Ab initio calculation of deformed nuclei with in-medium generator coordinate method

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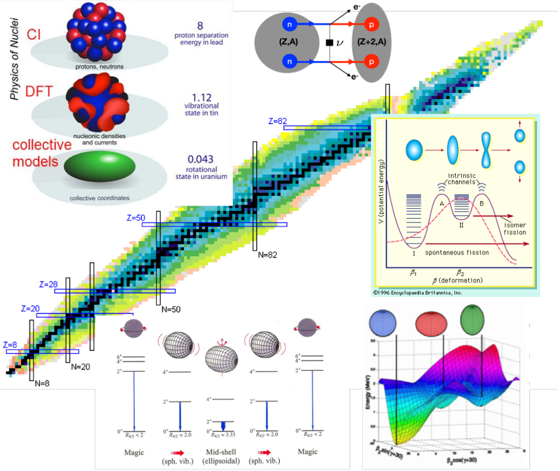
Nuclear shapes in modeling low-energy nuclear physics

- Deformation/collective correlations are relevant for understanding many phenomena of nuclear structure and reactions.
  - Evolution of shell structure and collectivity
  - Shape coexistence
  - Nuclear fission
  - (Double) beta decay
- Challenge to capture deformation effect for traditional shell models.
  - multi-particle-multi-hole excitation configurations



Capture deformation/collective correlations explicitly

Multi-reference energy density functionals

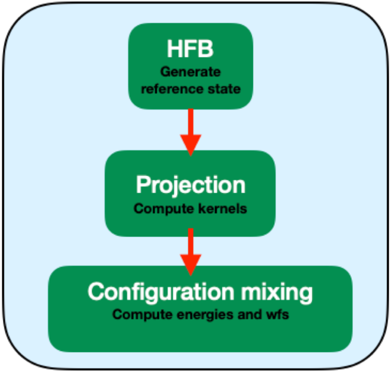
provides a successful microscopic tool for the low-energy spectroscopy of atomic nuclei with somewhat arbitrary shapes (with some unsolved issues).

- introduce collective correlations by breaking (rotation) symmetries in the fields/densities.
- recover symmetries for spectroscopic analysis with projection techniques
- consider additional correlations by mixing configurations of different shapes

- applications to nuclear reactions (fission)
- Implemented into shell-model calculations: MCSM/PSM
- An alternative way to perform configuration-interaction calculation

Recent review: Sheikh, Dobaczewski, Ring, Robledo, Yannouleas, arXiv:1901.06992 [nucl-th]

Generator coordinate method (GCM) in a nutshell



- The trial wave function of a GCM state

$$|\Phi^{JNZ\cdots}\rangle = \sum_Q F_Q^{JNZ} \hat{P}^J \hat{P}^N \hat{P}^Z \cdots |\Phi_Q\rangle$$

  $|\Phi_Q\rangle$ are a set of HFB wave functions from constraint calculations, Q is the so-called generator coordinate.

- The mixing weight F_Q^{JNZ} is determined from the Hill-Wheeler-Griffin equation:

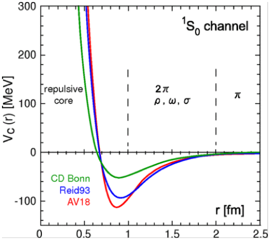
$$\sum_{Q'} \left[H^{JNZ}(Q, Q') - E^J N^{JNZ}(Q, Q') \right] F_{Q'}^{JNZ} = 0$$

Features (pros) of GCM

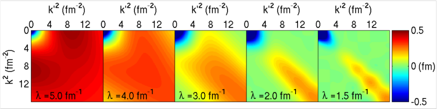
- The Hilbert space in which the H will be diagonalized is defined by the Q. Many-body correlations are controlled by the Q
- The Q is chosen as (collective) degrees of freedom relevant to the physics.
- Dimension of the space in GCM is generally much smaller than full CI calculations.

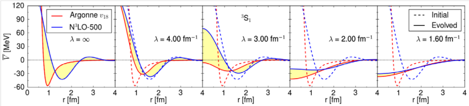
GCM calculations starting from a ...

