Decomposing and Factorizing Nuclear Forces

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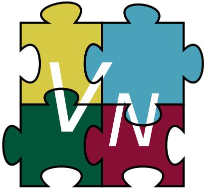
Cut my force into pieces...

Decompositions and factorizations of nuclear forces

- provide deeper insights into inner workings
- can be exploited to speed up computations
- give access to optimized operator basis?

Various techniques:

- Singular-Value Decomposition
- Tensor factorizations (CPD, THC, ...)
- Orthogonal Projections
- ...



This talk

- Decompose 3N forces to learn about the EM1.8/2.0 interaction.
- Implicit tensor factorizations as computational tool.

What's the magic in the magic interaction?

The "magic" EM1.8/2.0 interaction [Hebeler, Bogner, Furnstahl *et al.* PRC 83, 031301(R) (2011)]

- Predicts ground-state energies throughout nuclear chart, even for ^{208}Pb. [Simonis, Stroberg, Hebeler *et al.* PRC 96, 014303 (2017)] [Stroberg, priv. comm. (2019)]
- Construction:
  - NN-only SRG evolution of 2N force (Entem & Machleidt @ N^{3}LO).
  - Fit of c_D, c_E to triton g.s. and ^{4}He radius using unevolved 3N interaction @ N^{2}LO.
- Assumption: induced 3N terms can be absorbed into D and E contact terms.
  Never tested!

How?

Evolve EM2.0/2.0 and project evolved 3N onto N^{2}LO topologies.

Projection of three-body forces

- Chiral 3N topologies form basis of 3N operator subspace.

- Matrix representations in Jacobi-HO → basis $\{C_i\}$ of matrix subspace.

- Introduce Frobenius inner product $\langle U, V\rangle = \sum_{J\pi T} tr(U_{J\pi T}^{\mathsf{T}} V_{J\pi T})$.
  ⇒ Basis nonorthogonal, metric tensor $G_{ij} = \langle C_i, C_j\rangle$.

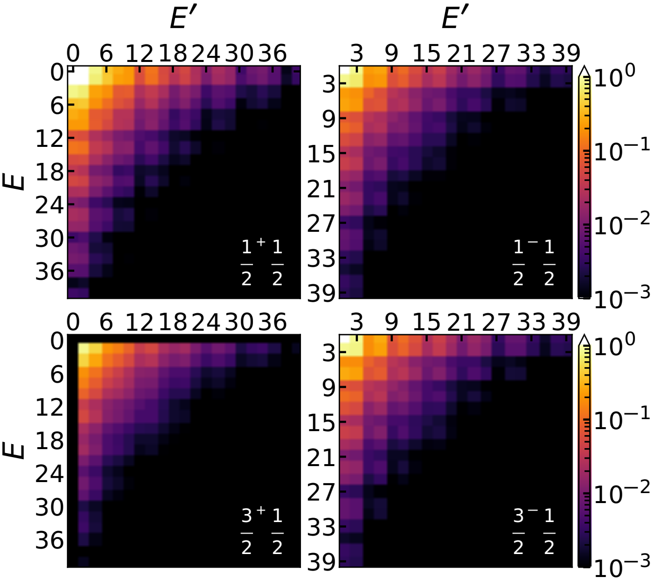
- To project force V, compute $y = (\langle C_1, V\rangle, \ldots, \langle C_n, V\rangle)^{\mathsf{T}}$ and solve

  $$\mathrm{G}c = y$$

  Vector c contains LECs of the projected V, projection solves least-squares problem of matrix elements

  $$\min_{\{c_i\}} \sum_{jk} \left(V_{jk} - \sum_i c_i (C_i)_{jk} \right)^2$$

Structure of N^{2}LO topologies



$\|C_3\|(E,E')$ [MeV]

$\hbar\Omega = 36\,\text{MeV}$

$\Lambda = 2.0\,\text{fm}^{-1}$

$n_{\text{reg}} = 4$

Low energy, low J.

Contacts:
C_D similar to C_3
C_E s-wave only!

