INTERACTIONS OF LIGHT NUCLEI FROM LATTICE QCD

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MIT

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THE INTENSITY FRONTIER

- Seek new physics through quantum effects
- Precise experiments
  - Sensitivity to probe the rarest interactions of the SM
  - Look for effects where there is no SM contribution
- Major component is nuclear targets
- Important focus of HEP/NP experimental program
  - Neutrino physics
  - Dark matter direct detection
  - Charged lepton flavour violation, EDMs, $\beta\beta$-decay,
LONG BASELINE NEUTRINO EXPERIMENTS

- Deep Underground Neutrino Experiment
  - Flagship facility for US HEP for next decades
  - Determine neutrino mass hierarchy and extract mixing parameters
- Neutrino scattering on argon target
  - Need fluxes/energies to high accuracy
  - Need to know interactions with argon over a wide range of energies
NUCLEI IN NEW PHYSICS

- Scalar currents
  - Dark matter direct detection
  - Lepton flavour violation: $\mu 2e$
  - Precision spectroscopy
- Tensor currents
  - Electric dipole moments of neutrons and nuclei
- Neutrinoless double beta decay
NUCLEAR UNCERTAINTIES

- How well do we know nuclear matrix elements?
- Gamow-Teller transitions in nuclei
  - Well measured for large range of nuclei (30<A<60)
  - Many nuclear structure calculations (shell-model,...) describe spectrum well
  - Matrix elements systematically off by 20-30%
  - “Correct” by “quenching” axial charge in nuclei ...
- Need a more fundamental understanding

Gamow-Teller amplitude


Points correspond to different nuclei
INTENSITY FRONTIER

PRECISION NUCLEAR PHYSICS

- Very challenging to explore all of NP from QCD
- Exploit effective degrees of freedom
- Establish quantitative control through linkages between different methods
  - QCD forms a foundation determines few body interactions & matrix elements
  - Match existing EFT and many body techniques onto QCD

Exact many body: GFMC, NCSM, lattice EFT
Shell model, coupled cluster, configuration interaction
Density Functional, Mean field
**QUANTITATIVE QCD**

- QCD is the “strong force”
- Interaction strength depends on energy
- At high energy, can use perturbative expansion

\[
\mathcal{O}_{\text{exact}} = \mathcal{O}_0 + \mathcal{O}_1 \alpha_s + \mathcal{O}_2 \alpha_s^2 + \ldots
\]

(also works beautifully in QED)

- At low energies/ long distances need another approach

\[
\alpha_s(Q) = 0.1184 \pm 0.0007
\]

April 2012
LATTICE QCD

- Strong coupling definition of QCD
- Numerical tool for nonperturbative QCD calculations
  - Discretise and compactify spacetime
  - Requires integration over $10^{12}$ degrees of freedom in current calculations!
- Major algorithmic and computational challenge
- Solve using importance sampling Monte Carlo
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HADRONS AND NUCLEI

HADRON MASSES

- Numerical LQCD entering precision era
- What is the mass of the proton?
- After 30 years, we calculated it
  \[ M_p = 936(25)(22) \text{ MeV} \]
  Cost: \(10^{21}\) floating point operations

- QCD is the theory of nonperturbative strong interactions

[Dürr et al, Science 322, 1224 (2008)]
HEAVY HADRONS

- QCD works for the proton mass
- Predictions for masses of baryons containing bottom/charm quarks
  - Test in experiment
QCD works for the proton mass

Predictions for masses of baryons containing bottom/charm quarks

Test in experiment
HADRONS AND NUCLEI

PROTON FEMTOGRAPHY

- LQCD also used to calculate the internal structure of hadrons
  - EM and weak probes
  - Partonic structure
- Pressure and shear distributions
  - Fundamental components of stress-energy tensor
- Experimental quark contributions
  [Burkert et al, Nature 2018]
- LQCD calculation of gluon contributions
  ➞ First complete determination

