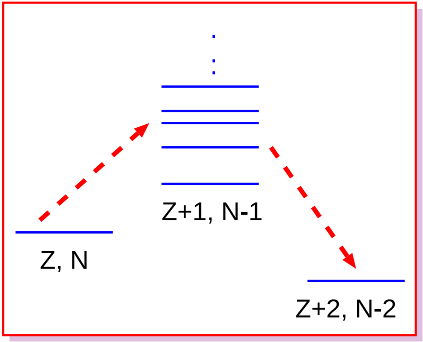
Computing Nuclear Matrix Elements for $\beta\beta$ Decay

J. Engel

University of North Carolina

October 7, 2014

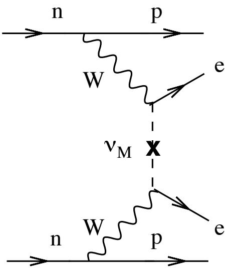
Neutrinolesss Double-Beta Decay



If energetics are right (ordinary beta decay forbidden)...

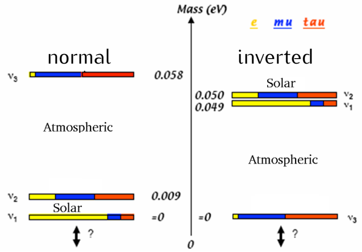
and neutrinos are their own antiparticles...

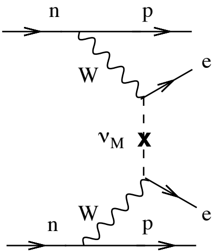
can observe two neutrons turning into protons, emitting two electrons and nothing else.



Why Double-Beta Decay Is Important

besides the ability to determine whether $\nu = \bar{\nu}$





In usual scenario, rate depends on square of "effective neutrino mass"

$$m_{\text{eff}} \equiv \sum_i m_i U_{ei}^2$$

If lightest neutrino is light:

- $m_{\text{eff}} \propto \sqrt{\Delta m^2_{\text{sol}}}$ normal
- $m_{\text{eff}} \propto \sqrt{\Delta m^2_{\text{atm}}}$ inverted

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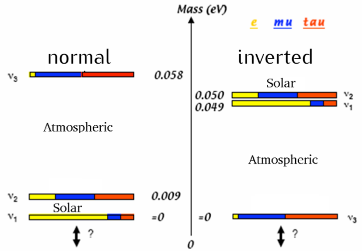

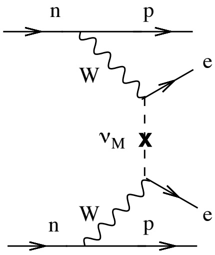

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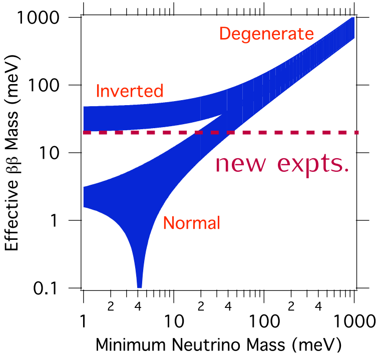

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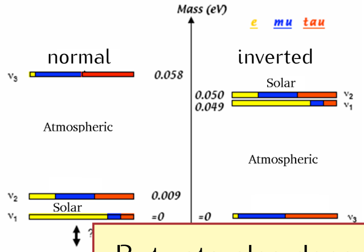

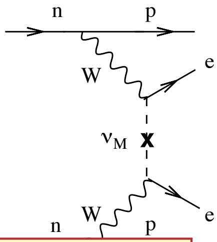

But rate also depends on a nuclear matrix element.

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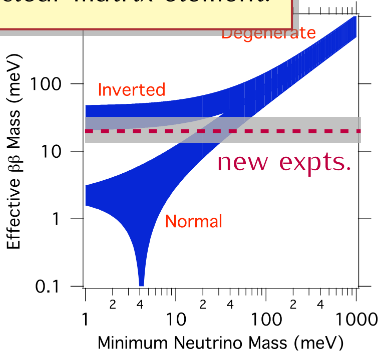


