Factorization of two- and three-body matrix elements for ab-initio calculations

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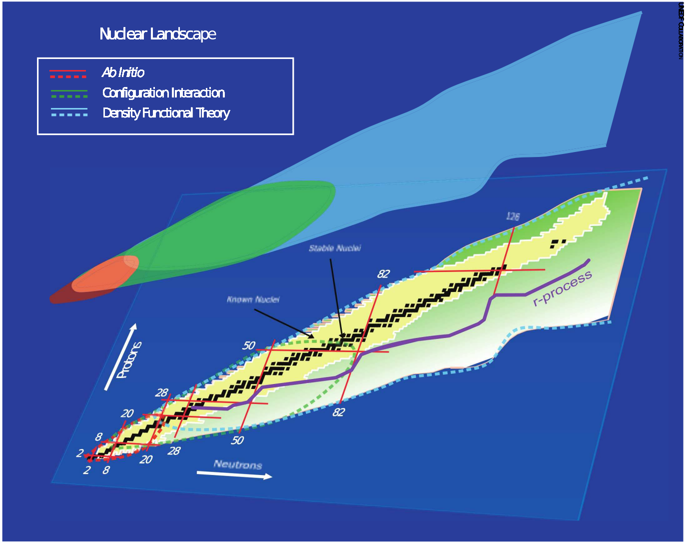
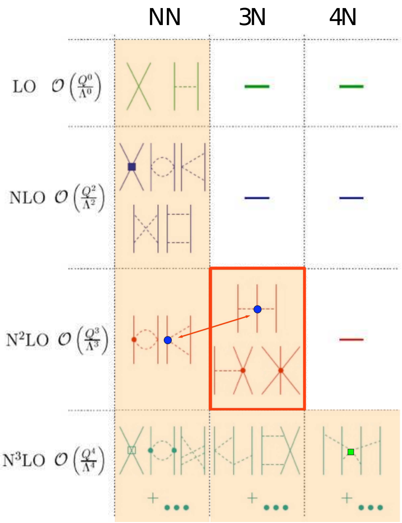
AG des théoriciens, IPN Orsay, 2014-12-16

Nuclear structure theory: methods



Nucleon Hamiltonian from chiral EFT



Ab-initio methods ?

- Renormalized interactions used in ab-initio schemes are promising

- Issues
  - Needs large bases to describe heavy nuclei or continuum
  - Three-body force currently limited to a few HO shells
    - ➡ Computationally expensive

➡ Separable expansions of V_{NN}, $V_{3\mathrm{N}}$

$V_{\mathrm{N^2LO,\ NN\langle N\rangle}}$

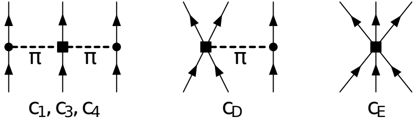
- NN + NNN Hamiltonian

$$\hat{V}_{NN} = \frac{1}{4}\overline{V}^{NN}_{ijkl}\, a^\dagger_i a^\dagger_j a_l a_k \qquad \hat{V}_{NNN} = \frac{1}{36}\overline{V}^{NNN}_{ijklmn}\, a^\dagger_i a^\dagger_j a^\dagger_k a_n a_m a_l$$

- First-order (Hartree-Fock-Bogolyubov) NN + NNN

$$\mathcal{E}_{\mathrm{int}} = \frac{1}{2}\overline{V}^{NN}_{ijkl}\ \rho_{ki}\rho_{lj} + \frac{1}{4}\overline{V}^{NN}_{ijkl}\ \kappa^*_{ij}\kappa_{kl} + \frac{1}{6}\overline{V}^{NNN}_{ijklmn}\ \rho_{li}\rho_{mj}\rho_{nk} + \frac{1}{4}\overline{V}^{NNN}_{ijklmn}\ \kappa^*_{ij}\kappa_{lm}\rho_{nk}$$

- NNN force in pp channel 3× that in ph (first order only)
- Start from N^{2}LO V_{NNN}



Separable $V_{\rm NN}$

- Principle: $|i\rangle$ s.p. basis, $1 < i < n_{\rm b}$, let $N = n_{\rm b}^2$

$$v_{ijkl} = \sum_a \lambda_a \, g_{ij}^{a*} \, g_{kl}^{a} = \sum_a \lambda'_a \, g'^{a}_{ik} \, g'^{a}_{jl}$$

