$0\nu\beta\beta$ Decay with Coupled Cluster Theory, and an analysis of the LO contact term

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Outline

Coupled Cluster $0\nu\beta\beta$ NME

$0\nu\beta\beta$ nuclear matrix element

$$\left|M^{0\nu}\right|^2 = \left|\langle \mathrm{f}|\,\hat{O}\,|\mathrm{i}\rangle\right|^2 = \langle \mathrm{f}|\,\hat{O}\,|\mathrm{i}\rangle\langle \mathrm{i}|\,\hat{O}^\dagger\,|\mathrm{f}\rangle$$

$$= \langle\Phi_0|\,\mathrm{e}^{-\hat{T}}\,\hat{L}_\mathrm{f}\hat{O}\,\mathrm{e}^{\hat{T}}\,|\Phi_0\rangle\langle\Phi_0|\,\mathrm{e}^{-\hat{T}}\,\hat{L}_0\,\hat{O}^\dagger\hat{R}_\mathrm{f}\,\mathrm{e}^{\hat{T}}\,|\Phi_0\rangle$$

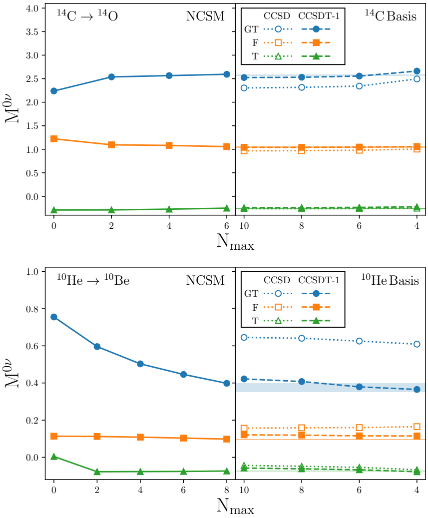
$$= \boxed{\langle\Phi_0|\,\hat{L}_\mathrm{f}\,\bar{O}\,|\Phi_0\rangle\langle\Phi_0|\,\hat{L}_0\,\bar{O}^\dagger\,\hat{R}_\mathrm{f}\,|\Phi_0\rangle}$$

Similarity-transformed beta-decay operator

$$\mathrm{e}^{-\hat{T}}\,\hat{O}\,\mathrm{e}^{\hat{T}} = \left(\hat{O}e^{\hat{T}}\right)_\mathrm{c}$$

$$\hat{O} = \hat{O}^{0\nu}_{\mathrm{GT}} + \hat{O}^{0\nu}_{\mathrm{F}} + \hat{O}^{0\nu}_{\mathrm{T}}$$

$0\nu\beta\beta$ Benchmarks in Light Nuclei: ^{14}C and ^{10}He

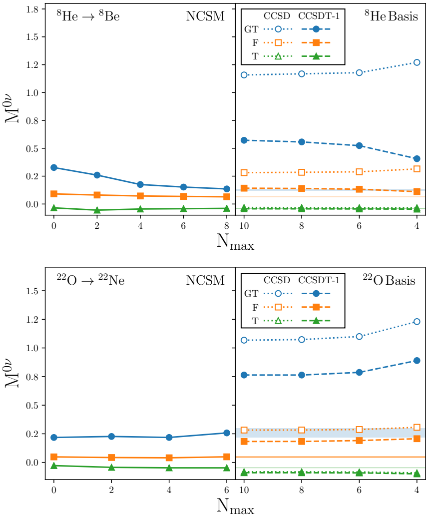


CC calculations of ^{14}C $\rightarrow$ ^{14}O agree well with NCSM. The mirror structure of the initial and final nuclei make this comparison somewhat trivial.

CC calculations of ^{10}He $\rightarrow$ ^{10}Be somewhat agree with NCSM. The final nuclei has an open-shell structure.

Both of these cases have relatively well-converged initial and final wavefunctions.

$0\nu\beta\beta$ Benchmarks in Light Nuclei: ^{8}He and ^{22}O

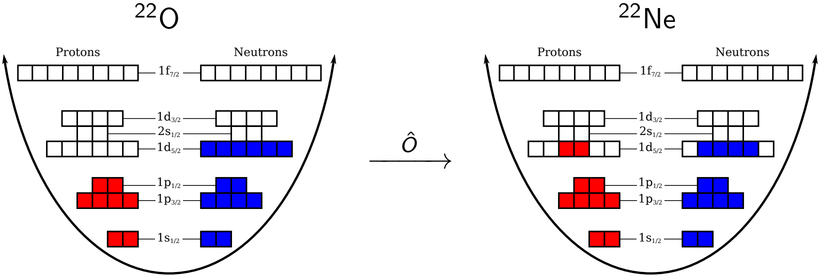


CC calculations of ^{8}He → ^{8}Be and ^{22}O → ^{22}Ne do not agree well with NCSM.

