# Calculating β Decay for the r Process

J. Engel

with

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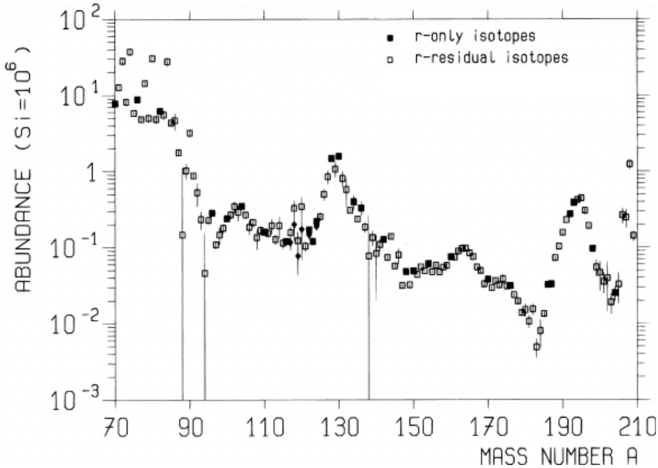
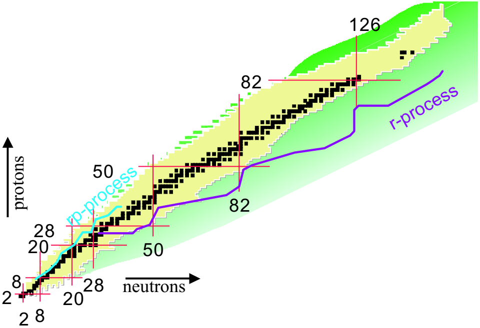
# R-Process Abundances



# Nuclear Landscape

To convincingly locate the site(s) of the *r* process, we need to know reaction rates and properties in very neutron-rich nuclei.



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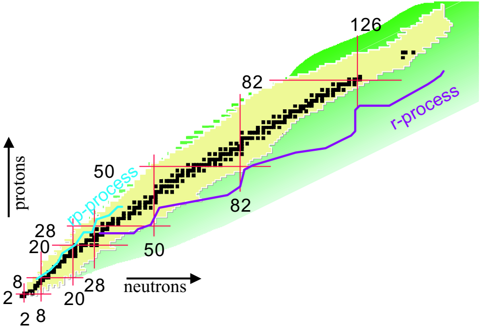


β decay is particularly important. Responsible for increasing *Z* throughout *r* process, and its competition with neutron capture during freeze-out can have large effect on abundances.

# Calculating β Decay is Hard

## Though, As We'll See, It Gets a Bit Easier in Neutron-Rich Nuclei

To calculate $\beta$ decay between two states, you need:

- an accurate value for the decay energy $\Delta E$ (since contribution to rate $\propto \Delta E^5$ for "allowed" decay).
- matrix elements of the decay operator $\boldsymbol{\sigma}\tau_-$ and "forbidden" operators $\mathbf{r}\tau_-$, $\mathbf{r}\boldsymbol{\sigma}\tau_-$ between the two states.

The operator $\tau_-$ turns a neutron into a proton; the allowed decay operator does that while flipping spin.

Most of the time the decay operator leaves you above threshold, by the way.

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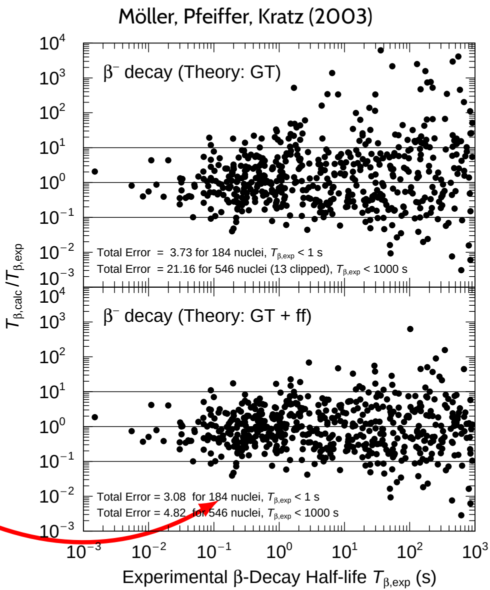
So nuclear structure model must do good job with masses, spectra, and wave functions, in many isotopes.

# What's Usually Been Used for β-Decay in Simulations

**Ancient but Still in Some Ways Unsurpassed Technology**

- Masses through "finite-range droplet model with shell corrections."
- "QRPA" with simple space-independent interaction.
- First forbidden decay (correction due to finite nuclear size) added very crude way in 2003. Shortens half lives.



