Hadron Interactions from LQCD

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Nuclear Physics Landscape

Mean Field Models
Density Functional

Shell Model(s)

Effective Interactions

Proton Number

1

10

100

Neutron Number

1

10

100

3He

4He

p

d

3H

n

Quark-Gluon Interaction

Microscopic Ab Initio

χEFT, EFT(α)

QCD

QCD Vacuum

chart adapted from G. Henning

figure by H. Greisshammer
Summary

- Overview of the physics project
  - Compute properties of hadron-hadron interactions on the lattice
- Describe the numerical problem
  - Cost estimate with today's algorithms
- Describe a new algorithm: Linear systems with multiple right hand sides
Nuclear physics

- Connect Nuclear physics to QCD
- QCD Scale: $1\text{GeV}$
- Nuclear binding energy $\sim \text{MeV}$
- Typical two scale problem
- Does it look hopeless?
- Not really!
Hadronic Interactions on the Lattice

- Effective field theory description of few nucleon systems
- Use lattice QCD to extract the low energy constants needed
  - Decay constants: $f_\pi$, $f_K$
  - Axial couplings: $g_A$, $g_{N\Delta}$, $g_{\Sigma\Sigma}$, $g_{\Xi\Xi}$, $g_{\Sigma\Lambda}$, ...
  - Scattering lengths: NPLQCD
- Lattice Nuclear physics [Lee et al., Borasoy et al.]
- Lattice offers flexibility!
  - Study quark mass dependence
  - Compute experimentally inaccessible quantities (Hyperons)
Hadronic Interactions

- Scattering processes from Lattice QCD are not straight forward
- Miani-Testa no-go theorem (‘90) [and C. Michael ‘89]
- Infinite Volume:
  - Euclidean → Minkowski
- Finite volume: discrete spectrum
  - Avoids Miani-Testa no-go theorem [M. Luscher]
Luscher Formula

Energy level shift in finite volume:

\[ \Delta E_n \equiv E_n - 2m = 2 \sqrt{p_n^2 + m^2} - 2m \]

For \( p_n \) solutions of:

\[
p \cot \delta(p) = \frac{1}{\pi L} S \left( \frac{p^2 L^2}{4\pi^2} \right)
\]

\[
p_n \cot \delta(p_n) = \frac{1}{a} + \cdots
\]

\[
\frac{1}{a} = \frac{1}{\pi L} S \left( \frac{p_0^2 L^2}{4\pi^2} \right) + \cdots
\]

Expansion at \( p \sim 0 \):

\[
\Delta E_0 = -\frac{4\pi a}{mL^3} \left[ 1 + c_1 \frac{a}{L} + c_2 \left( \frac{a}{L} \right)^2 \right] + O \left( \frac{1}{L^6} \right)
\]

\( c_1 \) and \( c_2 \) are universal constants

\( a \) is the scattering length
Scattering in One dimension

In center of mass coordinates

\[
\frac{1}{m} \frac{\partial^2 \Psi}{\partial x^2} + c(k) \delta(x) \Psi = E \Psi
\]

\[
\Psi = A \left( e^{-ik|x|} + e^{ik|x|} + 2i \delta(k) \right)
\]

\[
E = \frac{k^2}{m}
\]

- Wave functions are almost plane waves
- Finite length with periodic boundary conditions
- Wave function needs to be periodic and even under $x \rightarrow -x$
  (symmetric under particle exchange)
Scattering in One dimension

\[ c(k) = -\frac{1}{mk} \tan \delta(k) \]

\[ kL + 2\delta = 2n\pi \]
Realistic Calculations

- Include the vacuum polarization effects
  - 2 light (up down) 1 heavy (strange)

- Finite Volume
  - Compute in multiple and large volume

- Continuum Limit
  - Compute with several lattice spacings

- Chiral Limit
  - Compute with several values for the quark masses
  - Study quark mass dependence of QCD

- Need effective field theory for all the above
  - Light quark masses: $m_\pi < 400\text{MeV}$ (?)
The hybrid action program

