Benchmark Neutrinoless Double-Beta Decay ($0\nu\beta\beta$) Matrix Elements

For MR-IMSRG and NCSM ab initio approaches In a light nucleus

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R. A. M. Basili, J. M. Yao, J. Engel, H. Hergert, M. Lockner, P. Maris, and J. P. Vary, (2019), arXiv:1909.06501 [nucl-th] .

Why is Modeling $0\nu\beta\beta$-decay Important?

Neutrinos remain poorly understood, being extremely light & chargeless.

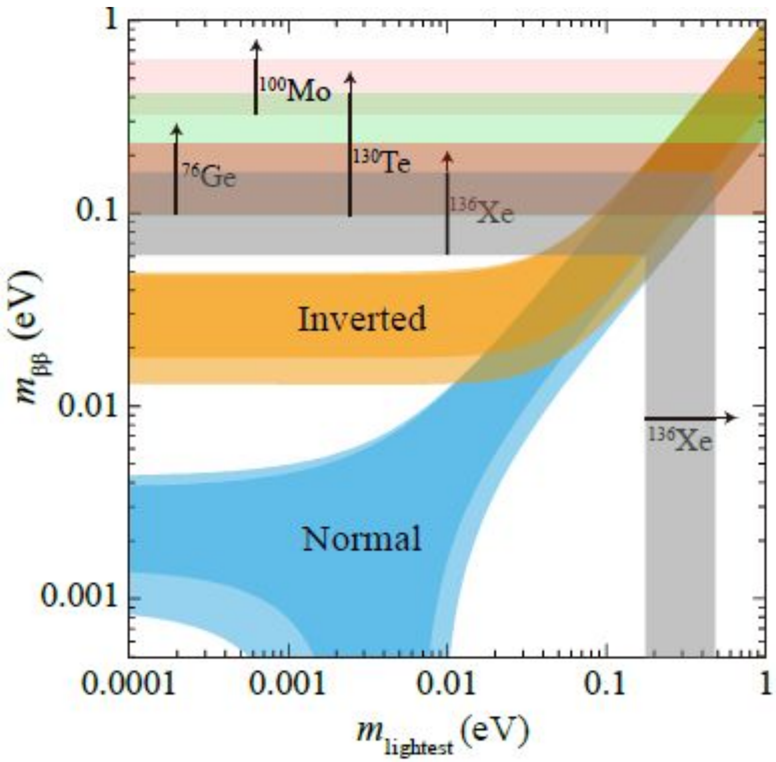
Observing $0\nu\beta\beta$ is considered one of the best ways to:

- Identify if neutrinos are *Majorana* fermions (i.e. their own anti-particle).
- Shed light on the neutrino mass hierarchy.
- Give insight on leptogenesis and the apparent matter-antimatter asymmetry of the universe.
- Determine whether a Lepton Number Violating (LNV) process exists.

But $0\nu\beta\beta$ (if it exists) is very rare.

Work on several experiments searching for $0\nu\beta\beta$ using ton-scale quantities of heavy nuclei (Ge-76 and up) continues to develop.

Bounds and Predictions from Experiment in 2020



Isotope, Q^a, NA^b MeV, %	$T_{1/2}^{2\nu\ c}$ 10^{19} y	$T_{1/2}^{0\nu}$ 10^{24} y	$m_{\beta\beta}$ eV	Experiment	Ref. Year
^{48}Ca, 4.268, 0.187	$4.4^{+0.6}_{-0.5}$	>0.058	<3.5–22	ELEGANT-IV	[49], 2008
		>0.062^d		CANDELS	[48], 2019
^{76}Ge, 2.039, 7.8	165^{+14}_{-12}	>90^d	<0.10–0.23^d	GERDA-II	[23], 2019
		> 27	<0.200–0.433	Majorana D.	[32], 2019
		>1000^e	<0.33–0.76^f	LEGEND-200	[33], 2021^f
		>10^{4e}	<0.017^e	LEGEND-1000	[33], 2025/6^f
^{82}Se, 2.998, 8.8	9.2±0.7	>0.36	<0.89–2.43	NEMO-3	[47], 2011
		>100	<0.05–0.1	SuperNEMO	[50], 2019^f
		>2.4	<0.376–0.770	CUPID-0	[41], 2018
^{100}Mo, 3.034, 9.7	0.71±0.04	>1.1	<0.33–0.62	NEMO-3	[24], 2015
		>0.095	<1.2–2.1	AMoRE-Pilot	[45], 2019
		>10^e	<0.12–0.2^e	AMoRE-I	[46], 2019^f
		>500^e	<0.017–0.029^e	AMoRE-II	[46], 2021^f
		>0.3^d	<0.715–1.19^d	CUPID-Mo	[42], 2019
		>1000^d	<20^d	CUPID	[43], 2025^f
^{130}Te, 2.528, 34.1	69±13	>23^d	<0.09–0.42^d	CUORE	[25], 2019
		>210^e	<0.03^g	SNO+	[28], 2020^f
^{136}Xe, 2.458, 8.9	219±6	>107	<0.061–0.165	KamL.-Zen400	[26], 2017
		>500^e	<0.028–0.076^e	KamL.-Zen800	[51], 2019
		>35	<0.093–0.286	EXO-200	[35], 2019
		>920^e	<0.009–0.018^e	nEXO	[52], 2027^f
		>0.21	<1.4–3.7	PandaX-II	[53], 2019
		>90^e	<0.06–0.18^e	PandaX-III	[38], 2020^f
		>90^e	<0.07–0.13^e	NEXT-100	[37], 2020^f

Next-gen $0\nu\beta\beta$ experiments predicted to enclose inverted band within next **half decade**!

Y.-H. Kim, (2020), arXiv:2004.02510 [hep-ex].

What do we need from Nuclear Structure?

Among other things, we need the **matrix elements (MEs) for the decay** to:

- Predict and model the decay.
- Provide the dependence on the LNV process(es) being observed.

$$\left[T^{0\nu}_{1/2}\right]^{-1} = G_{0\nu}(Q,Z)\,|M_{0\nu}|^2 \left|\sum_k m_k U^2_{ek}\right|^2$$

Decay rate — $\left[T^{0\nu}_{1/2}\right]^{-1}$

phase-space factor — $G_{0\nu}(Q,Z)$

Majorana mass eigenvalue — m_k

Element of neutrino mixing matrix — U^2_{ek}

BUT!

- The MEs require modeling the heavy nuclei used in experiment.
- The heavy nuclei can presently only be modeled with *effective* methods.
- Predictions of MEs differ by a factor of **2-3** between methods!!

We need to improve and validate our predictions by:

- Benchmarking and improving our current effective methods.
- Developing and benchmarking new candidate methods (preferably with strong *ab initio* roots) capable of modeling the heavy nuclei.

