Update on beta-decay calculations in DFT

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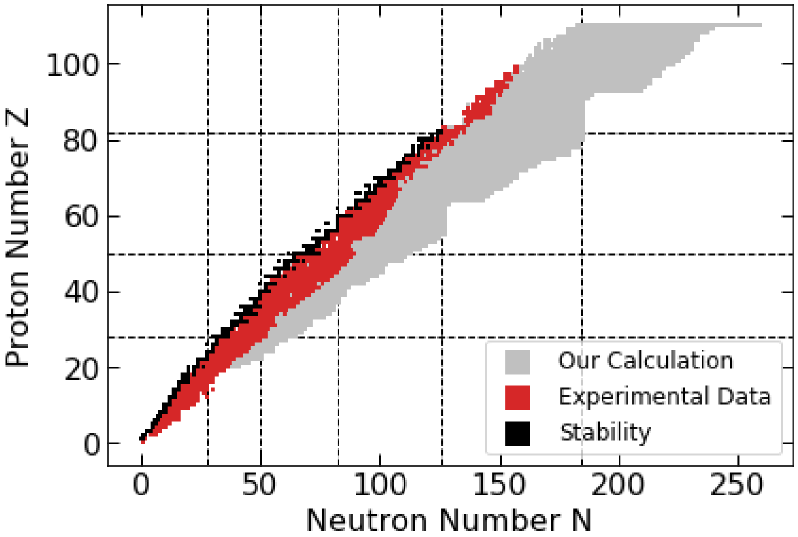
FIRE Collaboration Meeting

July 1, 2020

Beta Decay - What We're Doing

- **Beta decay for *r*-process simulations**
  - Many nuclei still beyond experimental reach
- **Density functional theory**
  - Self-consistent HFB + QRPA
  - Skyrme functionals
  - Axial deformations
- **Odd nuclei**
  - Break **time-reversal symmetry**.
  - Computationally expensive
  - Time-odd EDFs harder to constrain



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  - Break **time-reversal symmetry**.
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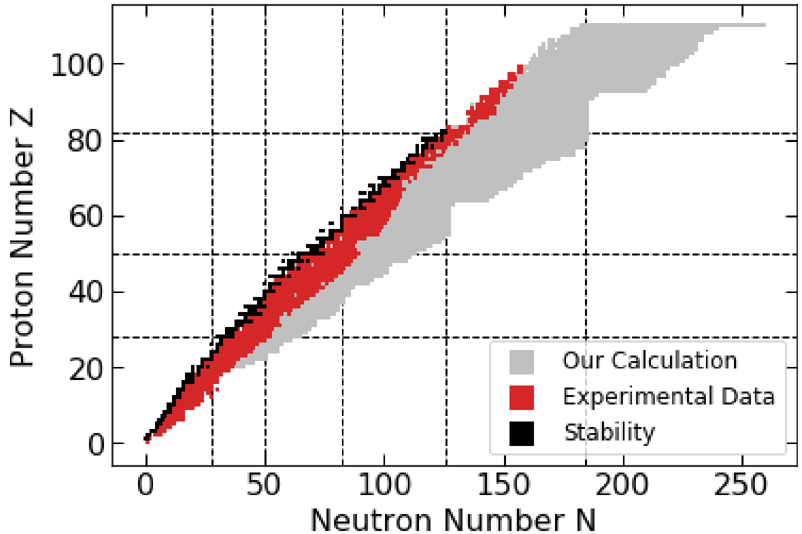
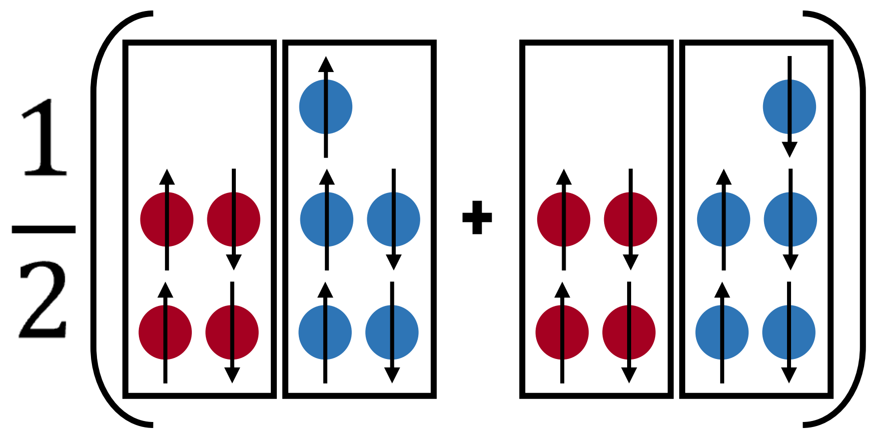
- **Equal filling approximation (EFA)**
  - Interpreted as a **statistical theory**
  - Impose equal occupations for odd state and time-reversed odd state
  - Use statistical QRPA to treat EFA ensemble self-consistently