[Shanahan, WD, PRL 2019]
QCD FOR NUCLEAR PHYSICS

- Nuclear physics is Standard Model physics
  - Can compute the mass of lead nucleus ... in principle

- Complex physics
  - Wide range of scales
  - Closely spaced excitations

- Numerical challenges:
  - Statistical sampling
  - Contraction complexity
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New algorithms enabling study of nuclei

Efficient contractions

Graph theory & recursions
[WD & Savage 2011; WD & Orginos 2012, Doi & Endres 2012; WD & Vachaspati 2014]

Signal-to-noise optimisation
[WD & Endres PRD 2014]

Better statistical estimators
[Wagman & Savage 2016; WD, Kanwar & Wagman 2018]

Machine learning for QFT
[Shanahan, Trewartha & WD 2018, Albergo et al. 2019]

... and lots of computing!

\[
\frac{\text{cost}(N A Z)}{\text{cost(proton)}} \sim (2Z + N)! (2N + Z)! / 2
\]

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Naive</th>
<th>Optimised</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^4\text{He})</td>
<td>250,000</td>
<td>~100</td>
</tr>
<tr>
<td>(^8\text{Be})</td>
<td>(10^{31})</td>
<td>(10^7)</td>
</tr>
<tr>
<td>(^{208}\text{Pb})</td>
<td>(10^{1300})</td>
<td>?</td>
</tr>
</tbody>
</table>
CASE STUDY: NUCLEI IN LQCD

NPLQCD: UNPHYSICAL NUCLEI

- Case study QCD with unphysical quark masses ($m_\pi \sim 800$ MeV, 450 MeV)

1. Spectrum and scattering of light nuclei ($A<5$) [PRD 87 (2013), 034506]


3. Nuclear reactions: $np \rightarrow d\gamma$ [PRL 115, 132001 (2015)]

4. Gamow-Teller transitions: $pp \rightarrow d\nu e$, $g_A(3H)$ [PRL 119 062002 (2017)]

5. Double $\beta$ decay: $pp \rightarrow nn$ [PRL 119, 062003 (2017)]

6. Gluon structure ($A<4$) [PRD 96 094512 (2017)]

7. Scalar/tensor currents ($A<4$) [PRL 2018]
HADRONS AND NUCLEI

NUCLEI (IN A HEAVY QUARK UNIVERSE, $M_\pi \sim 800$ MEV)

- 2013: first QCD calculation of nuclei (heavy masses as numerically cheaper)

<table>
<thead>
<tr>
<th>A</th>
<th>Nuclei</th>
<th>B [MeV]</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$H$, $n\Sigma(3/2)$, $d$, $nn$</td>
<td>0</td>
</tr>
<tr>
<td>3</td>
<td>$^3$He, $^3$H, $^\Lambda$He, $^\Lambda$He</td>
<td>-50</td>
</tr>
<tr>
<td>4</td>
<td>$^4$He, $^4$He, $^4$He</td>
<td>-100</td>
</tr>
<tr>
<td>5</td>
<td>$^5$He</td>
<td>-150</td>
</tr>
</tbody>
</table>

[NPLQCD collaboration, PRD 2013]
Combine LQCD and nucleon based many-body effective field theory (EFT) methods

Matching to LQCD determines NN, NNN interactions: allows predictions for larger nuclei

Further studies extend to complex nuclei such as $^{16}\text{O}$ [Contessi et al, Bansal et al.]

**NUCLEI (IN A HEAVY QUARK UNIVERSE, $M_\pi \sim 800$ MEV)**
NUCLEAR STRUCTURE

MAGNETIC STRUCTURE

- Hadron/nuclear energies are modified by presence of fixed external fields

- Eg: fixed B field

\[ E_{h;jz}(B) = \sqrt{M_h^2 + (2n + 1)|Q_{he}B| - \mu_h \cdot B - 2\pi \beta_0^{(M0)} |B|^2} + \ldots \]

- QCD calculations with multiple fields enable extraction of coefficients of response
  - Magnetic moments, polarisabilities, …
  - Not restricted to simple EM fields