- Domain wall fermions for valence (with hyp smeared links)
  - Chiral symmetry \(O(a^2)\) errors better scaling
  - Ward Identities (renormalization, power divergent mixing)
  - Match the pion mass to the staggered Goldstone pion mass

- Kogut-Susskind 2+1 Dynamical flavors
  - Improved KS action (Asqtad: \(O(a^4, g^2 a^2)\)) [KO, Sugar, Toussaint '99]
  - MILC has generated lattices

- Light quark masses: Lightest pion \(m_\pi \sim 250\text{MeV}\)

- Volumes: 2.6 to 3.2 fm

- Continuum extrapolation
  - MILC lattice spacings: \(a=0.125\text{fm}, 0.09\text{fm}\)
  - \(a=0.06\text{fm}\) in 1 - 2 years (..?)

- Problem: “Rooted” fermions? (Bernard, Golterman, Shamir, Sharpe, Durr, Creutz, Hassenfratz....)
**Pion 1=2 Scattering Length**

S. Bean P. Bedaque KO and M. Savage hep-lat/0506013

\[ C_{\pi^+}(t) = \sum_x \langle \pi^-(t, x) \pi^+(0, 0) \rangle \]

\[ C_{\pi^+\pi^+}(p, t) = \sum_{|p|=p} \sum_{x,y} e^{ip \cdot (x-y)} \langle \pi^-(t, x) \pi^-(t, y) \pi^+(0, 0) \pi^+(0, 0) \rangle \]

\[ G_{\pi\pi}(p, t) \equiv \frac{C_{\pi\pi}(p, t)}{C_{\pi}(t)^2} \rightarrow \sum_{n=0}^{\infty} A_n e^{-\Delta E_n} t \]

**Quenched**
- Sharpe et al '92
- Gupta et al '93
- Kuramashi et al '93
- Fugugita et al '94
- C. Liu et al '02
- J. Junk RBG '03
- CP-PACS

**Dynamical**
- CP-PACS '04 (Wilson)
- NPLQCD '05 (Hybrid)
- NPLQCD '07 (Hybrid)
The figure shows the correlator ratio $G_{\pi\pi}(t)$ as a function of time $t$ for different values of $m_\pi$: 295 MeV, 357 MeV, 495 MeV, and 595 MeV. The markers used are circles for $m_\pi = 295$ MeV, squares for $m_\pi = 357$ MeV, stars for $m_\pi = 495$ MeV, and triangles for $m_\pi = 595$ MeV. The plot illustrates how the correlator ratio decreases with increasing time for each mass value.
I=2 Pion Scattering

SU(2) ChiPT

One loop expression:

\[ m_\pi a_2 = -\frac{m_\pi^2}{8\pi f_\pi^2} \left[ 1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2} \left[ 3 \log \left( \frac{m_\pi^2}{\mu^2} \right) - 1 - l_{\pi\pi}(\mu) \right] \right] \]

Two loop expression:

\[ m_\pi a_2 = -\frac{m_\pi^2}{8\pi f_\pi^2} \left[ 1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2} \left[ 3 \log \left( \frac{m_\pi^2}{\mu^2} \right) - 1 - l_{\pi\pi}(\mu) + \frac{m_\pi^2}{4\pi^2 f_\pi^2} \left[ \frac{31}{6} \left( \log \left( \frac{m_\pi^2}{\mu^2} \right) \right)^2 + l^{(2)}(\mu) \log \left( \frac{m_\pi^2}{\mu^2} \right) + l^{(3)}(\mu) \right] \right] \}

Set the scale \( \mu \) to be \( f_\pi \) at the chiral limit (scale invariance)

\[ m_\pi a_2 = -\frac{m_\pi^2}{8\pi f_\pi^2} \left[ 1 + \frac{m_\pi^2}{16\pi^2 f_\pi^2} \left[ 3 \log \left( \frac{m_\pi^2}{f_\pi^2} \right) - 1 - l_{\pi\pi}(f_\pi) \right] \right] \]

Replace the ratio \( m_\pi/f_\pi \) by the lattice computed value on each quark mass. Amounts of modifications to higher order and in the case of the two loop formula modification of the second order counter terms.