Light-ν-Exchange Matrix Element

Lowest-order expressions

$$M_{0\nu} = M_{0\nu}^{GT} - \frac{g_V^2}{g_A^2} M_{0\nu}^{F} + \ldots$$

with

$$\begin{aligned} M_{0\nu}^{GT} &= \langle F \,|\sum_{i,j} H(r_{ij},\overline{E})\vec{\sigma}_i \cdot \vec{\sigma}_j \tau_i^+ \tau_j^+ \,|I\rangle + \ldots \\ M_{0\nu}^{F} &= \langle F \,|\sum_{i,j} H(r_{ij},\overline{E})\tau_i^+ \tau_j^+ \,|I\rangle + \ldots \end{aligned}$$

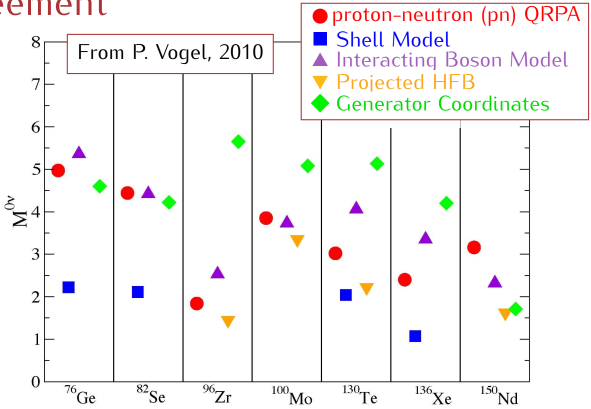
$$H(r,\overline{E}) \approx \frac{R}{r}$$

Corrections are from “forbidden” terms, weak nucleon form factors, 2-body currents (which give 3- and 4-body $\beta\beta$ operators) …

Recent Level of Agreement

Same level of agreement in 2014.

Not so great.



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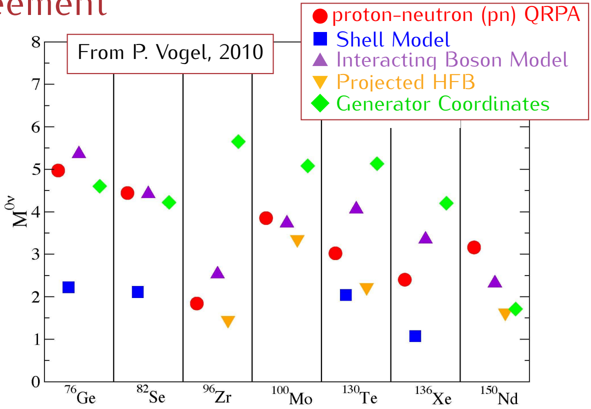

Major recent progress in nuclear-structure theory from increased computing power and new many-body methods.

We are in the process of improving all the models above, connecting them to *ab initio* work or including more correlations.

Focus here on shell model, QRPA, and GCM.

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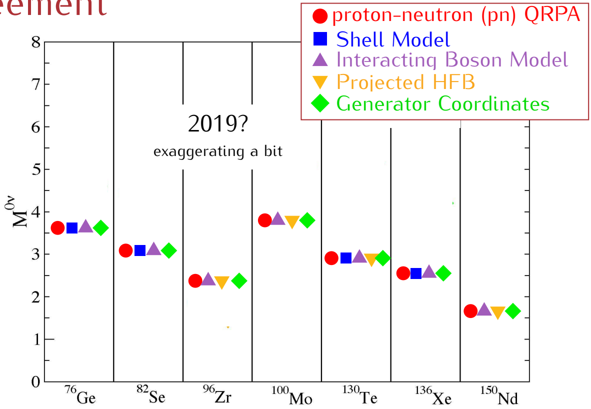

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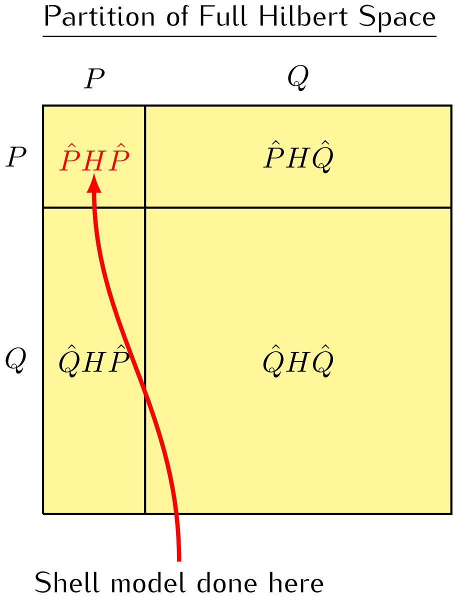