[NPLQCD PRL 2014, PRD 2014]
MAGNETIC STRUCTURE

- LQCD calculation of nuclear magnetic moments ($\mu$) and magnetic polarisabilities ($\beta$, deformation in B field)
- Simple shell model expectations
- Lattice results suggest heavy quark mass nuclei are shell-model like!
One nucleon coupling dominates
- Determine from nucleon matrix element calculations

Two nucleon contributions are sub-leading
- Study A=2,3,4,.. systems
- Determine nuclear effects

Example: 30% quenching of axial charge of medium mass nuclei relative to the proton
BIG BANG NUCLEOSYNTHESIS

- Light nuclei are formed during the initial few minutes after the Big Bang
- First nuclear reaction: slow neutron capture $np \rightarrow d\gamma$
  - 2015: First QCD calculation of a nuclear reaction
    - Reproduced measured rate
    - Ready to make predictions
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[NPLQCD, PRL 2015]
ELECTROWEAK PROCESSES

- Single $\beta$-decay
  2017: LQCD calculate of decay of tritium

- Double $\beta$-decay
  - Neutrinoful case is rarest process observed
  - Neutrinoless case
    - Majorana particles? Lepton number violation? Baryon asymmetry?
  - Rates depend on nuclear matrix elements
    - Currently quite uncertain
    - Important for design of future DBD search experiments
**PROTON–PROTON FUSION**

- First step in chain of reactions powering stars like the sun
- Intricate process involve all three SM forces
- Difficult to measure (Coulomb barrier)
- 2017: LQCD calculation of $pp$ fusion rate
  - Uncertainties competitive with phenomenological extractions
  - Next generation calculations will improve precision
    - Improve solar modelling
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DOUBLE BETA DECAY

- QCD calculation of subprocess
  \[ nn \rightarrow ppe^{-}e^{+}\bar{\nu}\nu \]
  [NPLQCD, PRL 2017b]
  - Revealed significant nuclear effects (even beyond \( g_{A} \) quenching)

- Beginning calculations of neutrinoless processes
  [WD, Murphy 1811.0554]
  - Disallowed pion transition as a test
    \[ \pi^{-} \rightarrow \pi^{+}e^{-}e^{-} \]
  - Light nuclei are next
DM direct detection experiments search for recoil of nucleus from DM scattering

One popular class of DM interactions is through scalar exchange

$$\mathcal{L} = \frac{G_F}{2} \sum_q \kappa_q (\bar{\chi} \chi)(\bar{q} q)$$

Direct detection depends on nuclear matrix element

$$\overline{m} \langle Z, N|\bar{u}u + \bar{d}d|Z, N \rangle$$

At hadronic/nuclear level
**INTENSITY FRONTIER**

**NUCLEON SCALAR COUPLING**

- Single nucleon contribution
- Calculated in LQCD
- Results from many groups

Summary from Shanahan 2016
NUCLEAR EFFECTS CAN BE BIG!

- LQCD study of scalar couplings for $A=1,2,3$
- Unexpectedly large ($\sim 10\%$) deviation from sum of nucleon matrix elements for $A=3$
- Naive extrapolation to $^{136}\text{Xe}$ implies significant consequences for dark matter detection sensitivity
GLUONIC STRUCTURE

- EMC effect: nuclear modification of partonic structure
- Access in LQCD by Mellin moments
  - Second moment of unpolarised gluon PDF (longitudinal momentum frac. carried by gluons)
    \[ \overline{O}_{\mu \nu} = G_{\mu \alpha} G^{\alpha}_{\nu} \]
  - Also additional leading twist gluon transversely PDF
- Calculate from ratio:
  \[ \frac{C^{(h)}_{\overline{O}}(t, \tau)}{C^{(h)}_{2}(t)} \propto \langle h | \overline{O}_{\mu \nu} | h \rangle \quad 0 \ll \tau \ll t \]
NUCLEAR STRUCTURE