Differences in Model Predictions

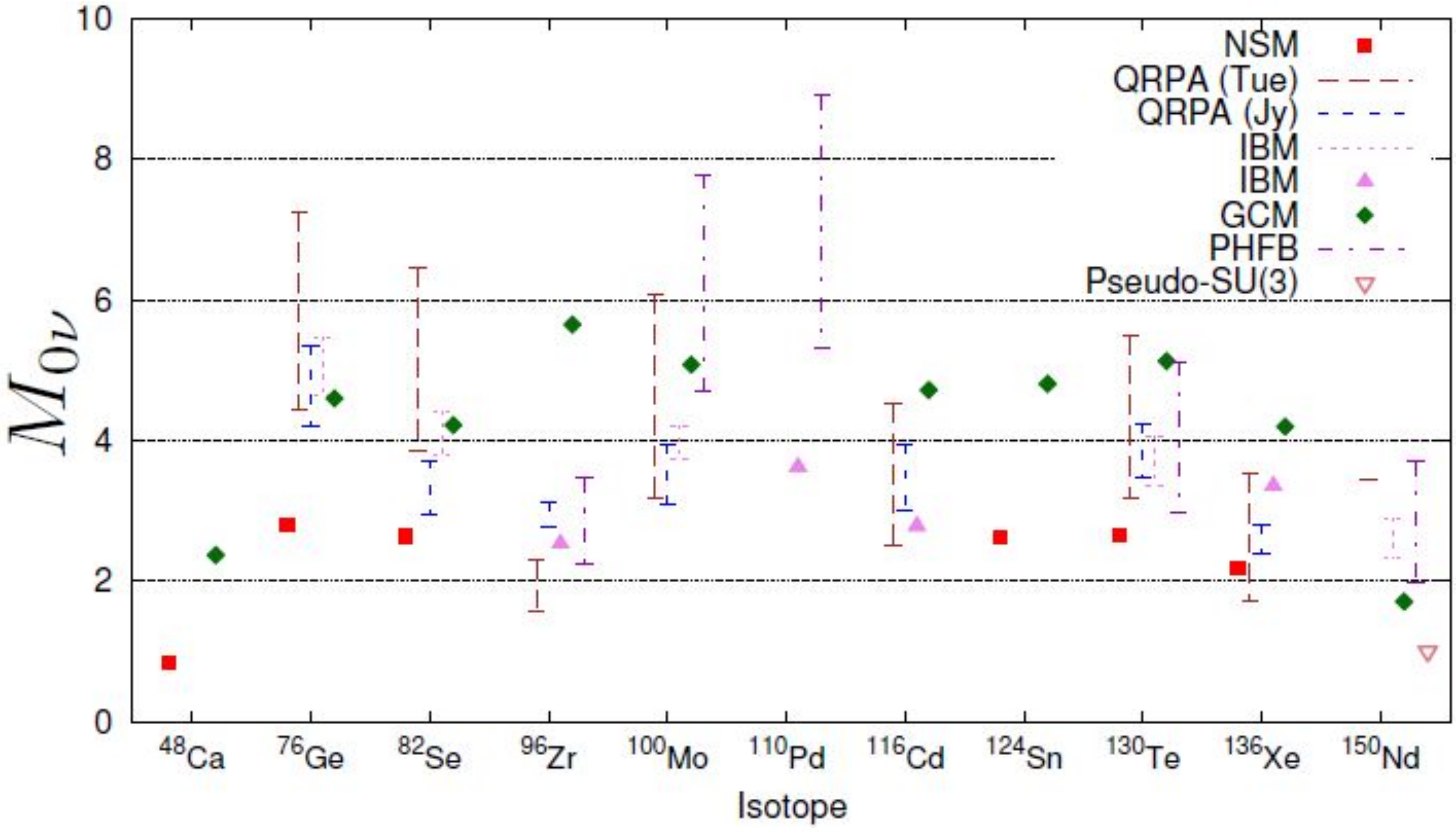


Figure from A. Dueck, W. Rodejohann and K.Zuber, Phys.Rev. D83 (2011) 113010

ab initio vs Effective Models

> *"All nuclear models are effective models; some are just more effective than others."*

ab initio: "from the beginning".

Effective: treated such that only a subset of the available information is preserved, that most often being just the resolution required for a given problem.

***ab initio* methods**: retain all the nucleon DoFs at the cost of greater complexity.

Effective methods: reduce DoFs/resolution at the potential cost of accuracy and/or general applicability.

<u>Example</u>: The Interacting Boson Model (IBM) is effective for modeling even-even nuclei, but isn't very accurate for bound states with unpaired nucleons.