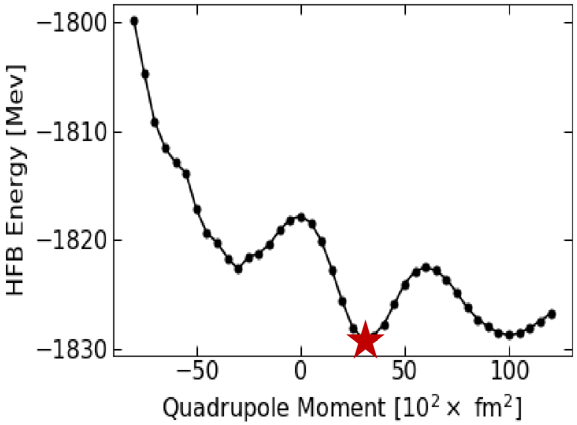




Beta Decay - How We're Doing It

Python Code: PyNFAM

Fortran Code: HFBTHO



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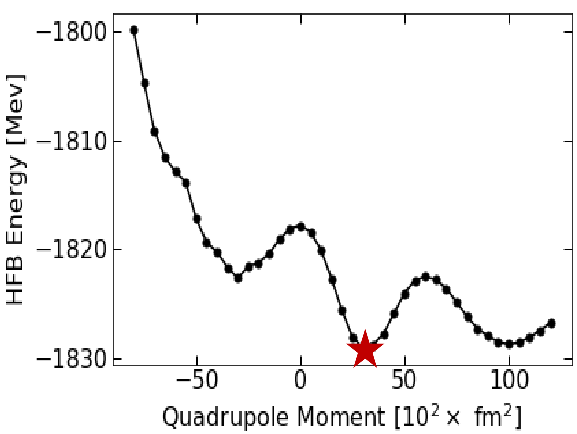

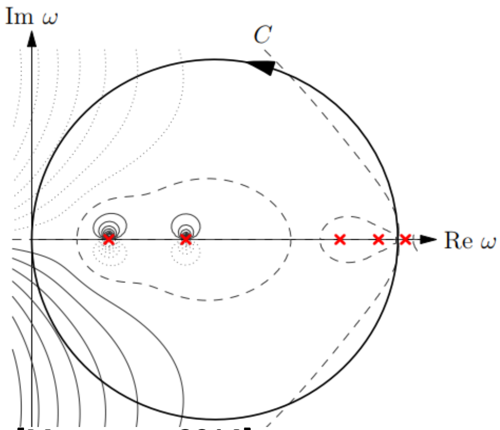

[Mustonen, 2014]

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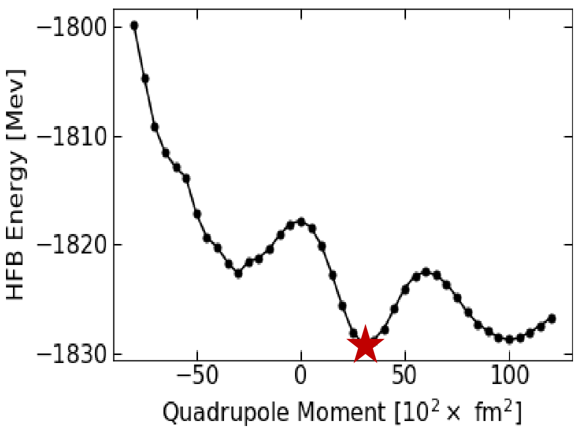

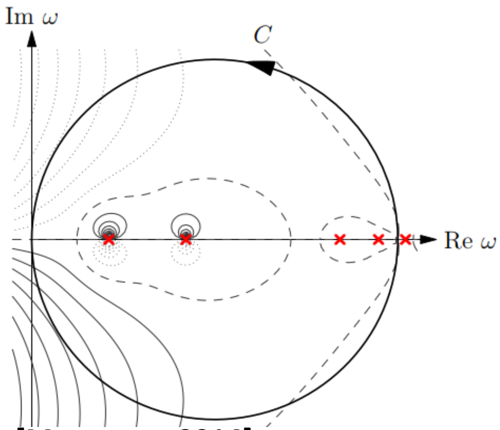

[Mustonen, 2014]

$$\lambda = \frac{\ln 2}{\kappa} \sum_f \left|\langle \mathrm{f\ e\ } \bar{\nu}_{\mathrm{e}} | \hat{\mathrm{H}}_\beta | \mathrm{i} \rangle\right|^2 \mathrm{f}(\mathrm{E_f})$$

