# Lecture IX: Ab Initio Nuclear Structure for Double-Beta Decay

J. Engel

November 1, 2017



#### Partition of Full Hilbert Space



*P* = valence space *Q* = the rest

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

Shell model done here.





*P* = valence space *Q* = the rest

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

Shell model done here.





*P* = valence space *Q* = the rest

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

For transition operator  $\hat{M}$ , must apply same transformation to get  $\hat{M}_{eff}$ .

#### Shell model done here.





P = valence space Q =the rest

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

For transition operator  $\hat{M}$ , must apply same transformation to get  $\hat{M}_{\text{eff.}}$ 

As difficult as solving full problem. But idea is that N-body effective operators may not be important for N > 2 or 3.

#### Method 1: Coupled-Cluster Theory

Ground state in closed-shell nucleus:

$$|\Psi_{0}\rangle = e^{T} |\phi_{0}\rangle \qquad T = \sum_{i,m} t_{i}^{m} a_{m}^{\dagger} a_{i} + \sum_{ij,mn} \frac{1}{4} t_{ij}^{mn} a_{m}^{\dagger} a_{n}^{\dagger} a_{i} a_{j} + \dots$$
Slater determinant
$$m,n > F \quad i,j < F$$

States in closed-shell + a few constructed in similar way.

#### Method 1: Coupled-Cluster Theory

Ground state in closed-shell nucleus:

$$|\Psi_{0}\rangle = e^{T} |\varphi_{0}\rangle \qquad T = \sum_{i,m} t_{i}^{m} a_{m}^{\dagger} a_{i} + \sum_{ij,mn} \frac{1}{4} t_{ij}^{mn} a_{m}^{\dagger} a_{i}^{\dagger} a_{j} a_{j} + \dots$$
Slater determinant
$$m,n > F \quad i,j < F$$

States in closed-shell + a few constructed in similar way.

Construction of Unitary Transformation to Shell Model for <sup>76</sup>Ge:

- 1. Calculate low-lying spectra of <sup>56</sup>Ni + 1 and 2 nucleons (and 3 nucleons in some approximation), where full calculation feasible.
- 2. Do Lee-Suzuki mapping of lowest eigenstates onto  $f_{5/2}pg_{9/2}$  shell, determine effective Hamiltonian and decay operator.

Lee-Suzuki maps d lowest eigenvectors to orthogonal vectors in shell model space in way that minimizes difference between mapped and original vectors.

3. Use these operators in shell-model calculation of matrix element for <sup>76</sup>Ge (with analogous plans for other elements).

#### **Option 2: In-Medium Similarity Renormalization Group**

Flow equation for effective Hamiltonian. Asymptotically decouples shell-model space.

 $\frac{d}{ds}H(s) = \left[\eta(s), H(s)\right], \qquad \eta(s) = \left[H_d(s), H_{od}(s)\right], \quad H(\infty) = H_{eff}$ 





Trick is to keep all 1- and 2-body terms in *H* at each step *after normal ordering*. Like truncation of coupled-clusters expansion.

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

#### Ab Initio Calculations of Spectra



# Coupled Cluster Test in Shell-Model Space: ${}^{48}Ca \longrightarrow {}^{48}Ti$

No Shell-Model Mapping



# Coupled Cluster Test in Shell-Model Space: ${}^{48}Ca \longrightarrow {}^{48}Ti$

No Shell-Model Mapping



#### Full Chiral NN + NNN Calculation (Preliminary) From G. Hagen

Method	E3 <sub>max</sub>	M <sup>0</sup> √
CC-EOM (2p2h)	0	1.23
CC-EOM (3p3h)	10	0.33
CC-EOM (3p3h)	12	0.45
CC-EOM (3p3h)	14	0.37
CC-EOM (3p3h)	16	0.36
SDPFMU-DB	-	1.12
SDPFMU	-	1.00

Last two are two-shell shell-model calculations with effective interactions.

#### Complementary Ideas: Density Functionals and GCM

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 $\beta_2\approx\pm.15$



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

We're now including crucial *isoscalar pairing amplitude* as collective coordinate...

#### Capturing Collectivity with Generator Coordinates

#### 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.



#### GCM Example: Proton-Neutron (pn) Pairing

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



Proton-neutron pairing significantly reduces matrix element.

