

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

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Nuclear shapes in modeling low-energy nuclear physics



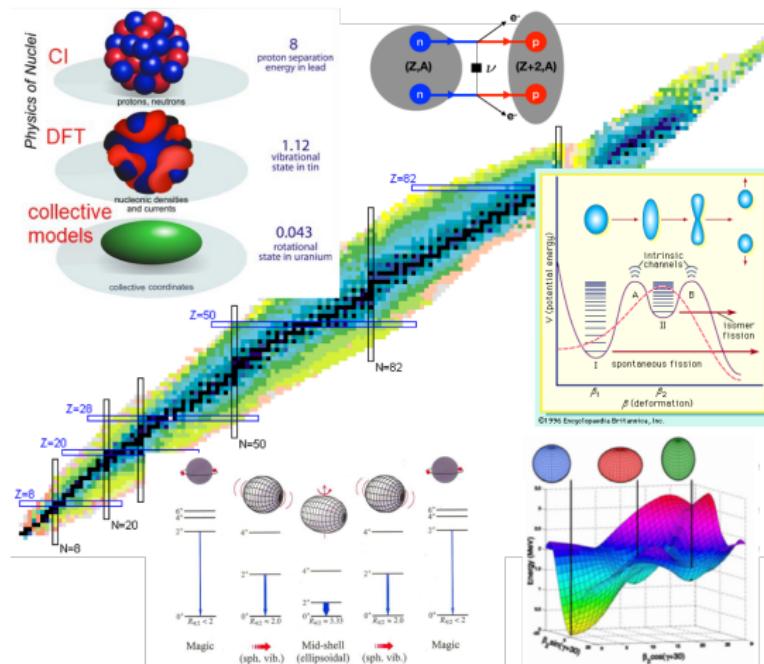
Modeling atomic nuclei

- single-particle dof: separation energy, shell structure
- globe dof: mass and radius, collective motions, fission

Nuclear models starting from effective nuclear interactions or energy density functionals have achieved a remarkable success in the past decades.

Nuclear shapes and symmetries

Nuclear shapes/deformation are relevant for understanding many phenomena of nuclear structure and reactions.



Capture deformation/collective correlations explicitly



advantage of introducing deformation dof

- mp-mh excitations, challenge for traditional nuclear shell models
- easier for mean-field/density based models by breaking rotation symmetries.

Symmetry restoration and shape mixing in EDFs

- recovering symmetries for spectroscopic analysis with projection techniques
- mixing configurations of different shapes with GCM

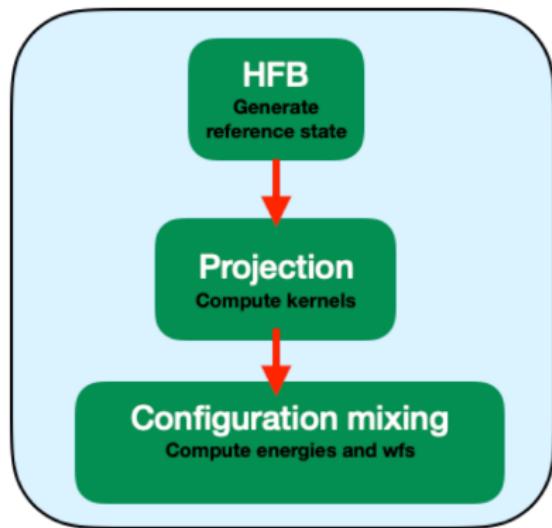
MR-EDF: provides a successful microscopic tool for the low-energy spectroscopy of atomic nuclei with somewhat arbitrary shapes (with some unsolved issues).

Caurier, Grammaticos, Bonche, Egido, Robledo, Heenen, Skalski, Rodriguez-Guzman, Valor, Anguiano, Bender, Satuła, Niksic, Rodriguez, Yao, Bally, Borrajo, Shimada, Bernard, Marevic, Konieczka, etc.

- 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

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

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

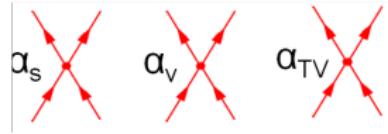
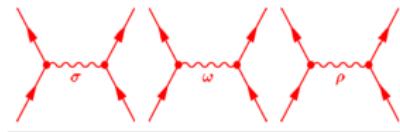
- The mixing weight F_Q^{JNZ} is determined from the Hill-Wheeler-Griffin equation:

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

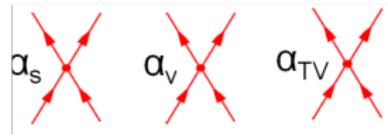
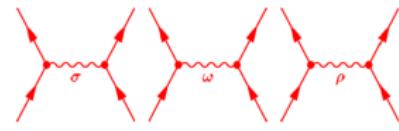
Features (pros) of GCM

- 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.

- relativistic EDF?



- relativistic EDF?

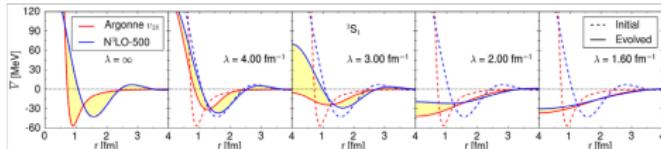
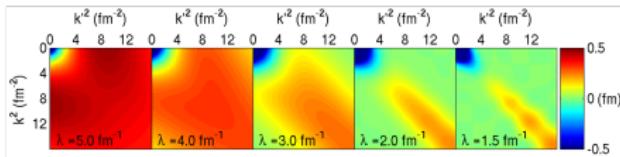


Not today !

