

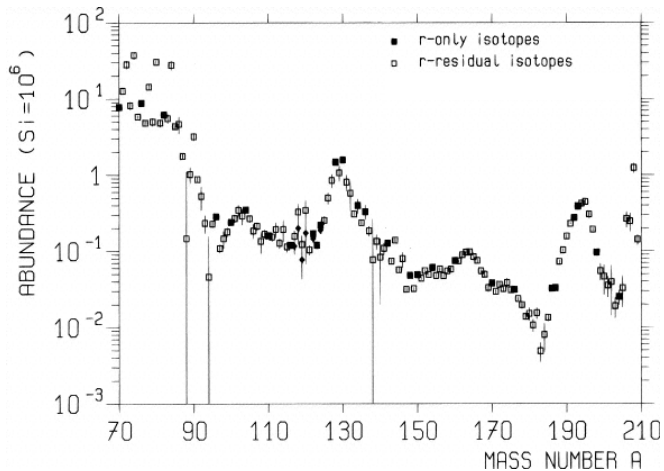
Weak Decay/Capture for Astrophysics

J. Engel

Work with M. Mustonen, T. Shafer, E. Ney, Q. Liu,
C. Fröhlich, D. Gambacurta, M. Grasso, G. McLaughlin, M. Mumpower,
N. Paar, A. Ravlić, N. Schunck, R. Surman, R. Zegers, ...

June 10, 2022

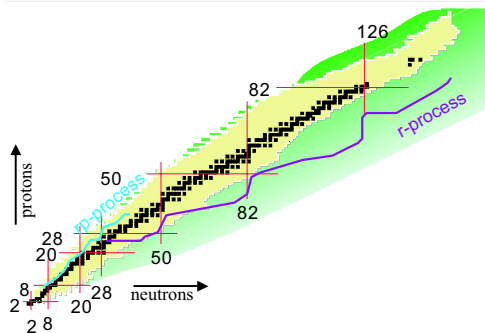
R-Process Abundances



Nuclear Landscape

To convincingly locate the site(s) of the r process, we need to know reaction rates, particularly β -decay rates, in neutron-rich nuclei.

To fully understand supernova evolution, we need to know electron-capture rates for lots of medium-mass nuclei.



Calculating These Rates is Hard

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

To calculate β decay between two states, you need:

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

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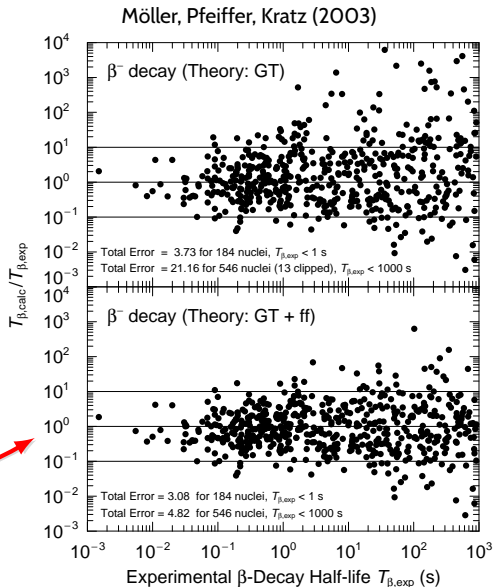
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Most of the time the decay operator leaves you above threshold, by the way.

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

What's Often Used for β -Decay in Simulations

- ▶ Masses through “finite-range droplet model with shell corrections.”
- ▶ QRPA with simple space-independent interaction.
- ▶ First forbidden decay included in approximate way. Shortens half lives.



Self-Consistent Version: Skyrme DFT

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

$$\begin{aligned}V_{\text{Skyrme}} = & t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \\ & + \frac{1}{2} t_1 (1 + x_1 P_\sigma) [(\nabla_1 - \nabla_2)^2 \delta(\mathbf{r}_1 - \mathbf{r}_2) + h.c.] \\ & + t_2 (1 + x_2 P_\sigma) (\nabla_1 - \nabla_2) \cdot \delta(\mathbf{r}_1 - \mathbf{r}_2) (\nabla_1 - \nabla_2) \\ & + \frac{1}{6} t_3 (1 + x_3 P_\sigma) \delta(\mathbf{r}_1 - \mathbf{r}_2) \rho^\alpha([\mathbf{r}_1 + \mathbf{r}_2]/2) \\ & + iW_0 (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot (\nabla_1 - \nabla_2) \times \delta(\mathbf{r}_1 - \mathbf{r}_2) (\nabla_1 - \nabla_2)\end{aligned}$$

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}_{odd} has no effect in mean-field description of time-reversal even states (e.g. ground states), but large effect in β decay.

Time-Even and Time-Odd Parts of Functional

Not including pairing:

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

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

Time-even densities:

ρ = usual density τ = kinetic density \mathbf{j} = spin-orbit current

Time-odd densities:

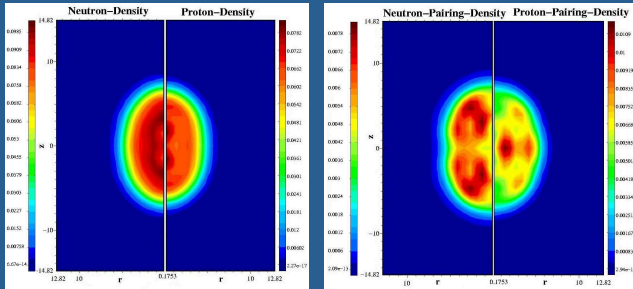
\mathbf{s} = spin current \mathbf{T} = kinetic spin current \mathbf{j} = usual current

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)

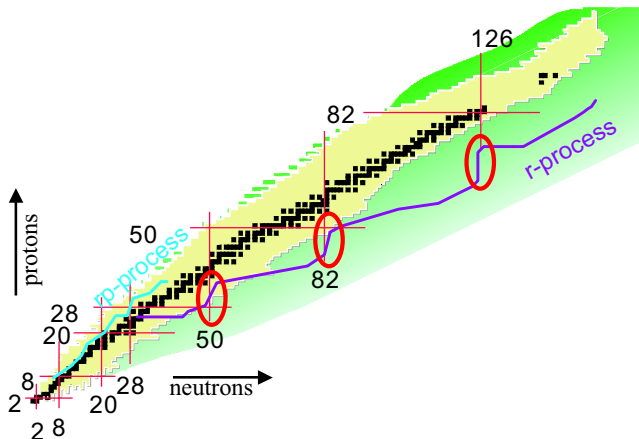
QRPA

Self-consistent QRPA is time-dependent HFB with small harmonic perturbation. Perturbing operator is β -decay transition operator. Decay matrix elements obtained from response of nucleus to perturbation.