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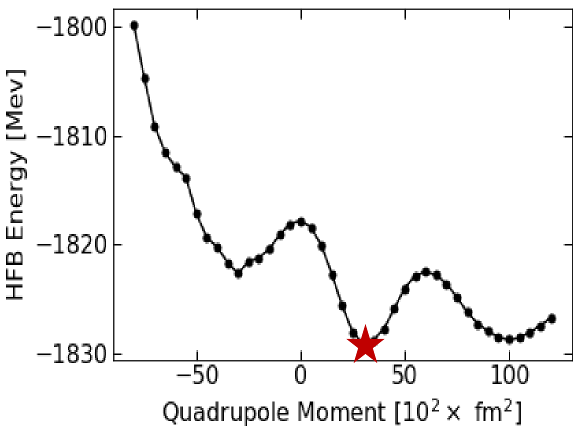

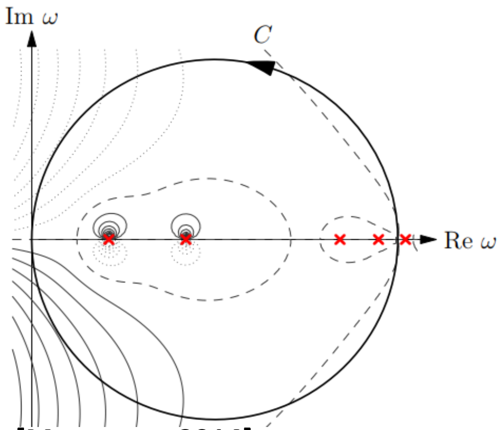

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BLAS accelerated construction of perturbed Hamiltonian
10x speed up per point [Li, Chen - MSU]

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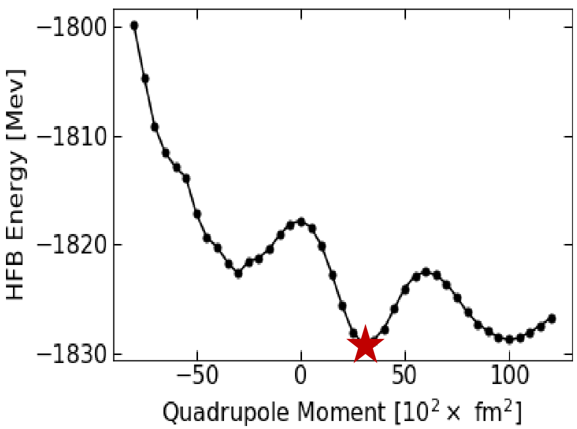

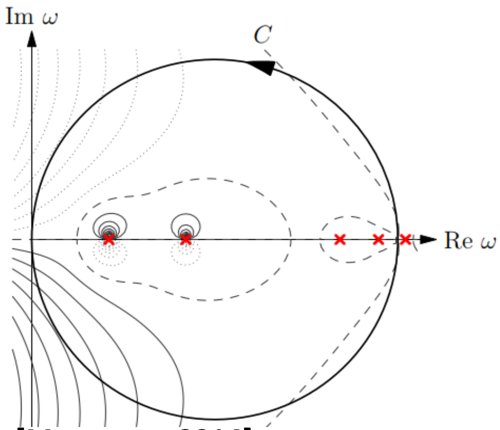

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10x speed up per point [Li, Chen - MSU]

