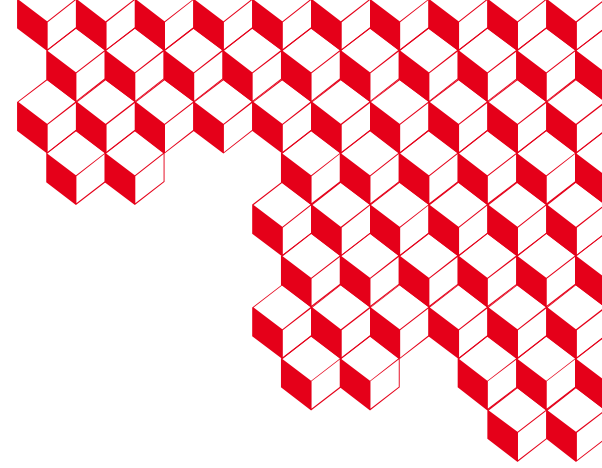




pnQRPA-FAM implementation for allowed beta-decay transitions using a Gogny interaction

Fast iterative pnQRPA calculations for beta-decay and beyond

Structure

- 1. Introduction**
- 2. Nuclear Models and Interactions**
- 3. pnQRPA-FAM**
- 4. Results**
- 5. Future Plans**



1 ■ Introduction

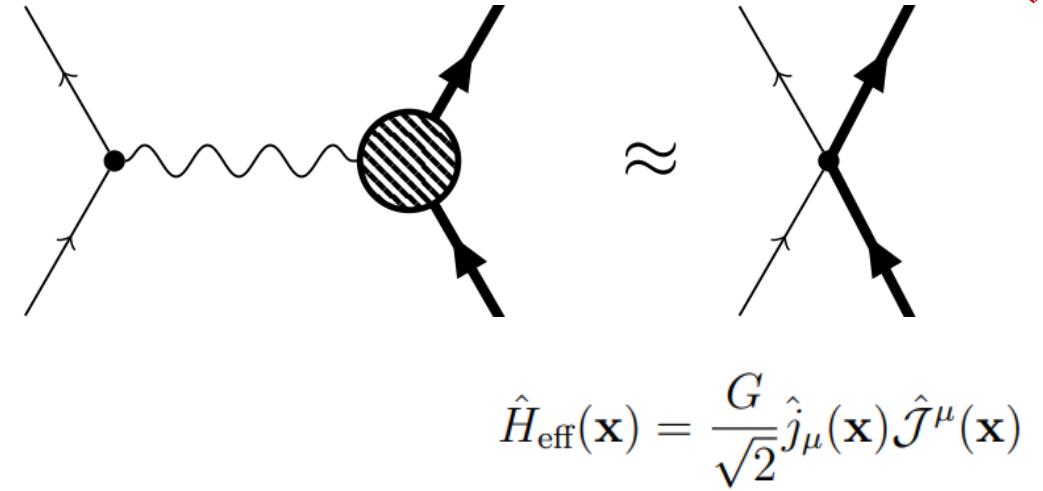
Some background

Nuclear beta decay from a nuclear model perspective

- Nuclear model inputs represent a major source of uncertainty in theoretical half-life calculations
- A variety of models have been developed along the years for the description of nuclei throughout the nuclear chart
- Many interesting nuclei are too short lived for half-life measurements (e.g. r-process nuclei), and theoretical estimates are the only data for their half-lives
- Intrinsic nuclear deformation and different approaches to angular momentum restoration in particular can greatly affect the resulting half-lives

Allowed beta decay

- Treatment of the nuclear beta decay starts from the general semi-leptonic weak interaction Hamiltonian
- At the lowest order (allowed limit) the operators mediating the process reduce to simple Fermi and Gamow-Teller operators



$$\hat{\mathcal{M}}_{JM}(|\mathbf{q}|) = \int d^3\mathbf{x} [j_J(|\mathbf{q}||\mathbf{x}|) Y_{JM}(\Omega_{\mathbf{x}})] \hat{\mathcal{J}}_0(\mathbf{x}),$$

$$\hat{\mathcal{L}}_{JM}(|\mathbf{q}|) = \frac{i}{|\mathbf{q}|} \int d^3\mathbf{x} \{ \nabla [j_J(|\mathbf{q}||\mathbf{x}|) Y_{JM}(\Omega_{\mathbf{x}})] \} \cdot \hat{\mathcal{J}}(\mathbf{x})$$

$$\hat{\mathcal{T}}_{JM}^{\text{el}}(|\mathbf{q}|) = \frac{1}{|\mathbf{q}|} \int d^3\mathbf{x} [\nabla \times j_J(|\mathbf{q}||\mathbf{x}|) \mathbf{Y}_{JJ1}(\Omega_{\mathbf{x}})] \cdot \hat{\mathcal{J}}(\mathbf{x})$$

$$\hat{\mathcal{T}}_{JM}^{\text{mag}}(|\mathbf{q}|) = \int d^3\mathbf{x} [j_J(|\mathbf{q}||\mathbf{x}|) \mathbf{Y}_{JJ1}(\Omega_{\mathbf{x}})] \cdot \hat{\mathcal{J}}(\mathbf{x})$$

Phys. Rep. **50**, 1 (1979)

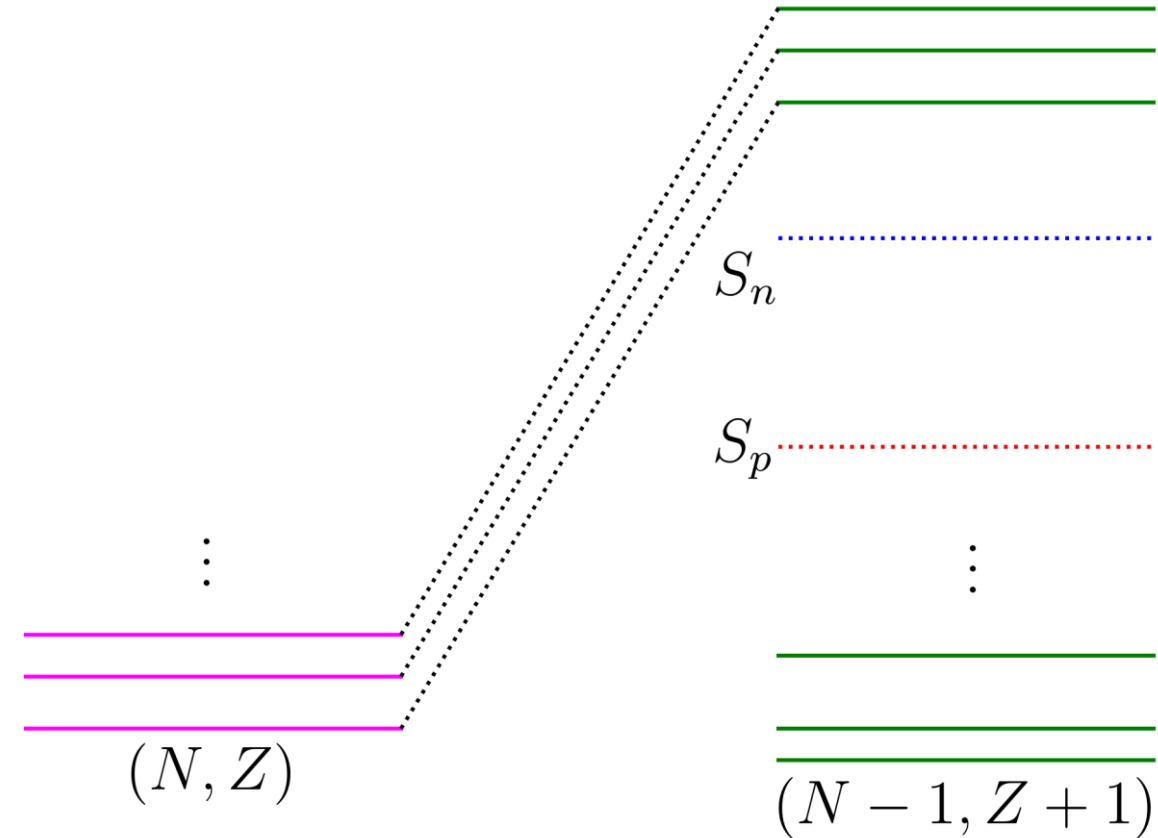
allowed limit
→

$$\hat{\mathcal{M}}_{00} = \frac{F_1}{\sqrt{4\pi}} \sum_{j=1}^A \tau_{\pm}(j)$$

$$\hat{\mathcal{L}}_{1M} = \frac{1}{\sqrt{2}} \hat{\mathcal{T}}_{1M}^{\text{el}} = \frac{iF_A}{\sqrt{12\pi}} \sum_{j=1}^A \tau_{\pm}(j) \sigma_{1M}(j)$$

