Ab initio treatment of collective correlations in neutrinoless double beta decay

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What's neutrinoless double beta decay?

At nuclear-structure level, it corresponds to the transition

 $^{A}Z \rightarrow ^{A} (Z + 2) + 2e^{-}$



Schechter-Valle theorem (1982): any diagram causing the $0\nu\beta\beta$ decay will generate a Majorana mass term for light neutrinos

- Beyond SM physics: nonzero neutrino mass
- Nature of neutrinos: Dirac or Majorana
- Origin of the matter-antimatter asymmetry: Lepton-number violation

V. Cirigliano+ (2020)





What kind of nuclei to observe the $0\nu\beta\beta$?





Single-beta decay is energetically forbidden

- Experimental interest
 - 1 Large $Q_{\beta\beta}$ value
 - 2 Large isotopic abundance
 - Low background in the energy region of interest

Features of candidate nuclei

The nuclei evolved in the $0\nu\beta\beta$ are mostly medium-mass open-shell (deformed) nuclei.

Current status on the studies of $0\nu\beta\beta$ decay



Based on the mechanism of exchange light Majorana neutrino, the inverse of half-life of $0\nu\beta\beta$ can be factorized as

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$$[T_{1/2}^{0\nu}]^{-1} = g_{A}^{4}G_{0\nu} \left| \frac{\langle m_{\beta\beta} \rangle}{m_{\theta}} \right|^{2} \left| M^{0\nu} \right|^{2}, \quad \langle m_{\beta\beta} \rangle = |\sum_{i=1,2,3} U_{ei}^{2}m_{i}|$$

A precise knowledge (from ab initio calculation) of the nuclear matrix element (NME) $M^{0\nu}$ is helpful to determine the neutrino effective mass $\langle m_{\beta\beta} \rangle$, if the process is measured eventually.

Nuclear matrix element for the $0\nu\beta\beta$ decay

• The NME for the $0\nu\beta\beta$ transition from $|0_I^+\rangle$ to $|0_F^+\rangle$

$$M^{0\nu}(0^+_I \to 0^+_F) = \langle 0^+_F | O^{0\nu} | 0^+_I \rangle$$



- the transition operator: exchange of light neutrinos and with closure approximation

$$\mathcal{O}^{0\nu} = \frac{4\pi R}{g_A^2} \int d^3 \vec{r}_1 \int d^3 \vec{r}_2 \int \frac{d^3 \vec{q}}{(2\pi)^3} \frac{e^{i\vec{q}\cdot(\vec{r}_1-\vec{r}_2)}}{q(q+E_d)} \mathcal{J}^{\dagger}_{\mu}(\vec{r}_1) \mathcal{J}^{\mu\dagger}(\vec{r}_2) \\
 = \sum_{K} \sum_{1,2} H_K(r_{12}, E_d) \tau_1^+ \tau_2^+ S_K$$
(1)

where $S_K = \{1, \sigma_1 \cdot \sigma_2, 3(\sigma_1 \cdot \hat{r}_{12})(\sigma_2 \cdot \hat{r}_{12}) - \sigma_1 \cdot \sigma_2\}$ for $K = \{F, GT, T\}$, respectively. The average excitation energy $E_d = \overline{E} - (E_i + E_f)/2 \sim 1.12A^{1/2}$. Only one-body current \mathcal{J}^{μ} is taken into account in the present study.

