The DBD Collaboration

and the

Multi-Reference In-Medium SRG

J. Engel

July 15, 2019

Collaboration Members who are Here

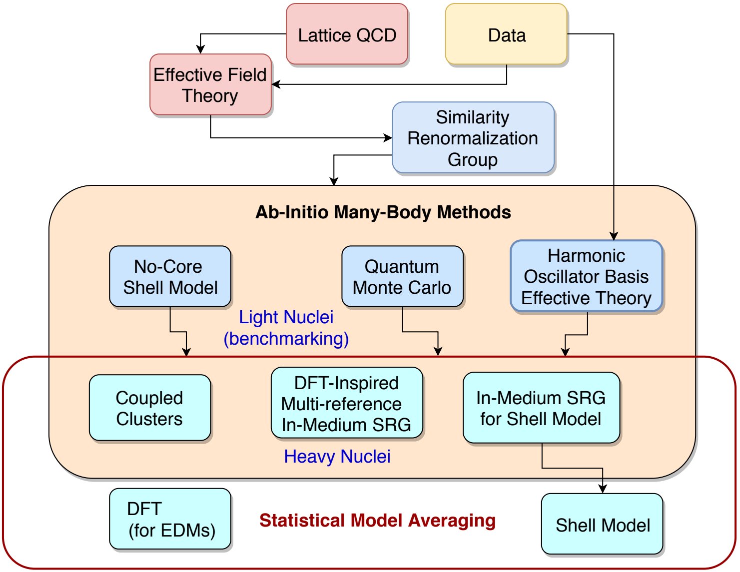
- Lattice QCD: H. Monge Camacho, A. Walker-Loud
- EFT: ~~V. Cirigliano~~, J. De Vries, E. Mereghetti
- Nuclear Structure:
  - HOBET: K. McElvain
  - QMC: S. Pastore
  - Coupled Clusters: S. Novario
  - Shell Model: M. Horoi
  - SM-IMSRG: J. Holt

Collaboration Members who are Here

- Lattice QCD: H. Monge Camacho, A. Walker-Loud
- EFT: ~~V. Cirigliano~~, J. De Vries, E. Mereghetti
- Nuclear Structure:
  - HOBET: K. McElvain
  - QMC: S. Pastore
  - Coupled Clusters: S. Novario
  - Shell Model: M. Horoi
  - SM-IMSRG: J. Holt
  - MR-IMSRG: Just me (so I'll talk about this after a brief review…)

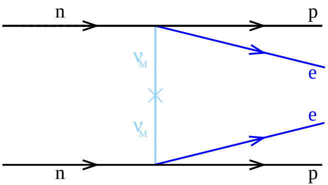
Part I: The Collaboration

Integrated Approach to $\beta\beta$ Decay



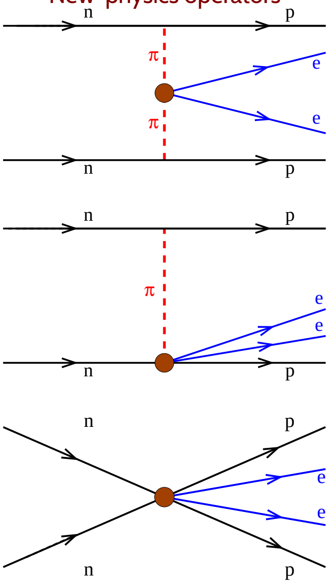
New Physics at Hadronic Level

Light-ν exchange:



+ corrections

New-physics operators

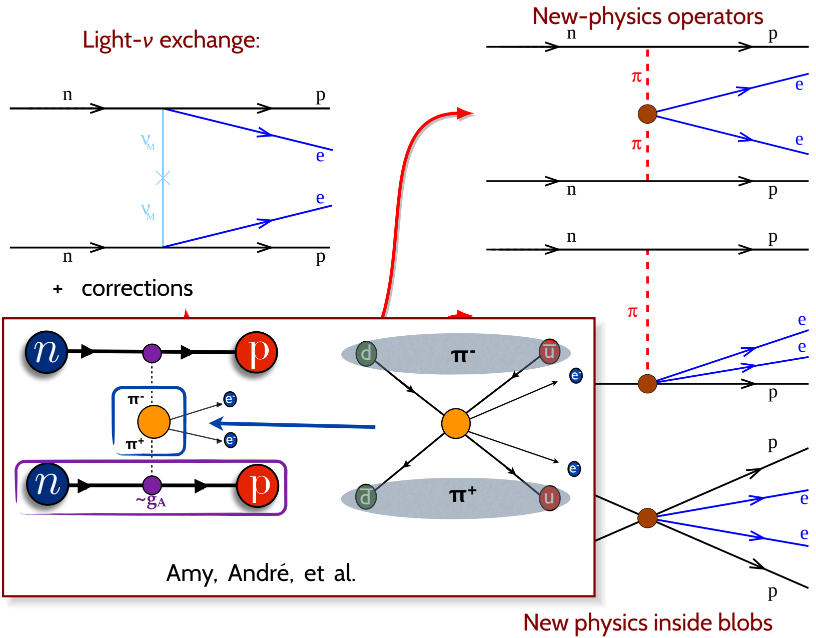


New physics inside blobs

Effective field theory lists pion-nucleon-level operators and determines their importance.

Lattice QCD can then compute dependence of blobs on new particle masses and couplings.

New Physics at Hadronic Level



Improving Nuclear Structure: Ab Initio Methods

Use most accurate methods:
No-Core Shell Model, Quantum Monte Carlo

in light nuclei to verify other methods:
Coupled Clusters, RG-based techniques

that are not quite as accurate but better able to treat heavy nuclei.

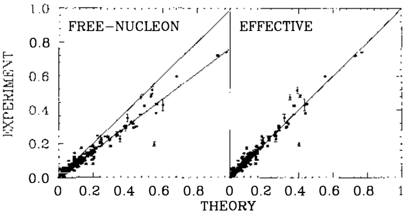
Improving Nuclear Structure: Ab Initio Methods

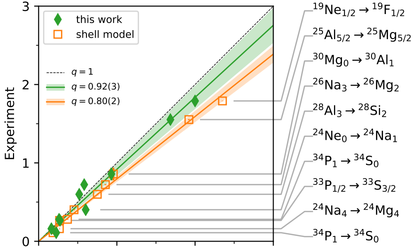
Use most accurate methods:
No-Core Shell Model, Quantum Monte Carlo

in light nuclei to verify other methods:
Coupled Clusters, RG-based techniques

that are not quite as accurate but better able to treat heavy nuclei.

> Practitioners have come together to explain most of the "g_A quenching" in ordinary β decay.





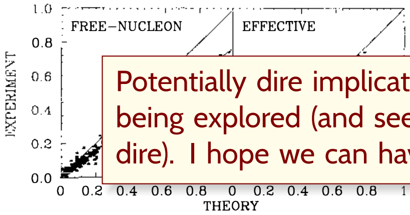
Improving Nuclear Structure: Ab Initio Methods

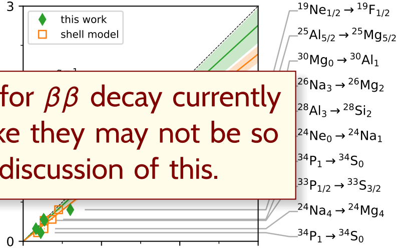
Use most accurate methods:
No-Core Shell Model, Quantum Monte Carlo

in light nuclei to verify other methods:
Coupled Clusters, RG-based techniques

that are not quite as accurate but better able to treat heavy nuclei.

Practitioners have come together to explain most of the "g_A quenching" in ordinary β decay.





Potentially dire implications for $\beta\beta$ decay currently being explored (and seem like they may not be so dire). I hope we can have a discussion of this.