Isobaric analogue states

- Fermi transitions can proceed from an initial mother nucleus state into a state of the daughter nucleus with analogous structure, but higher energy
- This isobaric analogue state (IAS) exhausts the vast majority of the transition sum rule
- IASes are formally simple to model, and provide a natural way to benchmark new methods and numerical codes



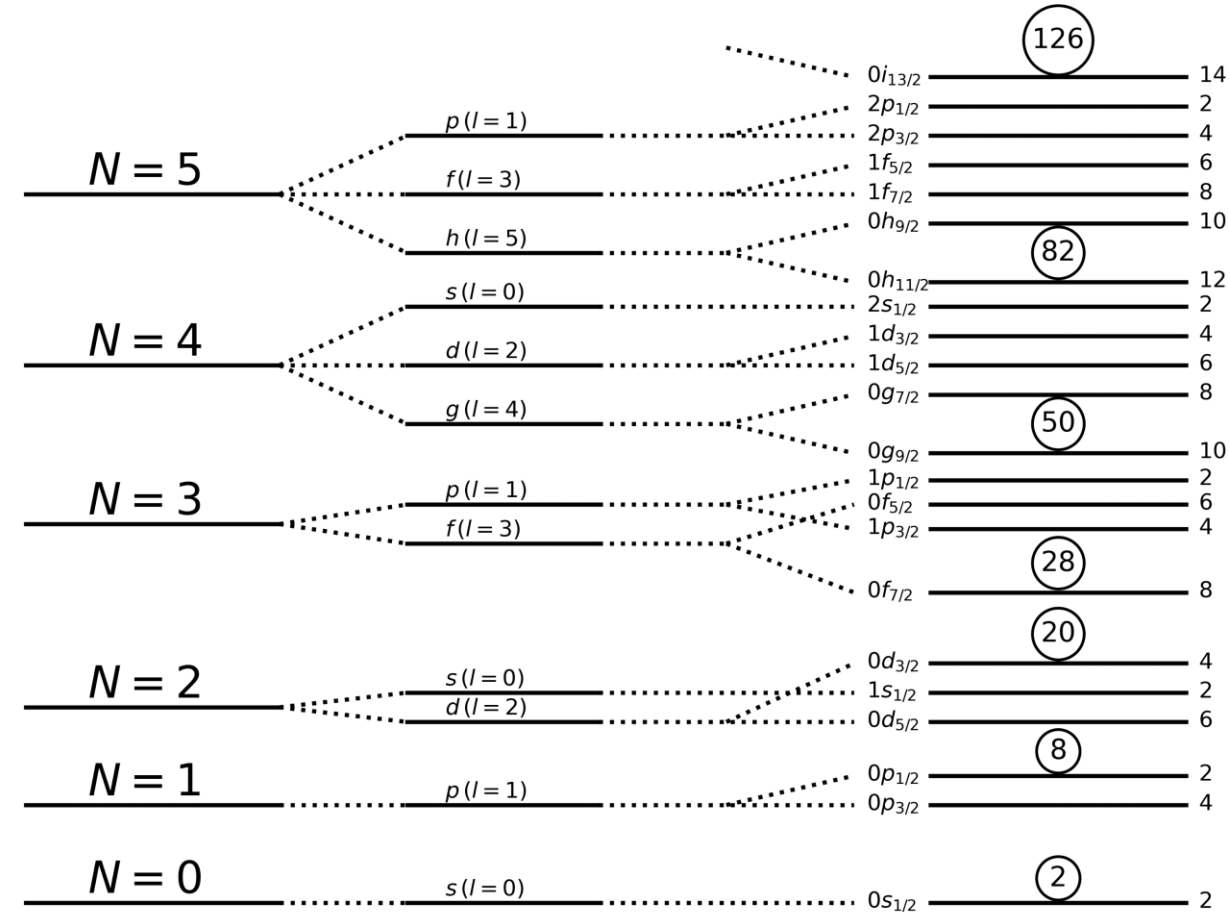


2 ■ Nuclear Models and Interactions

Motivations and justifications

The nuclear shell model

- Shell-model states are described in terms of configurations composed of protons and neutrons occupying specific orbitals
- Highly accurate for low-lying states in nearly magic nuclei
- Easy to interpret intuitively, when a state is composed of nearly entirely of a single configuration
- Very limited in number of shells, computational cost grows fast
- Completely incapable of describing many high-lying collective states, which can be important for beta decay



pnQRPA, and why it's so good

- Describes states as phonons built on top of a correlated ground state (or an effective vacuum)
- Treats single-particle and collective excitations on an equal footing
- Particularly suited for describing collective high-lying excitations
- Excellent overall description of the nuclear spectrum from low to high energies

pnQRPA, and why it's so bad

- Low-energy end of the spectra typically inferior to shell model results
- Computational cost for a large number of shells in the basis is massive without some truncations and cutoffs
- Some less consequential or “outside the scope of this talk” problems (presence of spurious modes, non-conservation of particle number, single-phonon configurations are not sufficient in describing states with a multiphonon character, not founded on a true variational principle, angular momentum restoration in the deformed case, etc.)

pnQRPA, and why it's so bad

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(It is what it is)

(This we can improve)

(Not our concern here)

The Gogny D1S EDF

- A popular energy density functional in the field of nuclear structure
- Differs from Skyrme EDFs by the inclusion of finite-range terms
- Particularly useful in studies on pairing and deformation
- Skyrme EDFs have been utilized in (pn)QRPA-FAM in the past, we present the first implementation for a Gogny force

$$\hat{V}(\mathbf{r}, \mathbf{R}) = \sum_{j=1}^2 e^{-\mathbf{r}^2/\mu_j^2} (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau) + t_3 (1 + x_0 P_\sigma) \delta(\mathbf{r}) \rho^\alpha(\mathbf{R}) \\ + iW_{LS} \delta(\mathbf{r}) \overleftarrow{\nabla}_{12} \times \overrightarrow{\nabla}_{12} \cdot (\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2) + e^2 (1 + 2\hat{\tau}_{1z}) (1 + 2\hat{\tau}_{2z}) |\mathbf{r}|^{-1}$$



3 ■ **pnQRPA-FAM**

pnQRPA, but fast

pnQRPA formalism

- Excited daughter nucleus states in pnQRPA are modelled as phonons built on top of a correlated mother nucleus ground state
- Phonons are built from quasiparticle creation and annihilation operators
- For the underlying quasiparticle vacuum (and effective pnQRPA vacuum), we are using the Hartree-Fock-Bogoliubov state
- HFB quasiparticle operators are obtained in the usual manner from single-particle operators via the generalized Bogoliubov transform
- The matrices U and V are obtained by solving the HFB equation

$$\mathcal{H}_{\text{s.p.}} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}, \quad \mathcal{H}_{\text{s.p.}} \equiv \begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h^* + \lambda \end{pmatrix}$$

$$|A_\omega\rangle \equiv Q_\omega^\dagger |\text{pnQRPA}\rangle$$

$$Q_\omega^\dagger = \sum_{\pi\nu} (X_{\pi\nu}^\omega \beta_\pi^\dagger \beta_\nu^\dagger - Y_{\pi\nu}^\omega \beta_\pi \beta_\nu)$$

$$|\text{HFB}\rangle = \prod_\mu \beta_\mu |0\rangle$$

$$\begin{cases} \beta_\mu^\dagger = \sum_a (U_{a\mu} c_a^\dagger + V_{a\mu} c_a) \\ \beta_\mu = \sum_a (V_{a\mu}^* c_a^\dagger + U_{a\mu}^* c_a) \end{cases}$$

pnQRPA-FAM introduction

- The pnQRPA equation can be derived by e.g. equations-of-motion method
- This yields the eigenenergies and phonon amplitudes, which can then be used to compute transition strengths

