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

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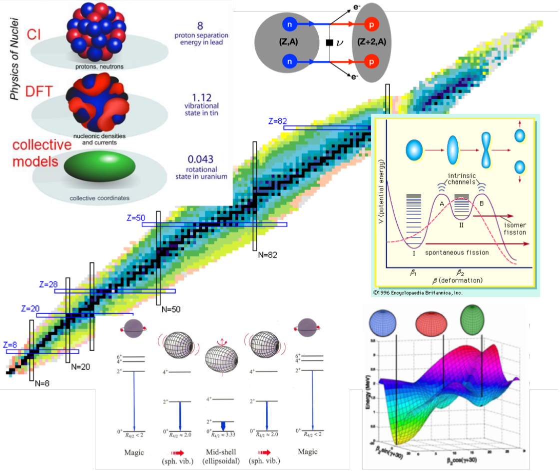
Nuclear shapes in modeling low-energy nuclear physics

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



Capture deformation/collective correlations explicitly

Multi-reference energy density functionals

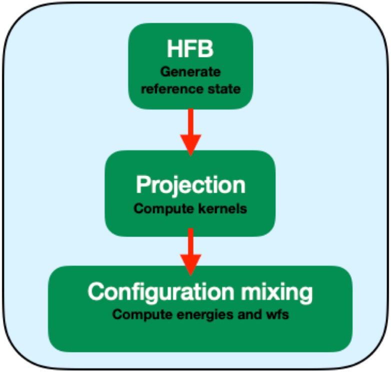
provides a successful microscopic tool for the low-energy spectroscopy of atomic nuclei with somewhat arbitrary shapes (with some unsolved issues).
Caurier, Grammaticos, Bonche, Egido, Robledo, Heenen, Skalski, Rodriguez-Guzman, Valor, Anguiano, Bender, Satuła, Niksic, Rodriguez, Yao, Bally, Borrajo, Shimada, Bernard, Marevic, Konieczka, etc.

- 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

- Also lots of applications to nuclear reactions (Bertsch, Descouvemont, etc)
- 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:

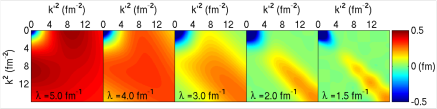
$$\sum_{Q'} \left[H^{JNZ}(Q, Q') - E^J N^{JNZ}(Q, Q') \right] F_{Q'}^{JNZ} = 0$$

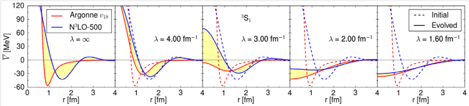
Features (pros) of GCM

- 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.

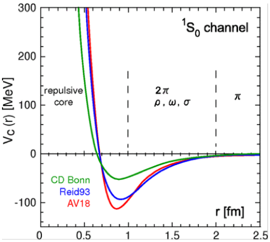
GCM calculations starting from a ...

- 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)

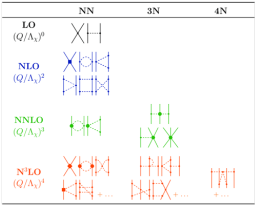




S. K. Bogner et al. (2010)

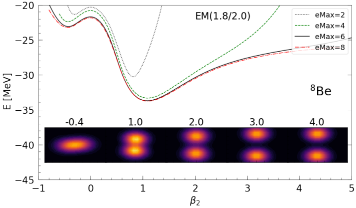


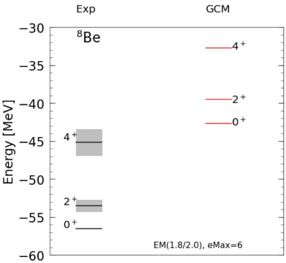
Phenomenological potentials



Potential from the chiral EFT

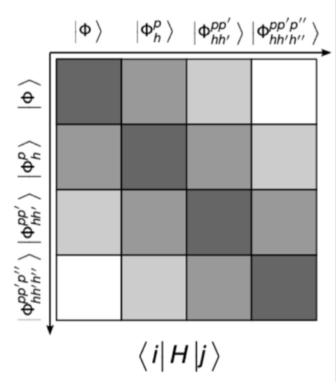
GCM calculations starting from a softened chiral interaction



