Spurious isospin symmmetry breaking in the IMSRG

Alexander Farren (supervised by Prof. Stroberg)

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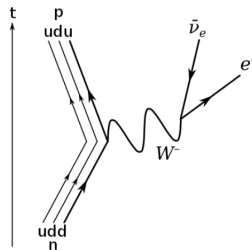June 2023

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Beta Decay

Three types of β-decay[1]:

- β^+: $p^+ \rightarrow n^0 + e^+ + \nu_e$
- β^-: $n^0 \rightarrow p^+ + e^- + \bar{\nu}_e$
- e^- capture:
  $^A_Z X + e^- \rightarrow ^A_{Z-1} Y + \nu_e$

Feynman Diagrams:

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Nuclear Shell Model

Can approximate nucleon energies as levels or shells

$$E_{n\ell} = \hbar\omega(2n + \ell + \tfrac{3}{2}) - V_0' + \text{Spin-Orbit} \ [2]$$

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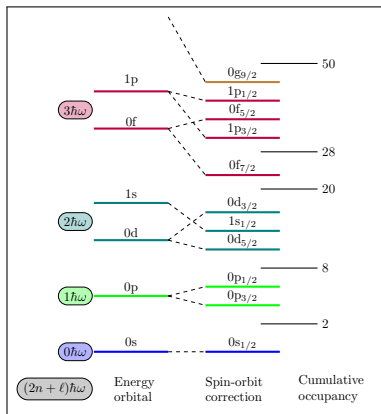
Isospin

Heisenberg introduced isospin t in 1932 because the proton and neutron are interchangeable with respect to

- mass: proton (938.28 MeV/c^2) and neutron (939.57 MeV/c^2)
- interaction with the nuclear force

Both nucleons have isospin $t = 1/2$.

n^0 ↑ ($t_z = +\frac{1}{2}$) isospin up   p$^+$ ↓ ($t_z = -\frac{1}{2}$) isospin down

Isospin has familiar angular momentum properties:

$$S^2|s\rangle = \hbar^2 s(s+1)|s\rangle \implies T^2|t\rangle = t(t+1)|t\rangle$$

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Isospin Symmetry Breaking

- Isospin is "rotated" ($T_\pm$) via β decay.

- Some properties of the nucleus are unchanged under this rotation, hence isospin *symmetry*.

- Symmetry is not exact (Coulomb interaction and pion exchange).

- Computational methods encounter *spurious* ISB, i.e. there are sources of ISB not predicted by theory, due to approximations.

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Why is this important?

Physicists want to know more about the universe. We are probing the limits of the SM, which predicts unitarity of CKM matrix

$$\begin{pmatrix} |d_{\mathsf{w}}\rangle \\ |s_{\mathsf{w}}\rangle \\ |b_{\mathsf{w}}\rangle \end{pmatrix} = \begin{pmatrix} V_{\mathsf{ud}} & V_{\mathsf{us}} & V_{\mathsf{ub}} \\ V_{\mathsf{cd}} & V_{\mathsf{cs}} & V_{\mathsf{cb}} \\ V_{\mathsf{td}} & V_{\mathsf{ts}} & V_{\mathsf{tb}} \end{pmatrix} \begin{pmatrix} |d_{\mathsf{s}}\rangle \\ |s_{\mathsf{s}}\rangle \\ |b_{\mathsf{s}}\rangle \end{pmatrix}$$

$$\implies |V_{\mathsf{ud}}|^2 + |V_{\mathsf{us}}|^2 + |V_{\mathsf{ub}}|^2 = 0.9985(05) \overset{!}{=} 1$$

$$|V_{\mathsf{ud}}|^2 \approx 0.97373(31)[3]$$

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Why is this important?

We can measure V_{ud}!

$$ft(1 + \delta'_{\mathsf{R}})(1 + \delta_{\mathsf{NS}} - \delta_{\mathsf{C}}) = \frac{K}{2G_{\mathsf{V}}^2 |V_{\mathsf{ud}}|^2 (1 + \Delta_{\mathsf{R}}^{\mathsf{V}})}$$

$$|M_{\mathsf{fi}}|^2 = \left| \langle \psi_{\mathsf{f}} | \, T_{\pm} | \psi_{\mathsf{i}} \rangle \right|^2 \equiv (1 - \delta_{\mathsf{C}}) \left| \langle \psi_{\mathsf{f}}^{\mathsf{iso}} | \, T_{\pm} | \psi_{\mathsf{i}}^{\mathsf{iso}} \rangle \right|^2 \underset{t=1}{=} 2(1 - \delta_{\mathsf{C}})$$

$$T_{\pm} \implies \delta_{\mathsf{C}} \implies V_{\mathsf{ud}} \implies \mathsf{BSM}$$

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What was the issue?