- potential determined from lattice QCD/phenomenological parametrization or chiral EFT with parameters determined by the data of NN scattering or 2B/3B systems. too “hard" to be used for mean-field-based approaches
- potential softened with SRG evolution (decoupling matrix elements between low- and high-momentum states)

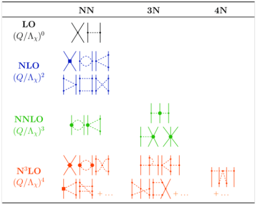


Phenomenological potentials



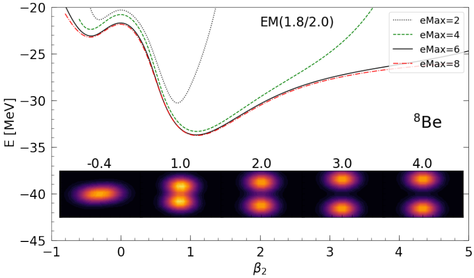


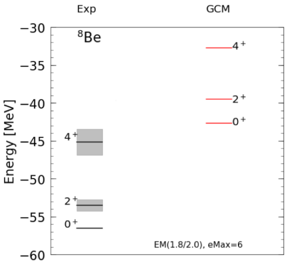
S. K. Bogner et al. (2010)



Potential from the chiral EFT

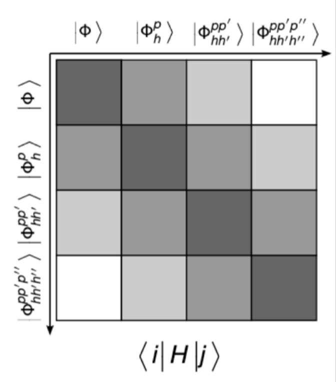
GCM calculations starting from a softened chiral interaction



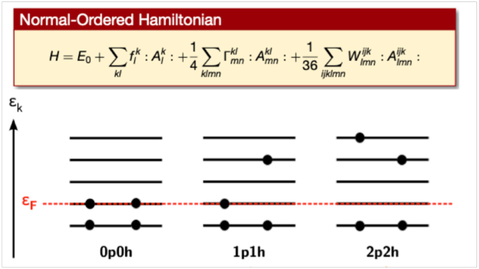


- The EM1.8/2.0 ($\hbar\omega = 16$ MeV) chiral interaction
  Hebeler, Bogner, Furnstahl, Nogga, Schwenk (2011)
- The collective properties are reasonably described. However, the entire spectrum is systematically shifted up to high energy.
- Some correlations missing

Missing correlations from ...



credit: H. Hergert



$$\langle \Phi^p_h | H | \Phi \rangle = \sum_{kl} f^k_l \langle \Phi | : A^h_p :: A^k_l : | \Phi \rangle$$

$$\langle \Phi^{pp'}_{hh'} | H | \Phi \rangle = \sum_{klmn} \Gamma^{kl}_{mn} \langle \Phi | : A^{hh'}_{pp'} :: A^{kl}_{mn} : | \Phi \rangle$$

- coupling of the reference state $|\Phi\rangle$ with other states by the H.

- A unitary transformation can be introduced to decouple the reference state from other states.

What's the unitary transformation?

For a given Hamiltonian H_0 with the bare nuclear interaction, the exact ground-state wave function $|\Psi_0\rangle$ is determined by

$$H_0|\Psi_0\rangle = E_{\mathrm{g.s.}}|\Psi_0\rangle$$

Let's assume this wave function is connected to the reference (or GCM) state $|\Phi\rangle$ with a unitary transformation

$$|\Psi_0\rangle = e^{-\Omega}|\Phi\rangle, \quad \Omega = -\Omega^\dagger = \Omega^{(1)} + \Omega^{(2)} + \cdots$$

It indicates that the $|\Phi\rangle$ is the ground-state of the effective Hamiltonian $H_{\mathrm{eff.}} = e^{\Omega}H_0e^{-\Omega}$,

$$H_{\mathrm{eff.}}|\Phi\rangle = E_{\mathrm{g.s.}}|\Phi\rangle.$$

- The mean-field based approaches (GCM) can still arrive at the correct solutions, provided that the unitary transformation e^{Ω} is known.
- The unitary transformation decouples the reference state from all other states.
- Many-body correlations are encoded into the effective Hamiltonian.
- The reference state $|\Phi\rangle$ can in principle be chosen as any state (not orthogonal to the exact ground state).