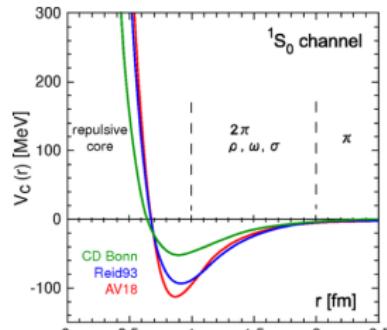
pls see talks by Anatoli Afanasjev, Elena Litvinova, Petar Marevic

GCM calculations starting from a ...

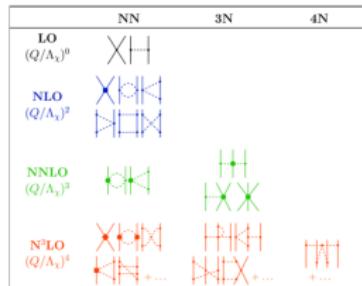
- potential determined from lattice
QCD/phenomenological parametrization or chiral EFT with parameters determined by the data of NN scattering or 2B/3B systems.
too "hard" to be used for mean-field-based approaches
- potential softened with SRG evolution
(decoupling matrix elements between low- and high-momentum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



S. K. Bogner et al. (2010)

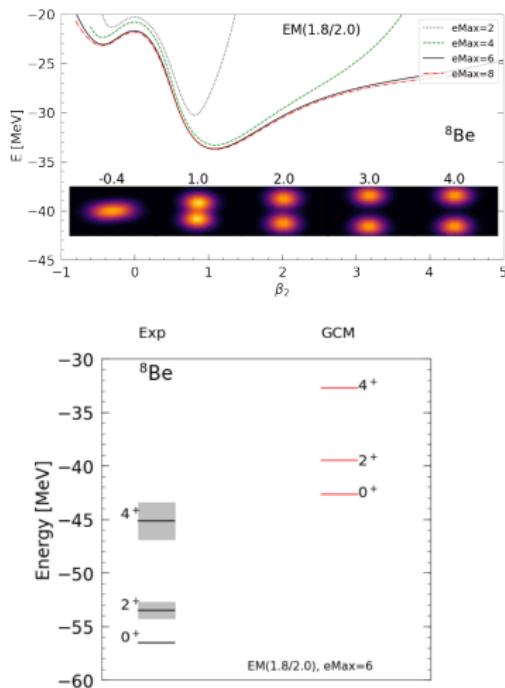


Phenomenological potentials



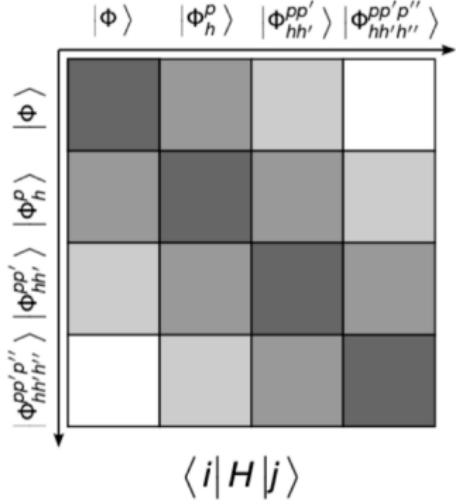
Potential from the chiral EFT

GCM calculations starting from a softened chiral interaction



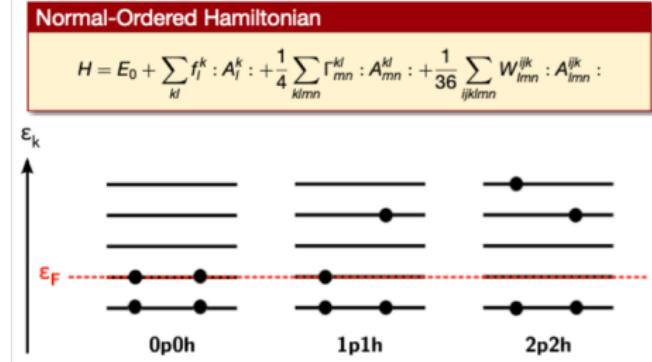
- The EM1.8/2.0 ($\hbar\omega = 16$ MeV) chiral interaction K. Hebeler et al PRC (2011)
- The collective properties are reasonably described. However, the entire spectrum is systematically shifted up to high energy.
- Enlarging the **eMax** value in the GCM calculation doesn't help to gain sufficient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

Missing more correlations from ...



credit: H. Hergert

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



$$\langle \overset{\textcolor{red}{p}}{h} | H | \Psi \rangle = \sum_{kl} f_l^k \langle \Psi | : A_p^h : : A_l^k : | \Psi \rangle = -n_h \bar{n}_p f_h^p$$

$$\langle \overset{\textcolor{red}{pp'}}{hh'} | H | \Psi \rangle = \sum_{klmn} \Gamma_{mn}^{kl} \langle \Psi | : A_{pp'}^{hh'} : : A_{mn}^{kl} : | \Psi \rangle \sim \Gamma_{hh'}^{pp'}$$

- 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

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

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 $H_{\text{eff.}} = e^{\Omega} H_0 e^{-\Omega}$,

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

- 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).