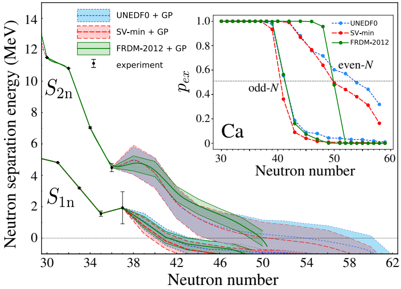
Finally: Error Quantification

PHYSICAL REVIEW LETTERS **122,** 062502 (2019)

Neutron Drip Line in the Ca Region from Bayesian Model Averaging

Léo Neufcourt,[1,2] Yuchen Cao (曹宇晨),[3] Witold Nazarewicz,[4] Erik Olsen,[2] and Frederi Viens[1]
[1]*Department of Statistics and Probability, Michigan State University, East Lansing, Michigan 48824, USA*
[2]*FRIB Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*
[3]*Department of Physics and Astronomy and NSCL Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*
[4]*Department of Physics and Astronomy and FRIB Laboratory, Michigan State University, East Lansing, Michigan 48824, USA*

(Received 12 September 2018; revised manuscript received 15 November 2018; published 14 February 2019)

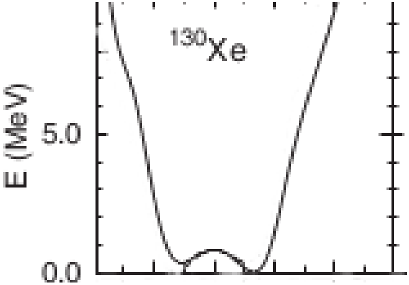


Will apply similar techniques to our ab-initio and DFT-based calculations.

Part II: The MR-IMSRG

Idea from DFT: Generator Coordinate Method

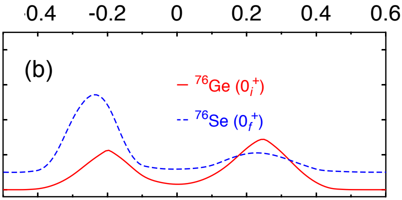
Construct set of mean fields by constraining coordinate(s), e.g. quadrupole moment $\langle Q_0 \rangle$. Then diagonalize H in space of symmetry-restored quasiparticle vacua with different $\langle Q_0 \rangle$.



β_2 = deformation

Robledo et al.: Minima at $\beta_2 \approx \pm.15$

Collective wave functions



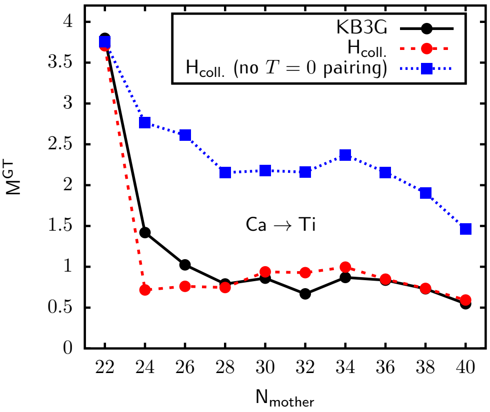
β_2

Rodriguez and Martinez-Pinedo: Wave functions peaked at $\beta_2 \approx \pm.2$

How Important are Collective Degrees of Freedom?

Can extract collective separable interaction –– monopole + pairing + isoscalar pairing + spin-isospin + quadrupole –– from shell model interaction, see how well it mimics full interaction for $\beta\beta$ matrix elements in light *pf*-shell nuclei.

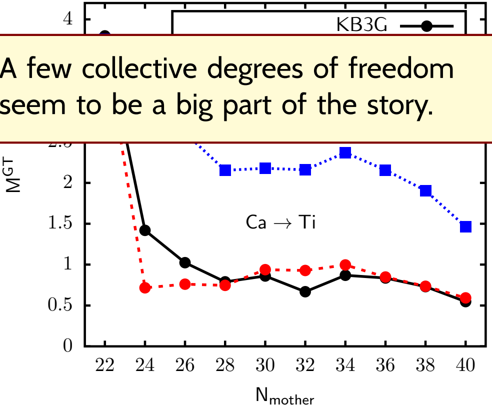
From Javier et al.



How Important are Collective Degrees of Freedom?

Can extract collective separable interaction –– monopole + pairing + isoscalar pairing + spin-isospin + quadrupole –– from shell model interaction, see how well it mimics full interaction for $\beta\beta$ matrix elements in light *pf*-shell nuclei.

From Javier et al.