# Modern Alternative: Skyrme Dens.-Func. Theory

Started as zero-range effective potential, treated in mean-field theory:

$$\begin{aligned}
V_{\text{Skyrme}} &= t_0\left(1 + x_0 P_\sigma\right)\delta(\mathbf{r}_1 - \mathbf{r}_2) \\
&+ \frac{1}{2}t_1\left(1 + x_1 P_\sigma\right)\left[(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)^2\delta(\mathbf{r}_1 - \mathbf{r}_2) + h.c.\right] \\
&+ t_2\left(1 + x_2 P_\sigma\right)\left(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2\right)\cdot\delta(\mathbf{r}_1 - \mathbf{r}_2)(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2) \\
&+ \frac{1}{6}t_3\left(1 + x_3 P_\sigma\right)\delta(\mathbf{r}_1 - \mathbf{r}_2)\rho^\alpha([\mathbf{r}_1 + \mathbf{r}_2]/2) \\
&+ iW_0\left(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2\right)\cdot\left(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2\right)\times\delta(\mathbf{r}_1 - \mathbf{r}_2)(\boldsymbol{\nabla}_1 - \boldsymbol{\nabla}_2)
\end{aligned}$$

where $P_\sigma \equiv \frac{1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2}{2}$.

Re-framed as density functional, which can then be extended:

$$\mathcal{E} = \int d^3r \left(\underbrace{\mathcal{H}_{\text{even}} + \mathcal{H}_{\text{odd}}}_{\mathcal{H}_{\text{Skyrme}}} + \mathcal{H}_{\text{kin.}} + \mathcal{H}_{\text{em}}\right)$$

$\mathcal{H}_{\text{odd}}$ has no effect in mean-field description of time-reversal even states (e.g. ground states), but large effect in $\beta$ decay.

# Time-Even and Time-Odd Parts of Functional

Not including pairing:

$$\mathcal{H}_{\text{even}} = \sum_{t=0}^{1} \sum_{t_3=-t}^{t} \Big\{ C_t^{\rho} \rho_{tt_3}^2 + C_t^{\Delta\rho} \rho_{tt_3} \nabla^2 \rho_{tt_3} + C_t^{\tau} \rho_{tt_3} \tau_{tt_3} + C_t^{\nabla J} \rho_{tt_3} \boldsymbol{\nabla} \cdot \mathbf{J}_{tt_3} + C_t^{J} \mathbf{J}_{tt_3}^2 \Big\}$$

$$\mathcal{H}_{\text{odd}} = \sum_{t=0}^{1} \sum_{t_3=-t}^{t} \Big\{ C_t^{s} \mathbf{s}_{tt_3}^2 + C_t^{\Delta s} \mathbf{s}_{tt_3} \cdot \nabla^2 \mathbf{s}_{tt_3} + C_t^{T} \mathbf{s}_{tt_3} \cdot \mathbf{T}_{tt_3} + C_t^{j} \mathbf{j}_{tt_3}^2 + C_t^{\nabla j} \mathbf{s}_{tt_3} \cdot \boldsymbol{\nabla} \times \mathbf{j}_{tt_3} + C_t^{F} \mathbf{s}_{tt_3} \cdot \mathbf{F}_{tt_3} + C_t^{\nabla s} \left( \boldsymbol{\nabla} \cdot \mathbf{s}_{tt_3} \right)^2 \Big\}$$

Time-even densities:

$\rho$ = usual density  $\tau$ = kinetic density  $\mathbf{J}$ = spin-orbit current

Time-odd densities:

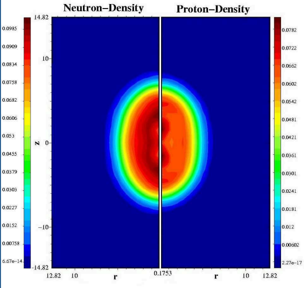
$\mathbf{s}$ = spin current  $\mathbf{T}$ = kinetic spin current  $\mathbf{j}$ = usual current

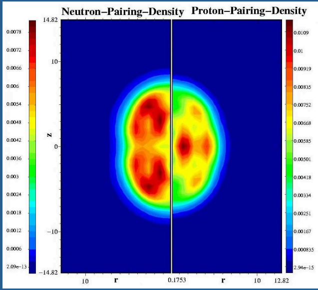
Couplings are connected by "Skyrme interaction," but can be set independently if working directly with density-functional.

# Starting Point: Mean-Field-Like Calculation (HFB)

Gives you ground state density, etc. This is where Skyrme functionals have made their living.

