Nuclear forces and their impact on structure, reactions and astrophysics

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Lectures for Week 3

- M. Many-body problem and basis considerations (as); Many-body perturbation theory (rjf)
- T. Neutron matter and astrophysics (as); MBPT + Operators (rjf)
- W. Operators + Nuclear matter (rjf); Student presentations
- Th. Impact on (exotic) nuclei (as); Student presentations
 - F. Impact on fundamental symmetries (as); From forces to density functionals (rjf)

Outline

Teaser: Skyrme vs. pionless, perturbative functional

Bethe-Brueckner-Goldstone Power Counting

Preview for MBPT applied in finite nuclei

Operators and resolution

"The limits of the nuclear landscape"

J. Erler et al., Nature 486, 509 (2012)



- Proton and neutron driplines predicted by Skyrme EDFs
 - Total: 6900 \pm 500 nuclei with Z \leq 120 (\approx 3000 known)
 - Estimate systematic errors by comparing models

Teaser: Comparing Skyrme and natural, pionless Functionals

• Textbook Skyrme EDF (for
$$N = Z$$
) $[\rho = \langle \psi^{\dagger}\psi \rangle, \tau = \langle \nabla\psi^{\dagger} \cdot \nabla\psi \rangle]$
 $E[\rho, \tau, \mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8} t_0 \rho^2 + \frac{1}{16} (3t_1 + 5t_2)\rho\tau + \frac{1}{64} (9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4} W_0 \rho \nabla \cdot \mathbf{J} + \frac{1}{16} t_3 \rho^{2+\alpha} + \cdots \right\}$

• Natural, pionless $\rho \tau \mathbf{J}$ energy density functional for $\nu = \mathbf{4}$

$$E[\rho,\tau,\mathbf{J}] = \int d^3x \left\{ \frac{\tau}{2M} + \frac{3}{8}C_0\rho^2 + \frac{1}{16}(3C_2 + 5C_2')\rho\tau + \frac{1}{64}(9C_2 - 5C_2')(\nabla\rho)^2 - \frac{3}{4}C_2''\rho\nabla\cdot\mathbf{J} + \frac{c_1}{2M}C_0^2\rho^{7/3} + \frac{c_2}{2M}C_0^3\rho^{8/3} + \frac{1}{16}D_0\rho^3 + \cdots \right\}$$

- Same functional as dilute Fermi gas with $t_i \leftrightarrow C_i$?
 - Is Skyrme missing non-analytic, NNN, long-range (pion), (and so on) terms? (But NDA works: C_i's are natural!)
 - Isn't this a "perturbative" expansion?

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DFT BBG Preview Operators

Compare Potential and G Matrix: AV18





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Compare Potential and G Matrix: AV18



TALENT: Nuclear forces

Compare Potential and G Matrix: N³LO (500 MeV)





Compare Potential and G Matrix: N³LO (500 MeV)





Hole-Line Expansion Revisited (Bethe, Day, ...)

• Consider ratio of fourth-order diagrams to third-order:



- "Conventional" G matrix still couples low-k and high-k
 - no new hole line \implies ratio $\approx -\chi(\mathbf{r} = \mathbf{0}) \approx -\mathbf{1} \implies$ sum all orders
 - add a hole line \implies ratio $\approx \sum_{n < k_F} \langle bn | (1/e)G | bn \rangle \approx \kappa \approx 0.15$
- Low-momentum potentials decouple low-k and high-k
 - add a hole line \implies still suppressed
 - no new hole line \implies also suppressed (limited phase space)
 - freedom to choose single-particle $U \Longrightarrow$ use for Kohn-Sham

 \implies Density functional theory (DFT) should work!