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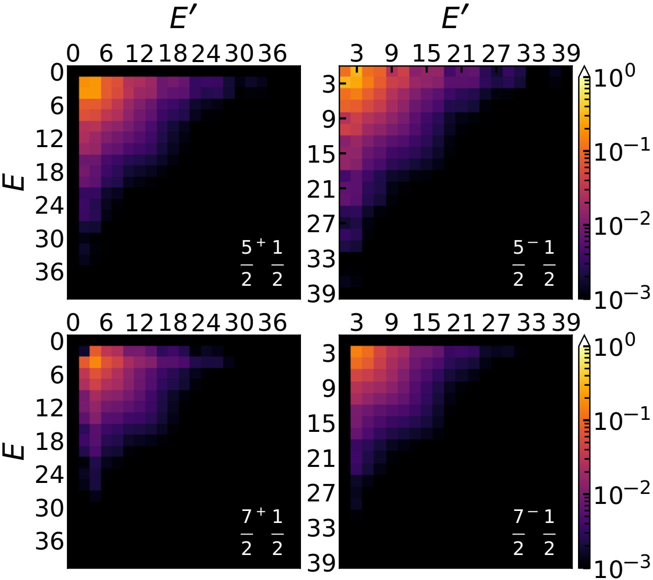

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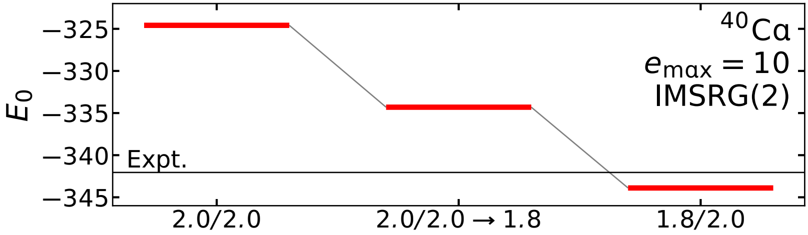
Evolving from 2.0 fm^{-1} to 1.8 fm^{-1}



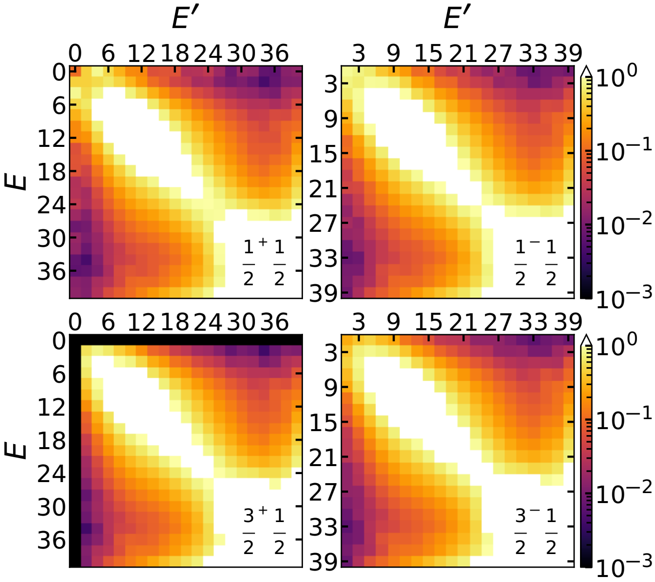
- Use SRG in three-body space

$$\frac{dH(\alpha)}{d\alpha} = [\eta(H(\alpha)), H(\alpha)] \qquad \frac{dU(\alpha)}{d\alpha} = -U(\alpha)\eta(H(\alpha))$$

  $\alpha = \lambda^{-4}$: SRG flow parameter

- SRG equations autonomous: start from EM2.0/2.0 and evolve to $\Delta\alpha = 1.8^{-4} - 2.0^{-4}$.
- 3N also evolves from $\Lambda = 2.0\,\mathrm{fm}^{-1}$
  $\Rightarrow$ Look at induced 3N from NN only: apply $U(\alpha)$ to V_{NN}.

Structure of induced 3N terms



$\|V_{2\to3,\mathrm{ind}}\|$ [MeV]

