+) \quad \Xi(1820) \quad D_{13} \quad 1/2(3/2^-) \quad \Xi(2370) \quad 1/2(?)^* \]

\[ \Xi^- \quad 1/2(1/2^+) \quad \Xi(1950) \quad 1/2(?)^* \quad \Xi(2500) \quad 1/2(?)^* \]

\[ \Xi(1530) \quad P_{13} \quad 1/2(3/2^+) \quad \Xi(2030) \quad 1/2(5/2^-) \quad \Xi(2120) \quad 1/2(?)^* \quad \Xi(2250) \quad 1/2(?)^* \]

---

\[ \Omega BARYONS \ (S = -3, \ I = 0) \]

\[ \Omega^- \quad 0(3/2^+) \quad \Omega(2250)^- \quad 0(?)^* \]

\[ \Omega(2380)^- \quad \Omega(2470)^- \quad \]

---
All baryon spin states wanted: \( j = 1/2, 3/2, 5/2, \ldots \)

Rotation symmetry is reduced due to discretization rotation \( O(3) \Rightarrow \text{octahedral } O_h \text{ group} \)

<table>
<thead>
<tr>
<th></th>
<th>I</th>
<th>J</th>
<th>6 C_4</th>
<th>8 C_6</th>
<th>8 C_3</th>
<th>6 C_9</th>
<th>6 C_9</th>
<th>12 C_4</th>
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Operator Design

- All baryon spin states wanted: $j = 1/2, 3/2, 5/2, \ldots$
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<th>$12 C_4'$</th>
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**Operator Design**

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<tr>
<td>$H$</td>
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<td>0</td>
<td>-1</td>
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</table>

![Graph showing 12 $C_4(3)$ symmetry group]
All baryon spin states wanted: \( j = 1/2, 3/2, 5/2, \ldots \)

Rotation symmetry is reduced due to discretization rotation \( O(3) \Rightarrow \text{octahedral } O_h \)

<table>
<thead>
<tr>
<th>( j )</th>
<th>Irreps</th>
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<td>( 1/2 )</td>
<td>( G_1 )</td>
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<tr>
<td>( 3/2 )</td>
<td>( H )</td>
</tr>
<tr>
<td>( 5/2 )</td>
<td>( G_2 \oplus H )</td>
</tr>
<tr>
<td>( 7/2 )</td>
<td>( G_1 \oplus G_2 \oplus H )</td>
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<tr>
<td>( 9/2 )</td>
<td>( G_1 \oplus 2H )</td>
</tr>
<tr>
<td>( 11/2 )</td>
<td>( G_1 \oplus G_2 \oplus 2H )</td>
</tr>
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<td>( 13/2 )</td>
<td>( G_1 \oplus 2G_2 \oplus 2H )</td>
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<td>( G_1 \oplus G_2 \oplus 3H )</td>
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<td>( 2G_1 \oplus G_2 \oplus 3H )</td>
</tr>
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<td>( 19/2 )</td>
<td>( 2G_1 \oplus 2G_2 \oplus 3H )</td>
</tr>
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<td>( 21/2 )</td>
<td>( G_1 \oplus 2G_2 \oplus 4H )</td>
</tr>
<tr>
<td>( 23/2 )</td>
<td>( 2G_1 \oplus 2G_2 \oplus 4H )</td>
</tr>
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Baryons
Operator Design

The basic building blocks

\[ B_{\alpha\beta\gamma}^{ABC}(x) = \bar{\psi}_\alpha A,i \bar{\psi}_\beta B,j \bar{\psi}_\gamma C,k \epsilon i,j,k \]

- A, B, C: quark flavor
- i, j, k: color
- \( \alpha, \beta, \gamma \): Dirac indices

Project onto irreducible representations (irreps)

\[ B_{\lambda}^{\Lambda,n}(x) = \Gamma_{\lambda}^{\Lambda,n}(\alpha, \beta, \gamma) B_{\alpha,\beta,\gamma}(x) \]

- \( \Lambda \): irrep
- \( \lambda \in [1, \text{dim}(\Lambda)] \)
- \( n \): element of interoperating op

Correlator matrix

\[ C_{\Lambda}^{\Lambda,n}(t) = \sum_{\vec{x}} \sum_{\lambda} \langle 0 \mid B_{\lambda}^{\Lambda,m}(\vec{x}, t) \bar{B}_{\lambda}^{\Lambda,n}(0) \mid 0 \rangle \]

For more details and extended-link operators:

Variational Method

Construct the matrix
\[ C_{ij}(t) = \langle 0 \mid \mathcal{O}_i(t)\mathcal{O}_j(0) \mid 0 \rangle \]

The \( O_i \) could be different choices of operator or smearing parameters.

