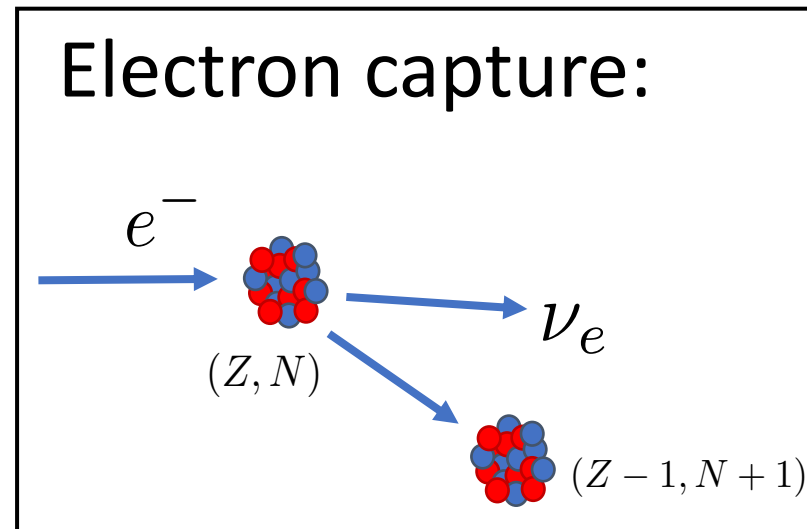
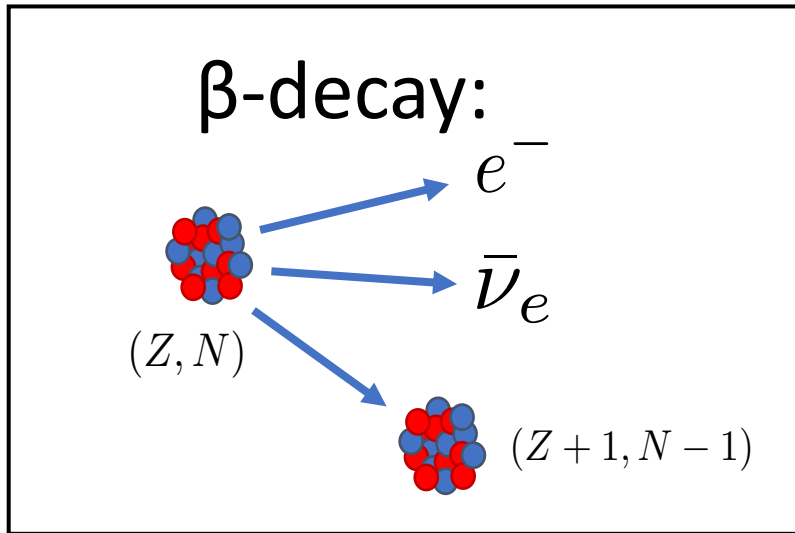


Investigating weak decays with nuclear density functional theory

Ante Ravlić (ravlic@frib.msu.edu)

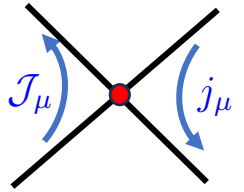
Facility for Rare Isotope Beams, Michigan State University
East Lansing, US





- Current-current form of weak-interaction Hamiltonian:

$$\hat{H}_W = \frac{G}{\sqrt{2}} \int d^3\mathbf{r} \mathcal{J}_\mu(\mathbf{r}) j^\mu(\mathbf{r})$$



- First-order time-dependent perturbation theory (Fermi rule):

EC:
$$\lambda_x = \frac{2\pi}{2J_i + 1} \sum_{M_i, M_f} \sum_{m_x s_\nu} \int d\Omega_\nu |\langle f | \hat{H}_W | i \rangle|^2 q_x^2 (2\pi)^{-3}$$

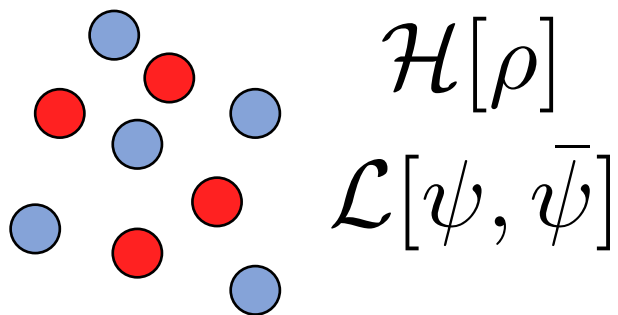
$q_x(m_e c^2) = E_0 + E_x$

β±:
$$\lambda_{\beta^\pm} = \frac{2\pi}{2J_i + 1} \underbrace{\sum_{M_i, M_f} \sum_{s_e, s_\nu}}_{\text{Depends on kinematics}} \int \int \int d\Omega_\nu d\Omega_e |\langle f | \hat{H}_W | i \rangle|^2 dp p^2 q^2 (2\pi)^{-6}$$

p **electron** momentum,
 q **neutrino** momentum

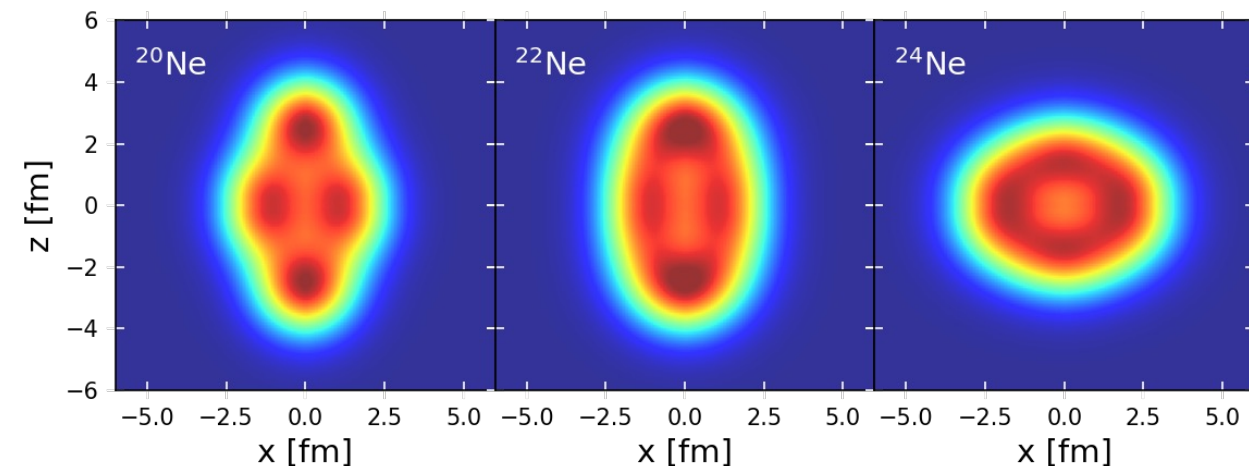
[W. Bambynek, H. Behrens, et al., Rev. Mod. Phys. 49, 77 (1977).]

Ground state



Density Functional Theory

$$\frac{\delta \mathcal{H}}{\delta \rho} \quad \frac{\delta \mathcal{L}}{\delta \psi^*} \quad \frac{\delta \mathcal{L}}{\delta \psi}$$



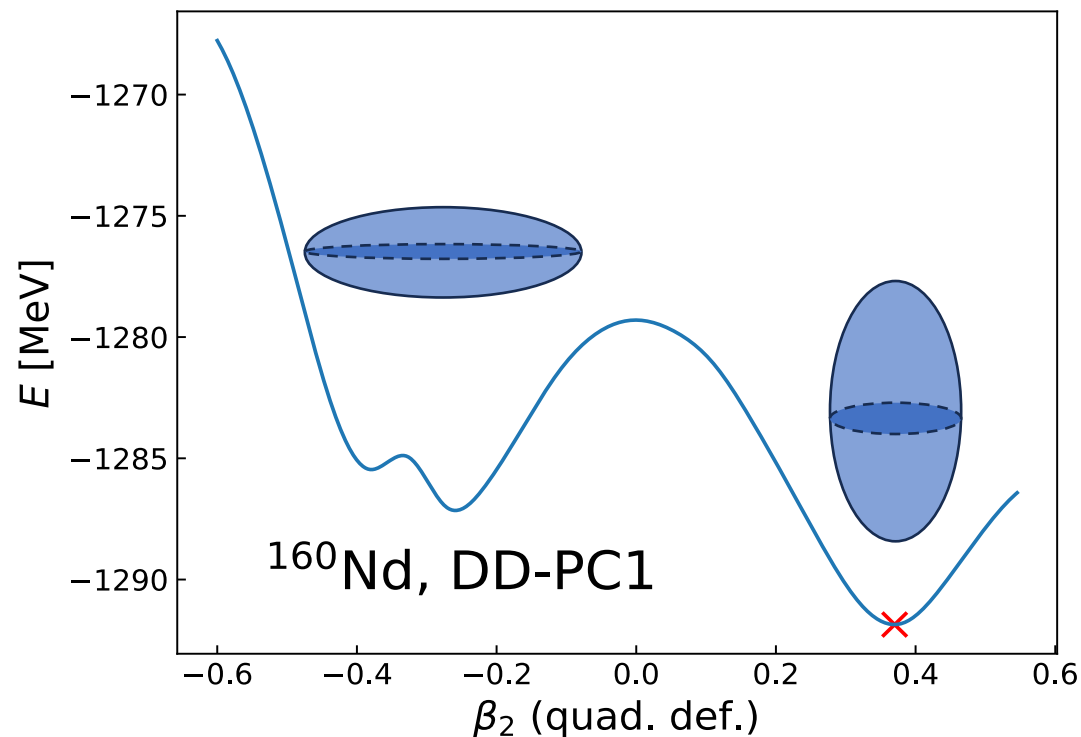
[J. Meng, *Relativistic density functional for nuclear structure*. Vol. 10. World Scientific (2016).]

Solve relativistic Hartree-Bogoliubov equation:

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -h + \lambda \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}$$

h : mean field, Δ : pairing field, E_k : q.p. energies

Quadrupole constraint (β_2) potential energy curve (PEC):

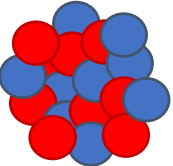
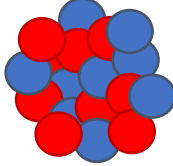


Excited states

Quasiparticle Random-Phase Approximation (QRPA)

$$\begin{array}{c} \nu \\ \text{blue circle} \end{array} \begin{array}{c} \nu' \\ \text{blue circle} \end{array} \begin{array}{c} \pi \\ \text{red circle} \end{array} \begin{array}{c} \pi' \\ \text{red circle} \end{array} \begin{array}{c} \mathbb{R} \end{array} = \begin{array}{c} \text{dotted line} \\ \mathbb{R}^0 \\ \text{dotted line} \end{array} + \begin{array}{c} \text{dotted line} \\ \boxed{\mathbb{W}} \\ \text{dotted line} \end{array}$$

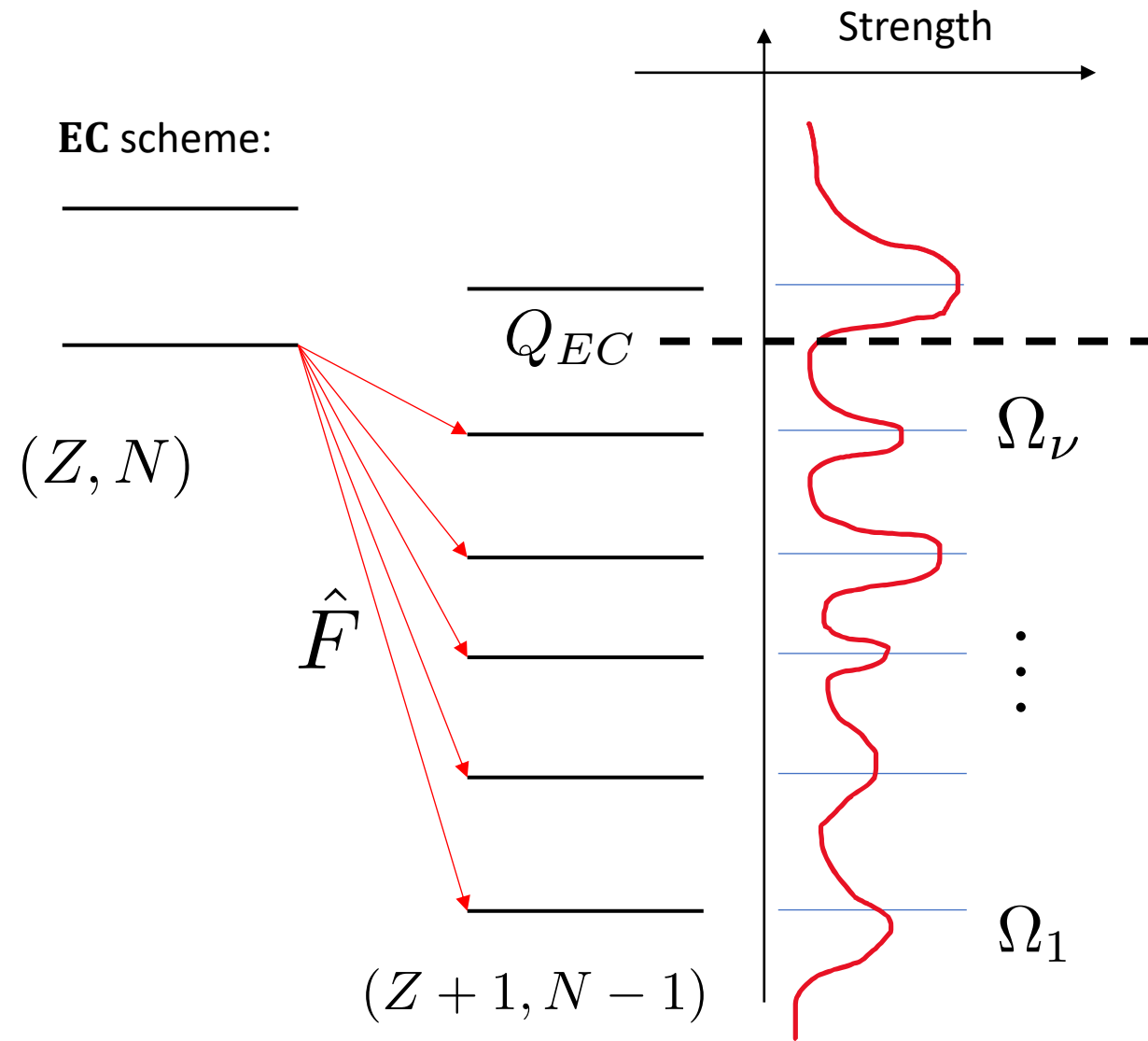
$$S(\omega) = -\frac{1}{\pi} \text{Im} \hat{F}^\dagger \mathbb{R} \hat{F}, \quad |\langle i | \hat{F} | 0 \rangle|^2 \sim S(\omega \rightarrow \Omega_i)$$


 $\hat{F} = \sum_{pn} F_{pn} a_p^\dagger a_n$


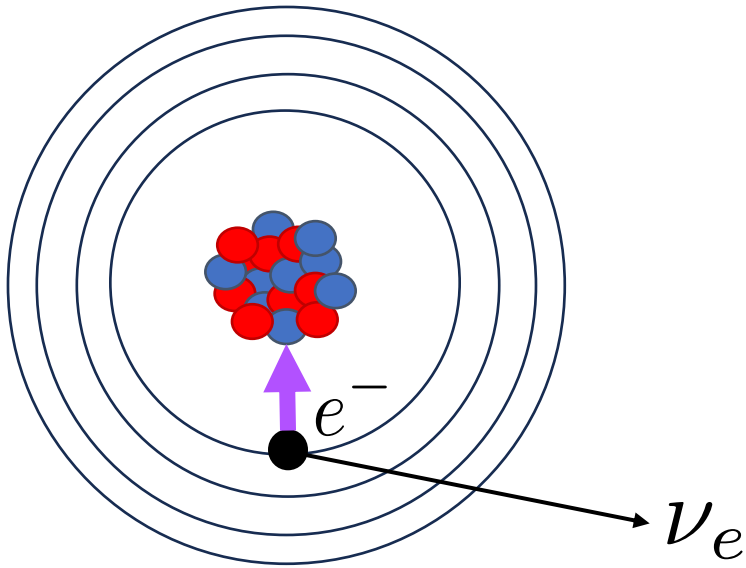
$$\rho_{g.s.} \rightarrow \rho_{g.s.} + \boxed{\delta\rho(\omega)} e^{-i\omega t} + \text{h.c.}$$

[A. Ravlić, Y.F. Niu et al., PRC 104, 064302 (2021).]

