Spurious isospin symmmetry breaking in the IMSRG

Alexander Farren (supervised by Prof. Stroberg)

University of Notre Dame

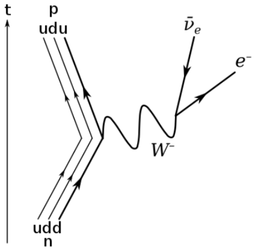
June 2023

Beta Decay

Three types of β-decay[1]:

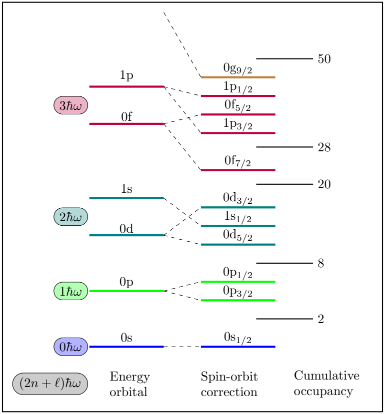
- β^+: $p^+ \rightarrow n^0 + e^+ + \nu_e$
- β^-: $n^0 \rightarrow p^+ + e^- + \bar{\nu}_e$
- e^- capture: ${}^A_Z X + e^- \rightarrow {}^A_{Z-1} Y + \nu_e$

Feynman Diagrams:



Nuclear Shell Model

Can approximate nucleon energies as levels or shells



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

Isospin

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

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

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

$\mathrm{n}^0 \uparrow (t_z = +\frac{1}{2})$ isospin up $\mathrm{p}^+ \downarrow (t_z = -\frac{1}{2})$ 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[3]

$$\begin{pmatrix} |d_w\rangle \\ |s_w\rangle \\ |b_w\rangle \end{pmatrix} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \begin{pmatrix} |d_s\rangle \\ |s_s\rangle \\ |b_s\rangle \end{pmatrix}$$

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

$$|V_{ud}|^2 \approx 0.97373(31)$$

Why is this important?

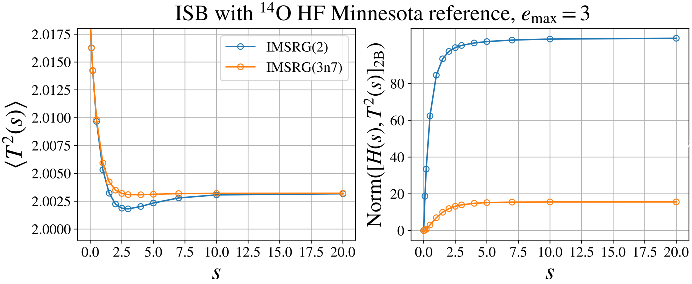
We can measure V_{ud}!

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

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

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

What was the issue?



(Left) $\langle T^2(s \to \infty)\rangle$ should be 2.
(Right) Norm$\left(\left[H(s), T^2(s)\right]_{2B}\right)$ should be 0.

IMSRG

Ab initio calculations for the nucleus are hard:

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

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

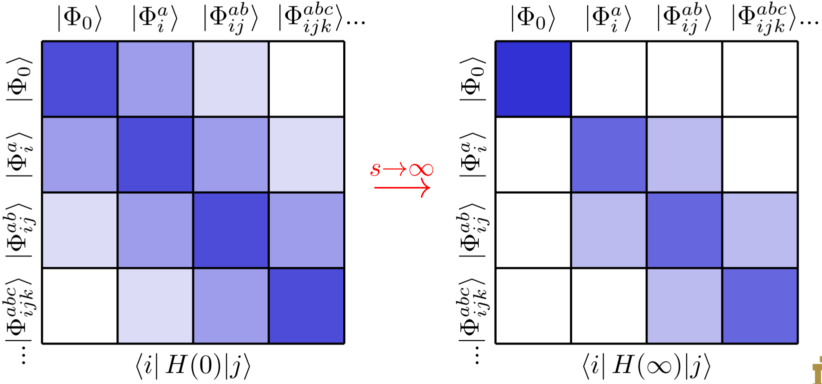
Simplify with in-medium similarity renormalisation group [4]:

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

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

IMSRG

$$\langle\Phi_0|H(s)|\Phi_0\rangle = \langle\Phi_0|U(s)H(0)U^\dagger(s)|\Phi_0\rangle \overset{s\to\infty}{=} \langle\psi|H(0)|\psi\rangle = E$$



Normal-ordering

In second-quantised form,

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

To make things simpler, adopt following notation.

