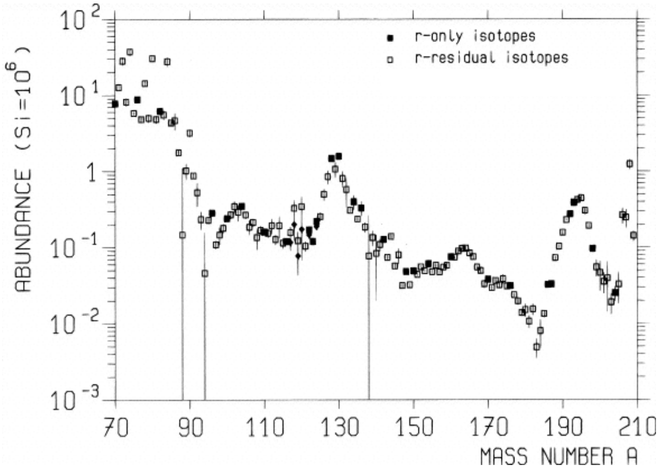
Developments in DFT for Weak Decay/Capture

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, …

May 24, 2023

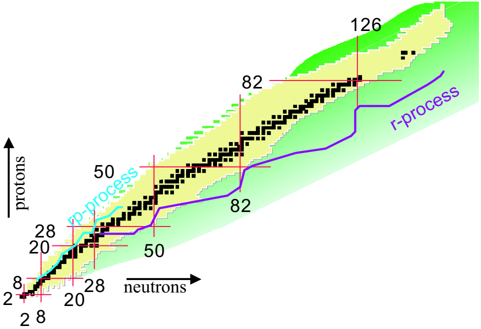
R-Process Abundances



Nuclear Landscape

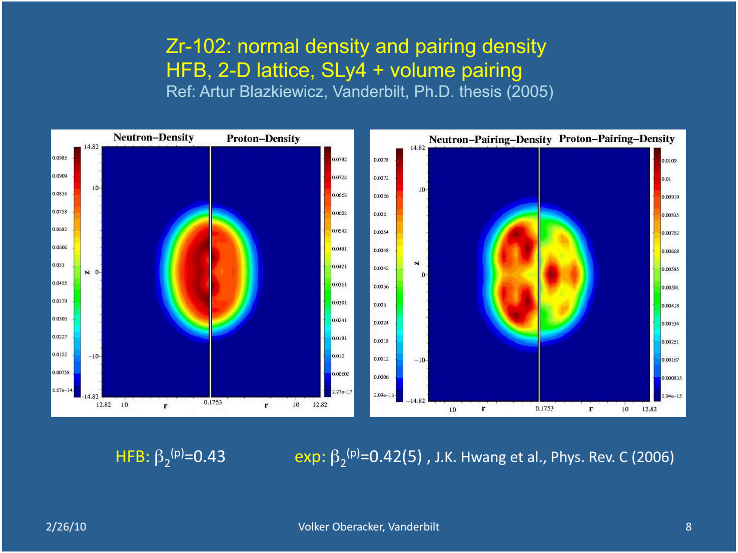
To convincingly locate the site(s) of the *r* process, we need to know reaction rates, particularly β-decay rates, in neutron-rich nuclei.

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



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

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

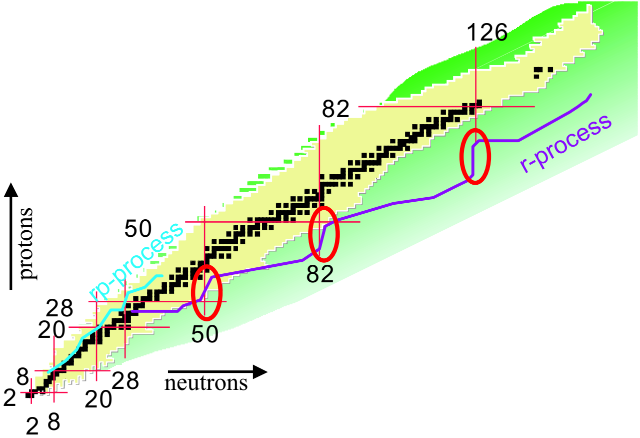


QRPA

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.