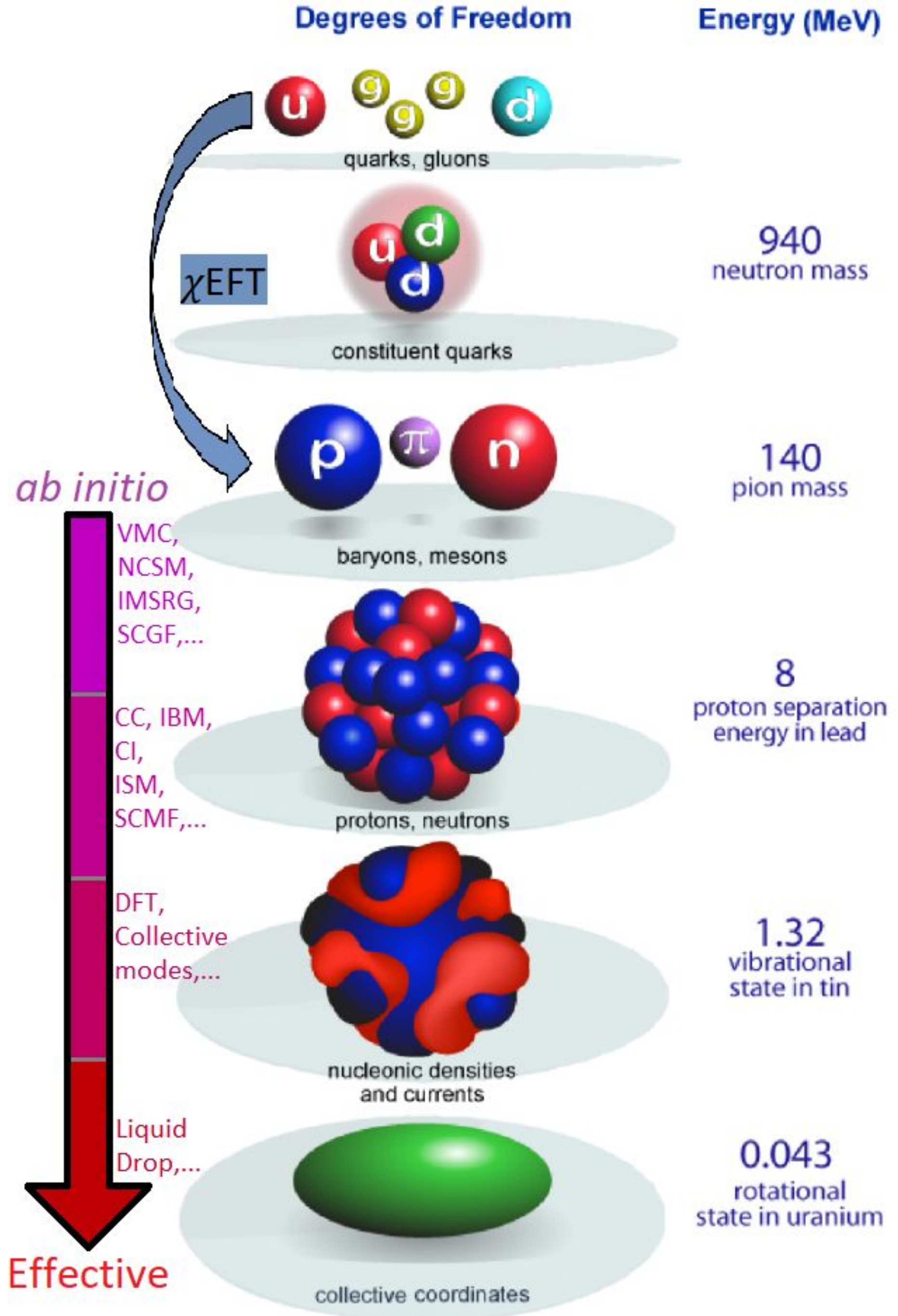
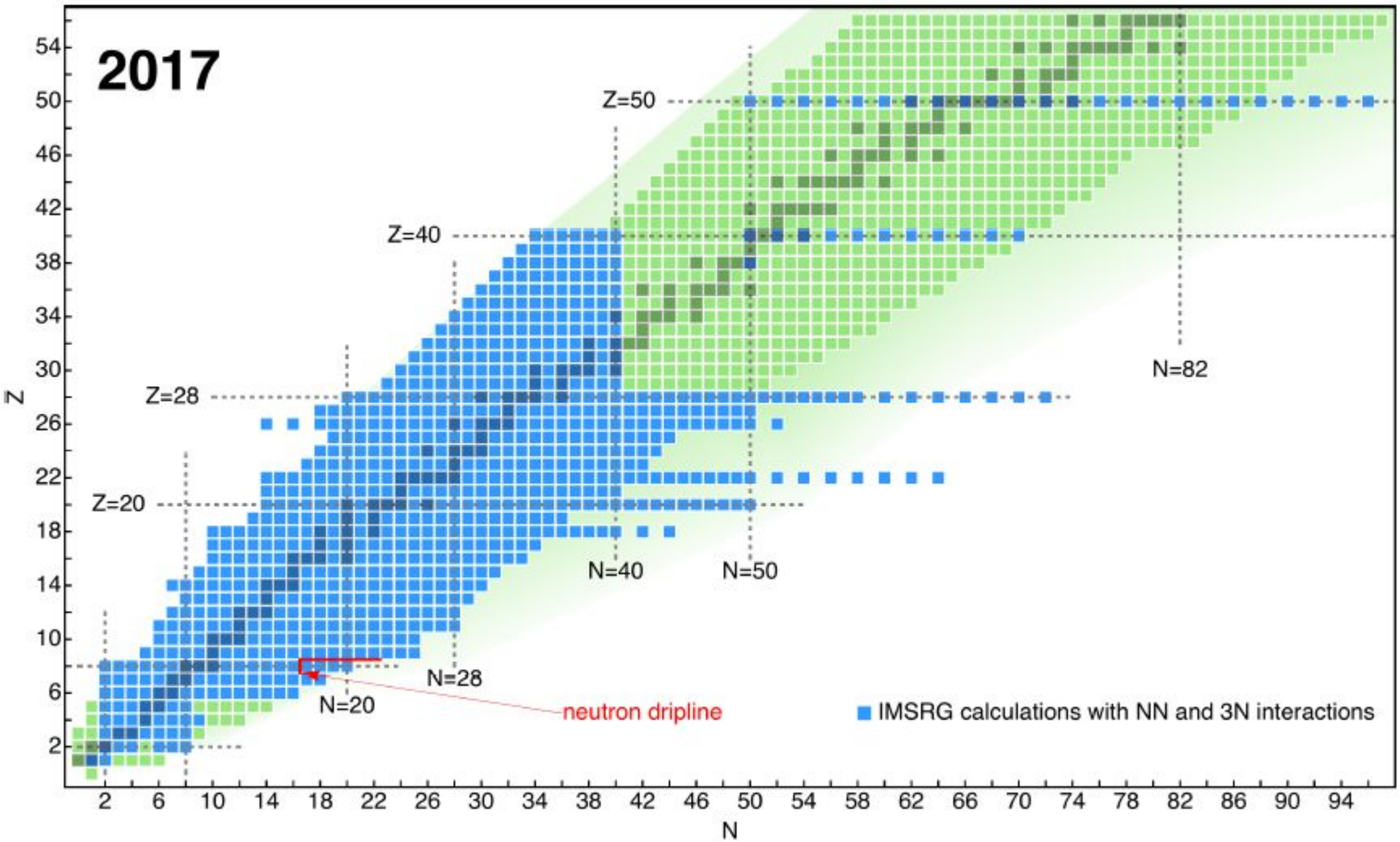


Figure adapted from R. J. Furnstahl, Nucl. Phys. Proc. Suppl. 228, 139 (2012), arXiv:1203.1779 [nucl-th].

IMSRG Low-Lying Spectra Progress (2017)



Multi-Reference In-Medium Similarity Renormalization Group (**MR-IMSRG**) is a variant approach that <u>may be capable of modeling $0\nu\beta\beta$-decay in heavy nuclei</u>.

H. Hergert, J. Yao, T. D. Morris, N. M. Parzuchowski, S. K. Bogner, and J. Engel. J. Phys. Conf. Ser. 1041, 012007 (2018), arXiv:1805.09221 [nucl-th] .

Benchmarking MR-IMSRG with NCSM

Goal: Compare NCSM and MR-IMSRG(2) results for a hypothetical case in a light nucleus, to gain insight on MR-IMSRG results in the heavy nuclei of interest.

MODEL DECAY: **$He^6 \rightarrow Be^6 + 2e^-$**

Details of Calculation:

- Compare **He^6** ground-state energy and proton, neutron, and matter radii.
- Calculate the groundstate-to-groundstate decay under isospin symmetry .
- Consider contribution from light-majorana exchange (ONLY).
- Use the N3LO-EM500, SRG-evolved to λ=2.0 fm^{-1}.
- Use HO NMEs calculated with neutrino potentials from UNC:

$$h_F(|\boldsymbol{q}|) \equiv -g_V^2(\boldsymbol{q}^2),$$

$$h_{GT}(|\boldsymbol{q}|) \equiv g_A^2(\boldsymbol{q}^2) - \frac{g_A(\boldsymbol{q}^2)g_P(\boldsymbol{q}^2)\boldsymbol{q}^2}{3m_N} + \frac{g_P^2(\boldsymbol{q}^2)\boldsymbol{q}^4}{12m_N^2} + \frac{g_M^2(\boldsymbol{q}^2)\boldsymbol{q}^2}{6m_N^2},$$