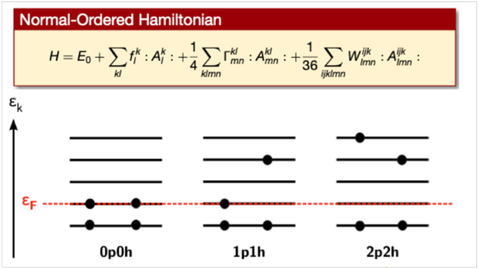


- The EM1.8/2.0 ($\hbar\omega = 16$ MeV) chiral interaction K. Hebeler et al PRC (2011)
- The collective properties are reasonably described. However, the entire spectrum is systematically shifted up to high energy.
- Enlarging the eMax value in the GCM calculation doesn't help to gain sufficient energy.
- 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

$$|\Psi_0\rangle = e^{-\Omega}|\Phi\rangle, \quad \Omega^\dagger = -\Omega$$

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 coded 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

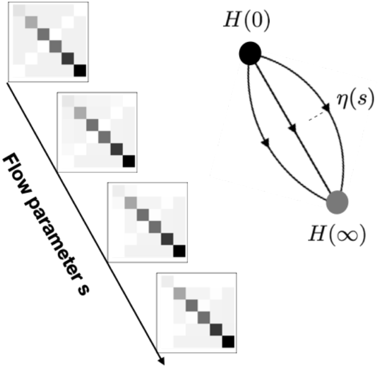
$$H(s) = U(s) H_0 U^\dagger(s)$$

- 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

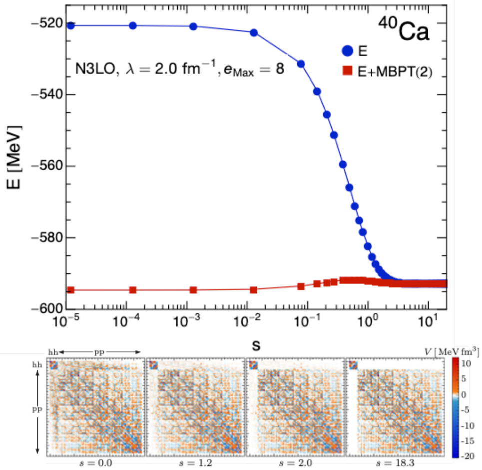
IMSRG for closed-shell nuclei

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

K. Tsukiyama et al., (2011)

Caution

- Higher-body operators are induced in the flow.
- Normal-ordering two-body (NO2B) approximation is adopted.



H. Hergert et al (2016)

IMSRG: a convenient way to derive the unitary transformation

MR-IMSRG for open-shell spherical nuclei

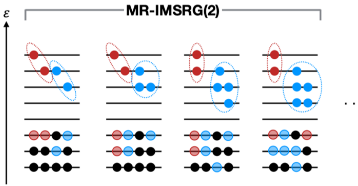
- Strong pairing correlations
- NO2B approximation on top of single-reference state is not sufficient
- Extension to multi-reference framework

H. Hergert et al (2013)

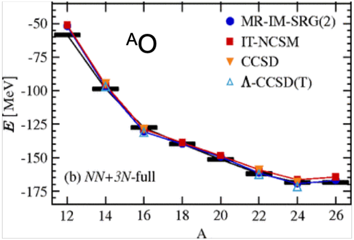
Valence-space IMSRG for open-shell nuclei

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

S.K. Bogner et al (2014);
S. R. Stroberg et al (2016)



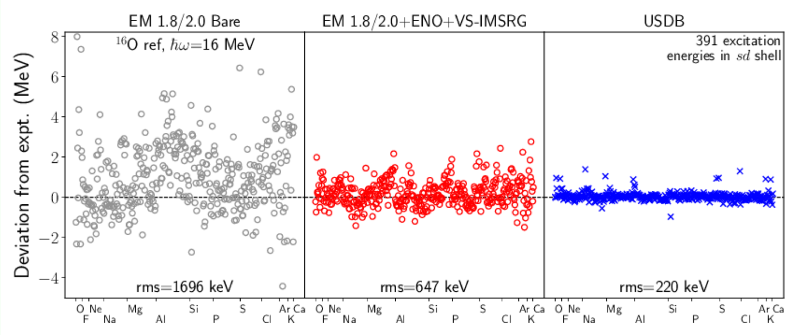
MR-IMSRG: build correlations on top of **already correlated** state (e.g., from a method that describes static correlation well)