Zr-102: normal density and pairing density
HFB, 2-D lattice, SLy4 + volume pairing
Ref: Artur Blazkiewicz, Vanderbilt, Ph.D. thesis (2005)



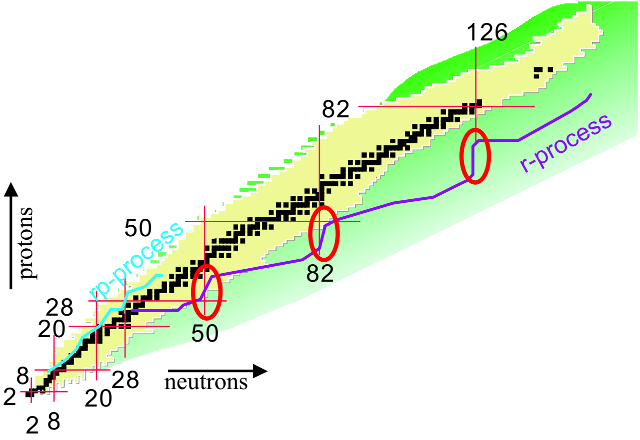

HFB: $\beta_2^{(p)}$=0.43 exp: $\beta_2^{(p)}$=0.42(5) , J.K. Hwang et al., Phys. Rev. C (2006)

# QRPA

QRPA done properly is time-dependent HFB with small harmonic perturbation. Perturbing operator is $\beta$-decay transition operator. Decay matrix elements obtained from response of nucleus to perturbation.

Schematic QRPA of Möller et al. is very simplified version of this.
No fully self-consistent mean-field calculation to start.
Nucleon-nucleon interaction is schematic.

# Initial Skyrme Application: Spherical QRPA

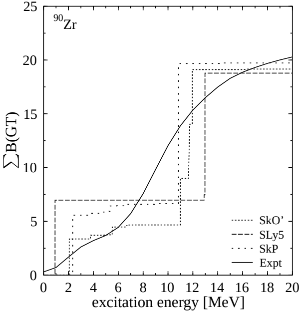



Closed shell nuclei are spherical.

# Initial Skyrme Application: Spherical QRPA

In nuclei near "waiting points," with no forbidden decay.

Chose functional corresponding to Skyrme interaction SkO′ because did best with GT distributions.



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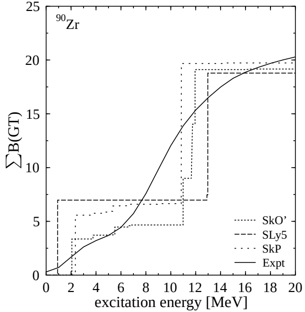
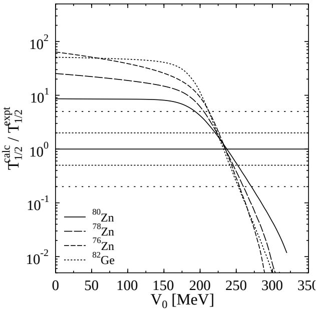


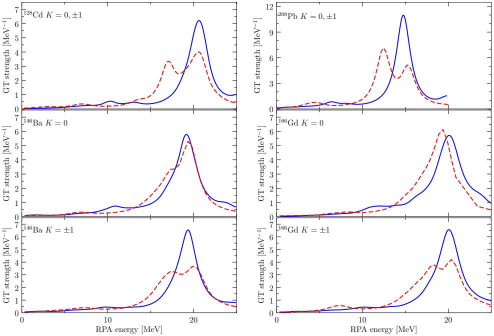

One free parameter: strength of proton-neutron spin-1 pairing (it's zero in schematic QRPA.) Adjusted in each of the three peak regions to reproduce measured lifetimes.



# New: Fast Skyrme QRPA in Deformed Nuclei

## Finite-Amplitude Method

Strength functions computed directly, in orders of magnitude less time than with matrix QRPA.



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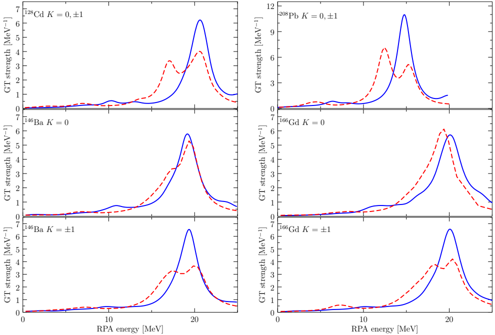
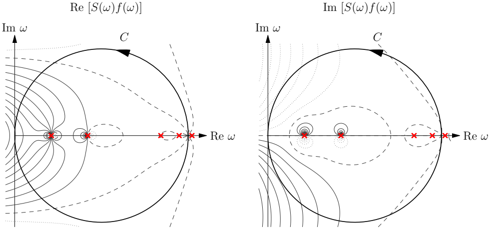



Beta-decay rates obtained by integrating strength with phase-space weighting function in contour around excited states below threshold.



