A Non-Empirical Approach to The Nuclear Shell Model Jason D. Holt

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Drip Lines and Magic Numbers: The Evolving Nuclear Landscape

Physics of exotic nuclei – era of coming decades

What are the limits of nuclear existence?

How do magic numbers form and evolve?

N=54 magic number in calcium?







Approaches to Nuclear Structure

"The first, the basic approach, is to study the elementary particles, their properties and mutual interaction. Thus one hopes to obtain knowledge of the nuclear forces. If the forces are known, one should, in principle, be able to calculate deductively the properties of individual nuclei. Only after this has been accomplished can one say that one completely understands nuclear structure...

The other approach is that of the experimentalist and consists in obtaining by direct experimentation as many data as possible for individual nuclei. One hopes in this way to find regularities and correlations which give a clue to the structure of the nucleus...The shell model, although proposed by theoreticians, really corresponds to the experimentalist's approach."

-M. Goeppert-Mayer, Nobel Lecture

Purpose of these lectures is to show how shell model can be based on the first approach!

To understand the properties of complex nuclei from fundamental interactions



To understand the properties of complex nuclei from elementary interactions



Two significant issues:

Interaction

Not well understood Not obtainable from QCD Too "hard" to be useful Multiple scales

Many-body Problem Not 'exactly' solvable above A~16 (ab-initio)

Here we focus on shell model

To understand the properties of complex nuclei from elementary interactions



How will we approach this problem:

QCD \rightarrow NN (3N) forces \rightarrow Renormalize \rightarrow Solve many-body problem \rightarrow Predictions

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Interaction Between Two Nucleons

"In the past quarter century physicists have devoted a huge amount of experimentation and mental labor to this problem – probably more manhours than have been given to any other scientific question in the history of mankind."

–H. Bethe

So let's burn a few more man-hours of mental labor on this!

To start, think to yourself what this should look like, and write it down...





Part I: The Nucleon-Nucleon Interaction

To understand the properties of complex nuclei from elementary interactions



How will we approach this problem:

QCD \rightarrow NN (3N) forces \rightarrow Renormalize \rightarrow Solve many-body problem \rightarrow Predictions

Meson-Exchange Potentials: Yukawa

- First field-theoretical model of nucleon interaction proposed by Yukawa 1935
- Pion discovered 1947





$$V(\mathbf{r}) = \Theta_{m_{\pi}^2}^{f_{\pi}^2} \left\{ \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 + C_T \left(1 + \frac{3}{m_{\alpha}r} + \frac{3}{(m_{\alpha}r)^2} \right) S_{12}(\hat{r}) \right\} \left(\frac{e^{-m_{\pi}r}}{m_{\pi}r} \right)$$

• Attractive, long range, spin dependent, non-central (tensor) part

- Successful in explaining scattering data, deuteron
- One pion is good, therefore more pions are better...
- Advanced to multi-pion theories in 1950's FAILED

One-Boson Exchange Potentials

- Heavy mesons discovered in 1950s theories developed based on these
- Intermediate range **attractive central, spin-orbit**

$$\mathbf{v}^{\sigma} = \mathbf{g}_{\sigma NN}^{2} \frac{1}{\mathbf{k}^{2} + m_{\sigma}^{2}} \left(-1 + \frac{\mathbf{q}^{2}}{2M_{N}^{2}} - \frac{\mathbf{k}^{2}}{8M_{N}^{2}} - \frac{\mathbf{LS}}{2M_{N}^{2}} \right)$$
$$\vec{q}_{i} = \vec{p}_{i}^{\prime} - \vec{p}_{i} \quad \vec{k}_{i} = \frac{1}{2} (\vec{p}_{i}^{\prime} + \vec{p}_{i})$$

Baryons	Mass (MeV)	Mesons	Mass (MeV)
p, n	938.926	π	138.03
Λ	1116.0	n	548.8
Σ	1197.3	σ	≈ 550.0
Δ	1232.0	ρ	770
Σ*	1385.0	ω	782.6
		δ	983.0
		К	495.8
		к*	895.0

One-Boson Exchange Potentials

- Heavy mesons discovered in 1950s theories developed based on these
- Short range; repulsive central force, attractive spin-orbit



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One-Boson Exchange Potentials

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- Short range; tensor force opposite sign of pion exchange



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Parameterizing the NN Interaction

Starting from any NN-interaction

We first solve scattering Lipmann-Schwinger scattering T-matrix equation:

$$T^{\alpha}_{ll'}(kk'K) = V^{\alpha}_{ll'}(kk') + \frac{2}{\pi} \sum_{l''} \int_0^\infty dq q^2 V^{\alpha}_{ll''}(kq) \frac{1}{k^2 - q^2 + i\epsilon} T^{\alpha}_{l''l'}(qk'K).$$

Where

$$T^{\alpha}_{ll'}(k,k';K) = \left\langle kK, lL; JST \middle| T \middle| k'K, l'L; JST \right\rangle$$

Parameterized in partial waves(α) – in relative / center of mass frame (K,L)

 $\tan\delta(p) = -pT(p,p)$

Fully-on-shell *T*-matrix directly related to experimental data

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Note intermediate momentum allowed to infinity (but cutoff by regulators) **Coupling of low-to-high momentum in** V

Constraining NN Scattering Phase Shifts

Phase shift is a function of relative momentum *k*; Figure shows *s*-wave Scattering from an attractive well potential