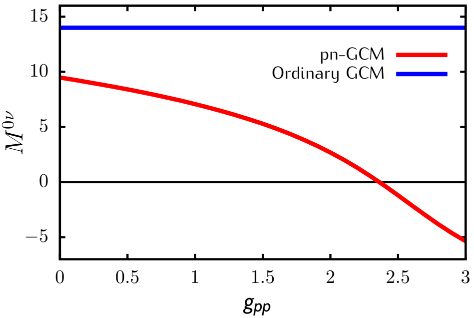


A few collective degrees of freedom seem to be a big part of the story.

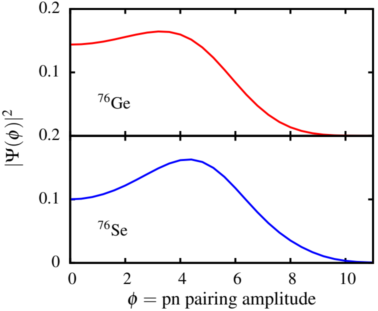
Example: Proton-Neutron Pairing in SO(8)

Can build possibility of pn correlations into mean field. They are frozen out in mean-field minimum, but included in GCM.

$0\nu\beta\beta$ matrix element

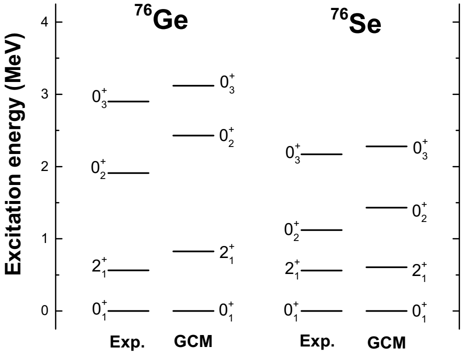


Collective pn-pairing wave functions



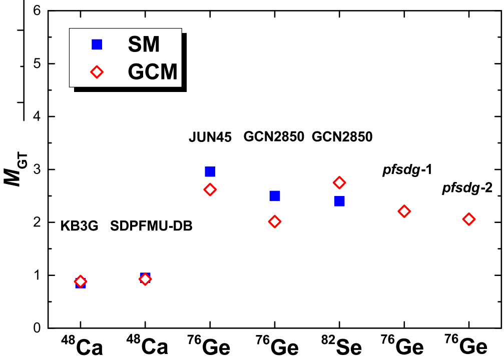
Proton-neutron pairing significantly reduces matrix element.

GCM in Shell-Model Spaces



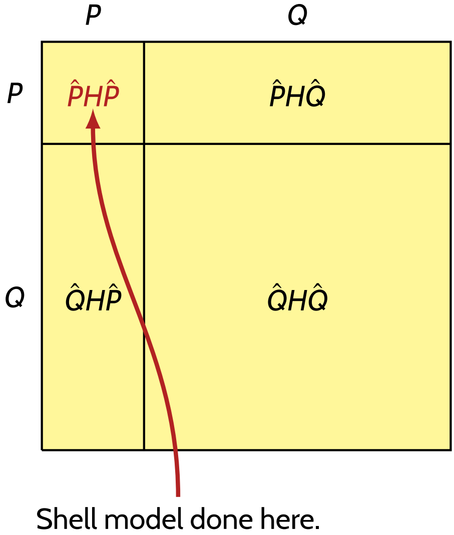
GCM Spectrum in 2 Shells

$\beta\beta$ Matrix Elements in 1 and 2 Shells



Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space

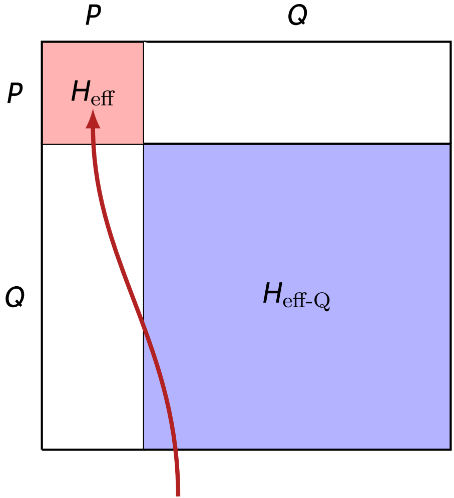


P = subspace you want
Q = the rest

Task: Find unitary transformation to make H block-diagonal in P and Q, with H_{eff} in P reproducing most important eigenvalues.

Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space



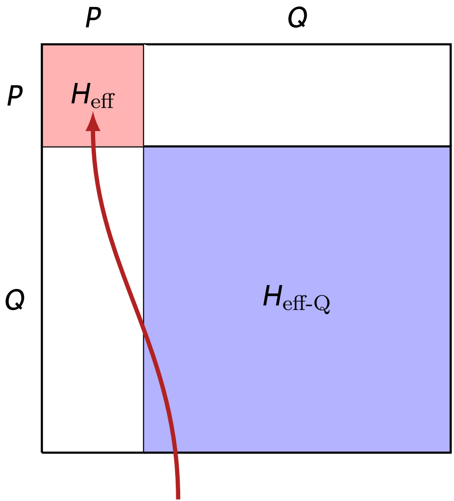
Shell model done here.

P = subspace you want
Q = the rest

Task: Find unitary transformation to make *H* block-diagonal in *P* and *Q*, with $H_{\rm eff}$ in *P* reproducing most important eigenvalues.

Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space



Shell model done here.

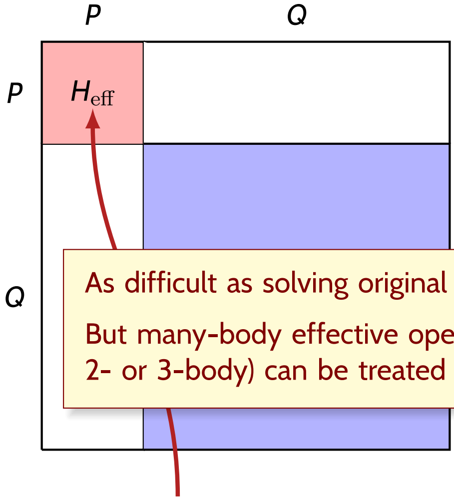
P = subspace you want
Q = the rest

Task: Find unitary transformation to make *H* block-diagonal in *P* and *Q*, with H_{eff} in *P* reproducing most important eigenvalues.

Must must apply same unitary transformation to transition operator.

Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space



Shell model done here.

P = subspace you want
Q = the rest

Task: Find unitary transformation to make H block-diagonal in P and Q, with H_{eff} in P reproducing most ...nvalues.

...ly same unitary ... to transition operator.

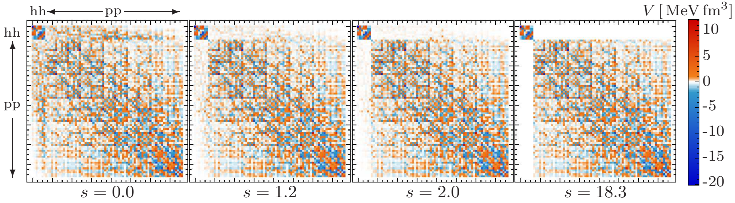
As difficult as solving original problem.

But many-body effective operators (beyond 2- or 3-body) can be treated approximately.

In-Medium Similarity Renormalization Group

One way to determine the transformation

Flow equation for effective Hamiltonian.
Gradually decouples selected set of states.



from H. Hergert

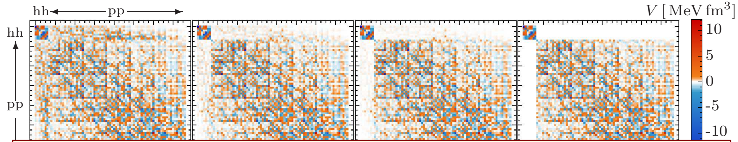
Trick is to keep all 1- and 2-body terms in *H* at each step *after normal ordering* (approximate treatment of 3-, 4-body …terms).

If selected set contains just a single state, approach yields ground-state energy. If it contains a typical valence space, result is effective shell-model interaction and operators.