GLUON STRUCTURE

- Statistically challenging!!
  - Consider many boosts and $H_4$ operator irreps
- Extract bare ME in $p$, $d$, $nn$, $^3$He
  - Fit $t$, $\tau$ dependence
- Mixes with singlet quark operator

\[
\overline{O}^{(E)} = Z^{gg} \overline{O}^{\text{ren.}} + Z^{qq} \overline{Q}^{\text{ren}}
\]

\[
\overline{Q}^{(E)}_{\mu_1 \mu_2} = \sum_{f = \{u,d,s\}} S \left[ \overline{\psi}_f \gamma_{\mu_1} \slashed{D}_{\mu_2} \psi_f \right]
\]

but \[ Z^{qq} = z_1 \alpha_s + \ldots \]
GLUON STRUCTURE

- Ratio of matrix elements in different hadrons almost scale and scheme independent

\[
\frac{\langle h| \mathcal{O}^{(E)} | h \rangle}{\langle N| \mathcal{O}^{(E)} | N \rangle} \approx \frac{\langle h| \mathcal{O}^{\text{ren}} | h \rangle}{\langle N| \mathcal{O}^{\text{ren}} | N \rangle} \left( 1 + \frac{Z^{gg}}{Z^{gg}} \left[ \frac{\langle h| \mathcal{Q}^{\text{ren}} | h \rangle}{\langle h| \mathcal{O}^{\text{ren}} | h \rangle} - \frac{\langle N| \mathcal{Q}^{\text{ren}} | N \rangle}{\langle N| \mathcal{O}^{\text{ren}} | N \rangle} \right] \right)
\]

- Gluonic EMC-like effect constrained to be <10-20%
Nuclei are under study directly from QCD

- Spectroscopy of light nuclei and exotic nuclei
- Structure: magnetic moments, parton structure
- Interactions: \( np \rightarrow d\gamma, \ pp \rightarrow d\ell+\nu, \ nn \rightarrow pp, \ DM \)

Prospect of a quantitative connection to QCD makes this an exciting time for nuclear physics

- Critical role in current and upcoming intensity frontier experimental program
- Exponential improvements needed for larger nuclei: machine learning
signal $\sim \langle C \rangle \sim \exp[-M_p t]$
Importance sampling of QCD functional integrals

- correlators determined stochastically

Proton

\[
\text{signal} \sim \langle C \rangle \sim \exp[-M_p t]
\]
STRICTED SAMPLING

- Importance sampling of QCD functional integrals
  - Correlators determined stochastically
- Proton
  - Signal: \( \langle C \rangle \sim \exp[-Mt] \)
  - Variance determined by:
    \[
    \sigma^2(C) = \langle CC^\dagger \rangle - |\langle C \rangle|^2
    \]
LQCD FOR NUCLEI

STATISTICAL SAMPLING

- Importance sampling of QCD functional integrals
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[Parisi 84, Lepage '89]
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- Proton
  
  \[
  \text{signal} \sim \langle C \rangle \sim \exp[-M_p t]
  \]
  
  \[
  \text{noise} \sim \sqrt{\langle CC^\dagger \rangle} \sim \exp[-3/2m_\pi t]
  \]
  
  \[
  \frac{\text{signal}}{\text{noise}} \sim \exp[-(M_p - 3/2m_\pi)t]
  \]

[Parisi 84, Lepage '89]
LQCD FOR NUCLEI

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  \]

- Signal to noise
  
  \[
  \frac{\text{signal}}{\text{noise}} \sim \exp[-(M_p - 3/2m_\pi) t]
  \]

- For nucleus A:
  
  \[
  \frac{\text{signal}}{\text{noise}} \sim \exp[-A(M_p - 3/2m_\pi) t]
  \]

[Parisi 84, Lepage '89]
CONTRACTIONS

- Quarks need to be tied together in all possible ways
  - \( N_{\text{contractions}} = N_u!N_d!N_s! \) (eg \( 10^{1500} \) for \(^{208}\text{Pb}\))