ISB with ^{14}O HF Minnesota reference, $e_{max} = 3$

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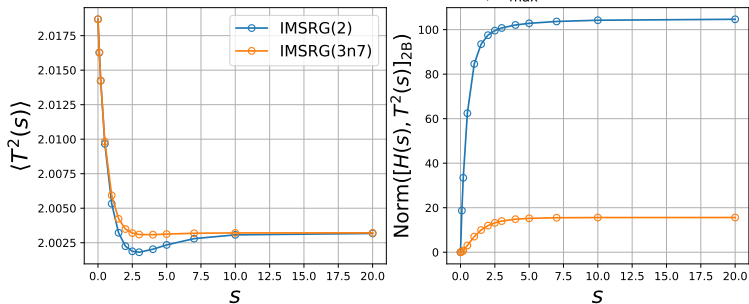
IMSRG

Ab initio calculations for the nucleus are hard:

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

$$\hat{H} = \sum_{i=1}^{N} \frac{1}{2m_i}\hat{P}_i^2 + \hat{V}(\hat{X}_1, ..., \hat{X}_N)$$

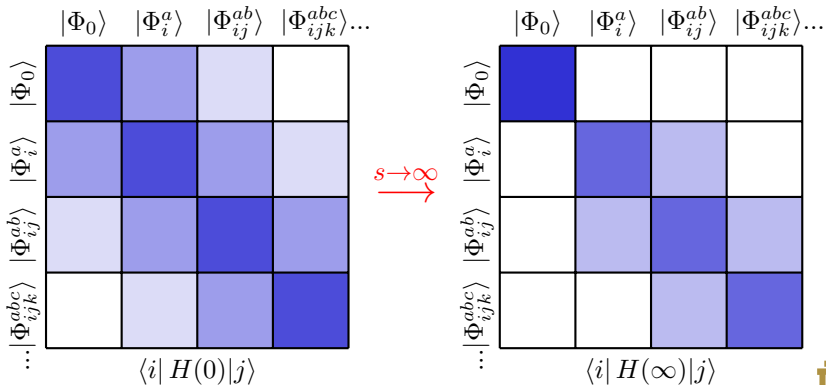Simplify with in-medium similarity renormalisation group [4]:

$$\hat{H}(s) = \hat{U}(s)\hat{H}(0)\hat{U}^\dagger(s)$$
$$= \hat{H}^{\mathsf{d}}(s) + \hat{H}^{\mathsf{od}}(s)$$

$$\hat{H}(s) \stackrel{s\to\infty}{=} \hat{H}^{\mathsf{d}}(s) \implies \text{Useful!}$$

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IMSRG

$$\langle \Phi_0 | \, H(s) | \Phi_0 \rangle = \langle \Phi_0 | \, U(s) H(0) U^\dagger(s) | \Phi_0 \rangle = \langle \psi | \, H(0) | \psi \rangle = E$$

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Normal-ordering

In second-quantised form,

$$\hat{H} = \sum_{\mu\lambda} \langle\mu|\,\hat{H}_{\text{1B}}|\lambda\rangle a_\mu^\dagger a_\lambda + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\,\hat{H}_{\text{2B}}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma + ...$$

To make things simpler, adopt following notation.

$$\{a_\mu^\dagger a_\lambda\} = a_\mu^\dagger a_\lambda - \langle\Phi_0|\, a_\mu^\dagger a_\lambda|\Phi_0\rangle$$

$$\implies \langle\Phi_0|\,\{a_\mu^\dagger a_\lambda\}|\Phi_0\rangle = 0$$

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Normal-ordering

$$\hat{H} = E_{\sf ref} + \overbrace{\sum_{pq} f_{pq}\{a_p^\dagger a_q\} + \underbrace{\frac{1}{4}\sum_{pqrs}\Gamma_{pqrs}\{a_p^\dagger a_q^\dagger a_s a_r\}}_{}}^{\text{IMSRG (2)}}+...$$