  - If $\lambda_a << \lambda_1$ for a > n: truncate

- HF: $\Gamma_{ij} = \frac{1}{2} \sum_a g'^{a}_{ij} \, \lambda'_a \, \breve{\rho}_a$, with $\breve{\rho}_a = \sum_{ij} g'^{a}_{ij} \, \rho_{ij}$
- HFB: $\Delta_{ij} = \frac{1}{4} \sum_a g^{a}_{ij} \, \lambda_a \, \breve{\kappa}_a$, with $\breve{\kappa}_a = \sum_{ij} g^{a}_{ij} \, \kappa_{ji}$
  - Cost $\mathcal{O}(nN)$ down from $\mathcal{O}(N^2) = \mathcal{O}(n_{\rm b}^4)$: gain n/N

$V_{\text{N}^2\text{LO, NN}\langle\text{N}\rangle}$

- NN low-momentum force ($\Lambda = 1.8$ fm^{-1}) pp-separable expansion
- 3N force ($\Lambda = 2.0$ fm^{-1})
  - Parameters (c_D, c_E) from fit on BE of ^{3}H and radius of ^{4}He
    S.K.Bogner et al., arXiv:0903.3366
  - Avg. over 3$^{\text{rd}}$ particle in INM (K. Hebeler, A. Schwenk, arXiv:0911.0483)
  - ➡ P-p separable representation in $^1S_0$ wave ($q, q' = \pm 1/2$ for n/p)

$$V^{^1S_0}_{qq\langle q'\rangle}(k, k'; k_{\text{F}}) = \sum_{\alpha,\beta=1}^{n} g_\alpha(k)\; \lambda_{\alpha\beta}(k_{\text{F},q'})\; g_\beta(k')$$

  - + Local Density Approximation (LDA):

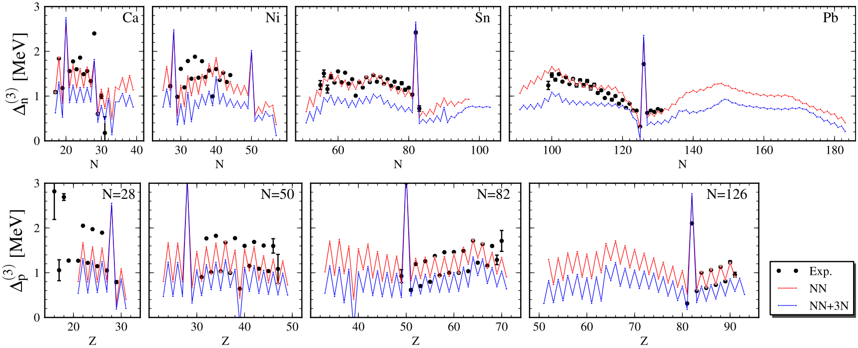
$$\lambda_{\alpha\beta} \to \lambda_{\alpha\beta}(\mathbf{R}) = \lambda_{\alpha\beta}\left(k_{\text{F},q'}(\mathbf{R})\right), \qquad k_{\text{F},q'}(\mathbf{r}) = \left(3\pi^2 \rho_{q'}(\mathbf{r})\right)^{1/3}$$

  - $\lambda_{\alpha\beta}\left(k_{\text{F}}\right) = \lambda^{(3)}_{\alpha\beta}\, k_{\text{F}}^3 + \lambda^{(4)}_{\alpha\beta}\, k_{\text{F}}^4$

Separable $V_{\rm NN}$: pairing systematics

- ph field from Skyrme quasi-local EDF
- m^* from INM HF with same $V_{\rm NN} + V_{\rm 3N}$

$$\Delta_{\rm n}^{(3)}(N,Z) = \frac{1}{2}(-1)^N \left[E(N-1,Z) - 2E(N,Z) + E(N+1,Z)\right]$$



- TL, K. Hebeler, T. Duguet and A. Schwenk, J. Phys. G 39 015108 (2012)