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

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

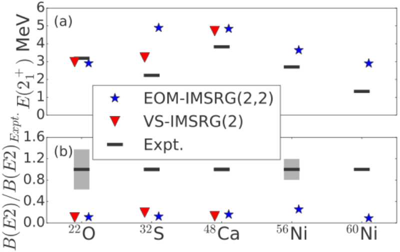
VS-IMSRG for excited states of *sd*-shell nuclei



Review: S. R. Stroberg, S. K. Bogner, H. Hergert, J. D. Holt (2019)

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.

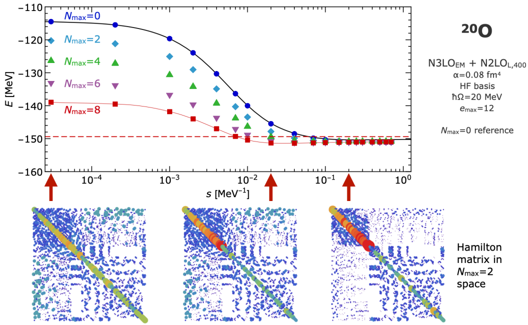
- The E2 transition strengths from ground state to the first 2+ state are systematically underestimated, indicating the truncation up to NO2B terms starting from a spherical HF/ ensemble reference state is difficult to capture collective correlations.

The E2 transition operator might not be decoupled into the small model space in the same manner as that of the interaction.
back to no-core calculation ...

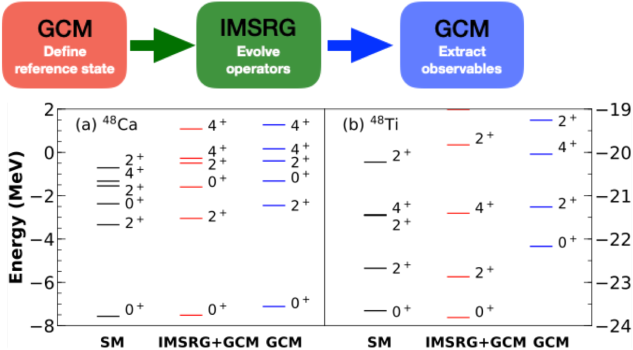
Speeding up the convergence of the NCSM with IMSRG

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.



E. Gebrerufael, K. Vobig, H. Hergert, and R. Roth (2017)



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

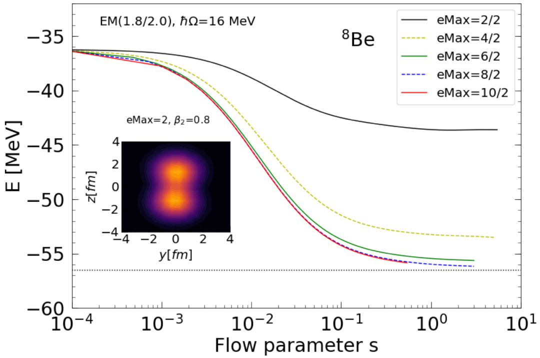
- benchmarked against the shell-model calculations for the low-lying energy spectra of 48Ca, 48Ti.
- The IMSRG overall improves the agreement with the shell-model results.