[Gasser-Leutwyler ‘84] [Colangelo et al. ‘01] [NPLQCD: hep-lat/0606023, KO: LATTICE 2006, LHPC:‘06 ‘07]
$I=2$ Pion Scattering

**SU(2) ChiPT**

$$m_{\pi} a_2 = - \frac{m_{\pi}^2}{8\pi f_{\pi}^2} \left[ 1 + \frac{m_{\pi}^2}{16\pi^2 f_{\pi}^2} \left[ 3 \log \left( \frac{m_{\pi}^2}{f_{\pi}^2} \right) - 1 - l_{\pi\pi}(f_{\pi}) \right] \right]$$

- Physical point -- Lighter three point fit: $m_{\pi} a_2 = -0.04196(12)$
- Physical point -- Lighter two point fit: $m_{\pi} a_2 = -0.04223(28)$
- Physical point -- Quadratic fit (higher order): $m_{\pi} a_2 = -0.0426(4)$
QCD results on $\pi$-$\pi$ scattering lengths

H. Leutwyler : hep-lat/0612112
I=2 Pion Scattering

- Preliminary result at the physical point: $m_\pi a_2 = -0.0426(4)$
- Experiment: $m_\pi a_2 = -0.0454(31)$
- Possible systematic errors:
  - Mixed action: $S\chi$PT has insignificant effect to the result
    - [Chen et al. ‘05], [A. Walker-Loud]
  - Finite volume correction:
    - At most 1% at the lightest mass
    - [Bedaque et.al ‘06], [A. Walker-Loud]
  - Finite range correction:
    - $p_n \cot \delta(p_n) = \frac{1}{a} + \cdots$
    - About 1% correction.
  - Lattice spacing errors:
    - Difficult to estimate without a second lattice spacing run. ~ 2-3% (?)
  - Charge symmetry breaking and electromagnetic effects:
    - May be the largest systematic: ~ 3%
I=1 Kaon-Kaon Scattering

\[ m_K a_1 = -\frac{m_K^2}{8\pi f_K^2} \left[ 1 + \frac{m_K^2}{16\pi^2 f_K^2} \left[ 2 \log \left( \frac{m_K^2}{f_\pi^2} \right) - \frac{2m_\pi^2}{3(m_\eta^2 - m_\pi^2)} \log \left( \frac{m_\eta^2}{f_\pi^2} \right) + \frac{2(20m_K^2 - 11m_\pi^2)}{27(m_\eta^2 - m_\pi^2)} \log \left( \frac{m_\eta^2}{f_\pi^2} \right) - \frac{14}{9} - 32(4\pi)^2 L_{KK}(f_\pi) \right] \right] \]

- Physical point -- Fit to all points : \( m_K a_1 = -0.374(4) \)
- Similar systematic errors as the pion scattering case
Kaon Pion Scattering Lengths

- Upcoming experiments on Kaon - pion molecules (DIRAC collab.)
- Continuum extrapolation still needed
$^{1}S_{0}$ channel

$^{3}S_{1}$ channel
Nucleon-Nucleon


BBSvK: Beane Bedaque Savage van Kolck ‘02
W: Weinberg ‘90; Weingberg ‘91; Ordonez et.al ‘95

Fukugita et al. ‘95: Quenched heavy pions
Computation break up

\[ \langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int \prod_{\mu,x} dU_\mu(x) \ O[U, D(U)^{-1}] \ \det (D(U)^\dagger D(U))^{n_f/2} \ e^{-S_g(U)} \]

- **Gauge field configuration generation:** The accelerator
  - Can be used by several collaborations
  - Thought to be the dominant cost