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

Initial Skyrme Application: Spherical QRPA

Even Isotopes Only

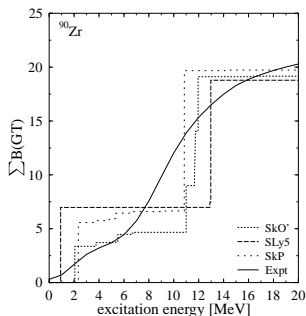


Closed shell nuclei are spherical.

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.

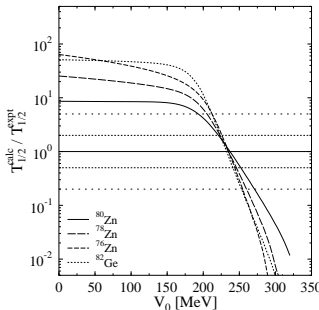
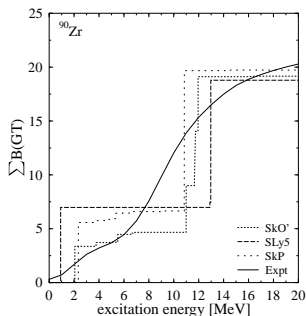


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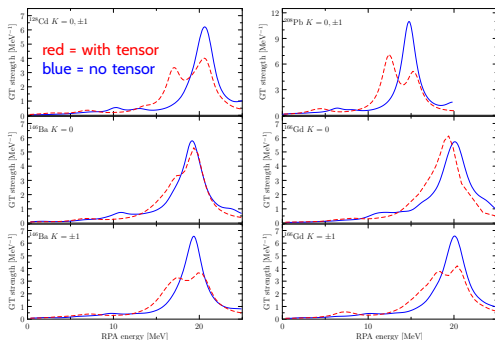
One free parameter: strength of proton-neutron spin-1 pairing (it's zero in schematic QRPA.) Adjusted in each of the three peak regions to reproduce measured lifetimes.



Later: Fast Skyrme QRPA in Deformed Nuclei

Finite-Amplitude Method – Nakatsukasa et al.

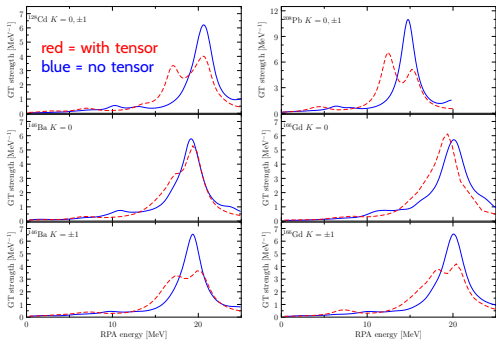
Strength functions
computed directly from
linear response, in orders
of magnitude less time
than with matrix QRPA.



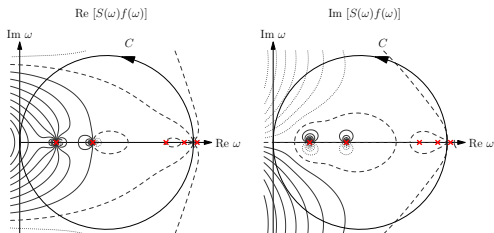
Later: Fast Skyrme QRPA in Deformed Nuclei

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



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



Rare-Earth Region

Tom Shafer

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

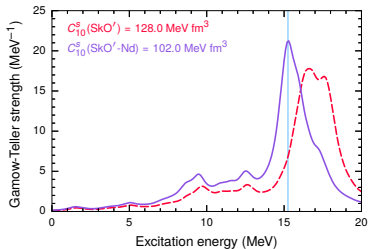
$$\mathcal{H}_{\text{odd}}^{\text{c.c.}} = C_1^S s_{11}^2 + C_1^{\Delta S} s_{11} \cdot \nabla^2 s_{11} + C_1^T s_{11} \cdot \mathbf{T}_{11} + C_1^j j_{11}^2 \\ + C_1^{\nabla j} j s_{11} \cdot \nabla \times j_{11} + C_1^F s_{11} \cdot \mathbf{F}_{11} + C_1^{\nabla s} (\nabla \cdot s_{11})^2 + V_0 \times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

Rare-Earth Region

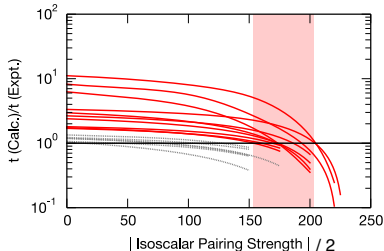
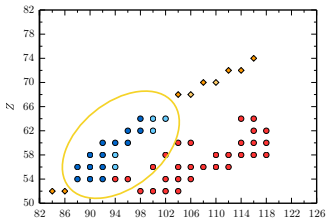
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Adjusting spin-isospin force