Scattering from repulsive core: phase shift opposite sign



Textbook nuclear potentials in **r**-space



Textbook nuclear potentials in **r**-space

Hard core, intermediate-range 2π -, long-range 1π exchange (OPE)



Textbook nuclear potentials in **r**-space

- Hard core, intermediate-range 2π , long-range 1π exchange Transform to momentum space via Fourier-Bessel Transformation

- Strong high-momentum repulsion, low-momentum attraction



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NN Interaction from QCD

Meson exchange described in QCD

Low-energy region non-perturbative – treat in the context of Lattice QCD Directly from QCD Lagrangian, solve numerically on discretized space-time



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Meson exchange described in QCD

Low-energy region non-perturbative – treat in the context of Lattice QCD Directly from QCD Lagrangian, solve numerically on discretized space-time



Lattice results give long-range OPE tail, hard core Not yet to physical pion mass – work in progress – so we're done, right?

Unique NN Potential?

What does this tell us in our quest for an NN-potential?

Expected form seems to be confirmed by QCD



OBE Potentials: Summary/Problems

First generation (1960-1990): Paris, Reid, Bonn-A,B,C $\chi^2/dof \approx 2$

High precision potentials (1990s): ~40 parameters fit to NN data $\chi^2/\text{dof} \approx 1$

ArgonneV18, Reid93, Nijmegen, CD-Bonn

NN problem "solved" !!

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- 1) Difficult (impossible) to assign theoretical error
- 2) 3N forces not consistent with NN forces
- 3) No clear connection to QCD
- 4) Clear model dependence...

Meson-Exchange Potentials and Phase Shifts

Examples of phase shift reproduction by NN potentials



Meson-Exchange Potentials and Phase Shifts

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Meson-Exchange Potentials and Phase Shifts

More model dependence: examples of phase shift reproduction by NN potentials



Agree well up to **pion-production threshold** ~350MeV Data sparse – most models don't fit above this point - **unconstrained**

From QCD to Nuclear Interactions

How do we determine interactions between nucleons?

$$H(\Lambda) = T + V_{\rm NN}(\Lambda) + V_{\rm 3N}(\Lambda) + V_{\rm 4N}(\Lambda) + \dots$$



Old view:

Multiple scales complicate life No meaningful way to connect them

Modern view:

Ratio of scales – small parameters Effective field theory at each scale connected by RG

Choose convenient resolution scale

Resolution scales



High energy probe resolves fine details

Need high-energy degrees of freedom

How do we determine interactions between nucleons?



Low-energy probe doesn't resolve such details

Don't need high-energy degrees of freedom – replace with something simpler **Use dof that are more convenient**, but preserve low-energy observables

Underlying theory with cutoff Λ_{∞} $V = V_L + V_S$

Known **long-distance physics** (like 1π -exchange) with some scale M_L

Short-distance physics (ρ, ω -exchange) with some scale M_S



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Say we want a **low-energy** *effective* theory describing physics up to some $M_L < \Lambda < M_S$

Integrate out states above Λ using **Renormalization Group (RG)**

General form of effective theory: $V_{eff} = V_L + \delta V_{c.t.}(\Lambda)$

$$\delta V_{c.t.}(\Lambda) = C_0(\Lambda)\delta^3(\vec{r}) + C_2(\Lambda)\nabla^2\delta^3(\vec{r}) + \cdots$$

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$$\delta V_{c.t.}(\Lambda) = C_0(\Lambda)\delta^3(\vec{r}) + C_2(\Lambda)\nabla^2\delta^3(\vec{r}) + \cdots$$

Encodes effects of high-E dof on low-energy observables Universal; depends only on symmetries

TWO choices:

Short distance structure of "true theory" captured in several numbers

- Calculate from underlying theory

When short-range physics is unknown or too complicated

- Extract from low-energy data

How do we apply these ideas to nuclear physics?

Chiral Effective Field Theory: Philosophy

"At each scale we have different degrees of freedom and different dynamics. Physics at a larger scale (largely) decouples from physics at a smaller scale... thus a theory at a larger scale remembers only finitely many parameters from the theories at smaller scales, and throws the rest of the details away.

More precisely, when we pass from a smaller scale to a larger scale, we average out irrelevant degrees of freedom... The general aim of the RG method is to explain how this decoupling takes place and why exactly information is transmitted from one scale to another through finitely many parameters." - *David Gross*

"The method in its most general form can.. be understood as a way to arrange in various theories that the degrees of freedom that you're talking about are the relevant degrees of freedom for the problem at hand." - *Steven Weinberg*

5 Steps to constructing the theory

Separation of Scales in Nuclear Physics

Step I: Identify appropriate separation of scales, degrees of freedom



Chiral EFT Symmetries

Step II: Identify relevant symmetries of underlying theory QCD

- SU(3) color symmetry from QCD (Nucleons and pions are color singlets)
- 2. Chiral symmetry: u and d quarks are almost massless
 - Left and right-handed (massless) quarks do not mix: SU(2)_L x SU(2)_R symmetry
 - Explicit symmetry breaking: u and d quarks have a small mass
 - Spontaneous breaking of chiral symmetry (no parity doublets observed in Nature)
 - SU(2)_L x SU(2)_R symmetry spontaneously broken to SU(2)_V
 - Pions are the Nambu-Goldstone bosons of spontaneously broken symmetry
 - Low-energy pion Lagrangian completely determined