Improved load balancing for multiple calculations

The Future of PyNFAM

Python Code: PyNFAM

Fortran Code: HFBTHO

Fortran Code: PNFAM

PyNFAM Post-Processing

The Future of PyNFAM

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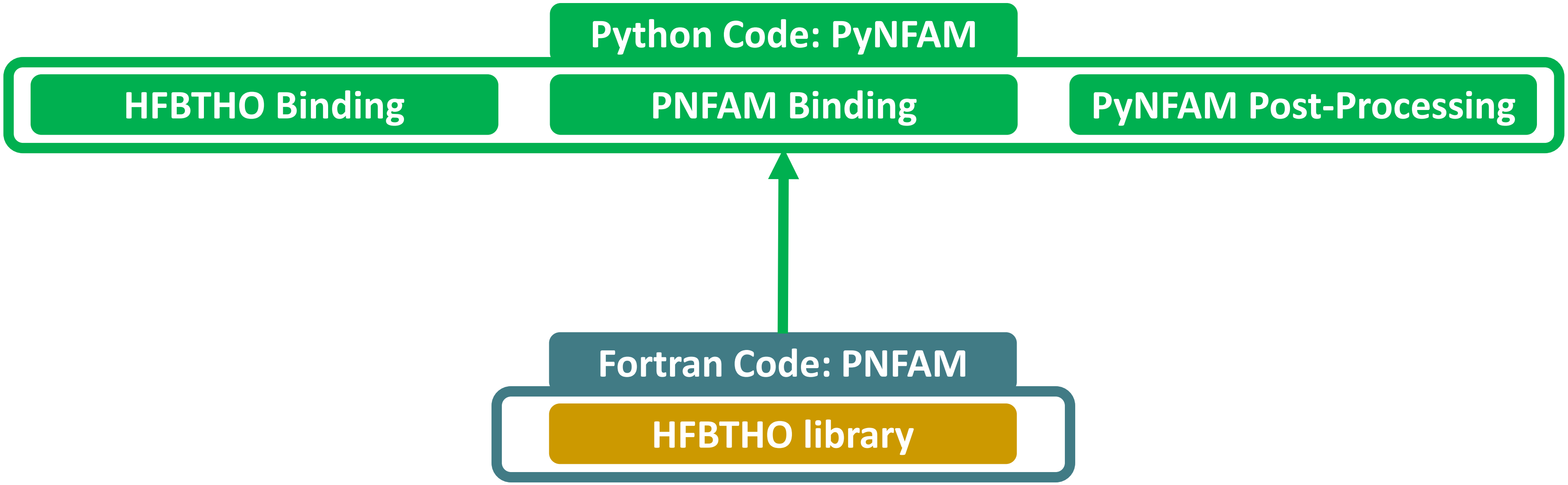
HFBTHO library

The Future of PyNFAM



Equal Filling Approximation Challenges

– Strength function contains **positive beta-minus** contributions as well as **negative beta-plus**.

QRPA Strength Function

$$\frac{dB}{d\omega} = -\frac{1}{\pi}\mathrm{Im}\left[-\sum_{\nu} \frac{|\langle \nu | \hat{\mathbf{F}} | 0 \rangle|^2}{E_\nu - \omega} + \frac{|\langle \nu | \hat{\mathbf{F}}^\dagger | 0 \rangle|^2}{E_\nu + \omega} \right]$$

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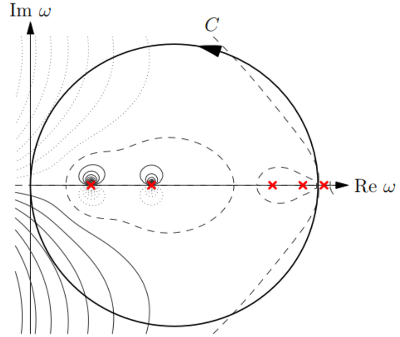

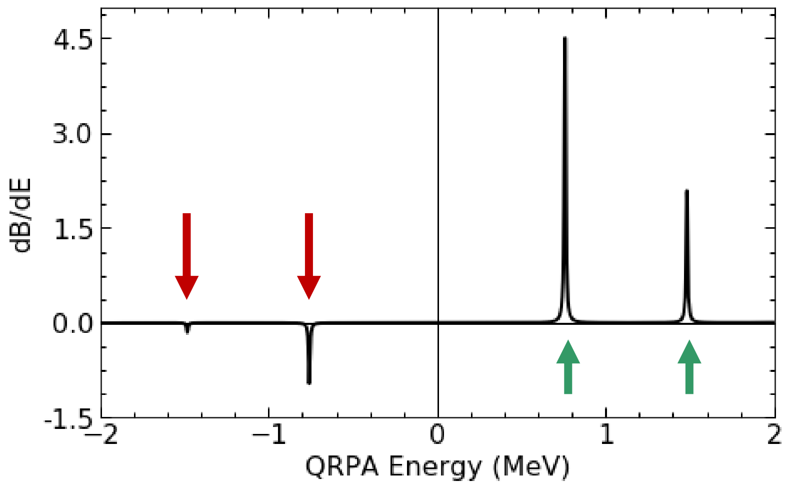

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– EFA can yield positive strength at negative energy (stable transitions to lower energy states)

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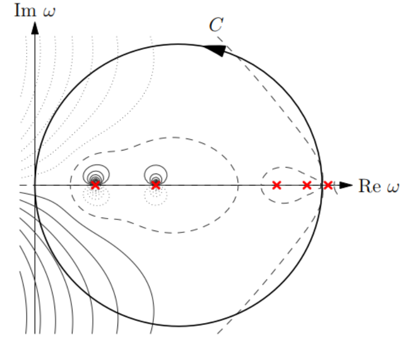