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

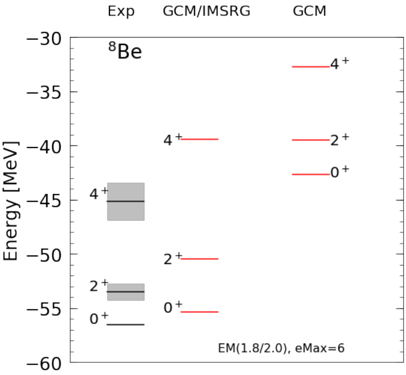
IMSRG+GCM calculations starting from a softened chiral interaction

GCM
define
reference state

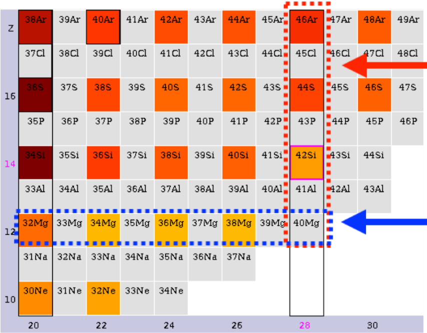
IMSRG
evolve
operators

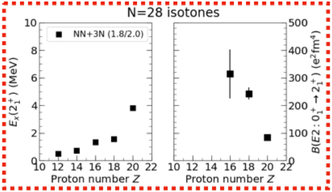


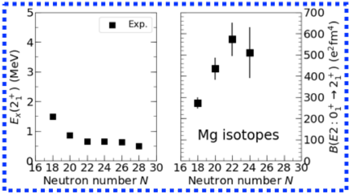

GCM
define
reference state
IMSRG
evolve
operators
GCM
extract
observables

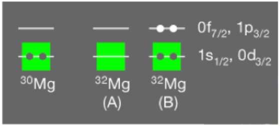

Exp
GCM/IMSRG
GCM
^{8}Be
Energy [MeV]
−30
−35
−40
−45
−50
−55
−60
4+
2+
0+
EM(1.8/2.0), eMax=6

Applications: onset of large deformation in “magic" nuclei









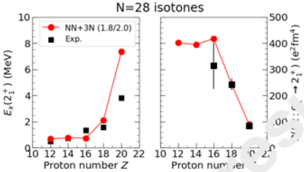
H. L. Crawford et al. (2019)

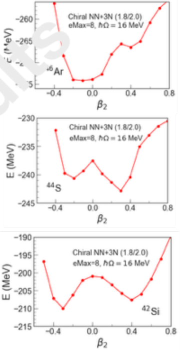
https://www.nndc.bnl.gov

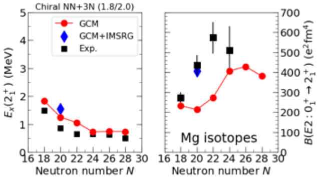
https://physics.aps.org

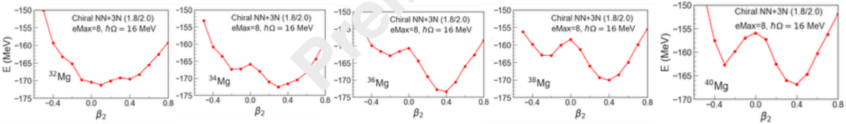
Applications: onset of large deformation in “magic" nuclei

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







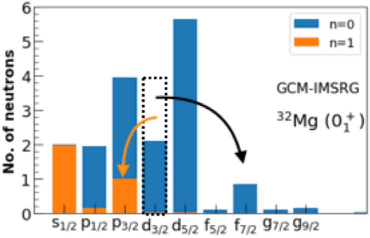


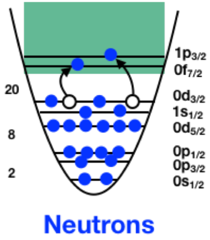
Applications: onset of large deformation in “magic" nuclei

- One-body density in natural basis

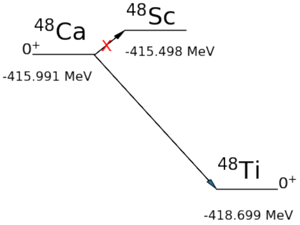
$$\begin{aligned}\rho_{ji}(s) &= \langle 0_1^+ | e^{\Omega(s)} [c_i^\dagger \tilde{c}_j]^0 e^{-\Omega(s)} | 0_1^+ \rangle \\ &= \langle 0_1^+ | [c_i^\dagger \tilde{c}_j]^0 | 0_1^+ \rangle + \langle 0_1^+ | [\Omega(s), [c_i^\dagger \tilde{c}_j]^0] | 0_1^+ \rangle + \cdots\end{aligned}$$

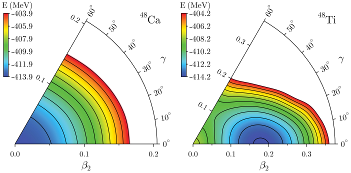
where the wave function $|0_1^+\rangle$ is from the GCM calculation with the $H(s) = e^{\Omega} H_0 e^{-\Omega}$.