$\hbar\Omega = 36\,\mathrm{MeV}$

$\lambda = 1.8\,\mathrm{fm}^{-1}$

All energies, approx. diagonal

Different from N^2LO 3N topologies

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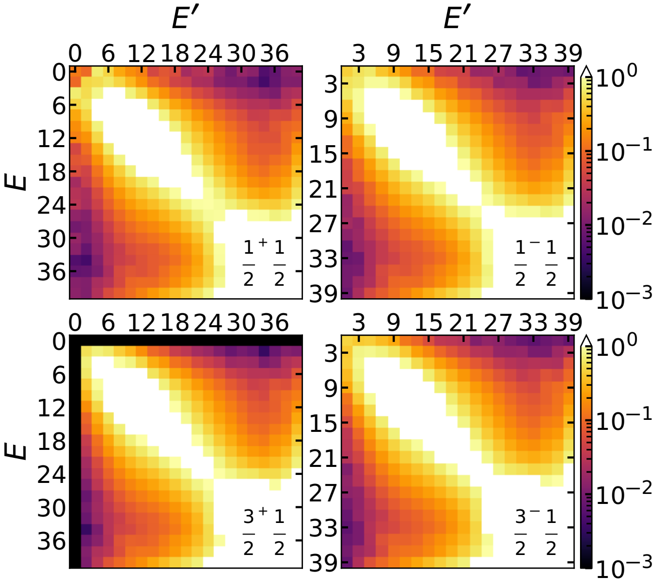

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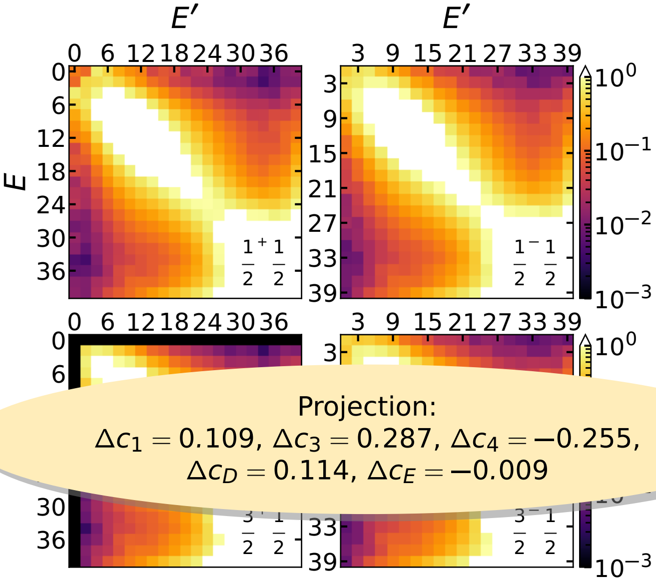

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Different from N^{2}LO 3N topologies

Projection:
$\Delta c_1 = 0.109$, $\Delta c_3 = 0.287$, $\Delta c_4 = -0.255$,
$\Delta c_D = 0.114$, $\Delta c_E = -0.009$

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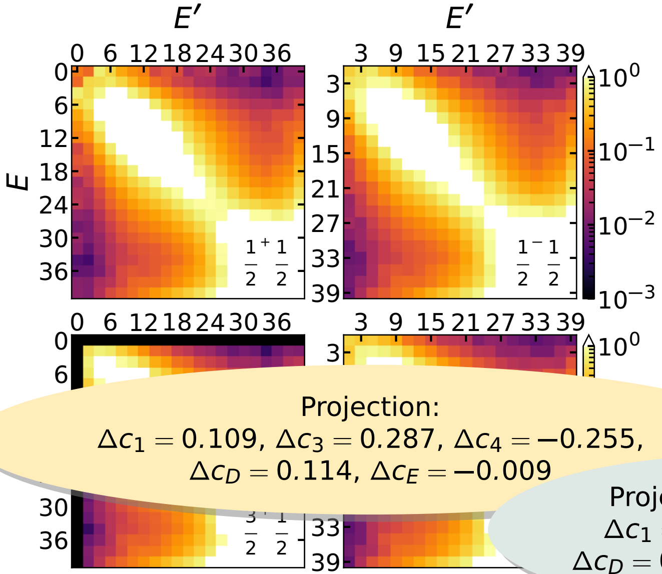

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Different from $\mathrm{N^2LO}$ 3N topologies