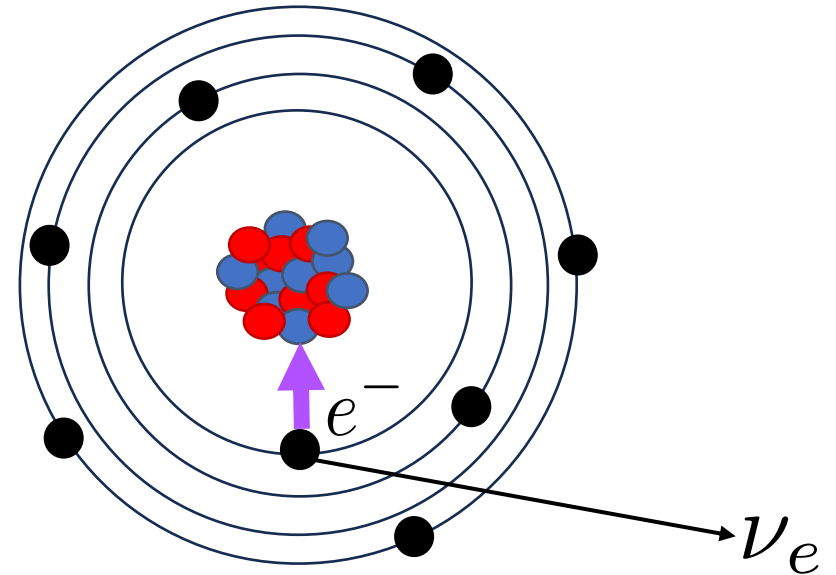
[A. Ravlić, T. Nikšić et al., PRC 110, 024323, (2024).]



What about leptons?

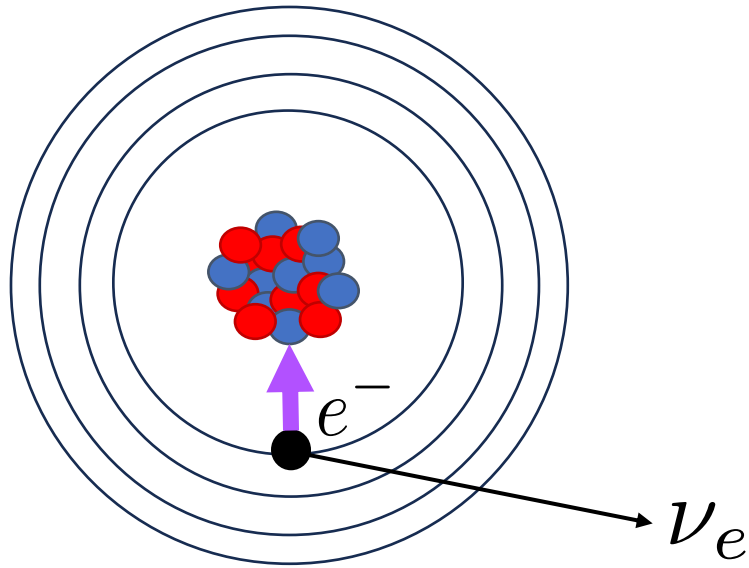


Single-particle orbital



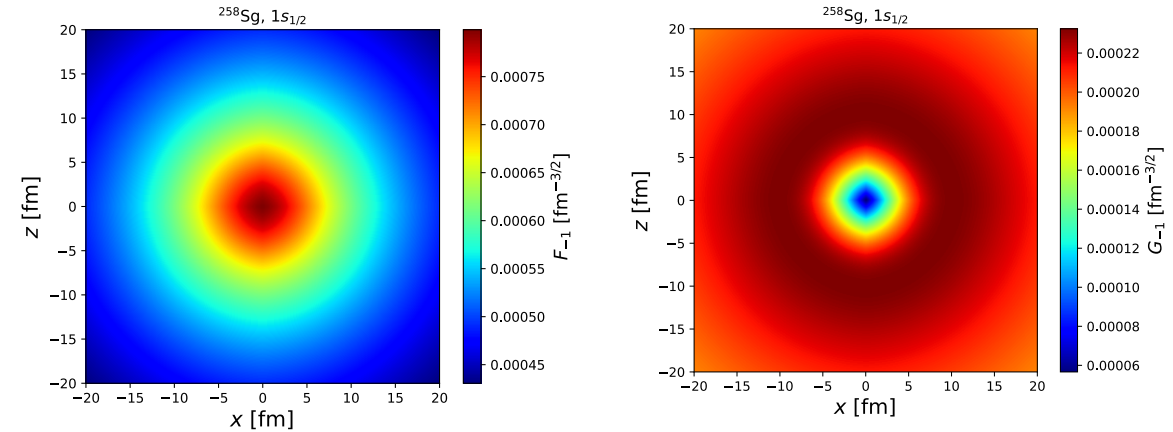
Multiple electrons in the cloud

What about leptons?

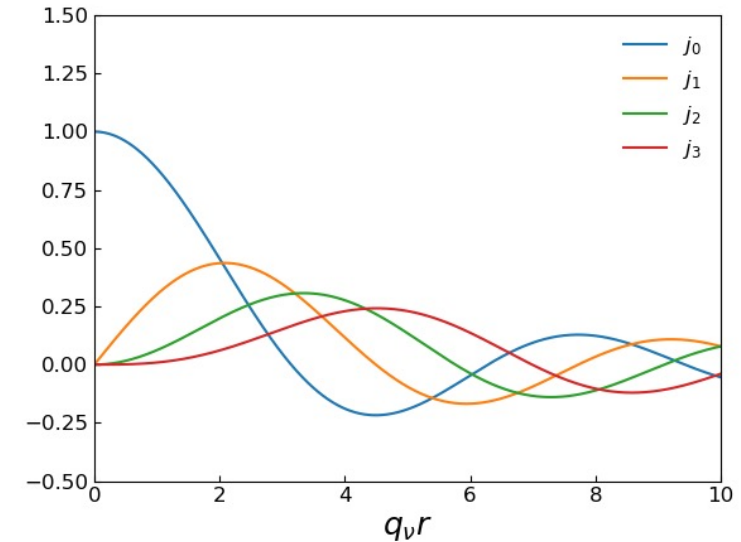


Single-particle orbital

- For **electron**: Solve the Dirac equation with nuclear charge distribution

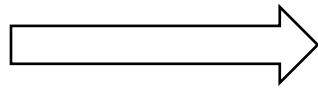


- For **neutrino**: expand into multipoles, spherical Bessel functions

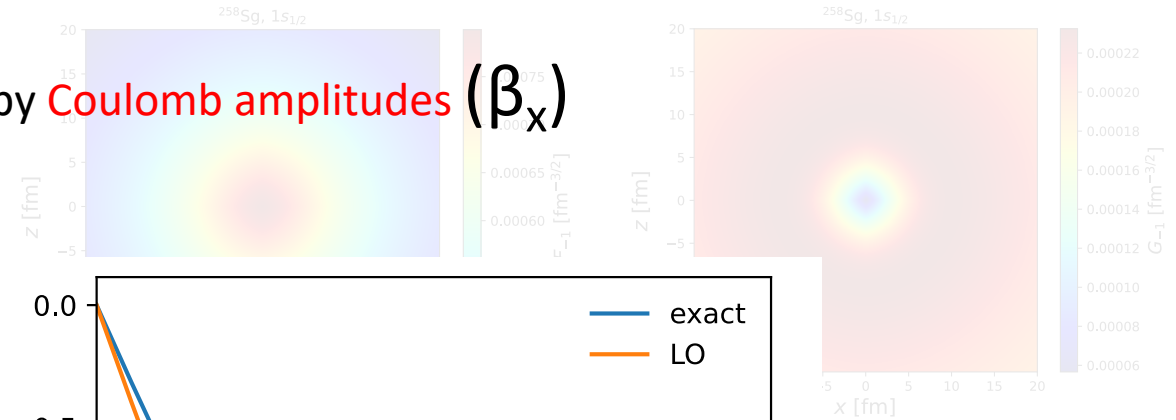
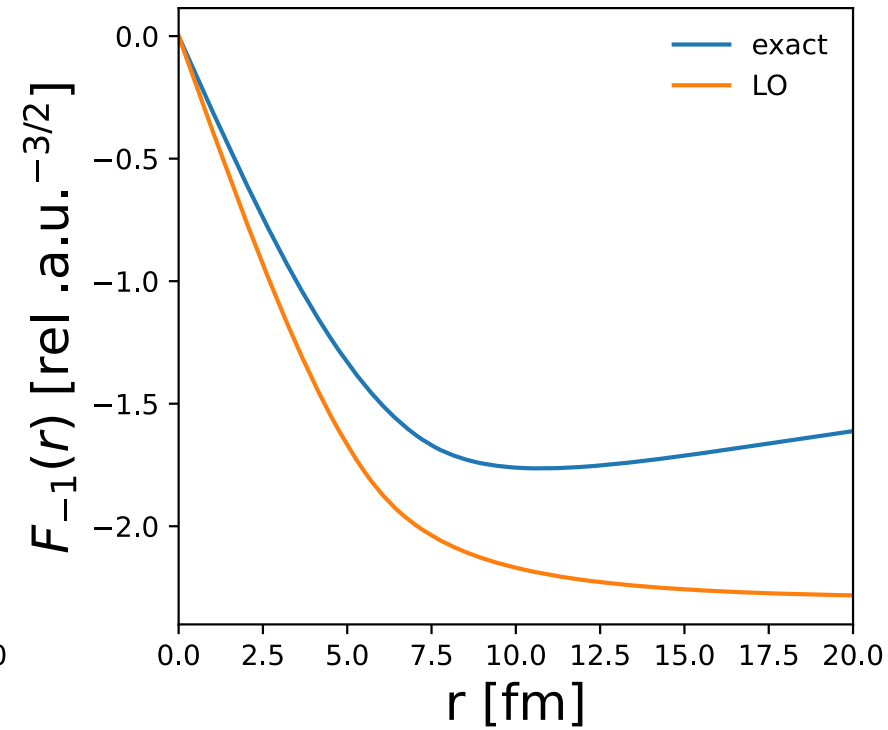
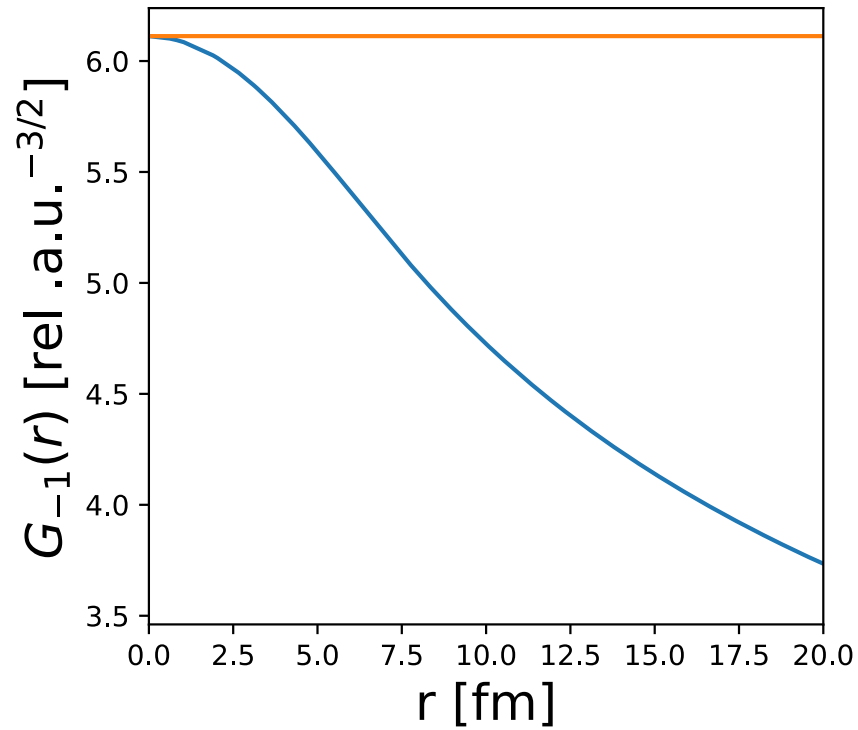


It is challenging to take full spatial distribution of lepton wave functions into account

What about leptons?



Parametrize atomic physics by **Coulomb amplitudes** (β_x)



LO expression for EC

$$\lambda_{EC} = \frac{\ln 2}{K} \sum_x \sum_{i,f} n_x C_x^{(i,f)} \underbrace{f_x(W_0^{(i,f)})}_{\text{phase-space factor:}} \quad W_0^{(i,f)} = E_i - E_f$$

[F. Salvat, et al., Comput. Phys. Commun. 90, 151 (1995).]

Coulomb amplitudes (RADIAL solver)

$f_x = \frac{\pi}{2} \beta_x^2 q_x^2$ neutrino transfer

→ Nuclear physics is contained in **shape-factor** $C_x^{(i,f)}$ with the form:

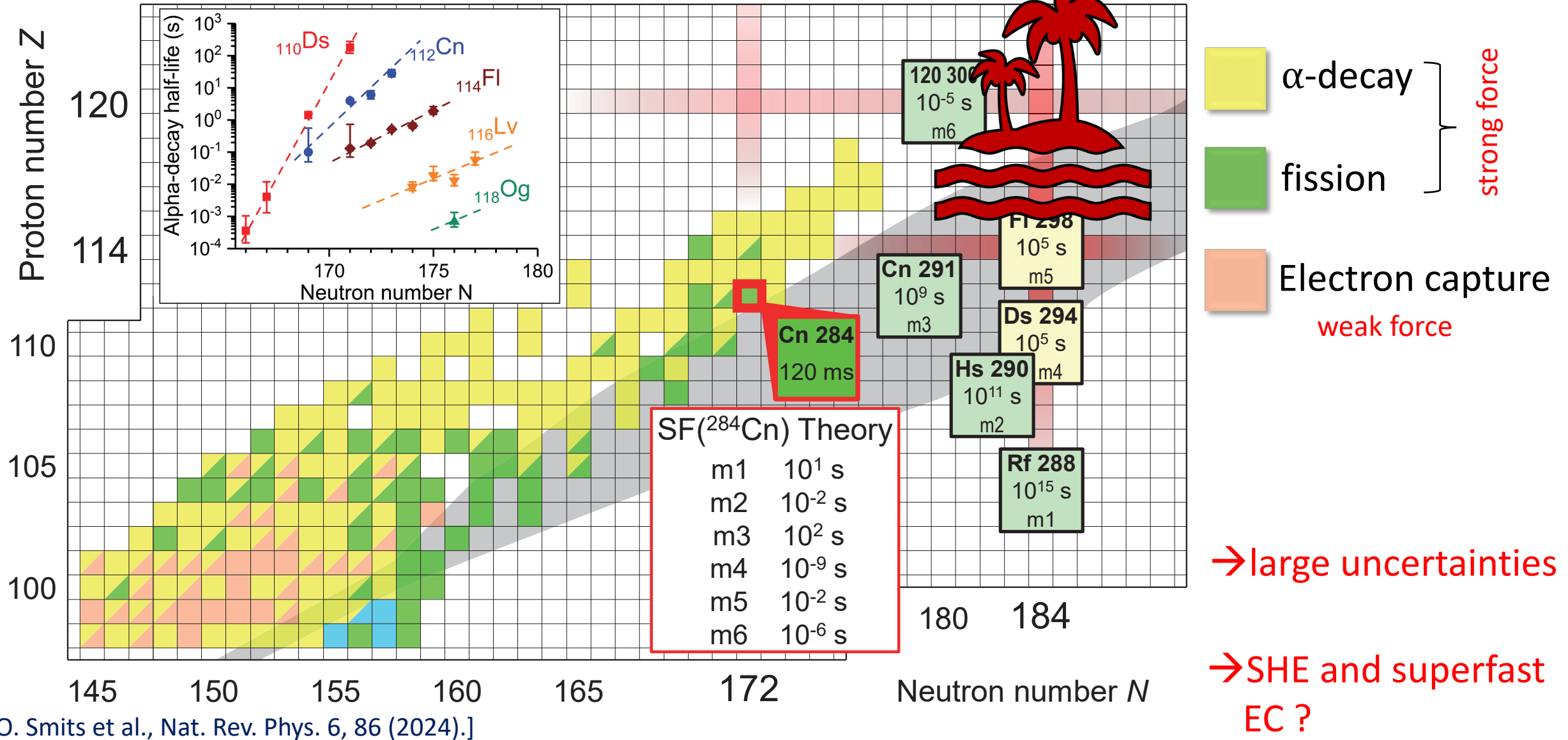
$$C_x(\omega) = \boxed{ka_x(\omega)} + 2\text{sgn}(\kappa_x) \boxed{kb_x(\omega)} + \boxed{kc_x(\omega)}, \quad \kappa_x = \pm 1$$

[W. Bambynek, H. Behrens, et al., Rev. Mod. Phys. 49, 77 (1977).]