IMSRG: a convenient way to derive the unitary transformation

- A set of continuous unitary transformations onto the Hamiltonian

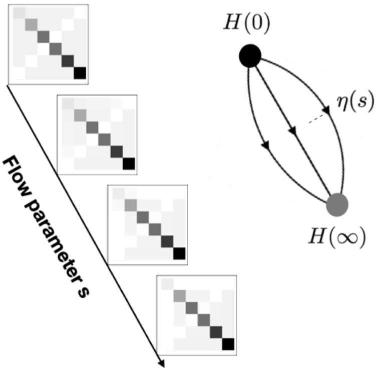
$$H(s) = U(s) H_0 U^{\dagger}(s)$$

- Flow equation for the Hamiltonian

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

where the $\eta(s)$ is the so-called generator chosen to decouple a given reference state from its excitations.

- Computation complexity scales polynomially with nuclear size



Tsukiyama, Bogner, and Schwenk (2011); Hergert, Bogner, Morris, Schwenk, Tsukiyama (2016)

Not necessary to construct the H matrix elements in many-body basis !

IMSRG: a convenient way to derive the unitary transformation

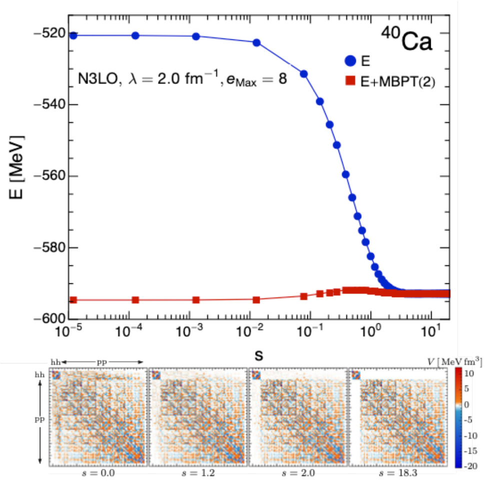
IMSRG for closed-shell nuclei

- The ref. state $|\Phi\rangle$ is chosen as a single-determinant (HF) state.
- Good agreement with other ab-initio calculations.

Tsukiyama, Bogner, Schwenk (2011)

Caveats

- Higher-body operators are induced in the flow.
- NO2B: truncation up to normal-ordered two-body terms



H. Hergert et al (2016)

IMSRG for open-shell nuclei

MR-IMSRG

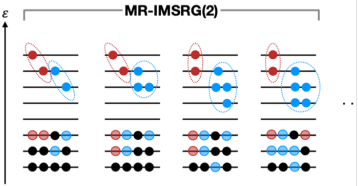
- Strong pairing correlations
- NO2B approximation on top of single-reference state is not sufficient
- Extension to multi-reference framework

Hergert, Binder, Calci, Langhammer, Roth (2013)

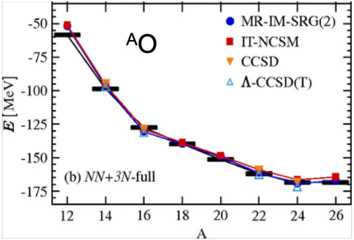
Valence-space IMSRG

- Decoupling the interaction into a small valence space
- Full CI in the valence space

Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth (2014);
Stroberg, Calci, Hergert, Holt, Bogner, Roth, Schwenk (2016)



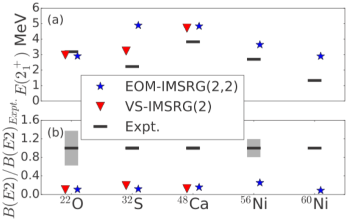
MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)



H. Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth (2013)

Extensions to excited states of open-shell nuclei: VS-IMSRG

- The valence-space IMSRG and EOM-IMSRG calculations using the effective interaction derived from a chiral NN+3N interaction with the IMSRG(2).



