Recent progress and attempts to describe beta decay based on nuclear DFT

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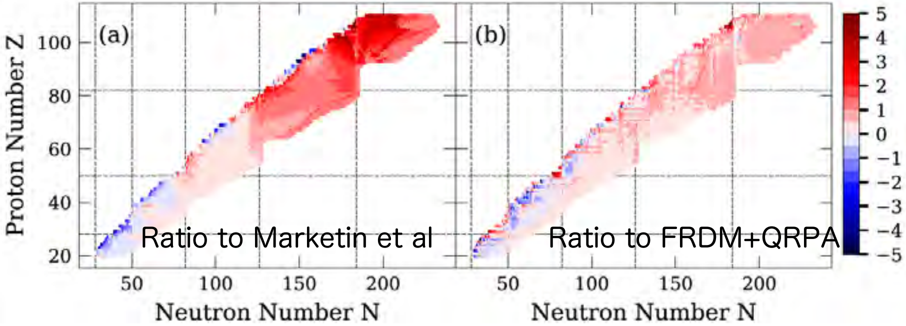
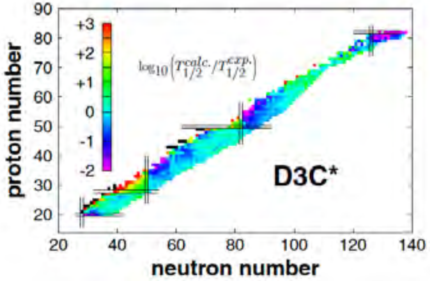
Global beta-decay calculation

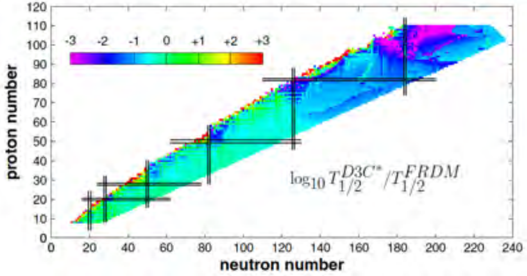
- r-process: neutron-star merger, supernovae… beta decay plays important role.
- Theoretical approaches: ab-initio, shell model, DFT
- DFT with deformation and pairing can cover whole r-process nuclei

Skyrme EDF: Ney et al., Phys. Rev. C **102**, 034326 (2020)
(Calculation within axial symmetry, odd: equal filling approx.)

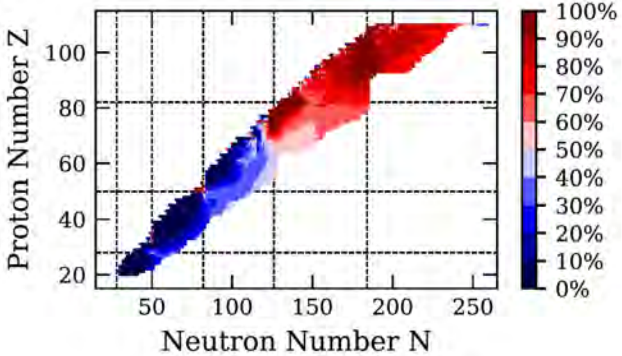


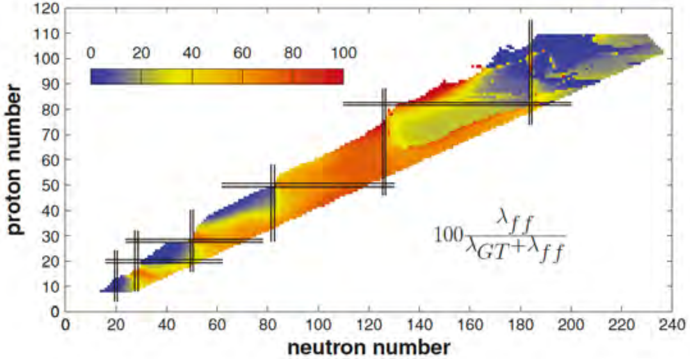
Covariant DFT: Marketin et al., Phys. Rev. C **93**, 025805 (2016)
(Calculation within spherical symmetry, odd: average number to odd)





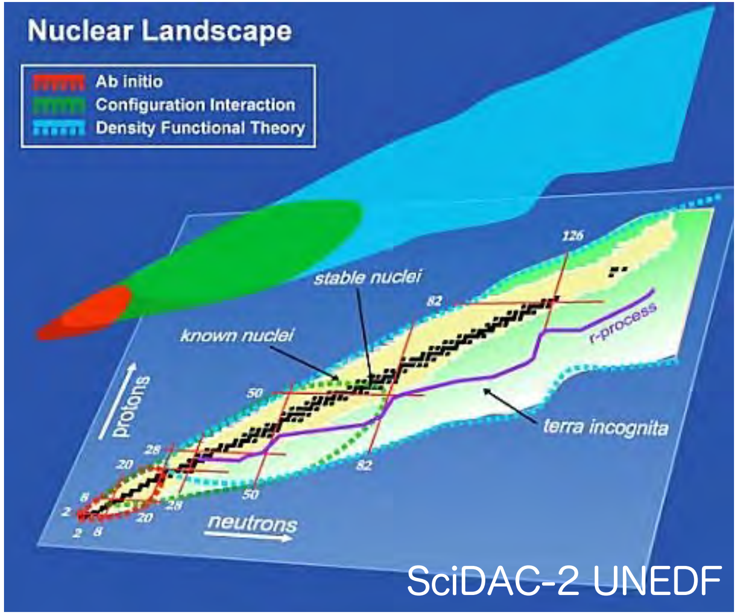
First forbidden percentage





Nuclear density functional theory (DFT)