Construct Lagrangian based on these symmetries

$$\mathcal{L}_{\rm eff} = \mathcal{L}_{\pi\pi} + \mathcal{L}_{N\pi} + \mathcal{L}_{NN}$$

Chiral EFT Lagrangian

Step III: Construct Lagrangian based on identified symmetries

Pion-pion Lagrangian: U is SU(2) matrix parameterized by three pion fields $\mathcal{L}_{\pi}^{(0)} = \frac{F^2}{4} \langle \nabla^{\mu} U \nabla_{\mu} U^{\dagger} + \chi_{+} \rangle,$

Leading-order pion-nucleon

 $\mathcal{L}_{\pi N}^{(0)} = \bar{N}(iv \cdot D + \mathring{g}_A u \cdot S)N,$

Leading-order nucleon-nucleon (encodes unknown short-range physics) $\mathcal{L}_{NN}^{(0)} = -\frac{1}{2}C_{S}(\bar{N}N)(\bar{N}N) + 2C_{T}(\bar{N}SN) \cdot (\bar{N}SN)$

EFT Power Counting

Step IV: Design an organized scheme to distinguish more from less important processes: Power Counting

Organize theory in powers of $\left(\frac{Q}{\Lambda_{\chi}}\right)$ where $Q \sim m_{\pi}$, typical momentum in nucleus

Expansion only valid for small expansion parameter, *i.e.*, low momentum

Irreducible time-ordered diagram has order $\left(\frac{Q}{\Lambda_{v}}\right)^{v}$, where

$$= -4 + 2N + 2L + \sum_{i} V_{i}\Delta_{i} \qquad \Delta_{i} = d_{i} + \frac{1}{2}n_{i} - 2$$
 "Chiral dimension"

N = Number of nucleons

V

L = Number of pion loops

 V_i = Number of vertices of type *i*

d = Number of derivatives or insertions of

n = Number of nucleon field operators m_{π}

Chiral EFT: Lowest Order (LO)

Step V: Calculate Feynmann diagrams to the desired accuracy

Leading order (v = 0)

•----**•**

One-pion exchange

$$V_{NN}^{(0)} = -\frac{g_A^2}{4F_\pi^2} \frac{\vec{\sigma}_1 \cdot \vec{q} \, \vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + M_\pi^2} \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

$$\vec{q}_i \equiv \vec{p}_i' - \vec{p}_i$$

$$g_A = 1.26$$

$$F_\pi = 92.4 \, \text{MeV}$$

Chiral EFT: Lowest Order (LO)

Step V: Calculate Feynmann diagrams to the desired accuracy

Leading order (v = 0)



One-pion exchange NN contact interaction

Two **low-energy constants (LECs)**: C_S, C_T

$$V_{NN}^{(0)} = -\frac{g_A^2}{4F_\pi^2} \frac{\vec{\sigma}_1 \cdot \vec{q} \,\vec{\sigma}_2 \cdot \vec{q}}{\vec{q}^2 + M_\pi^2} \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 + \underbrace{C_S}_{S} + \underbrace{C_T}_{T} \vec{\sigma}_1 \cdot \vec{\sigma}_2$$

 $\vec{q}_i \equiv \vec{p}'_i - \vec{p}_i$ $g_A = 1.26$ $F_\pi = 92.4 \text{ MeV}$

Chiral EFT

Step V: Calculate Feynmann diagrams to the desired accuracy

Question: What will v = 1 look like?

Answer: No contribution at this order

Chiral EFT: NLO

Step V: Calculate Feynmann diagrams to the desired accuracy Next-to-leading order (v = 2)



Higher order contact interaction: 7 new LECs, spin-orbit

 $+ (C_1 \vec{q}^2 + C_2 \vec{k}^2 + (C_3 \vec{q}^2 + C_4 \vec{k}^2) \vec{\sigma}_1 \cdot \vec{\sigma}_2$

$$+iC_{5}\frac{1}{2}(\vec{\sigma}_{1}+\vec{\sigma}_{2})\cdot\vec{q}\times\vec{k}+C_{6}\vec{q}\cdot\vec{\sigma}_{1}\vec{q}\cdot\vec{\sigma}_{2}$$

 $\cdot \vec{\sigma}_1 \vec{k} \cdot \vec{\sigma}_2$

Chiral EFT: N²LO

Step V: Calculate Feynmann diagrams to the desired accuracy

Next-to-next-to-leading order (v = 3)



3 new LECs from $\pi\pi$ NN vertex

$$\begin{split} V_{NN}^{(3)} &= -\frac{3g_A^2}{16\pi F_\pi^4} [2M_\pi^2 2c_1 + c_3 - c_3 \vec{q}^2] \\ &\times (2M_\pi^2 + \vec{q}^2) A^{\tilde{\Lambda}}(q) - \frac{g_A^2 c_4}{32\pi F_\pi^4} \tau_1 \cdot \tau_2 (4M_\pi^2 + q^2) A^{\tilde{\Lambda}}(q) (\vec{\sigma}_1 \cdot \vec{q} \vec{\sigma}_2 \cdot \vec{q} - \vec{q}^2 \vec{\sigma}_1 \cdot \vec{\sigma}_2), \end{split}$$