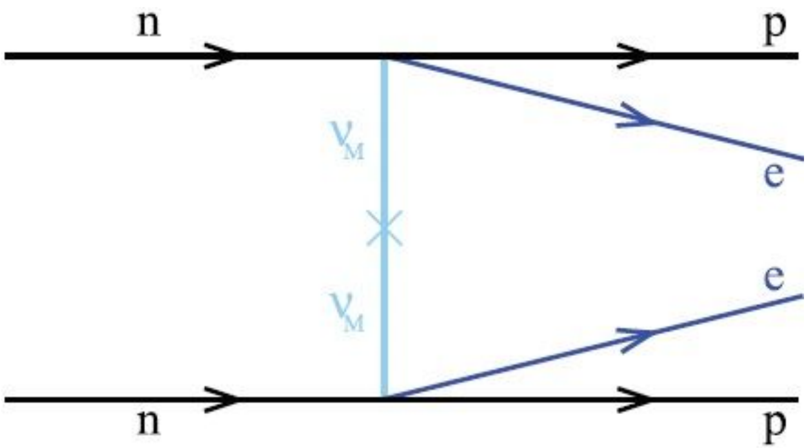
$$h_T(|\boldsymbol{q}|) \equiv \frac{g_A(\boldsymbol{q}^2)g_P(\boldsymbol{q}^2)\boldsymbol{q}^2}{3m_N} - \frac{g_P^2(\boldsymbol{q}^2)\boldsymbol{q}^4}{12m_N^2} + \frac{g_M^2(\boldsymbol{q}^2)\boldsymbol{q}^2}{12m_N^2},$$

J. Engel and J. Menèndez, Rept. Prog. Phys. 80, 046301 (2017), arXiv:1610.06548 [nucl-th].

The $0\nu\beta\beta$ Operator

$$O^{0,2}_{0,-2} = -\frac{1}{4\sqrt{3}}\sum_{abcd}\sum_{J}\left(\mathcal{N}_{ab}(J,1)\,\mathcal{N}_{cd}(J,1)\right)^{-1} \cdot (ab;J\,1|||O^{0,2}|||cd;J\,1)\cdot\left[\left[a^\dagger_a a^\dagger_b\right]^{J,1}\left[\hat{a}_c\hat{a}_d\right]^{J,1}\right]^{0,2}_{0,-2}$$

$$\mathcal{N}_{ij}(J,T) \equiv \sqrt{1-\delta_{ij}(-1)^{J+T}}/(1+\delta_{ij})$$



In transitions where ΔJ=0 (such as between the He-6 -> Be-6 groundstates), J'=J, and we write the components

$$M_{0\nu} = M^{F}_{0\nu} + M^{GT}_{0\nu} + M^{T}_{0\nu}$$

We solve for the HO matrix elements with the operators

$$O^{F}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_0(|\mathbf{q}|r)h_F(|\mathbf{q}|)}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+ ,$$

$$O^{GT}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_0(|\mathbf{q}|r)h_{GT}(|\mathbf{q}|)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+ ;$$

$$O^{T}_{0\nu}(r) = \frac{4R}{\pi g_A^2}\int_0^\infty |\mathbf{q}|d|\mathbf{q}|\frac{j_2(|\mathbf{q}|r)h_T(|\mathbf{q}|)\boldsymbol{S}_{12}}{|\mathbf{q}|+\bar{E}-(E_i+E_f)/2}\tau_1^+\tau_2^+ ,$$

J. Engel and J. Menèndez, Rept. Prog. Phys. 80, 046301 (2017), arXiv:1610.06548 [nucl-th].

ab initio No-Core Shell Model (NCSM)

Goal: Model nuclei microscopically from first principles with a finite matrix method.

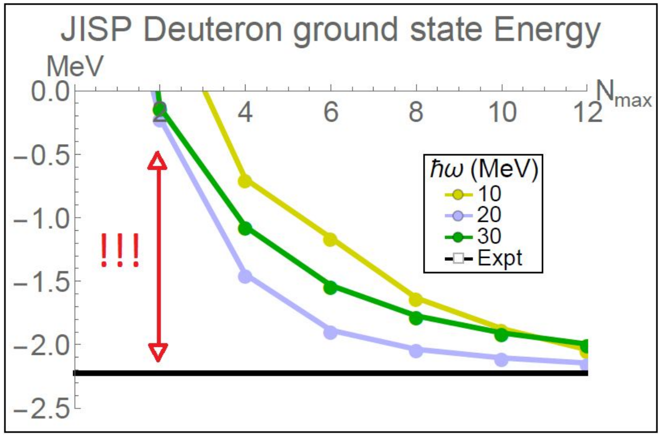
Key Directive: Treat all nucleons on equal footing.

General Process:

1. **Choose nucleus** and NN (& possibly 3N) **effective interaction(s)**.
2. **Construct** many-body (**mb**) **basis** from all possible Slater determinants of the Harmonic Oscillator (HO) single-particle (sp) basis states for the given nucleus.
3. **Construct** effective Hamiltonian, ***H*** as matrix in mb basis.
4. **Solve** large (but sparse) **eigenvalue problem** for H & other observables.
5. **Vary** basis cutoff N_{max} & energy scale $\hbar\Omega$ and **extrapolate**.
6. **Estimate** extrapolation **error** and **compare** results to **experiment**.

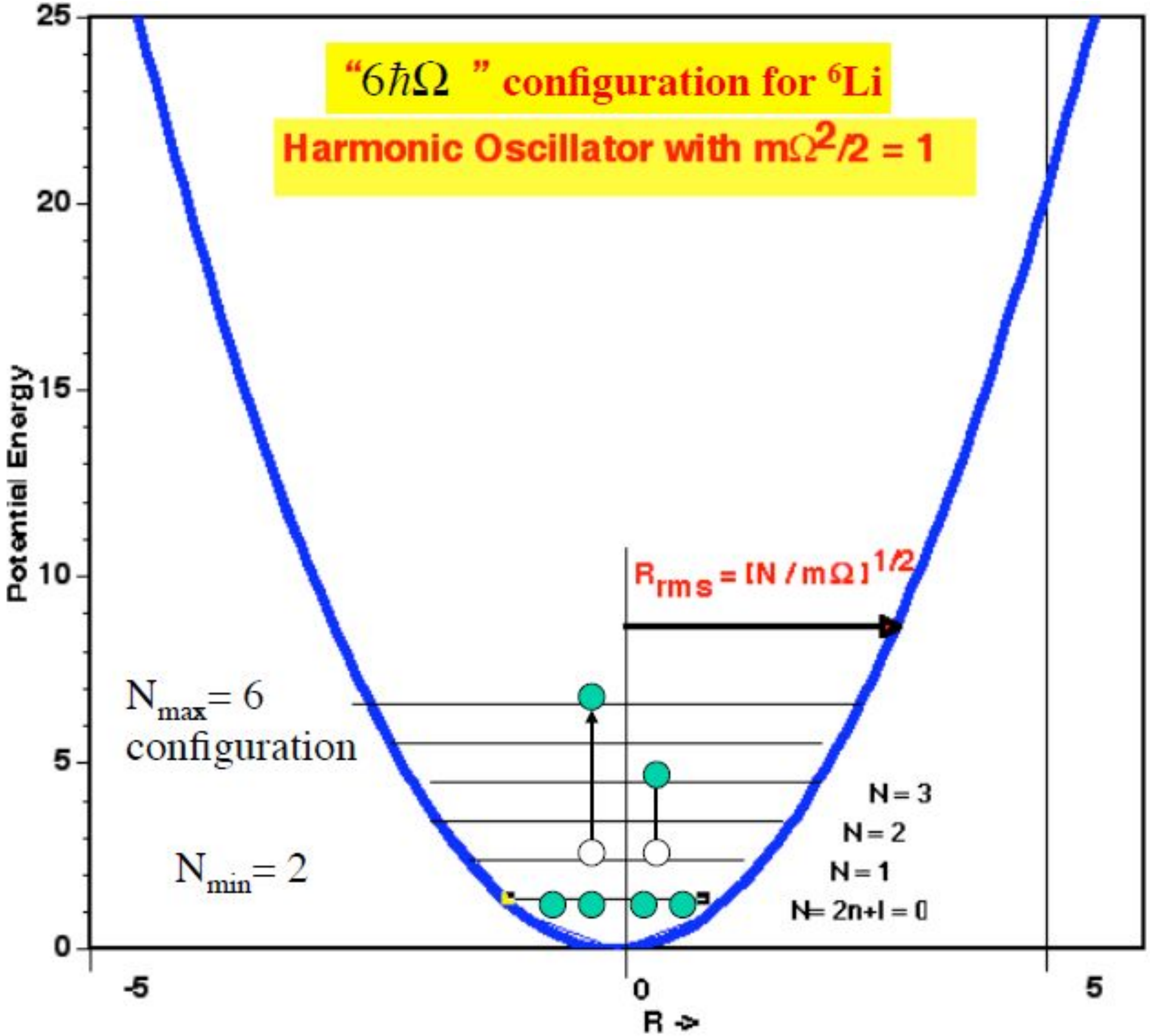
$N_{max} = 2n + l$ = maximum allowed excitation quanta in a basis state.