Superheavy nuclei

Superheavy nuclei

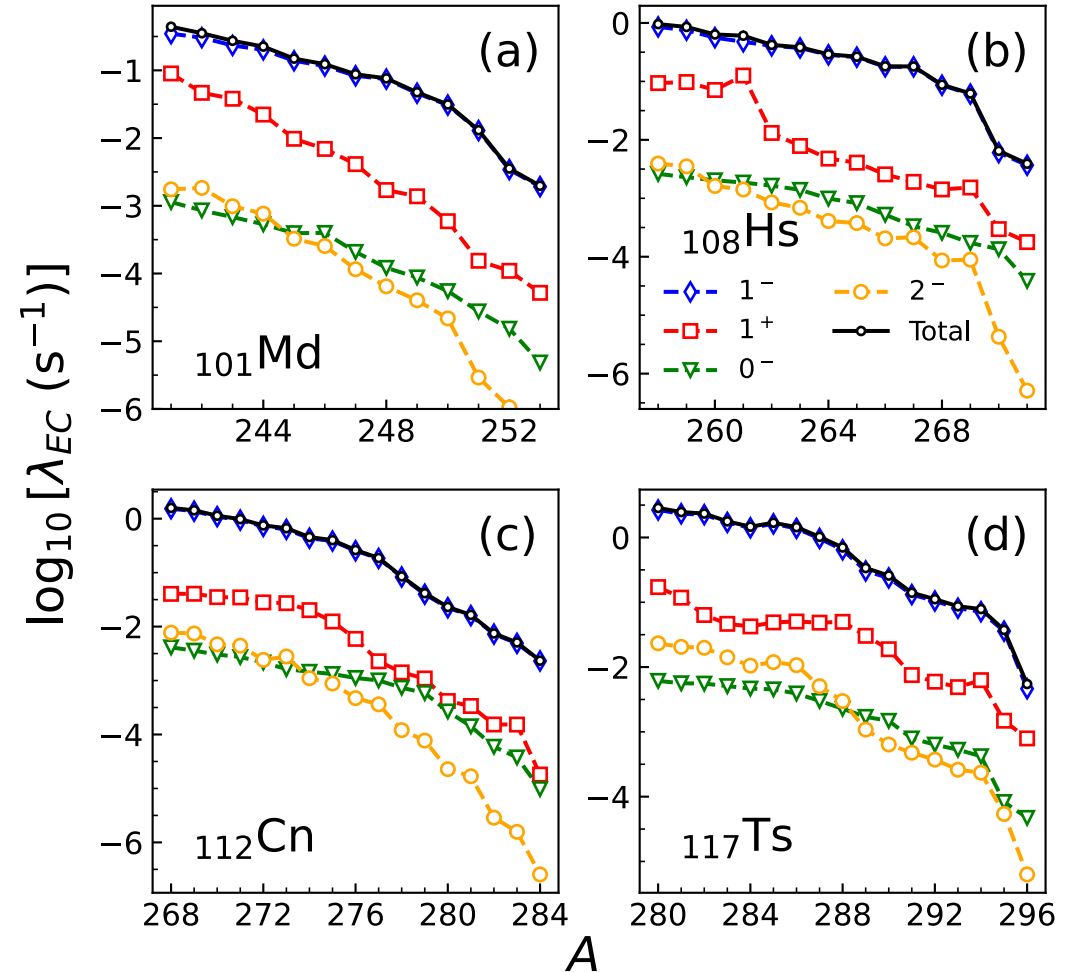
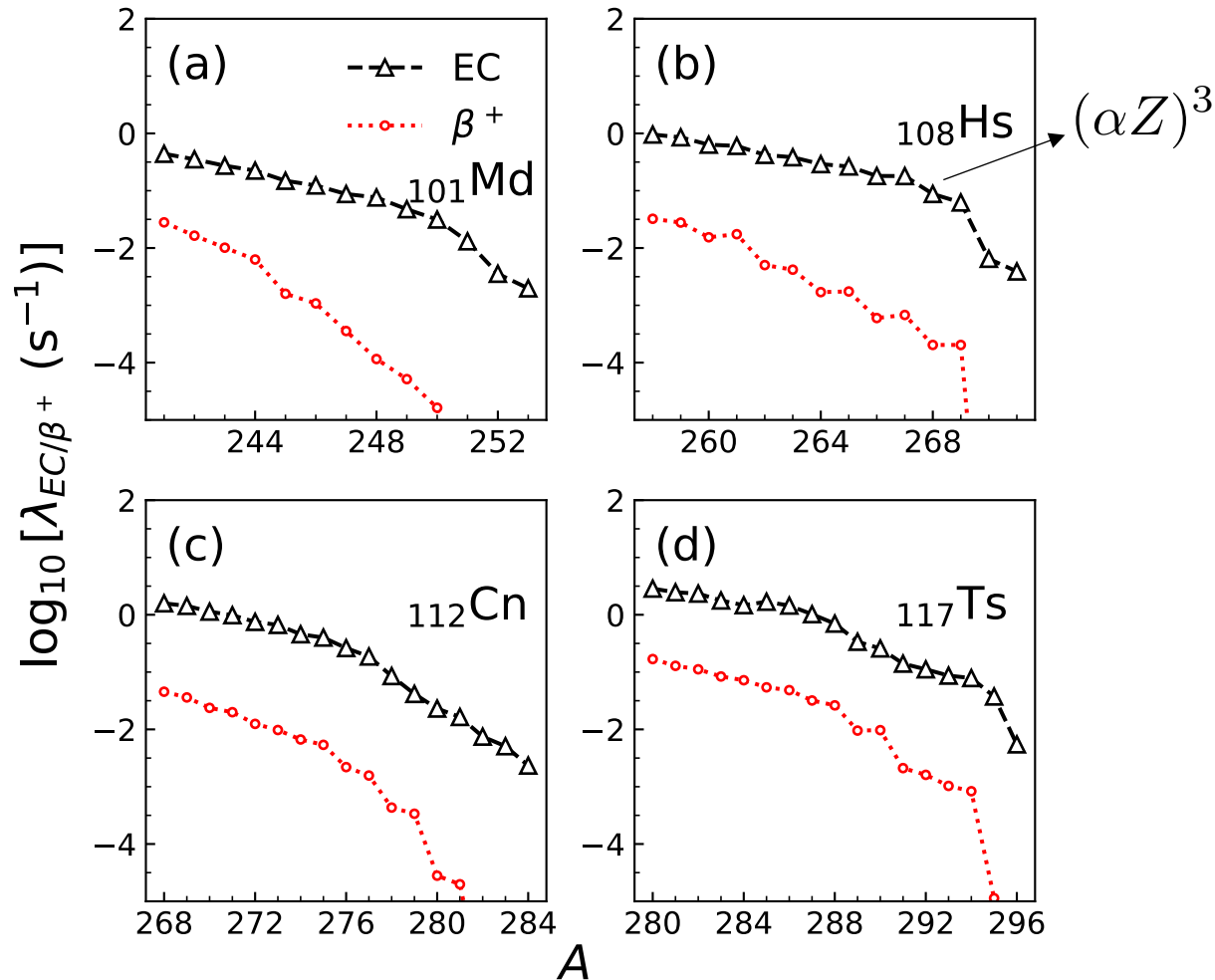
$$104 \leq Z \leq 118$$



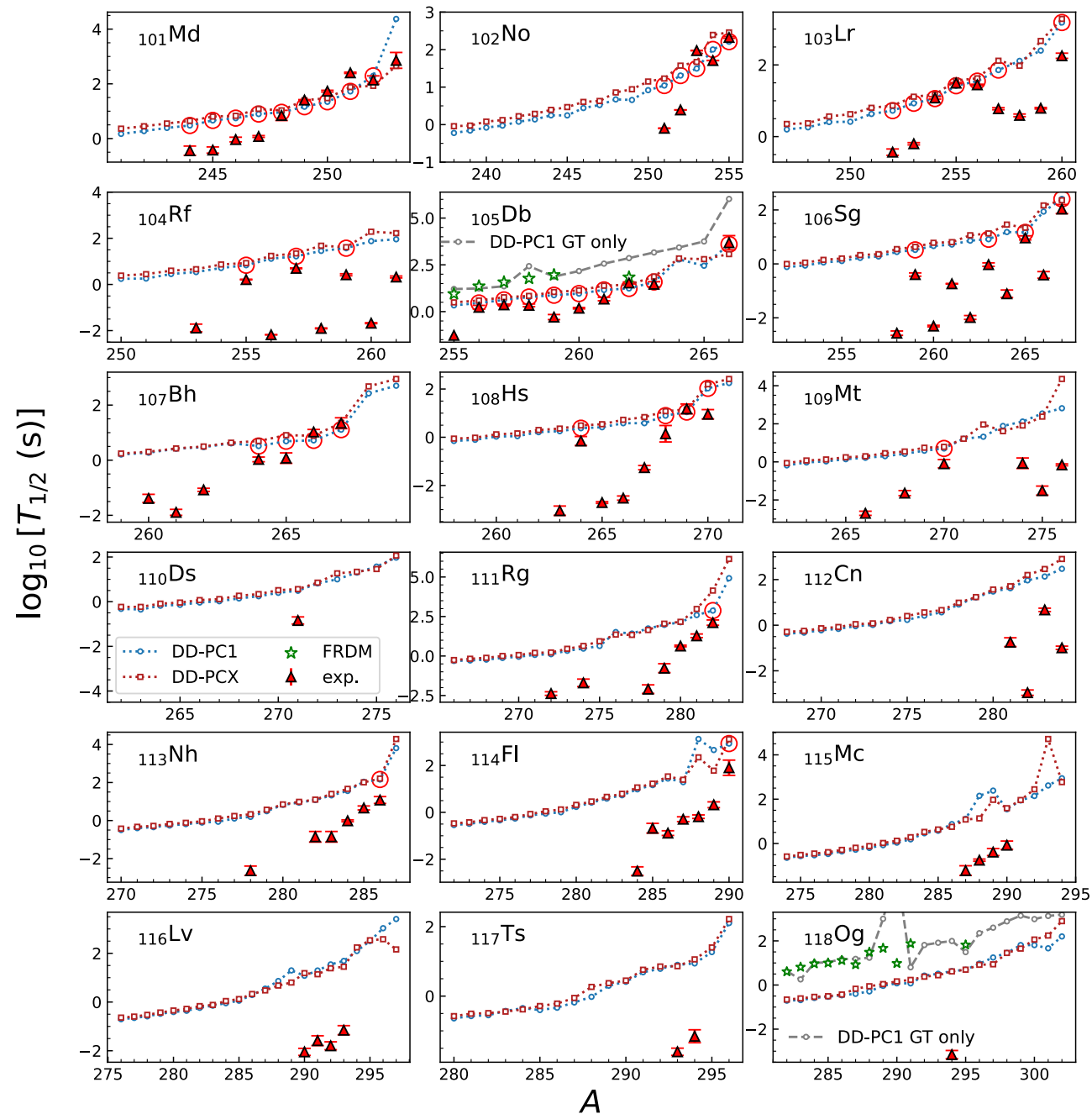
→ Goal: find candidates where EC could compete with fission and α -decay:

→ EC dominates over β^+ -decay:

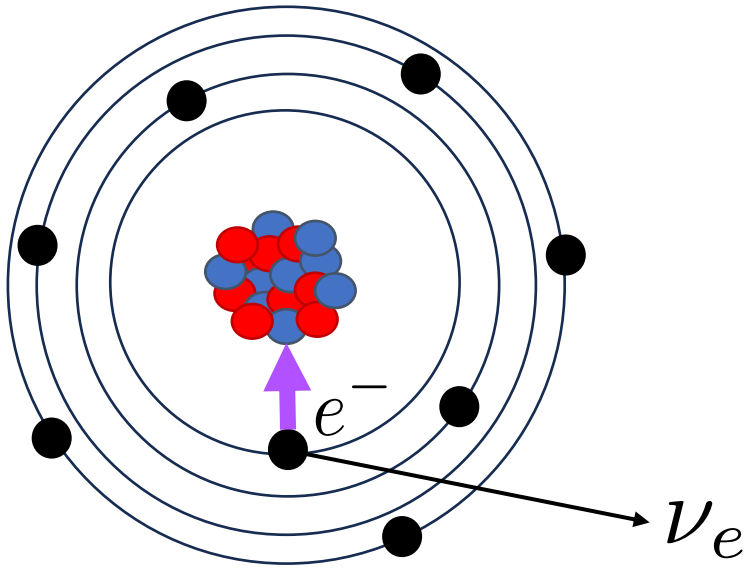
→ First-forbidden transitions dominate over allowed:



→ identify candidate where **EC** can compete with **α -decay** and **fission**
 → we consider two EDFs: **DD-PC1** and **DD-PCX**
 → Found candidates where EC could have branching **> 5%**
 → previous calculations miss important contribution of **FF transitions**



What if we take full radial dependence of lepton wavefunctions into account ?



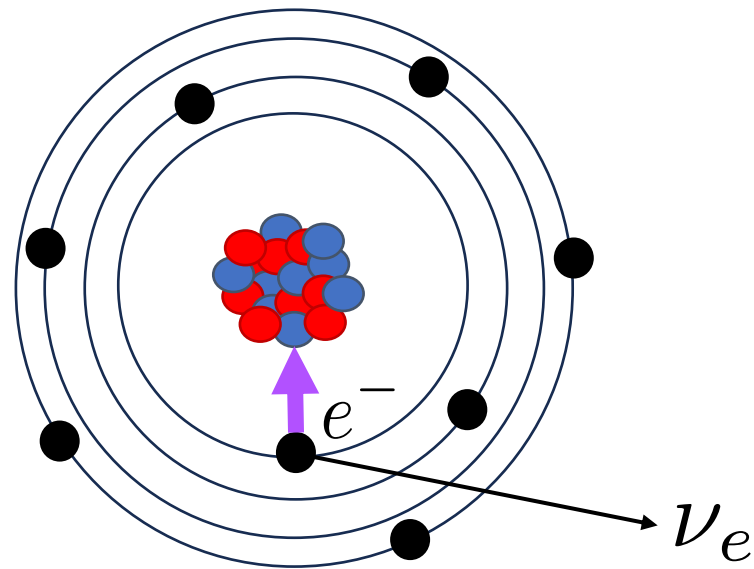
Multiple electrons in the cloud

- Solve the many-body problem

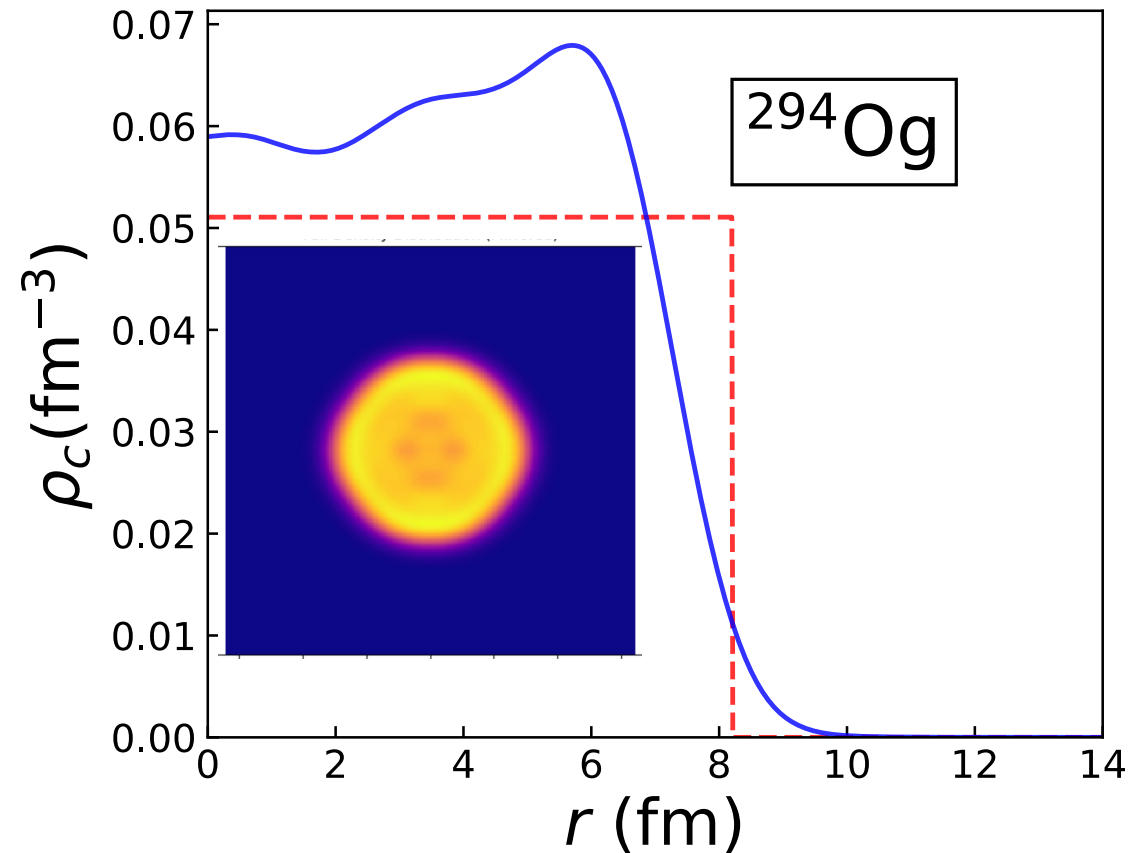
$$\hat{H} = \hat{H}_D + \hat{V}_{\text{nuc}} + \underbrace{\sum_{i=1}^{Z-1} \sum_{j=i+1}^Z \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}}_{\text{interaction between electrons}},$$