P = valence space
Q = the rest

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

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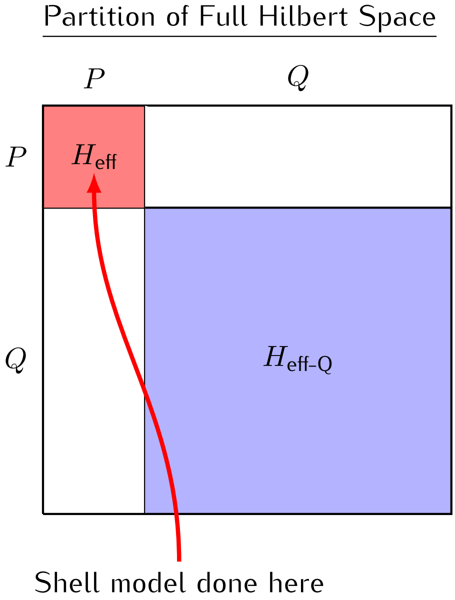

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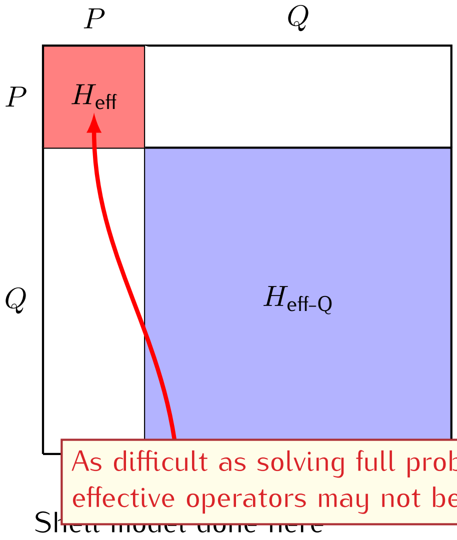
"Ab Initio" Shell Model

Partition of Full Hilbert Space



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Q = the rest

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

Some Options for Ab Initio Part

- **Coupled Clusters:**
  In closed shells

$$|GS\rangle = \exp\left(t_i^a a_a^\dagger a_i + t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j + \dots\right)|HF\rangle$$

$$a, b > F\,, \quad i, j < F$$

Excited states or states in nearby nuclei are excitations of $|GS\rangle$.

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- **In-Medium Similarity Renormalization Group:** Differential flow equation

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]\;, \tag{1}$$

  with η chosen to asymptotically decouple shell-model space from other states. Normal-ordered 1- and 2-body operators kept at each step. Can also obtain decay operator.

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- **No-Core Shell Model:** See Pieter Maris talk.

- **Auxiliary Diffusion Monte Carlo:** See Stefano Gandolfi talk.

Coupled-Clusers (CC) Procedure

1. Find good NN and NNN interactions, 1- and 2-body currents by matching EFT to data in NN scattering, He, triton decay,... ✓
2. Obtain ground state for closed-shell nucleus ^{56}Ni (28 protons, 28 neutrons). ✓
3. Use Equation-of-Motion (EOM) CC to obtain low-lying states in nuclei with $A = 57$ and 58, eventually 59. ✓
4. Do Lee-Suzuki mapping of low-lying eigenstates with $A = 57, 58$ onto $f_{5/2}p_{3/2}p_{1/3}g_{9/2}$ shell, determine shell-model Hamiltonian that reproduces energies. ✓
5. Do the same thing for the double-beta-decay operator, with 2-body current treated in normal-ordered 1-body approximation, at least initially.
6. Put more nucleons in the valence shell (20 for ^{76}Ge), shut up, and calculate (in the words, allegedly, of Feynman). ✓

✓ = done ✓ = done in lighter nuclei

Coupled Cluster Computing

About 50K core hours in 15 shells for ^{18}O.