A microscopic theory that can compute from all unstable nuclei to neutron star



Hartree-Fock-Bogoliubov equation for nuclear ground state

iterative eigenvalue problem (non-linear eq.)

$$\begin{pmatrix} h[\rho,\tilde{\rho}]-\lambda & \Delta[\rho,\tilde{\rho}] \\ -\Delta^*[\rho,\tilde{\rho}] & -h^*[\rho,\tilde{\rho}]+\lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

matrix elements (potential)

$$h[\rho,\tilde{\rho}] = \frac{\delta E}{\delta \rho} \qquad \Delta[\rho,\tilde{\rho}] = \frac{\partial E}{\partial \tilde{\rho}^*}$$

quasiparticle wave functions — densities

$$U, V \rightarrow \rho, \tilde{\rho}$$

Quasiparticle random-phase approximation (QRPA)

excited states (including beta decay) and dynamics

eigenvalue problem of large dimension (~10^6)

- Input of the nuclear DFT: energy density functional (EDF, E[ρ])
- EDF is determined phenomenologically (not directly derived from the nuclear force)
- EDF: kinetic energy + particle-hole energy + pairing energy + Coulomb

Quasiparticle random-phase approximation (QRPA)

QRPA: Microscopic theory for (the ground and) excited states of nuclei based on the nuclear DFT

QRPA equation (non-Hermitian eigenvalue problem)

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix} = \Omega_i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X^i \\ Y^i \end{pmatrix}$$

A: Hermitian matrix
B: symmetric matrix
Ω: excitation energy
(X,Y): wave functions

dimension: 10^5-10^6 full diagonalization is computationally demanding

i-th excited state:
(final state in beta decay)

$$|i\rangle = \hat{Q}_i^\dagger |0\rangle \qquad \hat{Q}_i^\dagger = \sum_{\pi\nu} X^i_{\pi\nu} \hat{a}_\pi^\dagger \hat{a}_\nu^\dagger - Y^i_{\pi\nu} \hat{a}_\nu \hat{a}_\pi$$

beta decay: we need transition strength for eigenstates below Q-value

$$\langle i|\hat{F}|0\rangle \approx \langle \mathrm{HFB}| \left[\hat{Q}_i, \hat{F}\right] |\mathrm{HFB}\rangle = \sum_{\pi\nu} (X^i_{\pi\nu} F^{20}_{\pi\nu} + Y^i_{\pi\nu} F^{02}_{\pi\nu})$$

F: decay operators

Solutions of Matrix QRPA:

basis reduction: truncation in the two-quasiparticle space (standard)
Lanczos method (Johnson, et al. Comp. Phys. Commun. **120**, 155 (1999))
iterative Arnoldi method (Toivanen et al. Phys. Rev. C **81**, 034312 (2010))

deformed QRPA calculation for beta-decay is computationally too time-consuming

Finite-amplitude method

Iterative solution of the QRPA

Nakatsukasa et al., Phys. Rev. C **76**, 024318 (2007)

Apply a weak time-dependent external one-body field

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

F: one-body operator
η: small number
ω: frequency of the external field (parameter)

$$\hat{F} = \sum_{\mu<\nu} F^{20}_{\mu\nu}\alpha^\dagger_\mu\alpha^\dagger_\nu + F^{02}_{\mu\nu}\alpha_\nu\alpha_\mu$$

time-dependent quasiparticles $\alpha^\dagger_\mu(t) = \sum_k \left[U_{k\mu}(t)c^\dagger_k + V_{k\mu}(t)c_k\right]$ $\alpha_\mu(t) = \{\alpha_\mu + \delta\alpha_\mu(t)\}e^{iE_\mu t}$

infinitesimal displacement from the HFB quasiparticles $\delta\alpha_\mu(t) = \eta\sum_\nu \alpha^\dagger_\nu\left[X_{\nu\mu}(\omega)e^{-i\omega t} + Y^*_{\nu\mu}(\omega)e^{i\omega t}\right]$

time propagation (TDHFB equation)

$$\delta\langle\Phi(t)|\hat{H} - i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle = 0$$

$$\hat{H}(t) = \hat{H}_0 + \eta\left[\delta\hat{H}(\omega)e^{-i\omega t} + \delta\hat{H}^\dagger(\omega)e^{i\omega t}\right]$$

$$\delta\hat{H}(\omega) = \sum_{\mu<\nu}\left[\delta H^{20}_{\mu\nu}(\omega)\alpha^\dagger_\mu\alpha^\dagger_\nu + \delta H^{02}_{\mu\nu}(\omega)\alpha_\nu\alpha_\mu\right]$$

