Multi-Reference In-medium Similarity Renormalization Group for the Nuclear Matrix Elements of Neutrinoless Double Beta Decay

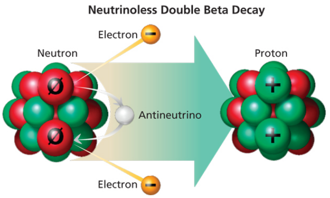
Jiangming Yao

Department of Physics and Astronomy, University of North Carolina at Chapel Hill, North Carolina, 27599-3255, USA

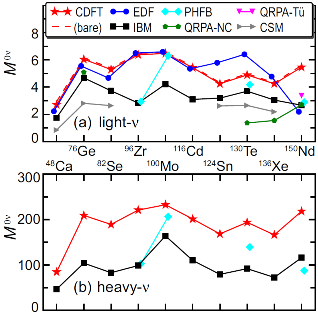
THE UNIVERSITY *of* NORTH CAROLINA *at* CHAPEL HILL

DOE topical collaboration "Nuclear Theory for Double-Beta Decay and Fundamental Symmetries", UMass Amherst, Feb.3, 2017

Nuclear Matrix Elements of $0\nu\beta\beta$ decay



$$M_i^{0\nu} = \langle 0_F^+ | \hat{O}_i^{0\nu} | 0_I^+ \rangle$$

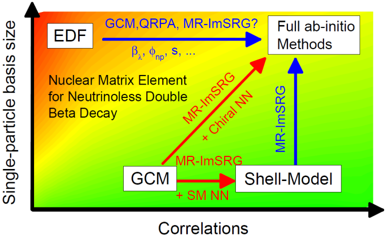


Song, JMY, Ring & Meng, PRC(2017)

- Decay mechanism: transition operator (limited to 1B current mostly, L/H ν)
- Nuclear structure: wave functions of initial and final nuclei

  Model-dependence (factor of 2-3)

Engel & Menendez, arXiv:1610.06548v1 [nucl-th]



ab initio approaches for heavy deformed nuclei

- Rapid developments in *ab initio* approaches (CC, SCGF, IMSRG) for nuclei
- Limitation: spherical or light nuclei
- Multi-Reference IMSRG: a promising approach for heavy deformed nuclei

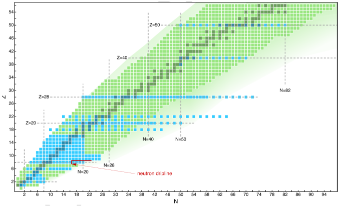
IMSRG: suppression H_{od} continuously

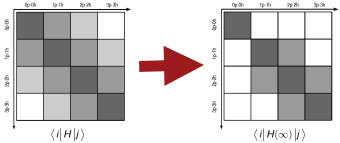
Unitary transformation $H(s) = U(s)H_0U^\dagger(s)$

$$\frac{dH(s)}{ds} = [\eta(s), H(s)],$$
$$\frac{dU(s)}{ds} = \eta(s)U(s)$$

Formal solution:

$$U(s) = \mathcal{S}\exp[\int_0^s ds'\eta(s')]$$





Hergert, Bogner, Morris, Schwenk, & Tsukiyama, PR

(2016)

IMSRG: Magnus expansion

- The Magnus expansion: rewriting $U(s) \equiv e^{\hat{\Omega}(s)}$ leads to the following ODE

$$\frac{d\hat{\Omega}(s)}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}^k_{\hat{\Omega}} \eta(s), \quad \Omega(0) = 0 \tag{1}$$

$\mathrm{ad}^0_{\Omega}\eta(s) = \eta(s), \mathrm{ad}^k_{\Omega}\eta(s) = [\Omega(s), \mathrm{ad}^{k-1}_{\Omega}]$ and B_k are the Bernoulli numbers.

$$\hat{\Omega}(s) = \int_0^s \eta(s_1) ds_1 + \frac{1}{2}\int_0^s ds_1 \int_0^{s_1} ds_2 [\eta(s_1), \eta(s_2)] + \cdots \tag{2}$$

The unitary of $U(s)$ is guaranteed by the anti-hermitian $\Omega(s)$.

- Operator $\hat{O}(s)$ (BCH expansion)

$$\begin{aligned} \hat{O}(s) &= e^{\hat{\Omega}(s)} \hat{O}_0 e^{-\hat{\Omega}(s)} = \sum_{k=0} \frac{1}{k!} \mathrm{ad}^k_{\hat{\Omega}(s)} \hat{O}_0 \\ &= \hat{O}_0 + [\hat{\Omega}(s), \hat{O}_0] + \frac{1}{2!}[\hat{\Omega}(s), [\hat{\Omega}(s), \hat{O}_0]] + \cdots \end{aligned} \tag{3}$$

Blanes, Casas, Oteo, Ros, PR(2009); Morries, Parzuchowski, Bogner, PRC (2015).