Scaling: EOM 2-particle attached: $N_p^5 N_h$

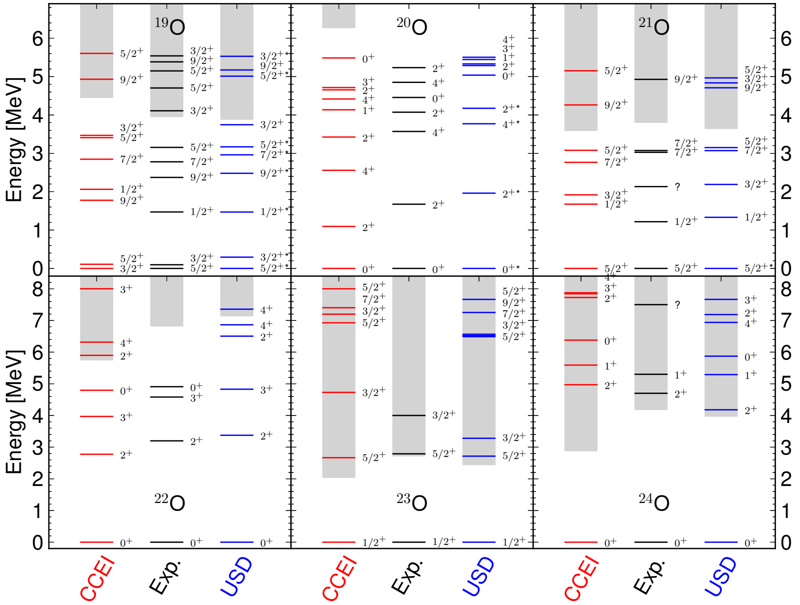
EOM 3-particle attached: $N_p^6 N_h$

TABLE III. Size of the many-body space in the diagonalization procedure in the Arnoldi algorithm for all states calculated in this work. All numbers are based on the angular-momentum-coupled representation (jj scheme).

State	$N_{\max}=10$	$N_{\max}=12$	$N_{\max}=14$	$N_{\max}=16$	$N_{\max}=18$	$N_{\max}=20$
^{6}He(0^+)	516 048	1 323 972	2 981 930	6 088 376	11 513 088	20 176 104
^{6}He(1^-)	1 507 930	3 894 028	8 808 688	18 040 354	34 190 482	60 011 982
^{6}He(2^+)	2 391 692	6 251 128	14 255 896	29 364 090	55 885 624	98 356 664
^{6}Li(0^+)	775 992	1 989 508	4 478 936	9 142 216	17 284 308	30 285 212
^{6}Li(1^+)	2 268 746	5 853 534	13 234 004	27 093 632	51 335 514	90 080 136
^{6}Li(2^+)	3 595 384	9 391 650	21 409 878	44 088 456	83 893 672	147 629 532
^{6}Li(3^+)	4 676 372	12 438 258	28 699 916	59 604 726	114 125 048	201 657 602
^{18}O(0^+)	1 908 474	5 022 710	11 485 808	23 680 034	45 071 990	79 331 610
^{18}O(1^-)	5 594 899	14 802 528	33 974 801	70 231 288	133 940 727	236 049 974
^{18}O(2^+)	8 891 923	23 794 936	55 036 119	114 391 274	219 038 683	387 077 788
^{18}O(2^-)	8 897 760	23 803 219	55 047 530	114 406 595	219 058 796	387 083 193
^{18}O(3^+)	11 613 562	31 596 862	73 906 056	154 840 950	298 237 942	529 098 382
^{18}O(3^-)	11 621 868	31 608 838	73 922 708	154 863 424	298 267 524	529 107 862
^{18}O(4^+)	13 629 562	37 905 214	89 982 332	190 504 054	369 757 342	659 327 780
^{18}F(0^+)	2 868 568	7 545 420	17 248 686	35 552 756	67 658 660	119 071 548
^{18}F(1^+)	8 403 602	22 228 738	51 009 366	105 427 688	201 040 066	354 285 892
^{18}F(2^+)	13 362 878	35 742 012	82 642 970	171 734 254	328 788 766	580 957 010
^{18}F(3^+)	17 451 568	47 458 334	110 973 350	232 452 890	447 659 068	794 095 862
^{18}F(4^+)	20 479 376	56 930 198	135 106 850	285 982 274	554 996 372	989 530 134
^{18}F(5^+)	22 363 324	63 896 228	154 444 460	331 158 558	648 765 300	1163 943 530

Coupled Clusters in sd Shell: Oxygen

G. Jansen, G. Hagen, A. Signoracci, JE



IMSRG

from Heiko Hergert

- Published results, which are similar to those from coupled clusters in oxygen, took only 200-500 hours per isotope.