N. M. Parzuchowski, S. R. Stroberg, P. Navrátil, H. Hergert, and S. K. Bogner (2017)

VS-IMSRG

Reference state is chosen as an ensemble of spherical HF states.

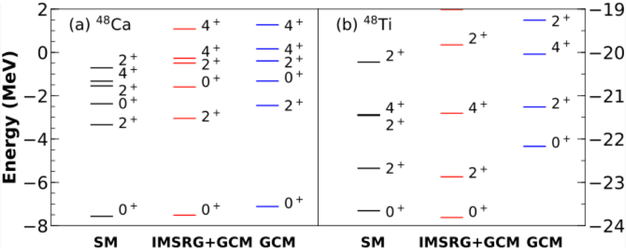
EOM-IMSRG

Reference state is chosen as a spherical HF state.

- The E2 transition strengths from ground state to the first 2+ state are systematically underestimated, indicating the truncation up to NO2B terms starting from a spherical HF/ ensemble reference state is difficult to capture collective correlations.

- The E2 transition operator might not be decoupled into the small model space in the same manner as that of the interaction.
- NO2B approximation starting from spherical HF state is not able to capture sufficient collective correlations.

Building many-body correlations into interaction with IMSRG



JMY, J. Engel, L.J. Wang, C.F. Jiao, H. Hergert (2018)

- benchmarked against the shell-model calculations for the low-lying energy spectra of 48Ca, 48Ti.
- The IMSRG overall improves the agreement with the shell-model results.

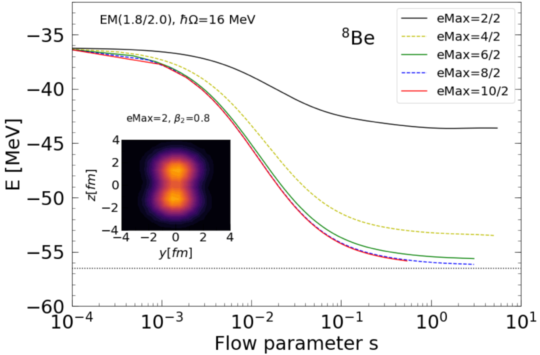
It encourages us to extend this approach by using interactions from chiral EFT.

IMSRG+GCM calculations starting from a softened chiral interaction

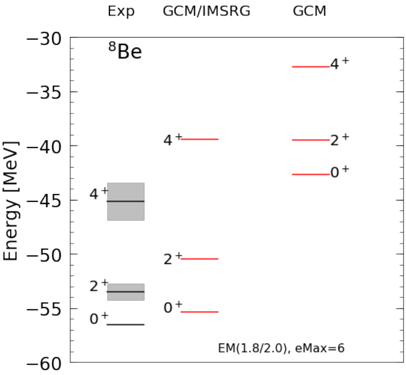
GCM
define
reference state

↓

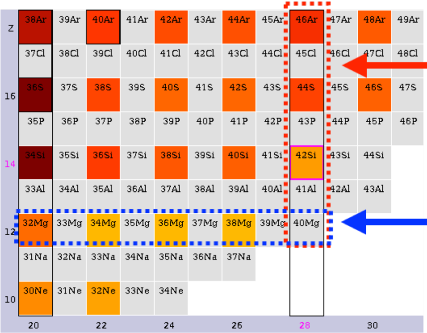
IMSRG
evolve
operators

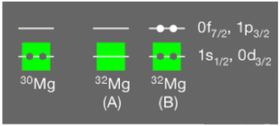


starting from a SRG softened chiral interaction

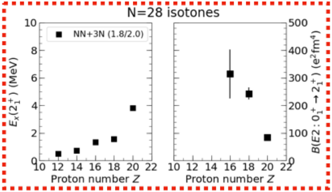


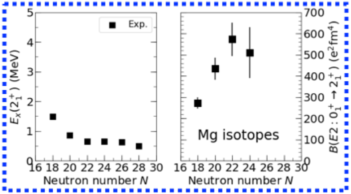
Applications: onset of large deformation in “magic" nuclei





https://physics.aps.org



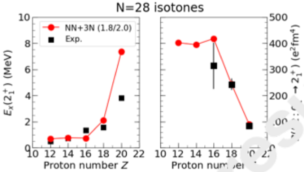


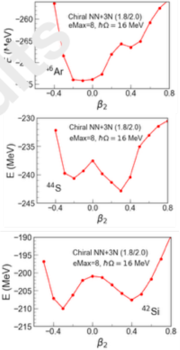
H. L. Crawford et al. (2019)