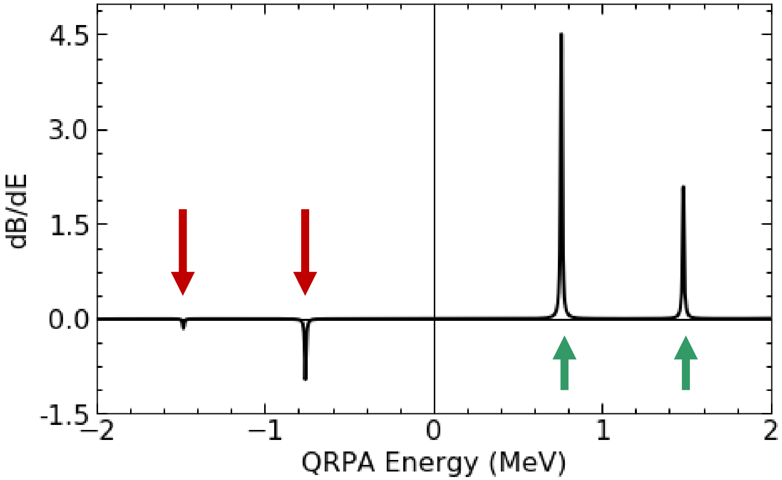

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- Positive strength at negative energy implies negative strength at positive energy

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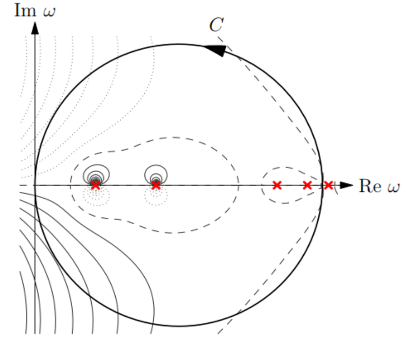

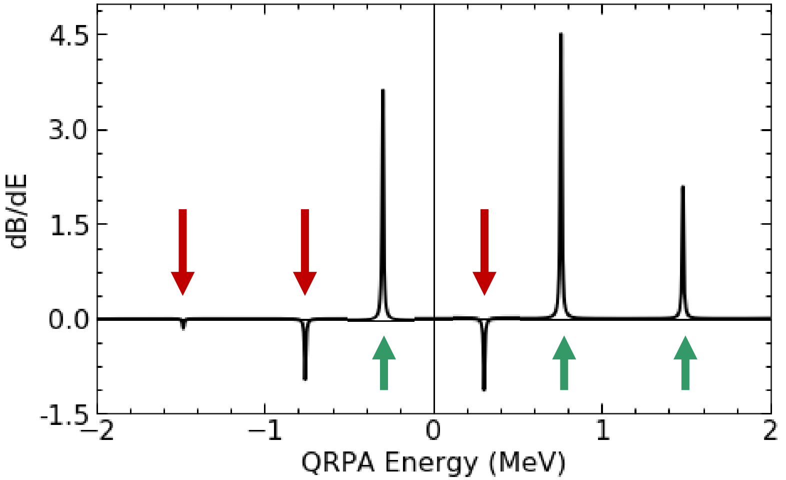

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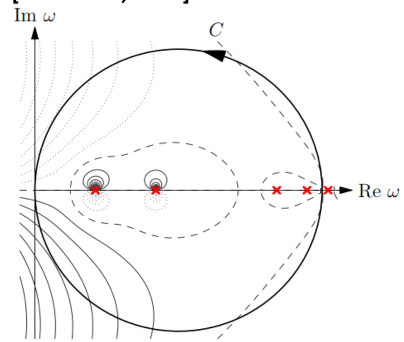

– EFA can yield positive strength at negative energy (stable transitions to lower energy states)

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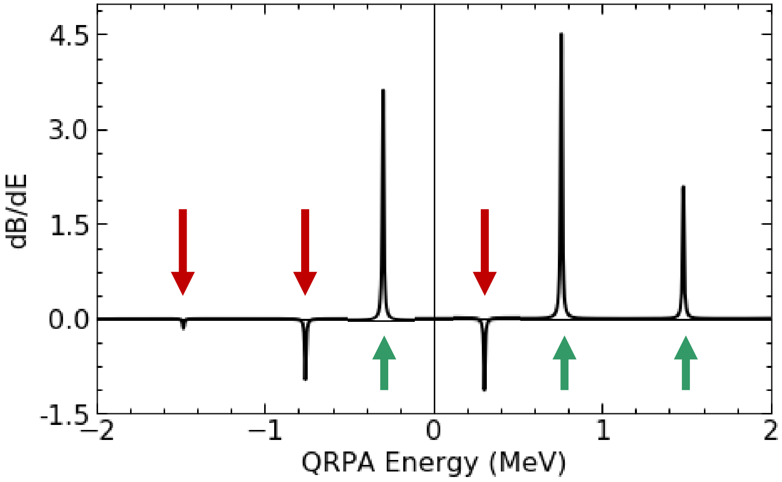
– Contour integration method is error prone