Solve for the generalized eigensystem of
\[ C(t_0)^{-1/2}C'(t)C(t_0)^{-1/2}v = \lambda(t, t_0)v \]

with eigenvalues
\[ \lambda_n(t, t_0) = e^{-(t-t_0)E_n}(1 + \mathcal{O}(e^{-|\delta E|(t-t_0)})) \]

At large \( t \), the signal of the desired state dominates.
Variational Method

Quenched Anisotropic ($a_t^{-1} \sim 6$ GeV)

- Clover action, 680 MeV pion
- Example: $5 \times 5$ smeared-smeared correlator matrices
- Fit them individually with exponential form (red bars)
- Plotted along with effective masses
Variational Method

Mixed Action \( (a_t^{-1} \sim 1.6 \text{ GeV}) \)

Example: (~350 MeV pion)

Omega \( 2 \times 2 \) smeared-smeared operator correlator matrices
Variational Method

Mixed Action ($a_t^{-1} \sim 1.6$ GeV)

Example: ($\sim 350$ MeV pion)

**Lambda** $4\times4$ smeared-smeared operator correlator matrices
Variational Method

Mixed Action \((a_t^{-1} \sim 1.6 \text{ GeV})\)

Example: (~350 MeV pion)

Nucleon \(3 \times 3\) smeared-smeared operator correlator matrices

Unfortunately, we cannot see a clear radial excited state
Ensembles and Parameters

- Mixed action: DWF on staggered sea
- Pion mass ranges 300–750 MeV
- $a \approx 0.125$ fm, $L_s = 16$, $M_5 = 1.7$
- Volume fixed at 2.6 fm, box size of $20^3 \times 32$ chopped
Ensembles and Parameters

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HYP-smeared gauge fields, Gaussian operator smearing

<table>
<thead>
<tr>
<th>ensem</th>
<th>m007</th>
<th>m010</th>
<th>m020</th>
<th>m030</th>
<th>m040</th>
<th>m050</th>
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<tr>
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<td>3693</td>
<td>1455</td>
<td>700</td>
<td>324</td>
<td>425</td>
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</table>
**Consistent Analyses**

- **Systematic error due to fit range**
- **Example: Nucleon @ 350 MeV**

\[ t_{\text{max}} = 26 \]

\[ t_{\text{min}} = 16 \]

- **Example: Delta @ 350 MeV**

\[ t_{\text{max}} = 26 \]

\[ t_{\text{min}} = 16 \]
Oscillating effective mass is related to transfer matrix with 5th-dimensional mass term → treat as a lattice artifact

Solution: oscillating term + one excited state

\[ C(t) = \sum_{n=0}^{1} A_n \exp[-M_n \times (t - t_{\text{src}})] + A_{\text{osc}} (-1)^t \exp[-M_{\text{osc}} \times (t - t_{\text{src}})]. \]

Example: Delta @ 350 MeV pion ensemble

\[ \chi^2/\text{dof} = 0.69 \]

“effective” mass

log corr. (ground-state removed)
**Consistent Analyses**

- Chopped lattice? Example: Delta @ 350 MeV
  - Set A: $20^3 \times 64$, 4 sources, 224 confs.
  - Set B: chopped $20^3 \times 32$, 620 confs.

Consistent results in both cases
Ground-State Results

work with

Lattice Hadron Physics Collaboration (LHPC)
Octets and Decuplets

Spin-1/2

Spin-3/2
Multiplet Mass Relations

- **SU(3) flavor symmetry breaking**
  - Gell-Mann-Okubo relation
    \[
    \Delta_{GMO} = \frac{3}{4} M_\Lambda + \frac{1}{4} M_\Sigma - \frac{1}{2} M_N - \frac{1}{2} M_\Xi
    \]
- **Decuplet Equal Spacing relation**
  \[
  \Delta_{DESI} = \frac{1}{2} (M_{\Sigma^*} - M_\Delta) + \frac{1}{2} (M_\Omega - M_{\Xi^*}) - M_{\Xi^*} + M_{\Sigma^*}
  \]
- Mass differences are close to experimental numbers
The non-strange baryons ($N$)

Symbols: $J^P = \frac{1}{2}^+ \, \Delta \, , \, \frac{1}{2}^- \, \nabla \, , \, 3/2^+ \, \Diamond \, , \, 3/2^- \, \Box$

$N \, \quad N(1535) \quad N(1720) \quad N(1520)$
The non-strange baryons ($N$ and $\Delta$)

Symbols: $J^P = 1/2^+$ △, $1/2^-\nabla$, $3/2^+ \Diamond$, $3/2^- \Box$

- $N$, $N(1535)$, $N(1720)$, $N(1520)$
- $\Delta(1620)$, $\Delta$, $\Delta(1700)$
The singly strange baryons: (\(\Sigma\) and \(\Lambda\))