Adjusting proton-neutron spin-1 pairing

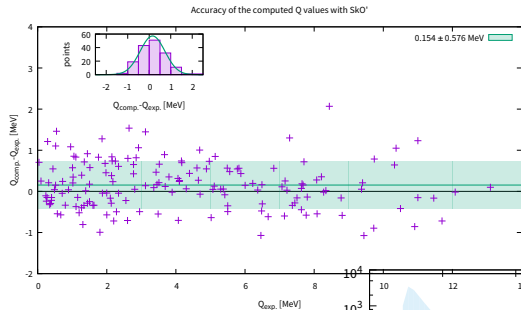


Global Skyrme Fit for Even Nuclei

Mika Mustonen

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

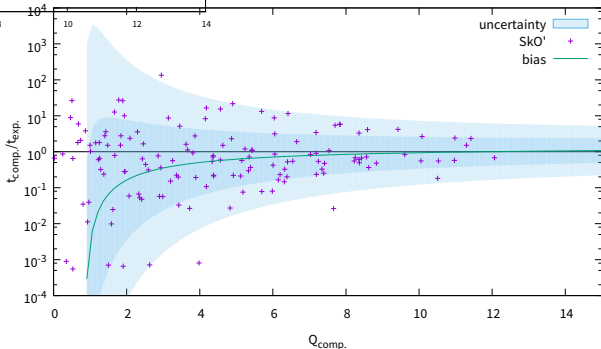
Initial Step: Two Parameters Again



Q values not given perfectly,
and β 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 ...

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

- ▶ Initial two-parameter fit

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- ▶ Initial two-parameter fit
- ▶ More comprehensive fit

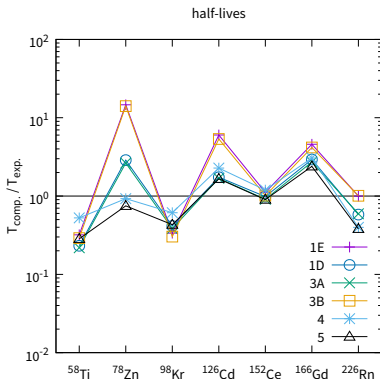
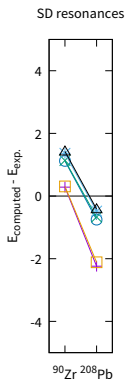
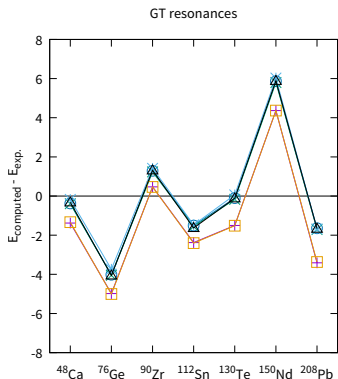
Fitting the Full Time-Odd Skyrme Functional

Charge-Changing Part, That is ...

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- ▶ 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

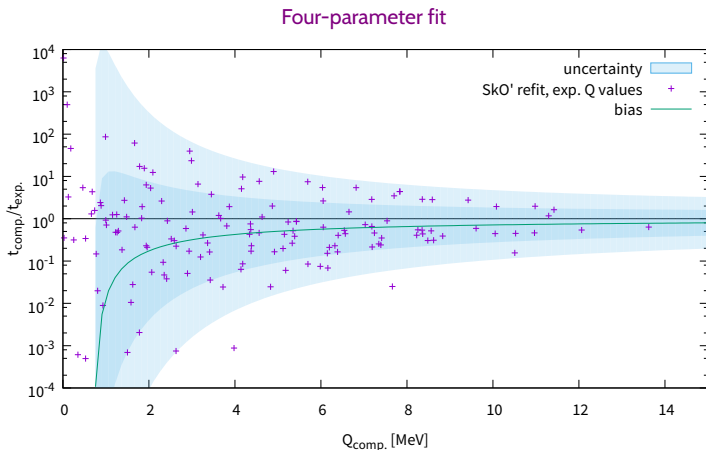
4 = Start with 3A, 3 more parameters

1D = Computed Q values, 2 parameters

3B = Experimental Q values, 4 parameters

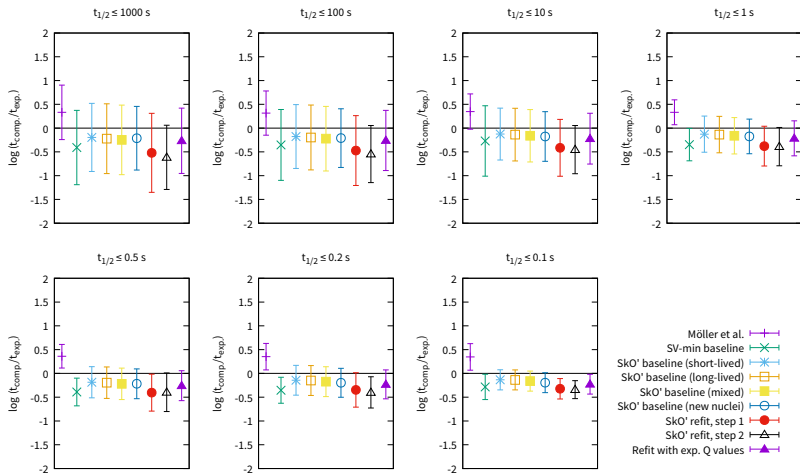
5 = Computed Q values, three more parameters

Results



Not significantly better than restricted two-parameter fit.

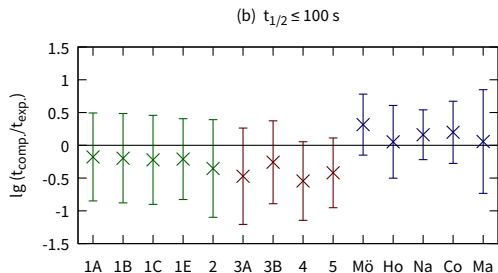
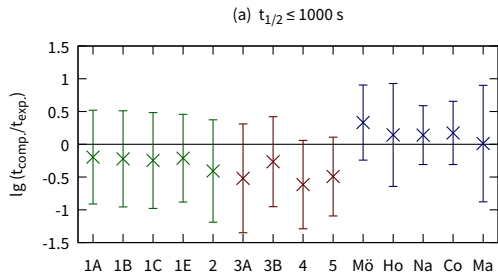
Summary of Fitting Performance



Not as good as we'd hoped.

Is the reason the limited correlations in the QRPA? Simplified current operators? Or will better UQ and more data help?