- A set of continuous **unitary transformations** onto the Hamiltonian

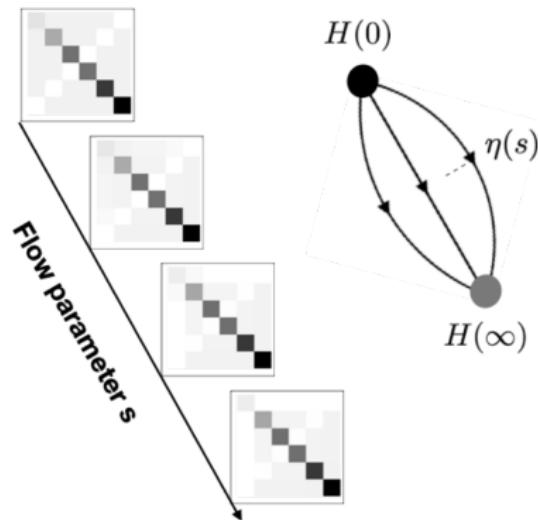
$$H(s) = U(s)H_0U^\dagger(s)$$

- 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 !

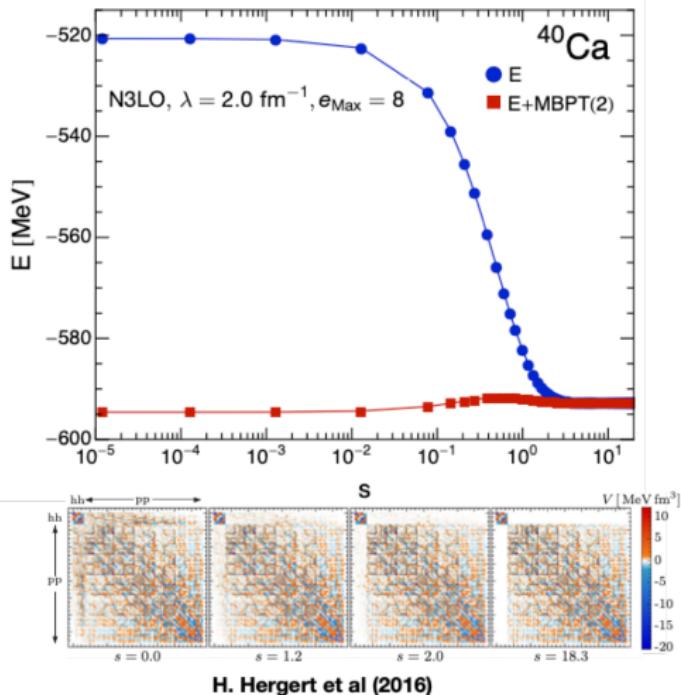
IMSRG for closed-shell nuclei

- A single-determinant (HF) state is chosen as the reference 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)

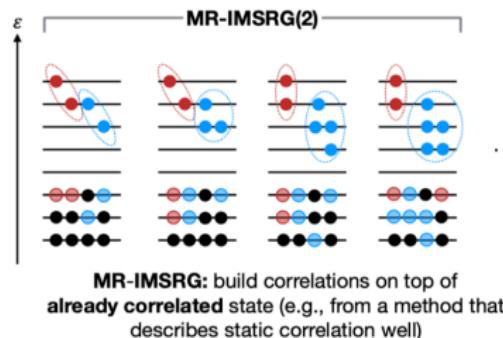
IMSRG: a convenient way to derive the unitary transformation



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

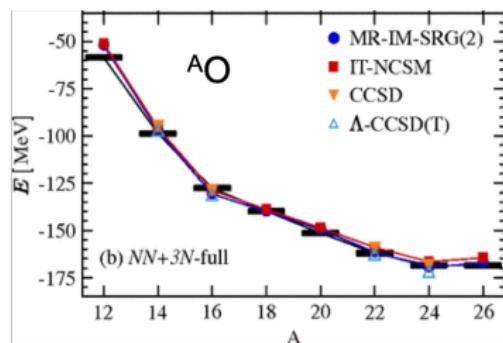
H. Hergert et al (2013)



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)