IMSRG (3)+

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Magnus formulation

$$U(s) \equiv e^{\Omega(s)} \qquad \frac{d}{ds}U(s) \equiv \eta(s)U(s)$$

$$\implies \hat{\mathcal{O}}(s) \approx \hat{\mathcal{O}}(0) + \left[\eta(s), \hat{\mathcal{O}}(0)\right] + \left[\eta(s), \left[\eta(s), \hat{\mathcal{O}}(0)\right]\right] + ...$$

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Locating spurious ISB

To identify sources of spurious ISB, needed to create scenario where no authentic ISB exists:

- Choose $^{14}_{8}$O Hartree-Fock (asymmetric) reference state.
- Swap realistic nuclear force for Minnesota potential

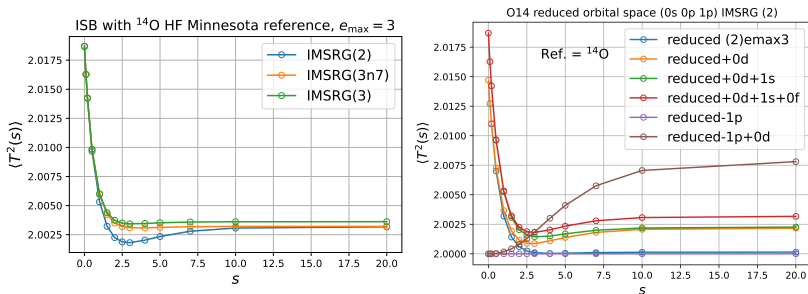$$\hat{H} \sim \text{ Kinetic Energy} + \text{ Minnesota} + \text{ Spin-Orbit}$$

- Treat only occupied states in reference as 'diagonal'
- Choose White generator $\hat{\eta}(s) = \hat{H}^{\text{od}}/\Delta$ [4]
- $\implies$ See where error in $\langle T^2(s) \rangle$ comes from...

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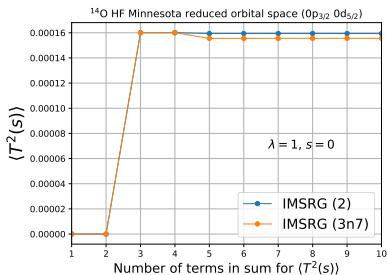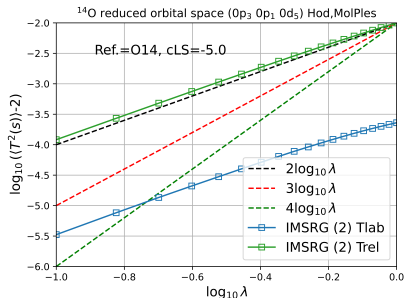
Locating spurious ISB

IMSRG truncation?

(Left) IMSRG truncation is relaxed yet the error does not decrease
(Right) Different orbital spaces display different convergence behaviours.

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Locating spurious ISB

Treat as perturbative scenario, with λH^{od}

(Left) Indicates error scales as λ^2. (Right) Shows problematic term $\langle [\eta(s), [\eta(s), T^2(0)]] \rangle$ indeed has two factors of H^{od}.

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Assessing spurious ISB

$$\langle[\eta(s),[\eta(s),T^2(0)]]\rangle = -2\,\langle\Phi_0|\,\eta_{2B}(s)T_{1B}^2(0)\eta_{2B}(s)|\Phi_0\rangle$$
$$-2\,\langle\Phi_0|\,\eta_{2B}(s)T_{2B}^2(0)\eta_{2B}(s)|\Phi_0\rangle$$

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Assessing spurious ISB

$$\langle[\eta(s),[\eta(s),T^2(0)]]\rangle = -2\,\langle\Phi_0|\,\eta_{2B}(s)T_{1B}^2(0)\eta_{2B}(s)|\Phi_0\rangle$$
$$-2\,\langle\Phi_0|\,\eta_{2B}(s)T_{2B}^2(0)\eta_{2B}(s)|\Phi_0\rangle$$

(trust me)

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Spurious isospin symmmetry breaking in the IMSRG