⇒

$$i\frac{\partial\alpha_\mu(t)}{\partial t} = [\hat{H}(t) + \hat{F}(t), \alpha_\mu(t)]$$

⇓

extract first-order terms in η

linear response equation (FAM)

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = -\begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

Note: X(ω)、Y(ω) are not the QRPA solutions (eigenvectors)
QRPA is obtained as a small-amplitude limit of the TDHFB (η <<1)

Finite-amplitude method

Nakatsukasa, Inakura, Yabana, Phys. Rev. C **76**, 024318 (2007)
Avogadro and Nakatsukasa, Phys. Rev. C **84**, 014314 (2011)

linear response equations:
linear equation of X and Y

$$\left[\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} - \omega \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right] \begin{pmatrix} X(\omega) \\ Y(\omega) \end{pmatrix} = - \begin{pmatrix} F^{20} \\ F^{02} \end{pmatrix}$$

ω and F are parameters

Solution 1: solve it as a simultaneous linear equations of X and Y (two-qp dim)

no need to diagonalize QRPA matrix (A,B)
need the matrix elements of A and B

Solution 2: iteration

displacement of quasiparticles

displacement of one-body mean-field Hamiltonian

$$(E_\mu + E_\nu - \omega) X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) = -F^{20}_{\mu\nu}$$
$$(E_\mu + E_\nu + \omega) Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) = -F^{02}_{\mu\nu}$$

$X(\omega), Y(\omega)$

$\delta H^{20}(\omega), \delta H^{02}(\omega)$

$$\delta H^{20}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} [A_{\mu\nu\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}] X_{\mu'\nu'}(\omega) + B_{\mu\nu\mu'\nu'} Y_{\mu'\nu'}(\omega)$$
$$\delta H^{02}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} [A^*_{\mu\nu\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}] Y_{\mu'\nu'}(\omega) + B^*_{\mu\nu\mu'\nu'} X_{\mu'\nu'}(\omega)$$

need the A and B matrix elements

Finite-amplitude method

Solution 3: FAM (iteration)

Nakatsukasa, Inakura, Yabana, Phys. Rev. C **76**, 024318 (2007)
Avogadro and Nakatsukasa, Phys. Rev. C **84**, 014314 (2011)

$$(E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) = -F^{20}_{\mu\nu}$$
$$(E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) = -F^{02}_{\mu\nu}$$

displacement of one-body mean-field Hamiltonian

$$\delta H^{20}(\omega), \delta H^{02}(\omega)$$

displacement of quasiparticles

$$X(\omega), Y(\omega)$$

$$\delta H^{20}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} [A_{\mu\nu\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}]X_{\mu'\nu'}(\omega) + B_{\mu\nu\mu'\nu'}Y_{\mu'\nu'}(\omega)$$
$$\delta H^{02}_{\mu\nu}(\omega) = \sum_{\mu'<\nu'} [A^*_{\mu\nu\mu'\nu'} - (E_\mu + E_\nu)\delta_{\mu\mu'}\delta_{\nu\nu'}]Y_{\mu'\nu'}(\omega) + B^*_{\mu\nu\mu'\nu'}X_{\mu'\nu'}(\omega)$$

A and B matrices are not necessary, but one-body displacement AX+BY and A*Y+B*X (vectors) are

$$A_{\rho\sigma,\mu\nu} = \delta_{\rho\mu}\delta_{\sigma\nu}(E_\mu + E_\nu) + \frac{\partial^2 \mathcal{E}'}{\partial\kappa^*_{\rho\sigma}\partial\kappa_{\mu\nu}},$$
$$B_{\rho\sigma,\mu\nu} = \frac{\partial^2 \mathcal{E}'}{\partial\kappa^*_{\rho\sigma}\partial\kappa^*_{\mu\nu}}.$$

$$A, B \approx \frac{\delta^2 E}{\delta\mathcal{R}^2} = \frac{\delta\mathcal{H}}{\delta\mathcal{R}}$$

A,B matrices:
second functional derivative of EDF
(first functional derivative of one-body potential)

displacement of the densities (δ R)

$$\delta\rho(\omega) = UX(\omega)V^T + V^*Y^T(\omega)U^\dagger$$
$$\delta\kappa^{(+)}(\omega) = UX(\omega)U^T + V^*Y^T(\omega)V^\dagger$$
$$\delta\kappa^{(-)}(\omega) = V^*X^\dagger(\omega)V^\dagger + UY^*(\omega)U^T$$