IMSRG: Brillouin Generator

- One-body term:

$$\eta_l^k(s) \equiv \langle\Phi|[\hat{H}(s), \tilde{A}_l^k]|\Phi\rangle \sim \lambda^{1B}, \lambda^{2B} \quad (4)$$

- Two-body term:

$$\eta_{mn}^{kl}(s) \equiv \langle\Phi|[\hat{H}(s), \tilde{A}_{mn}^{kl}]|\Phi\rangle \sim \lambda^{1B}, \lambda^{2B}, \lambda^{3B} \quad (5)$$

$\lambda^{1B}, \lambda^{2B}, \lambda^{3B}$: irreducible 1B, 2B, and 3B density matrices

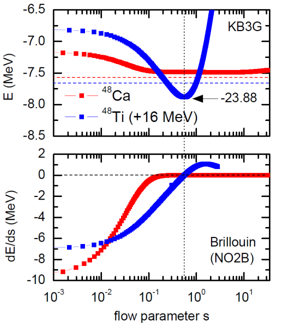
$$\lambda_j^i = \rho_j^i, \quad (6a)$$

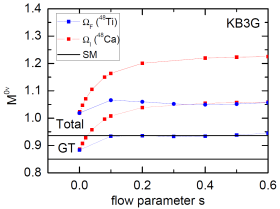
$$\lambda_{kl}^{ij} = \rho_{kl}^{ij} - \hat{\mathcal{A}}(\lambda_k^i \lambda_l^j), \quad (6b)$$

$$\lambda_{lmn}^{ijk} = \rho_{lmn}^{ijk} - \hat{\mathcal{A}}(\lambda_l^i \lambda_{mn}^{jk} + \lambda_l^i \lambda_m^j \lambda_n^k). \quad (6c)$$

- Hierarchy in irreducible DME: $\lambda^{1B} >> \lambda^{2B} >> \lambda^{3B} >> \cdots$
- Convergence: $\eta(\infty) = 0$ and $\frac{d\Omega(s)}{ds}|_{s=\infty} = 0$.

Brief summary of last talk at MSU





- $\lambda^i_j, \lambda^{ij}_{kl}$ from GCM $(\beta_2, \gamma, \phi_{pn})$
- NN Interaction: KB3G
- Minimum: $E(^{48}\text{Ti}) = -23.88$ MeV (SM: 23.66 MeV).

MR-IMSRG(2): does not work for ^{48}Ti?

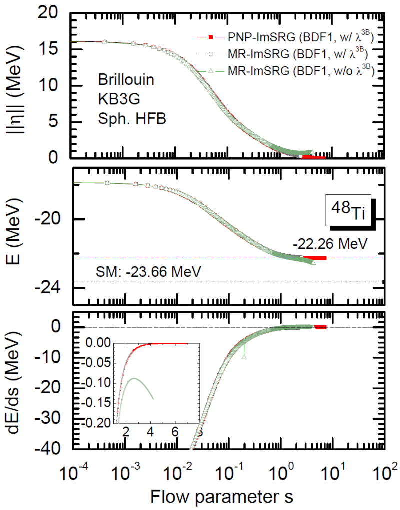
NME for $0\nu\beta\beta$

$$M^{0\nu} = \langle 0^+_F | e^{\hat{\Omega}_F(s)} \hat{O}^{0\nu} e^{-\hat{\Omega}_I(s)} | 0^+_I \rangle$$

	SM	GCM	ImSRG(2)(Ω_I)	ImSRG(2)(Ω_F)
GT	0.848	0.883	1.058	0.941
Fermi	0.146	0.207	0.233	0.172
Tensor	-0.058	-0.071	-0.067	-0.060
Total	0.936	1.019	1.224	1.053

Missing the irreducible λ^{3B} terms in $\eta^{(2B)}$?