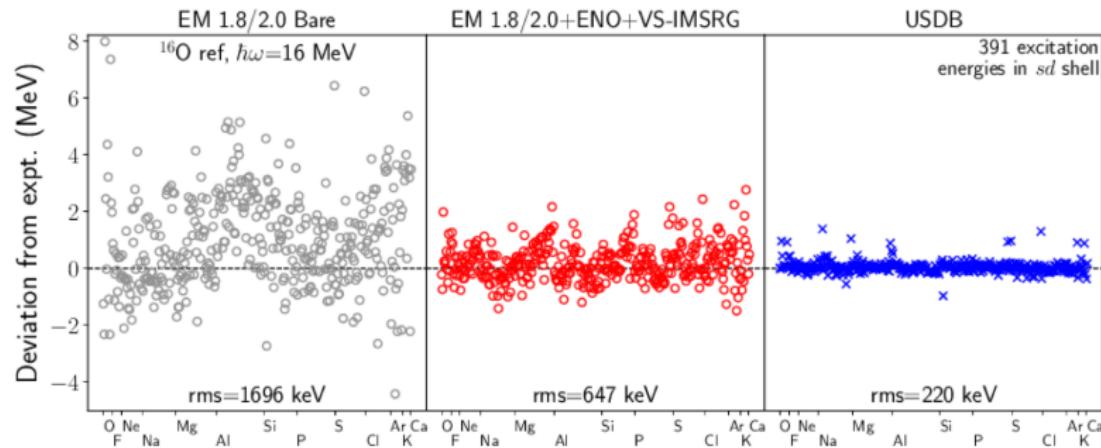


H. Hergert, S. Binder, A. Calci, J. Langhammer, and R. Roth (2013)

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



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

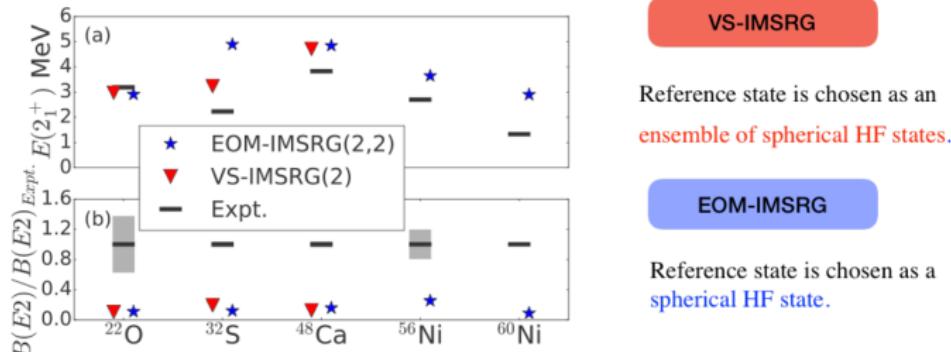


Review: S. R. Stroberg, S. K. Bogner, H. Hergert, J. D. Holt (2019)

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)

- 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.

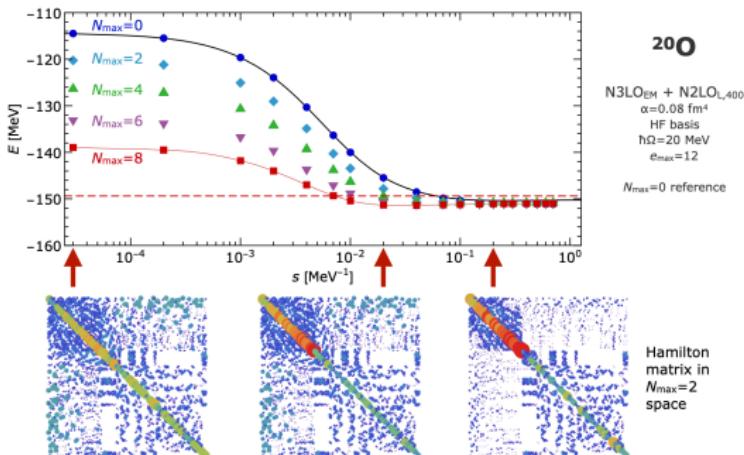
The E2 transition operator might not be decoupled into the small model space in the same manner as that of the interaction.
back to no-core calculation ...

Speeding up the convergence of the NCSM with IMSRG



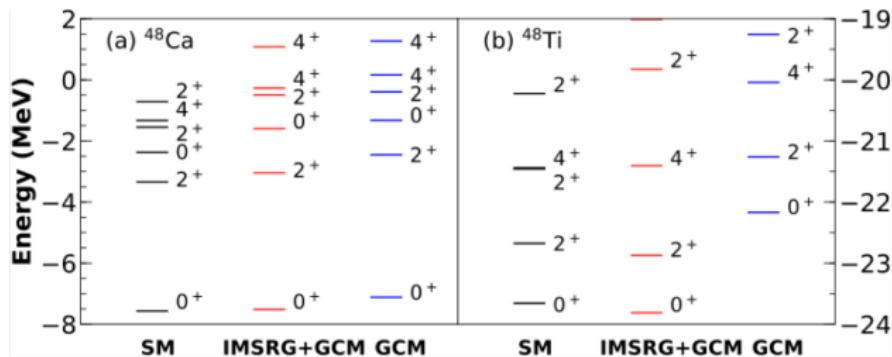
MR-IMSRG+NCSM

- 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)

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 ^{48}Ca , ^{48}Ti .
- ✓ The IMSRG overall improves the agreement with the shell-model results.

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

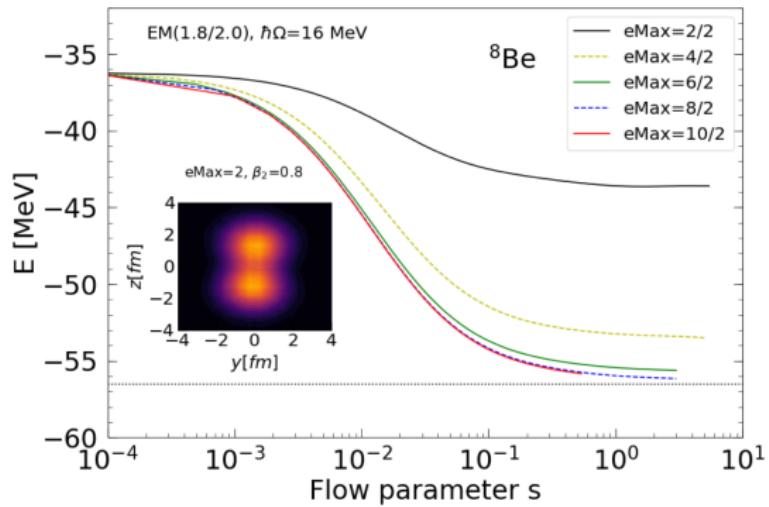
IMSRG+GCM calculations starting from a softened chiral interaction