Assessing spurious ISB

$$\langle\Phi_0|\,\eta_{2B}(s)T_{2B}^2(0)\eta_{2B}(s)|\Phi_0\rangle$$

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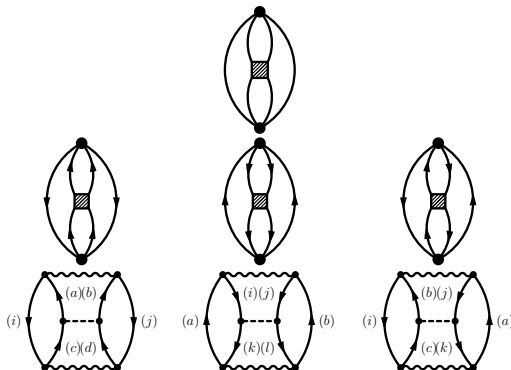
Assessing spurious ISB

$$\langle \Phi_0 | \, \eta_{2B}(s) T_{1B}^2(0) \eta_{2B}(s) | \Phi_0 \rangle$$

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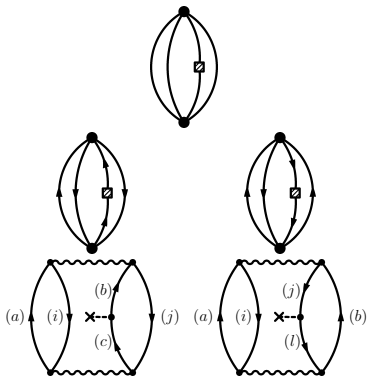
Assessing spurious ISB

$$\langle \big[\eta(s), \big[\eta(s), T^2(0) \big] \big] \rangle = ...$$

$$= \sum_{abij} \Big[\eta_{ijab} \big(\overbrace{\frac{1}{2}\eta_{abij}(n_{\bar{j}} - n_{\bar{b}})}^{T_{1B}^2} + \overbrace{\frac{1}{4}\eta_{\bar{a}\bar{b}ij}\overline{n}_{\bar{a}}\overline{n}_{\bar{b}}}^{T_{2B}^2 \text{ p ladder}} + \overbrace{\frac{1}{4}\eta_{ab\bar{i}\bar{j}}n_{\bar{i}}n_{\bar{j}}}^{T_{2B}^2 \text{ h ladder}}$$

$$\overbrace{-\eta_{a\bar{b}\bar{i}j}\overline{n}_{\bar{b}}n_{\bar{j}}}^{T_{2B}^2 \text{ ring}} \big) + \eta_{ija\bar{j}}\eta_{abi\bar{b}}\overline{n}_{\bar{j}}n_{\bar{b}} \Big]$$

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Assessing spurious ISB

$$\langle\left[\eta(s),\left[\eta(s),T^2(0)\right]\right]\rangle = ...$$

$$= \sum_{abij}\Big[\eta_{ijab}\big(\overbrace{\frac{1}{2}\eta_{abij}(n_{\bar{j}}-n_{\bar{b}})}^{T^2_{1B}}+\overbrace{\frac{1}{4}\eta_{\bar{a}\bar{b}ij}\overline{n}_{\bar{a}}\overline{n}_{\bar{b}}}^{T^2_{2B}\text{ p ladder}}+\overbrace{\frac{1}{4}\eta_{ab\bar{i}\bar{j}}n_{\bar{i}}n_{\bar{j}}}^{T^2_{2B}\text{ h ladder}}$$

$$\overbrace{-\eta_{ab\bar{i}\bar{j}}\overline{n}_{\bar{b}}n_{\bar{j}}}^{T^2_{2B}\text{ ring}}\big) + \eta_{ija\bar{j}}\eta_{abi\bar{b}}\overline{n}_{\bar{j}}n_{\bar{b}}\Big]$$

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Assessing spurious ISB

Having evaluated the problematic term, it was found that
Møller-Plesset and Epstein-Nesbet partitionings of Δ for
$\hat{\eta}(s) = \hat{H}^{\mathrm{od}}/\Delta$ both lead to spurious ISB. When η was switched to
the imaginary time generator [4], the error vanished for a
symmetric reference and $\hat{H}^{\mathrm{od}}$ (and thus η).

$$\implies \quad \text{makes sense}$$

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Sources of spurious ISB

- Δ of White generator
- Reference asymmetry
- H^{od} asymmetry

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Remedies for spurious ISB

- Δ of White generator Choose imaginary time instead
- Reference asymmetry Could be fixed with IMSRG(3)?
- H^{od} asymmetry Symmetrise core, diagonalise VS?

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Thank you

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