nucleus-electron
Coulomb
interaction

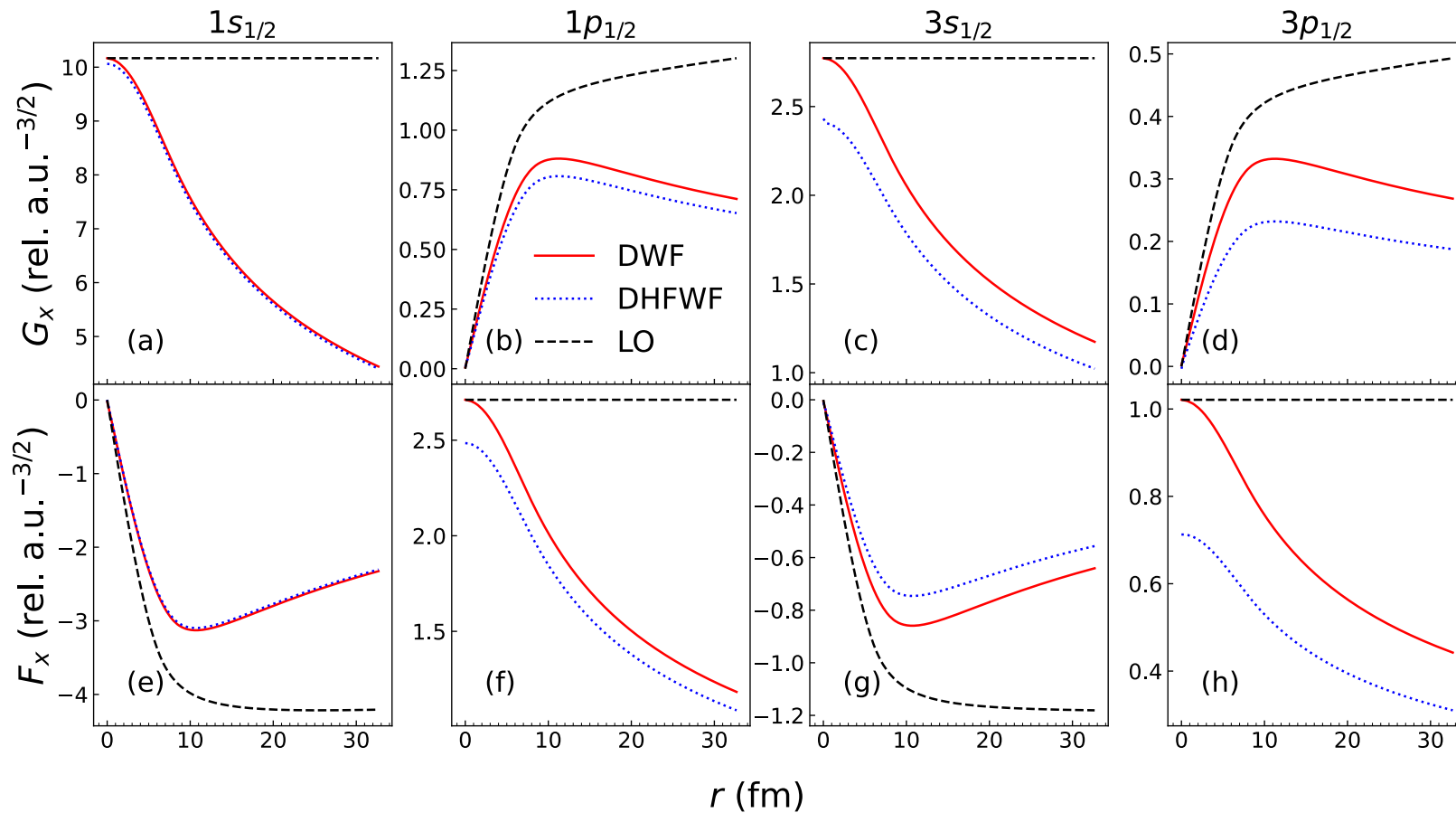
What if we take full radial dependence of lepton wavefunctions into account ?



Multiple electrons in the cloud



What if we take full radial dependence of lepton wavefunctions into account ?

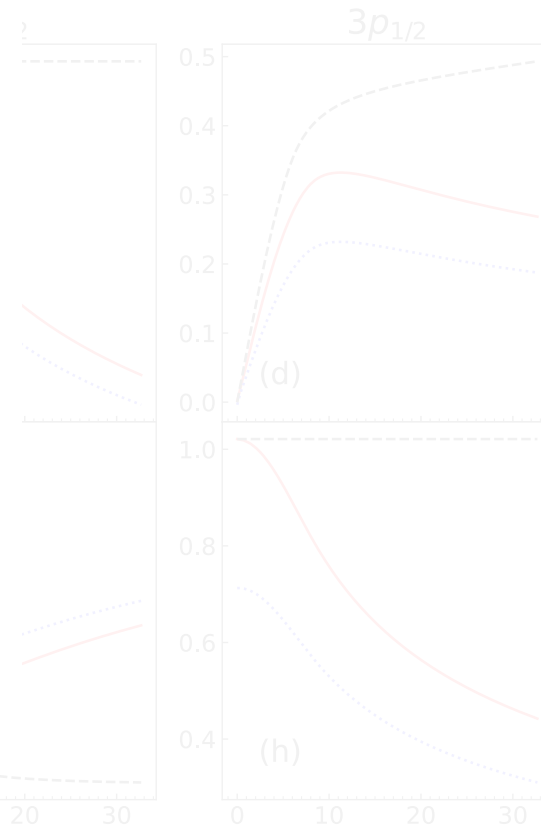
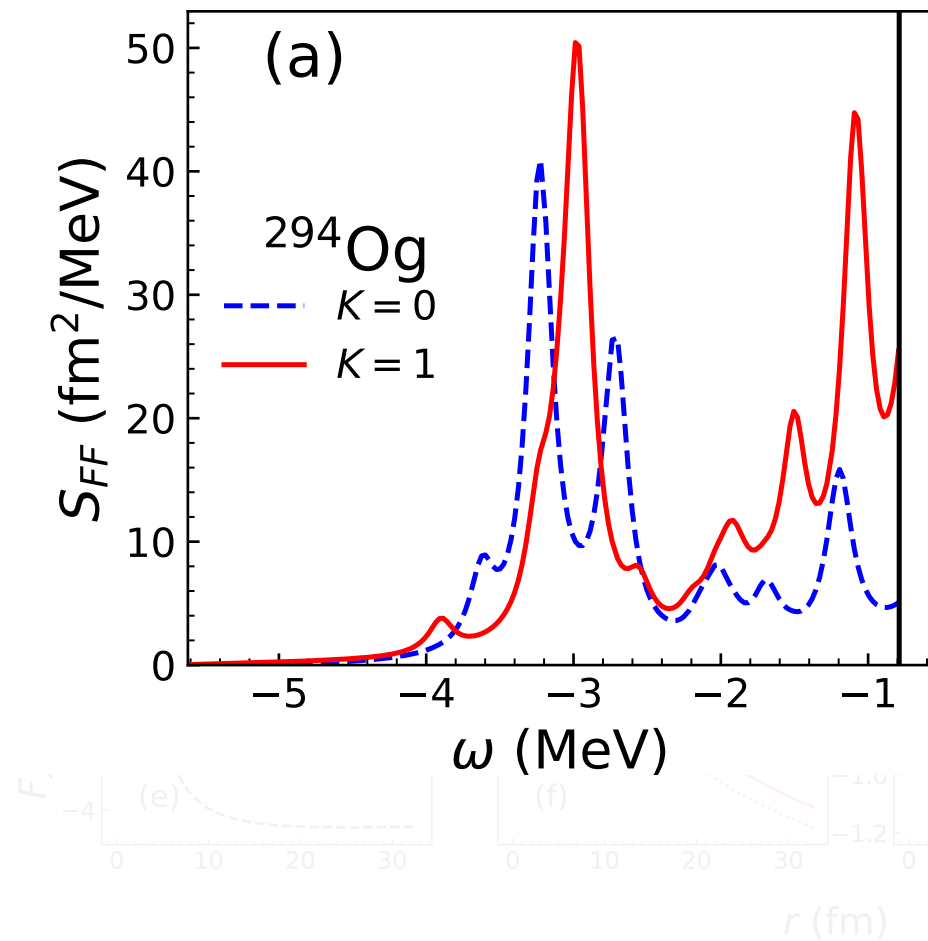


$$\Psi_{e^-}(\mathbf{r}) = \begin{pmatrix} G_{\kappa_x}(\mathbf{r})\chi_{\kappa_x\mu_x} \\ iF_{\kappa_x}(\mathbf{r})\chi_{\kappa_x\mu_x} \end{pmatrix},$$

DWF – Dirac single-particle
DHFWF – Dirac Hartree-Fock
LO – lowest order calculation

[A. Ravlic, P. Schwerdtfeger and W. Nazarewicz, PRC 111, 064323 (2025).]

What if we take full radial dependence of lepton wavefunctions into account ?

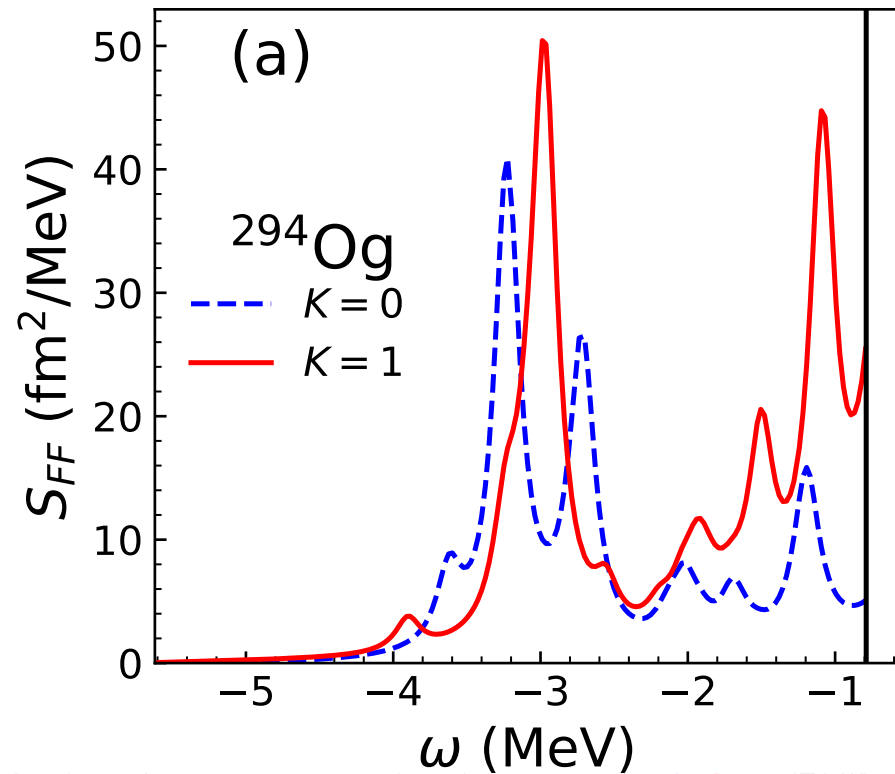


$$\Psi_{e^-}(\mathbf{r}) = \begin{pmatrix} G_{\kappa_x}(\mathbf{r})\chi_{\kappa_x\mu_x} \\ iF_{\kappa_x}(\mathbf{r})\chi_{\kappa_x\mu_x} \end{pmatrix},$$

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What if we take full radial dependence of lepton wavefunctions into account ?

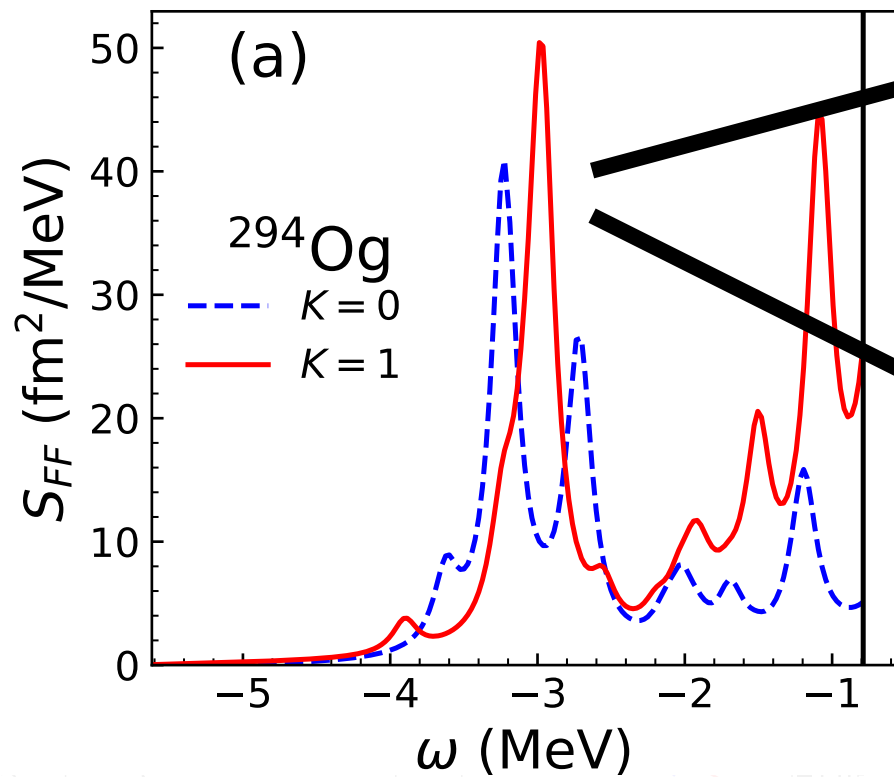


→ We can introduce transition density in the coordinate-space:

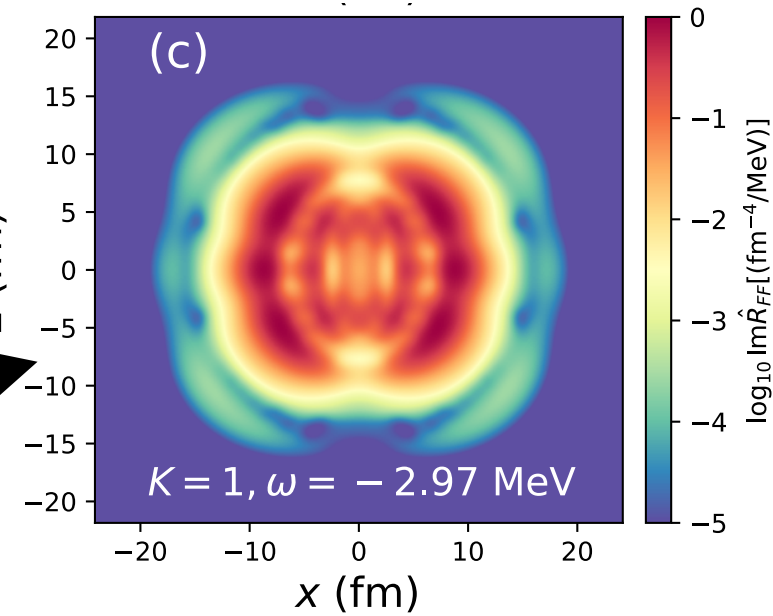
$$\langle 0 | \hat{F}_{JL} | \nu \rangle = \int d\mathbf{r} \delta\rho_{JL}(\Omega_\nu, \mathbf{r})$$

[A. Ravlic, P. Schwerdtfeger and W. Nazarewicz, PRC 111, 064323 (2025).]