In-Medium Similarity Renormalization Group

One way to determine the transformation

Flow equation for effective Hamiltonian.
Gradually decouples selected set of states.



We use GCM state – more precisely, and ensemble of initial and final states in $\beta\beta$ decay – as selected set.

Trick is to keep all 1- and 2-body terms in H at each step *after normal ordering* (approximate treatment of 3-, 4-body …terms).

If selected set contains just a single state, approach yields ground-state energy. If it contains a typical valence space, result is effective shell-model interaction and operators.

Generalized Normal Ordering

Begin with an arbitrary ground state $|\Phi\rangle$ (or density operator $\hat{\rho}$). Let

$$\rho^i_j = \langle\Phi|a^\dagger_i a_j|\Phi\rangle \qquad \rho^{ij}_{kl} = \langle\Phi|a^\dagger_i a^\dagger_j a_k a_l|\Phi\rangle \ .$$

Generalized Normal Ordering

Begin with an arbitrary ground state $|\Phi\rangle$ (or density operator $\hat{\rho}$). Let

$$\rho^i_j = \langle\Phi|a^\dagger_i a_j|\Phi\rangle \qquad \rho^{ij}_{kl} = \langle\Phi|a^\dagger_i a^\dagger_j a_k a_l|\Phi\rangle \ .$$

Define

$$\begin{aligned} :a^\dagger_p a_q: &= a^\dagger_p a_q - \rho^p_q \\ :a^\dagger_p a^\dagger_r a_q a_s: &= a^\dagger_p a^\dagger_r a_q a_s - \rho^p_q a^\dagger_r a_s - \text{permutations} - \rho^{pr}_{qs} \\ &\vdots \end{aligned}$$

Generalized Normal Ordering

Begin with an arbitrary ground state $|\Phi\rangle$ (or density operator $\hat{\rho}$). Let

$$\rho^i_j = \langle\Phi|a^\dagger_i a_j|\Phi\rangle \qquad\qquad \rho^{ij}_{kl} = \langle\Phi|a^\dagger_i a^\dagger_j a_k a_l|\Phi\rangle \; .$$

Define

$$\begin{aligned} :a^\dagger_p a_q: &= a^\dagger_p a_q - \rho^p_q \\ :a^\dagger_p a^\dagger_r a_q a_s: &= a^\dagger_p a^\dagger_r a_q a_s - \rho^p_q a^\dagger_r a_s - \text{permutations} - \rho^{pr}_{qs} \\ &\vdots \end{aligned}$$

which implies that

$$\langle\Phi| :a^\dagger_p a^\dagger_r \ldots a_q a_s \cdots: |\Phi\rangle = 0 \; .$$

Generalized Normal Ordering

Begin with an arbitrary ground state $|\Phi\rangle$ (or density operator $\hat{\rho}$). Let

$$\rho^i_j = \langle\Phi|a^\dagger_i a_j|\Phi\rangle \qquad \rho^{ij}_{kl} = \langle\Phi|a^\dagger_i a^\dagger_j a_k a_l|\Phi\rangle \ .$$

Define

$$\begin{aligned} :a^\dagger_p a_q: &= a^\dagger_p a_q - \rho^p_q \\ :a^\dagger_p a^\dagger_r a_q a_s: &= a^\dagger_p a^\dagger_r a_q a_s - \rho^p_q a^\dagger_r a_s - \text{permutations} - \rho^{pr}_{qs} \\ &\vdots \end{aligned}$$

which implies that

$$\langle\Phi| : a^\dagger_p a^\dagger_r \ldots a_q a_s \cdots : |\Phi\rangle = 0 \ .$$

And ∃ a useful Wick's theorem that relates products of (generalized) normal-ordered operators to sums of such operators.

MR-IMSRG

For properties of a single nucleus, we let $|\Phi\rangle$ be a GCM state, obtained from an ab initio calculation in 6 to 12 shells. The reference includes the collective correlations explicitly and the IMSRG builds in the rest.

For $\beta\beta$ decay we choose a reference ensemble,

$$\rho = \alpha \, |\Phi_I\rangle\langle\Phi_I| + (1-\alpha) \, |\Phi_F\rangle\langle\Phi_F| \; ,$$

where we can examine the dependence on α.