- **Correlation function calculation:** The detector
  - Used for specific calculations
  - Thought to be a small cost
Gauge Field Generation

\[ C = K \left( \frac{m_{PS}}{m_V} \right)^{-4} L^5 \frac{1}{a^7} \]

Lattice: \(24^3 \times 64, a=0.08\) fm

Urbach (ILFTN 3) hep-lat/0510064 hep-lat/0506011
Typical Calculations

\[ C_{2pt}(\vec{p}, t) = \langle J_{\vec{p}}(t) J(0) \rangle \]

1 propagator: 12 right hand sides

\[ C_{3pt}(\vec{p}, \vec{q}; t, \tau) = \langle J_{\vec{p}}(t) O(\vec{q}, \tau) J(0) \rangle \]

3 propagators: 36 right hand sides

- Multiple source locations per lattice to increase statistics
- For excited state spectroscopy we need multiple interpolating fields. Each source interpolating field needs a new propagator
- For three point functions we need new propagators every time we change the source or the sink interpolating field
- For typical production (hadronic form factors, spectrum) we typically need \( O(500) \) right hand sides. Many more in for increased statistics
- Optimization strategy: Reduce total cost of inversions by developing techniques for multiple right hand side problems.
Signal to Noise ratio for correlation functions

\[ C(t) = \langle N(t) \bar{N}(0) \rangle \sim E e^{-M_N t} \]

\[ \text{var}(C(t)) = \langle N \bar{N}(t) N \bar{N}(0) \rangle \sim A e^{-2M_N t} + B e^{-3m_\pi t} \]

\[ \text{StoN} = \frac{C(t)}{\sqrt{\text{var}(C(t))}} \sim A e^{-(M_N - 3/2m_\pi)t} \]

- The signal to noise ratio drops exponentially with time
- The signal to noise ratio drops exponentially with decreasing pion mass
Signal to noise ratio for single for Nucleon two point function

The red line is: Mnuc – 1.5 Mpion from the spectrum
The green point is the result for the $28^3$ lattices.
measured StoN = 1.06(6)
scaled up from small volume StoN = 1.02(11)
Scaling factor $\sqrt{28^3/20^3}$
What it takes

Based on signal to noise ratio 30 (at T=10)
What it really takes?

Based on signal to noise ratio 150 (at T=10)
Nucleon-Nucleon Interactions: Projected errors

- Errors on scattering nucleon-nucleon scattering length as function of computational resources
- Only cost for correlation function calculation presented
The Linear Algebra problem

Multiple right hand sides

- Basic problem in QCD: Compute the quark propagator

\[ D_{ss'}^{aa'} G_{s'k}^{ab} = \delta^{ab} \delta_{sk} \delta(x - y) \]

- Need \( N_s \times N_c \times V \) solutions of linear systems to get the propagator

- This cannot be done! (storage -- computation too much)

- In practice we solve exactly for the spin and color part and restrict the source to a fixed point (12 right hand sides)

- But this is not all! We need many more propagators per lattice for most calculations
Lesson:

Need to optimize the problem with solving linear systems with multiple right hand sides.

Where *multiple* really means a lot!
The problem of multiple right hand sides

- Appears in many numerical applications
  [Simoncini and Gallopoulos SIAM J. Sci. Comput. 16 (4)]
- It is difficult: i.e. no clear solution exists
- When the right hands sides are related it is somewhat simpler
- QCD: The right hand sides are orthogonal or nearly orthogonal
  - Probably the most difficult case of multiple right hand sides
- Early attempt for solution: de Forcrand and de Struler
Question

What is the maximal information that can be shared between solves with different right hand sides?

Answer:

The spectral properties of the Matrix

In practice this has been used for Lattice QCD. People compute eigenvectors and use them to deflate the iterative solver of choice.