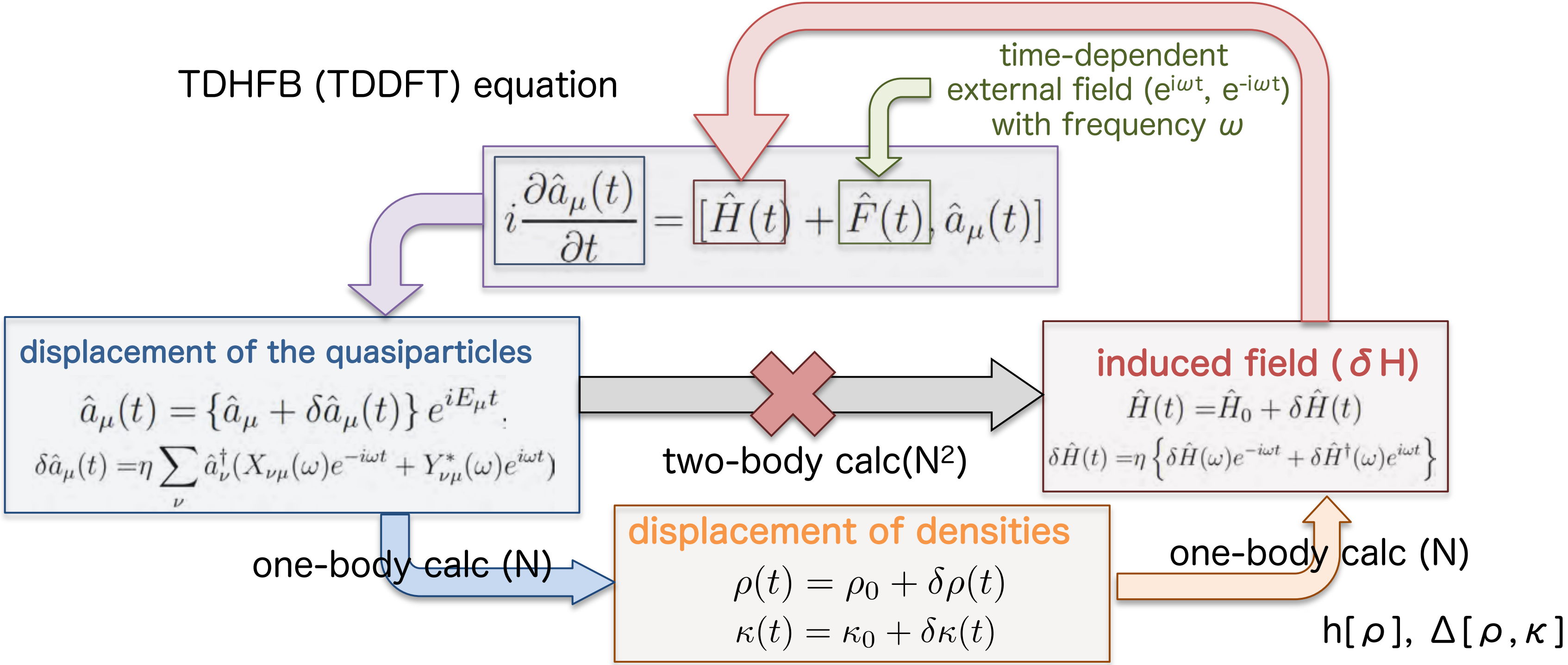
displacement of the one-body potential (δ H)

$$\delta h(\omega) = (h[\rho + \eta\delta\rho] - h[\rho])/\eta$$
$$\delta\Delta^{(\pm)}(\omega) = (\Delta[\rho + \eta\delta\rho, \kappa + \eta\delta\kappa^{(\pm)}, \kappa^* + \eta\delta\kappa^{(\mp)*}] - \Delta[\rho, \kappa, \kappa^*])/\eta$$

calculating A and B matrices avoided!

Finite-amplitude method

Nakatsukasa et al., Phys. Rev. C **76**, 024318 (2007)



- iterative solution of QRPA
- one-body induced field is calculated through one-body density displacement
- no need to evaluate A and B matrices
- one-body field subroutine for the mean-field calculation can be reused with minor extension

FAM for Gamow-Teller resonance and beta decay

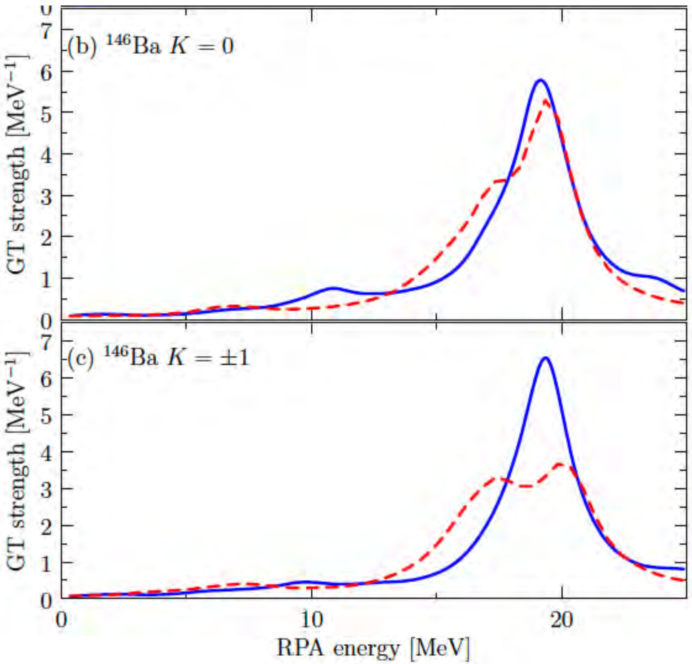
Mustonen et al., Phys. Rev. C **90**, 024308 (2014)

strength function $S(\hat{F},\omega) = \sum_{\mu<\nu} F^{20}_{\mu\nu} X_{\mu\nu}(\omega) + F^{02}_{\mu\nu} Y_{\mu\nu}(\omega)$