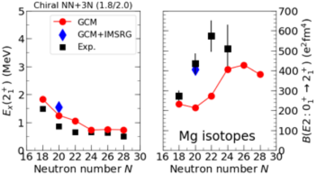
https://www.nndc.bnl.gov

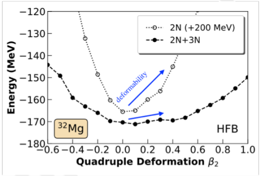
Applications: onset of large deformation in “magic" nuclei

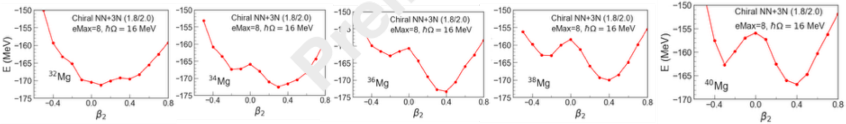
$\text{eMax} = 8, \hbar\Omega = 16 \text{ MeV}$

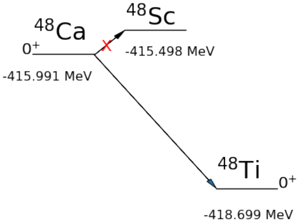


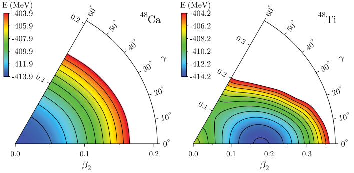


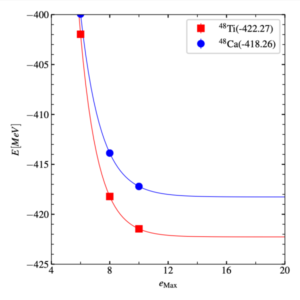










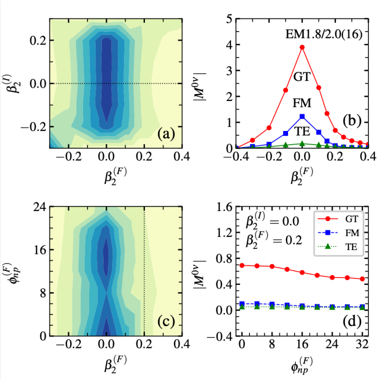


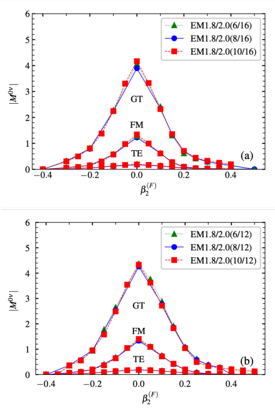
- PNVAP calculation with the IMSRG evolved chiral interaction.
- Extrapolation of the ground-state energy

JMY, B. Bally, J. Engel, R. Wirth, T.R. Rodríguez, H. Hergert, arXiv:1908.05424

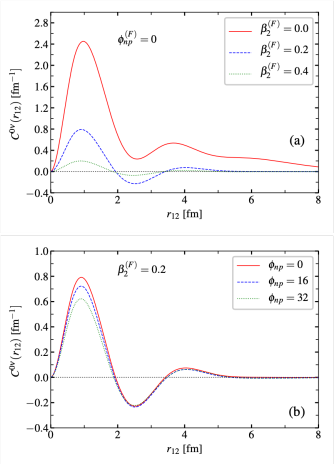
Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti

$$M^{0\nu} = \frac{4\pi R}{g_A^2}\int d^3\vec{r}_1 \int d^3\vec{r}_2 \int \frac{d^3\vec{q}}{(2\pi)^3}\frac{e^{i\vec{q}\cdot(\vec{r}_1-\vec{r}_2)}}{q[q+\bar{E}-(E_i+E_f)/2]}$$
$$\times\langle 0_F^+|e^{\Omega}\left[\mathcal{J}_\mu^\dagger(\vec{r}_1)\mathcal{J}^{\mu\dagger}(\vec{r}_2)\right]e^{-\Omega}|0_I^+\rangle$$





Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti



$$M^{0\nu} = \int dr_{12}\, C^{0\nu}(r_{12})$$

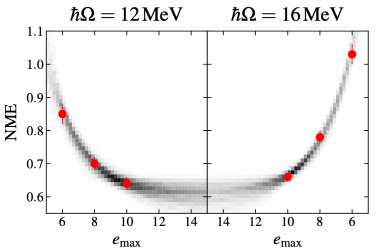
- The quadrupole deformation in ^{48}Ti changes both the short and long-range behaviors
- The neutron-proton isoscalar pairing is mainly a short-range effect

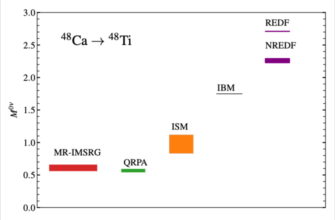
$$\phi_{np} = \langle \Phi | P_0^\dagger | \Phi \rangle + \langle \Phi | P_0 | \Phi \rangle$$

with

$$P_\mu^\dagger = \frac{1}{\sqrt{2}} \sum_\ell \hat{\ell} [a_\ell^\dagger a_\ell^\dagger]_{0\mu 0}^{L=0, J=1, T=0}$$

Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti





- The value from Markov-chain Monte-Carlo extrapolation is $M^{0\nu} = 0.61^{+0.05}_{-0.04}$
- The neutron-proton isoscalar pairing fluctuation quenches $\sim$17% further, which might be canceled out partially by the isovector pairing fluctuation.

Summary and outlook

Take-away messages:

- The IMSRG+GCM (IMGCM) opens a door to modeling deformed nuclei with realistic nuclear forces (from chiral EFT). Many interesting phenomena of low-energy physics (shape transition, coexistence, clustering structure) can be explored within this framework.
- The shape evolutions along $Z = 12$ and $N = 28$ chains are studied. The IMGCM shows promising results in the description of the systematics in the low-lying states.
- The NME for the neutrinoless double beta decay from spherical ^{48}Ca $\rightarrow$ deformed ^{48}Ti is calculated with the IMGCM. Deformation shows a strong quenching effect on the NME.

What's next:

- From IMSRG(2) to IMSRG(3)
- Extension to heavier nuclear systems:
  $M^{0\nu}$, single-β decay of nuclei relevant for r-process nucleosynthesis, etc

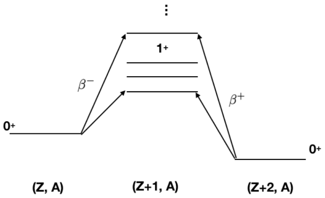
Recent development: GT transition to odd-odd nucleus

- a simple ansatz for the wave function for odd-odd nucleus

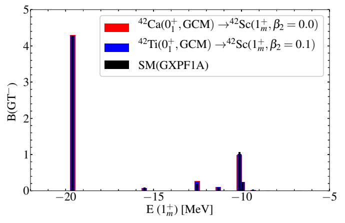
$$\left|{}^{42}\mathrm{Sc}; JNZ(\beta_2, \phi_{np})\right\rangle = \sum_{K,pn} f_K^{JNZ}(\beta_2)\hat{P}^N\hat{P}^Z\hat{P}^J_{MK}[\beta_p^\dagger\beta_n^\dagger]\left|{}^{42}\mathrm{Sc}; \mathrm{HFB}(\beta_2, \phi_{np})\right\rangle \quad (1)$$

The GT transition strength (g_A is taken as 1)