How can we compute eigenvalues and eigenvectors efficiently?
Eigenvectors and Deflation

- Goal: Reduce the cost of eigenvector computation
- Avoid it all together by constructing a basis to a space that has strong overlap with the low mode subspace
- Luscher’s deflation [arXiv:0706.2298]
- Algebraic Multigrid [M. Clark’s talk and Brannick et al arXiv:0707.4018]
- Produce eigenvectors during the solution of the linear system
- EigCG algorithm [Stathopoulos and KO arXiv:0707.0131]
Eigenvectors and Deflation

- Krylov linear system solvers and eigensolvers are closely related
- They produced Krylov space \( \{ r, Ar, \cdots A^n r \} \)
- Has overlap with extremal eigenvector space

GMRES \( \leftrightarrow \) Arnoldi

CG \( \leftrightarrow \) Lanczos
Conjugate Gradient and Lanczos

\[ k = 0; x_0 = 0; r_0 = b \]

**while** \( r_k \neq 0 \)

\[ k = k + 1 \]

**if** \( (k = 1) \)

\[ p_1 = r_0 \]

**else**

\[ \beta_k = \frac{r_{k-1}^\dagger r_{k-1}}{r_{k-2}^\dagger r_{k-2}} \]

\[ p_k = r_{k-1} + \beta_k p_{k-1} \]

**end**

\[ \alpha_k = \frac{r_{k-1}^\dagger r_{k-1}}{p_{k-1}^\dagger A p_k} \]

\[ x_k = x_{k-1} + \alpha_k p_k \]

\[ r_k = r_{k-1} - \alpha_k A p_k \]

**end**

\[ x = x_k \]

- Let \( A \) be a positive definite hermitian matrix
- Conjugate gradient produces a set of residual vectors \( r_k \) that are proportional to the Lanczos vectors \( r \)
- In the basis of the Lanczos vectors is \( A \) tri-diagonal
- Let \( T_k \) be the Lanczos tri-diagonal matrix at iteration step \( k \)
- The eigenvalues of \( T_k \) are approximations to the extremal eigenvalues of \( A \) (modulo precision issues)
- Eigenvectors can be constructed if the Lanczos vectors are stored.
The Lanczos Matrix

\[ T_m = \begin{bmatrix}
\frac{1}{\alpha_0} & \sqrt{\beta_0}/\alpha_0 \\
\sqrt{\beta_0}/\alpha_0 & 1/\alpha_1 + \beta_0/\alpha_0 \\
\vdots & \ddots & \ddots & \ddots \\
\sqrt{\beta_{m-2}}/\alpha_{m-2} & 1/\alpha_{m-1} + \beta_{m-2}/\alpha_{m-2}
\end{bmatrix}. \]

- Takes no effort to build during the conjugate gradient algorithm
- But we cannot really get eigenvectors this way
- Need to store all the residuals \( r_k \). This is impractical
- Finite precision introduces stability issues
The eigCG algorithm

Basic goals:

- Let CG do its job in solving the system
- Slowly accumulated few low eigenvectors of our matrix $A$ by interrupting CG without restarting it
- Use a “recurrence” relation that improves eigenvector convergence
- Use limited memory i.e. do not store all residual vectors that CG produces
The eigCG algorithm (\(N_{ev}, m\))

\[
k = 0; j = 0; x_0 = 0; r_0 = b
\]

while \(r_k \neq 0\)

\[
k = k + 1
\]

if \((k = 1)\)

\[
p_1 = r_0
\]

else

\[
\beta_k = \frac{r_{k-1}^\dagger r_{k-1}}{r_{k-2}^\dagger r_{k-2}}
\]

\[
p_k = r_{k-1} + \beta_k p_{k-1}
\]

end

\[
\alpha_k = \frac{r_{k-1}^\dagger r_{k-1}}{p_k^\dagger A p_k}
\]

\[
x_k = x_{k-1} + \alpha_k p_k
\]

\[
r_k = r_{k-1} - \alpha_k A p_k
\]

end

\[x = x_k\]
The eigCG algorithm

- Iterate the CG algorithm
- Save the residual vectors and fill in the tridiagonal matrix
- When max number of vectors reached: Diagonalize
- Keep only few low eigenpairs
- Continue the CG filling in the tridiagonal matrix and saving the new residual vectors

\[ N_{ev} = 2 \quad m = 9 \]
The init-CG (deflation)