- Managed using algorithmic trickery [WD & Savage, WD & Orginos; Doi & Endres, Günther et al]
  - Study up to \( N=72 \) pion systems, \( A=5 \) (and 28) nuclei
**NUCLEAR SPECTROSCOPY**

**NN BOUND STATES**

- Potential for fake plateaus? [Iritani et al.]
  - Scattering states combine with relative signs to give negative-shifted flat behaviour
  - Very unlikely
- Study at 3 volumes with same source structure
- Negative shifted states
  - Correlators fully consistent at L=24, 32, 48
- Excited state
  - Scales as 1/L^3 consistent with scattering state
Thermal neutron capture cross-section: $np \rightarrow d\gamma$

- Critical process in Big Bang Nucleosynthesis
- Historically important: 2-body contributions $\sim 10$
- First QCD nuclear reaction!
NP→Dγ IN PIONLESS EFT

- Cross-section at threshold calculated in pionless EFT
  \[ \sigma(np \rightarrow d\gamma) = \frac{e^2(\gamma_0^2 + |p|^2)^3}{M^4\gamma_0^3|p|} |\tilde{X}_{M1}|^2 + ... \]

- EFT expansion at LO given by mag. moments
  NLO contributions from short-distance two nucleon operators
  \[ \tilde{X}_{M1} = \frac{Z_d}{-\frac{1}{a_1} + \frac{1}{2}r_1|p|^2 - i|p|} \times \left[ \frac{\kappa_1\gamma_0^2}{\gamma_0^2 + |p|^2} \left( \gamma_0 - \frac{1}{a_1} + \frac{1}{2}r_1|p|^2 \right) + \frac{\gamma_0^2}{2}l_1 \right] \]

- Phenomenological description with 1% accuracy for E< 1MeV
  - Short distance (MEC) contributes ~10%

\[ Z_d = 1/\sqrt{1 - \gamma_0r_3} \]

**MECs:**
Consider QCD in the presence of a constant background magnetic field

Implement by adding term to the action (careful with boundaries)

Shifts spin-1/2 particle masses

\[ M_{\uparrow\downarrow} = M_0 \pm \mu |B| + 4\pi \beta |B|^2 + \ldots \]

Changing strength of background field allows \( \mu, \beta \) to be extracted

Two nucleon states

Levels split and mix

Similar for electro-weak fields and twist-two fields
ENERGY LEVELS IN BF

- Background field modifies eigenvalue equation for $m=\pm 1$ states

\[ p \cot \delta(p) - \frac{1}{\pi L} S \left( \frac{L^2}{4\pi^2} \left[ p^2 \pm e|B|\kappa_0 \right] \right) = \frac{e|B|}{2} (L_2 - r_3\kappa_0) = 0 \]

- Asymptotic expansion of lowest scattering level

\[ E_0^{m=\pm 1} = \pm \frac{e|B|\kappa_0}{M} + \frac{4\pi A_3}{ML^3} \left[ 1 - c_1 \frac{A_3}{L} + c_2 \left( \frac{A_3}{L} \right)^2 + \ldots \right] \]

where \[ \frac{1}{A_3} = \frac{1}{a_3} \pm \frac{e|B|L_2}{2} \]

- Mixes $^1S_0$ and $^3S_1$ $m=0$ states (coupled channels - but perturbative)

\[ \left[ p \cot \delta_1(p) - \frac{S_+ + S_-}{\pi L} \right] \left[ p \cot \delta_3(p) - \frac{S_+ + S_-}{\pi L} \right] = \left[ \frac{e|B|L_1}{2} + \frac{S_+ - S_-}{2\pi L} \right]^2 \]

where \[ S_\pm = S \left( \frac{L^2}{4\pi^2} \left[ p^2 \pm e|B|\kappa_1 \right] + \ldots \right) \]