Comparison



Mö = P. Möller, B. Pfeiffer, and K.-L. Kratz, *PRC* **67**, 055802 (2003)

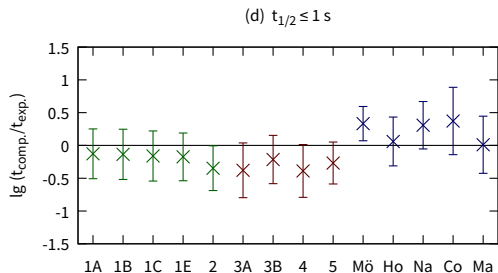
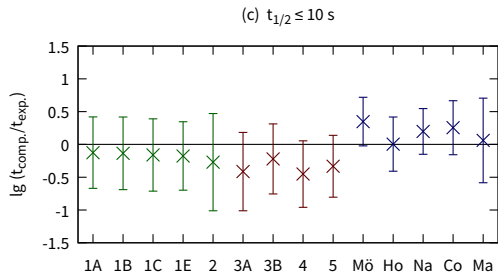
Ho = H. Homma, E. Bender, M. Hirsch, K. Muto, H. V. Klapdor-Kleingrothaus, and T. Oda, *PRC* **54**, 2972 (1996)

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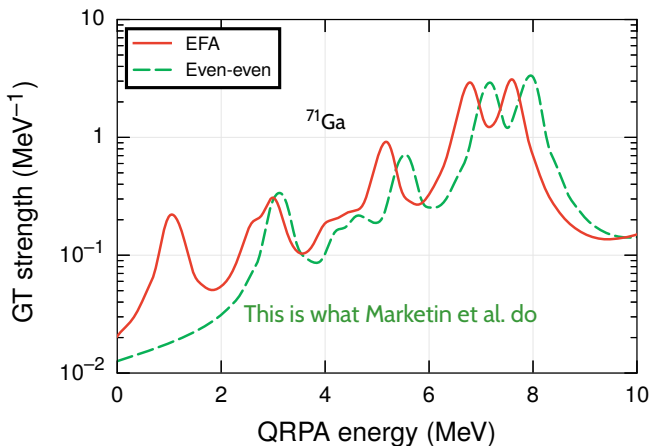
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Odd and Odd-Odd Nuclei

These have $J \neq 0$

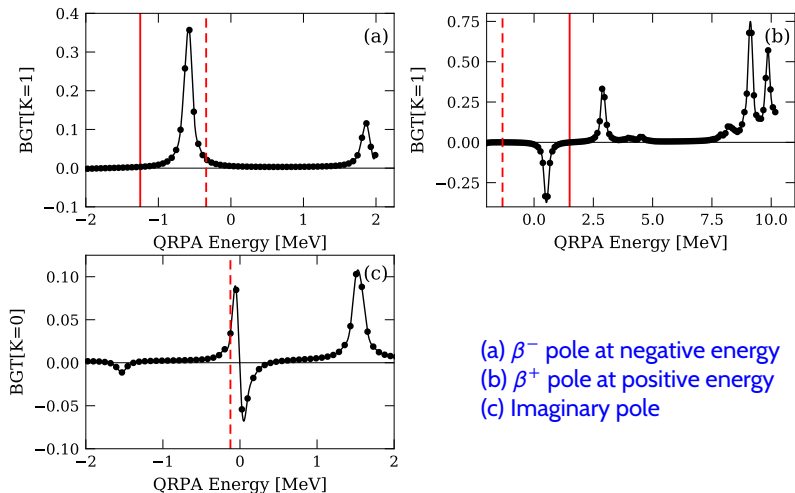
Treat resulting degeneracy of substates as ensemble (Equal Filling Approximation). Time-dependent version gives Equal-Filling FAM.



Problems with Equal Filling

Evan Ney

$$S(F, \omega) = - \sum_n \left(\frac{|\langle n | \hat{F} | 0 \rangle|^2}{\Omega_n - \omega} + \frac{|\langle n | \hat{F}^\dagger | 0 \rangle|^2}{\Omega_n + \omega} \right)$$



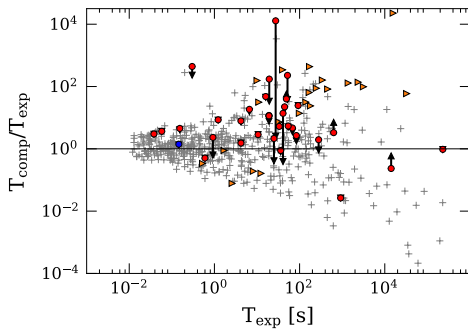
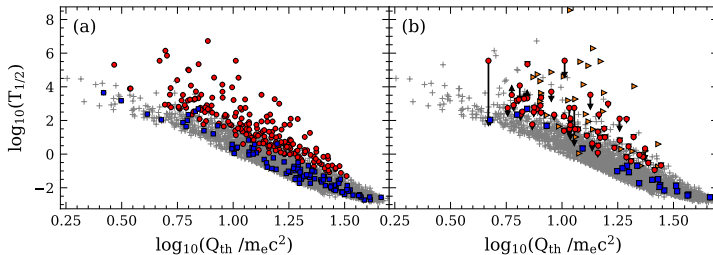
- (a) β^- pole at negative energy
- (b) β^+ pole at positive energy
- (c) Imaginary pole

We can often correct such cases by hand...

