Spurious isospin symmmetry breaking in the IMSRG

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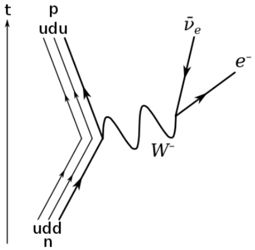
Beta Decay

Three types of β-decay[1]:

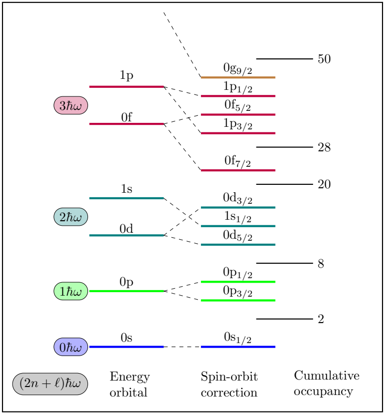
- β^+: $\mathrm{p}^+ \rightarrow \mathrm{n}^0 + e^+ + \nu_e$
- β^-: $\mathrm{n}^0 \rightarrow \mathrm{p}^+ + e^- + \bar{\nu}_e$
- e^- capture:
  ${}^{A}_{Z}X + e^- \rightarrow {}^{A}_{Z-1}Y + \nu_e$

Feynman Diagrams:



Nuclear Shell Model

Can approximate nucleon energies as



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

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 $\uparrow$ $(t_z = +\frac{1}{2})$ isospin up   p$^+$ $\downarrow$ $(t_z = -\frac{1}{2})$ isospin down

Isospin has familiar angular momentum properties:

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

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.

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

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

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

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

Why is this important?

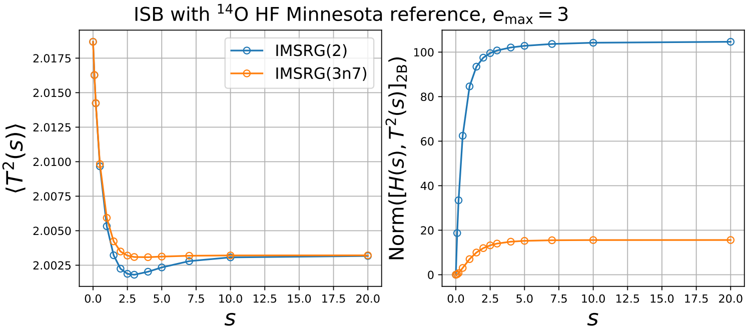
We can measure V_{ud}!

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

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

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

What was the issue?



IMSRG

Ab initio calculations for the nucleus are hard:

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

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

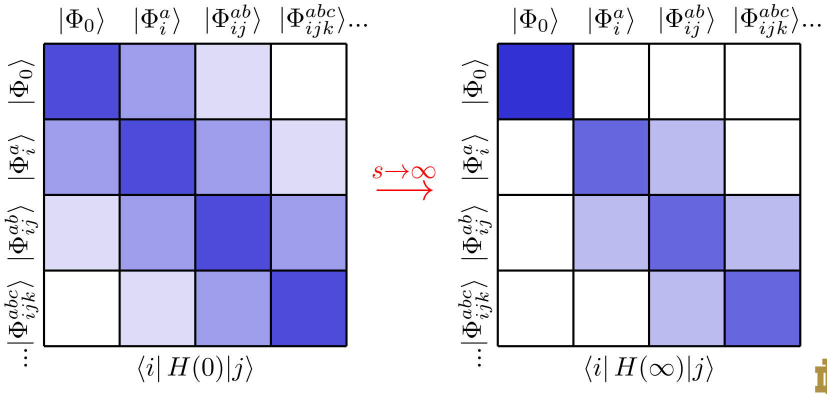
Simplify with in-medium similarity renormalisation group [4]:

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

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

IMSRG

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



Normal-ordering

In second-quantised form,

$$\hat{H} = \sum_{\mu\lambda} \langle\mu| \hat{H}_{\mathsf{1B}} |\lambda\rangle a^\dagger_\mu a_\lambda + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta| \hat{H}_{\mathsf{2B}} |\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta + \ldots$$

To make things simpler, adopt following notation.

$$\{a^\dagger_\mu a_\lambda\} = a^\dagger_\mu a_\lambda - \langle\Phi_0| a^\dagger_\mu a_\lambda |\Phi_0\rangle$$

$$\implies \langle\Phi_0| \{a^\dagger_\mu a_\lambda\} |\Phi_0\rangle = 0$$

Normal-ordering

$$\hat{H} = \overbrace{E_{\text{ref}} + \sum_{pq} f_{pq}\{a_p^\dagger a_q\} + \frac{1}{4}\sum_{pqrs}\Gamma_{pqrs}\{a_p^\dagger a_q^\dagger a_s a_r\}}^{\text{IMSRG (2)}}\!\underbrace{\phantom{E_{\text{ref}} + \sum_{pq} f_{pq}\{a_p^\dagger a_q\} + \frac{1}{4}\sum_{pqrs}\Gamma_{pqrs}\{a_p^\dagger a_q^\dagger a_s a_r\}} + \ldots}_{\text{IMSRG (3)+}}$$