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X^\omega \\ Y^\omega \end{pmatrix} = \Omega_\omega \begin{pmatrix} X^\omega \\ Y^\omega \end{pmatrix} \quad B_\chi(F) = | \langle A_\chi | \hat{F} | \text{pnQRPA} \rangle |^2$$

- Solving the pnQRPA equation is computationally very expensive, both in terms of computational time and memory requirements
- pnQRPA-FAM forgoes the exact solution to the eigenvalue problem, and instead solves directly the transition strength for a chosen energy
- Solution by iterative means using the GMRES (generalized minimal residue) method
- FAM was originally developed for RPA strength calculations [PRC **76**, 024318 (2007)]
- Later expanded to QRPA and pnQRPA [PRC **84**, 014314 (2011)], [PRC **90**, 024308 (2014)]

pnQRPA-FAM formalism

- pnQRPA-FAM is based on a linear response of the system to a weak time-dependent external field mediating the transition of interest
- Here we consider the Fermi operator(s) of allowed beta decay
- Starting point is the time-dependent HFB equation for the generalized density matrix
- The field induces time-dependent perturbations in the H and R matrices
- We get an equation for the perturbations of R in quasiparticle basis

$$\hat{F}(t) = \eta(\hat{F}e^{-i\omega t} + \hat{F}^\dagger e^{i\omega t})$$

$$\hat{F}_- = \sum_{pn} f_{pn} c_p^\dagger c_n, \quad \text{and} \quad \hat{F}_+ = \sum_{pn} f_{np} c_n^\dagger c_p$$

$$i\dot{\mathcal{R}}_{\text{s.p.}}(t) = [\mathcal{H}_{\text{s.p.}}[\mathcal{R}_{\text{s.p.}}(t)] + \mathcal{F}_{\text{s.p.}}(t), \mathcal{R}_{\text{s.p.}}(t)]$$

$$\mathcal{R}_{\text{s.p.}} \equiv \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1 - \rho^* \end{pmatrix} \quad \begin{aligned} \rho_{ij} &= \langle \text{HFB} | c_j^\dagger c_i | \text{HFB} \rangle \\ \kappa_{ij} &= \langle \text{HFB} | c_j c_i | \text{HFB} \rangle \end{aligned}$$

$$\begin{cases} (E_\pi + E_\nu - \omega)X_{\pi\nu}(\hat{F}; \omega) + \delta H_{\pi\nu}^{20}(\hat{F}; \omega) = -F_{\pi\nu}^{20} \\ (E_\pi + E_\nu + \omega)Y_{\pi\nu}(\hat{F}; \omega) + \delta H_{\pi\nu}^{02}(\hat{F}; \omega) = -F_{\pi\nu}^{02} \end{cases}$$

pnQRPA-FAM strength functions

- The pnFAM strength function S can be written in terms of the perturbations X and Y

$$S(\hat{F}; \omega) = \sum_{\pi\nu} \left[F_{\pi\nu}^{20*} X_{\pi\nu}(\hat{F}; \omega) + F_{\pi\nu}^{02*} Y_{\pi\nu}(\hat{F}; \omega) \right]$$

- The S function can be alternatively written as a sum of physical (and unphysical) transition strengths

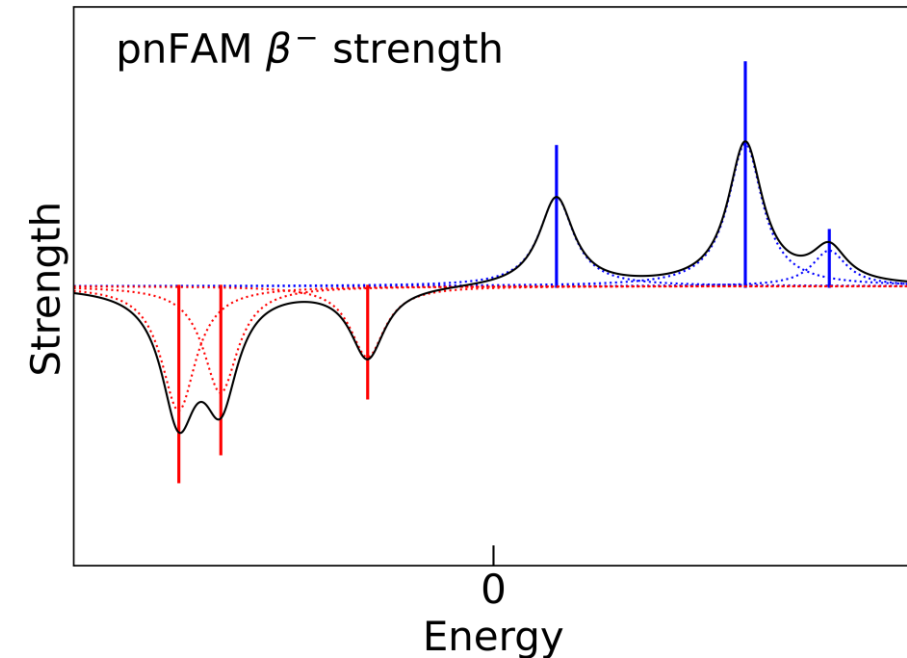
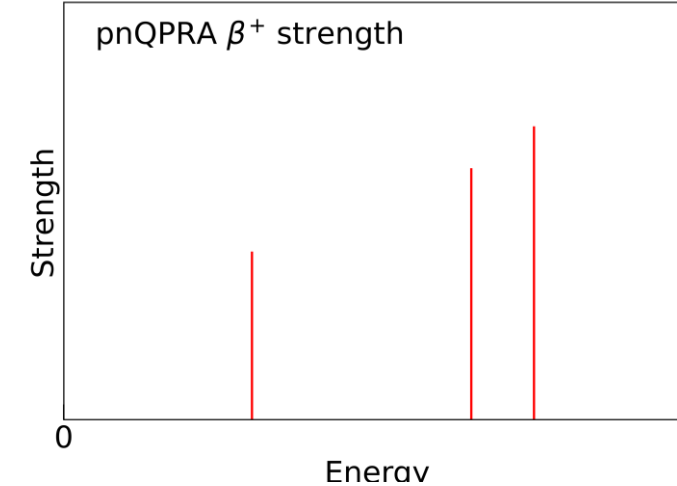
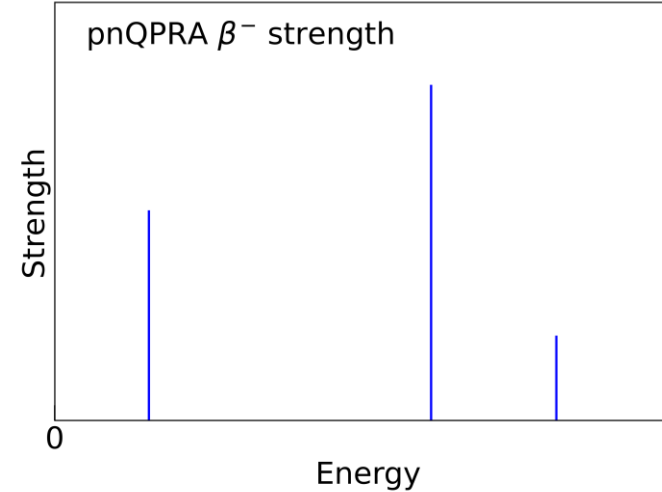
$$\omega = \Omega + i\gamma$$

$$-\frac{1}{\pi} \text{Im } S(F; \omega) = \frac{\gamma}{\pi} \sum_{\chi} \left[\frac{|\langle A_{\chi} | \hat{F} | \text{pnQRPA} \rangle|^2}{(\Omega - \Omega_{\chi})^2 + \gamma^2} - \frac{|\langle A_{\chi} | \hat{F}^{\dagger} | \text{pnQRPA} \rangle|^2}{(\Omega + \Omega_{\chi})^2 + \gamma^2} \right]$$

What does the pnFAM strength represent?