# Rare-Earth Region

Local fit of two parameters: strengths of spin-isospin force and proton-neutron spin-1 pairing force, with several functionals.

$$\mathcal{H}^{c.c.}_{\text{odd}} = C_1^s\, \mathbf{s}_{11}^2 + C_1^{\Delta s}\, \mathbf{s}_{11} \cdot \nabla^2 \mathbf{s}_{11} + C_1^T \mathbf{s}_{11} \cdot \mathbf{T}_{11} + C_1^j\, \mathbf{j}_{11}^2$$
$$+ C_1^{\nabla j}\, \mathbf{s}_{11} \cdot \boldsymbol{\nabla} \times \mathbf{j}_{11} + C_1^F\, \mathbf{s}_{11} \cdot \mathbf{F}_{11} + C_1^{\nabla s} \left(\boldsymbol{\nabla} \cdot \mathbf{s}_{11}\right)^2 + V_0 \times pn \text{ pair.}$$

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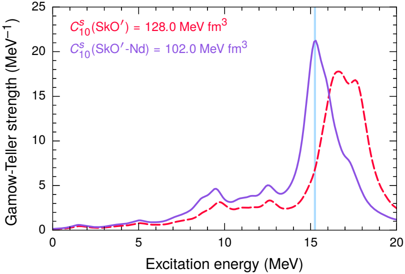
Local fit of two parameters: strengths of spin-isospin force and proton-neutron spin-1 pairing force, with several functionals.

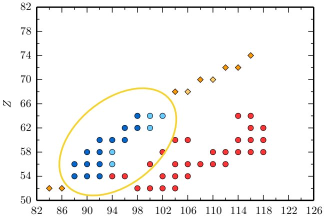
## Adjusting spin-isospin force

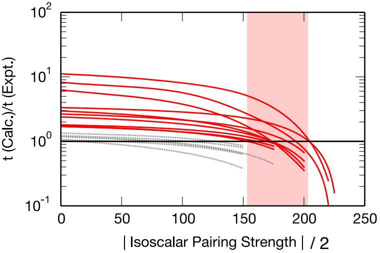



$C_1^T s_{11} \cdot T_{11} + C_1^j j_{11}^2$

$s_{11} \cdot F_{11} + C_1^{\nabla s} (\nabla \cdot s_{11})^2 + V_0 \times pn$ pair.

## Adjusting proton-neutron spin-1 pairing

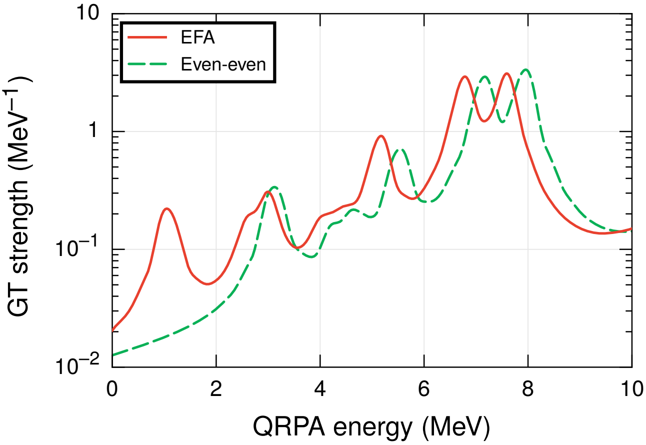


# Odd Nuclei

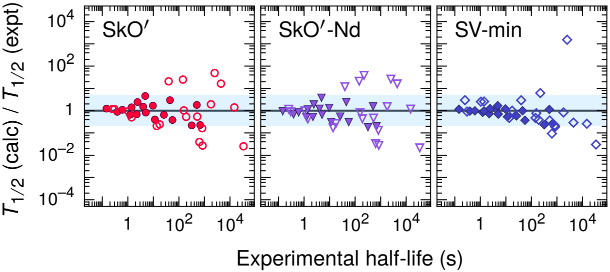
Have $J \neq 0$

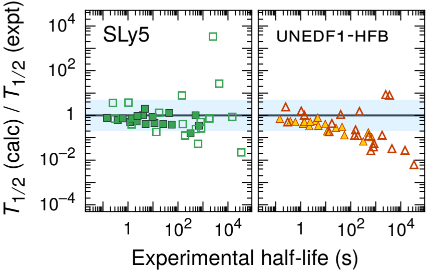
Treat degeneracy as ensemble of state and angular-momentum-flipped partner (Equal Filling Approximation).