MR-IMSRG(2): Benchmark Calc. from a Spherical State

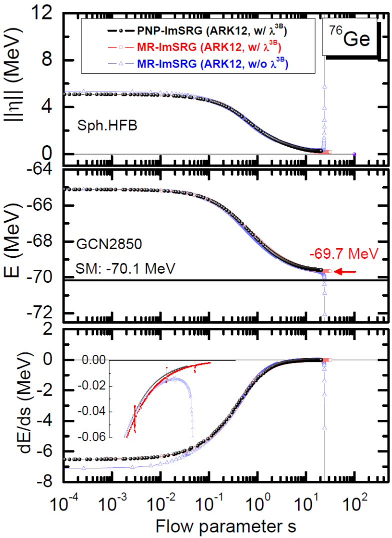


Numerical Details

- Reference state: spherical HFB
- *NN* Interaction: shell-model KB3G
- Techniques: PNP-ImSRG and MR-ImSRG

Better convergence $w/\ \lambda^{3B}$ in $\eta(s)$

MR-IMSRG(2): Benchmark Calc. from a Spherical State



Numerical Details

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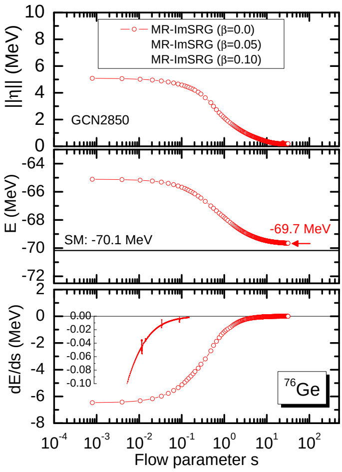
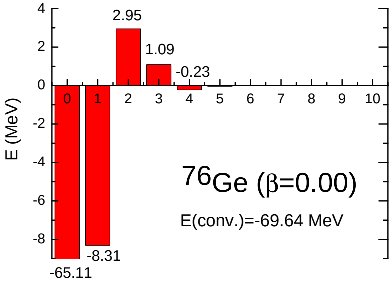
Better convergence $w/\ \lambda^{3B}$ in $\eta(s)$

MR-IMSRG(2): Benchmark Calc. from a Deformed State

$$E(s) \;=\; E(0) + \frac{1}{1!}[\hat{\Omega}(s), \hat{H}_0]^{0B} + \frac{1}{2!}[\hat{\Omega}(s), [\hat{\Omega}(s), \hat{H}_0]]^{0B} + \frac{1}{3!}[\hat{\Omega}(s), [\hat{\Omega}(s), [\hat{\Omega}(s), \hat{H}_0]]]^{0B} + \ldots$$



- λ^{3B} to energy ($\beta = 0.00$ case): $\sim +1 \times 10^{-3}$ MeV



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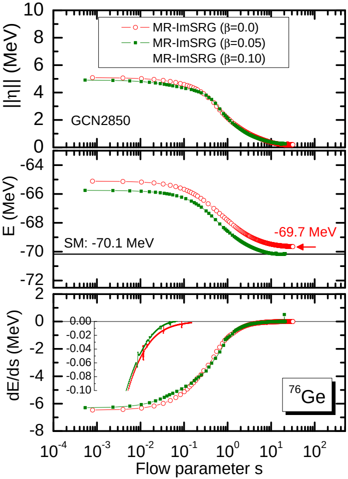
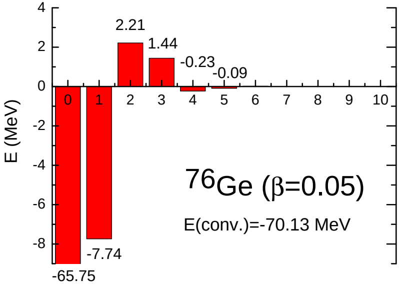
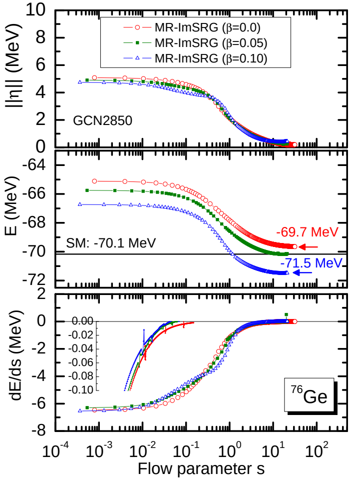


- λ^{3B} to energy ($\beta = 0.05$ case): $\sim +4 \times 10^{-3}$ MeV

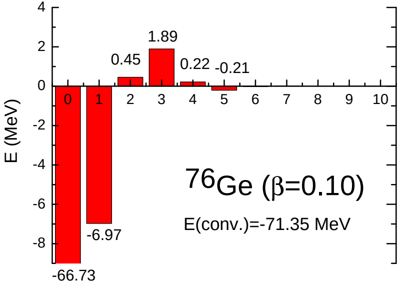


MR-IMSRG(2): Benchmark Calc. from a Deformed State

$$E(s) = E(0) + \frac{1}{1!}[\hat{\Omega}(s), \hat{H}_0]^{0B} + \frac{1}{2!}[\hat{\Omega}(s), [\hat{\Omega}(s), \hat{H}_0]]^{0B} + \frac{1}{3!}[\hat{\Omega}(s), [\hat{\Omega}(s), [\hat{\Omega}(s), \hat{H}_0]]]^{0B} + \dots$$



- λ^{3B} to energy ($\beta = 0.10$ case): $\sim +0.15$ MeV. $[\hat{\Omega}(s), \hat{H}_0]^{3B}$?