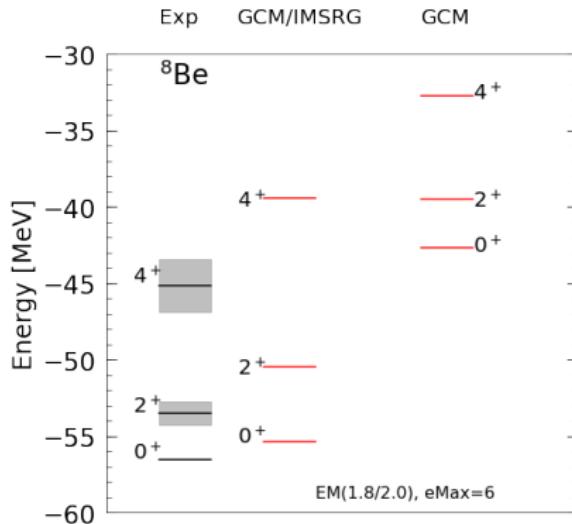


GCM
define
reference state

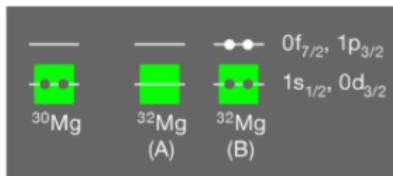
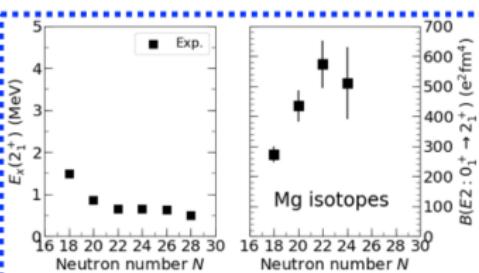
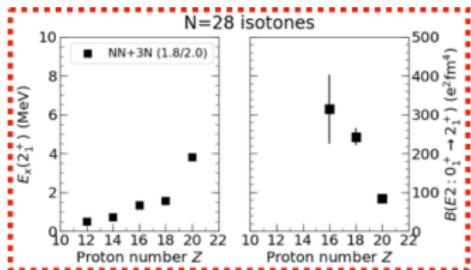
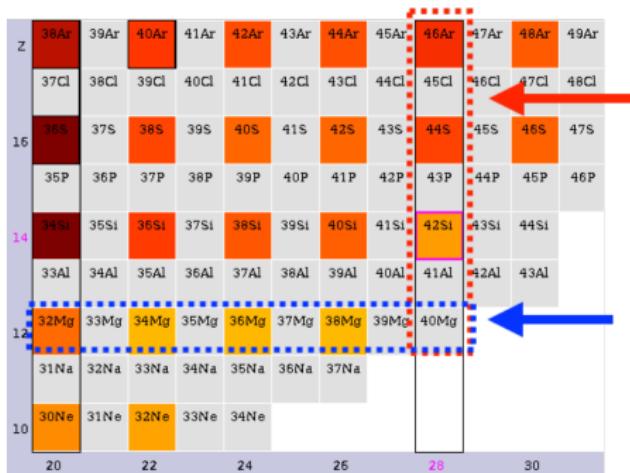


IMSRG
evolve
operators





Applications: onset of large deformation in “magic” nuclei



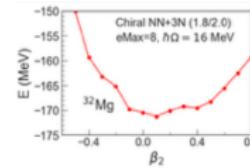
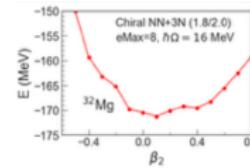
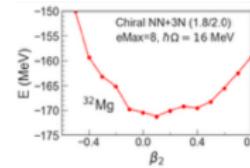
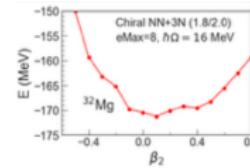
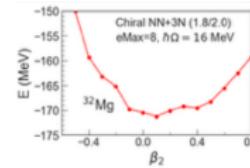
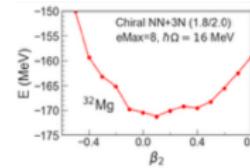
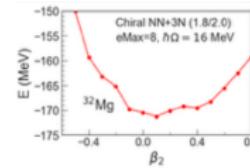
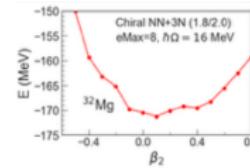
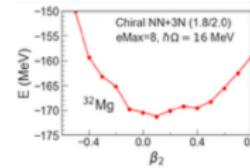
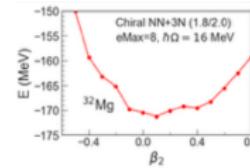
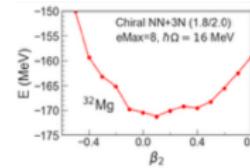
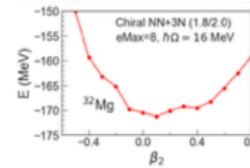
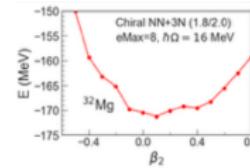
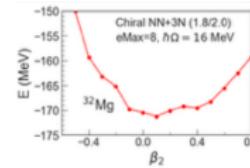
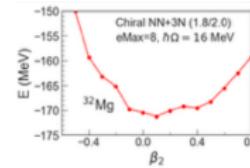
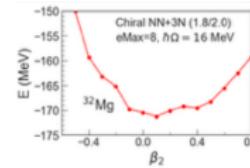
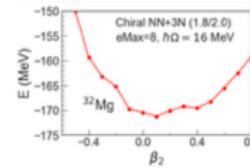
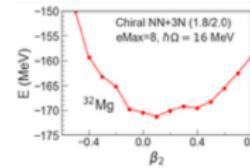
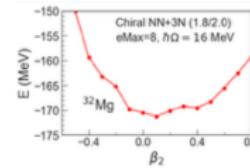
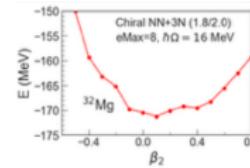
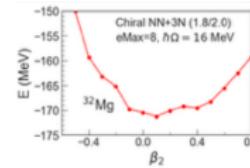
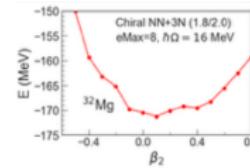
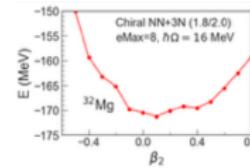
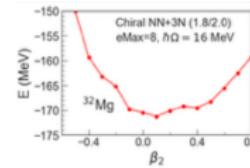
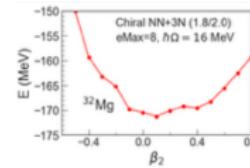
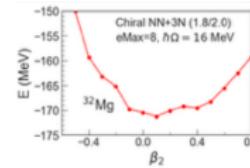
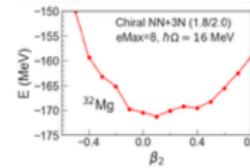
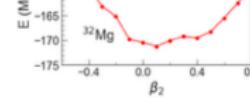
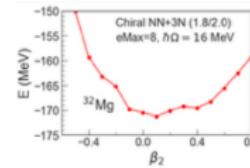
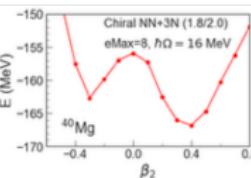
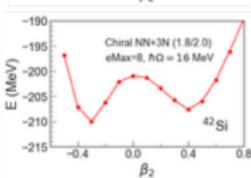
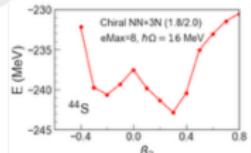
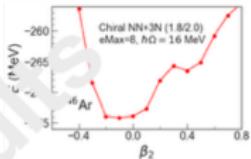
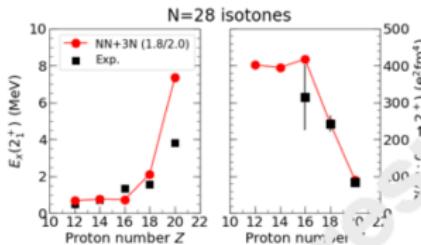
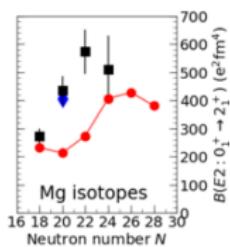
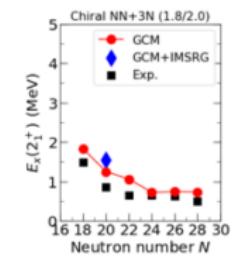
<https://physics.aps.org>