(X, Y: FAM amplitudes)

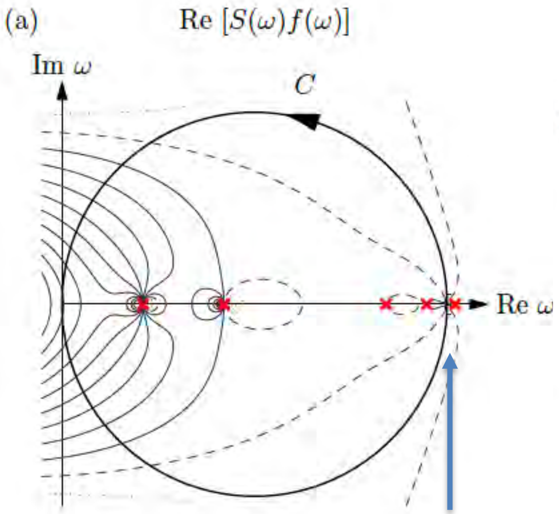
$$\frac{dB}{d\omega}(\hat{F},\omega) = -\frac{1}{\pi}\mathrm{Im}S(\hat{F},\omega) = \frac{\gamma}{\pi}\sum_{\nu}\left\{\frac{|\langle\nu|\hat{F}|0\rangle|^2}{(\Omega_i-\omega)^2+\gamma^2} - \frac{|\langle 0|\hat{F}|\nu\rangle|^2}{(\Omega_i+\omega)^2+\gamma^2}\right\}$$

Gamow-Teller resonance



beta decay rate

$$B_n(F) = |\langle n|F|0\rangle|^2 = \mathrm{Res}[S(F),\Omega_n],$$



$$\lambda_{1+} = \frac{\ln 2}{\kappa}\sum_n f(\Omega_n) B_n^{(\mathrm{GT})}$$
$$\approx \frac{\ln 2}{\kappa}\sum_n f_{\mathrm{poly}}(\Omega_n)\,\mathrm{Res}[S(\sigma\tau_-),\Omega_n]$$
$$= \frac{\ln 2}{\kappa}\sum_n \mathrm{Res}[f_{\mathrm{poly}} S(\sigma\tau_-),\Omega_n]$$
$$= \frac{\ln 2}{\kappa}\frac{1}{2\pi i}\oint_C d\omega\, f_{\mathrm{poly}}(\omega) S(\sigma\tau_-;\omega),$$

$$\omega_{\max} = Q + E_{\mathrm{g.s.}} = \lambda_n - \lambda_p + \Delta M_{\text{n-H}}.$$

Quasiparticle-phonon coupling

Liu et al., Phys. Rev. C **109**, 044308 (2024)

QRPA: includes coupling to two-quasiparticle states (Landau damping)
no coupling to more complex configurations (multi-quasiparticles) (spreading width)
in the current HO basis no two-quasiparticle states coupling to continuum (escaping width)

QPVC(quasiparticle vibration coupling): coupling with phonon, a part of spreading width included

GTR: Niu et al., Phys. Rev. C **94**, 064328 (2016), beta decay: Niu et al Phys. Lett. B **780**, 325 (2018)

$$|M\rangle = Q_M^\dagger |0\rangle \qquad Q_M^\dagger = \sum_{\pi\nu} \left(X_{\pi\nu}^M \alpha_\pi^\dagger \alpha_\nu^\dagger - Y_{\pi\nu}^M \alpha_\nu \alpha_\pi + \sum_N \tilde{X}_{\pi\nu N}^M \alpha_\pi^\dagger \alpha_\nu^\dagger Q_N^\dagger - \tilde{Y}_{\pi\nu N}^M Q_N \alpha_\nu \alpha_\pi \right).$$

charge-changing QRPA level amplitude

beyond QRPA amplitudes

N-th like-particle phonon

In the FAM equations

$$X_{\pi\nu}(\omega) = -\frac{\delta H_{\pi\nu}^{20} + [\tilde{W}(\omega)X(\omega)]_{\pi\nu} + F_{\pi\nu}^{20}}{\varepsilon_\pi + \varepsilon_\nu - \omega}, \qquad [\tilde{W}(\omega)X(\omega)]_{\pi\nu} = \sum_{\pi'\nu'} \tilde{W}_{\pi\nu,\pi'\nu'}(\omega) X_{\pi'\nu'}(\omega),$$

$$Y_{\pi\nu}(\omega) = -\frac{\delta H_{\pi\nu}^{02} + [\tilde{W}^*(-\omega)Y(\omega)]_{\pi\nu} + F_{\pi\nu}^{02}}{\varepsilon_\pi + \varepsilon_\nu + \omega}, \qquad [\tilde{W}^*(-\omega)Y(\omega)]_{\pi\nu} = \sum_{\pi'\nu'} \tilde{W}_{\pi\nu,\pi'\nu'}^*(-\omega) Y_{\pi'\nu'}(\omega).$$

spreading matrix $\tilde{W}(\omega) = W(\omega) - W(0)$ (subtraction procedure. reduces to QRPA at ω=0)