Magnus formulation

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

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

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

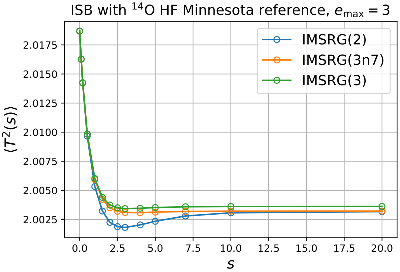
$$\hat{H} \sim \text{ Kinetic Energy} + \text{ Minnesota} + \text{ Spin-Orbit}$$

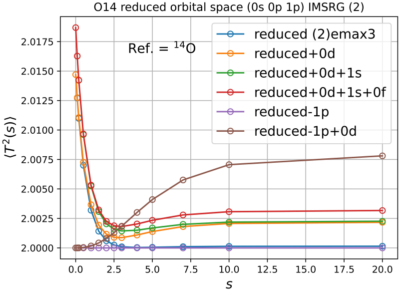
- Treat only occupied states in reference as 'diagonal'
- Choose White generator $\hat{\eta}(s) = \hat{H}^{\text{od}}/\Delta$ [4]

$\implies$ See where error in $\langle T^2(s) \rangle$ comes from...

Locating spurious ISB

IMSRG truncation?

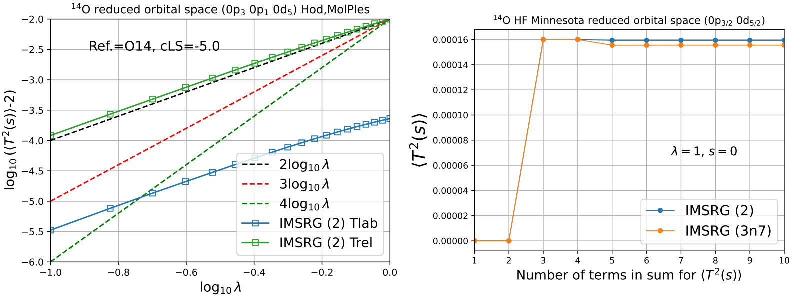




(Left) IMSRG truncation is relaxed yet the error does not decrease
(Right) Different orbital spaces display different convergence behaviours.

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}.

Assessing spurious ISB

$$
\begin{aligned}
\langle [\eta(s), [\eta(s), T^2(0)]] \rangle = & -2 \langle \Phi_0 | \, \eta_{\text{2B}}(s) T^2_{\text{1B}}(0) \eta_{\text{2B}}(s) | \Phi_0 \rangle \\
& -2 \langle \Phi_0 | \, \eta_{\text{2B}}(s) T^2_{\text{2B}}(0) \eta_{\text{2B}}(s) | \Phi_0 \rangle
\end{aligned}
$$

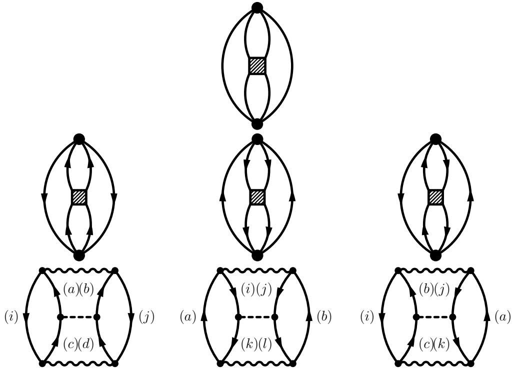
Assessing spurious ISB

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

(trust me)

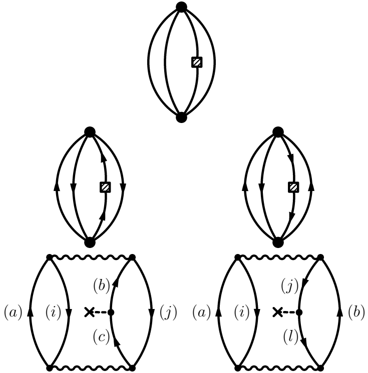
Assessing spurious ISB

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



Assessing spurious ISB

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



Assessing spurious ISB

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

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

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

Assessing spurious ISB

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

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

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

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).

$\Longrightarrow$ makes sense

Sources of spurious ISB

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

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