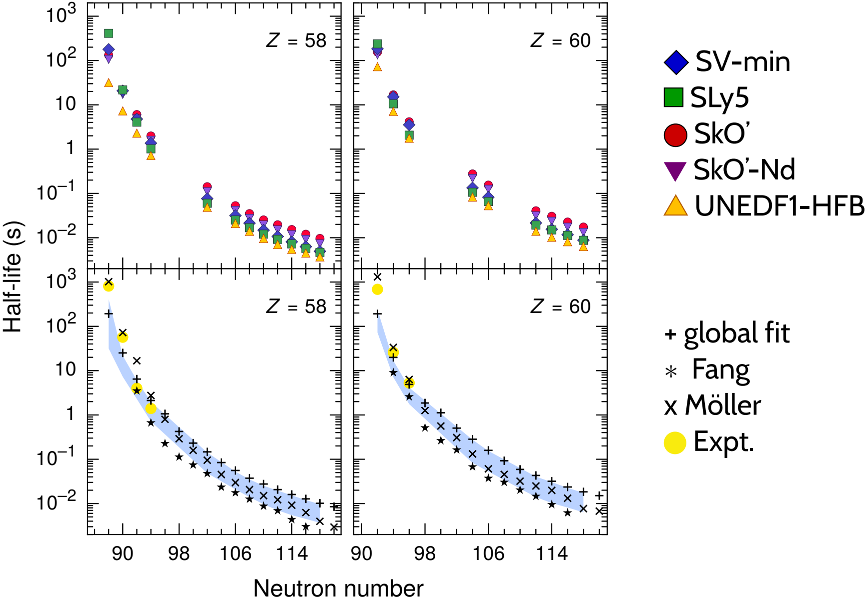
# How Do We Do?

Open symbols mean used in fit

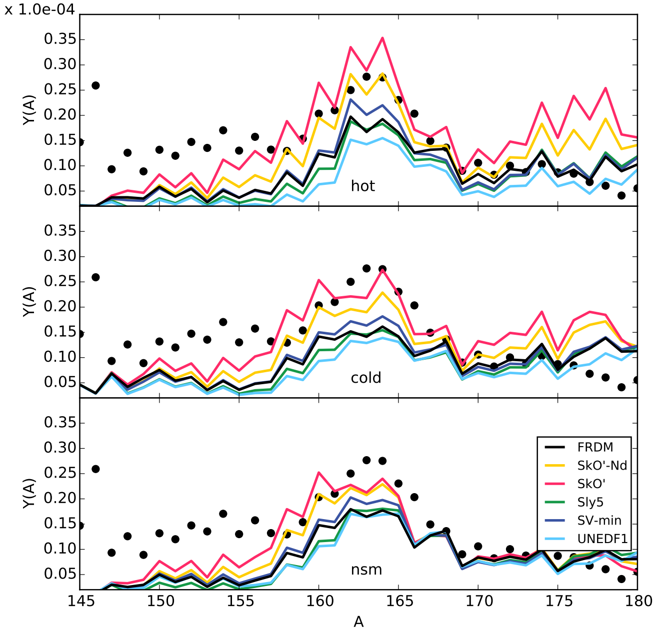


# Predicted Half Lives



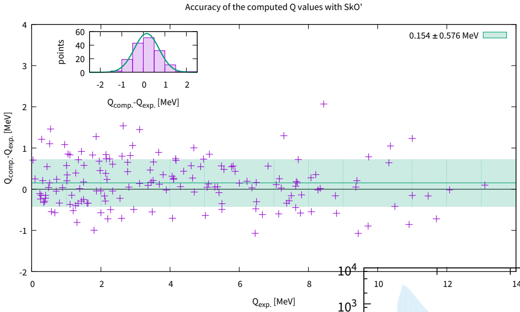
# What's the Effect?



# Fast QRPA Now Allows Global Skyrme Fit

Fit to 7 GT resonance energies, 2 spin-dipole resonance energies, 7 $\beta$-decay rates in selected spherical and well-deformed nuclei from light to heavy.

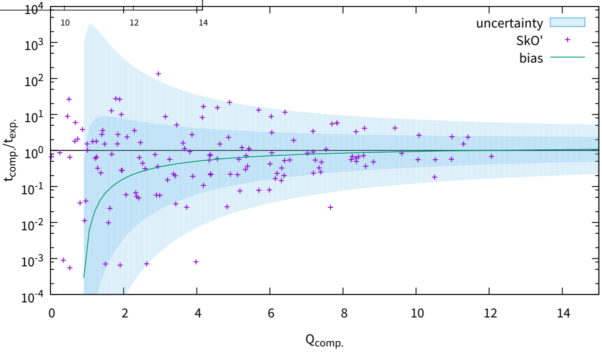
# Initial Step: Two Parameters Again




$Q$ values not given perfectly, and $\beta$ rate roughly $\propto Q^5$.

Initially adjusted only $C_1^s$, which moves GT resonance, and isoscalar pairing strength.

Uncertainty decreases with increasing $Q$.