- Defect wf χ(r) for particular kinematics (k = 0, P_{cm} = 0)
- AV18: "Wound integral" provides expansion parameter



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High-order Rayleigh-Schrödinger MBPT in finite nuclei

- R. Roth et al.
- Excitation energies in ⁷Li
- Degenerate R-S MBPT
- SRG with two resolutions from N³LO 2NF
- Fixed HO model space

⁷Li 14 12 10 E* [MeV] $\alpha = 0.04 \, \text{fm}^4$ $\alpha = 0.16 \, \text{fm}^4$ $\Lambda \approx 2.24 \, \text{fm}^{-1}$ $\Lambda \approx 1.58 \, \text{fm}^{-1}$ p = 8Exp. NCSM v = 2p = 30 = 4NCSM Exp. Padé Padé 0

Order p = 2, 3, 4, and 8 compared to experiment, exact NCSM calculations, and the Padé resummed result \implies note the good agreement of the last two!

The shell model revisited

Configuration interaction techniques

- · light and heavy nuclei
- detailed spectroscopy
- quantum correlations (lab-system description)



Confronting theory and experiment to both driplines

- Precision mass measurements test impact of chiral 3NF
- Proton rich [Holt et al., arXiv:1207.1509]
- Neutron rich [Gallant et al., arXiv:1204.1987]
- Many new tests possible!





- Shell model description using chiral potential evolved to V_{low k} plus 3NF fit to A = 3, 4
- Excitations outside valence space included in 3rd order MBPT

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Non-empirical shell model [from J. Holt]

Solving the Nuclear Many-Body Problem

Nuclei understood as many-body system starting from closed shell, add nucleons Interaction and energies of valence space orbitals from original $V_{\text{low }k}$ **This alone does not reproduce experimental data**



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

Hjorth-Jensen, Kuo, Osnes (1995)



DFT BBG Preview Operators

Chiral 3NFs meet the shell model [from J. Holt] Drip Lines and Magic Numbers: The Evolving Nuclear Landscape



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Chiral 3NFs meet the shell model [from J. Holt] 3N Forces for Valence-Shell Theories

Normal-ordered 3N: contribution to valence neutron interactions



Combine with microscopic NN: eliminate empirical adjustments

OFT BBG Preview Operators

Chiral 3NFs meet the shell model [from J. Holt] Drip Lines and Magic Numbers: 3N Forces in Medium-Mass Nuclei

Important in light nuclei, nuclear matter...

What are the limits of nuclear existence?

How do magic numbers form and evolve?



N=28 magic number in calcium



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Operators and resolution

Unevolved long-distance operators change slowly with λ

- Matrix elements dominated by long range run slowly for λ ≥ 2 fm⁻¹
- Here: examples from the deuteron (compressed scales)
- Which is the correct answer?
- Are we using the complete operator for the experimental quadrupole moment?





Deuteron electromagnetic form factors

- *G_C*, *G_Q*, *G_M* in deuteron with chiral EFT at leading order (Valderrama et al.)
- NNLO 550/600 MeV potential
- Unchanged at low *q* with unevolved operators
- Independent of λ with evolved operators





'Non-observables' vs. Scheme-dependent observables

- Some quantities are *in principle* not observable
 - T.D. Lee: "The root of all symmetry principles lies in the assumption that it is impossible to observe certain basic quantities; these will be called 'non-observables'."
 - E.g., you can't measure absolute position or time or a gauge

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- Directly measurable quantities are "clean" observables
 - E.g., cross sections and energies
 - Note: Association with a Hermitian operator is not enough!

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 - Note: Association with a Hermitian operator is not enough!
- Scale- and scheme-dependent derived quantities
 - Critical questions to address for each quantity:
 - What is the ambiguity or convention dependence?
 - Can one convert between different prescriptions?
 - Is there a consistent extraction from experiment such that they can be compared with other processes and theory?
 - Physical quantities can be *in-practice* clean observables if scheme dependence is negligible (e.g., (*e*, 2*e*) from atoms)
 - How do we deal with dependence on the Hamiltonian?