MR-IMSRG

For properties of a single nucleus, we let $|\Phi\rangle$ be a GCM state, obtained from an ab initio calculation in 6 to 12 shells. The reference includes the collective correlations explicitly and the IMSRG builds in the rest.

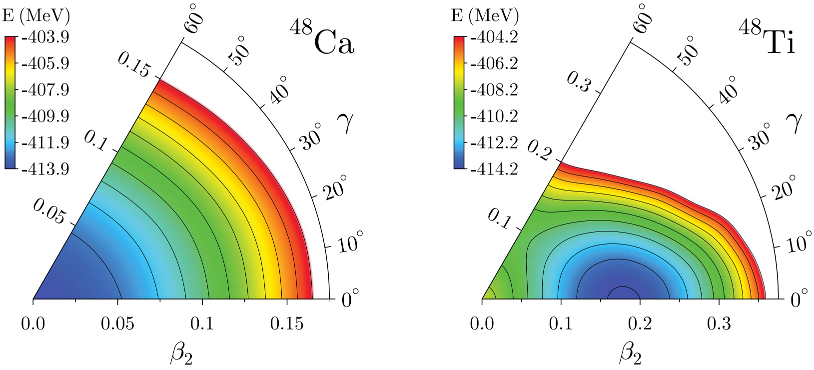
For $\beta\beta$ decay we choose a reference ensemble,

$$\rho = \alpha\,|\Phi_I\rangle\langle\Phi_I| + (1-\alpha)\,|\Phi_F\rangle\langle\Phi_F|\ ,$$

where we can examine the dependence on α.

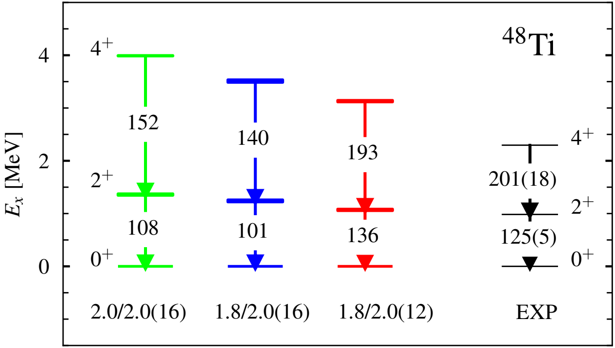
With and ensemble, the IMSRG flow makes neither $|\Phi_I\rangle$ nor $|\Phi_F\rangle$ exact ground states of the transformed H, so we do a second GCM calculation with the evolved Hamiltonian in both nuclei and compute the $\beta\beta$ matrix element with the evolved decay operator.

Deformation Energy



^{48}Ca is spherical and ^{48}Ti can be represented well by an axially-symmetric state.

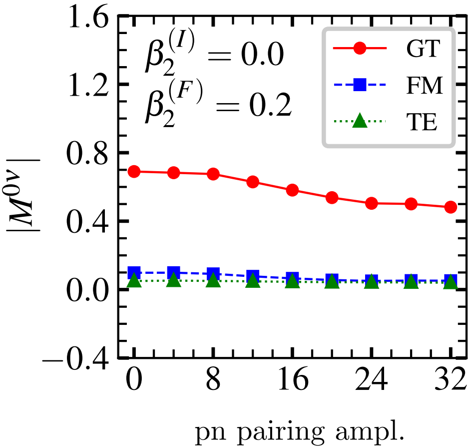
Spectrum in ^{48}Ti



In 9 shells

Smaller $\hbar\omega$ gives a bit more collectivity.

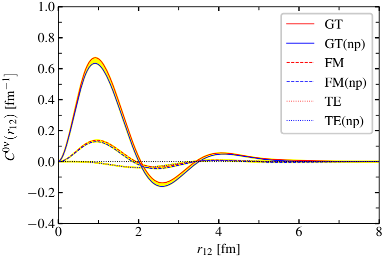
Effects of Isoscalar (pn) Pairing



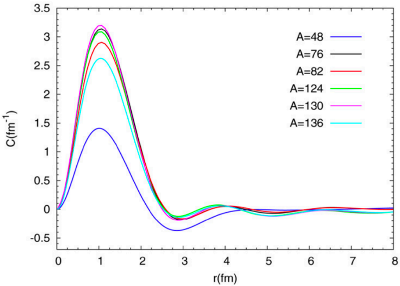
Weaker effect than shell-model and SO(8) results indicate.