# Fitting the Full Time-Odd Skyrme Functional

## Charge-Changing Part, That is …

$$
\begin{aligned}
\mathcal{H}^{c.c.}_{\text{odd}} = & C_1^{s}\,\mathbf{s}_{11}^2 + C_1^{\Delta s}\,\mathbf{s}_{11}\cdot\nabla^2\mathbf{s}_{11} + C_1^{T}\mathbf{s}_{11}\cdot\mathbf{T}_{11} + C_1^{j}\,\mathbf{j}_{11}^2 \\
& + C_1^{\nabla j}\,\mathbf{s}_{11}\cdot\boldsymbol{\nabla}\times\mathbf{j}_{11} + C_1^{F}\,\mathbf{s}_{11}\cdot\mathbf{F}_{11} + C_1^{\nabla s}\,\left(\boldsymbol{\nabla}\cdot\mathbf{s}_{11}\right)^2 + V_0 \times pn \text{ pair.}
\end{aligned}
$$

- Initial two-parameter fit

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- Initial two-parameter fit
- More comprehensive fit

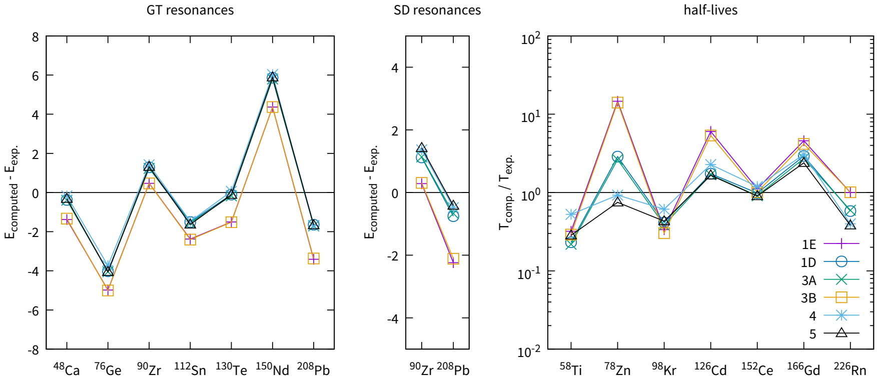
# Fitting the Full Time-Odd Skyrme Functional

## Charge-Changing Part, That is …

$$\begin{aligned}\mathcal{H}^{c.c.}_{\text{odd}} = & C^s_1 \, \mathbf{s}^2_{11} + C^{\Delta s}_1 \, \mathbf{s}_{11} \cdot \nabla^2 \mathbf{s}_{11} + C^T_1 \mathbf{s}_{11} \cdot \mathbf{T}_{11} + C^j_1 \, \mathbf{j}^2_{11} \\ & + C^{\nabla j}_1 \, \mathbf{s}_{11} \cdot \boldsymbol{\nabla} \times \mathbf{j}_{11} + C^F_1 \, \mathbf{s}_{11} \cdot \mathbf{F}_{11} + C^{\nabla s}_1 \, (\boldsymbol{\nabla} \cdot \mathbf{s}_{11})^2 + V_0 \times pn \text{ pair.}\end{aligned}$$

- Initial two-parameter fit
- More comprehensive fit
- Additional adjustment

# Tried Lots of Things…

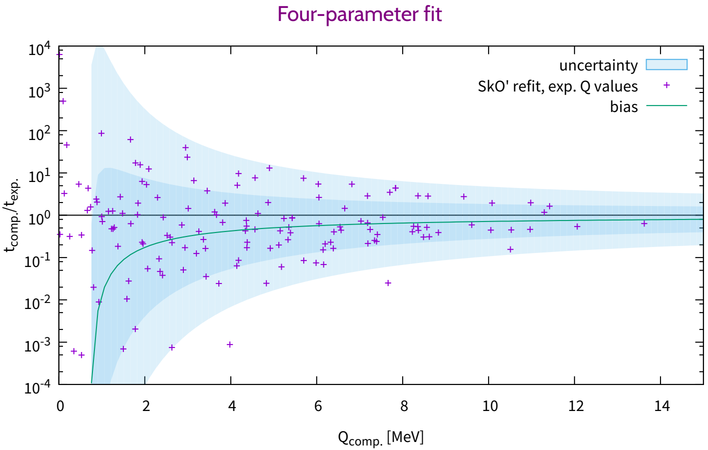



All SkO'

1E = Experimental *Q* values, 2 parameters
3A = Computed *Q* values, 4 parameters
4 = Start with 3A, 3 more parameters