H. L. Crawford et al. (2019)
<https://www.nndc.bnl.gov>

Applications: onset of large deformation in “magic” nuclei



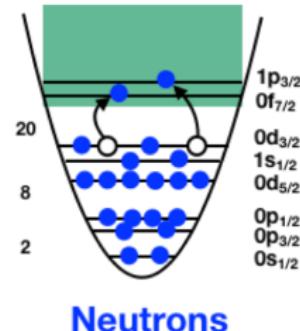
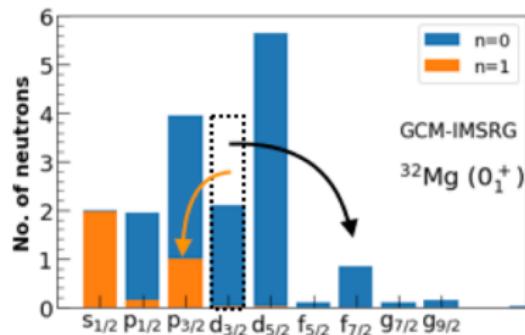
$e_{\text{Max}} = 8, \hbar\Omega = 16 \text{ MeV}$



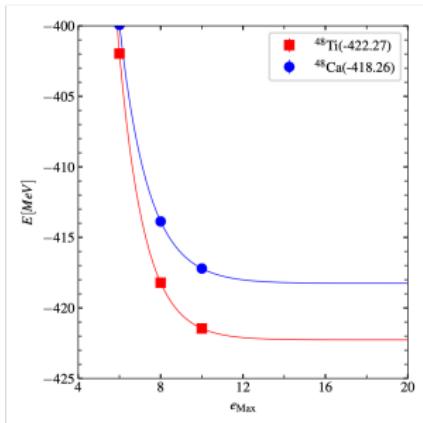
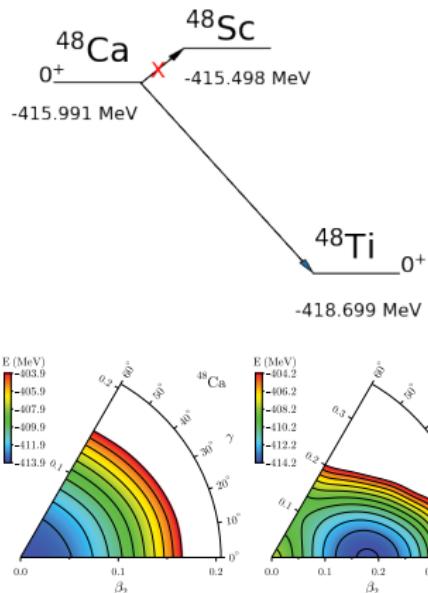
- One-body density in natural basis