V. I. Tselyaev, Phys. Rev. C **88**, 054301 (2013).

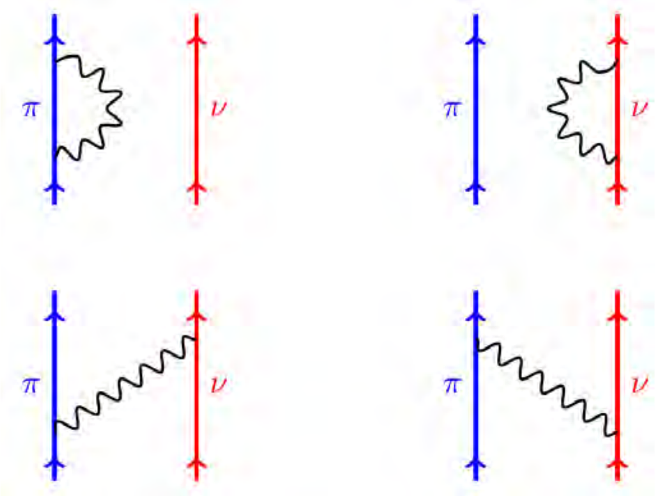
Quasiparticle-phonon coupling

Liu et al., Phys. Rev. C **109**, 044308 (2024)

$$W_{\pi\nu,\pi'\nu'}(\omega) = \sum_N \Bigg\{ \sum_{\pi_1} \langle\pi|H|\pi_1, N\rangle \frac{1}{\omega - [\omega_N + (\varepsilon_{\pi_1} + \varepsilon_\nu)]} \langle\pi'|H|\pi_1, N\rangle^* \delta_{\nu'\nu}$$

$$+ \sum_{\nu_1} \langle\nu|H|\nu_1, N\rangle \frac{1}{\omega - [\omega_N + (\varepsilon_\pi + \varepsilon_{\nu_1})]} \langle\nu'|H|\nu_1, N\rangle^* \delta_{\pi'\pi} + \langle\pi|H|\pi', N\rangle \frac{1}{\omega - [\omega_N + (\varepsilon_{\pi'} + \varepsilon_\nu)]} \langle\nu'|H|\nu, N\rangle^*$$

$$+ \langle\nu|H|\nu', N\rangle \frac{1}{\omega - [\omega_N + (\varepsilon_\pi + \varepsilon_{\nu'})]} \langle\pi'|H|\pi, N\rangle^* \Bigg\}. \quad (12)$$



ω_N: phonon energy

$<\pi'|H|\pi, N>$: coupling with proton quasiparticle

Phonon (like-particle QRPA)

Liu et al., Phys. Rev. C **109**, 044308 (2024)

Operator to excite like-particle phonon (isoscalar/isovector multipole operators)

$$G = \sum_{pp'} G_{pp'} a_p^\dagger a_{p'} + \sum_{nn'} G_{nn'} a_n^\dagger a_{n'},$$

$$G_{LK}^{T=0} = \sum_i r_i^L Y_{LK}(\theta_i, \varphi_i), \quad G_{LK}^{T=1} = \sum_i r_i^L Y_{LK}(\theta_i, \varphi_i)\tau_z(i),$$

Coupling with quasiparticles

$$\langle \beta | H | \beta_1, N \rangle = i \lim_{\Delta \to 0} \frac{\Delta}{\langle N | G | 0 \rangle} \delta H^{11}_{\beta\beta_1}(\Omega_N + i\Delta).$$

strength

$$S_G(\omega) = -\sum_N \left(\frac{|\langle N|G|0\rangle|^2}{\omega_N - \omega} - \frac{|\langle N|G^\dagger|0\rangle|^2}{\omega_N + \omega} \right)$$