Quenches matrix element by only about 17%.

Spatial Dependence



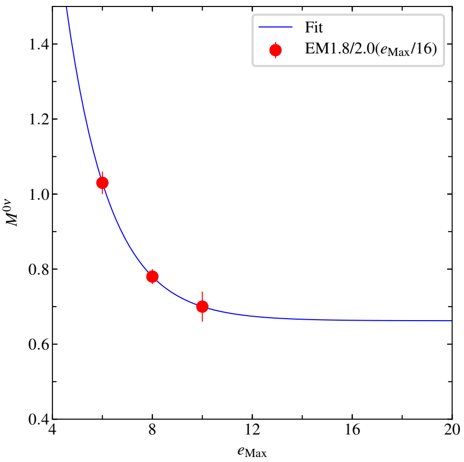
Our calculation



Shell model

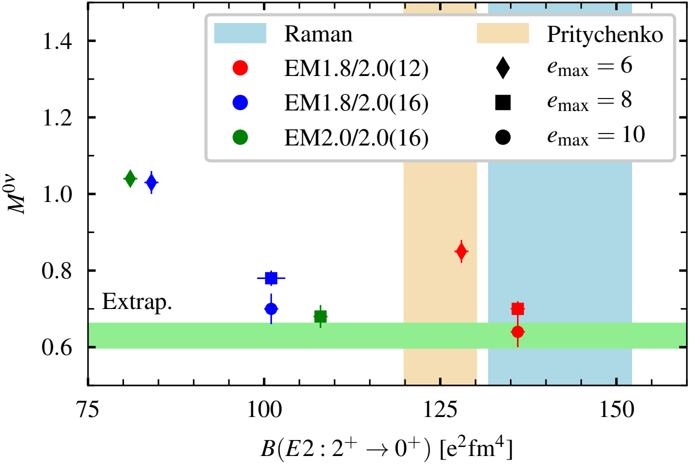
Similar shape, different amplitude

Increasing Size of Single-Particle Space



10 shells seems to be nearly good enough.

Variation with BE2 and Summary of Results



The green band is our best (preliminary) guess for the matrix element.

Uncertainty and Things to Do

Hard to quantify uncertainty right now. On the GCM front, need to test effects of fluctuations in

- like-particle pairing gap
- isovector pn pairing gap
- triaxiality (though its effect is likely small here)

and include a few more shells. This may require a better way to generate and select HFB vacua.

Uncertainty and Things to Do

Hard to quantify uncertainty right now. On the GCM front, need to test effects of fluctuations in

- like-particle pairing gap
- isovector pn pairing gap
- triaxiality (though its effect is likely small here)

and include a few more shells. This may require a better way to generate and select HFB vacua.

On the IMSRG front, need to incorporate three-body operators into flow equations. We're getting there (well . . . , not me, exactly).

In Sum ...

- The DBD collaboration is great!
- Jiangming Yao, Benjamin Bally, Tomás Rodríguez, Roland Wirth, Heiko Hergert, and I have done and an ab initio calculation of the (light) ν-exchange matrix element for the decay of ^{48}Ca. We haven't included absolutely everything but don't expect the number to change too much when we do.
- The method is applicable to other deformed open-shell nuclei, even those with shape coexistence. ^{76}Ge is next!

In Sum ...

- The DBD collaboration is great!
- Jiangming Yao, Benjamin Bally, Tomás Rodríguez, Roland Wirth, Heiko Hergert, and I have done and an ab initio calculation of the (light) ν-exchange matrix element for the decay of ^{48}Ca. We haven't included absolutely everything but don't expect the number to change too much when we do.
- The method is applicable to other deformed open-shell nuclei, even those with shape coexistence. ^{76}Ge is next!

That's all. Thanks very much for your kind attention!