- A pnQRPA-FAM calculation yields the S-function, but no phonons (energies or amplitudes)
- The S-function is the sum of all strength for the given operator smeared by a Lorentzian at a given energy
- **HOWEVER!** It also contains the sum of all strength for the Hermitian conjugate of the operator of interest
- The states contributing to the former are located at their pnQRPA eigenvalues, while the latter at their negative eigenvalues

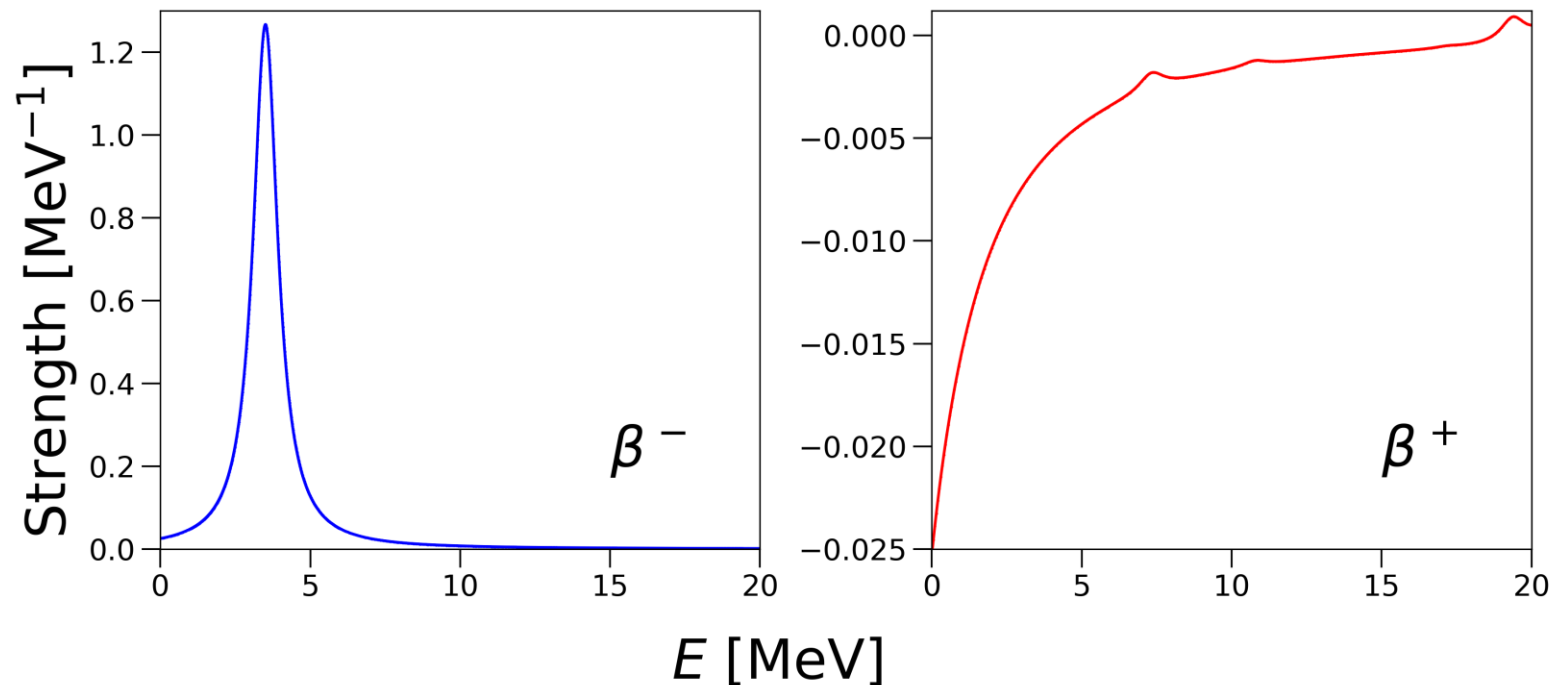
$$\frac{\gamma}{\pi} \sum_{\chi} \left[\frac{|\langle A_{\chi} | \hat{F} | \text{pnQRPA} \rangle|^2}{(\Omega - \Omega_{\chi})^2 + \gamma^2} - \frac{|\langle A_{\chi} | \hat{F}^{\dagger} | \text{pnQRPA} \rangle|^2}{(\Omega + \Omega_{\chi})^2 + \gamma^2} \right]$$



What does this mean for Fermi transitions?

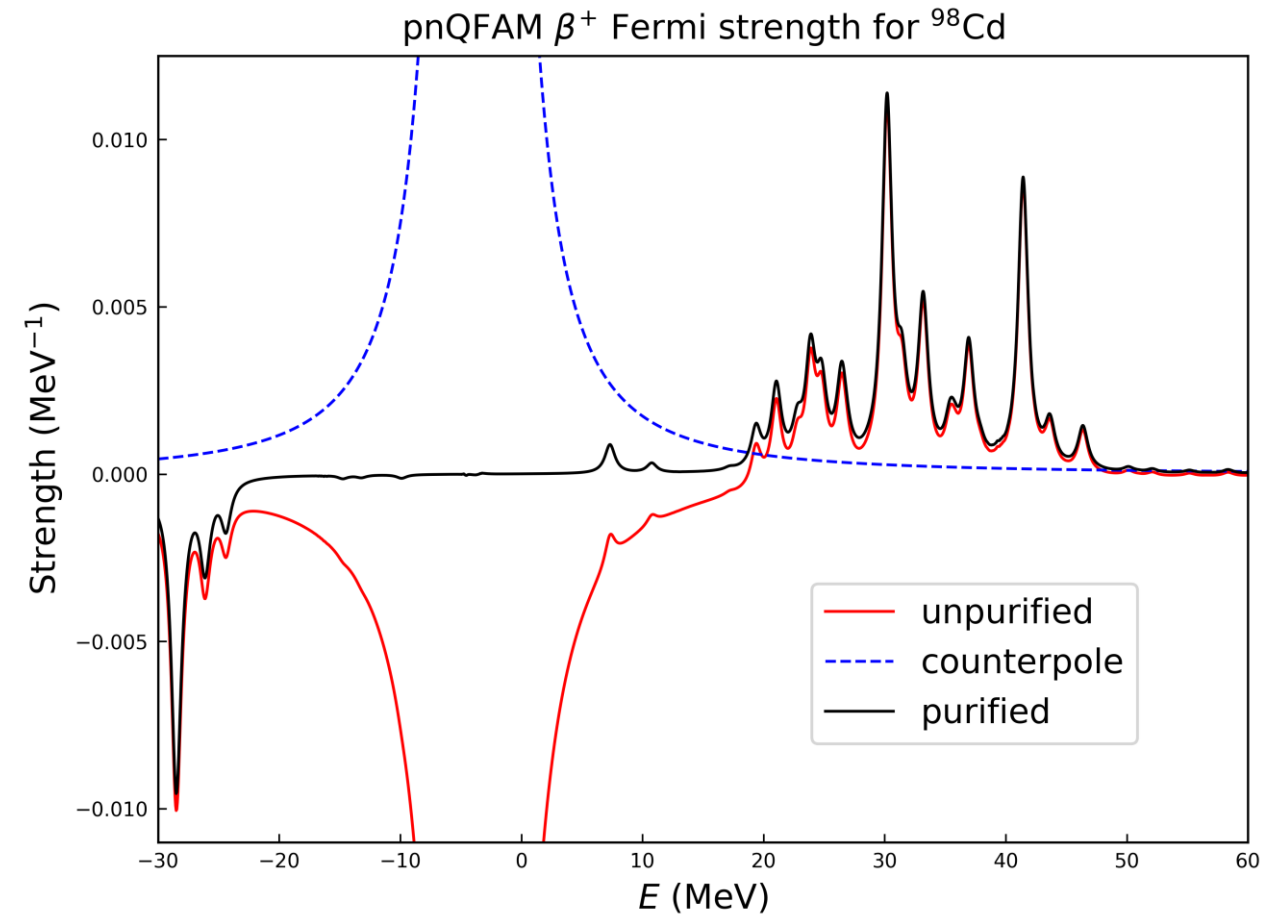
- In charge-conserving FAM operators are Hermitian, and the physical and unphysical strengths are typically of equal magnitude
- In pnFAM the Hermitian conjugate of the Fermi operator represents a transition into the opposite direction
- When there is an asymmetry between N and Z, there is a preferred direction, and pnFAM strength to the opposite is completely drowned out by the other

pnQFAM Fermi β^- and β^+ strengths for ^{98}Cd



Purification of the strength

- If the contamination is mostly due to single state (e.g. the IAS), the contaminations from other states can be neglected
- If the strength contribution and energy of this state are then known, the pnFAM strength can be purified by an equal, but opposite contribution at this exact energy
- This procedure removes the contribution of that state from the strength entirely
- Works well when there is only one or at most a few of such states, less practical when many unphysical states contribute
- Nevertheless, the strength contribution and energy need to be obtained somehow