$V_{\text{low }k}$, NN, ($\Lambda = 2.0$ fm^{-1}) particle-hole channel

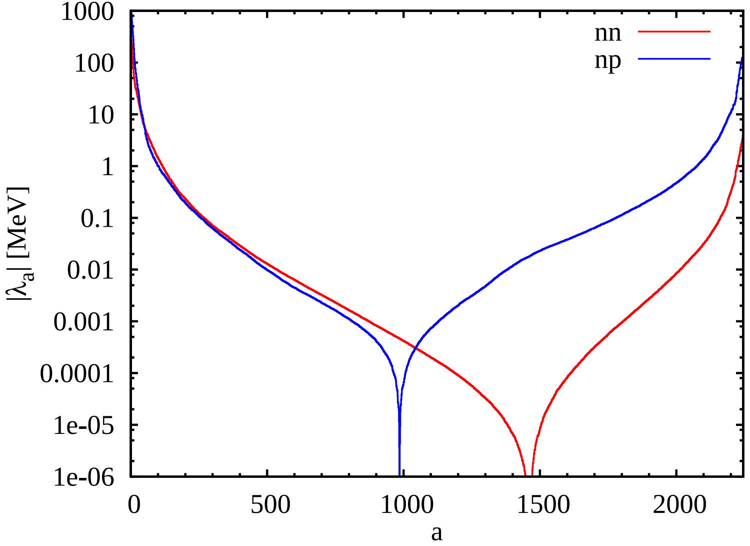
- What about p-h mean field ?
  - ➨ s.p.e. (range, surface, spin-orbit, tensor ?)
  - ➨ deformation properties...
  - ✘ No coordinate-space separable expansion (Galilei)

- Basis: spherical Bessel, $R_{\text{box}} = 15$ fm, $k_{\text{cut}} = 2.5$ fm^{-1}, $l_{\text{cut}} = 20$
- $N = 2245$ for $J^\pi = 0^+$, similar to 22 HO shells
- Obtain ph-separable form

$$\langle n_1 l_1 j_1 \; n_2 l_2 j_2 | \overline{V}_{\text{NN},T_z} | n_1' l_1' j_1' \; n_2' l_2' j_2' \rangle^{(J)} = \sum_a \lambda_a^{JT_z} \, g^{JT_z,a}_{(n_1 l_1 j_1, n_1' l_1' j_1')} \, g^{JT_z,a}_{(n_2 l_2 j_2, n_2' l_2' j_2')}$$

- Eigenvalue decomposition: ScaLAPACK PDSYEV

$V_{\mathrm{low}\ k}$, NN, particle-hole channel



HF computation time

- Skyrme-HF calculation time per iteration is about 20 ms.
- Expect strong overbinding due to lack of three-body force

			^{16}O		^{132}Sn	
ε	$n_{\text{sv}}^{\text{nn}}$	$n_{\text{sv}}^{\text{np}}$	E [MeV]	[ms/it.]	E [MeV]	[ms/it.]
1E-2	76	91	-196.96411	63	-3353.88187	58
3E-3	145	161	-197.28190	83	-3351.94746	78
1E-3	228	273	-197.22297	128	-3352.62366	107
1E-4	546	727	-197.22733	336	-3352.70369	367
1E-5	1047	1369	-197.22716	775	-3352.71063	690
1E-6	1597	1932	-197.22716	1102	-3352.71065	987
0	2245	2245	-197.22716	1343	-3352.71065	1255

$V_{3\mathrm{N}}$?

- Can we use a similar technique for 3N forces ?

Higher-Order Singular Value Decomposition (HOSVD)

- L. De Lathauwer, B. De Moor and J. Vandewalle, SIAM J. Matrix Anal. Appl. 21, 1253 (2000)
- For a symmetric rank-3 tensor: $T_{pqr} = \sum_{stu} S_{stu} U_{sp} U_{tq} U_{ur}$ with
  - U an orthogonal (unitary) matrix
  - All-orthogonality: $\sum_{rs} S^*_{prs} S_{qrs} = \sigma_p^2 \delta_{pq}$
  - Ordering: $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_N$

- ph and pp factorizations: HF scaling $\mathcal{O}(N^3) = \mathcal{O}(n_\mathrm{b}^6) \to \mathcal{O}(n^3) + \mathcal{O}(nN)$: gain $(n/N)^3$

$$v^{(3)}_{ijklmn} = \sum_{abc} \lambda_{abc}\, g^{a*}_{ij}\, g^{b}_{lm}\, g'^{c}_{kn} = \sum_{abc} \lambda'_{abc}\, g'^{a}_{il}\, g'^{b}_{jm}\, g'^{c}_{kn}$$

1. Define $A_{pI} = T_{pqr}$, with $I = (q, r)$ and SVD $A_{pI} = \sum_s U_{ps} \sigma_s V^*_{Is}$
2. Core tensor:
   - Use $S_{pqr} = \sum_{stu} U^*_{ps} U^*_{qt} U^*_{ru} T_{stu}$, cost $\mathcal{O}(N^5)$
   - Invert $\sum_{stu} U_{sp} U_{tq} U_{ur} S_{stu} = T_{pqr}$, cost $\mathcal{O}(n^9)$

$V_{3\mathrm{N}}$?