Chiral EFT: N³LO

Step V: Calculate Feynmann diagrams to the desired accuracy

Next-to-next-to-next-to-leading order ($\nu = 4$)



Higher order contact interaction: 15 new LECs

Regularization of Chiral potentials

Remember: constructing potential involves solving L-S equation All NN potentials cutoff loop momenta at some value > 1GeV Impose exponential regulator, Λ , in Chiral EFT potentials – not in integral

$$\widehat{T}(\vec{p}\,',\vec{p}) = \widehat{V}(\vec{p}\,',\vec{p}) + \int d^3 p''\,\widehat{V}(\vec{p}\,',\vec{p}\,'')\,\frac{M}{p^2 - p''^2 + i\epsilon}\,\widehat{T}(\vec{p}\,'',\vec{p})$$

$$\widehat{V}(\vec{p}',\vec{p}) \longrightarrow \widehat{V}(\vec{p}',\vec{p}) e^{-(p'/\Lambda)^{2n}} e^{-(p/\Lambda)^{2n}}$$

LECs will depend on regularization approach and Λ Infinitely many ways to do this

Infinitely many chiral potentials

Indeed, many on the market – some fit well to phase shifts, others not

Chiral EFT: Resulting fits to Phase shifts

Systematic improvement of chiral EFT potentials fit to phase shifts

Cutoff variation – information about missing physics

NLO: dashed band9 ParametersN²LO: light band12 ParametersN³LO: dark band27 Parameters

Generally decreasing error and increasing accuracy – not entirely...



Chiral Effective Field Theory: Nuclear Forces



Chiral NN Potentials

Two chiral potentials with regulators of 500MeV and 600MeV Still low-to-high momentum coupling: poor convergence, non perturbative, etc.



How do these compare to the potential you drew?

Lesson: Infinitely many phase-shift equivalent potentials $E_n = \langle \Psi_n | H | \Psi_n \rangle = (\langle \Psi_n | U^{\dagger}) U H U^{\dagger} (U | \Psi_n \rangle) = \langle \widetilde{\Psi}_n | \widetilde{H} | \widetilde{\Psi}_n \rangle$

NN interaction not observableLow-to-high momentum makes life difficult for
low-energy nuclear theorists

Part II: RG and Low-Momentum Interactions

To understand the properties of complex nuclei from elementary interactions



Ok, high momentum is a pain. I wonder what would happen to low-energy observables...

Low-to-high momentum makes life difficult for low-energy nuclear theorists

Can we just make a sharp cut and see if it works?



 $V_{filter}(k',k) \equiv 0 \quad k,k' > 2.2 \text{ fm}^{-1}$

Can we just make a sharp cut without renormalizing?



Low and high k are coupled by quantum fluctuations (virtual states) $\langle k|V|k'\rangle + \sum_{q=0}^{\Lambda} \frac{\langle k|V|q\rangle\langle q|V|k'\rangle}{\epsilon_{k'} - \epsilon_q} + \sum_{q=\Lambda}^{\infty} \frac{\langle k|V|q\rangle\langle q|V|k'\rangle}{\epsilon_{k'} - \epsilon_q}$

Can't simply drop high q without changing low k observables.

To do properly: from *T*-matrix equation, define **low-momentum** equation:



Leads to **renormalization group** equation for low-momentum interaction

$$\frac{\mathrm{d}}{\mathrm{d}\Lambda} V^{\Lambda}_{\mathrm{low}\,k}(k',k) = \frac{2}{\pi} \frac{V^{\Lambda}_{\mathrm{low}\,k}(k',\Lambda) T^{\Lambda}(\Lambda,k;\Lambda^2)}{1-(k/\Lambda)^2}$$

Run cutoff to lower values – decouples high-momentum modes





These are all our favorite OBE NN potentials...

These are all our favorite OBE NN potentials... **at low momentum**

Renormalization of Chiral EFT Potentials



These are all our favorite Chiral EFT NN potentials...

These are all our favorite Chiral EFT NN potentials... **at low momentum**

Differences remain in off-diagonal matrix elements Sensitive to agreement for phase shifts (not all fit perfectly)

Renormalization of NN Potentials



 $V_{eff} = V_L + \delta V_{c.t.}(\Lambda)$

Long-range tail of deuteron wavefunction preserved Main effect is shift in momentum space – delta function Removes hard core!

Renormalization of Nuclear Interactions

Short-distance behaviour of the deuteron – striking difference between potentials



- A) Argonne is correct: Short range repulsion prohibits nucleons from
- B) Vlowk is correct: the nucleons really will overlap in space
- C) Some superposition of these
- D) It doesn't matter

Renormalization of Nuclear Interactions

$$H(\Lambda) = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \dots$$

Evolve momentum resolution scale of chiral interactions from initial Λ_{χ} Remove coupling to high momenta, low-energy physics unchanged



 $V_{\text{low }k}(\Lambda)$: lower cutoffs advantageous for nuclear structure calculations

Smooth vs. Sharp Cutoffs

$$H(\Lambda) = T + V_{NN}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \dots$$

Can have sharp as well as smooth cutoffs (codes only do sharp) Remove coupling to high momenta, low-energy physics unchanged Bogner, Kuo, Schwenk, Furnstahl



Similar but not exact same results – will be differences in calculations

Benefits of Lower Cutoffs

Also use cutoff dependence to assess missing physics: return to Tjon line Varying cutoff moves along line