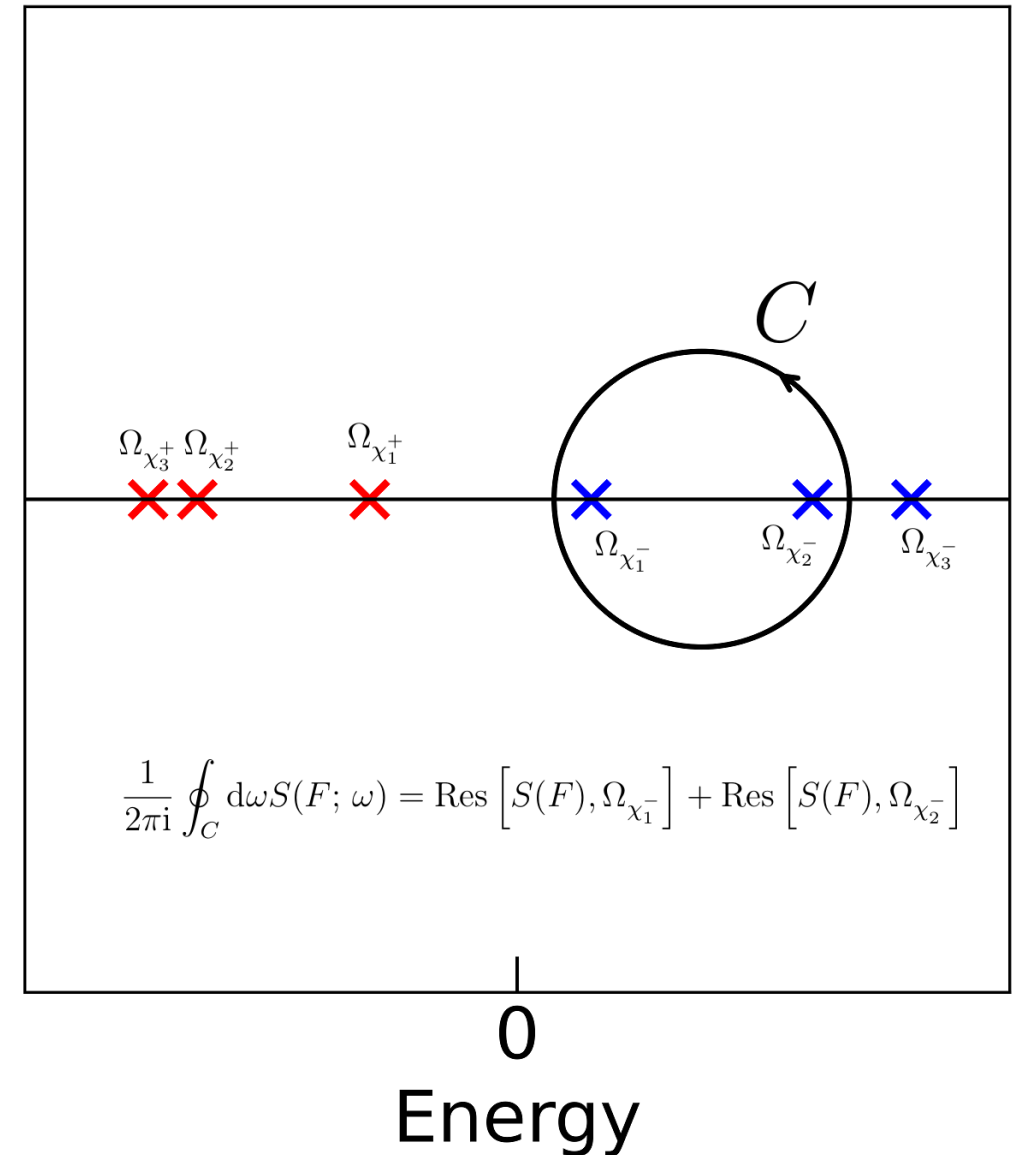


About contour integration

- Complex contour integration can be used to obtain the exact strengths
- An integral around a contour C gives the sum of the strengths from all of the poles (final states) enclosed by the contour
- The IAS energy and the strength associated with it can then be obtained via integration around an appropriately chosen contour

$$B_{\chi}(F) = |\langle A_{\chi} | \hat{F} | \text{pnQRPA} \rangle|^2 = \text{Res} [S(F), \Omega_{\chi}]$$

$$\text{Res} [S(F), \Omega_{\chi}] = \frac{1}{2\pi i} \oint_C d\omega S(F; \omega)$$