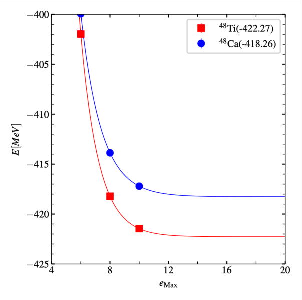




Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti





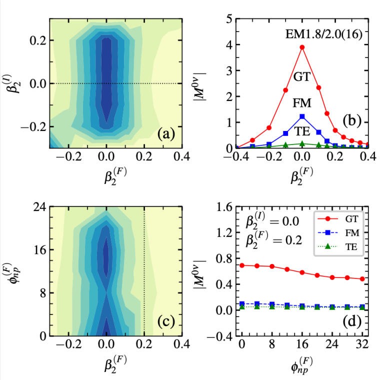


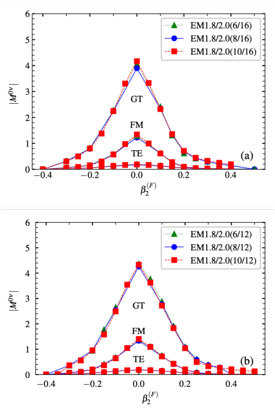
- PNVAP calculation with the IMSRG evolved chiral interaction.
- Extrapolation of the ground-state energy

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

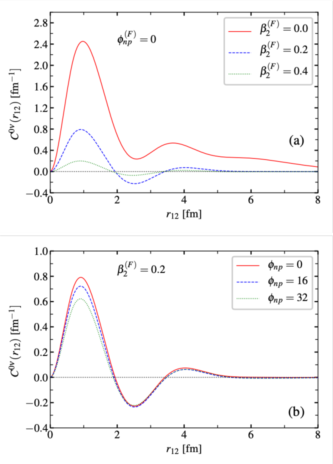
Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti

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



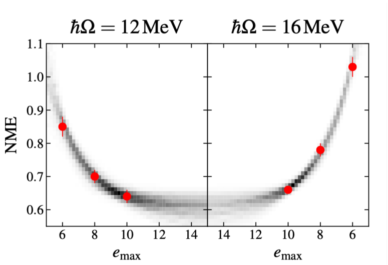


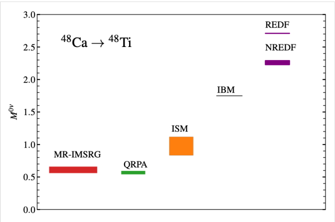
Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti



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

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





- 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 MR-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, cluster 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.

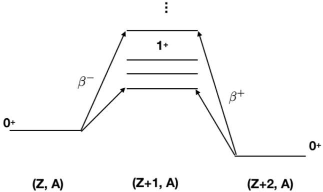
What's next:

- Extension to heavier nuclear systems
- From IMSRG(2) to IMSRG(3)
- Extension to odd-mass and odd-odd nuclei and the single-beta decay

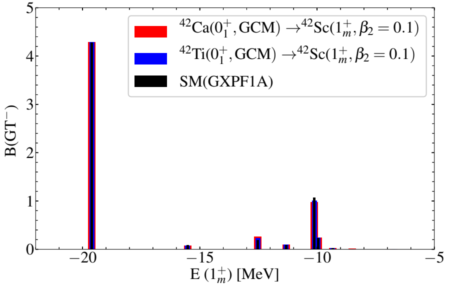
Outlook: GT transition to odd-odd nucleus

- GCM calculation for GT transition (simple ansatz)