Never breaks off to experiment

31 a $\Lambda = 1.6 \text{ fm}$ Lesson:Variation in 30 $\Lambda = 2.1 \text{ fm}$ physical observables Λ=1.9 fm 29 with cutoff denotes E(⁴He) [MeV] $\Lambda=1.3 \text{ fm}^{-1}$ 28 Exp. missing physics $\Lambda=3.0 \text{ fm}^{-1}$ beyond NN 27 bare" CD-Bonn 26 $\Lambda=1.0 \text{ fm}^{-1}$ Tool, not a parameter! $V_{low \, k} \, AV18$ 25 V_{low k} CD-Bonn bare" AV18 24 8.2 8.4 7.6 8.0 8.8 7.8 8.6 $E(^{3}H)$ [MeV]
Benefits of Lower Cutoffs

Removes coupling from low-to-high harmonic oscillator states Expect to speed convergence in HO basis



Benefits of Lower Cutoffs

Exactly what happens in no-core shell model calculations Probably equally helpful in normal shell model calculations Come back to this later...



Standard method for softening interaction in nuclear structure for decades:



Infinite summation of ladder diagrams

Need two model spaces:

1) **M** space in which we will want to calculate (excitations allowed in M)

2) Large space \mathbf{Q} in which particle excitations are allowed

To avoid double counting, can't overlap – matrix elements depend on M

Standard method for softening interaction in nuclear structure for decades:



Iterative procedure Dependence on arbitrary starting energy!

Standard method for softening interaction in nuclear structure for decades:



Results of **G-matrix** renormalization:



Removes some diagonal high-momentum components Still large low-to-high coupling in both interactions No indication of universality

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Summary

Low-momentum interactions can be constructed from any V_{NN} via RG



- Low-to-high momentum coupling not desirable in low-energy nuclear physics Evolve to low-momentum while preserving low-energy physics
- Universality attained near cutoff of data
- Low-momentum cutoffs remove low-to-high harmonic oscillator couplings Cutoff variation assesses missing physics at the level of interactions: tool not a parameter

Part III: Many-Body Perturbation Theory

To understand the properties of complex nuclei from elementary interactions



Solving the Many-Body Problem

Matrix elements now given in momentum space, partial waves

 $\langle kK, lL; JST | V | k'K, l'L; JS'T \rangle$

To go to finite nuclei begin from Hamiltonian

$$H|\psi\rangle = (T+V)|\psi\rangle = E|\psi\rangle$$

Assume many particles in the nucleus generate a **mean field** *U*: *U* a one-body potential simple to solve (typically Harmonic Oscillator)

$$H = H_0 + H_1$$
 $H_0 = T + U$ $H_1 = V - U$

So transform from momentum space to Harmonic Oscillator Basis

$$|nl,NL;JST\rangle = \int k^2 dk \ K^2 dK \ R_{nl}(\sqrt{2\alpha}k)R_{NL}(\sqrt{1/2\alpha}K)|kl,KL;JST\rangle$$

One more (ugly) transformation from center-of-mass to lab frame: $\langle ab; JT | V | cd; JT \rangle$



Nuclei understood as many-body system starting from closed shell, add nucleons

Recipe



Now have interaction and energies of valence space orbitals from original V **This alone does not reproduce experimental data**



Now have interaction and energies of valence space orbitals from original V This alone does not reproduce experimental data



Now have interaction and energies of valence space orbitals from original V This alone does not reproduce experimental data

Effective two-body matrix elements Single-particle energies (SPEs)





Many-Body Perturbation Theory

How do we calculate valence space interactions and SPEs??

Define operator P that projects onto the model space

$$P = \sum_{i=1}^{D} |\psi_i\rangle \langle \psi_i| \qquad Q = \sum_{i=1+D}^{\infty} |\psi_i\rangle \langle \psi_i|$$

With relations:

$$PQ = 0 \qquad P^2 = P \qquad Q^2 = Q \qquad P + Q = 1$$

Project full Schrodinger equation into model space eqn that's easy to solve:

$$PH_{eff}P\psi = EP\psi; \quad H_{eff} = H_0 + V_{eff}$$

Need to construct Veff

Many-Body Perturbation Theory

To construct the effective interaction, define \hat{Q} -box = sum of all possible topologically distinct diagrams which are **irreducible** and **valence linked**:



Single-particle energies can be calculated from one-body part Traditionally taken from experimental one-particle spectrum or empirical values

Calculation Details

Convergence in terms of Harmonic Oscillator basis size

NN matrix elements derived from:

- Chiral N³LO (Machleidt, 500 MeV) using smooth-regulator $V_{\text{low }k}$
- 3^{rd} -order in perturbation theory
- 13 major shells for intermediate state configurations (converged)



Calculation Details

Convergence in terms of Harmonic Oscillator basis size

NN matrix elements derived from:

- Chiral N³LO (Machleidt, 500 MeV) using smooth-regulator $V_{\text{low }k}$
- 3^{rd} -order in perturbation theory
- 13 major shells for intermediate state configurations (converged)



Monopole Part of Valence-Space Interactions

Microscopic MBPT – effective interaction in chosen model space Works near closed shells: deteriorates beyond this Deficiencies improved adjusting particular two-body matrix elements

Monopoles: Angular average of interaction

$$V_{ab}^{T} = \frac{\sum_{J} (2J+1) V_{abab}^{JT}}{\sum_{J} (2J+1)}$$

Determines interaction of orbit a with b: evolution of orbital energies



$$\Delta \varepsilon_a = V_{ab} n_b$$

Microscopic low-momentum interactions Phenomenological USD interactions Clear shifts in low-lying orbitals: -T=1 repulsive shift

Phenomenological vs. Microscopic



Compare monopoles from: *Microscopic* low-momentum interactions *Phenomenological* KB3G, GXPF1 interactions Shifts in low-lying orbitals: -T=1 repulsive shift

Limits of Nuclear Existence: Oxygen Anomaly

Where is the nuclear dripline?