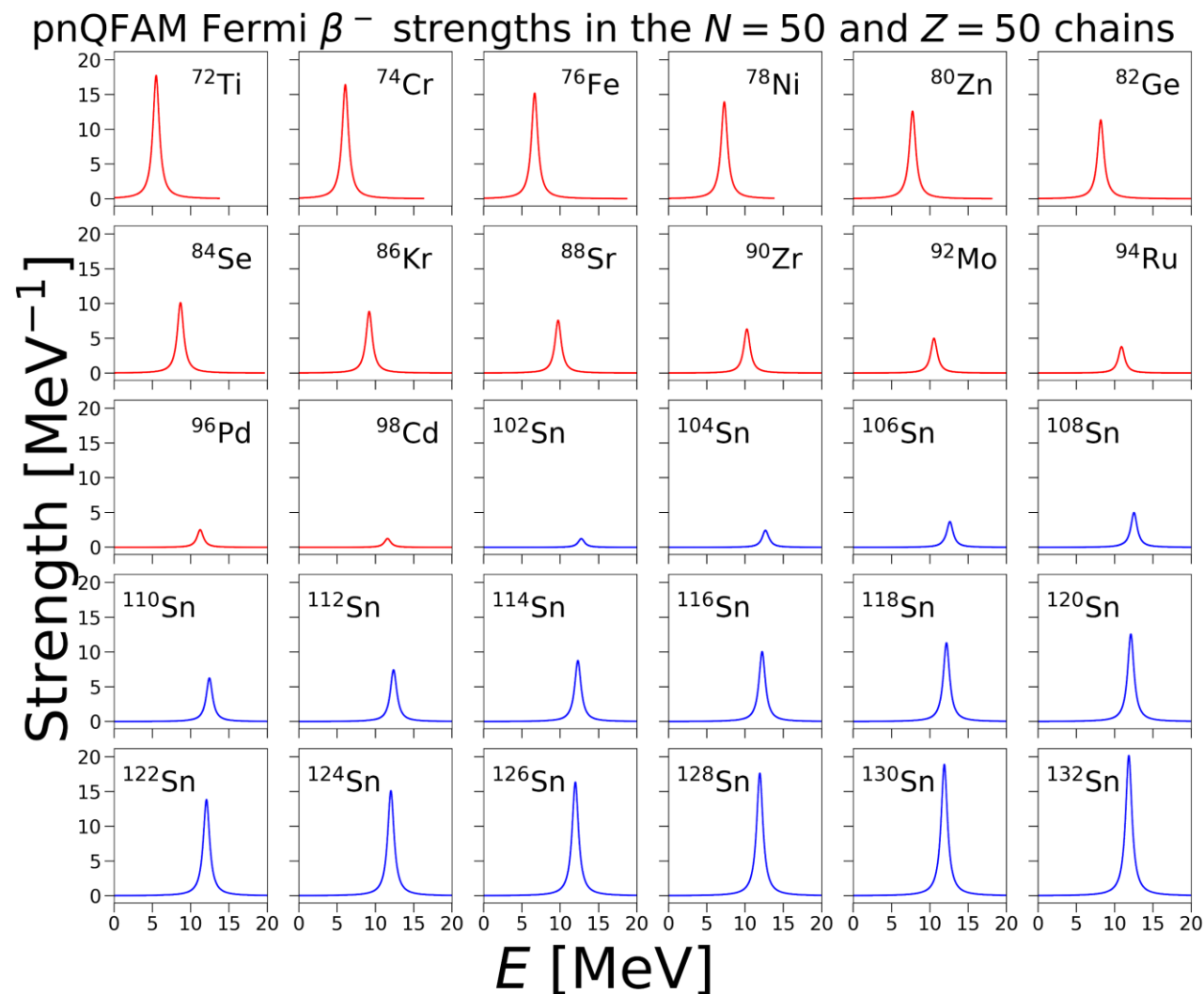


4 ■ Results

What all this amounted to

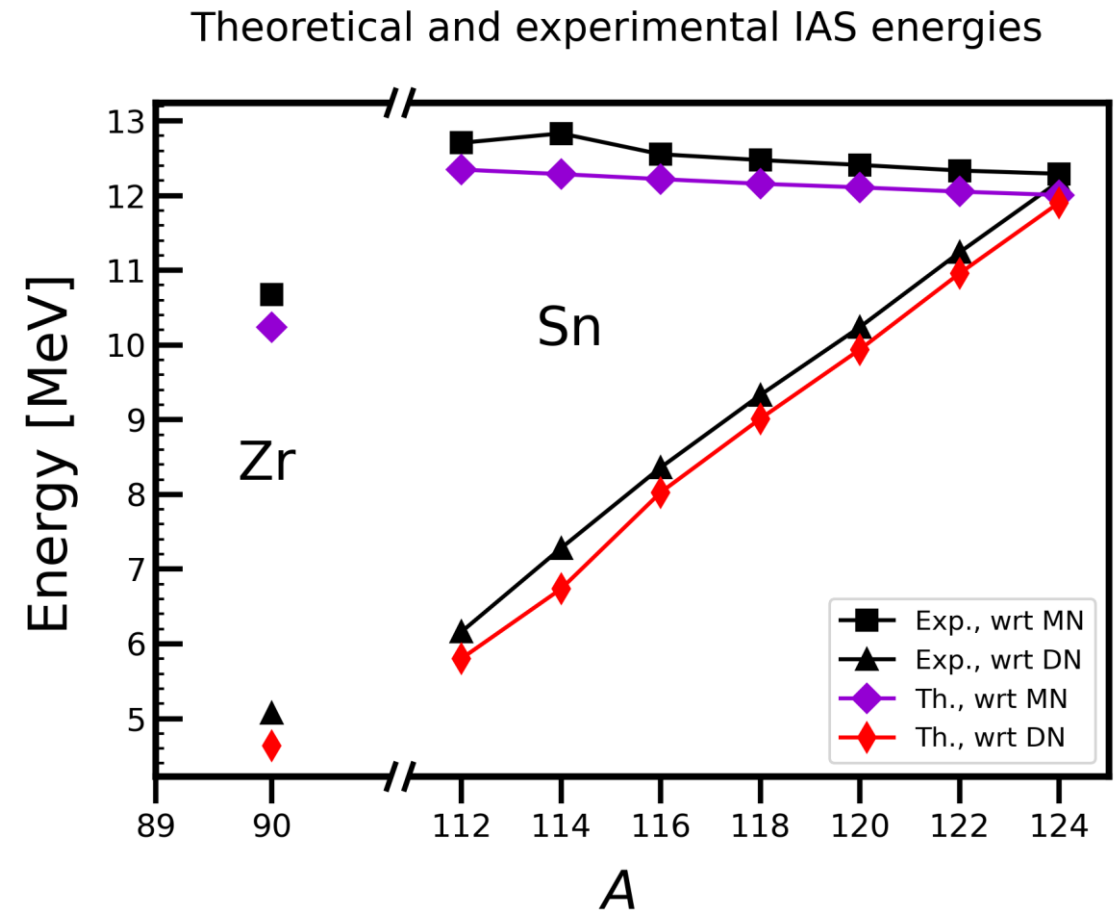
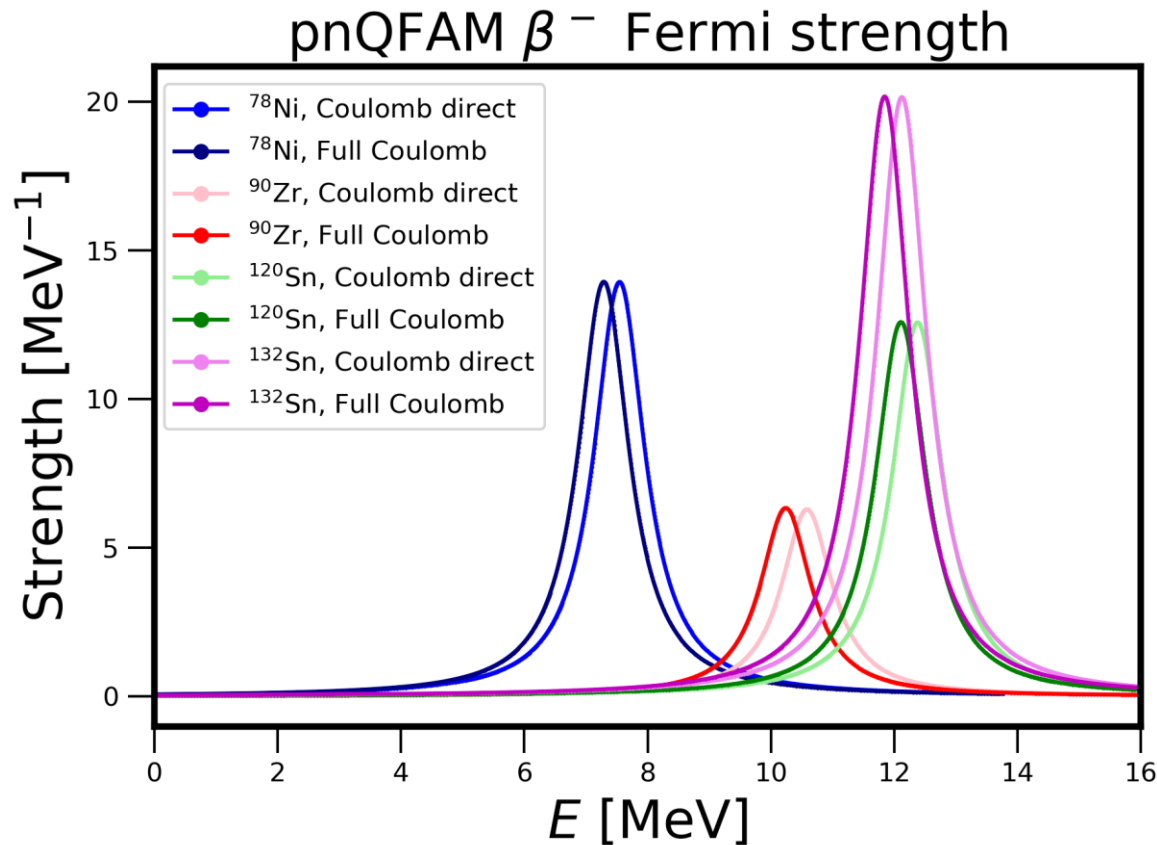
Beta minus strengths for N=50 and Z=50 nuclei