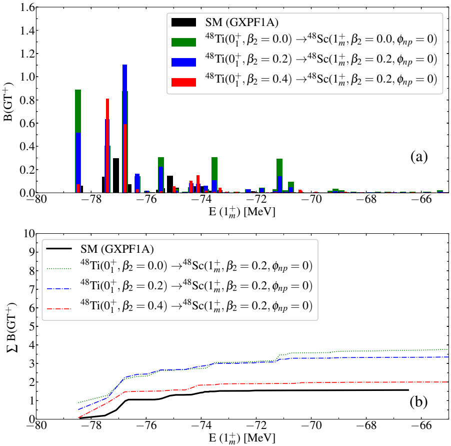
$$B(GT^- : 0_1^+ \to 1_m^+) = \left|\langle 1_m^+ || \hat{O}^-_{\mathrm{GT}} || 0_1^+\rangle\right|^2 \quad (2)$$



Benchmark calculation with a SM interaction

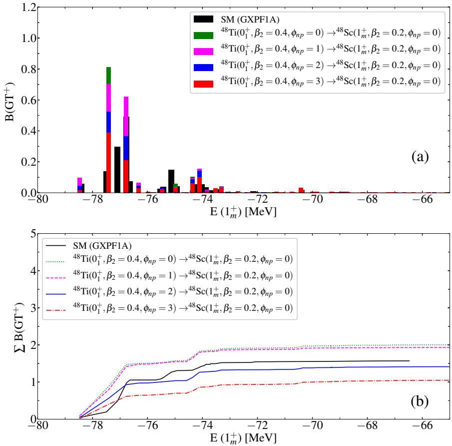


Recent development: deformation effect in ^{48}Ti on $B(GT^+)$



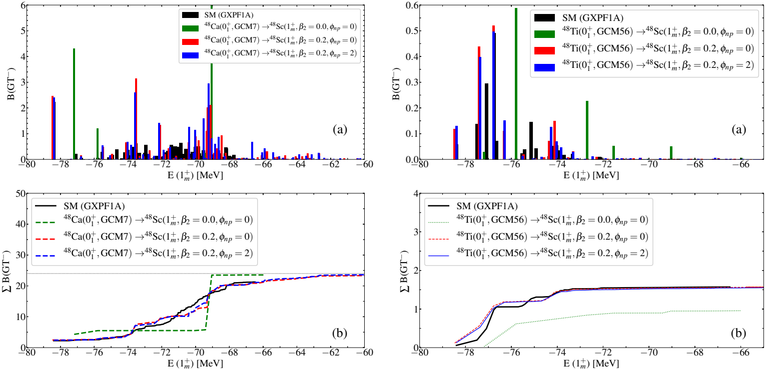
- Quadrupole deformation in ^{48}Ti reduces the $B(GT^+)$

Recent development: np pairing effect in ^{48}Ti on $B(GT^{+})$



- neutron-proton isoscalar pairing in ^{48}Ti reduces significantly the $B(\mathrm{GT}^+ : ^{48}\mathrm{Ti} \to ^{48}\mathrm{Sc})$.

Recent development: deformation/np pairing effects in ^{48}Sc

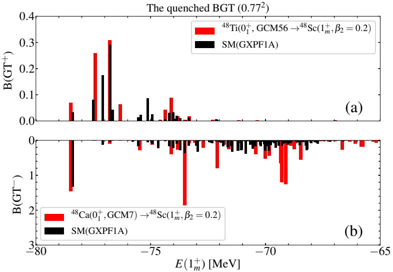


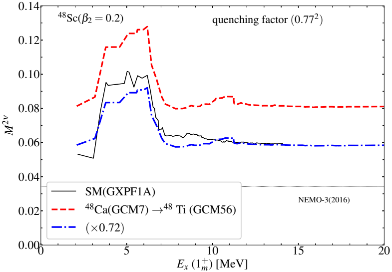
- Quadrupole deformation in ^{48}Sc is essential to reproduce the $B(GT^+)$
- *np* pairing in ^{48}Sc reduces slightly the $B(GT^+)$