Limits defined as last isotope with positive neutron separation energy

- Nucleons "drip" out of nucleus

Neutron dripline experimentally established to Z=8 (Oxygen)



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Microscopic picture: **NN-forces too attractive** Incorrect prediction of dripline

Physics in Oxygen Isotopes

Calculate evolution of *sd*-orbital energies from interactions



 $d_{3/2}$ orbit bound to ²⁸O $d_{3/2}$ orbit unbound

Physics in Oxygen Isotopes

Calculate evolution of sd-orbital energies from interactions



Comparison to Coupled Cluster

Many-body method insufficient?

Benchmark against *ab-initio* Coupled Cluster at NN-only level



SPEs: one-particle attached CC energies in ¹⁷O and ⁴¹Ca Small difference in many-body methods

Include **3N forces** to improve agreement with experiment

The Challenge of Microscopic Nuclear Theory

To understand the properties of complex nuclei from elementary interactions



Why Three-Body Forces?

Tidal Bulges from Moon and Sun



Earth not point particle Experiences tidal forces from sun *and* moon Lead to 3-body forces in E-M-S system

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Tidal Bulges from Moon and Sun



Earth not point particle Experiences tidal forces from sun *and* moon Lead to 3-body forces in E-M-S system

Nucleons are composite particles Can be excited to resonances



Leads to non-negligible effects

Chiral Effective Field Theory: Summary



Nucleons interact via pion exchanges and contact interactions

Hierarchy: $V_{NN} > V_{3N} > \dots$

Consistent treatment of NN, 3N, ... electroweak operators

Weinberg, van Kolck, Kaplan, Savage, Wise, Epelbaum, Kaiser, Meissner,...

Chiral Effective Field Theory: Nuclear Forces



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Chiral EFT: N²LO

First non-vanishing 3N contributions

Next-to-next-to-leading order (v = 3)



$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left(-\frac{4c_1 M_{\pi}^2}{F_{\pi}^2} + \frac{2c_3}{F_{\pi}^2} \vec{q}_i \cdot \vec{q}_j \right) + \sum_{\gamma} \frac{c_4}{F_{\pi}^2} \varepsilon^{\alpha\beta\gamma} \tau_k^{\gamma} \vec{\sigma}_k \cdot \left(\vec{q}_i \times \vec{q}_j \right)$$

Chiral EFT: N²LO

First non-vanishing 3N contributions

Next-to-next-to-leading order (v = 3)



3 LECs – determined from NN fit



Chiral EFT: N²LO

First non-vanishing 3N contributions

Next-to-next-to-leading order (v = 3)



$$\vec{q}_i \equiv \vec{p}'_i - \vec{p}_i$$
$$g_A = 1.26$$
$$F_{\pi} = 92.4 \text{ MeV}$$

$$V_{1\pi,\,\text{cont}}^{(3)} = -\sum_{i\neq j\neq k} \left(\frac{g_A}{8F_\pi}\right)^2 \underbrace{\mathcal{O}}_{\vec{q}_j^2 + M_\pi^2} \left(\vec{\sigma}_j \cdot \vec{\tau}_j\right) \left(\vec{\sigma}_i \cdot \vec{\sigma}_j\right)$$

$$V_{\text{cont}}^{(3)} = \frac{1}{2} \sum_{j \neq k} E(\tau_j \cdot \tau_k)$$

Two new unconstrained couplings D,E: what should we fit to?
Chiral EFT: N³LO



Good news: no new constants

Bad news: it's not obvious?

Cutoff Variation with 3N Forces

Use cutoff variation to assess missing physics in few body systems Radii of triton and alpha particle calculated from NN+3N forces



Clearly minimal cutoff variation

Chiral Three-Body Forces in Light Nuclei

Importance of chiral 3N forces established in light nuclei $A \le 12$ Converged No-core shell model Navratil et al., 2007



They work! What about medium-mass and exotic nuclei?

3N Forces for Valence-Shell Theories

Normal-ordered 3N: contribution to valence neutron interactions

Effective two-body

Effective one-body



Combine with microscopic NN: eliminate empirical adjustments

3N Forces for Valence-Shell Theories

Effects of residual 3N between 3 valence nucleons?

Normal-ordered 3N: microscopic contributions to inputs for CI Hamiltonian Effects of residual 3N between 3 valence nucleons?



