The DBD Collaboration

and the

Multi-Reference In-Medium SRG

J. Engel

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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
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  - **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

- Lattice QCD
- Data
- Effective Field Theory
- Similarity Renormalization Group

Ab-Initio Many-Body Methods

- No-Core Shell Model
- Quantum Monte Carlo
- Harmonic Oscillator Basis Effective Theory

Light Nuclei (benchmarking)

Heavy Nuclei

- Coupled Clusters
- DFT-Inspired Multi-reference In-Medium SRG
- In-Medium SRG for Shell Model

Statistical Model Averaging

- DFT (for EDMs)
- Shell Model
New Physics at Hadronic Level

Light-$\nu$ exchange:

$\nu_M$ + corrections

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 operators

New physics inside blobs
New Physics at Hadronic Level

Light-$\nu$ exchange:

\[ p \rightarrow p + \text{corrections} \]

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 operators

New physics inside blobs

This is the matrix element we need to calculate using LQCD.

Amy, André, et al.
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

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No-Core Shell Model, Quantum Monte Carlo

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Practitioners have come together to explain most of the “$g_A$ quenching” in ordinary $\beta$ 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:
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Practitioners have come together to explain most of the “$g_A$ quenching” in ordinary $\beta$ 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

Neutron Drip Line in the Ca Region from Bayesian Model Averaging

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We apply the Bayesian method to provide a full quantification of the uncertainty surrounding the point estimate. For instance, the posterior mean of the separation energy becomes negative, depending on the choice of credibility level. For instance, the posterior mean of the separation energy becomes negative, depending on the choice of credibility level. For instance, the posterior mean of the separation energy becomes negative, depending on the choice of credibility level. For instance, the posterior mean of the separation energy becomes negative, depending on the choice of credibility level.

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 $\langle Q_0 \rangle$.

Robledo et al.: Minima at $\beta_2 \approx \pm 0.15$

Collective wave functions

Rodriguez and Martinez-Pinedo: Wave functions peaked at $\beta_2 \approx \pm 0.2$
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.

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.

$$M^{0\nu}$$ matrix element

Collective pn-pairing wave functions

Proton-neutron pairing significantly reduces matrix element.
GCM in Shell-Model Spaces

**FIG. 1:** The calculated $M_{0\beta\beta}$ of the $0^{+}\beta\beta$ decay, compared with those by the shell-model (SM) calculation with JUN45 interaction [1], with the GCN2850 interaction [2], with KB3G interaction [3], and with the SDPFMU-DB interaction [4]. "pfsdg-1" denotes the pfsdg-shell interaction in which the 3N forces are normal ordered with respect to $^{40}\text{Ca}$, while "pfsdg-2" denotes the pfsdg-shell interaction with respect to $^{56}\text{Ni}$.

**FIG. 2:** Calculated low-lying excitation spectra of $^{76}\text{Ge}$ and $^{76}\text{Se}$ given by pfsdg-2 interaction, compared with experimental data [5].

**FIG. 3:** The calculated occupancies of valence neutron and proton orbits for $^{76}\text{Ge}$ and $^{76}\text{Se}$, compared with the experimental occupancies of valence orbits [6, 7].

**ββ Matrix Elements in 1 and 2 Shells**

**GCM Spectrum in 2 Shells**
Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space

\[ \hat{P} H \hat{P} \quad \hat{P} H \hat{Q} \]

\[ \hat{Q} H \hat{P} \quad \hat{Q} H \hat{Q} \]

\( P = \) subspace you want
\( Q = \) the rest

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

Shell model done here.
Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space

\[ P \]  \[ \text{H}_{\text{eff}} \]  \[ Q \]

\[ P = \text{subspace you want} \]
\[ Q = \text{the rest} \]

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

Must must apply same unitary transformation to transition operator.

Shell model done here.
Brief Detour: Ab Initio Many-Body Methods

Partition of Full Hilbert Space

\[ P = \text{subspace you want} \]
\[ Q = \text{the rest} \]

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

As difficult as solving original problem.

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

Shell model done here.
In-Medium Similarity Renormalization Group

One way to determine the transformation

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

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.

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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

$$\rho^i_j = \langle \Phi | a_i^\dagger a_j | \Phi \rangle \quad \rho^{ij}_{kl} = \langle \Phi | a_i^\dagger a_j^\dagger a_k a_l | \Phi \rangle .$$
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Define

$$\begin{align*}
: a_p^\dagger a_q : &= a_p^\dagger a_q - \rho_q^p \\
: a_p^\dagger a_r^\dagger a_q a_s : &= a_p^\dagger a_r^\dagger a_q a_s - \rho_q^p a_r^\dagger a_s - \text{permutations} - \rho_{qs}^{pr} \\
&\vdots
\end{align*}$$
Generalized Normal Ordering

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$$\rho^i_j = \langle \Phi | a_i^\dagger a_j | \Phi \rangle \quad \rho^{ij}_{kl} = \langle \Phi | a_i^\dagger a_j^\dagger a_k a_l | \Phi \rangle .$$

Define

$$\alpha^\dagger_p a_q : = a_p^\dagger a_q - \rho^p_q$$

$$\alpha^\dagger_p a_r^\dagger a_q a_s : = a_p^\dagger a_r^\dagger a_q a_s - \rho^p_q a_r^\dagger a_s - \text{permutations} - \rho^{pr}_{qs}$$

which implies that

$$\langle \Phi | : a_p^\dagger a_r^\dagger \ldots a_q a_s \ldots : | \Phi \rangle = 0 .$$
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Define

$$: a^\dagger_p a_q : = a^\dagger_p a_q - \rho^p_q$$

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$$: \cdots :$$

which implies that

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

And $\exists$ a useful Wick’s theorem that relates products of (generalized) normal-ordered operators to sums of such operators.
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,

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

where we can examine the dependence on $a$. 
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With an 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.
\(^{48}\text{Ca}\) is spherical and \(^{48}\text{Ti}\) 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.
The green band is our best (preliminary) guess for the matrix element.
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.
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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).
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) $\nu$-exchange matrix element for the decay of $^{48}\text{Ca}$. 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. $^{76}\text{Ge}$ 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) $\nu$-exchange matrix element for the decay of $^{48}\text{Ca}$. 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. $^{76}\text{Ge}$ is next!

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