[WD & MJ Savage Nucl Phys A 743, 170]
NUCLEAR INTERACTIONS

NP $\rightarrow$ Dγ

- Presence of magnetic field mixes $I_z=J_z=0$ $^3S_1$ and $^1S_0$ np systems

- Wigner SU(4) super-multiplet (spin-flavour) symmetry relates $^3S_1$ and $^1S_0$ states (diagonal elements approximately equal)
  - Shift of eigenvalues determined by transition amplitude
    \[
    \Delta E_{^3S_1,^1S_0} = \mp (\kappa_1 + \bar{L}_1) \frac{eB}{M} + \ldots
    \]
  - More generally eigenvalues depend on transition amplitude

[NPLQCD PRL 115, 1320031 (2015)]
\[ \text{NP} \rightarrow D \gamma \]

- \( L_z = J_z = 0 \) correlation matrix

\[
\mathbf{C}(t; \mathbf{B}) = \begin{pmatrix}
C_{3S_1,3S_1}(t; \mathbf{B}) & C_{3S_1,1S_0}(t; \mathbf{B}) \\
C_{1S_0,3S_1}(t; \mathbf{B}) & C_{1S_0,1S_0}(t; \mathbf{B})
\end{pmatrix}
\]

- Generalised eigenvalue problem

\[
[\mathbf{C}(t_0; \mathbf{B})]^{-1/2} \mathbf{C}(t; \mathbf{B}) [\mathbf{C}(t_0; \mathbf{B})]^{-1/2} \nu = \lambda(t; \mathbf{B}) \nu
\]

- Ratio of correlator ratios to extract 2-body

\[
R_{3S_1,1S_0}(t; \mathbf{B}) = \frac{\lambda_+(t; \mathbf{B})}{\lambda_-(t; \mathbf{B})} \xrightarrow{t \to \infty} \hat{Z} \exp \left[ 2 \Delta E_{3S_1,1S_0} t \right]
\]

\[
\delta R_{3S_1,1S_0}(t; \mathbf{B}) = \frac{R_{3S_1,1S_0}(t; \mathbf{B})}{\Delta R_p(t; \mathbf{B})/\Delta R_n(t; \mathbf{B})} \rightarrow A \ e^{-\delta E_{3S_1,1S_0}(\mathbf{B}) t}
\]

\[
\delta E_{3S_1,1S_0} \equiv \Delta E_{3S_1,1S_0} - \left[ E_{p,\uparrow} - E_{p,\downarrow} \right] + \left[ E_{n,\uparrow} - E_{n,\downarrow} \right]
\rightarrow 2L_1|e\mathbf{B}|/M + \mathcal{O}(\mathbf{B}^2)
\]
Correlator ratios for different field strengths

- $m_\pi = 450$ MeV
- $m_\pi = 800$ MeV

Field strength & mass dependence

Slopes give $\Gamma_I$
NUCLEAR INTERACTIONS

[NPLQCD PRL 115, 1320031 (2015)]

NP $\rightarrow$ Dɣ

- Extracted short-distance contribution at physical mass

$$\bar{L}_{1}^{\text{lqcd}} = 0.285 (^{+0.63}_{-0.00}) \text{ nNM}$$

$$l_{1}^{\text{lqcd}} = -4.48 (^{+0.16}_{-0.15}) \text{ fm}$$

- Combine with phenomenological nucleon magnetic moment, scattering parameters at incident neutron velocity $v=2,200 \text{ m/s}$

$$\sigma^{\text{lqcd}}(np \rightarrow d\gamma) = 307.8 (1 + 0.273 \bar{L}_{1}^{\text{lqcd}}) \text{ mb}$$

$$\sigma^{\text{lqcd}}(np \rightarrow d\gamma) = 332.4 (^{+5.4}_{-4.7}) \text{ mb}$$

c.f. phenomenological value

$$\sigma^{\text{expt}}(np \rightarrow d\gamma) = 334.2 (0.5) \text{ mb}$$

- NB: at $m_\pi=800 \text{ MeV}$, use LQCD for all inputs (ab initio)

$$\sigma^{800 \text{ MeV}}(np \rightarrow d\gamma) \sim 10 \text{ mb}$$