While the initial wavefunctions are well-converged, the spherical basis does not capture the deformed, open-shell final states.

Describing these states would require correlations beyond double and triple excitations.

Hartree Fock Basis: Spherical

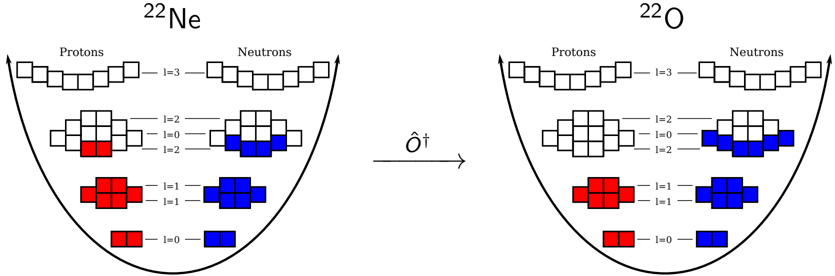


1) Compute spherical HF basis of initial nucleus
2) Decouple initial nucleus ground state
3) Diagonalize EOM ground state of final nucleus

Pros: Maintains total angular momentum and is computationally efficient.

Cons: Cannot feasibly calculate open-shell, deformed nuclei.

Hartree Fock Basis: Deformed

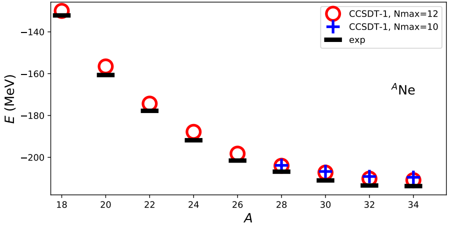


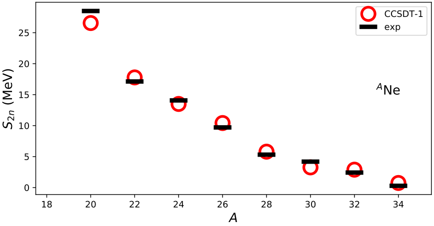
1) Compute deformed natural orbital basis of final nucleus (Tichai et al 2018)
2) Decouple final nucleus ground state
3) Diagonalize EOM ground state of initial nucleus

Pros: Can calculate open-shell, deformed nuclei without EOM diagonalization.

Cons: Doesn't preserve total angular momentum and is more computationally expensive.

Deformed Basis Example: Even-even Isotopes

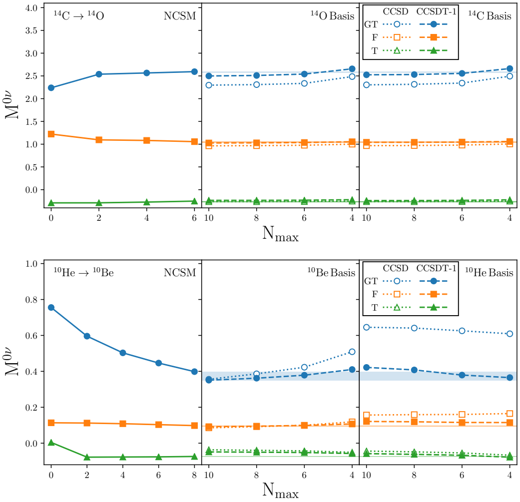




Deformed CC calculations of even-even neon isotopes reproduce binding energies and two-neutron separation energies.

Realistic spectra requires symmetry restoration.