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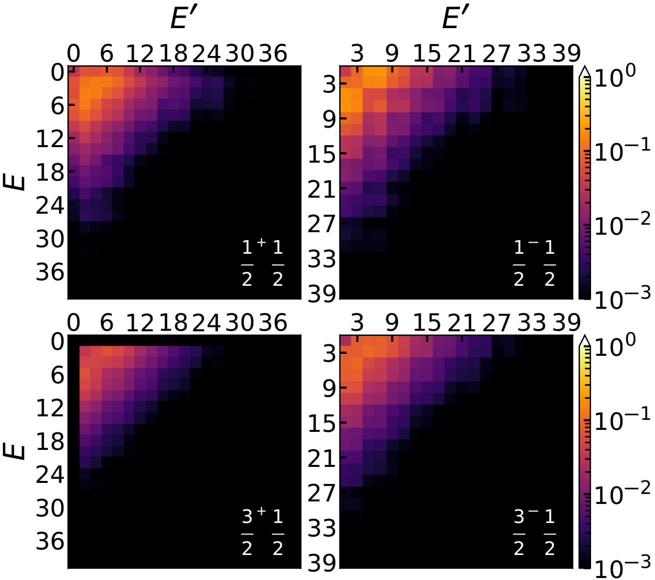
$\Delta c_1 = 0.109$, $\Delta c_3 = 0.287$, $\Delta c_4 = -0.255$,
$\Delta c_D = 0.114$, $\Delta c_E = -0.009$

Projection on c_D, c_E:
$\Delta c_1 = \Delta c_3 = \Delta c_4 = 0$,
$\Delta c_D = 0.160$, $\Delta c_E = 0.007$

Structure of induced 3N terms



$\|V_{3\to3,\mathrm{ind}}\|$ [MeV]

$\hbar\Omega = 36\,\mathrm{MeV}$

$\lambda = 1.8\,\mathrm{fm}^{-1}$

Shape similar to initial 3N

Generally weak

Projection of the evolved interaction

LEC	2.0/2.0	2.0/2.0 → 1.8		1.8/2.0
		Full	c_D, c_E	
c_1	−0.81	−0.673	−0.81	−0.81
c_3	−3.20	−2.928	−3.20	−3.20
c_4	5.40	5.139	5.40	5.40
c_D	1.264	1.381	1.446	1.271
c_E	−0.120	−0.133	−0.115	−0.131

- Full: c_i's get $\sim 10\,\%$ correction, 2PE suppressed, contacts enhanced.
- c_D, c_E: D term enhanced, E term suppressed.
- Values quite different from 1.8/2.0.

Conclusions?

- Induced 3N vastly different from N2LO topologies. Cannot absorb into LECs.
- Magic in the EM1.8/2.0 is an accidential cancellation: Suppose chiral EFT eventually converges, then, at $\lambda = 1.8\,\mathrm{fm}^{-1}$,

$$V_\chi = V_{1.8} + (V_{3,\mathrm{SRG}} - V_{3,\delta DE}) + V_{2,\mathrm{N^4LO+}} + V_{3,\mathrm{N^3LO+}} + V_4 + \cdots$$

Since $\langle T_{\mathrm{int}} + V_{1.8} \rangle_{\mathrm{g.s.}} \approx \langle T_{\mathrm{int}} + V_\chi \rangle_{\mathrm{g.s.}}$,

$$\langle V_{3,\delta DE} \rangle_{\mathrm{g.s.}} \approx \langle V_{3,\mathrm{SRG}} + V_{2,\mathrm{N^4LO+}} + V_{3,\mathrm{N^3LO+}} + V_4 + \cdots \rangle_{\mathrm{g.s.}}\,.$$

- Induced terms and higher orders cancel in g.s. expectation value, except for contact-like part.
- EM1.8/2.0: Contacts have right strength to fit few-body observables and provide correct shift in *E/A* once saturated.

Factorizations and random embeddings

Factorizing a Hamiltonian

- Nuclear Hamiltonian is superposition of few operators.
- Some operators are simple (contacts, kinetic energy), some more complicated
- Can we divide operators into simpler objects?
  ⇒ Lower-scaling many-body methods.
  ⇒ Inclusion of explicit 3N/4N terms.

We can try tensor factorizations!

Canonical Polyadic Decomposition

Simple factorization: Write Hamiltonian as

$$H_{abcd} = \sum_{\alpha=1}^{r} \lambda_\alpha A^{(1)}_{a,\alpha} A^{(2)}_{b,\alpha} A^{(3)}_{c,\alpha} A^{(4)}_{d,\alpha}$$

Changes scaling of many-body methods, e.g.,

$$\sum_{abcd} H_{abcd} H_{abcd} = \sum_{\alpha,\beta=1}^{r} \lambda_\alpha \lambda_\beta \sum_{a} A^{(1)}_{a,\alpha} A^{(1)}_{a,\beta} \cdots \sum_{d} A^{(4)}_{d,\alpha} A^{(4)}_{d,\beta}$$

Complexity $\mathcal{O}(N^4) \rightarrow \mathcal{O}(4Nr^2)$

See [Tichai, Schutski, Scuseria, Duguet. PRC 99, 034320 (2019)]

How to compute? Alternating Least-Squares!