Results **have no basis dependence** at continuum limit.



B. Barrett, P. Navratil and J. Vary, Prog. Part. Nucl. Phys. 69, (2013).

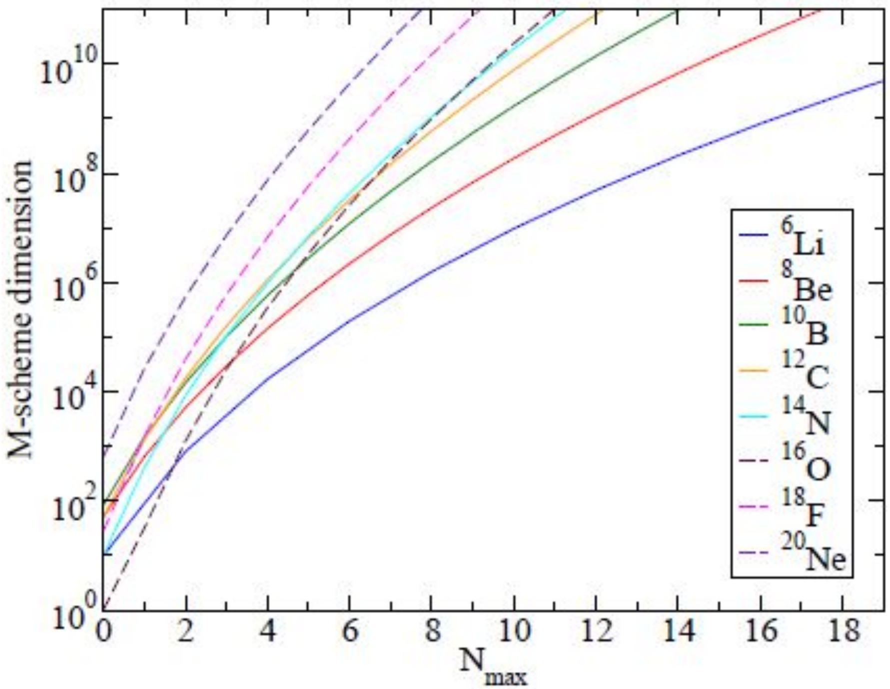
Example Li-6 mp Configuration



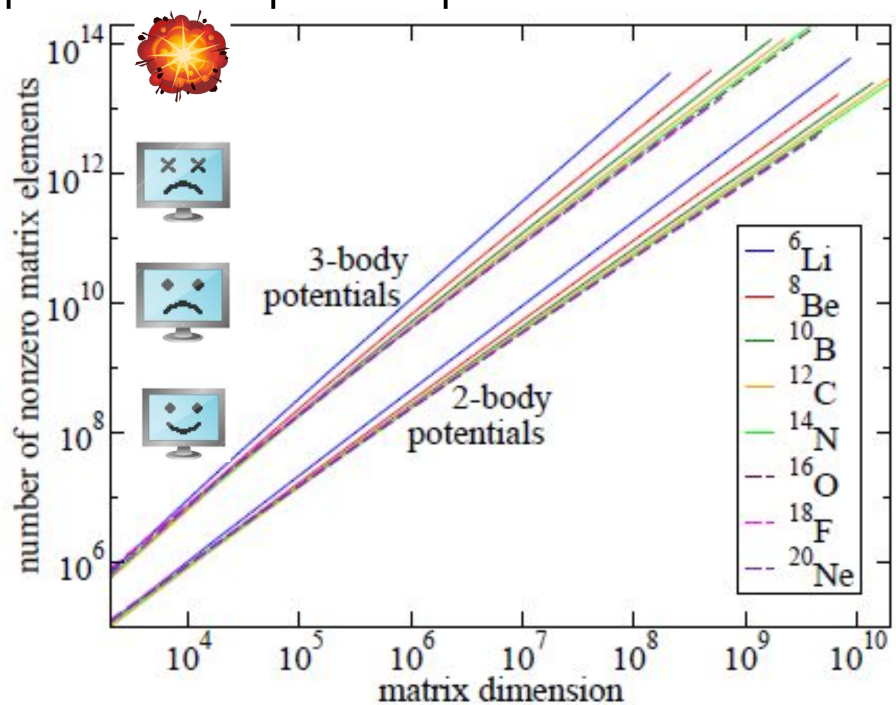
Limitations of NCSM Calculations

Primary Limiting Factor: COMPUTATIONAL RESOURCES

- memory increases rapidly with N_{max} , mb forces, and nucleon count, *A*.
- Quickly outscales the world's most powerful supercomputers.



The mb basis dimension rising with the number of allowed HO excitation quanta, N_{max}, for each case of the listed nuclei.



Number of nonzero matrix elements (nnz) rising with dimension for listed nuclei with and without 3NFs.