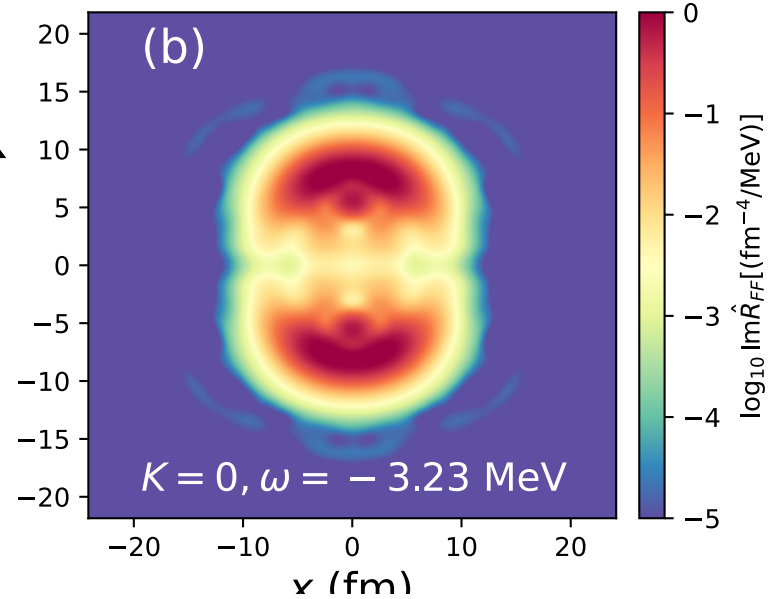
What if we take full radi
wavefunctions into accc



$z \text{ (fm)}$



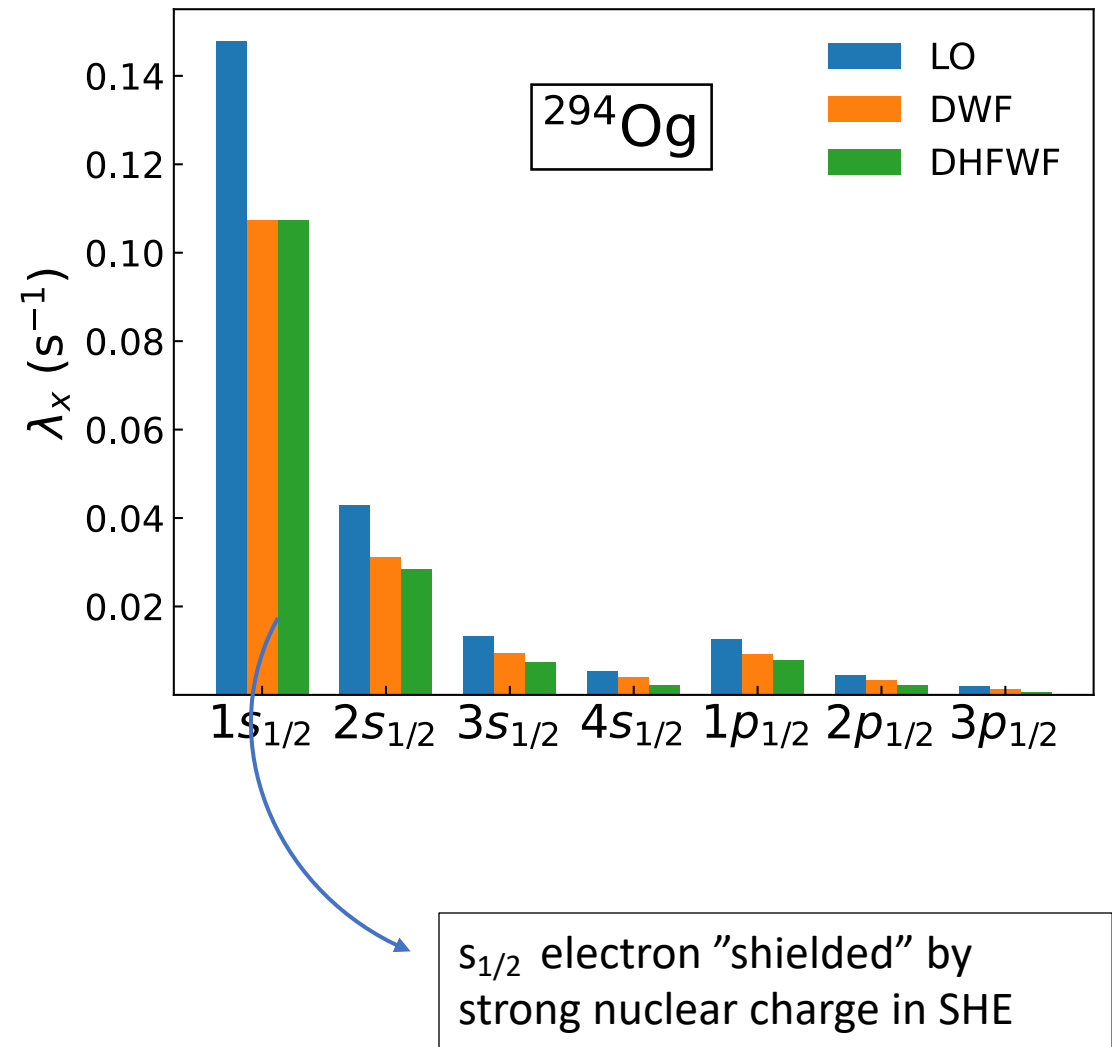
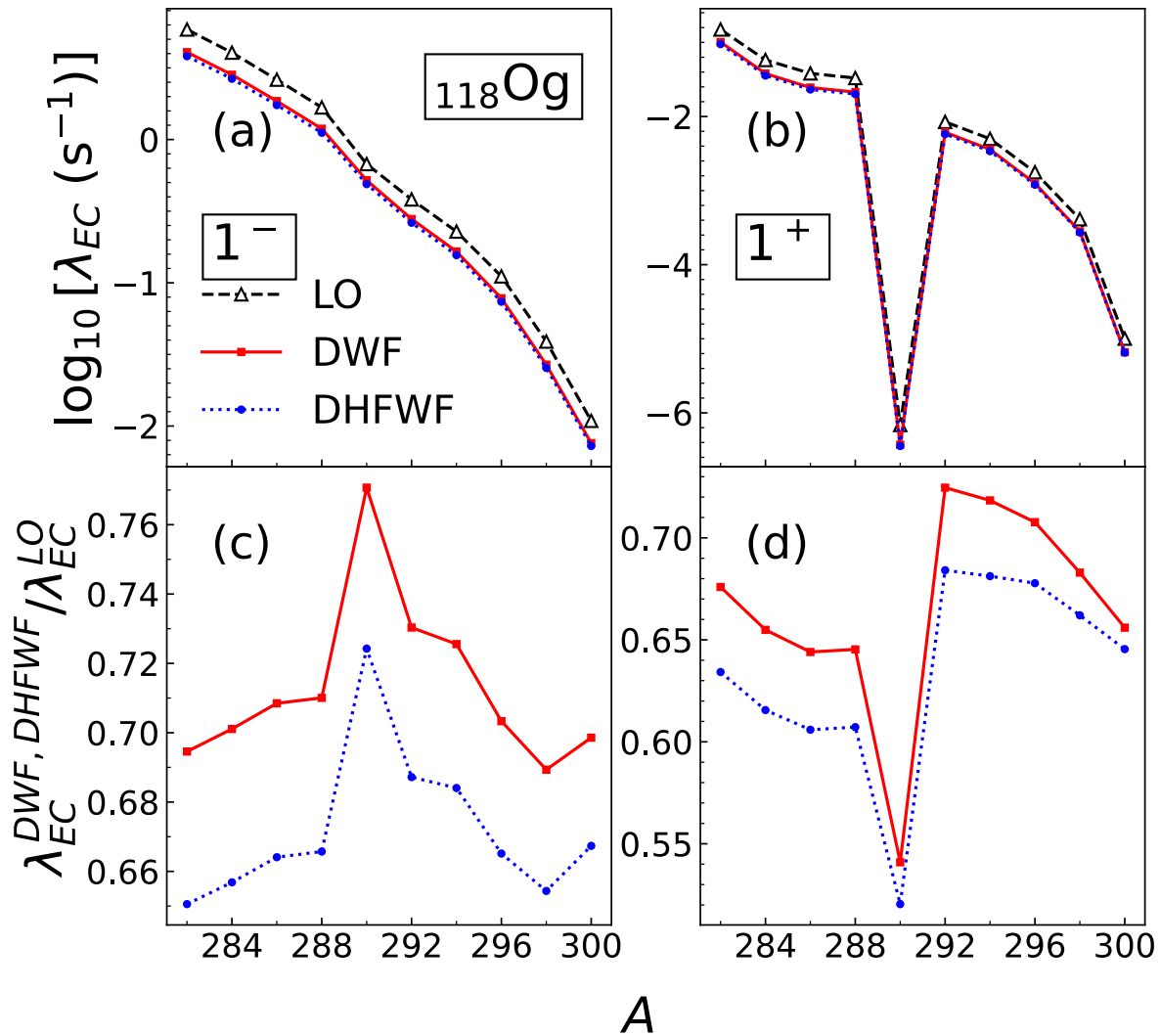
$z \text{ (fm)}$



$$\begin{pmatrix} G_{\kappa_x}(\mathbf{r}) \chi_{\kappa_x \mu_x} \\ i F_{\kappa_x}(\mathbf{r}) \chi_{\kappa_x \mu_x} \end{pmatrix},$$

DWF – Dirac single-particle
c Hartree-Fock
order calculation

werdtfeiger and W.
:111, 064323 (2025).]

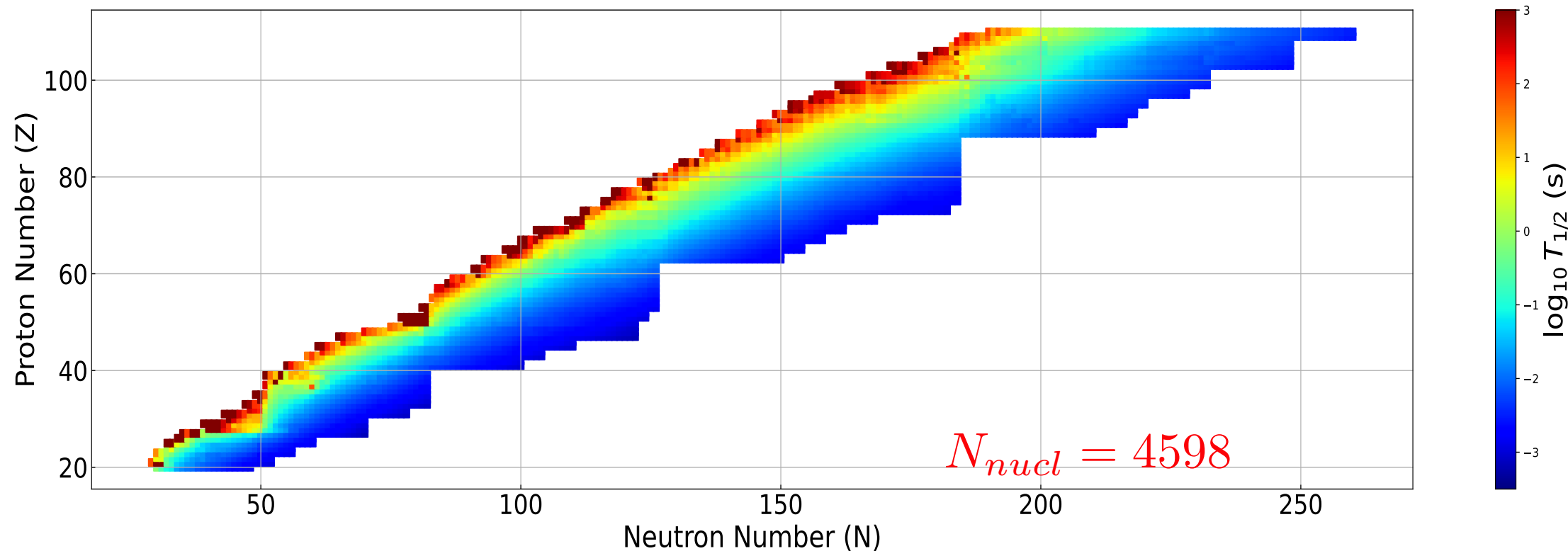


[A. Ravlic, P. Schwerdtfeger and W. Nazarewicz, PRC 111, 064323 (2025).]

Global calculations of β -decay rates

DD-PC1(X) + optimized time-odd terms

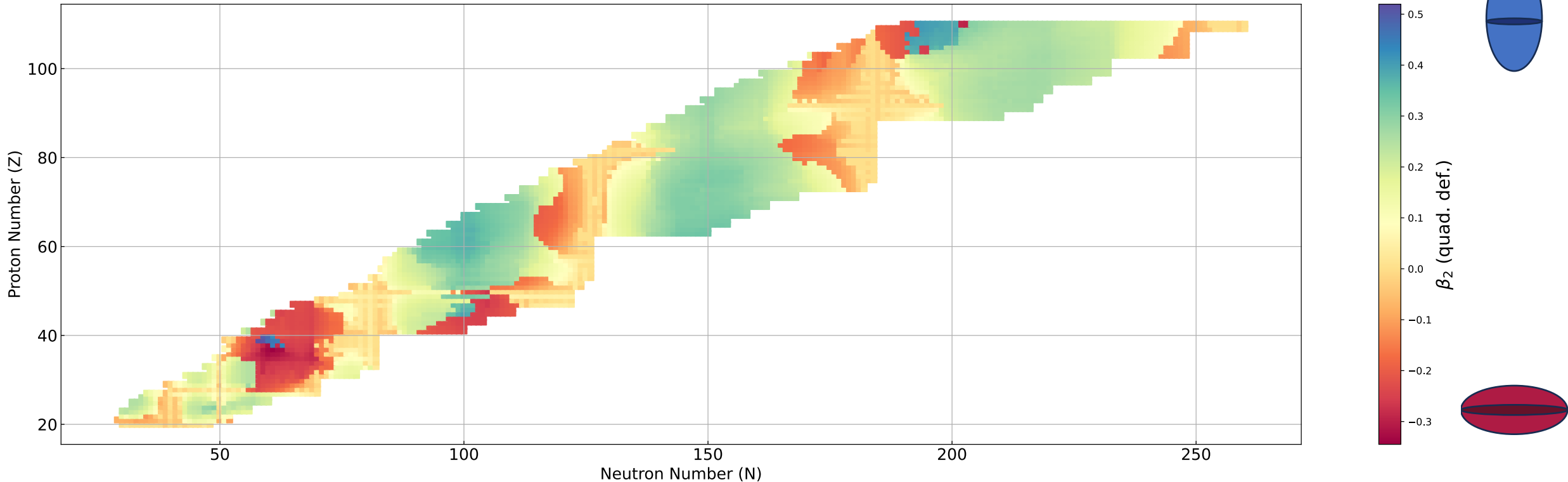
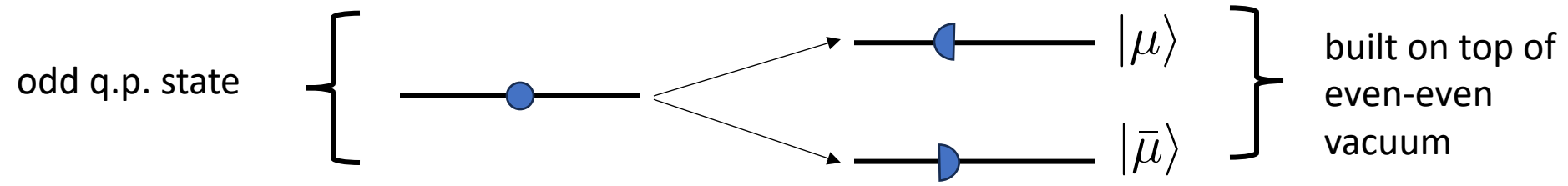
GT(1^+) + first forbidden (0^- , 1^- , 2^-)



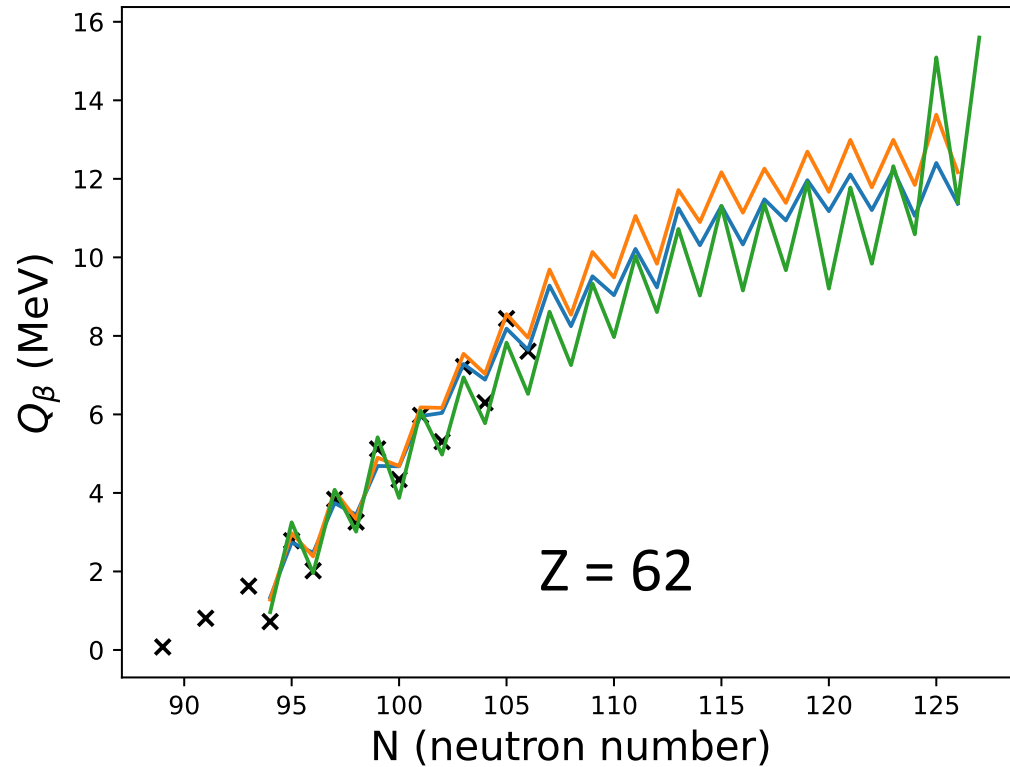
See Yukiya Saito's talk on Thursday !