Coupled-Cluster theory with 3N: benchmark of ⁴He

0- 1- and 2-body of 3NF dominate
Residual 3N can be neglected
Work on ¹⁶O in progress

Approximated residual 3N by summing over valence nucleon - Nucleus-dependent: effect small, not negligible by $^{24}{\rm O}$

Two-body 3N: Monopoles in sd-shell



First calculations to show missing monopole strength due to neglected 3N

Future: Improved treatment of high-lying orbits

Oxygen Anomaly



Oxygen Anomaly



One-Body 3N: Single Particle Energies

NN-only microscopic SPEs yield poor results – rely on empirical adjustments



sd-shell: SPEs much too bound, unreasonable splitting

Orbit	"Exp"	USDb	$T + V_{NN}$
<i>d</i> _{5/2}	-4.14	-3.93	-5.43
s _{1/2}	-3.27	-3.21	-5.32
d _{3/2}	0.944	2.11	-0.97

One-Body 3N: Single Particle Energies

NN-only microscopic SPEs yield poor results – rely on empirical adjustments



sd-shell: SPEs much too bound, unreasonable splitting **3N forces**: additional repulsion – reasonable values!

Orbit	USDb	$T+V_{NN}+V_{3N}$
<i>d</i> _{5/2}	-3.93	-3.82
s _{1/2}	-3.21	-2.14
d _{3/2}	2.11	2.01

One-Body 3N: Single Particle Energies

Effects of correlations beyond one major oscillator shell:



Fully microscopic framework and extended valence space

Ground-State Energies of Oxygen Isotopes

Valence-space interaction and SPEs from NN+3N



JDH, Menendez, Schwenk, EPJA (2013)

Repulsive character improves agreement with experiment *sd*-shell results underbound; improved in **extended space** $sdf_{7/2} p_{3/2}$

Impact on Spectra: ²³O

Neutron-rich oxygen spectra with NN+3N





Drip Lines and Magic Numbers: The Evolving Nuclear Landscape

Physics of exotic nuclei – era of coming decades

What are the limits of nuclear existence?

How do magic numbers form and evolve?

N=34 magic number in calcium?



Shell Formation/Evolution in Calcium Isotopes



Calcium Isotope Physics: Magic Numbers



GXPF1: Honma, Otsuka, Brown, Mizusaki (2004) KB3G: Poves, Sanchez-Solano, Caurier, Nowacki (2001)



Phenomenological Forces Large gap at ⁴⁸Ca Discrepancy at N=34
Microscopic NNTheory Small gap at ⁴⁸Ca

N=28: first standard magic number not reproduced in microscopic NN theories

Evolution of Shell Structure

SPE evolution with 3N forces in *pf* and *pfg*_{9/2} spaces:



NN+3N *pf*-shell:

JDH, Otsuka, Schwenk, Suzuki JPG (2012)

Trend across: improved binding energies Increased gap at ⁴⁸Ca: enhanced closed-shell features

Include $g_{9/2}$ orbit, calculated SPEs

Different behavior of ESPEs (not observable, model dependent)

Small gap can give large 2^+ energy: due to many-body correlations

Duguet, Hagen, PRC (2012)

N=28 Magic Number in Calcium

First excited 2^+ energies in calcium isotopes with NN+3N



pf-shell: robust but modest improvement in 2^+ energies, below experiment *pfg*_{9/2}-shell: reproduce experimental 2^+ in 48 Ca Both 3N and extended space essential

Evolution of Magic Numbers: N=34

N=34 magic number in calcium?



GXPF1: Honma, Otsuka, Brown, Mizusaki (2004) KB3G: Poves, Sanchez-Solano, Caurier, Nowacki (2001)

Significant phenomenological disagreement for neutron-rich calcium

Evolution of Magic Numbers: N=34

First excited 2^+ energies in calcium isotopes with NN+3N



pf-shell: Very pronounced closed-shell properties $pfg_{9/2}$ -shell: More modest, similar to ⁵²Ca

Evolution of Magic Numbers: N=40

First excited 2^+ energies in calcium isotopes with NN+3N



Holt, Otsuka, Schwenk, Suzuki arXiv:1009.5984

Robust prediction of closed-shell

Neutron-Rich Ca Spectra Near N=34

Neutron-rich calcium spectra with NN+3N



JDH, Menendez, Simonis, Schwenk, in prep.

Different predictions from phenomenology NN+3N similar to KB3G – weak signature of *N*=*34* magic number **Consistent with predictions from Coupled-Cluster theory New measurements from RIKEN** Steppenbeck, priv. comm.

Impact on Spectra: ⁵¹Ca

Neutron-rich calcium spectra with NN+3N



Possibility to assign spin/parity where unknown Gamma-ray spectroscopy needed

Calcium Ground State Energies and Dripline

Ground state energies using NN+3N

NN-only: overbinds beyond $\sim {}^{46}Ca$



Holt, Otsuka, Schwenk, Suzuki, JPG (2012)

pf-shell: 3N forces correct binding energies; good experimental agreement $pfg_{9/2}$ -shell: calculate to ⁷⁰Ca; modest overbinding near ⁵²Ca Heaviest calcium isotope ~ ⁵⁸⁻⁶⁰Ca; flat behavior past ⁵⁴Ca

N=28 Magic Number: *M1* Transition Strength

 $B(M1:0_{gs}^{+} \rightarrow 1^{+})$ concentration indicates a single particle (spin-flip) transition Not reproduced in phenomenology von Neumann-Coesel, *et al.* (1998)

NN-only: highly fragmented strength, well below experiment



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pf-shell:

3N concentrates strength Peaks below experiment

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JDH, Otsuka, Schwenk, Suzuki, JPG (2012)

 $pfg_{9/2}$ -shell:

3N gives additional concentration Peak close to experimental energy

Supports N=28 magic number

Experimental Connection: Mass of 52Ca

 S_{2n} energies for exotic calcium isotopes:



NN-only

poor experimental agreement

NN+3N

Improvement for lighter calcium, wrong behavior past 50 Ca

Experimental Connection: Mass of 52Ca

New mass measurements of 51,52Ca at TITAN: Penning trap experiment



NN-only

poor experimental agreement

NN+3N

Improved agreement with new experimental trend

TITAN Measurement ⁵²Ca mass 1.75MeV **more** bound than AME2003 value!