Partial list of 'non-observables' references

- Equivalent Hamiltonians in scattering theory, H. Ekstein, (1960)
- Measurability of the deuteron D state probability, J.L. Friar, (1979)
- Problems in determining nuclear bound state wave functions, R.D. Amado, (1979)
- Nucleon nucleon bremsstrahlung: An example of the impossibility of measuring off-shell amplitudes, H.W. Fearing, (1998)
- Are occupation numbers observable?, rjf and H.-W. Hammer, (2002)
- Unitary correlation in nuclear reaction theory: Separation of nuclear reactions and spectroscopic factors, A.M. Mukhamedzhanov and A.S. Kadyrov, (2010)
- Non-observability of spectroscopic factors, B.K. Jennings, (2011)
- How should one formulate, extract, and interpret 'non-observables' for nuclei?, rjf and A. Schwenk, (2010) [in J. Phys. G focus issue on Open Problems in Nuclear Structure Theory, edited by J. Dobaczewski]

Source of scale-dependence for low-E structure

- Measured cross section as convolution: reaction \otimes structure
 - but separate parts are not unique, only the combination
- Short-range unitary transformation U leaves m.e.'s invariant:

$$\boldsymbol{O}_{mn} \equiv \langle \Psi_m | \widehat{\boldsymbol{O}} | \Psi_n \rangle = \left(\langle \Psi_m | \boldsymbol{U}^{\dagger} \right) \, \boldsymbol{U} \widehat{\boldsymbol{O}} \boldsymbol{U}^{\dagger} \left(\boldsymbol{U} | \Psi_n \rangle \right) = \langle \widetilde{\Psi}_m | \widetilde{\boldsymbol{O}} | \widetilde{\Psi}_n \rangle \equiv \widetilde{\boldsymbol{O}}_{\widetilde{m}\widetilde{n}}$$

Note: matrix elements of operator \widehat{O} itself between the transformed states are in general modified:

$$O_{\widetilde{m}\widetilde{n}} \equiv \langle \widetilde{\Psi}_m | O | \widetilde{\Psi}_n \rangle \neq O_{mn} \implies \text{e.g., } \langle \Psi_n^{\mathcal{A}-1} | a_\alpha | \Psi_0^{\mathcal{A}} \rangle \text{ changes}$$

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- In a low-energy effective theory, transformations that modify short-range unresolved physics ⇒ equally valid states.
 So Õ_{mn} ≠ O_{mn} ⇒ scale/scheme dependent observables.
- [Field theory version: the equivalence principle says that only on-shell quantities can be measured. Field redefinitions change off-shell dependence only. E.g., see rjf, Hammer, PLB **531**, 203 (2002).]
- RG unitary transformations change the decoupling scale change the factorization scale. Use to characterize and explore scale and scheme and process dependence!

All pieces mix with unitary transformation

• A one-body current becomes many-body (cf. EFT current):

$$\widehat{U}\widehat{\rho}(\mathbf{q})\widehat{U}^{\dagger} = \mathbf{W} + \alpha \mathbf{W} + \cdots$$

• New wf correlations have appeared (or disappeared):



- Similarly with $|\Psi_f\rangle = a_p^{\dagger}|\Psi_n^{A-1}\rangle$
- Thus spectroscopic factors are scale dependent
- Final state interactions (FSI) are also modified by \widehat{U}
- Bottom line: the cross section is unchanged *only* if all pieces are included, *with the same U*: H(λ), current operator, FSI, ...

Deuteron scale-(in)dependent observables



- V_{low k} RG transformations labeled by Λ (different V_Λ's)
 ⇒ soften interactions by lowering resolution (scale)
 ⇒ reduced short-range and tensor correlations
- Energy and asymptotic D-S ratio are unchanged (cf. ANC's)
- But D-state probability changes (cf. spectroscopic factors)
- Plan: Make analogous calculations for *A* > 2 quantities (like SFs)



- ANC's, like phase shifts, are asymptotic properties
 short-range unitary transformations do not alter them [e.g., see Mukhamedzhanov/Kadyrov, PRC 82 (2010)]
- In contrast, SF's rely on interior wave function overlap
- (Note difference in S-wave and D-wave ambiguities)

Why are ANC's different?