[A. Ravlic, Y. Saito and W. Nazarewicz, in preparation (2025)]

- axially-deformed RHB state with reflection symmetry
- Equal Filling Approximation blocking RHB+QRPA for odd-A and odd-odd nuclei



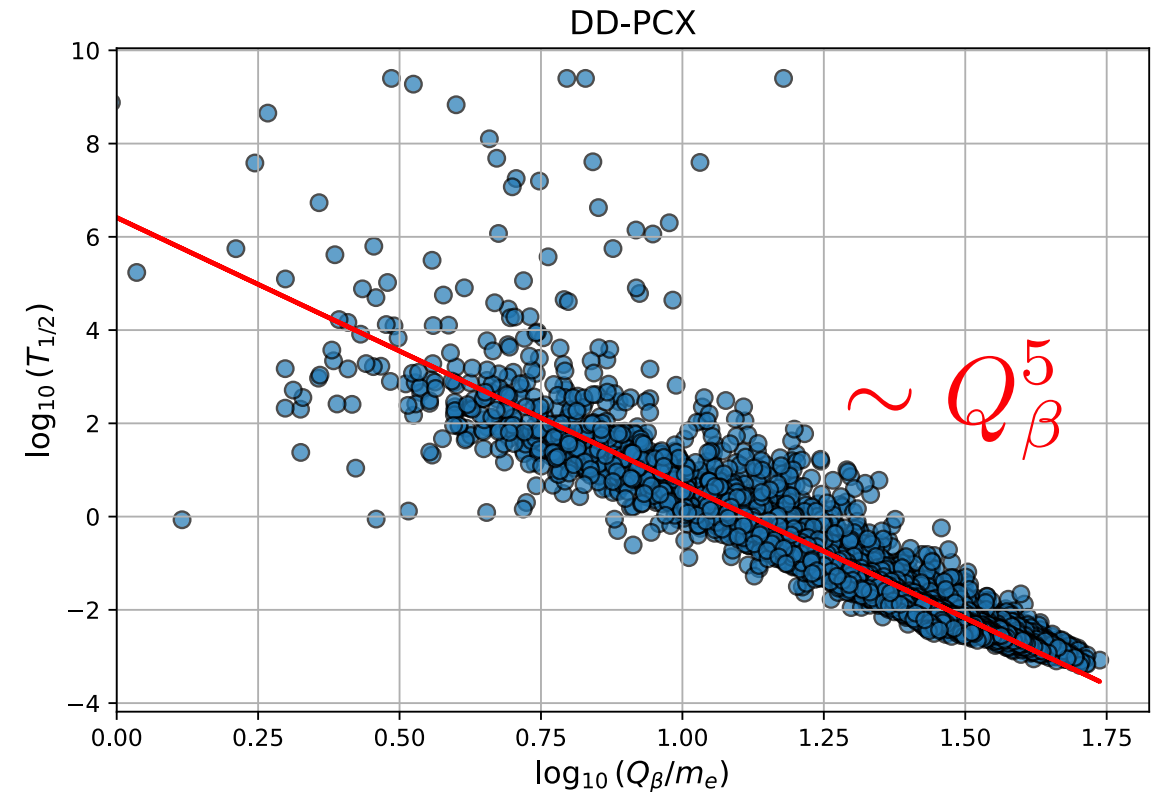
Q-values calculated self-consistently within the model:



Overall RMSE (micro-average)
DD-PC1: 0.9818 (N=959)
DD-PCX: 0.7687 (N=959)
Sk0: 0.8278 (N=958)

} in MeV

Half-lives vs Q-values:



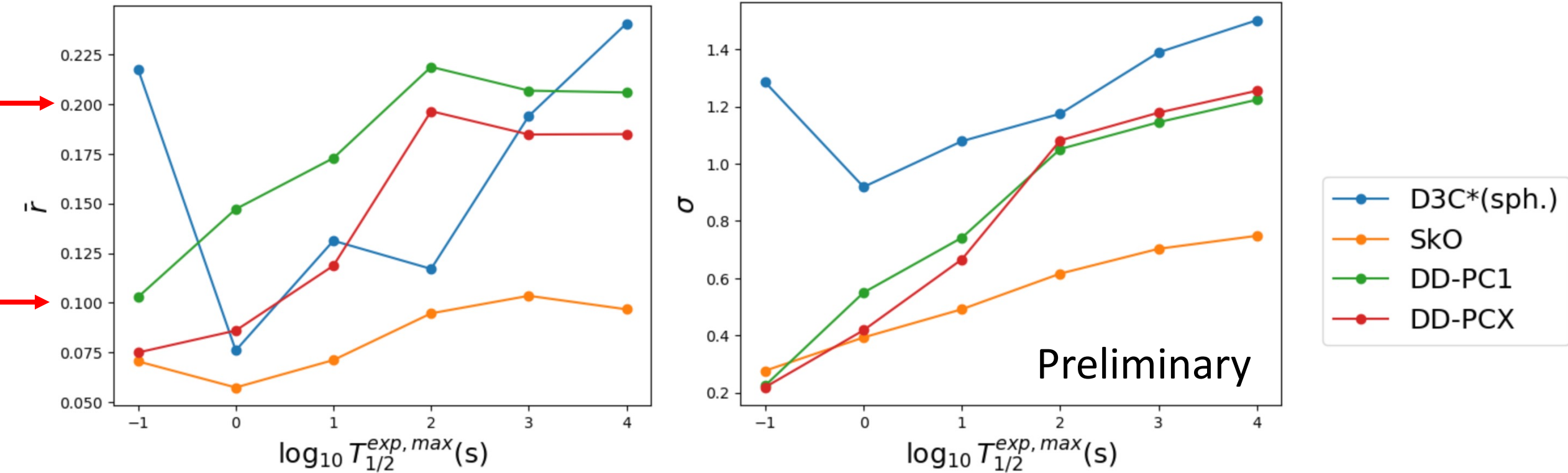
See discussion in:

[E. M. Ney, J. Engel, T. Li, N. Schunck, Phys. Rev. C 102, 034326 (2020)]

Performance on experimental data (NUBASE2020):

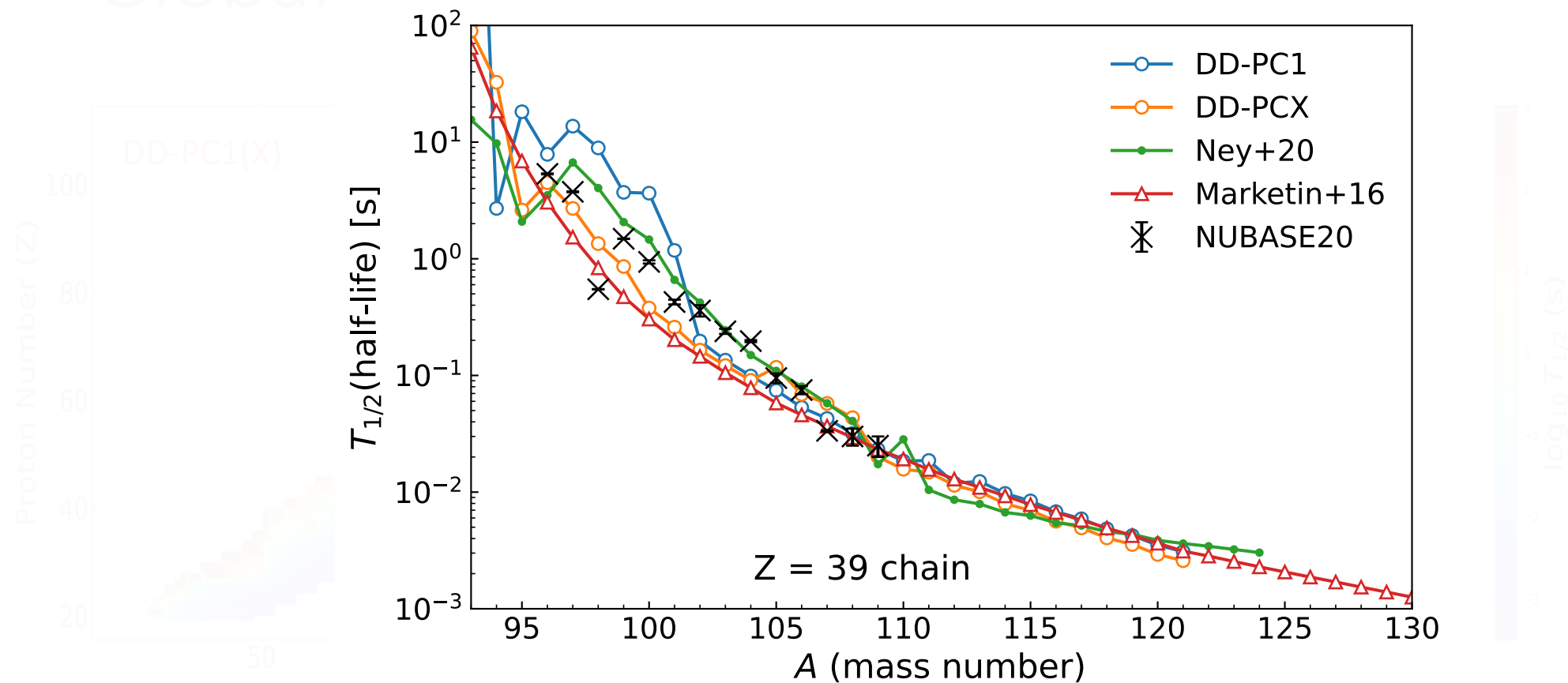
$$\bar{r} = \frac{1}{N} \sum_{i=1}^N r_i, \quad r_i = \log_{10} \frac{T_{1/2}^{calc}}{T_{1/2}^{exp}}$$

$$\sigma = \sqrt{\frac{1}{N} \sum_{i=1}^N (r_i - \bar{r})^2}$$



Half-life is just the moment of distribution, it hides a lot of underlying structure

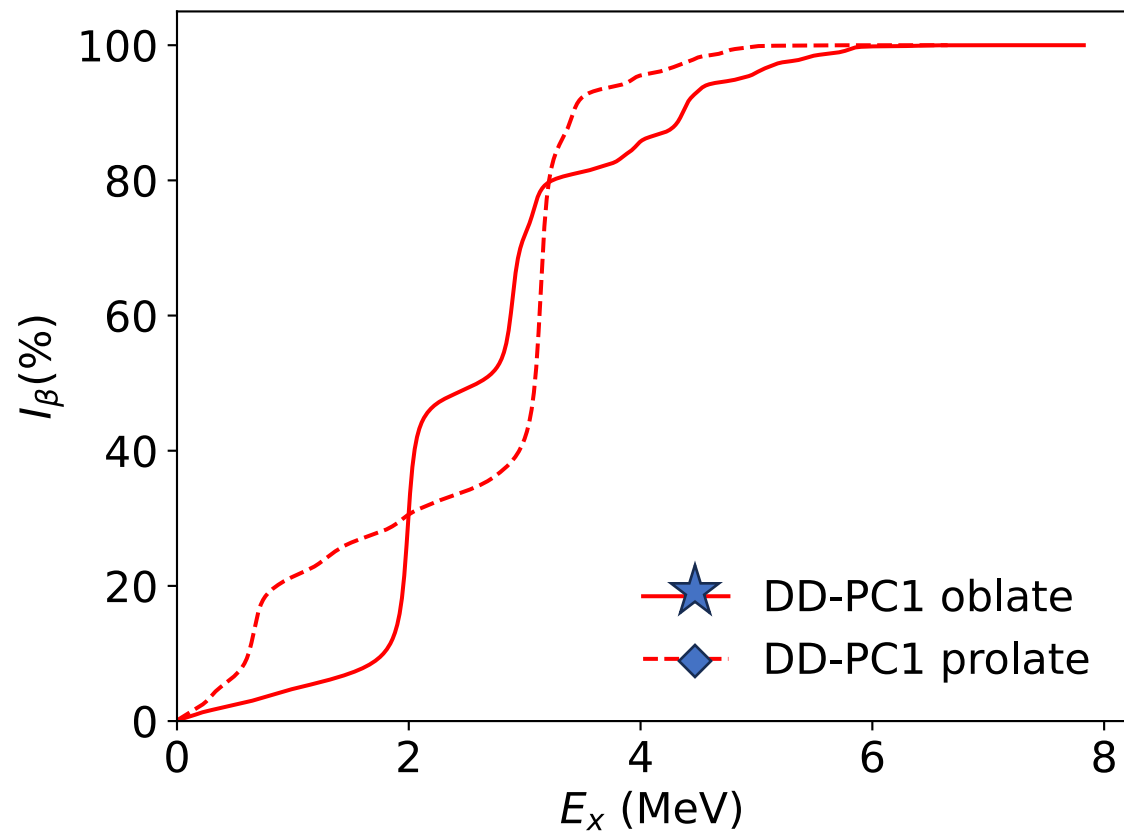
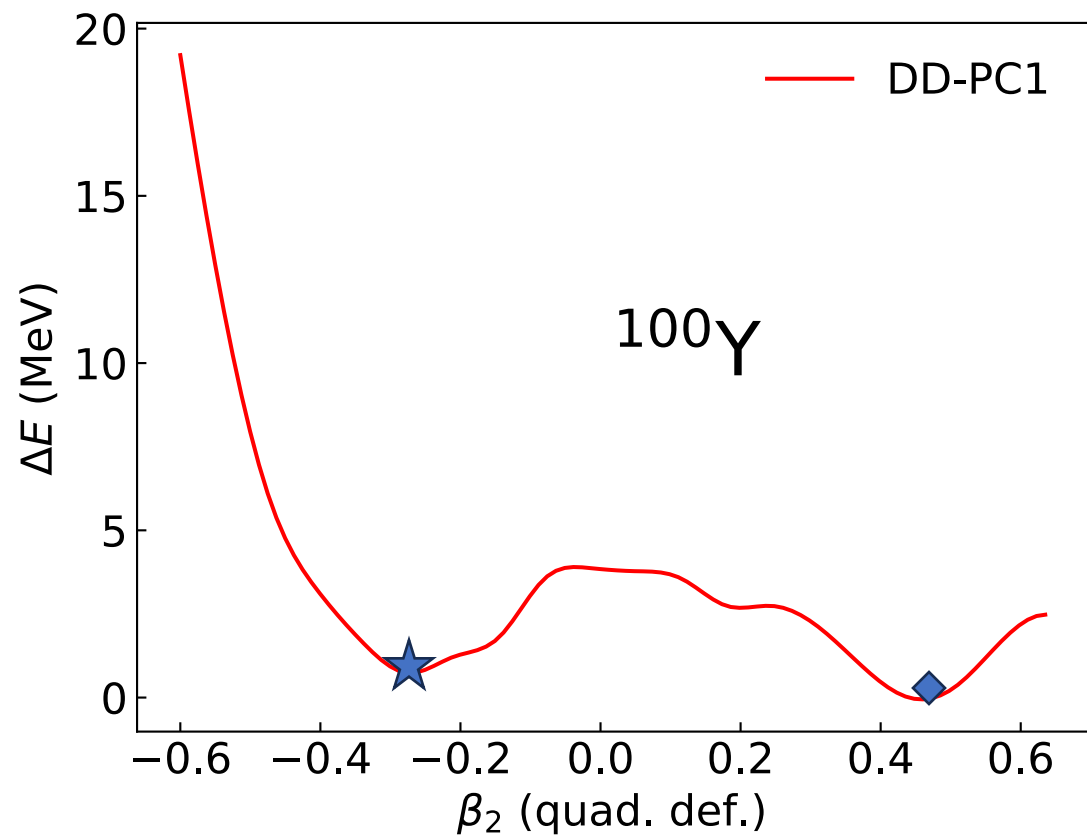
Global β -decay calculations