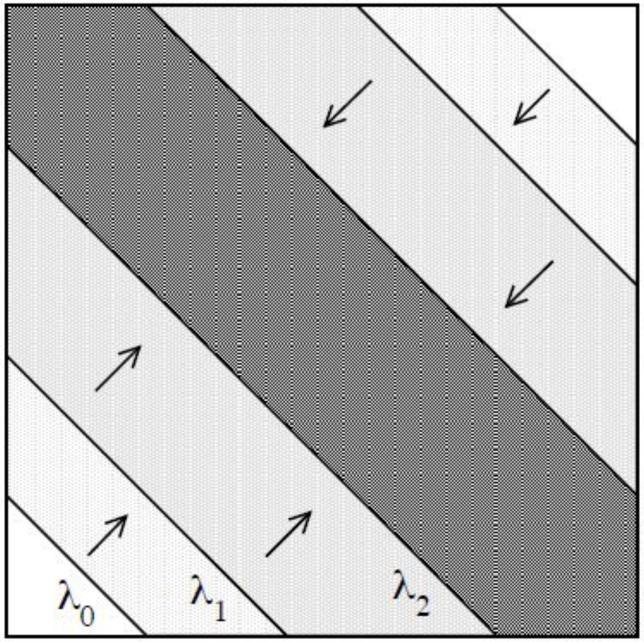
We need ways to reduce resource needs with minimal loss in accuracy.

Figure adapted from M. Shao, H. Aktulga, C. Yang, E. G. Ng, P. Maris, and J. P. Vary, Computer Physics Communications 222, 1 (2018)..

SRG in Brief

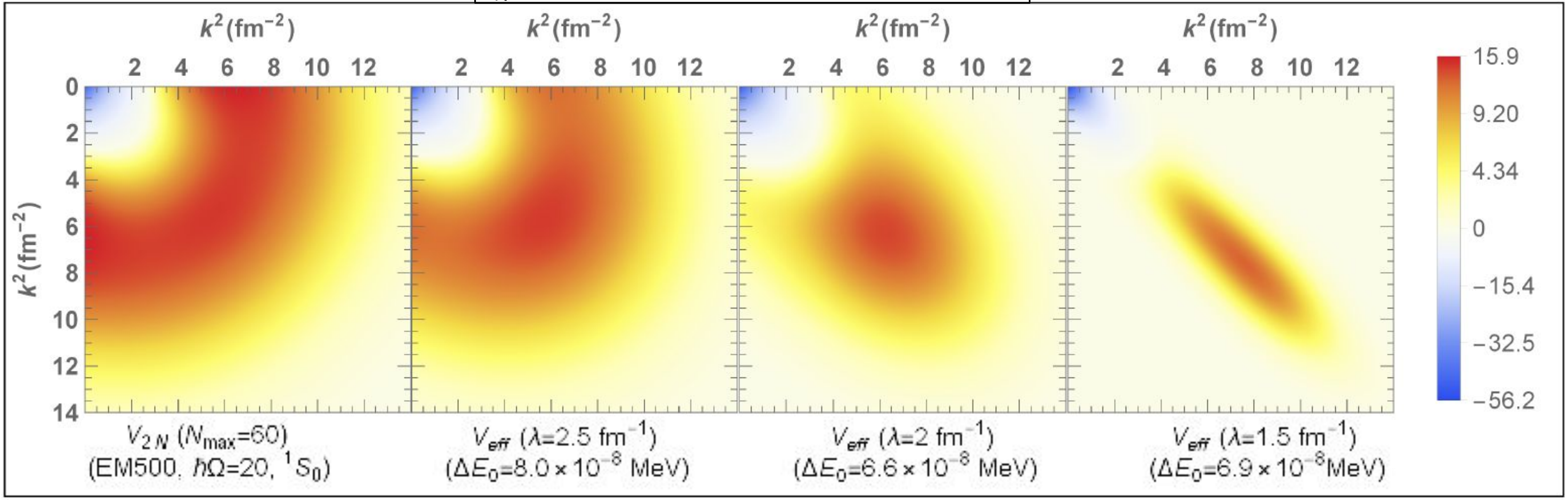
Similarity Renormalization Group (SRG) Procedure:

1. Choose generator: $\eta_\lambda = [V_\lambda, T_{rel}]$
2. Evolve Hamiltonian iteratively with flow equation: $\frac{dH_\lambda}{d\lambda} = -\frac{4}{\lambda^5}[H_\lambda, \eta_\lambda]$



Pulls off-diagonal contributions into the diagonal band.

V_λ SRG-evolution in momentum space



IMSRG in Brief

The Magnus formulation of SRG

Instead of evolving *H*, evolve the SRG-transform using the Magnus expansion

$$\frac{d\hat{H}(s)}{ds} = [\hat{\eta}(s), \hat{H}(s)] \rightarrow \frac{d\hat{U}(s)}{ds} = \hat{\eta}(s)\hat{U}(s) \rightarrow \frac{d\hat{\Omega}(s)}{ds} = \sum_{n=0}^{\infty} \frac{B_n}{n!}[\hat{\Omega}(s), \hat{\eta}(s)]^{(n)}$$

$$\hat{U}(s) \equiv e^{\hat{\Omega}(s)}$$

$$\left[\hat{\Omega}(s), \hat{\eta}(s)\right]^{(0)} = \hat{\eta}(s)\,,$$

$$\left[\hat{\Omega}(s), \hat{\eta}(s)\right]^{(n)} = \left[\hat{\Omega}(s), \left[\hat{\Omega}(s), \hat{\eta}(s)\right]^{(n-1)}\right]$$

Then mb operator O may be evaluated using the Baker-Campbell-Hausdor (BCH) formula

$$e^{\hat{\Omega}(s)}\hat{O}(0)e^{-\hat{\Omega}(s)} = \sum_{n=0}^{\infty} \frac{1}{n!}[\hat{\Omega}(s), \hat{O}(0)]^{(n)}$$

The IMSRG(2) many-body truncation

Use a White generator η that is diagonal in 2-particle 2-hole (2p2h) space to decouple from the valence space.

- Induced many-body terms beyond the IMSRG truncation are discarded.
- Can be improved to 3p3h, 4p4h, etc., at the cost of increased computation.

H. Hergert, S. K. Bogner, T. D. Morris, A. Schwenk, and K. Tsukiyama, Phys. Rept. 621, 165 (2016), arXiv:1512.06956 [nucl-th].

Multi-Reference IMSRG in Brief

Problem: The mb wavefunction of the heavy nuclei of interest cannot be described even approximately using a Slater Determinant.

Solution: Solve for an ***effective*** many-body wavefunction instead.

If we consider the Schrodinger equation when using an SRG evolved potential

$$\left[U(s)HU^{\dagger}(s)\right]U(s)\left|\Psi_k\right\rangle = E_k U(s)\left|\Psi_k\right\rangle$$

Now we're approximating $\boldsymbol{U\Psi_k}$ instead of $\boldsymbol{\Psi_k}$ when doing IMSRG.