Initial Skyrme Application: Spherical QRPA

Even Isotopes Only

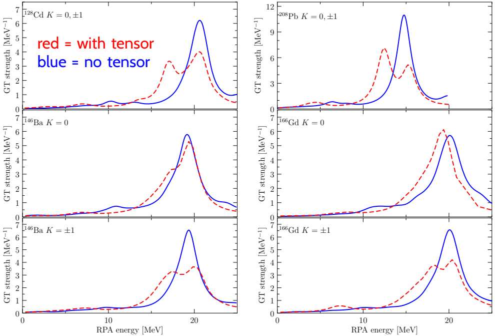


Closed shell nuclei are spherical.

Later: Fast Skyrme QRPA in Deformed Nuclei

Finite-Amplitude Method (FAM) — Nakatsukasa et al.

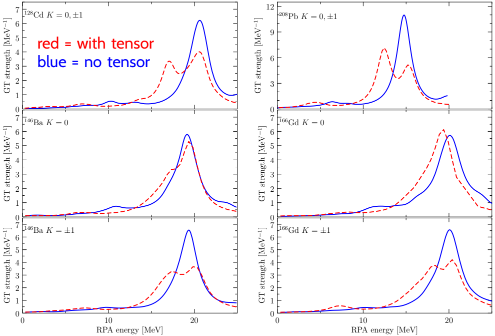
Strength functions computed directly from linear response, in orders of magnitude less time than with matrix QRPA.



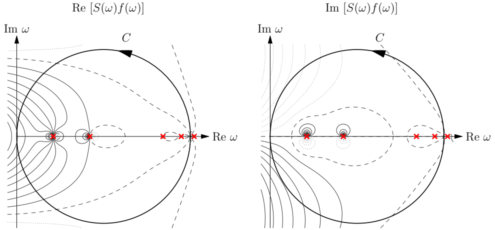
Later: Fast Skyrme QRPA in Deformed Nuclei

Finite-Amplitude Method (FAM) — Nakatsukasa et al.

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.



Global Skyrme Fit for Even Nuclei

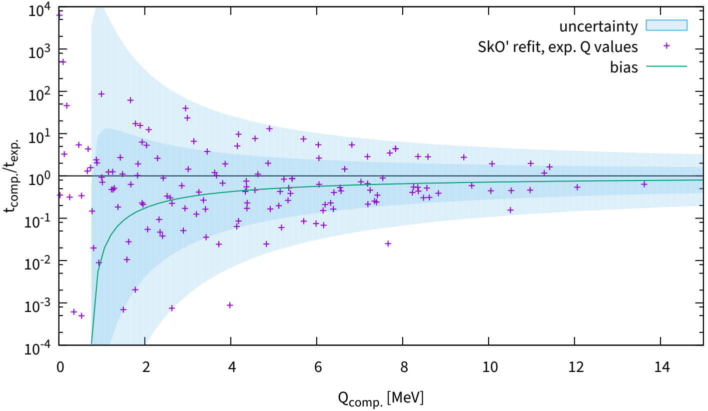
Mika Mustonen

Fit the charge-changing time-odd functional

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

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

Results

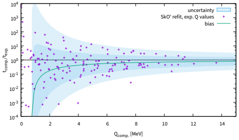


uncertainty
SkO' refit, exp. Q values
bias
$t_{comp.}/t_{exp.}$
$Q_{comp.}$ [MeV]
10^4
10^3
10^2
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
0
2
4
6
8
10
12
14

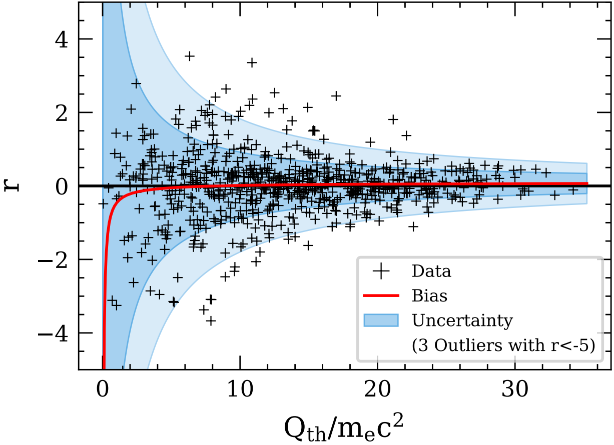
Results with All Nuclei

Evan Ney

Figured out how to adapt FAM to treat odd-A and odd-odd nuclei.