  50K total hours needed to produce oxygen isotopes, vs 500K coupled-cluster hours.

- ^{76}Ge in the $f_{5/2}p_{1/2}p_{3/2}g_{9/2}$ space would increase time by a factor of 5 to 10[1].

  Overall cost would be be less than that of the subsequent shell-model calculations for ^{76}Ge.

- 3-body induced operators not possible in the near future. Need for data sharing makes parallelization with MPI difficult.

- New methods (the "Magnus expansion") may enable perturbative evolution of 3-body operators, however. The group is hopeful.

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[1]A caveat: there are issues with extended valence spaces that could increase the time to convergence or stall the calculation entirely.

Shell Model Diagonalization (Lanczos)

from Mihai Horoi

Model Space	Dimension	Comments
No Core in 6 major shells, $N_{\text{max}} = 2$		
^{48}Ca	3.0×10^9	doable with 3-body
$f_{7/2}, f_{5/2}, p_{3/2}$ $p_{1/2}, g_{9/2}, g_{7/2}$		
^{76}Ge n=1[2]	2.5×10^{10}	may be doable with 3-body
^{76}Ge n=2	4.3×10^{11}	next gen., 2-body and 3-body
^{82}Se n=1	3.0×10^9	doable with 3-body
^{82}Se n=2	6.4×10^{10}	next gen., 2-body and 3-body
$g_{9/2}, g_{7/2}, d_{3/2}$ $d_{1/2}, s_{1/2}, h_{11/2}, h_{9/2}$		
^{136}Xe n=1[3]	1.6×10^9	done with 2-body, 3-body doable
^{136}Xe n=2	8.6×10^{10}	next gen., 2-body and 3-body
^{130}Te n=1	7.6×10^{10}	next gen., 2-body and 3-body

[2] n is the number of particles excited from $f_{7/2}$ and to $g_{7/2}$

[3] n is the number of particles excited from $g_{9/2}$ and to $h_{9/2}$

AFDMC (Not Via Shell Model)

Aiming initially at calculation of decay of ^{48}Ca

Now can include 3-body (Urbana UIX and similar) forces almost exactly, implementing chiral Hamiltonians up to N2LO. Any other operator, including 2-body currents, should incur just a small extra cost.

Very conservative estimate for the ground state calculation of ^{48}Ca: 100,000-150,000 core hours. Includes optimization of initial variational wave-function and then projection in imaginary time.

Larger nuclei and mid-shell nuclei still a complete unknown.

Heavy Deformed Nuclei: Large-Scale QRPA

pn-QRPA inserts complete set of states in intermediate nucleus, provides single-beta matrix elements from ground states of initial and final nuclei to this complete set.

Used modern Skyrme functional with tranditional matrix methods, consumed $\approx$ 7M CPU hours.

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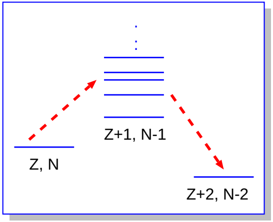
Worth noting:

QRPA gives two sets of intermediate-nucleus energies and strengths (for transitions involving initial/final nuclei) but not corresponding wave functions. Doesn't tell you how the two sets of states are related.

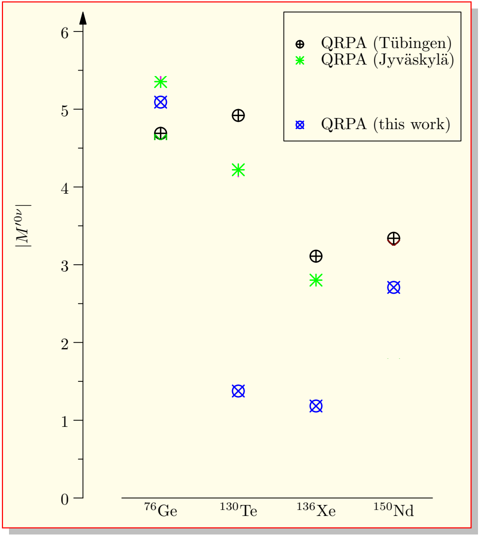


J. Terasaki tryng to avoid probelm by replacing boson vaccuum with quasiparticle coupled-cluster state

$$|\text{“}QRPA\text{”}\rangle \propto \exp([YX^{-1}]^*_{abcd} b^\dagger_{ab} b^\dagger_{cd}) \, |0\rangle$$

$$\Longrightarrow \mathcal{N} \exp\left([YX^{-1}]^*_{abcd} \alpha^\dagger_a \alpha^\dagger_b \alpha^\dagger_c \alpha^\dagger_d\right) |HFB\rangle$$