Accounting for Problems

Suspicious (red) and random (blue) nuclei

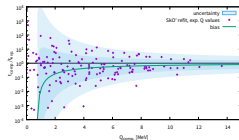
Corrections



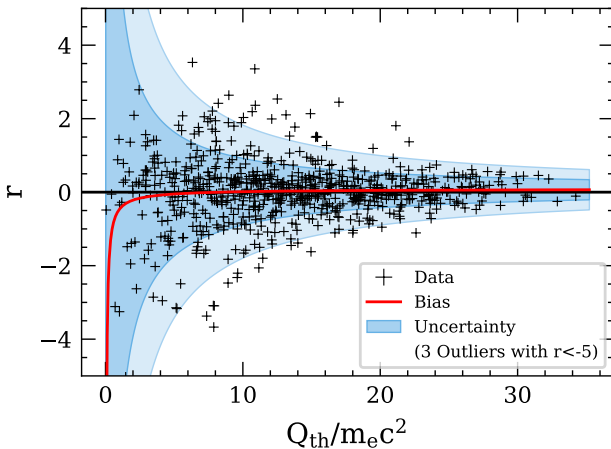
Corrections vs. experiment

Results with All Nuclei

Evan Ney



Even-even results



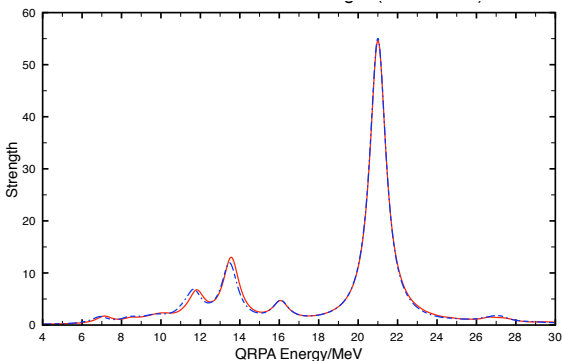
But For High- Q /Fast Decays ...

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

But For High-Q/Fast Decays ...

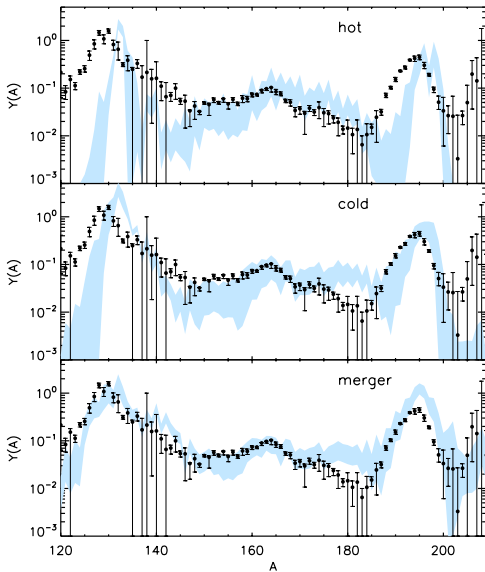
- ▶ These are the most important for the r process.
- ▶ And they are easier to predict:

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



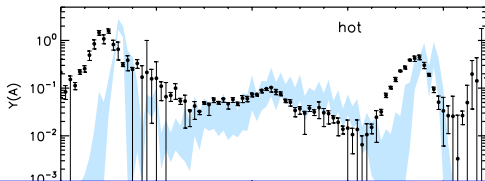
What's at Stake Here?

Significance of Factor-of-Two Uncertainty

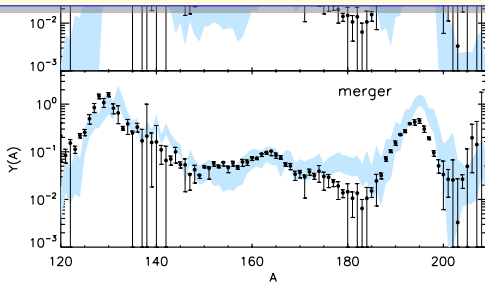


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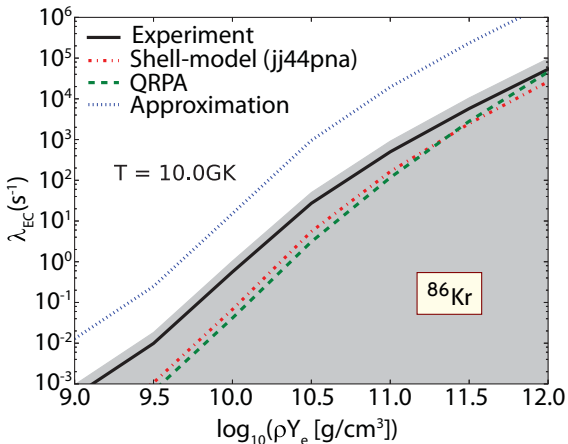


Real uncertainty is larger, though.



Electron Capture

Evan Ney



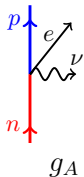
For terrestrial or astrophysical environments.

Developed a non-zero-temperature FAM.

Most Recently: Two-Body Current

Evan Ney

Leading order:

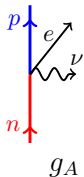


Usual β -decay current

Most Recently: Two-Body Current

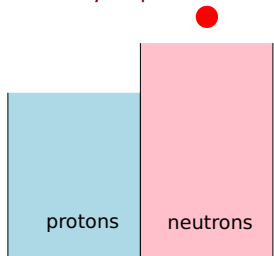
Evan Ney

Leading order:



Usual β -decay current

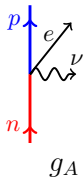
Consider very simple wave function



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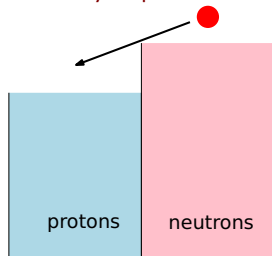
Evan Ney

Leading order:



Usual β -decay current

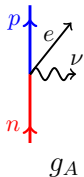
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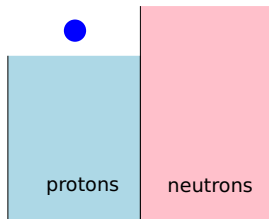
Evan Ney

Leading order:



Usual β -decay current

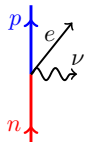
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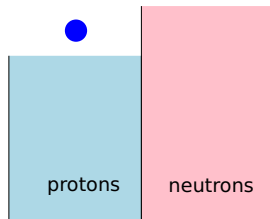
Leading order:



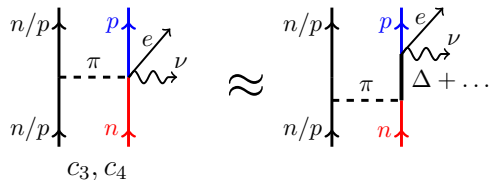
g_A

Usual β -decay current

Consider very simple wave function



Higher order:

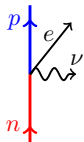


There are also contact terms...