#### GCM in Shell-Model Spaces



#### Combining DFT-like and Ab Initio Methods

GCM incorporates some correlations that are hard to capture automatically (e.g. shape coexistence). So use it to construct initial "reference" state, let IMSRG, do the rest.



Test in single shell for "simple" nucleus.

In progress:

- Improving GCM-based flow.
- Coding IMSRG-evolved  $\beta\beta$  transition operator.
- To do: applying with DFT-based GCM.

## Improving RPA/QRPA

RPA produces states in intermediate nucleus, but form is restricted to 1p-1h excitations of ground state. Second RPA adds 2p-2h states.



#### Issue Facing All Models: "g<sub>A</sub>"

<u>40-Year-Old Problem:</u> Effective  $g_A$  needed for single-beta and two-neutrino double-beta decay in shell model and QRPA.



from F. Iachello

If Ov matrix elements quenched by same amount as 2v matrix elements, experiments will be much less sensitive; rates go like fourth power of  $g_A$ .

#### Arguments Suggesting Strong Quenching of Ov

- Both β and 2νββ rates are strongly quenched, by consistent factors.
- Forbidden (2<sup>-</sup>) decay among low-lying states appears to exhibit similar quenching.
- Quenching due to correlations shows weak momentum dependence in low-order perturbation theory.

#### Arguments Suggesting Weak Quenching of $0\nu$

- Many-body currents seem to suppress  $2\nu$  more than  $0\nu$ .
- Enlarging shell model space to include some effects of high-j spin-orbit partners reduces 2v more than 0v.
- Neutron-proton pairing, related to spin-orbit partners and investigated pretty carefully, suppresses 2v more than Ov.



# Effects of Closure on Quenching



$$M_{\beta\,\beta} = \frac{M_{\beta}^2}{E_0} \qquad \qquad M_{\beta\,\beta}^{cl} = M_{\beta}^2$$

In full calculation, low and high-energy states mix:

$$\begin{split} |\mathsf{O}'\rangle &= \cos\theta \, |\mathsf{O}\rangle + \sin\theta \, |\mathsf{1}\rangle \\ |\mathsf{1}'\rangle &= -\sin\theta \, |\mathsf{O}\rangle + \cos\theta \, |\mathsf{1}\rangle \end{split}$$

in all three nuclei. Then we get

$$\begin{split} \mathbf{M}_{\beta}' &= \mathbf{M}_{\beta} (\cos^2 \theta - \alpha \sin^2 \theta)^2 \\ \mathbf{M}_{2\nu}' &= \mathbf{M}_{\beta}'^2 \left( \frac{1}{E_0} + \frac{(\alpha + 1)^2 \sin^2 \theta \cos^2 \theta}{E_1} \right) \\ \mathbf{M}_{2\nu}'^{\,\text{cl}} &= \mathbf{M}_{\beta}'^2 \left( 1 + (\alpha + 1)^2 \sin^2 \theta \cos^2 \theta \right) \end{split}$$

In full calculation, low and high-energy states mix:

$$\begin{split} |\mathsf{O}'\rangle &= \cos\theta \, |\mathsf{O}\rangle + \sin\theta \, |\mathsf{1}\rangle \\ |\mathsf{1}'\rangle &= -\sin\theta \, |\mathsf{O}\rangle + \cos\theta \, |\mathsf{1}\rangle \end{split}$$

in all three nuclei. Then we get

$$\begin{split} \mathbf{M}_{\beta}' &= \mathbf{M}_{\beta} (\cos^2 \theta - \alpha \sin^2 \theta)^2 \qquad < \mathbf{M}_{\beta} \\ \mathbf{M}_{2\nu}' &= \mathbf{M}_{\beta}'^2 \left( \frac{1}{E_0} + \frac{(\alpha + 1)^2 \sin^2 \theta \cos^2 \theta}{E_1} \right) \\ \mathbf{M}_{2\nu}'^{\text{cl}} &= \mathbf{M}_{\beta}'^2 \left( 1 + (\alpha + 1)^2 \sin^2 \theta \cos^2 \theta \right) \end{split}$$