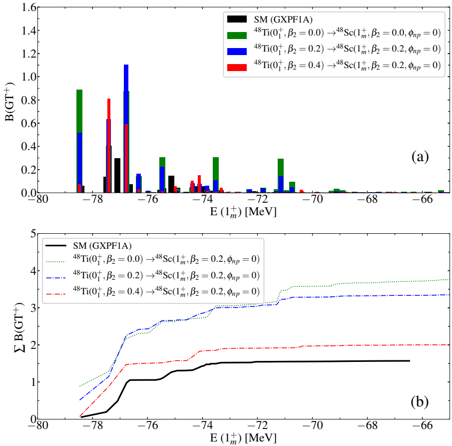
$$|^{42}\mathrm{Sc}(\beta_2)\rangle = \hat{P}^N \hat{P}^Z \hat{P}^J [\beta_p^\dagger \beta_n^\dagger] |\mathrm{HFB}(\beta_2)\rangle \quad (1)$$



Benchmark calculation with a SM interaction

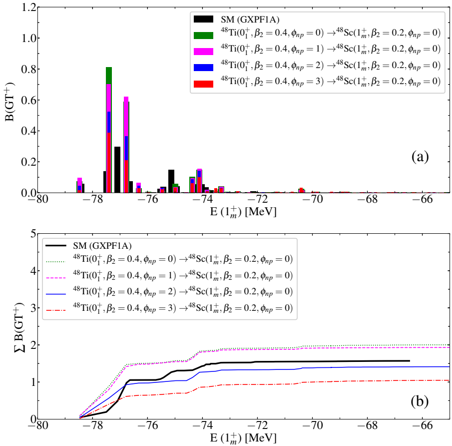


deformation effect in ^{48}Ti on $B(GT^+)$



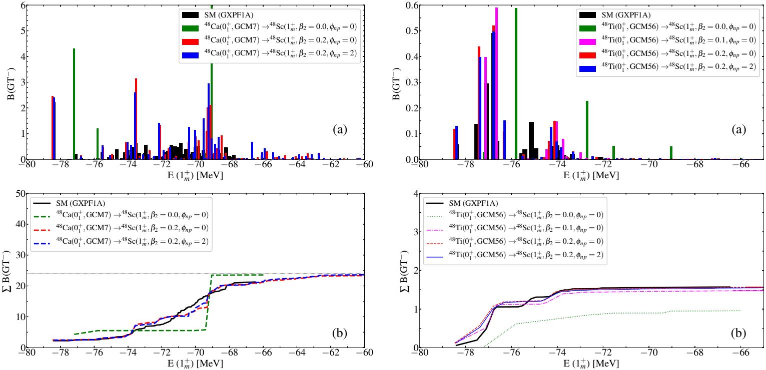
- Quadrupole eformation in ^{48}Ti reduces the $B(GT^+)$

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



- neutron-proton isoscalar pairing in ^{48}Ti reduces the $B(GT^+)$

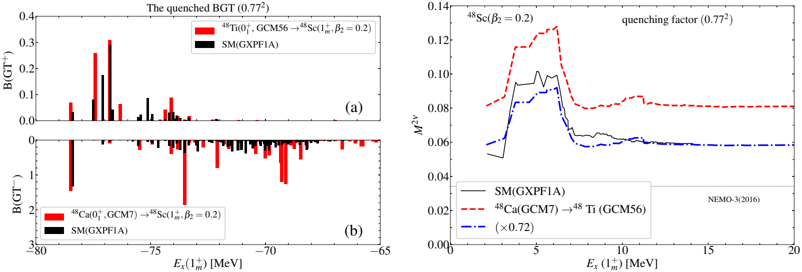
deformation/np pairing effects in ^{48}Sc



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

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

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



- 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

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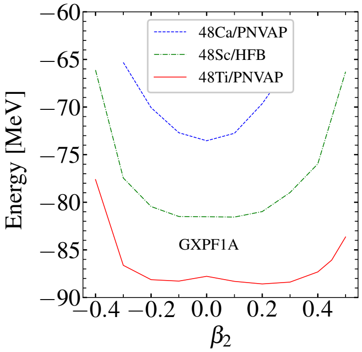
Thank your for your attention!

PESs



−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