Most Recently: Two-Body Current

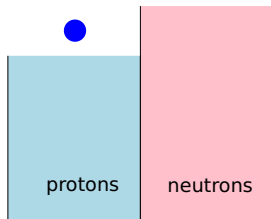
Evan Ney

Leading order:

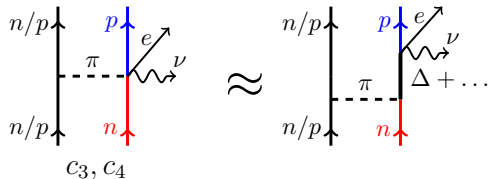


Usual β -decay current

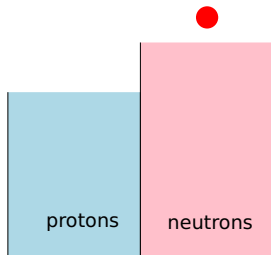
Consider very simple wave function



Higher order:



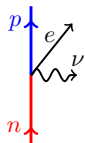
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Most Recently: Two-Body Current

Evan Ney

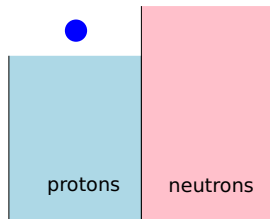
Leading order:



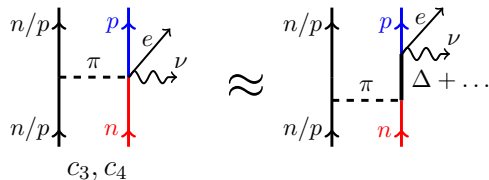
g_A

Usual β -decay current

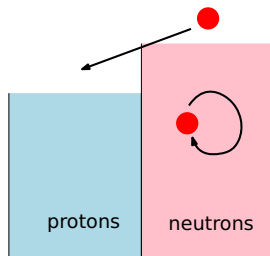
Consider very simple wave function



Higher order:



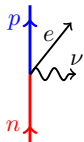
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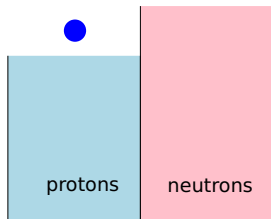
Leading order:



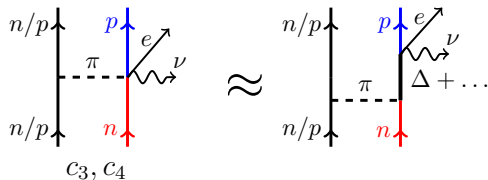
g_A

Usual β -decay current

Consider very simple wave function

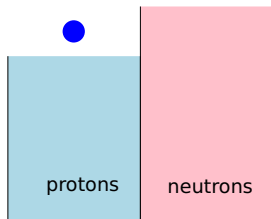


Higher order:

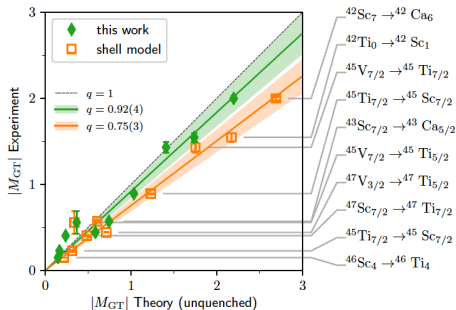
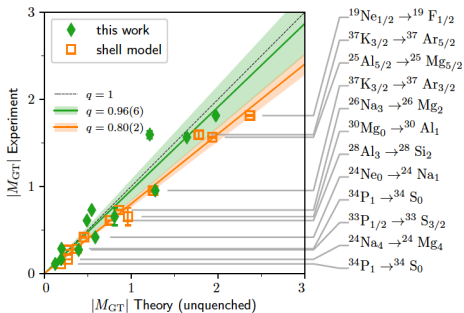


C_3, C_4

There are also contact terms...



Quenching in the *sd* and *pf* Shells

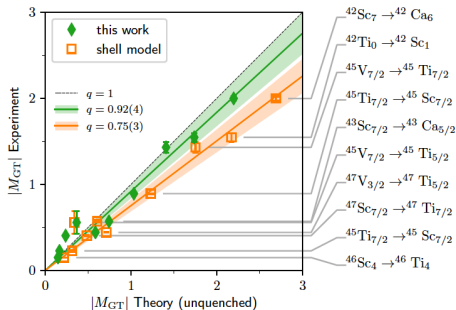
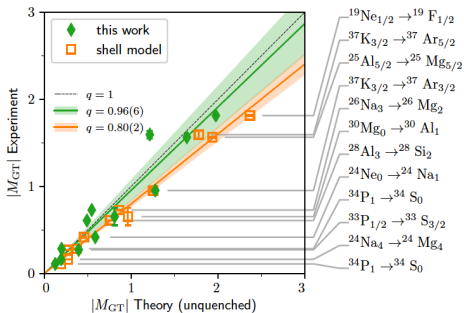


IMSRG calculation, Gysbers et al

Some quenching from correlations omitted by the shell model.

But a lot comes from the two-body current.

Quenching in the *sd* and *pf* Shells



IMSRG calculation, Gysbers et al

Some quenching from correlations omitted by the shell model.

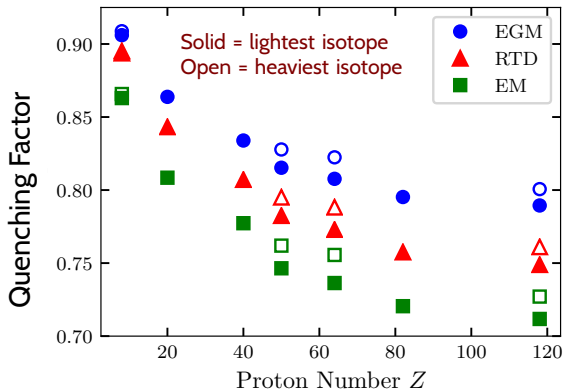
But a lot comes from the two-body current.