ab initio calculations of nuclear structure



- The wave functions of initial and final nuclei require the calculation from ab initio methods:
 - starts from a bare nucleon-nucleon interaction (fitted to data of NN scattering/few-body systems)
 - Isolves Schroedinger equation (for the many-body system) with a controllable accuracy of approximations
- Benchmark calculations in light nuclei:
- Variational Monte Carlo calculation starting from the Argonne v18 two-nucleon potential and Illinois-7 three-nucleon interaction for light nuclei
 S. Pastore et al. (2017)
- V No-core shell model calculations starting from chiral NN+3N interactions for light nuclei P. Gysbers et al., R. A. Basili et al. (2019)
- Extension to medium-mass candidate nuclei:
- \checkmark Application of coupled-cluster (S. Novario, G. Hagen, T. Papenbrock et al.) and valence-space in-medium similarity renormalization group (IMSRG) (Antoine Belley, R. Stroberg, J. Holt et al.) method starting from chiral NN+3N interactions for $0\nu\beta\beta$ -candidate nuclei
- √ Merging the multi-reference IMSRG with generator coordinate method (GCM) starting from chiral NN+3N interactions for 0νββ-candidate nuclei JMY, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, H. Hergert, arXiv:1908.05424

The method: basic idea of IMSRG

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 $\eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s)$ 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 !



Extension of the IMSRG for the NMEs of $0\nu\beta\beta$: challenges



open-shell nuclei with collective correlations: mp-mh excitation configurations



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

■ different unitary transformation for the initial and final nuclei: $U_I(s) \neq U_F(s)$. Computation of the following matrix element

$$M^{0\nu} = \langle \Phi_F | U_F(s) O^{0\nu} U_I^{\dagger}(s) | \Phi_I \rangle = \langle \Phi_F | e^{\Omega_F(s)} O^{0\nu} e^{-\Omega_I(s)} | \Phi_I \rangle$$
⁽²⁾

with truncation error controllable is challenge.

choose the reference state $|\Phi\rangle$ as an ensemble of the initial and final nuclei

The IMSRG+GCM method: procedure

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- Generation of a reference state with collective correlations
 - Constrained deformed HFB calculation with variation after particle-number projection
 - projection onto the right quantum numbers (NZ,J)
 - 3 computing many-body density matrices of the reference state
- Normal-ordering all the operators with respect to the reference state and solve the IMSRG flow equation
 - Ensemble normal-ordering (NO2B)
 - 2 Computing all the RG evolved operators
- Diagonalization of the evolved Hamiltonian with GCM
 - Generate a set of non-orthogonal quantum-number projected HFB states with different coll. correlations
 - 2 mixing of these states with GCM
 - Computing observables with the GCM wave functions using the corresponding evolved operators

A benchmark of the method



- model space: pf shell
- KB3G interaction



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

Computation time for the many-body density matrices increases significantly while using chiral interactions in full model space.

Many-body density matrices in a small model space



Prescription

- Construct density matrix elements in a small model space (defined by emax)
- Normal-order the H and solve the IMSRG flow in a large model space (eMax)





An illustrative calculation for deformed nuclei: ⁸Be





 HFB potential energy surface by the SRG softened chiral interaction EM1.8/2.0(ħΩ = 16 MeV)

Starting from the reference state with two-α structure, the IMSRG(2) is converged to ground state.

Applications to neutrinoless double beta decay



- Benchmark calculations of light nuclei:
 - 1 transition between $\Delta T = 0$ states: ⁶He \rightarrow ⁶Be, and ¹⁰Be \rightarrow ¹⁰C 2 transition between $\Delta T = 2$ states: ⁸He \rightarrow ⁸Be, and ²²O \rightarrow ²²Ne
- Application to candidate $0\nu\beta\beta$ process ($\Delta T = 2$):
 - 1 ${}^{48}Ca \rightarrow {}^{48}Ti$ 2 ${}^{76}Ge \rightarrow {}^{76}Se$

0 uetaeta from ⁶He and ⁶Be ($\Delta T = 0$)



- SRG softened two-body NN interaction: EM2.0/500
- make use of isospin symmetry in the wave functions of initial and final nuclei



R.A. M Basili, JMY, J. Engel, H. Hergert, M. Lockner, P. Maris, J.P. Vary, arXiv:1909.06501

$0\nu\beta\beta$ from ⁶He and ⁶Be ($\Delta T = 0$)



chiral 2N+3N interaction(EM1.8/2.0), isospin symmetry is NOT assumed in the wfs



- $M^{0\nu}$ is weakly sensitive to the shapes/deformations of concerned
- $M^{0\nu}$ (GT/F/TE)= 3.18/0.88/-0.05
- VMC (AV18+IL17): M⁰^v (GT/F/TE)=3.688/0.946/-0.025 [S. Pastore+(2018)] discrepancy contributed from both wfs and transition operators.