1. Fix $A^{(2)},\ldots,A^{(4)}$. Build LS problem for $A^{(1)}$ ($\mathcal{O}(N^4 r)$).
2. Solve LS problem for $A^{(1)}$.
3. Repeat for $A^{(2)},\ldots,A^{(4)}$.
4. Repeat 1 - 3 until convergence (100's of iterations)

The Johnson-Lindenstrauss lemma

- Computing CPD is expensive.
- Use existence of low-rank CPD without actually computing it?
  $\hookrightarrow$ Many-body methods care about inner products, not matrix elements.

Johnson-Lindenstrauss lemma (paraphrased)

We can find a projection matrix $P \in \mathbb{R}^{m \times N}$ with *random elements* that preserves norms of a set of vectors $S = \{\vec{x}_i\}$ up to some adjustable error ϵ with high probability if $m \geq m_0(\epsilon, |S|)$:

$$\|P\vec{x}_i\| = (1 + \epsilon_i)\|\vec{x}_i\|, \qquad |\epsilon_i| < \epsilon$$

Using $\vec{u} \cdot \vec{v} = 1/4(\|\vec{u} + \vec{v}\|^2 - \|\vec{u} - \vec{v}\|^2)$, this translates to preservation of scalar products.

Random embeddings

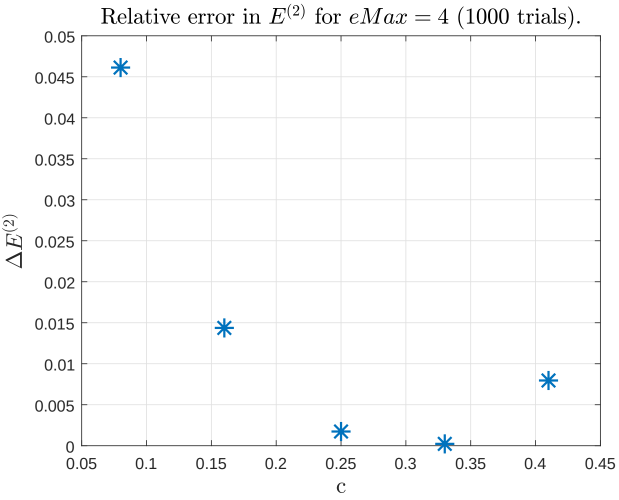
- Existence of CPD: $r(3r-1)/2$ vectors to preserve in each mode.
- Apply Johnson-Lindenstrauss modewise

[Iwen, Needell, Rebrova, Zare. arXiv:1912.08294]

$$\tilde{H}_{\alpha\beta\gamma\delta} = \sum_{abcd} H_{abcd} P^{(1)}_{a,\alpha} P^{(2)}_{b,\beta} P^{(3)}_{c,\gamma} P^{(4)}_{d,\delta}$$

- Turns N^4 matrix elements into m^4. Compression factor $c = m/N$.
- Savings depend on m required for given precision ϵ.

Results: Many-Body Perturbation Theory



[Zare, RW, *et al. in prep.*]

^{16}O

$\hbar\Omega = 24\,\mathrm{MeV}$

$\Lambda_{3N} = 400\,\mathrm{MeV/c}$

$\alpha_{\mathrm{SRG}} = 0.08\,\mathrm{fm}^4$

Entem & Machleidt + local 3NF

$$\Delta E^{(2)} = \left| \frac{\tilde{E}^{(2)} - E^{(2)}}{E^{(2)}} \right|$$

averaged over 1000 trials

$c = 0.25$ sufficient for $1\,\%$ accuracy

Computational savings $1/4^4 = 4 \times 10^{-3}$

Conclusions

Tensor Factorizations

- Factorizations can yield low-scaling many-body methods.
- Drawback: initial cost.

JL Embeddings

- Use existence of factorization implicitly.
- Computationally cheap.
- Reduce index length by factor $c = m/N$.
- Drawback: scaling does not change
  (In fact, c becomes smaller with increasing model space)

Future: combine both to reduce factorization cost.
Gain improved scaling and shorter indices.

...this was my workshop talk

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    University of Washington

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- **Thank you for your attention!**

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