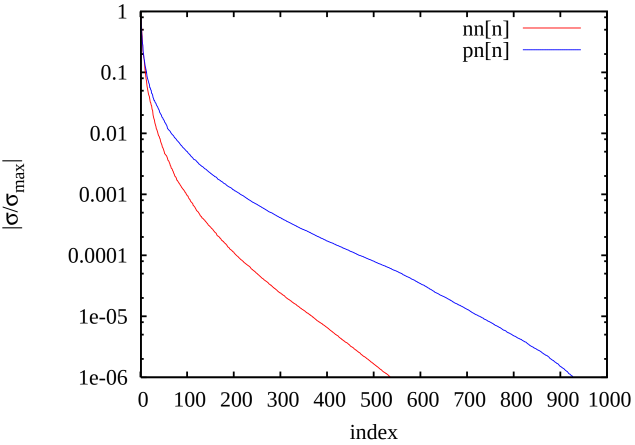
- Define $A_{pI} = T_{pqr}$, with $I = (q, r)$ and SVD $A_{pI} = \sum_s U_{ps} \sigma_s V_{Is}$
- Use EVD of $\sum_I A_{pI} A^*_{qI} = \sum_s U_{ps} \sigma^2_s U^*_{qs}$
- Choose convenient representation:
  $\sum_I A_{pI} A^*_{qI} = \sum_{IJK} A_{pI} W^*_{JI} W_{JK} A^*_{qK}$

$$\langle \vec{k}_1 \sigma_1 \vec{k}_2 \sigma_2 (\vec{k}'_1 \sigma'_1)^{-1} (\vec{k}'_2 \sigma'_2)^{-1} | V_{3N} | (l_3 j_3 n_3)^{-1} l'_3 j'_3 n'_3 \rangle^{(J)}$$

- Basis: spherical Bessel, $R_{\mathrm{box}} = 15$ fm, $k_{\mathrm{cut}} = 2.5$ fm^{-1}, $l_{\mathrm{cut}} = 12$
  - $N = 1909$ for $J^\pi = 0^+$
- V_{3N} chiral N2LO, $\Lambda_\chi = 700$ MeV, $\Lambda_{3N} = 2.0$ fm^{-1}
  ($c_1 = -0.76,\ c_3 = -4.78,\ c_4 = 3.96,\ c_D = -2.785,\ c_E = -0.822$)

$V_{3\mathrm{N}}$ ph expansion (PRELIMINARY)

- Chiral (N2LO) 3N interaction deduced from NN PWA (c_i), ^{3}He binding E and ^{4}He radius (c_D, c_E), $\Lambda_{3\mathrm{N}} = 2.0\mathrm{fm}^{-1}$



- Next: core tensor, implement in HFB, SCGoGF, CC, etc...

Separable expansions beyond first order ?

- Ex: MP2 correction

$$E_{MP2} = \frac{1}{4}\sum_{ijab} \frac{|\langle ij|v|ab\rangle|^2}{e_a + e_b - e_i - e_j}$$

- Matrix element

$$\langle ij|v|ab\rangle = \sum_{\alpha} g^{\alpha}_{ij} \lambda_\alpha g^{\alpha}_{ab}$$

- Energy Denominator ? (B. Khomoromskij et al.)

$$\frac{1}{e_a + e_b - e_i - e_j} = \int_0^\infty dx\, e^{-x(e_a+e_b-e_i-e_j)}$$
$$\simeq \sum_\beta w_\beta\, e^{x_\beta(e_i+e_j)}\, e^{-x_\beta(e_a+e_b)}$$

➡ Factorize the expression

$$E_{\mathrm{MP2}} = \frac{1}{4}\sum_{\alpha\beta\gamma} \lambda_\alpha\, w_\beta\, \lambda_\gamma\, L_{\alpha\beta\gamma}\, L'_{\alpha\beta\gamma}, \qquad L_{\alpha\beta\gamma} = \sum_{ij} g^{\alpha}_{ij}\, e^{x_\beta(e_i+e_j)}\, g^{\gamma}_{ij}$$

Summary and outlook

- Separable form of NN+3N low-k interactions promising ingredient
  - NN+3N pp-separable form shows interesting physics for pairing near the drip line
  - NN ph-separable form usable almost as efficiently as a contact effective interaction
  - 3N ph-separable form looks promising

  - Speedup of tensor contractions occuring in common many-body schemes
    - Heavier nuclei
    - Symmetry breaking/restoration: T. Duguet, arXiv:1406.7183
    - Ab-initio DFT

      J. E. Drut, L. Platter, PRC 84, 014318 (2011)

      T. Lesinski, PRC 89, 044305 (2014)