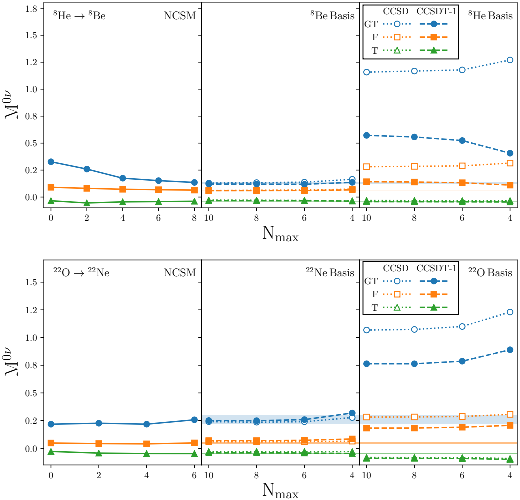
$0\nu\beta\beta$ Benchmarks in Light Nuclei: ^{14}C and ^{10}He



Deformed CC calculations of ^{14}C → ^{14}O and ^{10}He → ^{10}Be still agree well with NCSM.

In the deformed basis, ^{10}Be can be computed much more easily, and the small differences between NCSM are resolved.

$0\nu\beta\beta$ Benchmarks in Light Nuclei: ^{8}He and ^{22}O

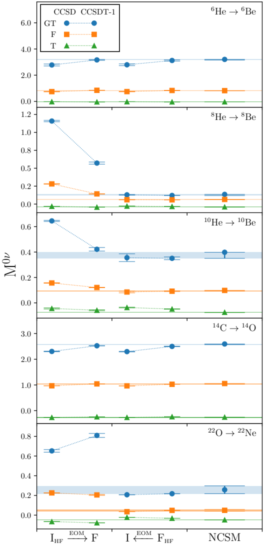


Deformed CC calculations of ^{8}He → ^{8}Be and ^{22}O → ^{22}Ne agree well with NCSM.

The final deformed nuclei are well described without triples corrections.

The initial spherical nuclei is sufficiently described in the deformed basis.

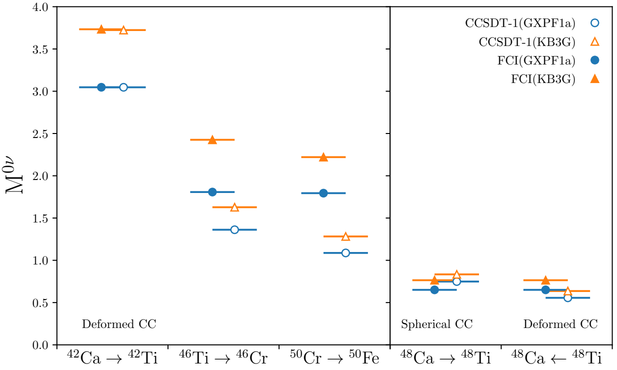
$0\nu\beta\beta$ Benchmarks in Light Nuclei



Triples correlations and deformed basis both address deformation in daughter nuclei and should give confidence in calculation of ^{48}Ca.

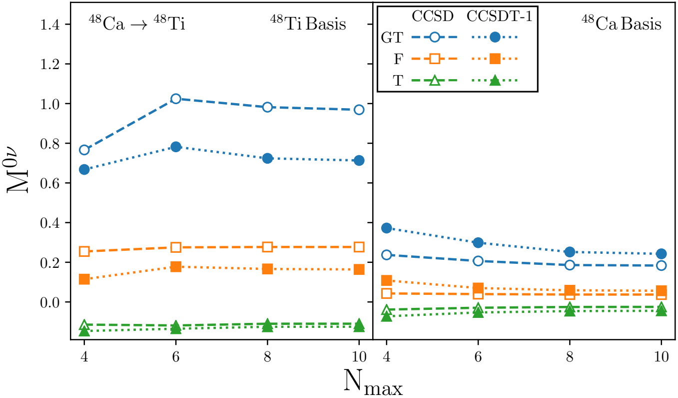
$0\nu\beta\beta$ Decay of ^{48}Ca with FCI

Comparing with exact FCI (Javier Menendez) in pf-shell with phenomenological interactions.



The spherical and deformed calculations give upper and lower bounds to the NME. Symmetry restoration is needed.