– These errors will **decrease rates/increase half-lives**

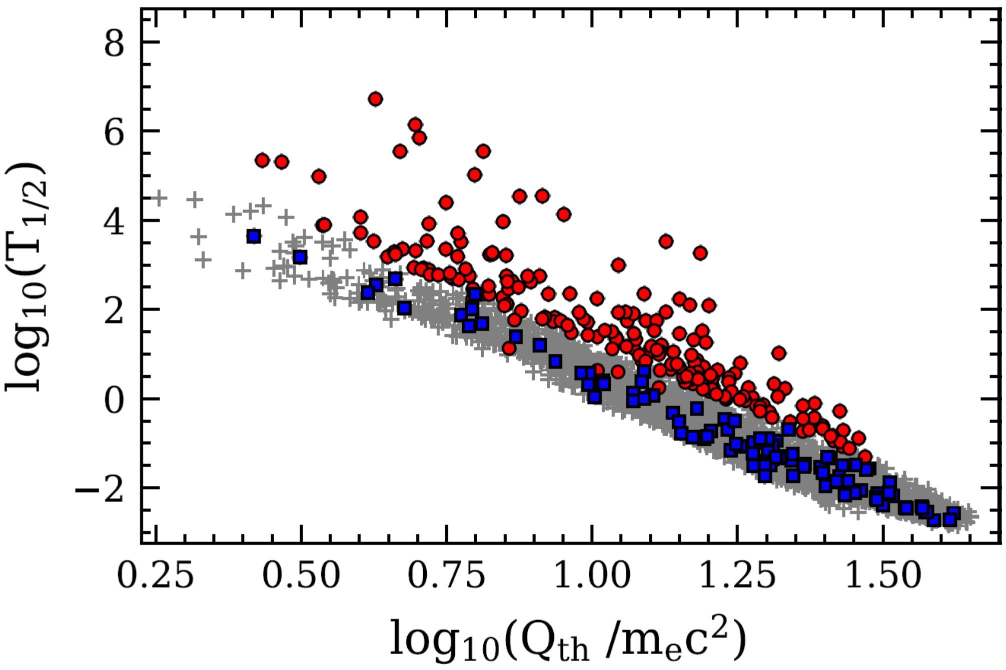


Equal Filling Approximation Corrections

Computing strength near the real axis is expensive!

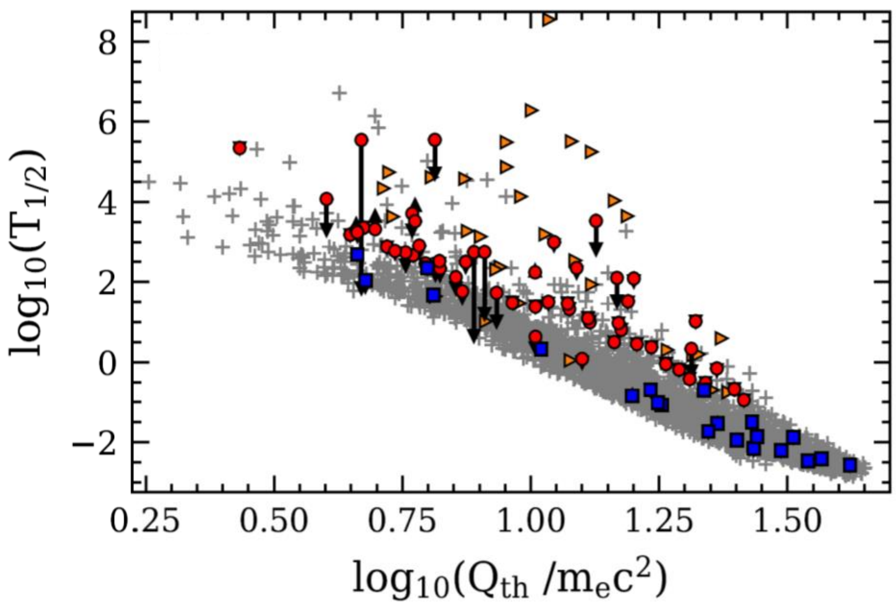
Feasible approach:

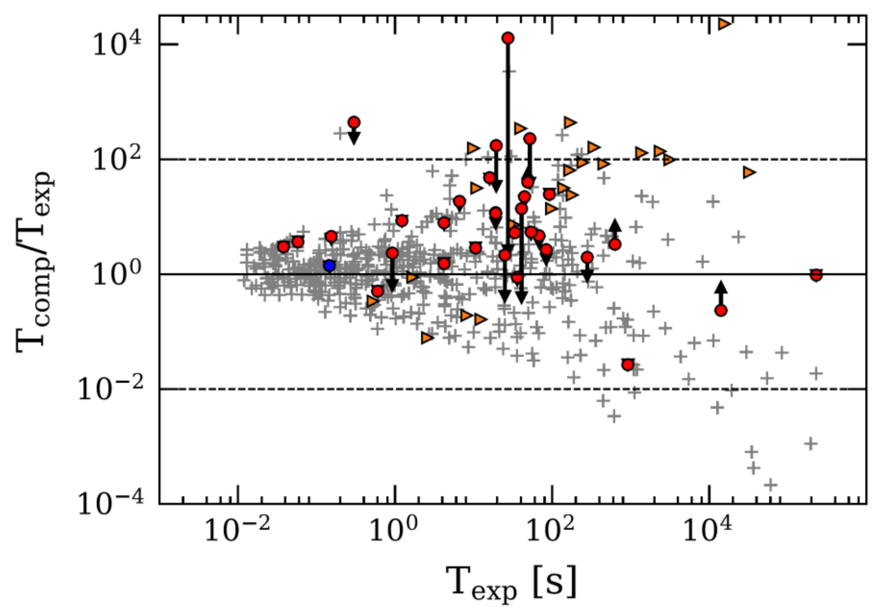
1. Estimate transitions without QRPA residual interaction
2. Conduct contour calculation
3. Compute strength near the real axis for a subset of nuclei
4. Estimate errors



Equal Filling Approximation Corrections

- More than half of examined lifetimes were already correct
- Only a few lifetimes change significantly once corrected
- Remaining corrections likely very small