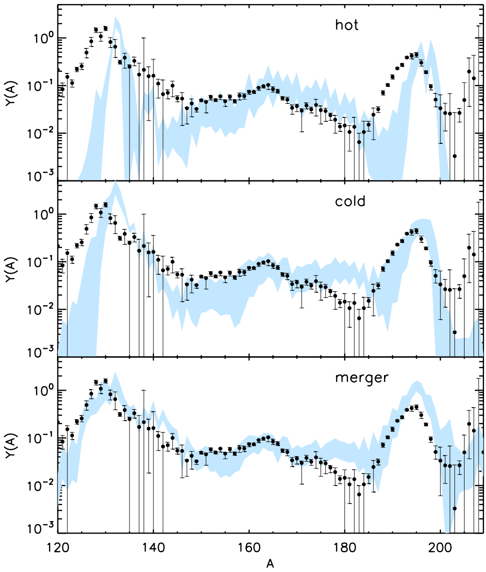


Even-even results



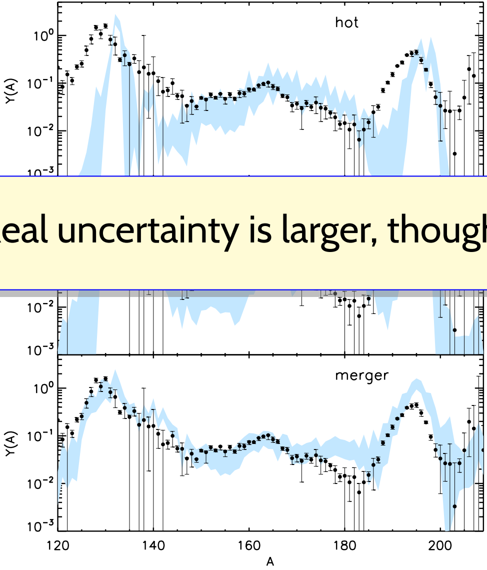
What's at Stake Here?

Significance of Factor-of-Two Uncertainty



What's at Stake Here?

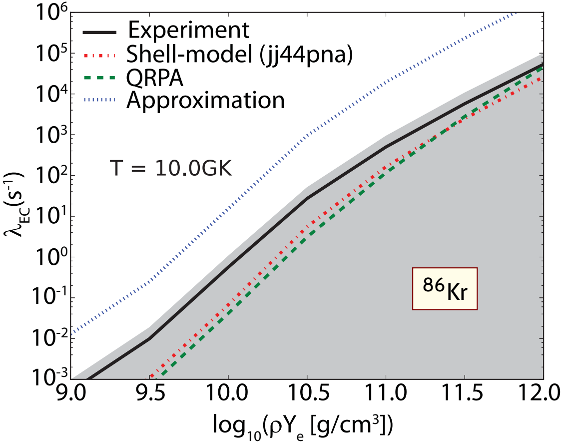
Significance of Factor-of-Two Uncertainty



Real uncertainty is larger, though.

Electron Capture

Evan Ney



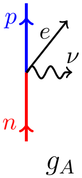
For terrestrial or astrophysical environments.

Developed a non-zero-temperature FAM.

Most Recently: Two-Body Current

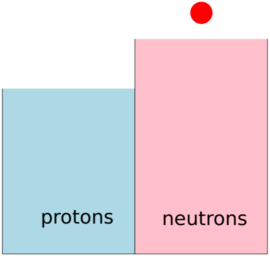
Evan Ney

Leading order:



Usual β-decay current

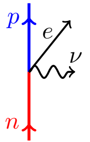
Consider very simple wave function



Most Recently: Two-Body Current

Evan Ney

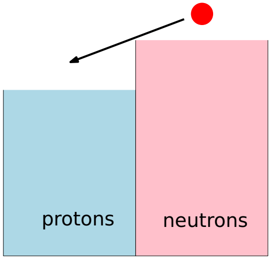
Leading order:



g_A

Usual β-decay current

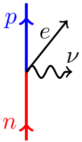
Consider very simple wave function



Most Recently: Two-Body Current

Evan Ney

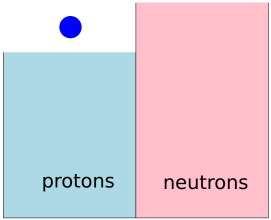
Leading order:



g_A

Usual β-decay current

Consider very simple wave function

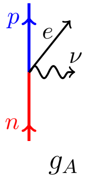


Most Recently: Two-Body Current

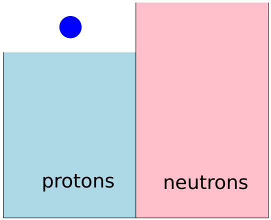
Evan Ney

Consider very simple wave function

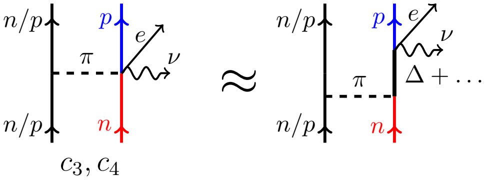
Leading order:

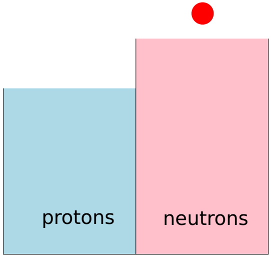


Usual β-decay current



Higher order:



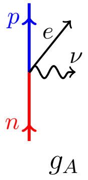


There are also contact terms…

Most Recently: Two-Body Current

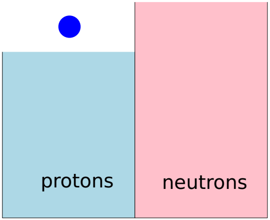
Evan Ney

Leading order:

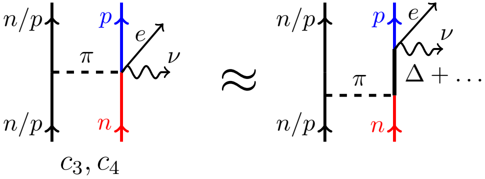


Usual β-decay current

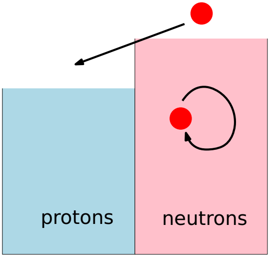
Consider very simple wave function



Higher order:



There are also contact terms…

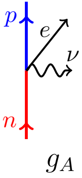


Most Recently: Two-Body Current

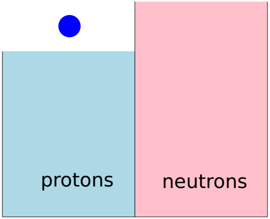
Evan Ney

Consider very simple wave function

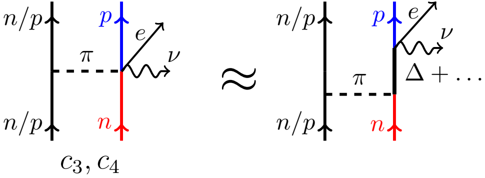
Leading order:



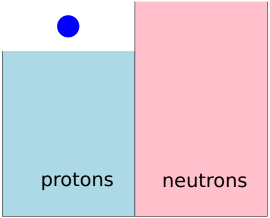
Usual β-decay current



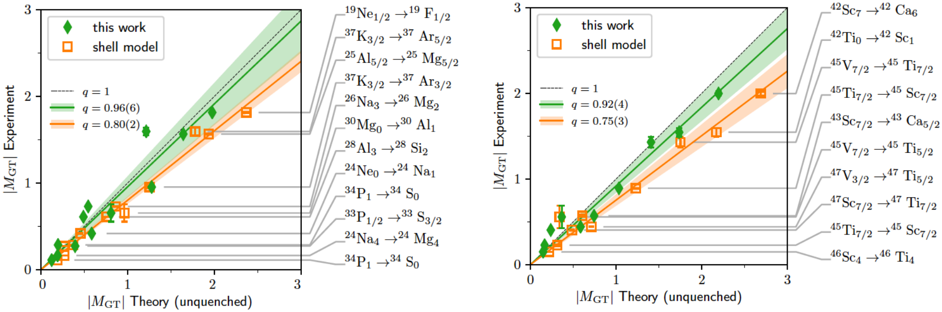
Higher order:



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.

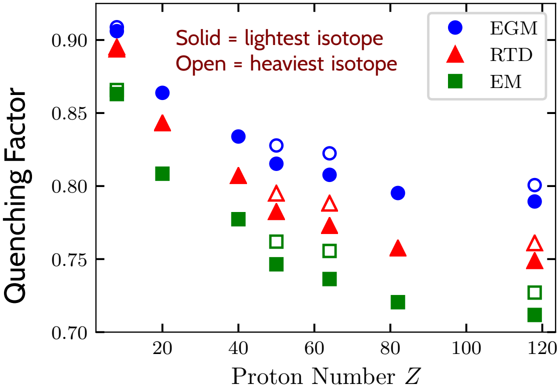
But a lot comes from the two-body current.

