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

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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]
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)
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 ...

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

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

\[ \langle \Phi^{pp'}_{hh'} | H | \Phi \rangle = \sum_{klmn} \Gamma^k_{lm} \langle \Phi | : A^{hh'}_{pp'} : : A^k_{mn} : | \Phi \rangle \]

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

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

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 $e^{\Omega}$ 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).
- 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: 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
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)
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).

![Graph showing comparisons between EOM-IMSRG and VS-IMSRG](image)

- 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.

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- 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.
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Building many-body correlations into interaction with IMSRG

GCM
Define reference state

IMSRG
Evolve operators

GCM
Extract observables

- 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

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**Graph**
- Title: $^8\text{Be}$
- $h\Omega = 16$ MeV
- EM(1.8/2.0)
- Flow parameter $s$
- Energy $E$ [MeV]
- $e_{\text{Max}}=2/2$, $e_{\text{Max}}=4/2$, $e_{\text{Max}}=6/2$, $e_{\text{Max}}=8/2$, $e_{\text{Max}}=10/2$
- $\beta_2 = 0.8$

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Ab initio calculation of deformed nuclei
starting from a SRG softened chiral interaction

GCM
- define reference state

IMSRG
- evolve operators

GCM
- extract observables

\[
\begin{aligned}
\text{Exp} & \\
\text{GCM/IMSRG} & \\
\text{GCM} & \\
\end{aligned}
\]

\[
\begin{array}{ccc}
\text{Energy [MeV]} & \text{4}^+ & \text{2}^+ & \text{0}^+ \\
\text{8Be} & \text{Exp} & \text{GCM/IMSRG} & \text{GCM} \\
\end{array}
\]

EM(1.8/2.0), eMax=6
Applications: onset of large deformation in “magic” nuclei

H. L. Crawford et al. (2019)

https://physics.aps.org
Applications: onset of large deformation in “magic” nuclei

e_{\text{Max}} = 8, \hbar \Omega = 16 \text{ MeV}
Application: $0\nu\beta\beta$ from $^{48}\text{Ca}$ to $^{48}\text{Ti}$

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

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

$$M^{0\nu} = \frac{4\pi R}{g_A^2} \int d^3\vec{r}_1 \int d^3\vec{r}_2 \int d^3\vec{q} \frac{e^{i\vec{q} \cdot (\vec{r}_1 - \vec{r}_2)}}{(2\pi)^3} \frac{e^{i\vec{q} \cdot (\vec{r}_1 - \vec{r}_2)}}{q + \bar{E} - (E_i + E_f)/2} \times \langle 0^+_F | e^{\Omega} \left[ \mathcal{J}_{\mu}^\dagger (\vec{r}_1) \mathcal{J}_{\mu}^\dagger (\vec{r}_2) \right] e^{-\Omega} | 0^+_i \rangle$$
Application: $0\nu\beta\beta$ from $^{48}\text{Ca}$ to $^{48}\text{Ti}$

\[ M^{0\nu} = \int dr_{12} \; C^{0\nu}(r_{12}) \]

- The quadrupole deformation in $^{48}\text{Ti}$ 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 $^{48}\text{Ca} \rightarrow$ deformed $^{48}\text{Ti}$ 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-$\beta$ 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

\[ \left| ^{42}_{\text{Sc}}; JNZ(\beta_2, \phi_{np}) \right\rangle = \sum_{K, pn} f_{K}^{JNZ}(\beta_2) \hat{P}^{N} \hat{P}^{Z} \hat{P}_{MK}^{J}[\beta_2, \beta_{np}^{\dagger}] \left| ^{42}_{\text{Sc}}; \text{HFB}(\beta_2, \phi_{np}) \right\rangle \]  

(1)

The GT transition strength \((g_A\) is taken as 1)

\[ B(GT^- : 0_1^+ \rightarrow 1_m^+) = \left| \left\langle 1_m^+ | \hat{O}_{GT}^- | 0_1^+ \right\rangle \right|^2 \] 

(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 $B(GT^+)$ of $^{48}$Ti $\rightarrow$ $^{48}$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

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

- 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 you for your attention!
PESs

Energy [MeV]

GXPF1A

48Ca/PNVAP

48Sc/HFB

48Ti/PNVAP

$\beta_2$

Energy [MeV]

GXPF1A
Speeding up the convergence of the NCSM with IMSRG

**MR-IMSRG+NCSM**

- NCSM with $N_{\text{max}} = 0$ 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 \textit{sd}-shell nuclei

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 Hamiltonian \( H(s) = e^{\Omega} H_0 e^{-\Omega} \).