Benefits:

- Much smaller induced terms
- May be optimized for collective correlations

Drawbacks:

- Adds additional contraction terms
- Hamiltonian can become rank-deficient (only ground-state is guaranteed to be orthogonal)

H. Hergert, Phys. Scripta 92, 023002 (2017), arXiv:1607.06882 [nucl-th].

Special Considerations for Comparison

- To enable calculation, consider mirror nuclei under good isospin symmetry:

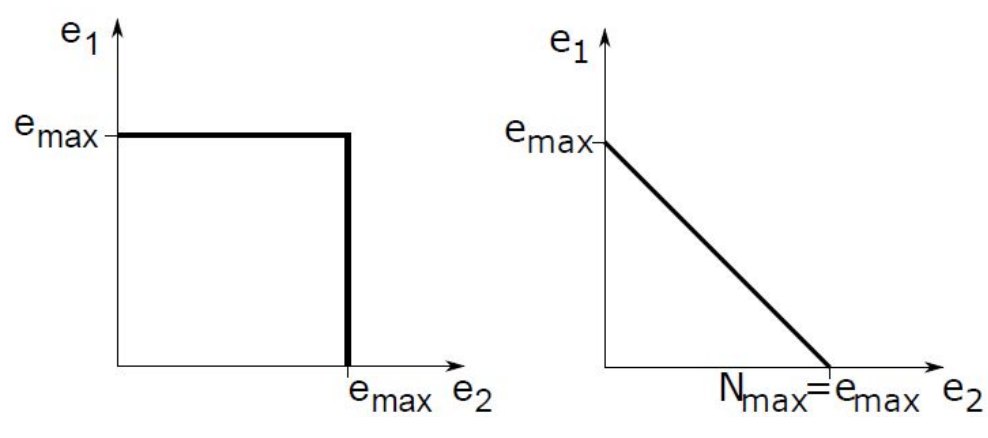
$$\langle {}^6\mathrm{Be}| \left[\left[a_a^\dagger a_b^\dagger \right]^{J,1} \left[\hat{a}_d \hat{a}_c \right]^{J,1} \right]^{0,2}_{0,-2} |{}^6\mathrm{He}\rangle \simeq \sqrt{6} \langle {}^6\mathrm{He}| \left[\left[a_a^\dagger a_b^\dagger \right]^{J,1} \left[\hat{a}_d \hat{a}_c \right]^{J,1} \right]^{0,2}_{0,0} |{}^6\mathrm{He}\rangle$$

$$M_{0\nu}^{\lambda 0} = M_{0\nu}^{\lambda 0}(nn) + M_{0\nu}^{\lambda 0}(pp) - 2M_{0\nu}^{\lambda 0}(pn)$$

- To enable comparison, map the differing cutoff parameters as

$$e_{\max} \equiv N_{\max} + 1$$

- This way the highest number of quanta possessed by any single particle (for ^{6}**He**) matches between bases.



Extrapolation Procedure

Using respective cutoff parameter, extrapolate using non-linear least-squares fit to a given functional form.

- Extrapolate energy with: $f\left(X_{\max}\right)=a+b\cdot e^{-cX_{\max}}$

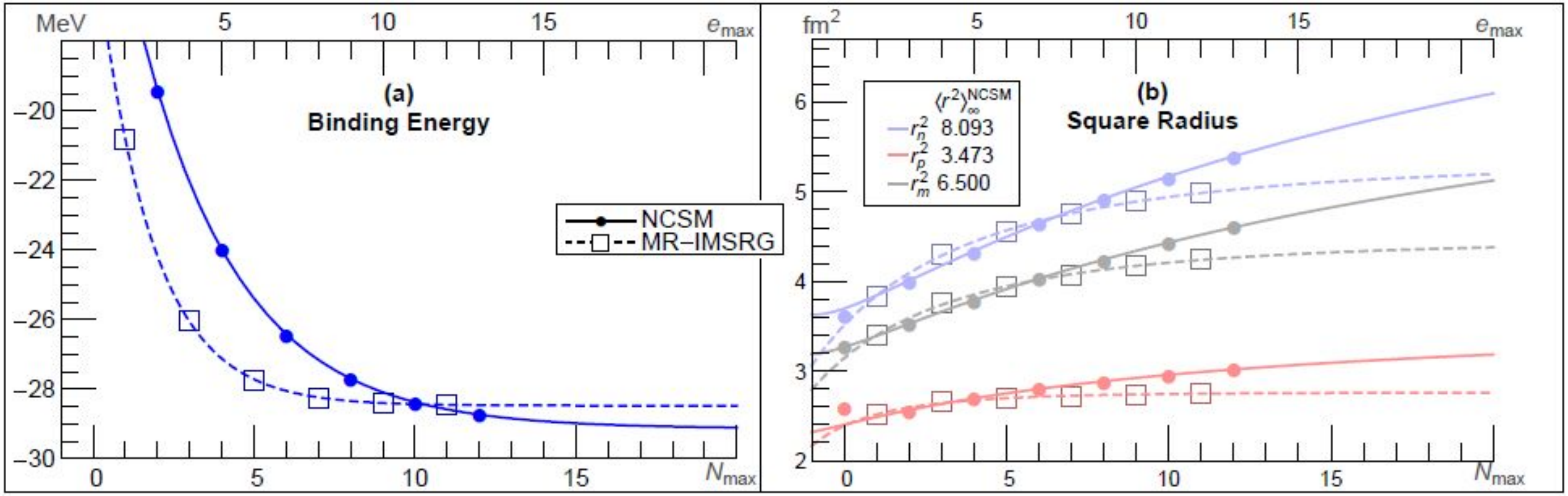
- Extrapolate square radii with: $\langle r^2\rangle=\langle r^2\rangle_\infty-\left(c_0\beta+c_1\beta^3\right)e^{-\beta}$

$$\beta\equiv 2k_\infty\frac{\hbar}{m\Omega}\left[\sqrt{2X_{\max}+5}+0.54437\left(2X_{\max}+5\right)^{1/6}\right]$$

- $0\nu\beta\beta$-decay extrapolation forms have not yet been studied.
- Noting observed similarities in r-dependence of NMEs to energy, we opt to apply the same extrapolation (when feasible).

F. Simkovic, A. Faessler, V. Rodin, P. Vogel, and J. Engel, Phys. Rev. C77, 045503 (2008), arXiv:0710.2055 [nucl-th].
Extrapolations formulated in R. J. Furnstahl, G. Hagen, and T. Papenbrock, Phys. Rev. C86, 031301(R) (2012), arXiv:1207.6100 [nucl-th].