- Fermi strengths in the selected nuclear chains
- HFB calculations conducted using the PAN@CEA numerical suite
- Spherical harmonic oscillator basis, 10 shells, BM-parametrization for oscillator length
- Parity, isospin and axial symmetry at HFB level
- 1b2b CoM correction
- Full D1S interaction (Coulomb direct + exchange)
- Average particle numbers constrained to that of the nucleus of interest



Comparison with experiment

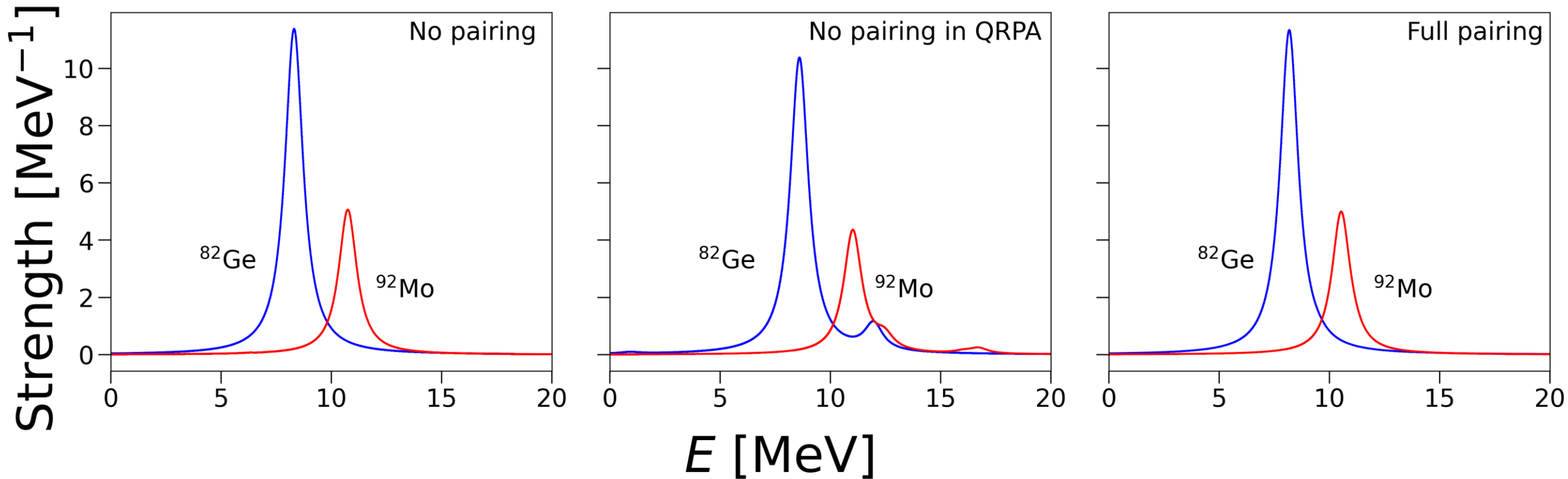
- Good agreement with experiment
- Small systematic difference due to the Coulomb term



Self-consistency considerations

- Consistency in the treatment of the pairing-channel interaction can be important for obtaining a single IAS peak and avoiding fragmentation

pnQFAM Fermi β^- strengths for different treatments of the pairing-channel interaction

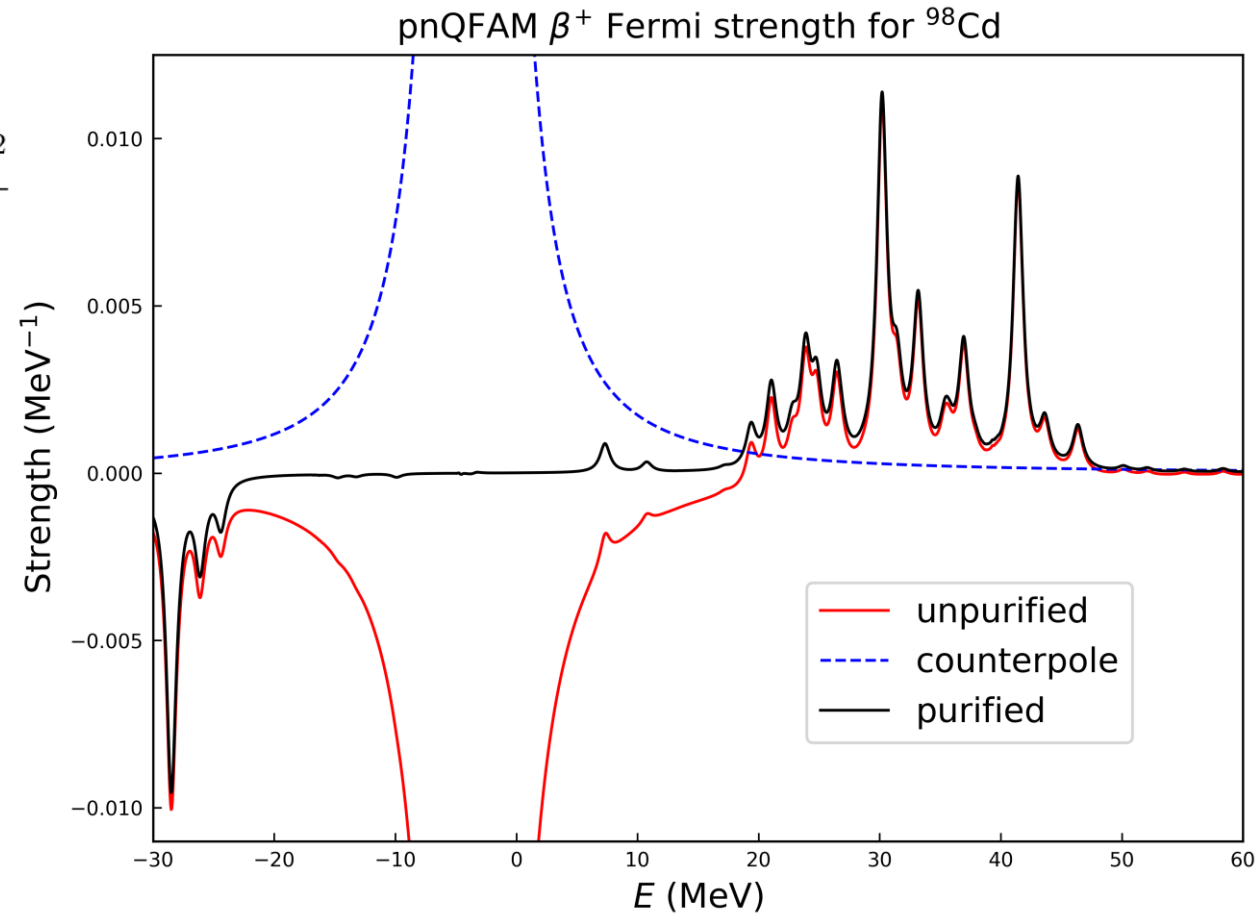


Decontaminating the beta+ Fermi strength

- The unphysical contamination is essentially solely due to the IAS, so we approximate