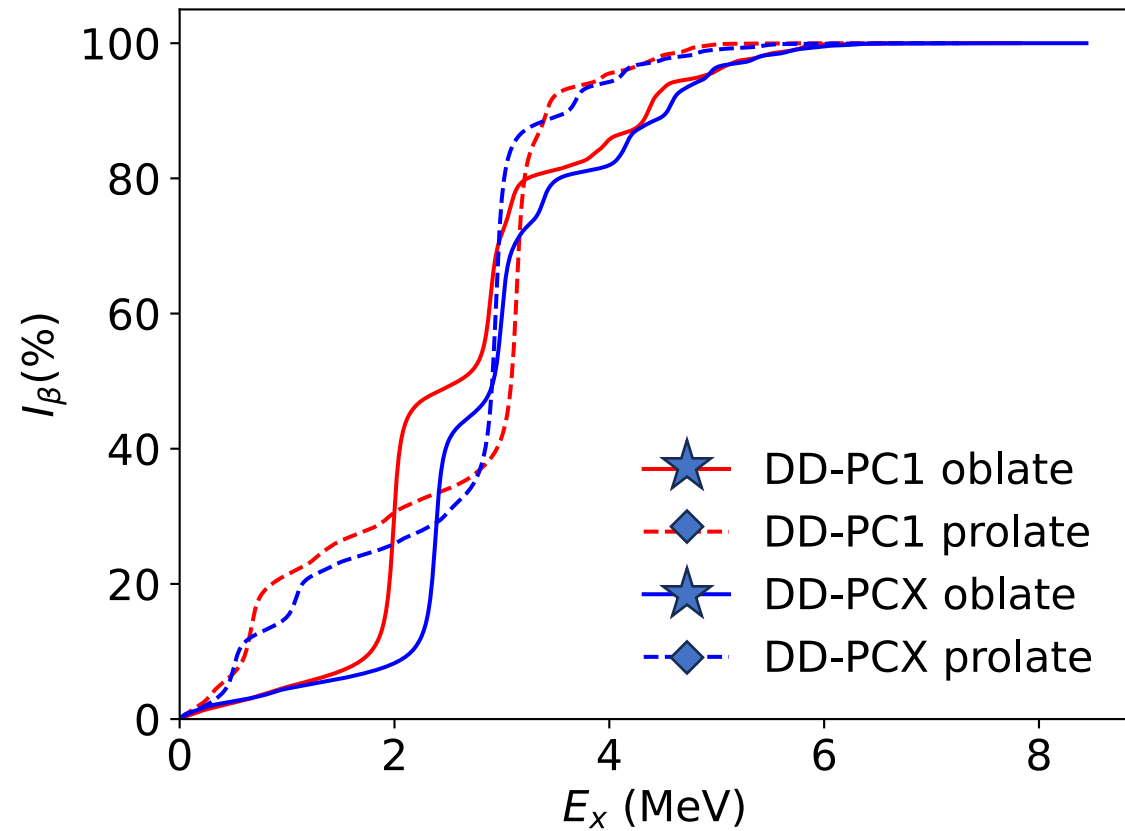
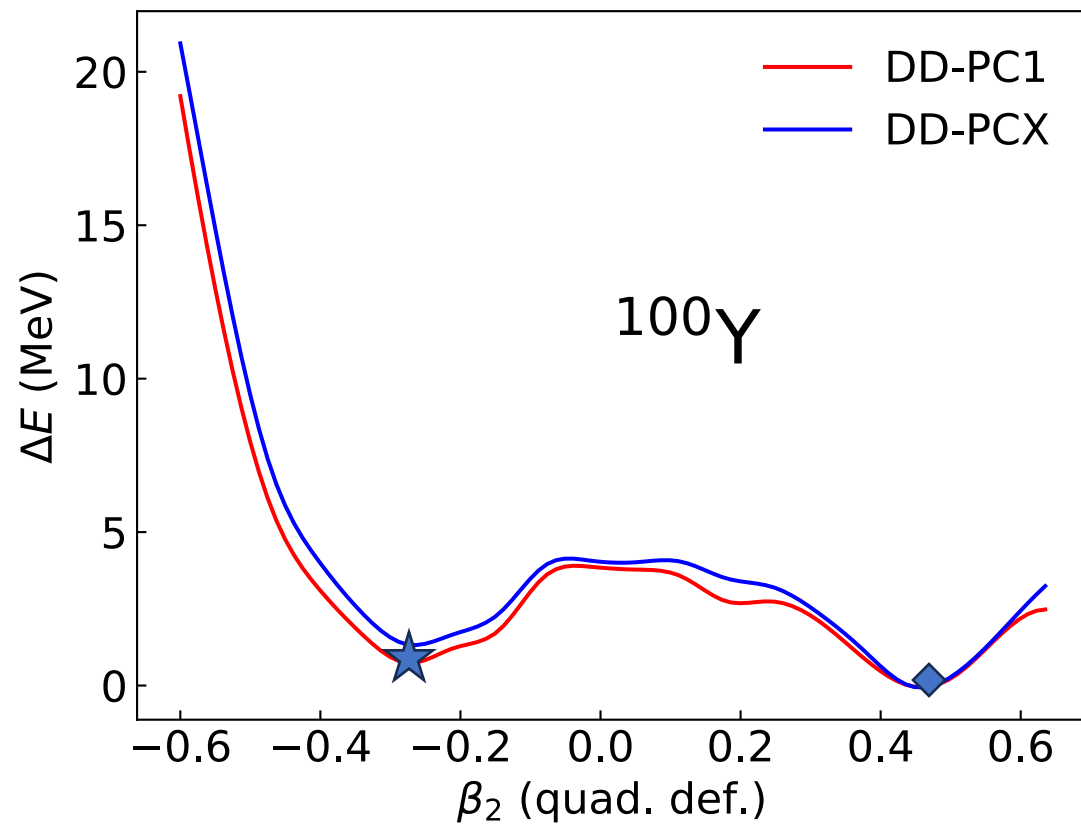
[A. Ravlic, Y. Saito and W. Nazarewicz, in preparation (2025)]

[T. Marketin, L. Huther, G. Martinez-Pinedo, PRC 93, 025805 (2016)]

[E. M. Ney, J. Engel, T. Li, N. Schunck, Phys. Rev. C 102, 034326 (2020)]



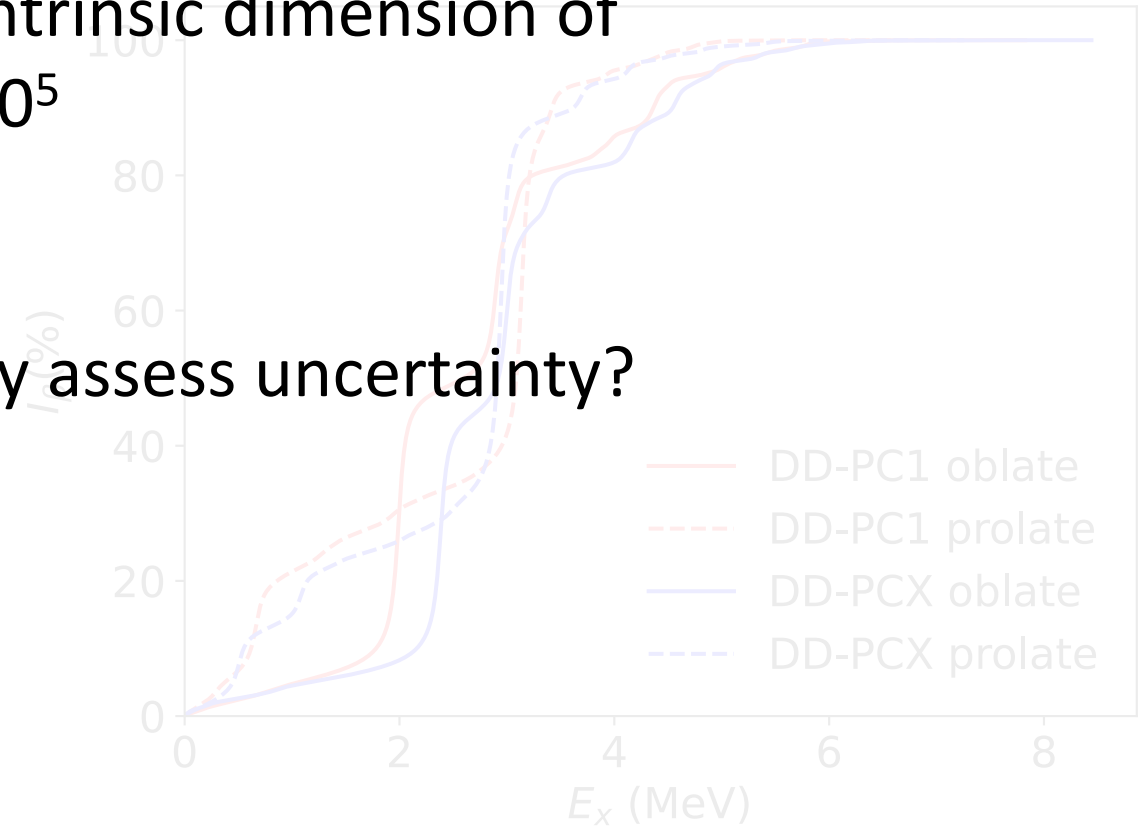
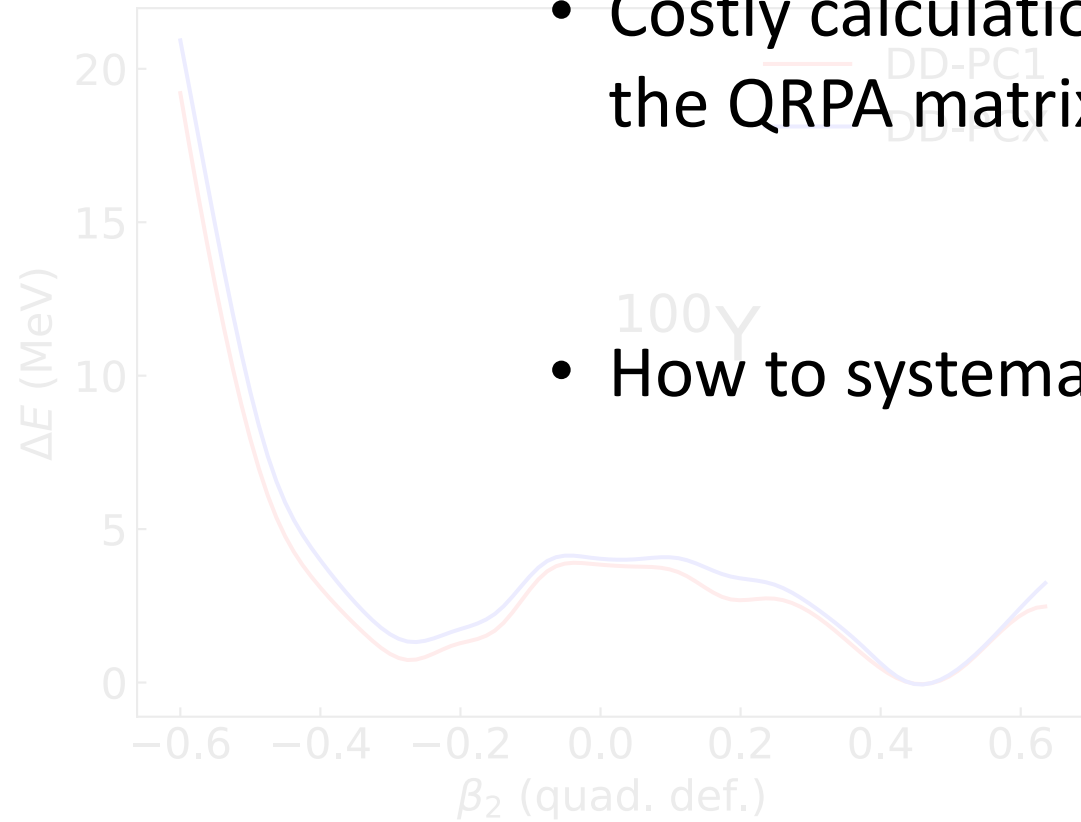
[A. Ravlic, Y. Saito and W. Nazarewicz, in preparation (2025)]



[A. Ravlic, Y. Saito and W. Nazarewicz, in preparation (2025)]

- Costly calculations, intrinsic dimension of the QRPA matrix $\cong 10^5$

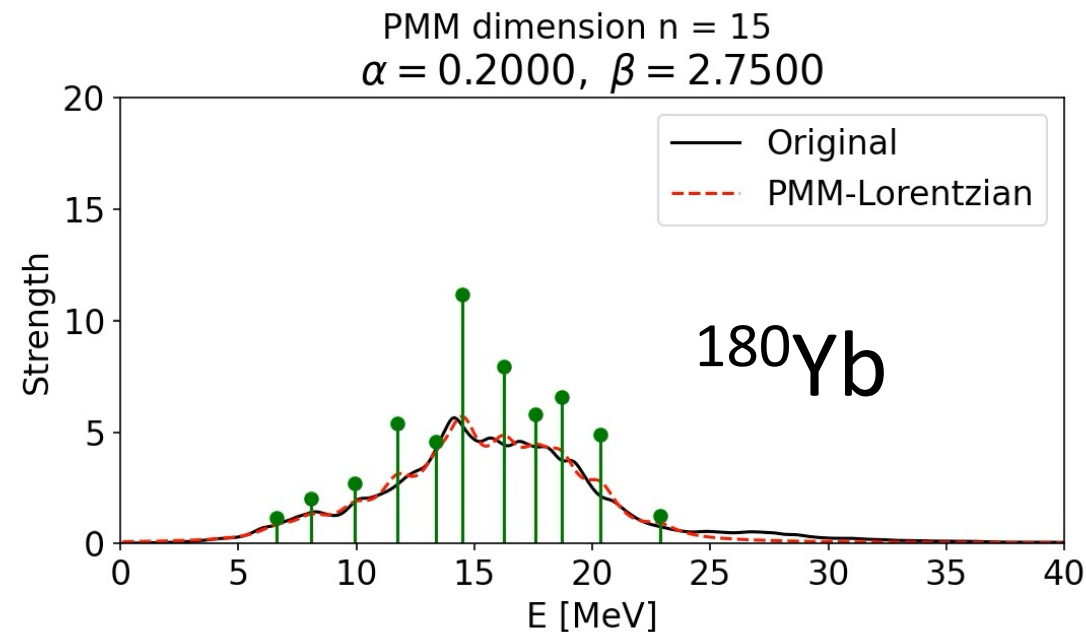
- How to systematically assess uncertainty?



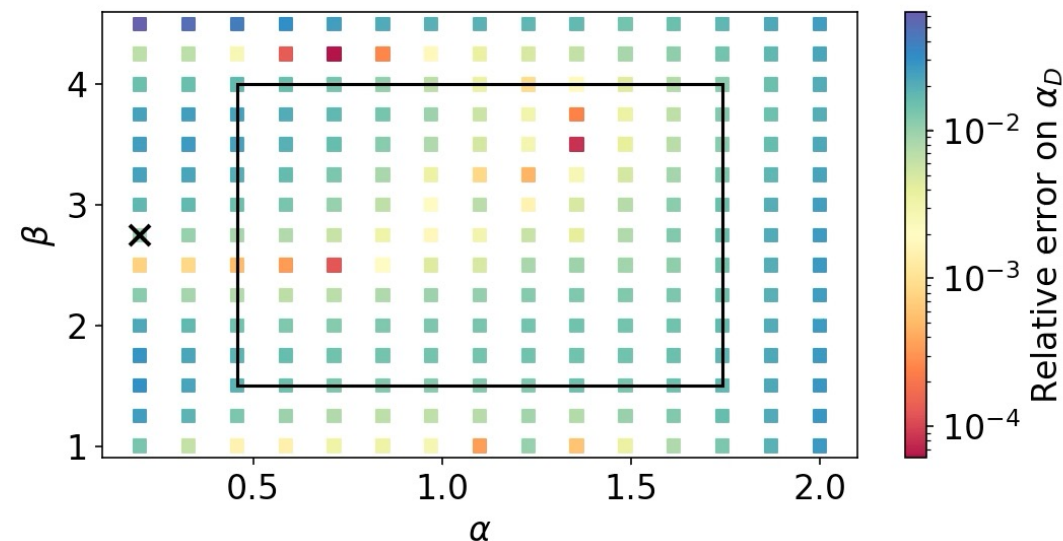
Full-order model: $\mathcal{N} \sim 10^5$

$$\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E \begin{pmatrix} X \\ Y \end{pmatrix}$$

$$B = \left| \mathcal{F}^\dagger \begin{pmatrix} X \\ Y \end{pmatrix} \right|^2$$



Work by Lauren Jin @ MSU



Emulator: $n \sim 10$

$$\hat{\mathcal{M}} = \mathcal{M}_0 + \sum_{j=1}^k f(\alpha_j) \mathcal{M}_j \quad \hat{\mathcal{M}}v = \Omega v$$

$$\hat{B} = \left| \hat{\mathcal{F}}(\boldsymbol{\alpha})^\dagger v \right|^2$$

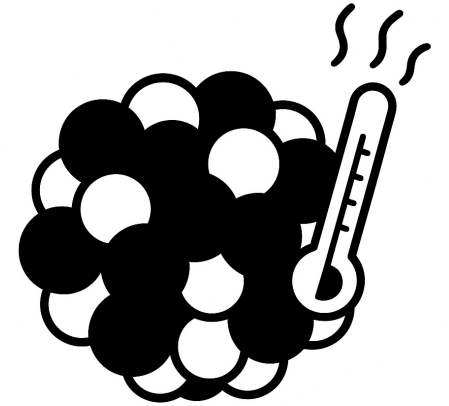
[P. Cook, D. Jammooa, M. Hjorth-Jensen, D. D. Lee, D. Lee, Nat. Commun. 16 5929 (2025).]