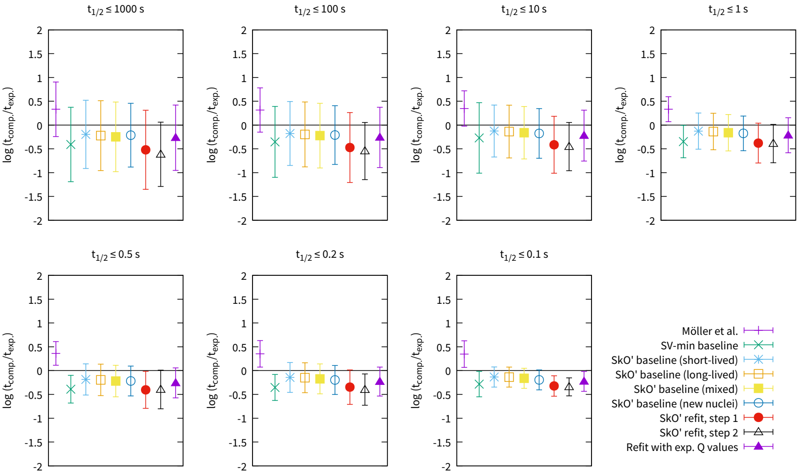
1D = Computed *Q* values, 2 parameters
3A = Experimental *Q* values, 4 parameters
5 = Computed *Q* values, three more parameters

# Results



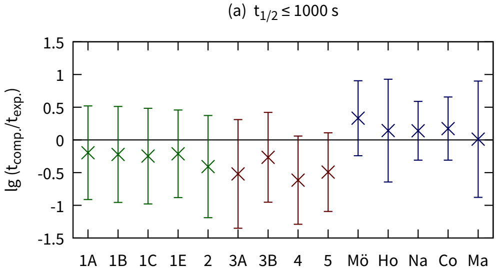

Not significantly better than restricted two-parameter fit.

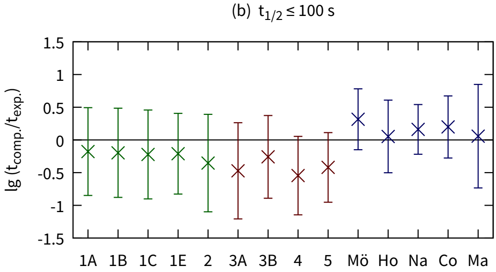
# Summary of Fitting So Far




Meh…. Not doing as well as we'd hoped. Is the reason the limited correlations in the QRPA? Or will better fitting and more data help?

# Comparison with Other Groups



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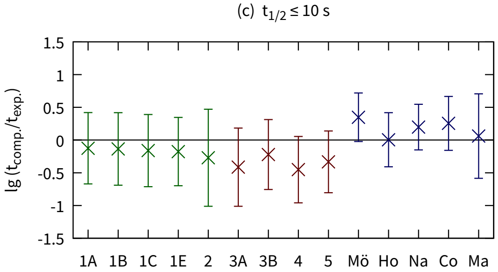
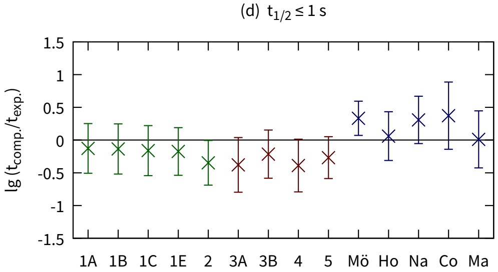


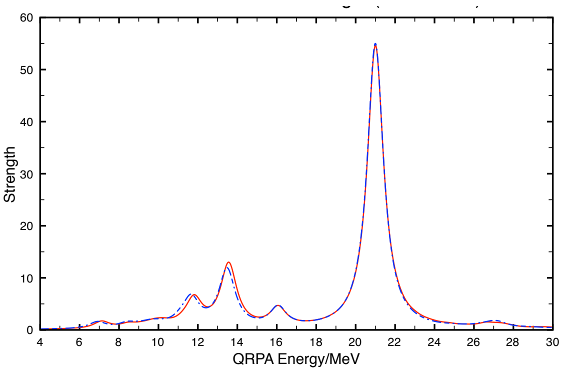
# But We Really Care About High-Q/Fast Decays

- These are the most important for the *r* process.

# But We Really Care About High-Q/Fast Decays

- These are the most important for the *r* process.
- And they are easier to predict:

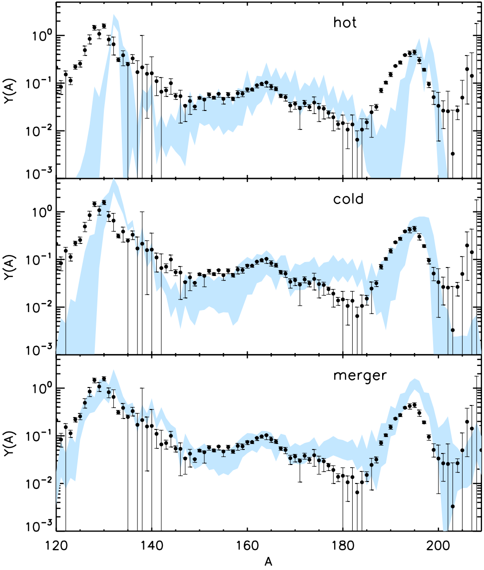
$$\frac{(\Delta E + \delta)^5}{(\Delta E)^5} = 1 + 4\frac{\delta}{\Delta E} + \ldots$$




Can more be measured?