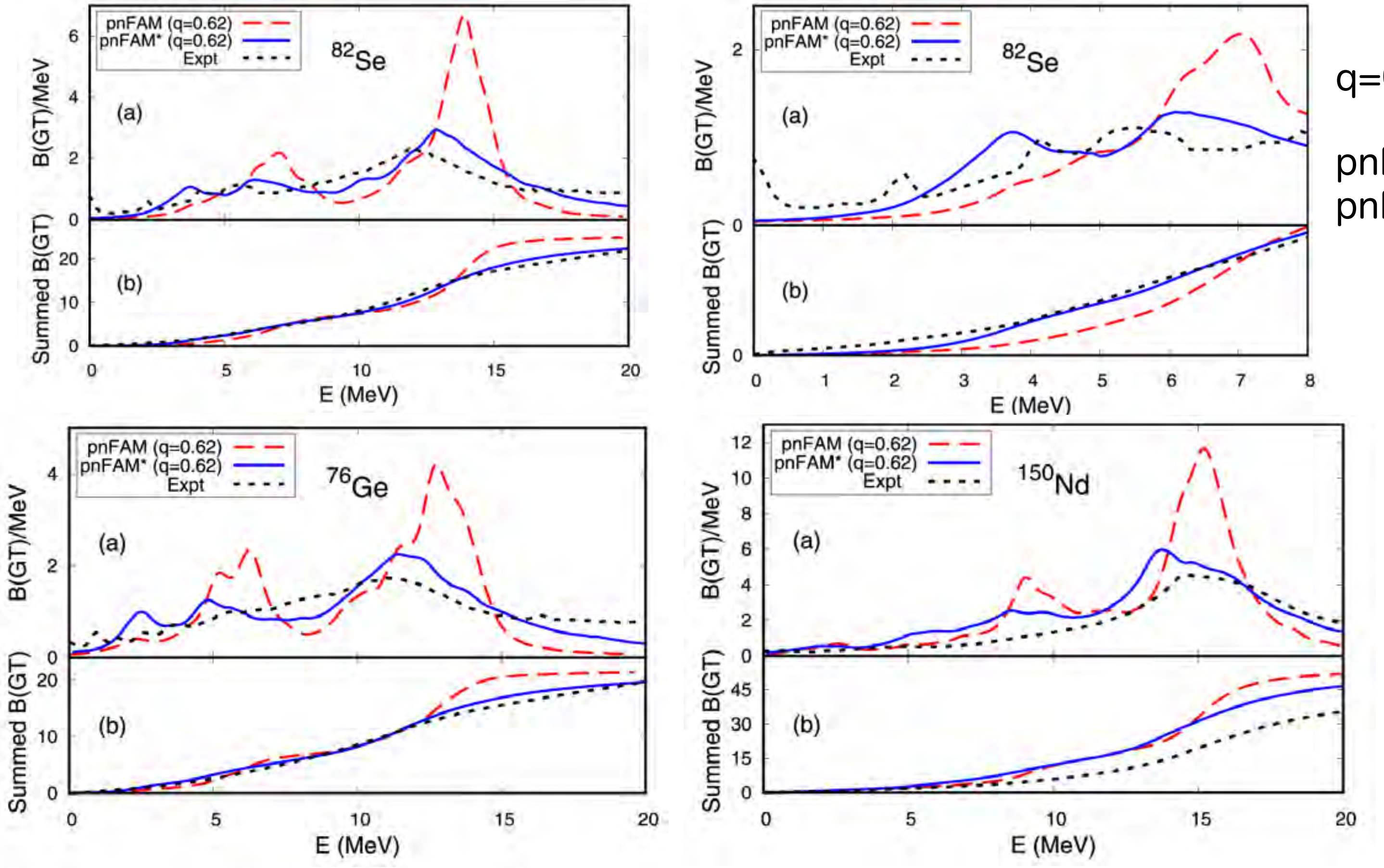
$$\langle N|G|0\rangle = \lim_{\Delta \to 0} \sqrt{i\Delta S_G(\omega_N + i\Delta)}.$$

Like-particle phonon search

- FAM with Im ω = 0.5 MeV, 40 points in the range Re ω = 0 - 20 MeV
- for each T=0, 1, L(Lmax=6), K operator
- typical number of phonons: 150 (^{82}Se)

Gamow-Teller resonance

Liu et al., Phys. Rev. C **109**, 044308 (2024)



$q=0.62 \sim g_A=1.0$

pnFAM: pnQRPA
pnFAM*: pnQRPA+QPVC

Convergence

How many phonons do we need to take into account?

Liu et al., Phys. Rev. C **109**, 044308 (2024)