In these $A < 50$ nuclei, β -decay quenching doesn't much depend on Z and N . But what about in heavier nuclei?

Z- and N-Dependence of Quenching

Integrated GT Strength

Three sets of chiral parameters, no contact



EGM - E. Epelbaum, W. Glöckle, and U.-G. Meißner, Nucl. Phys. A 747, 362 (2005).

RTS - M. C. M. Rentmeester, R. G. E. Timmermans, and J. J. de Swart, Phys. Rev. C 67, 044001 (2003)

EM - D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001(R) (2003).

$$g_A = 1 \quad \longrightarrow \quad q = .79$$

Density-Matrix Expansion of Exchange Term

$$\vec{O}(\vec{r}) = \frac{g_A}{m_N f_\pi^2} \vec{\sigma} \tau_\pm \left\{ \bar{C} \left[1 - m_\pi^2 F[k_F(\vec{r})] - \frac{1}{10} m_\pi^2 G[k_F(\vec{r})] \right] \rho(\vec{r}) - \bar{D} \rho(\vec{r}) - \frac{1}{6} \frac{\bar{C} m_\pi^2}{k_F^2(\vec{r})} G[k_F(\vec{r})] \left[\frac{1}{4} \nabla^2 \rho(\vec{r}) - \tau(\vec{r}) \right] \right\},$$

with $\bar{C} = \frac{1}{3} \left(2\bar{c}_4 - \bar{c}_3 + \frac{1}{2} \right)$ and $\bar{D} \equiv \bar{d}_1 - 2\bar{d}_2$.

$$F[k] = \frac{3}{2k^2} \left[1 - \frac{m_\pi}{k} \tan^{-1} \left(\frac{2k}{m_\pi} \right) + \frac{m_\pi^2}{4k^2} \ln \left(1 + 4 \frac{k^2}{m_\pi^2} \right) \right]$$

$$G[k] = \frac{3}{2k^2} \left[1 + 8 \frac{k^2}{4k^2 + m_\pi^2} - \frac{m_\pi^2}{k^2} \ln \left(1 + 4 \frac{k^2}{m_\pi^2} \right) \right]$$

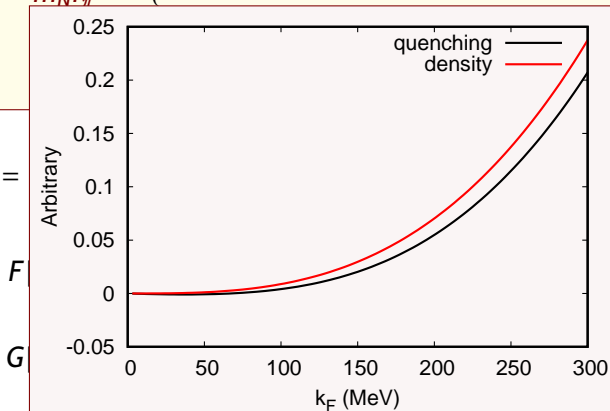
and $k_F(\vec{r}) \equiv [3\pi^2 \rho(\vec{r})/2]^{1/3}$ is the local Fermi momentum.

Non-contact direct terms are much less important.

Density-Matrix Expansion of Exchange Term

$$\vec{O}(\vec{r}) = \frac{g_A}{m_N f_\pi^2} \vec{\sigma} \tau_\pm \left\{ \bar{C} \left[1 - m_\pi^2 F[k_F(\vec{r})] - \frac{1}{10} m_\pi^2 G[k_F(\vec{r})] \right] \rho(\vec{r}) \right.$$

with $\bar{C} =$



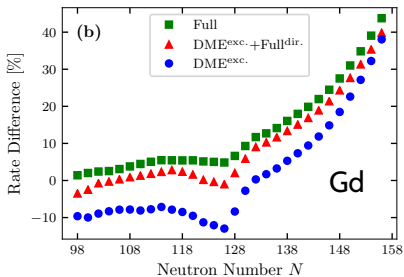
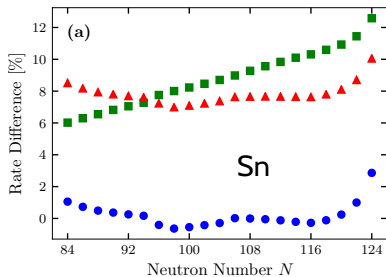
and $k_F(\vec{r})$

Quenching compared with density at constant density

Non-contact direct terms are much less important.

Effect on β -Decay Rates

Difference from rate with one-body operator, with $g_A = 1.0$



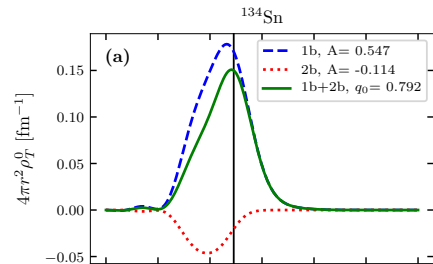
Conclusions:

- ▶ DME is a good approximation to exchange current.
- ▶ Use of two body current more important in neutron-rich nuclei. Quenching of rates decreases and can even become enhancement near the drip line. *Why?*

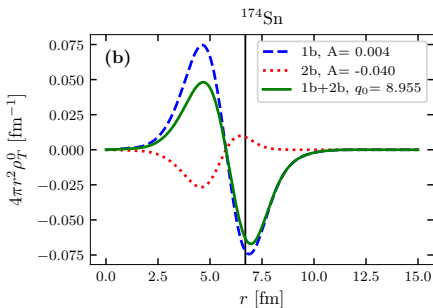
Enhancement of Low-Lying Strength

Can occur in neutron-rich isotopes

Density-dependence of current means it does very little beyond the nuclear surface.