Results



QRPA (Tübingen)
QRPA (Jyväskylä)
QRPA (this work)
$|M'^{0\nu}|$
0
1
2
3
4
5
6
^{76}Ge
^{130}Te
^{136}Xe
^{150}Nd

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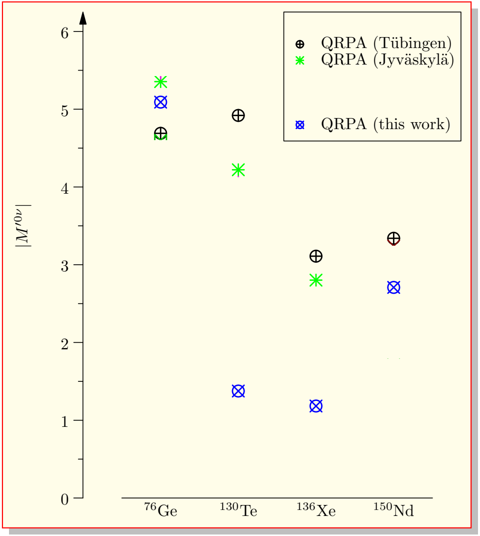
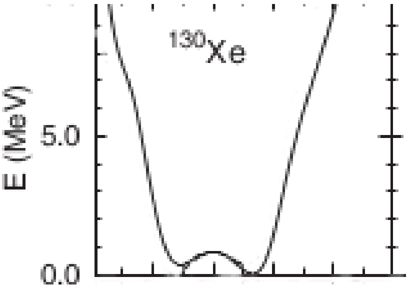


Robledo et al.:

Energy minima at $\beta_2 \approx \pm .15$



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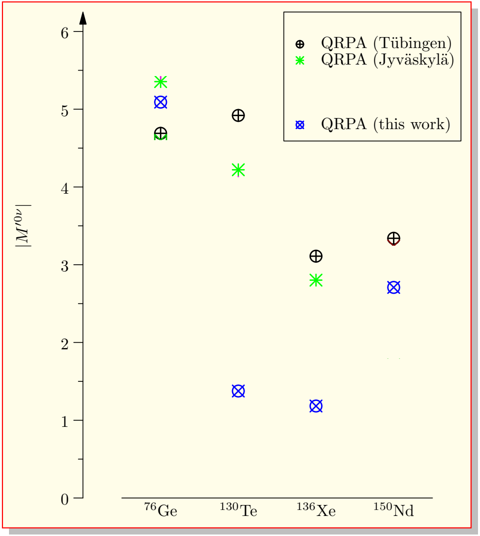

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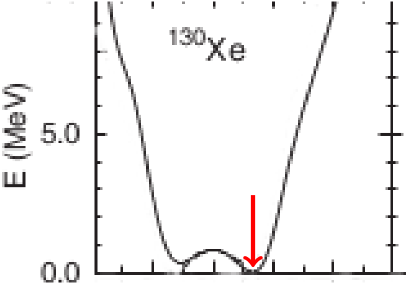

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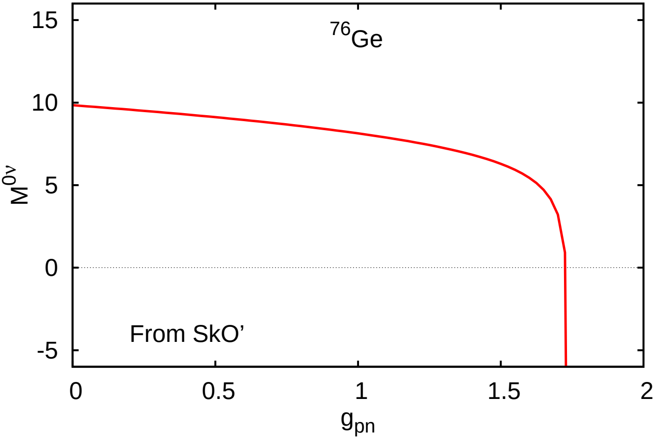
QRPA Also Challenged by Proton-Neutron Pairing



Simplified interaction in two major shells

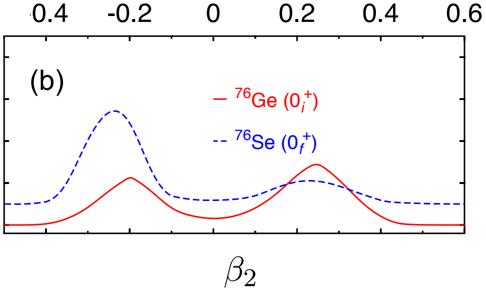
Amplitude blows up when mean field state on which it's based changes from normal like-particle pair condensate to proton-neutron pair condensate.