$$v_N \equiv \frac{\langle V \rangle_N}{\omega_N}.$$

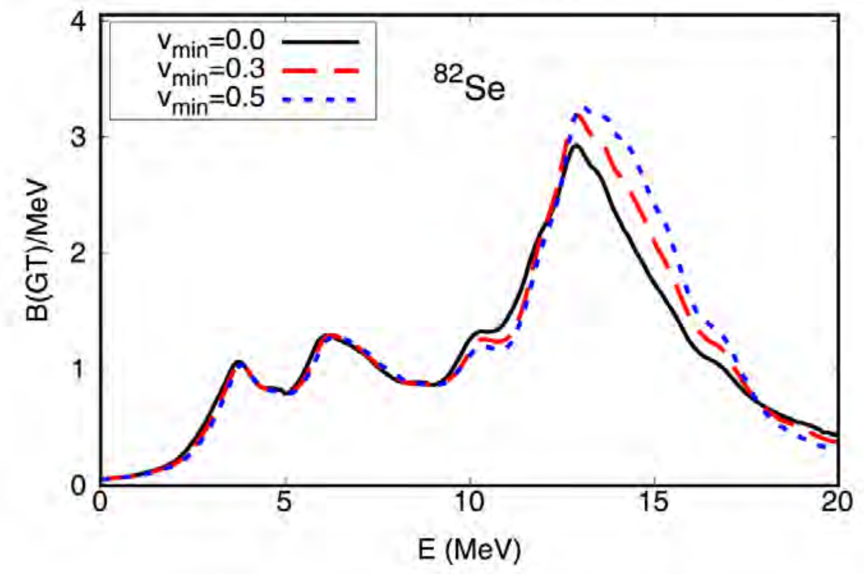
v_n large: collective

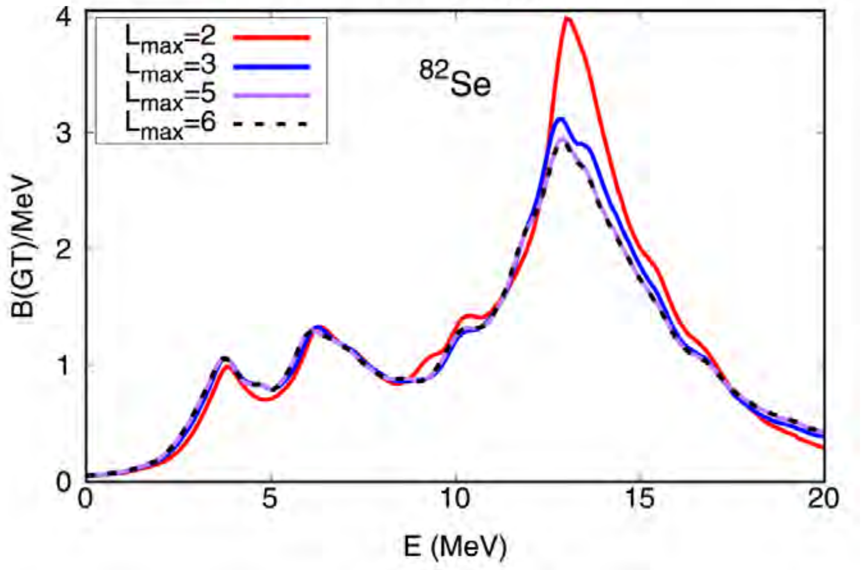
$$v_N = 1 - \frac{1}{\omega_N} \sum_{\alpha\beta} (\varepsilon_\alpha + \varepsilon_\beta) \left(\left| \mathcal{X}^N_{\alpha\beta} \right|^2 + \left| \mathcal{Y}^N_{\alpha\beta} \right|^2 \right).$$

FAM amplitudes

$$\mathcal{X}^N_{\alpha\beta} = -i \lim_{\Delta\to 0} \frac{\Delta}{\langle N|G|0\rangle} \mathcal{X}_{\alpha\beta}(\omega_N + i\Delta),$$

$$\mathcal{Y}^N_{\alpha\beta} = -i \lim_{\Delta\to 0} \frac{\Delta}{\langle N|G|0\rangle} \mathcal{Y}_{\alpha\beta}(\omega_N + i\Delta).$$





- ☐ Phonons with small vn contributes to GTR, less contributes to low-lying states
- ☐ v_{min}=0.0: 150 phonons, v_{min}=0.3: 62 phonons, v_{min}=0.5: 35 phonons

Beta decay

Liu et al., Phys. Rev. C **109**, 044308 (2024)

- isoscalar pn pairing was globally fitted to beta decay half-life within pnQRPA
  Mustonen and Engel, Phys. Rev. C **93**, 014304 (2016)

TABLE I. Deformation parameter, experimental half-life in seconds, pnFAM half-life with the Skyrme functional SGII, pnFAM* half-life with the same functional, and pnFAM* half-life when phonons with $v_N < 0.3$ are excluded, for 11 deformed isotopes.

Isotope	β	$t_{1/2}^{\text{Exp.}}$ (s)	$t_{1/2}^{\text{pnFAM}}$ (s)	$t_{1/2}^{\text{pnFAM*}}$ (s)	$t_{1/2}^{\prime\,\text{pnFAM*}}$ (s)
^{78}Zn	0.12	1.47	408	3.77	4.80
^{168}Gd	0.31	3.03	381	37.1	39.7
^{152}Ce	0.29	1.40	93.1	19.0	20.3
^{156}Nd	0.32	5.49	470	53.5	59.2
^{164}Sm	0.33	1.42	142	17.2	18.5
^{154}Ce	0.30	0.30	19.2	7.26	7.89
^{112}Mo	−0.18	0.15	1.92	2.47	2.31
^{94}Kr	−0.22	0.21	1.48	3.23	3.01
^{112}Ru	−0.21	1.75	93	27.0	31.0
^{106}Mo	−0.20	8.73	62.8	38.0	49.6
^{96}Sr	−0.21	1.07	23.8	20.0	25.9

- qp vibration coupling increases allowed beta decay rate (same as isoscalar pairing)
- isoscalar pairing (~strength similar to isovector) reduces
  40% of pnFAM half-life, 20% of pnFAM* half-life (^{112}Ru)
  45% (pnFAM) and 30% (pnFAM*) for ^{95}Sr

Summary

- Global calculation of beta-decay half-life using nuclear DFT
    - FAM allows up to compute global deformed calculations
    - Quasiparticle-phonon coupling improves the GT strength distribution, beta decay
    - Reduced basis method to speed up the QRPA phonon calculations

Collaborators

- MSU : Xilin Zhang
- UNC Chapel Hill: Qunqun Liu, Jon Engel
- Jyvaskyla: Markus Kortelainen