$r = b - Ax$

$x_1 = x + \sum_{j=1}^{N_{ev}} \frac{e_j^\dagger r}{\lambda_j} e_j$

- $x_1$ is now the starting solution of the subsequent CG
- It is the optimal solution in the subspace of $N_{ev}$ (approximate) eigenvectors
- Needs one matvec operation and $N_{ev}$ dot products
- Cost is negligible compared to full CG solve for reasonable number of eigenvectors
The Incremental eigCG

For the first $s_1$ right hand sides do:

$$U = \lfloor \rfloor, \Lambda = \lfloor \rfloor$$  // accumulated eigenpairs
for $i = 1 : s_1$
$$x_0 = U \Lambda^{-1} U^\dagger b_i$$  // for $s_1$ initial rhs
$$[x_i, V, M] = \text{eigCG}(N_{ev}, m, A, x_0, b_i)$$  // the init-CG part
$$[U, \Lambda] = \text{RayleighRitz}([U, V]);$$  // eigCG with initial guess $x_0$
end

- Most of the cost is in Rayleigh-Ritz
- Needs $N_{ev}$ MatVec operations and several dot products
- Ultimate size of $U$ is determined by how much cost you can amortize for a given number of right hand sides
- Lots of the flops can be done efficiently using level 3 BLAS
Descriptions of the test cases

- Dynamical Wilson fermions ($N_f=2$)
- Anisotropic lattice ($a_s \sim 0.108\text{fm}, a_t \sim 1/3 a_s$)
- Dynamical pion mass $\sim 400(36)\text{MeV}$
- Two volumes: $16^3 \times 64$ and $24^3 \times 64$
  - Degrees of freedom: $N=3 \times 10^6$ and $N=10 \times 10^6$
- Critical mass: $-0.4188$
- Range of masses tested ($m_{\text{crit}} --- -0.4000$)
Results for QCD

$N_{ev}=10$, $m=100$

- **Valence Quark mass equals to sea quark mass**
Results for QCD

Convergence of 48 successive linear systems
Incremental eigCG on the first 24, then Init–CG with restarting at 2.5e−5

Case: $16^3 \times 64$. Mass = −0.4000

Convergence of 48 successive linear systems
Incremental eigCG on the first 24, then Init–CG with restarting at 5e−5

Case: $24^3 \times 64$. Mass = −0.4000

$N_{ev}=10$, $m=100$
Results for QCD

$N_{ev}=10, \ m=100$

Convergence of 48 successive linear systems
Incremental eigCG on the first 24, then Init–CG with restarting at $2.5\times10^{-5}$

Case: $16^3\times64$. Mass = $-0.4200$

Convergence of 48 successive linear systems
Incremental eigCG on the first 24, then Init–CG with restarting at $5\times10^{-5}$

Case: $24^3\times64$. Mass = $-0.4180$
Critical slowing down (or lack off)

For sufficiently large number of right hand sides:

- Small volume factor of 8 speed up at \( m_{\text{sea}} = m_{\text{val}} \)
- Large volume factor of 6 speed up at \( m_{\text{sea}} = m_{\text{val}} \)
Conclusions

- Observables related to Hadronic interactions are now being computed
  - Meson-Meson sector: Precision results already exist
  - Baryon sector: A lot needs to be done...

- New algorithms are needed for calculation of observables
  - The eigCG/Incremental CG algorithm seems to be a viable way to treat the multiple right hand sides problem for QCD [Bean, Detmold, Savage] (theory)  
  - Multi-particle systems: n-Bosons in a box
    - $\Delta E$ up to $O(1/L^6)$ [Stathopoulis, KO]  
  - Petaflop computing is around the corner
    - Precision will be reached in the baryon sector
    - Will takes us long ways in understanding the nuclear force

arXiv:0707.031 [Stathopoulis, KO]
arXiv:0710.1827: NPLQCD (results for up to 5 pions)