Summary and outlook

Summary

- The MR-IMSRG(2) based on shell-model interactions works well for near-spherical Ref. states, but not for large deformed ones.
- The more correlation is included in the Ref. state, the more important is the high-rank irreducible density ($\lambda^{2B}, \lambda^{3B}, \cdots$).
- Extension of the MR-IMSRG(2) to MR-IMSRG(2*) or MR-IMSRG(3) is needed for deformed nuclei.

Outlook

- MR-IMSRG based on chiral NN interaction with the MR-IMSRG(2*).
- Calculation of the NME for $0\nu\beta\beta$ with the MR-IMSRG(2*).

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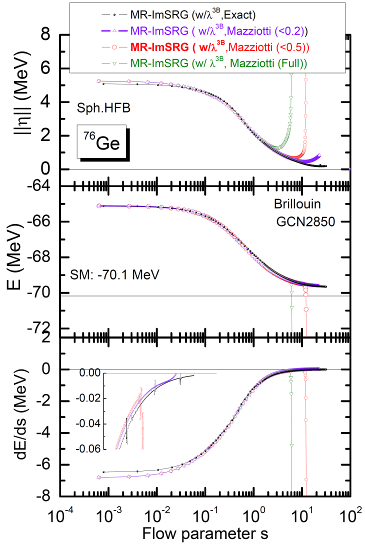
Thanks for your attention

SciDAC Scientific Discovery through Advanced Computing NUCLEI Nuclear Computational Low-Energy Initiative NERSC

MR-IMSRG: Benchmark Calculation from a Spherical State



Mazziotti's prescription for λ^{3B}

$$\lambda^{pqr}_{stu} \simeq -[n^{pqr}_{stu}]^{-1}\frac{1}{4}\sum_{a}\hat{\mathcal{A}}(\lambda^{pa}_{st}\lambda^{qr}_{au}) \quad (7)$$

with

$$n^{pqr}_{stu} = \sum_{a=p,q,r,s,t,u}\lambda^{a}_{a} - 3 \quad (8)$$

D. A. Mazziotti, PRA (1999)

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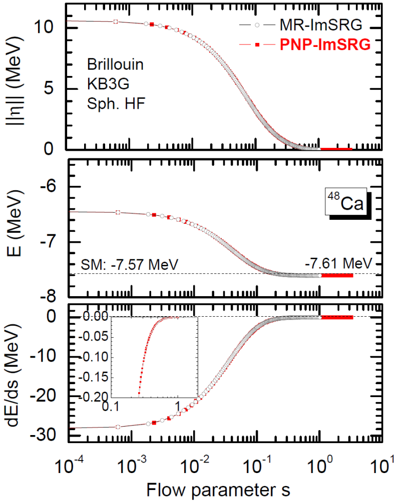
MR-IMSRG(2): Benchmark Calc. from a Spherical State

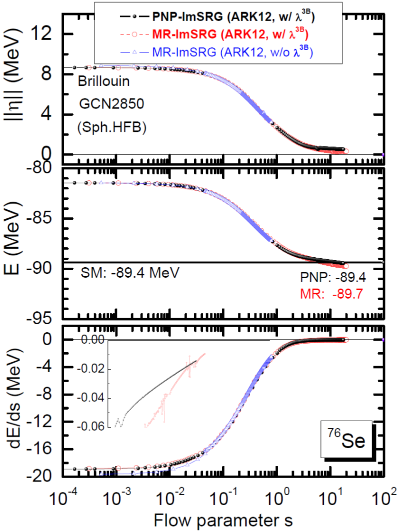


Numerical Details

- Reference state: spherical HF state: λ^{2B}, λ^{3B} are zero.
- *NN* Interaction: shell-model KB3G
- Techniques: PNP-ImSRG and MR-ImSRG

MR-IMSRG(2) works for this case

MR-IMSRG(2): Benchmark Calc. from a Spherical State



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