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 from Currents

Integrated GT Strength

Three sets of chiral parameters, no contact



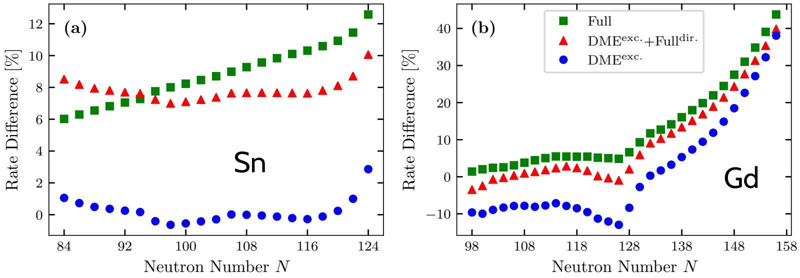
EGM - E. Epelbaum, W. Glöckle, and U.-G. Meißner, Nucl. Phys. A 747, 362 (2005).
RTS - M. C. M. Rentmeester, R. G. E. Timmermans, and J. J. de Swart, Phys. Rev. C 67, 044001 (2003)
EM - D. R. Entem and R. Machleidt, Phys. Rev. C 68, 041001(R) (2003).

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

Effect on β-Decay Rates

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

Focus on green squares

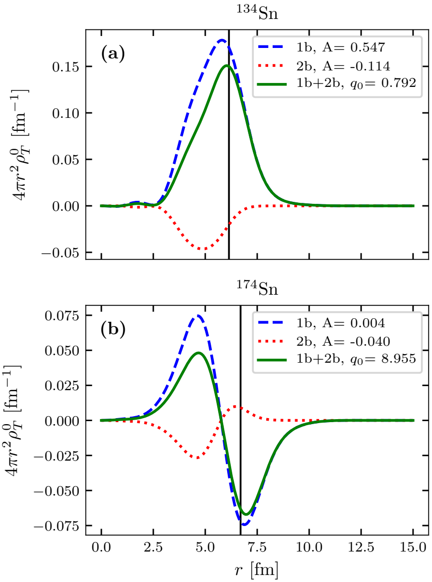


Two-body current has larger effect in neutron-rich nuclei. Quenching of rates decreases and can even become enhancement near the drip line.

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 ^{134}Sn

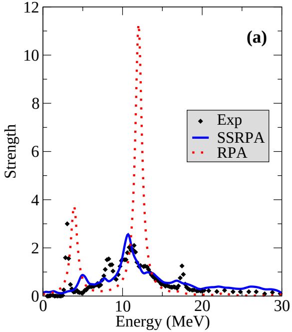
← Unusual (and lowest-lying) transition in ^{174}Sn

Beyond QRPA

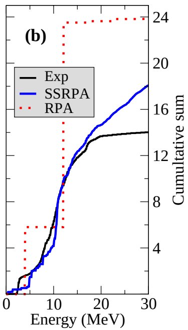
Second RPA with D. Gambacurta and M. Grasso

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

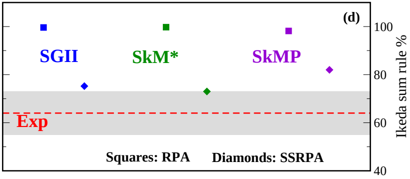
GT strength in ^{48}Ca



Summed strength

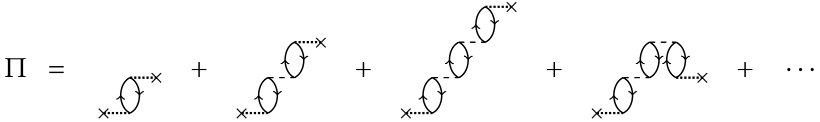


Percentage of Ikeda sum below 30 MeV



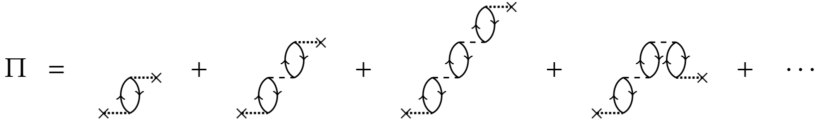
Simpler Version: QRPA + Quasiparticle-Vibration Coupling