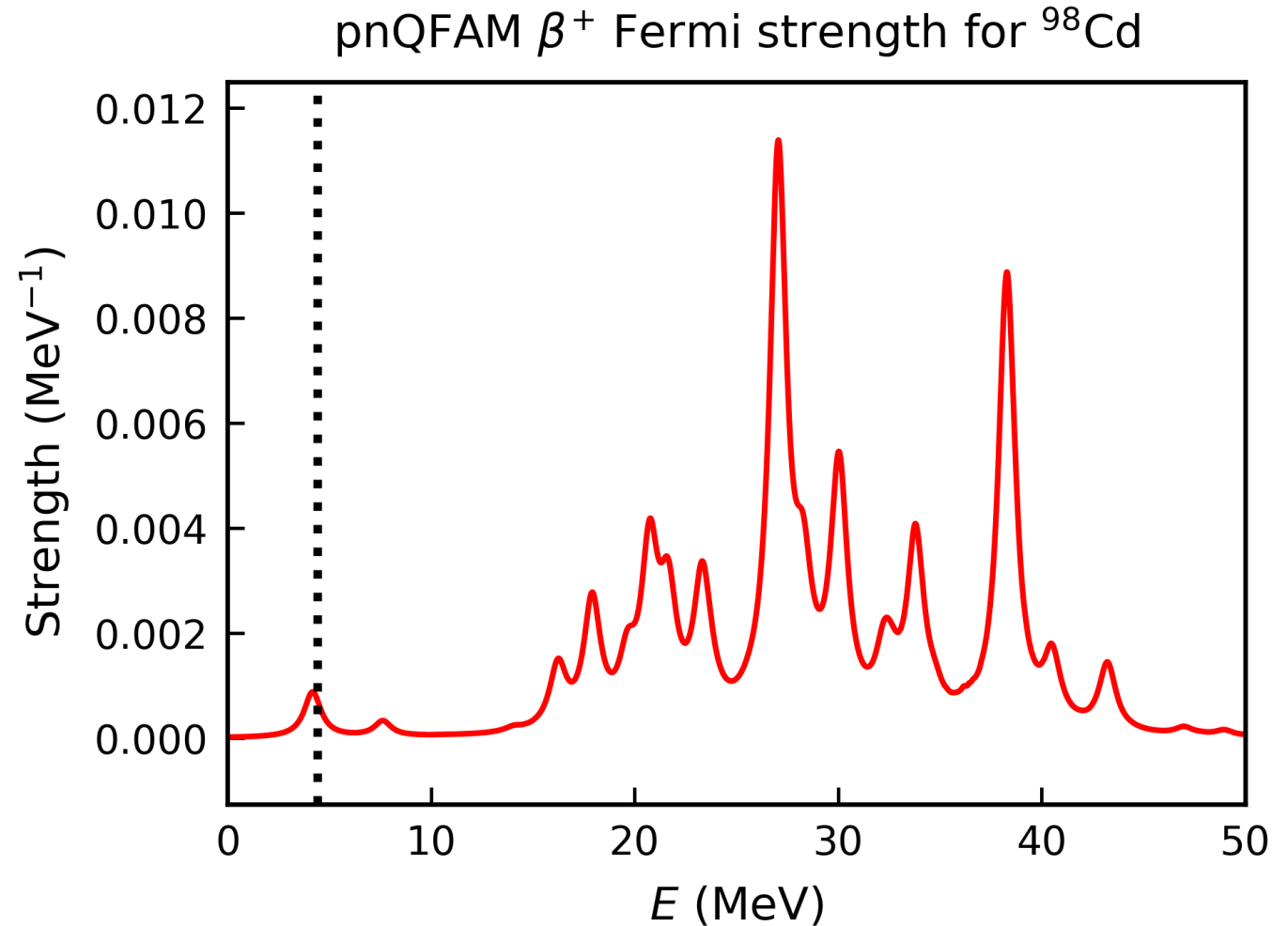
$$-\frac{1}{\pi} \text{Im } S(F; \omega) \approx \frac{\gamma}{\pi} \sum_{\chi} \frac{|\langle A_{\chi} | \hat{F} | \text{QRPA} \rangle|^2}{(\Omega - \Omega_{\chi})^2 + \gamma^2} - \frac{|\langle A_{\text{IAS}} | \hat{F}^{\dagger} | \text{QRPA} \rangle|^2}{(\Omega + \Omega_{\text{IAS}})^2 + \gamma^2}$$

- By adding a term to the strength equal to the rightmost term, but opposite in sign its contribution can be directly removed
- The energy and strength of the IAS were obtained via contour integration using adaptive integration with a circular contour of radius 50 keV
- The exact energy was further fine-tuned by hand to match the counterpole as close to the IAS pole in the strength plot



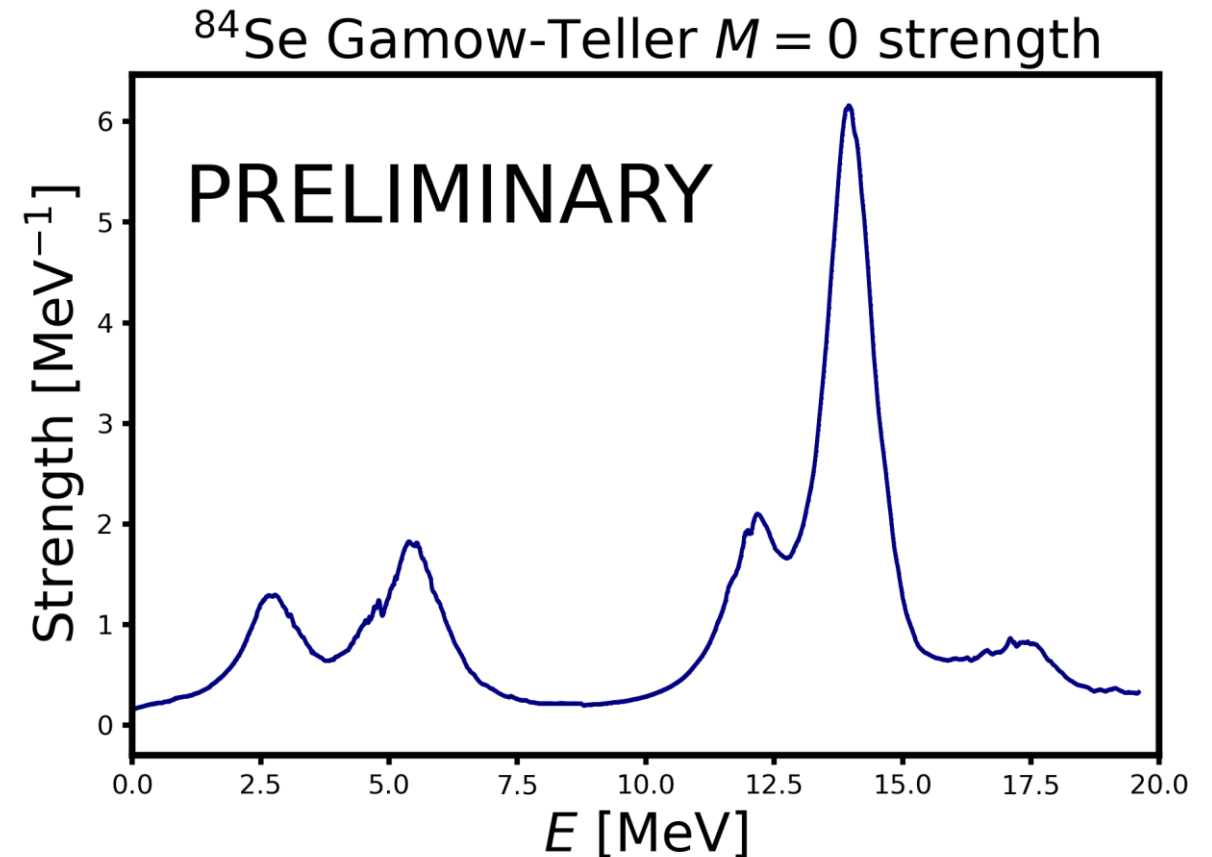
Beta plus strength

- Direct removal works well when there is a small number of highly contributing unphysical states, such as the IAS
- Less practical when there are many states that contribute
- Relies on information about the strengths and energies of singular eigenstates
- Methods which give these could work in conjunction



Gamow-Teller preliminary results

- 10 shells too few for proper convergence, need more (16 or so)
- Deformation entails angular momentum restoration
- The approach to this should be simple, and work without explicit eigenvalues (e.g. the needle approximation)





5 ■ Conlusions and Future Plans

What we plan to do next

What we plan to do next

The great benefit of pnQRPA-FAM is its use in pnQRPA calculations with very large numbers of shells and without truncations and cutoffs. To this end, we plan to utilize it towards the following goals:

- Conduct and report calculations for Gamow-Teller strengths
- Implement Fermi function for contour integration half-life calculations
- Implement first-forbidden beta decay operators and other formalism for calculations involving these
- Explore the possibility of using pnQRPA-FAM for other weak semi-leptonic nuclear processes (e.g. muon capture, low-energy neutrino scattering)
- Conduct a systematic study (Fermi and/or GT) of strengths for nuclei that are of particular interest, and construct a database of the results

Thank you for listening

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