A Better Approach: Generator Coordinates?

Generator Coordinate Method is perhaps best approach if nuclei don't have definite shape, can't be approximated by single mean field.

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 $\langle Q_0 \rangle$.

Collective wave functions



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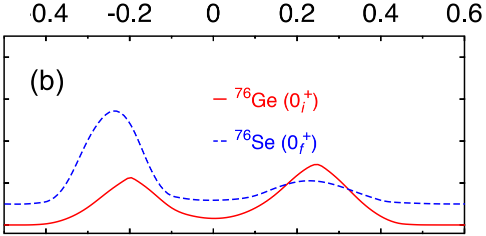

β_2

But other important non-shape degrees of freedom still missing.

Adding Proton-Neutron Correlations to GCM

GCM missing physics that affects pn-QRPA calculations.

So we generalize GCM in a way that avoids wild QRPA behavior:

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So we generalize GCM in a way that avoids wild QRPA behavior:

1. pp and nn pairing currently treated in mean-field theory, but not pn pairing. So use quasiparticles that mix not only particles and holes, but also protons and neutrons.
2. Constrain pn pairing as well as deformation, i.e. minimize

$$H' = H - \lambda_Q \langle Q_0 \rangle - \lambda_P \langle P_0^\dagger \rangle$$

with

$$P_0^\dagger = \sum_l \left[a_l^\dagger a_l^\dagger \right]^{L=0, S=1, T=0}_{M_S=0}$$

The pn operators have zero expectation value at HFB minimum, but we add HFB states constrained to have non-zero values.

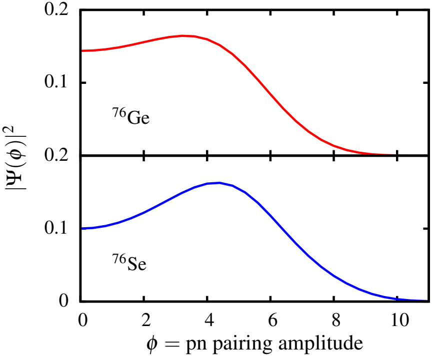
Results for ^{76}Ge

N. Hinohara and JE

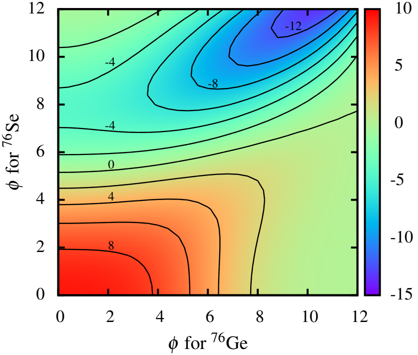
Can build pn correlations into mean field. Frozen out in mean field minimum, but included dynamically in GCM.

Work with several-term separable interaction in two shells.

Collective pn-pairing wave functions



$0\nu\beta\beta$ matrix element

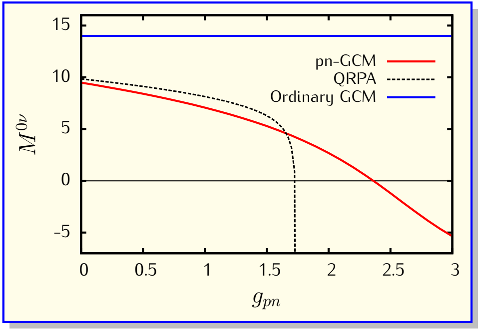


Simplified calculation, no quadrupole coordinate

Proton-neutron pairing significantly reduces matrix element.