He^6 Binding and Square radius Comparison

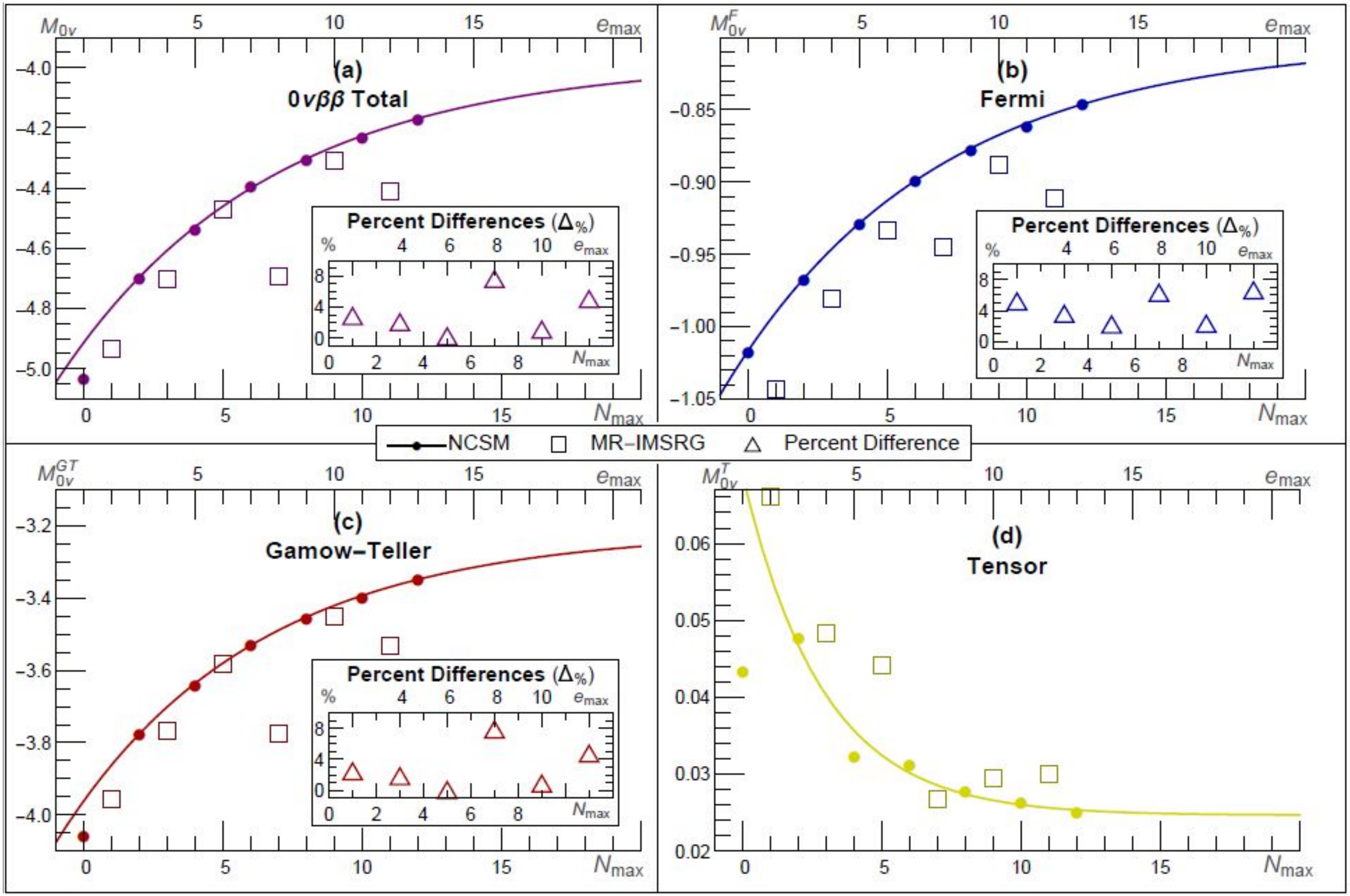


Energy differs by ~**2.3%**; square radii differ ~**21-34**%

- Differences reflect how well He^6 ground-state is modeled using just 1p1h & 2p2h correlations.
- Fast convergence of r^2 suggests 1p1h & 2p2h correlations well-accounted for by e_{max}=12, 24, and difference comes from MR-IMSRG(2) cutoff.

R. A. M. Basili, J. M. Yao, J. Engel, H. Hergert, M. Lockner, P. Maris, and J. P. Vary, (2019), arXiv:1909.06501 [nucl-th] .

He6 -> Be6 $0\nu\beta\beta$ Result Comparison



R. A. M. Basili, J. M. Yao, J. Engel, H. Hergert, M. Lockner, P. Maris, and J. P. Vary, (2019), arXiv:1909.06501 [nucl-th] .

Observations and Takeaways

- Meaningful differences in **square radius** results.
- $0\nu\beta\beta$ results appear to share **similar convergence pattern**.
- MR-IMSRG $0\nu\beta\beta$ results appear **less smooth** as function of basis cutoff.
- ME is **~80\20% GT\Fermi**. Tensor component is small and of opposite sign.
- **~15% smaller GT\Fermi** NMEs than VMC results using av18 w/ 3NF.
- Total $0\nu\beta\beta$ ME results match between the two methods within **<9%** for all paired bases considered.

Takeaway: Looks fairly promising so far!

For VMC results, see S. Pastore, et. al., Phys. Rev. C97, 014606 (2018), arXiv:1710.05026 [nucl-th].

Future Study

- Here we considered a **0^+, ΔT=0** decay, but experimental decays are **0^+, ΔT=2**.
- Recent study has demonstrated significant $0\nu\beta\beta$ NME sensitivity (up to ~**300%**!) to node in transition density (such as when ΔT=2).

Comparing ΔT=2 case would provide a much more robust benchmark.

Other Improvements

- Go to higher cutoffs.
- Include 3N interaction.
- Do MR-IMSRG(3).
- Developing robust $0\nu\beta\beta$ extrapolation would allow better comparison and uncertainty estimation.

	ΔT=0		ΔT=2	
	$^{10}Be(0_1^+)\to{}^{10}C(0_1^+)$ F	GT	$^{12}Be(0_1^+)\to{}^{12}C(0_1^+)$ F	GT
VMC-1	−1.001(40)	2.273(91)	−0.100(4)	0.257(10)
VMC-2	–	–	−0.113(5)	0.274(11)
$SM_{H.O.}$(w/o SRC, *p*)	−1.127	2.616	−0.183	1.228
SM_{WS}(w/o SRC, *p*)	−0.980	2.269	−0.147	1.023
$SM_{H.O.}$(w/o SRC, *psd*)	−1.274	3.228	−0.271	0.770
SM_{WS}(w/o SRC, *psd*)	−1.100	2.783	−0.198	0.570
$SM_{H.O.}$(M.S. SRC, *psd*)	−1.085	2.659	−0.157	0.431
$SM_{H.O.}$(CCM SRC, *psd*)	−1.226	3.075	−0.234	0.659
$SM_{H.O.}$(CVMC SRC, *psd*)	−1.131	2.799	−0.185	0.513
$SM_{H.O.}$(Fab SRC, *psd*)	−1.118	2.762	−0.181	0.501
$SM_{H.O.}$(Fab+abc SRC, *psd*)	−1.079	2.658	−0.169	0.467
SM_{WS}(M.S. SRC, *psd*)	−0.967	2.381	−0.122	0.342
SM_{WS}(CCM SRC, *psd*)	−1.069	2.683	−0.175	0.499
SM_{WS}(CVMC SRC, *psd*)	−0.992	2.457	−0.141	0.398
SM_{WS}(Fab, *psd*)	−0.988	2.449	−0.138	0.388
SM_{WS}(Fab+abc, *psd*)	−0.957	2.362	−0.128	0.361

X. Wang, A. Hayes, J. Carlson, G. Dong, E. Mereghetti, S. Pastore, and R. Wiringa, Physics Letters B 798, 134974 (2019).

Thank You!
Questions?

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