Recent development: two-neutrino double-beta decay

- GCM calculation for the NME of two-neutrino double-beta decay transition

$$M^{2\nu} = \sum_m \frac{\langle 0_f^+ || \sigma\tau^- || 1_m^+ \rangle \langle 1_m^+ || \sigma\tau^- || 0_i^+ \rangle}{E(1_m^+) - [E(0_i^+) + E(0_f^+)]/2} \quad (3)$$





- The $M^{2\nu}$ is dominated by the transition through the first 1^+ state in the intermediate nucleus (overestimated).
- The model space is still not sufficient (expected to decrease the NME).
- Interest to see the results with the IMSRG+GCM starting from a chiral interaction

Collaborators and acknowledgement

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- Benjamin Bally
- Jonanthan Engel

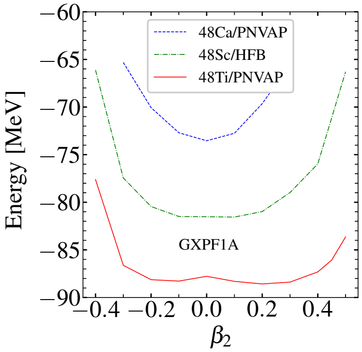
Iowa State University

- Robert A. Basili
- James P. Vary

Southwest University

- Longjun Wang

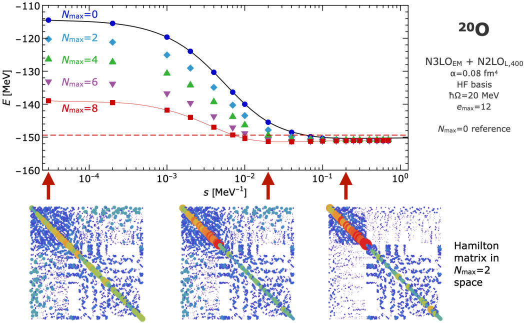
Thank your for your attention!


−60
−65
−70
−75
−80
−85
−90
Energy [MeV]
−0.4
−0.2
0.0
0.2
0.4
β_2
48Ca/PNVAP
48Sc/HFB
48Ti/PNVAP
GXPF1A

Speeding up the convergence of the NCSM with IMSRG

MR-IMSRG+NCSM

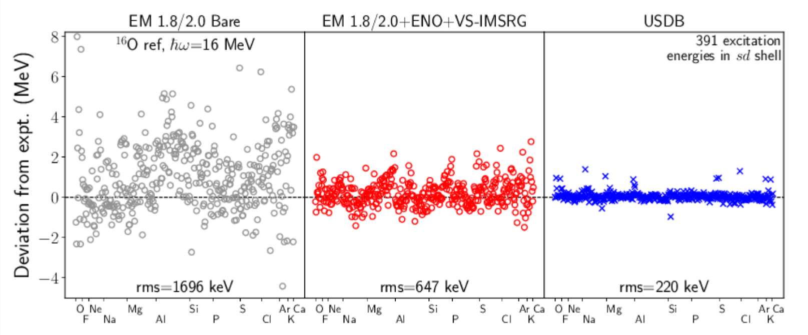
- NCSM with $N_{\max} = 0$ for the reference state
- MR-IMSRG evolution in a large model space
- Convergence of the NCSM with the evolved interaction is speeded up.



Gebrerufael, Vobig, Hergert, Roth (2017)

Extensions to excited states of open-shell nuclei: VS-IMSRG

VS-IMSRG for excited states of *sd*-shell nuclei



Review: Stroberg, Bogner, Hergert, Holt (2019)

Applications: onset of large deformation in “magic" nuclei

- One-body density in natural basis

$$\rho_{ji}(s) = \langle 0_1^+ | e^{\Omega(s)} [c_i^\dagger \tilde{c}_j]^0 e^{-\Omega(s)} | 0_1^+ \rangle$$
$$= \langle 0_1^+ | [c_i^\dagger \tilde{c}_j]^0 | 0_1^+ \rangle + \langle 0_1^+ | [\Omega(s), [c_i^\dagger \tilde{c}_j]^0] | 0_1^+ \rangle + \cdots$$

where the wave function $|0_1^+\rangle$ is from the GCM calculation with the $H(s) = e^{\Omega} H_0 e^{-\Omega}$.