RPA response function

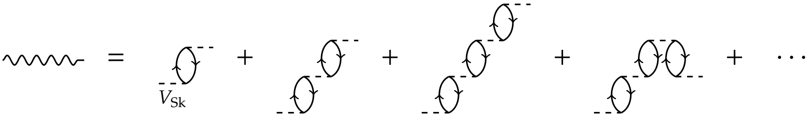


Simpler Version: QRPA + Quasiparticle-Vibration Coupling

RPA response function

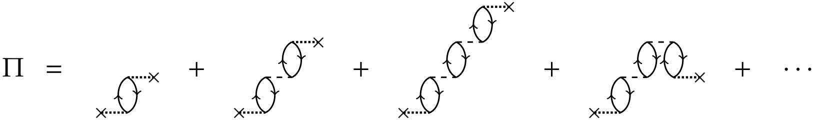


Phonon-exchange potential

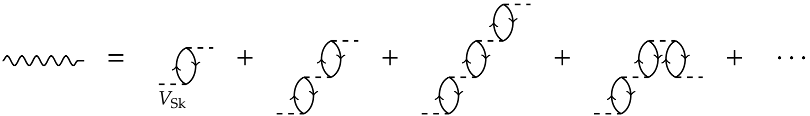


Simpler Version: QRPA + Quasiparticle-Vibration Coupling

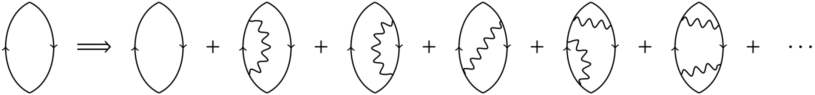
RPA response function



Phonon-exchange potential

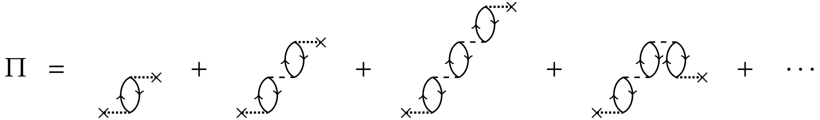


Modification of particle-hole bubble by QVC



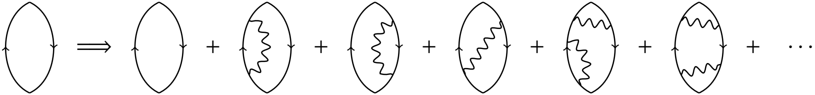
Simpler Version: QRPA + Quasiparticle-Vibration Coupling

RPA response function



Has been applied in spherical nuclei, but never deformed ones. We figured out how to build it into the FAM.

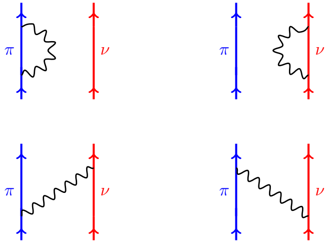
Modification of particle-hole bubble by QVC



QVC Results

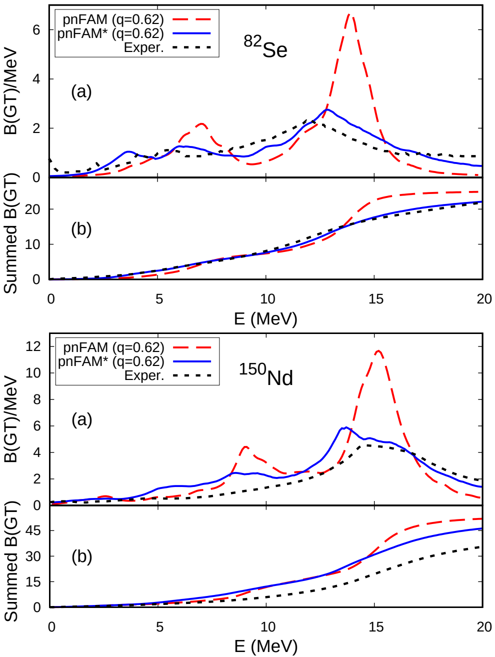
Called pnFAM* Here

Phonon-exchange diagrams: phonons are like-particle excitations



With Q. Liu

GT Distributions ($g_A = 1$)



Next

All these developments will require refitting of the time-odd functional (and constants in the current) and UQ. There's still a lot to do on the road to more realistic DFT-based β-decay rates!

Whatever one can measure far from stability related to β decay,

- GT distributions
- charge-changing dipole and spin-dipole distributions
- β-decay half lives
- $\vdots$

will be helpful.

Next

All these developments will require refitting of the time-odd functional (and constants in the current) and UQ. There's still a lot to do on the road to more realistic DFT-based β-decay rates!

Whatever one can measure far from stability related to β decay,

- GT distributions
- charge-changing dipole and spin-dipole distributions
- β-decay half lives
- ⋮

will be helpful.

Thanks for Listening