← Typical transition in ¹³⁴Sn

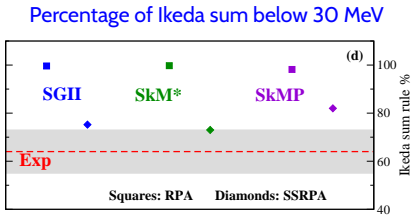
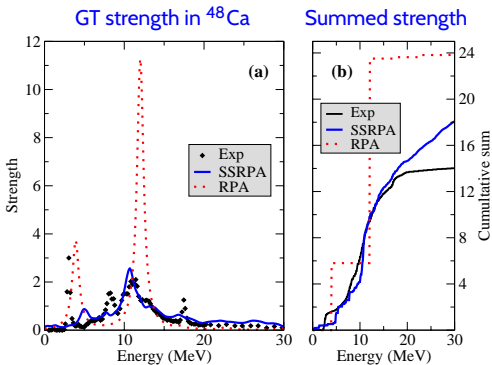


← Unusual (and lowest-lying) transition in ¹⁷⁴Sn

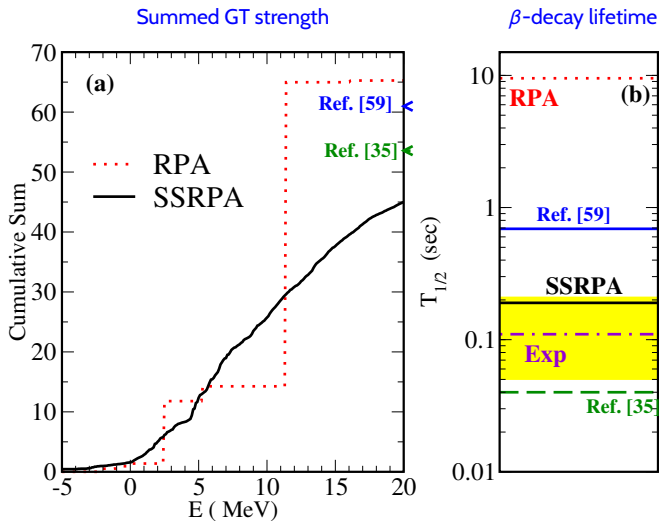
Beyond QRPA

Second RPA with D. Gambacurta and M. Grasso

Second RPA: Add 4p-4h basic excitations to RPA 2q-2h excitations.
Should better describe spreading widths and low-lying strength.



β Decay of ^{78}Ni in Second RPA



Ref. [35] = C. Robin and E. Litvinova, *Phys. Rev. C* **98**, 051301(R) (2018)

Ref. [59] = Y. F. Niu, Z. M. Niu, G. Colò, and E. Vigezzi, *Phys. Rev. Lett.* **114**, 142501 (2015)

Simpler Version: "Time Blocking" Approximation

Equivalent to Quasiparticle-Phonon Model

RPA response function

$$\Pi = \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \dots$$

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Phonon-exchange potential

$$\text{Wavy line} = V_{\text{Sk}} + \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \dots$$

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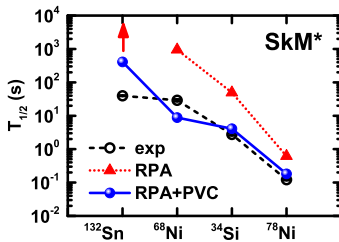
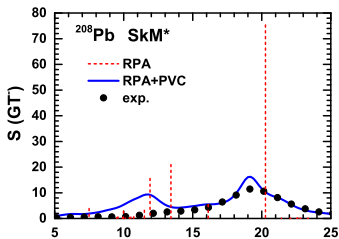
$$\text{Wavy line} = V_{\text{Sk}} \text{Diagram 1} + \text{Diagram 2} + \text{Diagram 3} + \text{Diagram 4} + \dots$$

Time-blocking modification of response

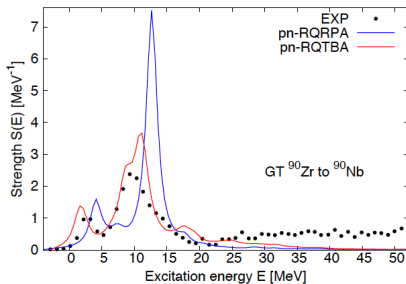
$$\text{Loop} \Rightarrow \text{Loop} + \text{Loop with wavy line} + \text{Loop with wavy line} + \text{Loop with wavy line} + \text{Loop with wavy line} + \text{Loop with wavy line} + \dots$$

Use for Beta Decay

Niu et al. in Skyrme DFT



Litvinova in relativistic DFT



Deformed Time-Blocking QRPA

In progress: Qunqun Liu

A modified FAM is the best hope for a global calculation.

$$X_{\mu\nu}(\omega) = -\frac{\delta H_{\mu\nu}^{20}(\omega) + F_{\mu\nu}^{20} + [W(\omega)X(\omega)]_{\mu\nu}}{E_{\mu} + E_{\nu} + \omega}$$
$$Y_{\mu\nu}(\omega) = -\frac{\delta H_{\mu\nu}^{20}(\omega) + F_{\mu\nu}^{20} + [W^*(-\omega)Y(\omega)]_{\mu\nu}}{E_{\mu} + E_{\nu} + \omega},$$

where W is the phonon propagator, and, e.g.,

$$[W(\omega)X(\omega)]_{\mu\nu} = \sum_{\mu' < \nu'} W_{\mu\nu, \mu'\nu'}(\omega) X_{\mu'\nu'}(\omega)$$

Assemble W from qp-phonon vertices and qp energies on the fly. The qp-phonon vertices come from like-particle FAM. Use contour-integral technique of N. Hinohara and collaborators to obtain them from residues of δH_{11} . [Litvinova and Zhang, PRC 104, 044303 \(2021\)](#)

Too hard to find all relevant poles in all isotopes. Ultimately need FAM to generate QRPA matrix. [Avogadro and Nakatsukasa, PRC 87 014331 \(2013\)](#)

Finally...

All these developments will require refitting and UQ. There's still a lot to do on the road to more realistic DFT-based β -decay rates!

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Thanks for Listening