# What's at Stake Here?

## Significance of Factor-of-Two Uncertainty



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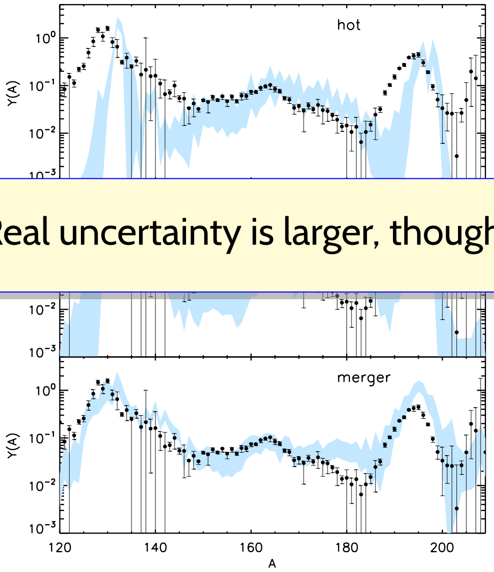
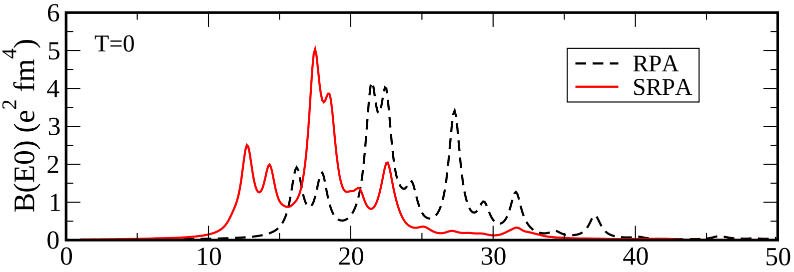



Real uncertainty is larger, though.

# The Future: Second (Q)RPA

Add two-phonon states to RPA's one-phonon states; should describe spreading width of resonances and low-lying strength much better.

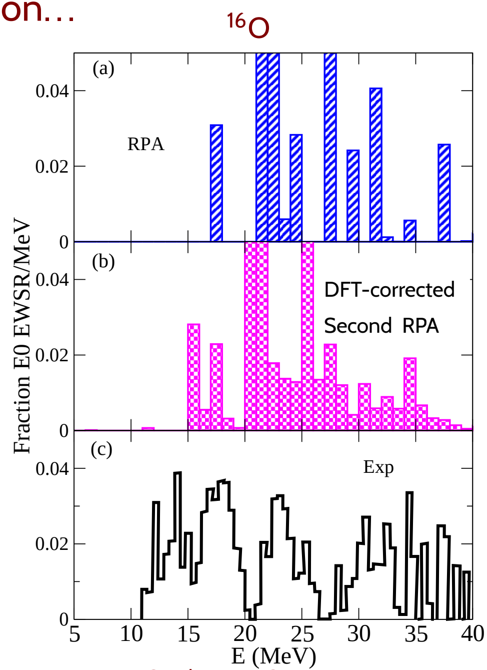
But…




Argghh!

RPA gets location of resonances about right (spreading width inserted by hand). Second RPA lowers them by several MeV. But problem turns out to be due to insconsistency with DFT…

# With Correction…

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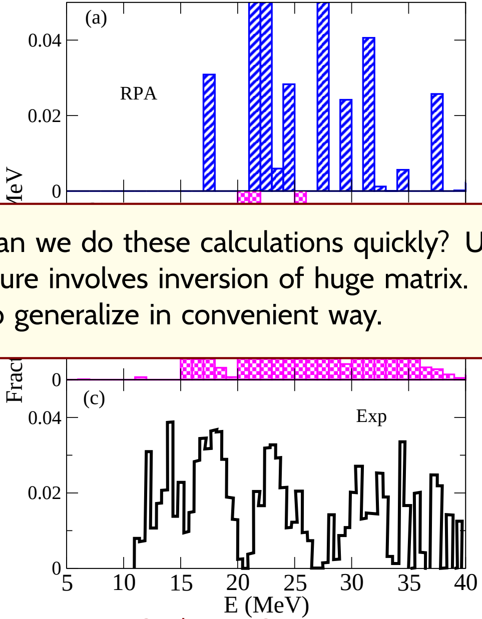
# With Correction…

$^{16}O$




How can we do these calculations quickly? Usual procedure involves inversion of huge matrix. FAM hard to generalize in convenient way.

Gambacurta, Grasso, JE

# Finally…

# The End

Thanks for your kind attention.