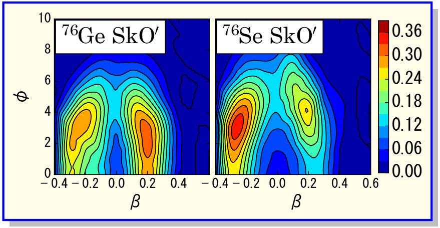
More Results in ^{76}Ge

No deformation coordinate



(Realistic value of g_{pn} about 1.5 — 1.6.)

Two-dimensional calculation with both pn pairing amplitude and deformation as coordinates



2-d collective wave funcions

Matrx element about the same with and without deformation coordinate.

Next steps: combine with DFT or *ab initio* interaction, include other collective and non-collective degrees of freedom (jacking up computing needs).

GCM Computing

Most time in calculation of matrix elements of H and $\beta\beta$ operator between symmetry-projected states. Our calculation used about 40K hours for each set of Hamiltonian parameters.

From Tomas Rodriguez, re his Gogny-based GCM calculations:

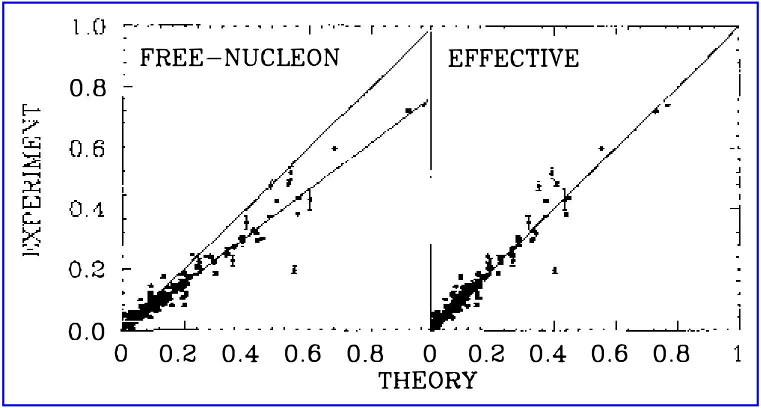
triaxial	pp/nn pairing	pn pairing	# GCM points	Core hours
✓	—	—	60	7.2×10^4
✓	✓	—	300	1.8×10^6
✓	✓	✓	1500	4.4×10^7

Will add more coordinates as well as additional states, including noncollective excitations, to this variational bais. Problem size grows rapidly but scales well; ship matrix elements of H and $\beta\beta$ operator to independent processors.

Finally: "Renormalization of g_A"

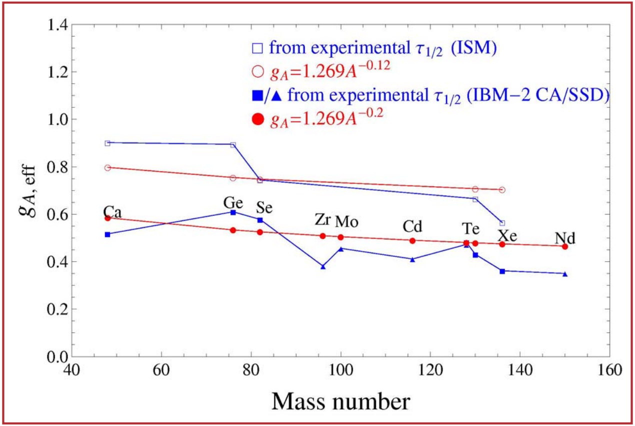
Forty(?)-year old problem: Single-beta rates, 2ν double-beta rates, related observables over-predicted.

Brown & Wildenthall: Beta-decay strengths in *sd* shell



Problem Particularly Important for $\beta\beta$ Decay

Effective g_A needed for two-neutrino decay in shell model and IBM-2



F. Iachello, MEDEX'13 meeting

If neutrinoless matrix elements quenched by same amount, experiments are in trouble; rates go like $(g_A)^4$.

Resolving the Issue

Typical practice: "Renormalize" g_A only for 2ν decay. Assume 0ν decay unaffected.

Better practice: Understand reasons for over-prediction of β and 2ν $\beta\beta$ rates. Must be due to

1. Many-body weak currents, either modeled explicitly as π, ρ exchange, etc., or from effective-field-theory fits. Conventional wisdom says meson-exchange effects in β decay are small; chiral-EFT folk suggest they may not be.

   More careful EFT work, in progress, should settle question.

2. Truncation of model space.

   Will be fixed, e.g., in ab-initio shell model.

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That's all; thanks.