[based on R.D. Amado, PRC 19 (1979)]

$$\begin{array}{l} \bullet \quad \frac{k^2}{2\mu} \langle \mathbf{k} | \psi_n \rangle + \langle \mathbf{k} | \mathbf{V} | \psi_n \rangle &= -\frac{\gamma_n^2}{2\mu} \langle \mathbf{k} | \psi_n \rangle \\ \Longrightarrow \langle \mathbf{k} | \psi_n \rangle &= -\frac{2\mu \langle \mathbf{k} | \mathbf{V} | \psi_n \rangle}{k^2 + \gamma_n^2} \\ \bullet \quad \langle \mathbf{r} | \psi_n \rangle &= \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k} \cdot \mathbf{r}} \langle \mathbf{k} | \psi_n \rangle \\ & \stackrel{|\mathbf{r}| \to \infty}{\longrightarrow} A_n e^{-\gamma_n r} / r \end{array}$$



• extrapolate $\langle {f k} | {m V} | \psi_n
angle$ to $k^2 = -\gamma_n^2$



Momentum space

- Or, residue from extrapolating on-shell T-matrix to deuteron pole
 invariant under unitary transformations
- Next vertex singularity at $-(\gamma + m_{\pi})^2 \Longrightarrow$ same for FSI

How should one choose a scale/scheme?

- To make calculations easier or more convergent
 - QCD running coupling and scale: improved perturbation theory; choosing a gauge: e.g., Coulomb or Lorentz
 - Low-k potential: improve CI or MBPT convergence, or to make microscopic connection to shell model or ...
 - (Near-) local potential: quantum Monte Carlo methods work
- Better interpretation or intuition \Longrightarrow predictability
 - SRC phenomenology?
- Cleanest extraction from experiment
 - Can one "optimize" validity of impulse approximation?
 - Ideally extract at one scale, evolve to others using RG
- Plan: use range of scales to test calculations and physics
 - Use renormalization group to consistently relate scales and quantitatively probe ambiguities (e.g., in spectroscopic factors)
 - Match Hamiltonians and operators (EFT) and then use RG

Operator flow in practice [e.g., see arXiv:1008.1569]

Evolution with s of any operator O is given by:

$$O_{s} = U_{s}OU_{s}^{\dagger}$$

so Os evolves via

$$\frac{dO_s}{ds} = [[G_s, H_s], O_s]$$

- $U_s = \sum_i |\psi_i(s)\rangle \langle \psi_i(0)|$ or solve dU_s/ds flow
- Matrix elements of evolved operators are unchanged
- Consider momentum distribution $\langle \psi_d | a_q^{\dagger} a_q | \psi_d \rangle$ at q = 0.34 and 3.0 fm^{-1} in deuteron



High and low momentum operators in deuteron





• Induced two-body operator \approx regularized delta function:

High and low momentum operators in deuteron





- Integrated value does not change, but nature of operator does
- Similar for other operators: $\langle r^2 \rangle$, $\langle Q_d \rangle$, $\langle 1/r \rangle \langle \frac{1}{r} \rangle$, $\langle G_C \rangle$, ...

Is the tail of n(k) for nuclei measurable? (cf. SRC's)



- E.g., extract from electron scattering?
- Scale- and schemedependent high-momentum tail!
- n(k) from V_{SRG} has no high-momentum components!
- No region where 1/a_s « k « 1/R (cf. large k limit for unitary gas)

What parts of wf's can be extracted from experiment?

- Measurable: asymptotic (IR) properties like phase shifts, ANC's
- Not observables, but well-defined theoretically given a Hamiltonian: interior quantities like spectroscopic factors
 - These depend on the scale and the scheme
 - Extraction from experiment requires robust factorization of structure and reaction; only the combination is scale/scheme independent (e.g., cross sections) [What if weakly dependent?]
- What about the high-momentum tails of momentum distributions?
 - Consider cold atoms in the unitary regime
 - Compare to nuclear case
- Short-range correlations (SRCs) depend on the Hamiltonian *and* the resolution scale (cf. parton distribution functions)
- So might expect Hamiltonian- and resolution-dependent but *A*-independent high-momentum tails of wave functions
 - Universal extrapolation for different A, but λ_{SRG} dependent