Symbols: \(J^P = 1/2^+ \bigtriangleup, 1/2^- \blacktriangleleft, 3/2^+ \blacklozenge, 3/2^- \square\)

\(\Sigma\) \(\Sigma(1620)\) \(\Sigma^*\) \(\Sigma(1580)\)

\(\Lambda\) \(\Lambda(1405)\) \(\Lambda(1890)\) \(\Lambda(1520)\)
General Spectroscopy

The less known baryons ($\Xi$)

Symbols: $J^P = \frac{1}{2}^+, \Delta$, $\frac{1}{2}^-, \nabla$, $\frac{3}{2}^+, \Diamond$, $\frac{3}{2}^-$

$\Xi, \Xi(1690)?, \Xi(1530), \Xi(1820)$
The less known baryons (Ξ)

Symbols: $J^P = \frac{1}{2}^+, \quad \triangle, \quad \frac{1}{2}^- \quad \blacktriangle, \quad \frac{3}{2}^+ \quad \diamondsuit, \quad \frac{3}{2}^- \quad \square$

$\Xi$, $\Xi(1690)$? $\Xi(1530)$ $\Xi(1820)$

Babar at MENU 2007:
$\Xi(1690)^0$ negative parity
$-1/2$
**General Spectroscopy**

- The less known baryons (Ξ and Ω)
- Symbols: $J^P = 1/2^+ \triangle, 1/2^- \nabla, 3/2^+ \diamond, 3/2^- \square$
- $\Xi, \Xi(1690), \Xi(1530), \Xi(1820)$
- Could they be $\Omega(2250), \Omega(2380), \Omega(2470)$?
Excited-State Results

Roper Puzzles
What is the Roper?

- First positive-parity excited state of the nucleon
- Unusual feature: 1st excited state is lower than its negative-parity partner!
- Long-standing puzzle
  - Quark-gluonic (hybrid) state [C. Carlson et al. (1991)]
  - Five-quark (meson-baryon) state [O. Krehl et al. (1999)]
  - Constituent quark models (many different specific approaches)
  - and many other models…

- Lattice gauge theory
  - Many early quenched calculations failed to extract the correct Roper mass
  - Kentucky group (with lightest pion mass = 180 MeV) got $M_{Roper} = 1462(157)$ MeV
Kentucky’s calculation
- Quenched Iwasaki, overlap
  (ghost contributions are included in analysis)
- Volume: 2.4 and 3.6 fm
- Large range of $m_\pi$

Conclusive?
- Many groups fail to see similar behaviour
- War still going on...
Roper in Full QCD

- Attempt to extract Roper mass from our current data
- Analysis: oscillating term is necessary for small $t$

$$C(t) = \sum_{n=0}^{1} A_n e^{p[-M_n \times (t - t_{src})]} + A_{osc} (-1)^t e^{p[-M_{osc} \times (t - t_{src})]}.$$ 

- Example plot (300 MeV ensemble)

“effective” mass

log corr. (ground-state removed)

- Reasonable $\chi^2$/dof < 0.6
- Systematic error due to lack of 2nd-excited state in the fit?
Roper in Full QCD

Results from mixed action

Symbols: $J^P$

1/2$^+$  ◊
1/2$^-$  △
1/2$^+$  △

No sign of crossover occurs here

Finite-volume effects starting at 350 MeV pion?
Summary/Outlook — I

What we have done:
- 2+1-flavor calculations with volume around 2.6 fm
- Preliminary study with lightest pion mass 300 MeV
- Ground states of \( G_{1g/u} \) and \( H_{g/u} \) for each flavor
- Roper state calculated;
  - correct mass-ordering pattern is not yet seen

Currently in progress:
- Mixed action chiral extrapolation for octet and decuplet
- Open-minded for extrapolation to physical pion mass for other states

In the future:
- Lower pion masses to confirm chiral logarithm drops
The Future
Physical-Pion Era

Physical pion mass ensembles are near
Chiral perturbation theory will no longer be a guide, but can be judged against predictions of QCD

Three major gauge-generation projects within US community
- Chiral fermions:
  DWF on Iwasaki gauge, 0.093 fm (RBC+LHPC+UKQCD)
  Designing next generation with IBM (RBC+UKQCD)
- Staggered fermions: MILC
  Considering HISQ instead of the asqtad
- Anisotropic clover lattices: LHPC
  2+1-flavor dynamical runs
Anisotropic Clover Fermions

Solution: increase resolution

- Excited-state resonances and form factors
- Glueballs, hybrids, etc.
- Nucleon scattering, four-point Green functions

Roadmap:
- 2012: physical pion at $a \sim 0.10$ fm $(72^3)$
- 2014: physical pion at $a \sim 0.08$ fm $(96^3)$