In full calculation, low and high-energy states mix:

$$\begin{split} |\mathsf{O}'\rangle &= \cos\theta \, |\mathsf{O}\rangle + \sin\theta \, |\mathsf{1}\rangle \\ |\mathsf{1}'\rangle &= -\sin\theta \, |\mathsf{O}\rangle + \cos\theta \, |\mathsf{1}\rangle \end{split}$$

in all three nuclei. Then we get

$$\begin{split} M'_{\beta} &= M_{\beta} (\cos^2 \theta - \alpha \sin^2 \theta)^2 &< M_{\beta} \\ M'_{2\nu} &= M'_{\beta}^2 \left( \frac{1}{E_0} + \frac{(\alpha + 1)^2 \sin^2 \theta \cos^2 \theta}{E_1} \right)^{E_0 \ll E_1} &\approx \frac{M'_{\beta}^2}{E_0} \\ M'_{2\nu}^{cl} &= M'_{\beta}^2 \left( 1 + (\alpha + 1)^2 \sin^2 \theta \cos^2 \theta \right) \end{split}$$

In full calculation, low and high-energy states mix:

$$\begin{split} |\mathsf{O}'\rangle &= \cos\theta \, |\mathsf{O}\rangle + \sin\theta \, |\mathsf{1}\rangle \\ |\mathsf{1}'\rangle &= -\sin\theta \, |\mathsf{O}\rangle + \cos\theta \, |\mathsf{1}\rangle \end{split}$$

in all three nuclei. Then we get

$$\begin{split} M'_{\beta} &= M_{\beta} (\cos^2 \theta - \alpha \sin^2 \theta)^2 &< M_{\beta} \\ M'_{2\nu} &= M'_{\beta}^2 \left( \frac{1}{E_0} + \frac{(\alpha + 1)^2 \sin^2 \theta \cos^2 \theta}{E_1} \right)^{E_0 \ll E_1} &\approx \frac{M'_{\beta}^2}{E_0} \\ M'_{2\nu}^{cl} &= M'_{\beta}^2 \left( 1 + (\alpha + 1)^2 \sin^2 \theta \cos^2 \theta \right) &> M'_{\beta}^2 \\ &= M_{2\nu}^{cl}, \quad \alpha = 1 \end{split}$$

So if  $\alpha = 1$ , the closure matrix element is not suppressed at all. If  $\alpha = 0$ , it's suppressed as much as the single- $\beta$  matrix element, but still less than the non-closure  $\beta\beta$  matrix element.

#### We Hope to Resolve the Issue Soon

Problem must be due to some combination of:

1. Truncation of model space.

Should be fixable in ab-initio shell model, which compensates effects of truncation via effective operators.

2. Many-body weak currents.

Size still not clear, particularly for  $0\nu\beta\beta$  decay, where current is needed at finite momentum transfer *q*.

Leading terms in chiral EFT for finite *q* only recently worked out. Careful fits and use in decay computations will happen in next year or two.

## **Benchmarking and Error Estimation**

#### Systematic Error:

- 1. Calculate and benchmark spectra and transition rates (including  $\beta$  decay) with all good methods.
- Calculate β, 2νββ and Ονββ matrix elements in light nuclei <sup>6</sup>He, <sup>8</sup>He, <sup>22</sup>O, <sup>24</sup>O – with methods discussed here plus no-core shell model and quantum Monte Carlo.
- 3. Do the same in <sup>48</sup>Ca.
- 4. Test effects of "next order" in EFT Hamilton, coupled-cluster truncation, restrictions to *N*-body operators, etc.
- 5. Benchmark methods against spectra and electromagnetic transitions in A = 76, 82, 100, 130, 136, 150.

#### Statistical Error:

Chiral-EFT Hamiltonians contain many parameters, fit to data. Posterior distributions (for Bayesian analysis) or covariance matrices (for linear regression) developed to quantify statistical errors for  $\beta\beta$  matrix elements.

#### Finally...

Existence of topical collaboration will speed progress in next few years.

Goal is accurate matrix elements with quantified uncertainty by end of collaboration (5 years from now).

# That's all; thanks for listening.

#### Finally...

Existence of topical collaboration will speed progress in next few years.

Goal is accurate matrix elements with quantified uncertainty by end of collaboration (5 years from now).

# That's all; thanks for listening.