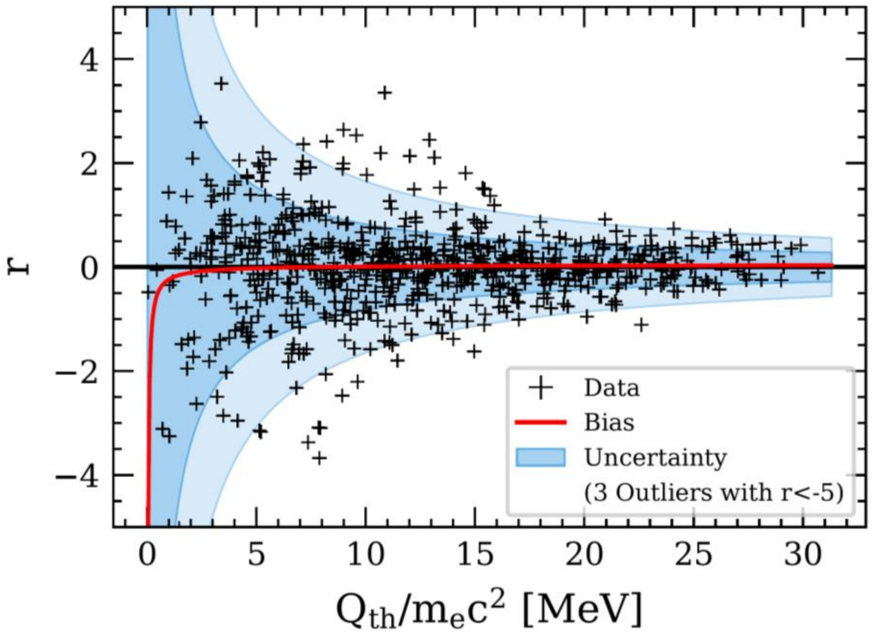


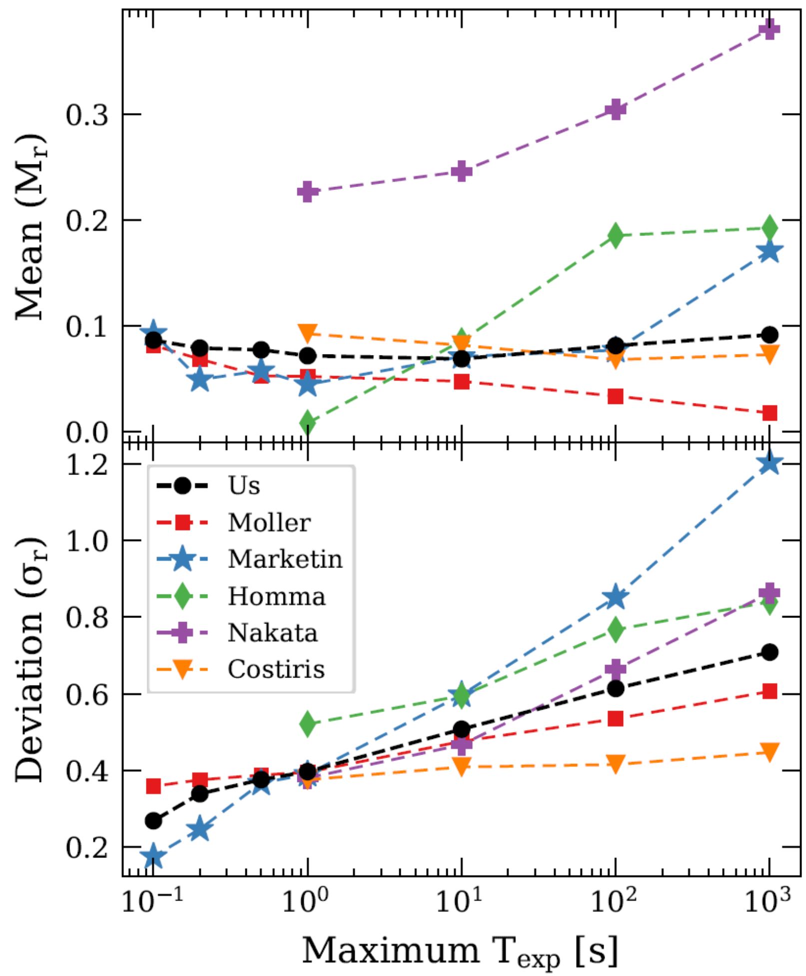


Results and Comparisons

$$r_i = \log_{10}\left(\frac{t_{\mathrm{th}}}{t_{\mathrm{exp}}}\right)$$

$$r_i(q^{\mathrm{th}}_{\mathrm{g.s.}}) = b_c + f^P_r(q^{\mathrm{th}}_{\mathrm{g.s.}})b_q + \mathcal{N}(0, \sigma_r)$$

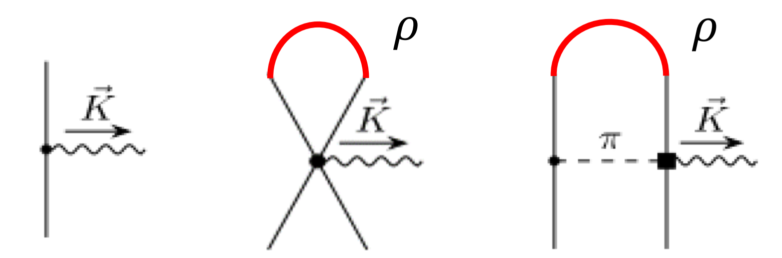




Improving the Description of Beta Decay

- **QRPA response to two-body currents with pnFAM**
  - Two-body currents responsible for a large portion of quenching of axial vector coupling
  - Compute two-body matrix elements for axial current in HO basis
  - Use pnFAM to compute response to effective one-body operator
  - How much will a more detailed account of the nuclear density affect results? Pairing? Deformation?

2BC effective one-body operator



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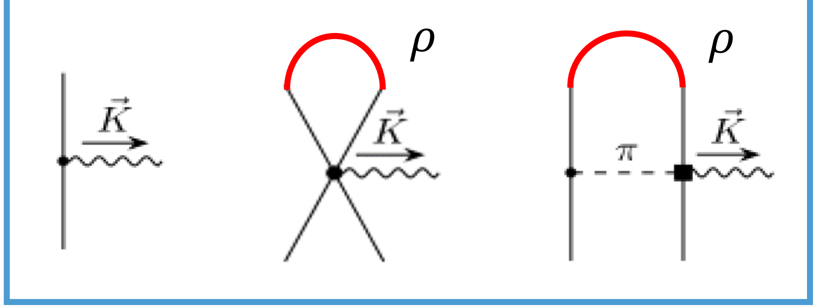
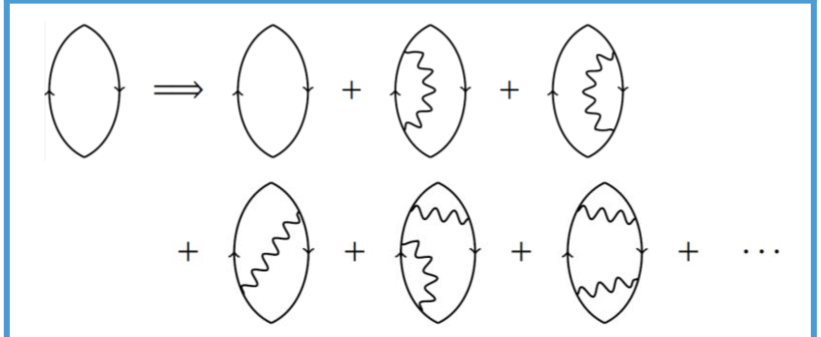
  - How much will a more detailed account of the nuclear density affect results? Pairing? Deformation?
- **Developing a FAM for beyond QRPA**
  - Multi-phonon physics can improve the ability to capture low-lying strength
  - An extension of the FAM will open the door for feasible global calculations that include correlations beyond QRPA

2BC effective one-body operator



P-H propagator with phonon exchange



THANK YOU!

<u>Special thanks to collaborators</u>

Jonathan Engel

Nicolas Schunck

Tong Li

Mengzhi Chen