Experimental Connection: Mass of 52Ca

New mass measurements of ^{51,52}Ca at **TITAN**: Penning trap experiment



NN-only

Poor experimental agreement

TITAN Measurement

⁵²Ca mass 1.75MeV *more* bound than AME2003 value!

NN+3N

Agreement with new measurements Reduced uncertainty from SPEs Good reproduction of pairing gaps

Ground-State Energies of N=8 Isotones



Ground-State Energies of N=8 Isotones



Data limited – use phenomenological isobaric multiplet mass equation (IMME) $E(A,T,T_{z}) = E(A,T,-T_{z}) + 2b(A,T)T_{z}$ $b = 0.7068A^{2/3} - 0.9133$ **NN-only**: overbound **NN+3N**: improved agreement with experiment/IMME Extended space important $\sim A = 21$

er A JDH, Menendez, Schwenk, PRL (2013)

Dripline unclear: ²²Si unbound in AME, NN+3N; bound in IMME

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Dripline unclear: ²²Si unbound in AME, NN+3N; bound in IMME

²² Si possible two-proton emitter	C	IMME	NN+3N (sd)	NN+3N ($sdf_{7/2}p_{3/2}$)
Measurement needed	S _{2p}	0.01 MeV	-1.63 MeV	-0.12 MeV

Spectra of N=8 Isotones



JDH, Menendez, Schwenk, PRL (2012)

NN+3N: reasonable agreement with experiment

New measurement: excited state in ²⁰Mg close to predicted 4⁺-2⁺ doublet Predictions for proton-rich ²¹Al, ²²Si spectra Closed sub-shell signature in ²²Si

Ground-State Energies of N=20 Isotones



Ground-State Energies of N=20 Isotones



Dripline: Predicted to be ⁴⁶Fe in all calculations



C	Expt.	NN+3N (<i>pf</i>)	NN+3N ($pfg_{9/2}$)
S _{2p}	-1.28(6) MeV	-2.73 MeV	-1.02 MeV

Prediction for ⁴⁸Ni within 300keV of experiment

Dossat et al (2005); Pomorski et al (2012)
In-medium NN interactions

JWH, N. Kaiser, W. Weise, PRC (2009)



$$V_{3N}^{(2\pi)} = \sum_{i \neq j \neq k} \frac{g_A^2}{8f_\pi^4} \frac{\vec{\sigma}_i \cdot \vec{q}_i \,\vec{\sigma}_j \cdot \vec{q}_j}{(\vec{q}_i^{\ 2} + m_\pi^2)(\vec{q}_j^{\ 2} + m_\pi^2)} F_{ijk}^{\alpha\beta} \tau_i^{\alpha} \tau_j^{\beta}}$$
$$F_{ijk}^{\alpha\beta} = \delta^{\alpha\beta} \left(-4c_1 m_\pi^2 + 2c_3 \vec{q}_i \cdot \vec{q}_j \right) + c_4 \epsilon^{\alpha\beta\gamma} \tau_k^{\gamma} \vec{\sigma}_k \cdot (\vec{q}_i \times \vec{q}_j)$$

N³LO:
$$c_1 = -0.81$$
, $c_3 = -3.2$, $c_4 = 5.4$ [GeV⁻¹]
 $V_{\rm low-k}(2.1)$: $c_1 = -0.76$, $c_3 = -4.78$, $c_4 = 3.96$ [GeV⁻¹]







$$V_{3N}^{(1\pi)} = -\sum_{i \neq j \neq k} \frac{g_A c_D}{8 f_\pi^4 \Lambda_\chi} \frac{\vec{\sigma}_j \cdot \vec{q}_j}{\vec{q}_j^2 + m_\pi^2} \vec{\sigma}_i \cdot \vec{q}_j \, \vec{\tau}_i \cdot \vec{\tau}_j$$

$$c_D(N^3LO) = -0.2$$

 $c_D(2.1 \text{ fm}^{-1}) = -2.06$



$$V_{3N}^{(\rm ct)} = \sum_{i \neq j \neq k} \frac{c_E}{2f_\pi^4 \Lambda_\chi} \vec{\tau}_i \cdot \vec{\tau}_j$$

 $c_E(N^3LO) = -0.205$ $c_E(2.1 \text{ fm}^{-1}) = -0.63$







The Challenge of Microscopic Nuclear Theory

To understand the properties of complex nuclei from elementary interactions



QCD \rightarrow NN (3N) forces \rightarrow Renormalize \rightarrow Solve many-body problem \rightarrow Predictions

Chiral Effective Field Theory: Philosophy

"Very soft potentials must be excluded because they do not give saturation; they give too much binding and too high density." - *H. Bethe*

How might you respond?