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

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

Normal-ordering

IMSRG (2)

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

IMSRG (3)+

Magnus formulation

Impose definition on transformation

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

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

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

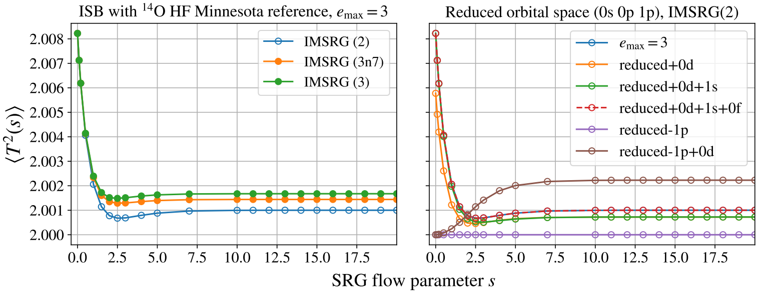
$$\hat{H} \sim \text{ Kinetic Energy} + \text{ Minnesota} + \text{ Spin-Orbit}$$

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

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

Locating spurious ISB

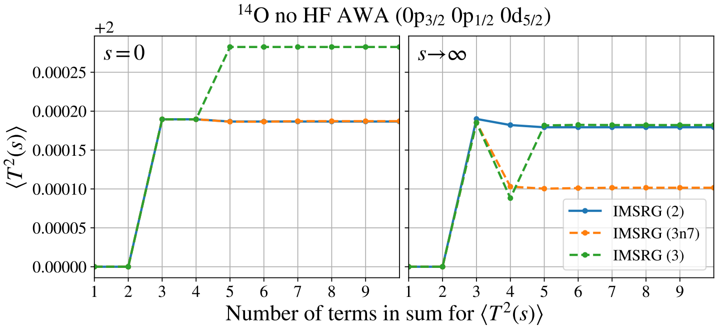
IMSRG truncation?



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

Locating spurious ISB

Pinpoint source of ISB in 0s 0p 0d reduced orbital space



Shows problematic term $\langle [\eta(s), [\eta(s), T^2(0)]] \rangle$ persists under IMSRG flow. What is it?

Assessing spurious ISB

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

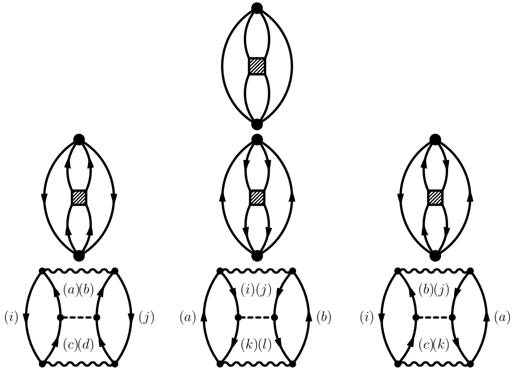
Assessing spurious ISB

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

(trust me)

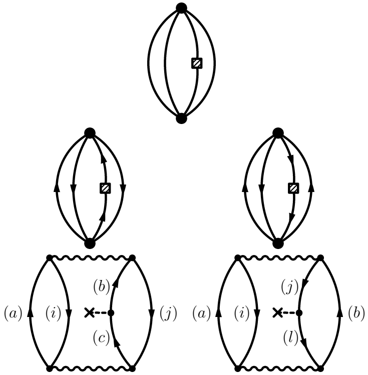
Assessing spurious ISB

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



Assessing spurious ISB

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



Assessing spurious ISB

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

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

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

Assessing spurious ISB

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

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

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

Assessing spurious ISB

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

$\implies$ 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?

Acknowledgements

- Prof. Ragnar Stroberg
- Jonathan Riess
- The Physics and Astronomy Department
- The Naughton Foundation
- A fantastic REU cohort

References

[1] K. S, *Introductory Nuclear Physics*. Wiley India, 2008. [Online]. Available: https://books.google.com/books?id=Cxt0CgAAQBAJ.

[2] P. Cappellaro, *Introduction to applied nuclear physics*, Massachusetts Institute of Technology: MIT OpenCouseWare, https://ocw.mit.edu/, Spring 2012.

[3] J. C. Hardy and I. S. Towner, “Superallowed $0^+ \rightarrow 0^+$ nuclear β decays: 2020 critical survey, with implications for V_{ud} and ckm unitarity,” *Phys. Rev. C*, vol. 102, p. 045 501, 4 Oct. 2020. [Online]. Available: https://link.aps.org/doi/10.1103/PhysRevC.102.045501.

[4] H. Hergert, “A guided tour of ab initio nuclear many-body theory,” *Frontiers in Physics*, vol. 8, Oct. 2020. [Online]. Available: https://doi.org/10.3389%2Ffphy.2020.00379.

Thank you