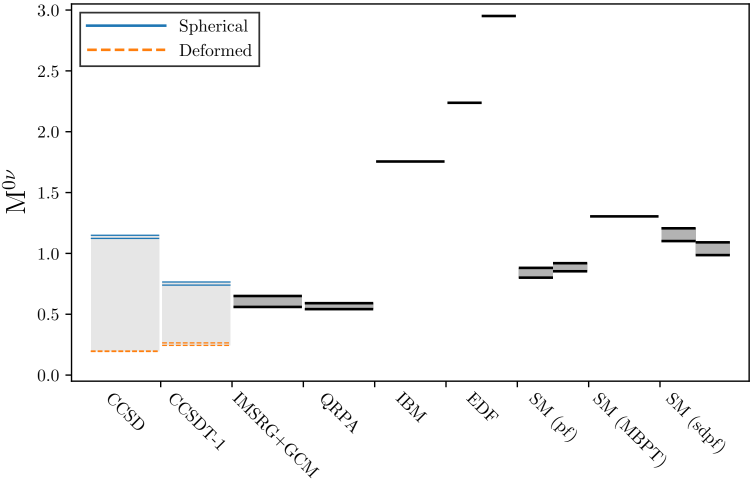
Ab Initio $0\nu\beta\beta$ Decay of ^{48}Ca



$0\nu\beta\beta$ NME of ^{48}Ca → ^{48}Ti $\sim 0.25 - 0.75$.

NME is consistent with phenomenological models and IM-SRG+GCM at ~ 0.6.

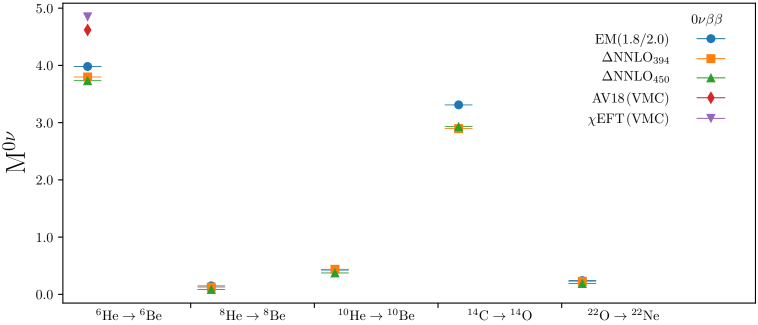
Ab Initio $0\nu\beta\beta$ Decay of ^{48}Ca



Determining the Unknown Contact

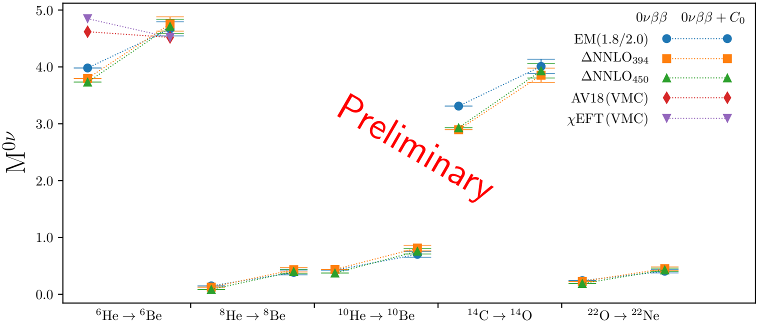
- $0\nu\beta\beta$ NME should be cutoff invariant when LO contact is included.
- LECs can be determined by minimizing the spread of the NMEs from different interactions?
- Using benchmarked cases, find g_i to minimize $\chi^2 = \sum_a \sum_{i \neq j} \left(L_{i,a} + g_i S_{i,a} - L_{j,a} - g_j S_{j,a}\right)^2$.
- Contact term defined as $C_0 = g_i \delta^3 \left(\mathbf{r}\right)$

LO Contact in Light Benchmark Nuclei



Included VMC results from V. Cirigliano et al (2019)

LO Contact in Light Benchmark Nuclei



Solutions enhance the $0\nu\beta\beta$ NMEs and agree with similar analysis of VMC results from V. Cirigliano et al (2019)

Still need to apply to ^{48}Ca → ^{48}Ti.

Summary

- Coupled cluster $0\nu\beta\beta$ calculations agree well with NCSM benchmarks of light nuclei with well-described final states.
- Deformed coupled cluster can address problems involving open-shell, deformed nuclei.
- The deformed ground state of ^{48}Ti is not easily obtained without symmetry restoration.
- NME for ^{48}Ca $\rightarrow$ ^{48}Ti with CC provides upper and lower bounds.
- Missing contact term seems to enhance the $0\nu\beta\beta$ NME.

Current and Future Work

- Investigate quadrupole deformation and symmetry restoration of ^{48}Ti.
- Continue analysis of missing LO contact term.
- Use developed machinery for $2\nu\beta\beta$ decays.
- Use deformed basis to calculate previously intractable case of ^{76}Ge.

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