$0\nu\beta\beta$ from ⁶He and ⁶Be ($\Delta T = 0$)



$$M^{0\nu} = \int_0^\infty C^{0\nu}(r_{12}) dr_{12}$$





Summary of the NMEs in light nuclei





consistent with the findings in the "exact" calculations with VMC (AV18+IL17) S. Pastore et al (2018); X.B. Wang (2019) and NCSM (EM1.8/2.0) P. Gysbers et al.









- IMSRG+GCM: Low-energy structure of ⁴⁸Ti is reasonably reproduced (spectrum stretched). Inclusion of non-collective configurations from neutron-proton isoscalar pairing fluctuation can compress the spectra further by about 6%.
- IMSRG+CI(T0 → T1): the spectrum becomes more stretched in a larger model space (more collective correlations).







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

- The quadrupole deformation in ⁴⁸Ti 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 ~17% further, which might be canceled out partially by the isovector pairing fluctuation.

$0\nu\beta\beta$ from ⁷⁶Ge to ⁷⁶Se (preliminary results)







	⁷⁶ Ge		⁷⁶ Se	
eMax	E2 (e ² fm ⁴)	$E_x(2_1^+)$ (MeV)	E2 (e ² fm ⁴)	$E_x(2^+_1)$ (MeV)
6	255(3)	1.03(4)	412(11)	0.73(1)
8	287(3)	1.17(7)	468(6)	0.70(1)
Exp.	547(6)	0.563	864(22)	0.559

The above $B(E2: 2^+ \rightarrow 0^+)$ values are evaluated with the evolved one-body E2 operator only.

$0\nu\beta\beta$ from ⁷⁶Ge to ⁷⁶Se (preliminary results)





renormalization effect on the transition operator:

- 1 The renormalization effect is mainly contributed from $\Omega^{(2)}$
- The pp/hh diagrams enhance the NME (GT)

$$\sum_{ab} O^{0\nu}_{pp'ab} \Omega_{abnn'} (1 - n_a - n_b) + (\Omega \leftrightarrow O^{0\nu})$$
(3)

while the ph diagrams quench the NME.

enhances the transition from ⁴⁸Ca to ⁴⁸Ti and quenches that from ⁷⁶Ge to ⁷⁶Se.

Summary of NMEs from IMSRG calculations





- The unpublished results of VS-IMSRG are from (A. Belley, R. Stroberg, J. Holt et al.)
- Uncertainties from different sources (model truncation, chiral expansion, contact operator, two-body currents) are to be included.

Summary and outlook



- The mass ordering of neutrinos is expected to be disclosed with the development of ton-scale $0\nu\beta\beta$ decay experiments in the next few years, depending on the values of the NMEs.
- The NMEs governing the $0\nu\beta\beta$ are essential to determine the neutrino effective mass. Several ab initio methods have begun to calculate the NMEs starting from first principles.
- We develop a novel multi-reference framework of IMSRG+GCM which opens a door to modeling deformed nuclei with realistic nuclear forces.
- The NMEs for several unphysical process in light nuclei and those for candidate process in medium-mass nuclei ⁴⁸Ca and ⁷⁶Ge(preliminary) are calculated. The NMEs in both cases are smaller than the predictions by (most) phenomenological models.
- More benchmarks among different *ab initio* calculations for the NMEs are underway.
- Quantification of uncertainties from different sources: systematic and statistic (open for comments/suggestions)

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Thank your for your attention!

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Ab initio calculation of $0\nu\beta\beta$