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

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



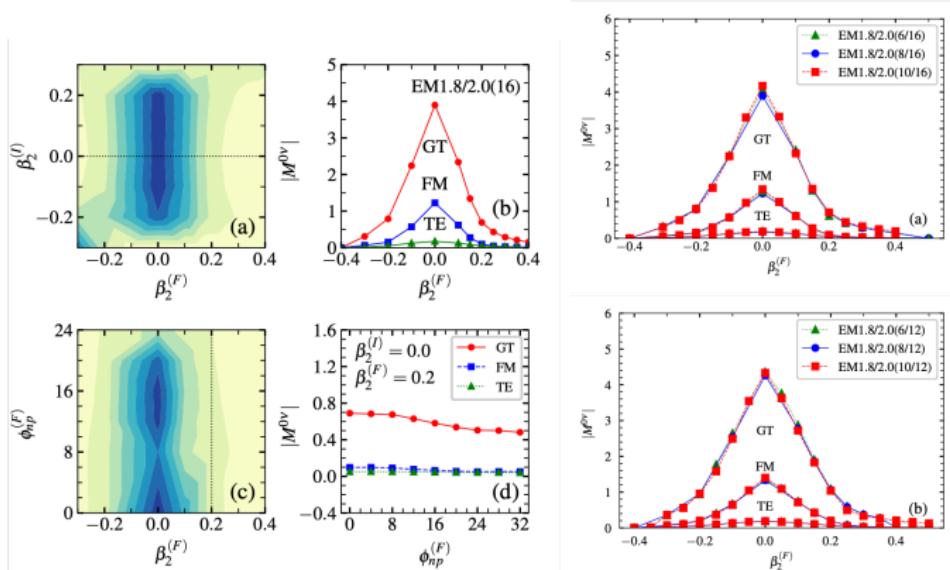
- PNVAP calculation with the IMSRG evolved chiral interaction.
- Extrapolation of the ground-state energy

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

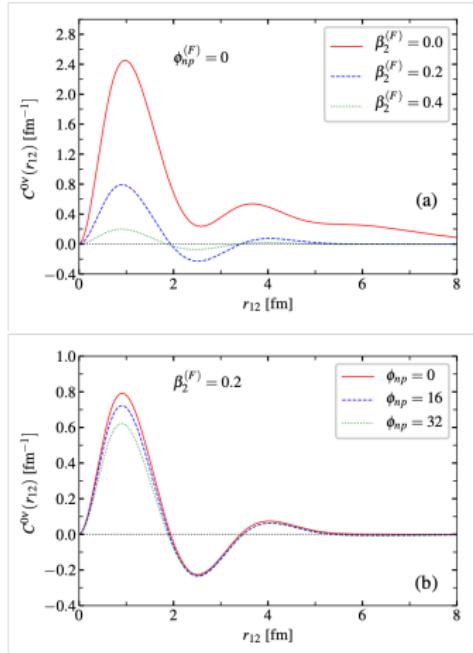
Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti



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



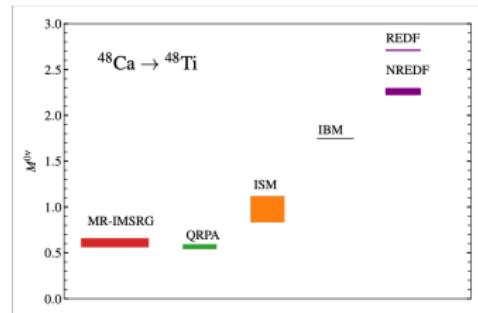
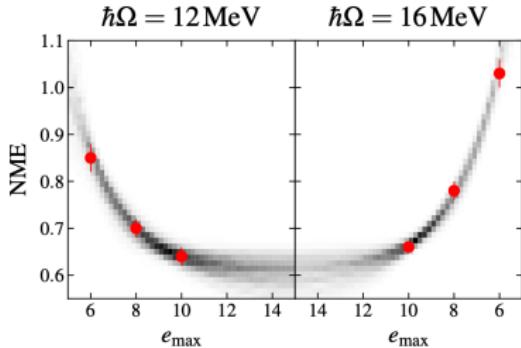
Application: $0\nu\beta\beta$ from ^{48}Ca to ^{48}Ti



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

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

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.

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 $^{48}\text{Ca} \rightarrow$ deformed ^{48}Ti is calculated with the IMGCM. Deformation shows a strong quenching effect on the NME.

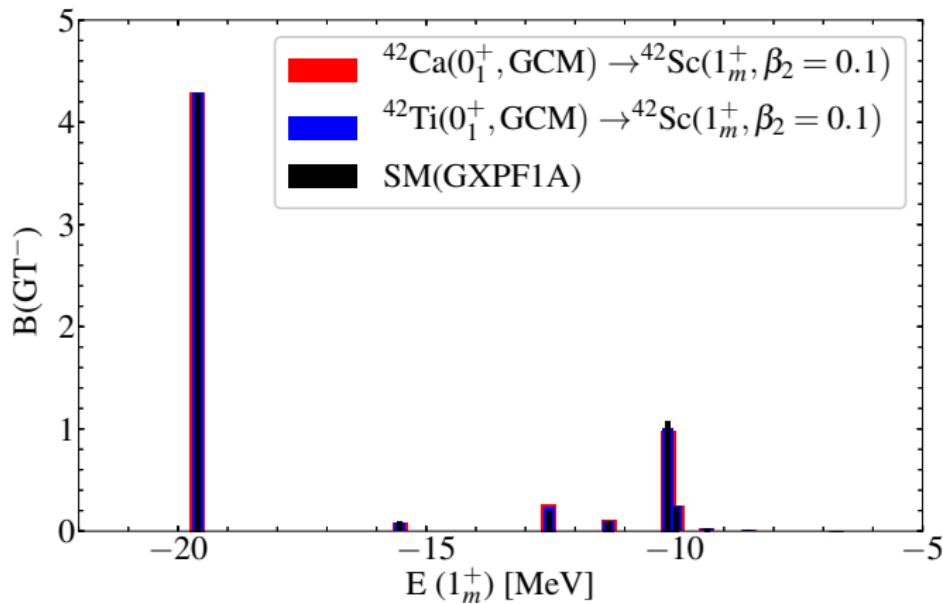
What's next:

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

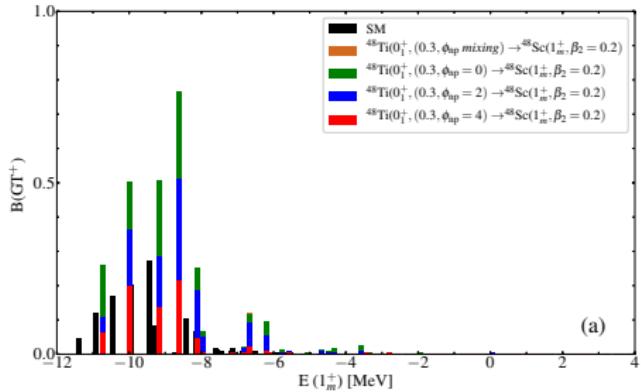
Summary and outlook

- GCM calculation for GT transition

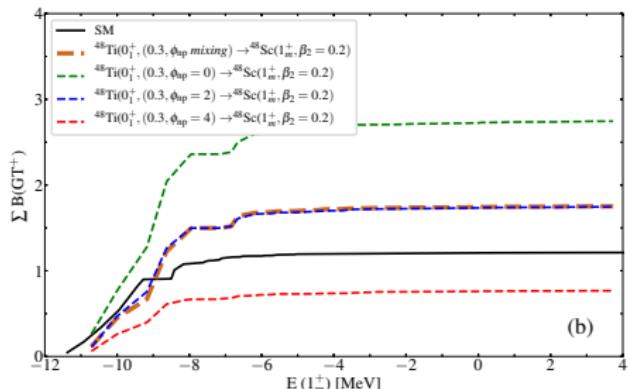
Benchmark calculation with a shell-model interaction



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



(a)

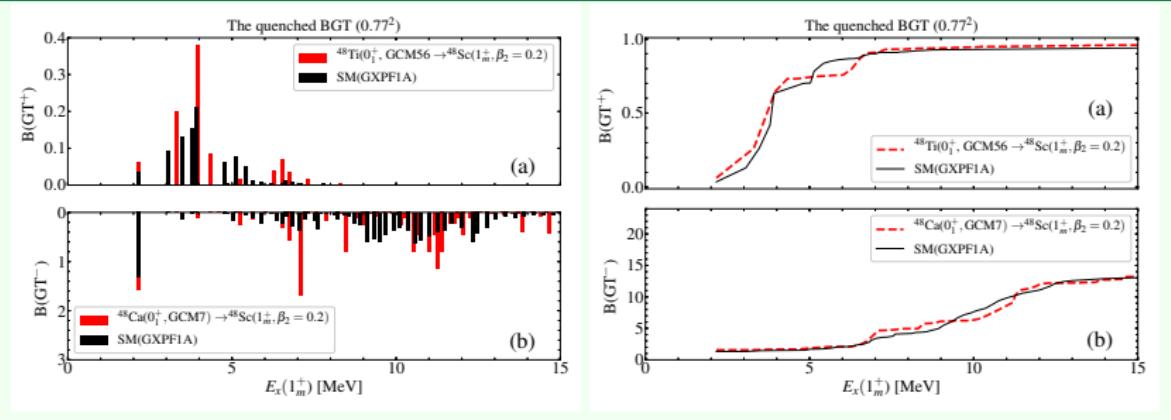


(b)

Summary and outlook

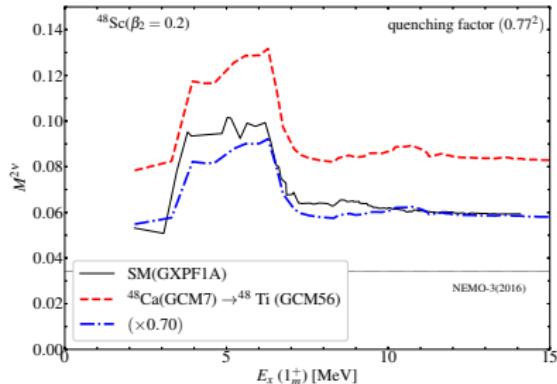
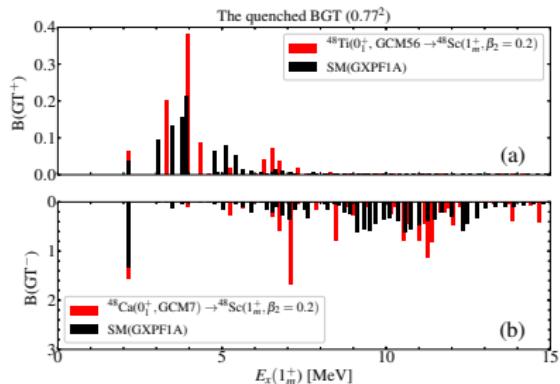
- GCM calculation for two-neutrino double-beta decay transition

Benchmark calculation with a shell-model interaction



Summary and outlook

- GCM calculation for two-neutrino double-beta decay transition



- The $M^{2\nu}$ is dominated by the transition through the first 1^+ state in the intermediate nucleus.
- The model-space in the GCM calculation for the intermediate states is still not sufficient. The inclusion of neutron-proton pairing correlation is expected to decrease the NME.

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Thank you for your attention!