[L. Jin, A. Ravlic, P. Giuliani, K. Godbey and W. Nazarewicz, in prep (2025)]

Weak decays in stellar conditions

Expression for electron capture rate in stellar environment:

$$\lambda_{ec} = \frac{(m_e c^2)^3}{\pi^2 \hbar^3} \frac{1}{Z} \sum_{if} e^{\beta E_i} \int_{W_0^{th(i,f)}}^{\infty} pW \sigma_{ec}^{(i,f)}(W) f_e(W, \mu_e) dW$$



$$\sigma_{ec}^{(i,f)}$$

Requires knowledge on nuclear matrix elements at finite-temperature

$$k_B T > 0$$

→ Calculated using **finite-temperature** QRPA (FT-QRPA)

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} \quad \longrightarrow \quad \begin{pmatrix} C & a & b & D \\ a^\dagger & A & B & b^T \\ b^\dagger & B^* & A^* & a^T \\ D^* & b^* & a^* & C^* \end{pmatrix} \begin{pmatrix} P \\ X \\ Y \\ Q \end{pmatrix} = E \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} P \\ X \\ Y \\ Q \end{pmatrix}$$

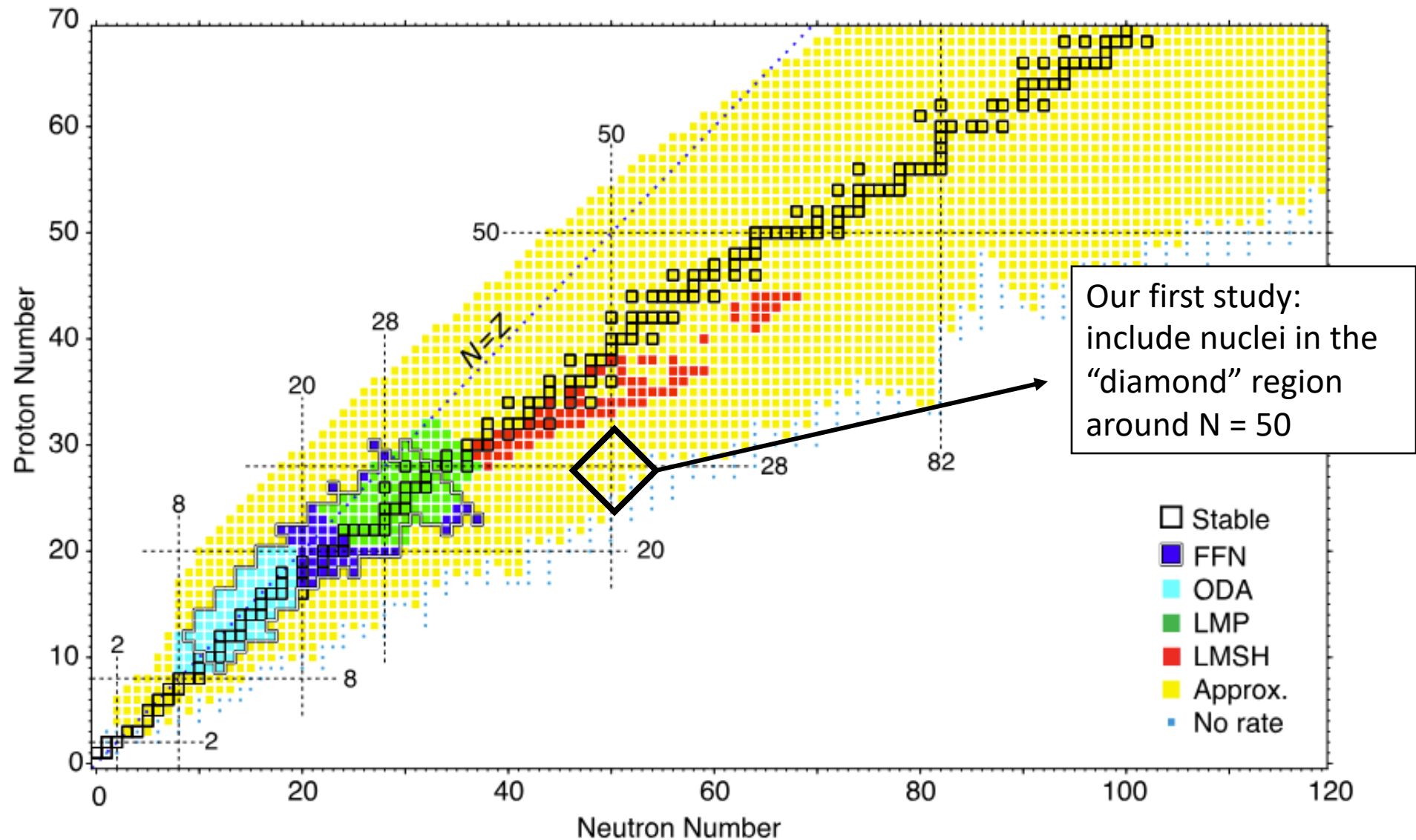
$$f_e(W, \mu_e)$$

Fermi-Dirac factor – takes into account density dependence of rates

[A. Ravlic, E. M. Ney, J. Engel, and N. Paar, Eur. Phys. J A 61(2) 37 (2025).]

[A. Ravlic, E. Yüksel et al. PRC 102, 065804 (2020).]

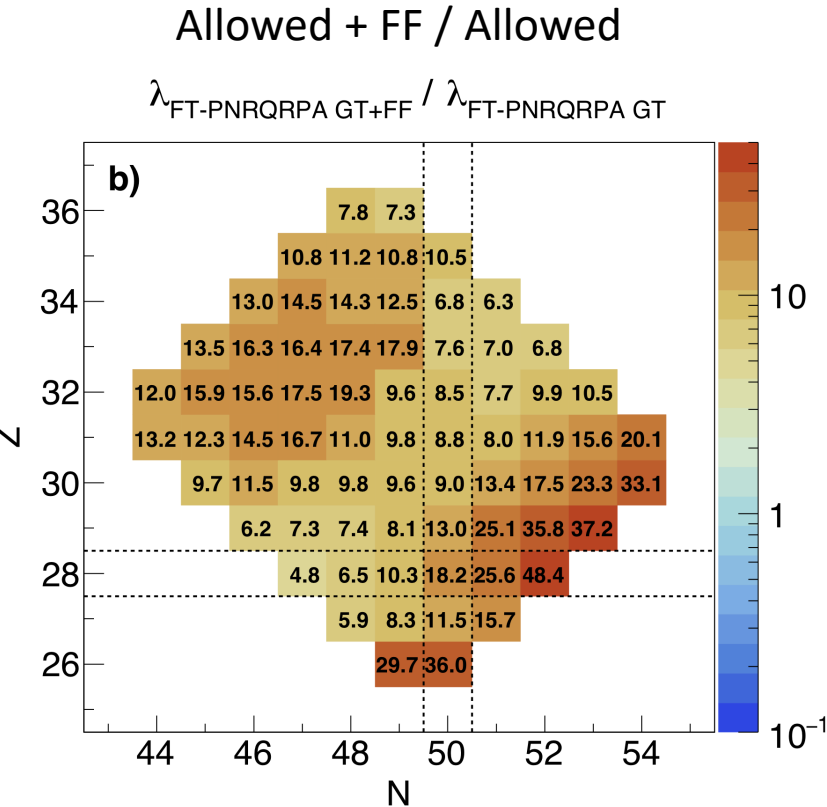
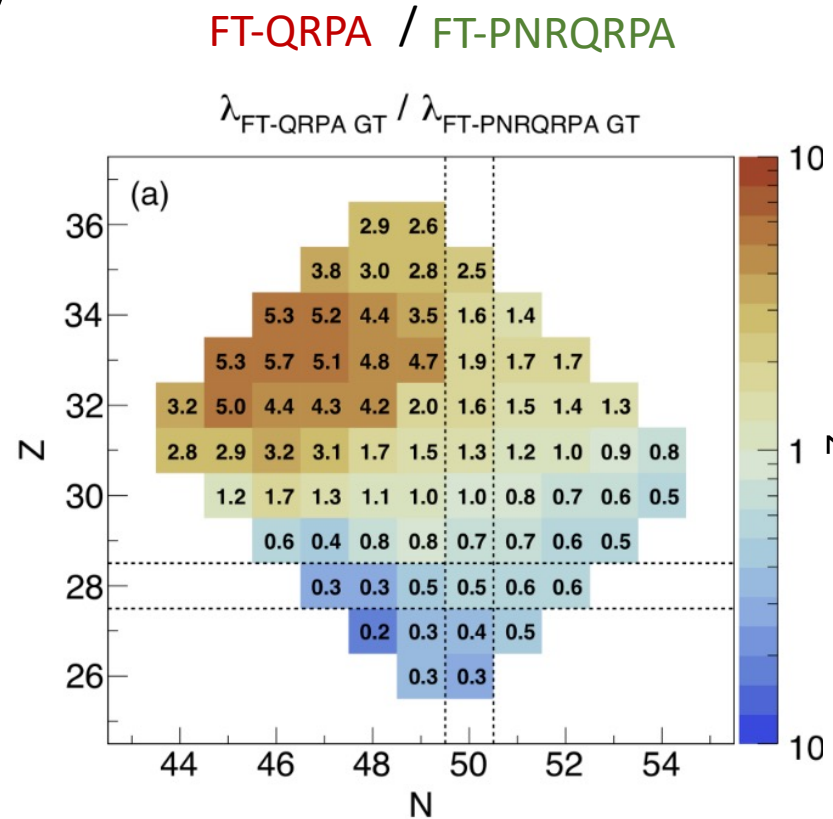
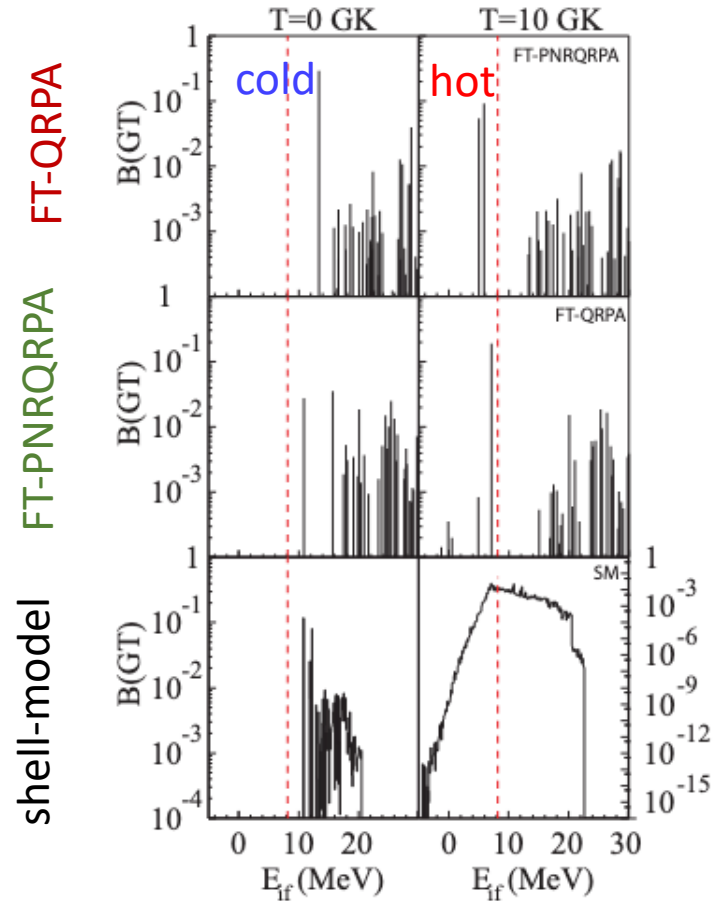
Different microscopic EC calculations (based on shell-model):



[C. Sullivan, E. O'Connor, R. Zegers et al. ApJ 816(1), 44 (2016).]

We employed 3 theoretical models:

- non-relativistic **FT-QRPA** (SkO')
- relativistic **FT-PNRQRPA** (D3C*)
- shell-model for ^{86}Kr

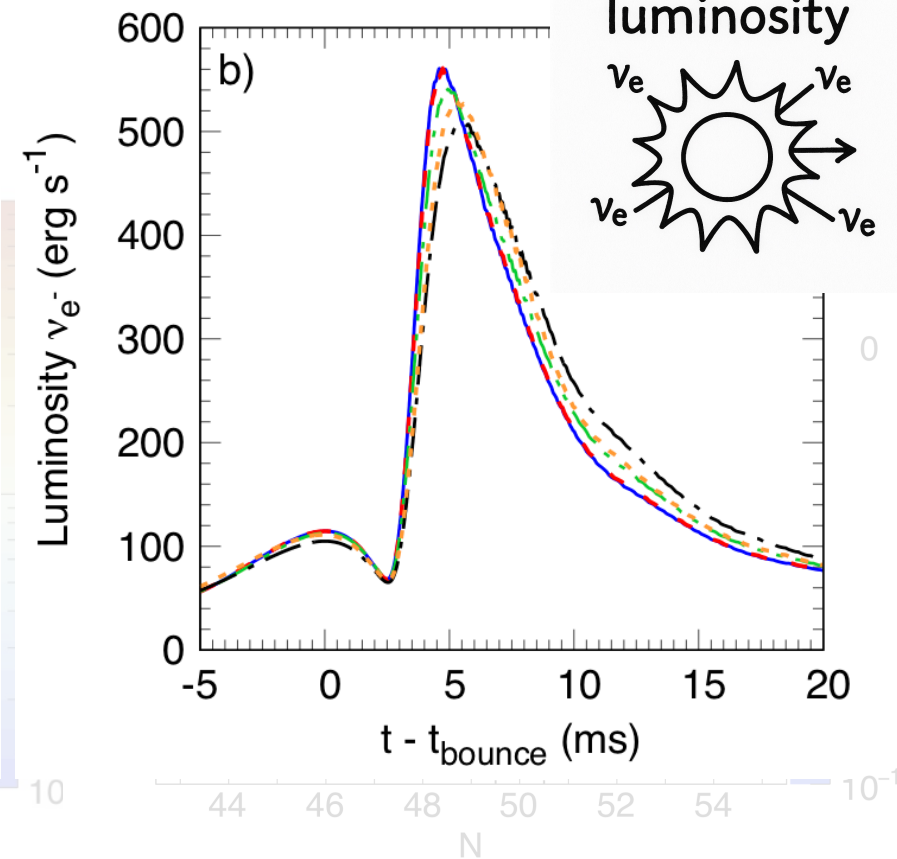
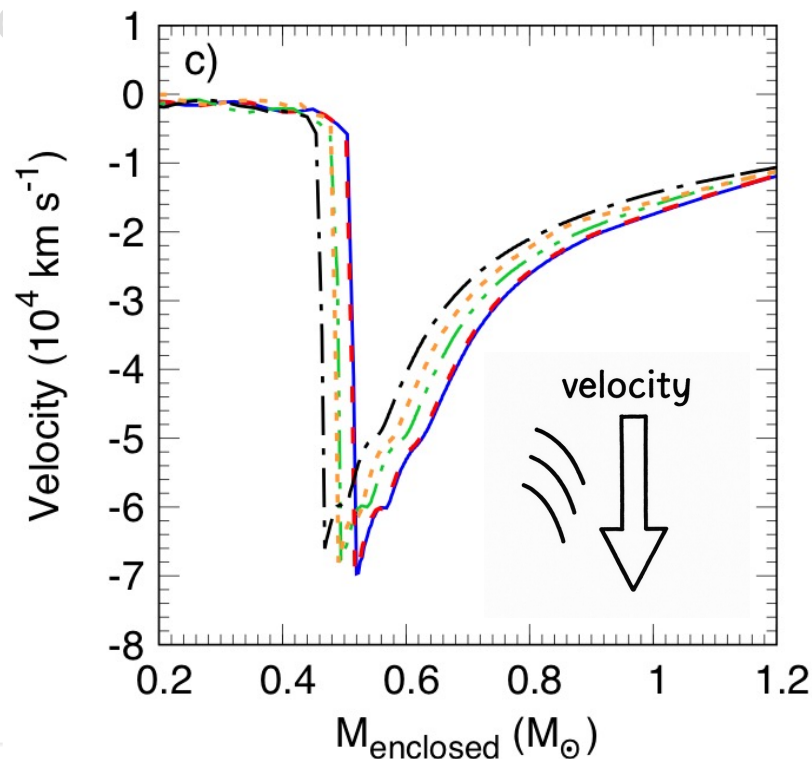
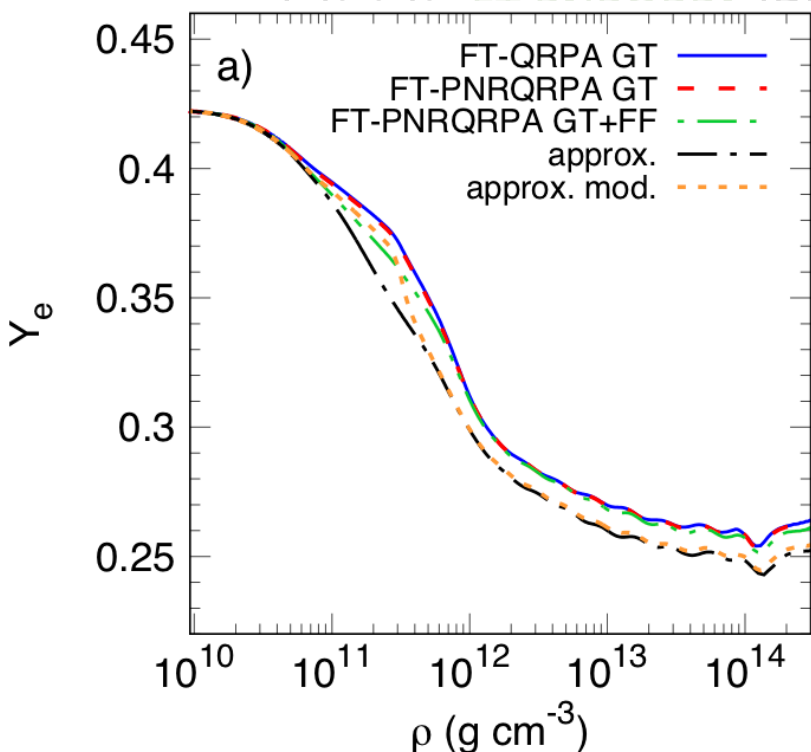


[S. Giraud, E.M. Ney, A. Ravlic et al. PRC 105, 055801 (2022).]

We employed 3 theoretical models:

Results for main CCSNe observables:

- non-relativistic FT-QRPA (SkO')



shell-model

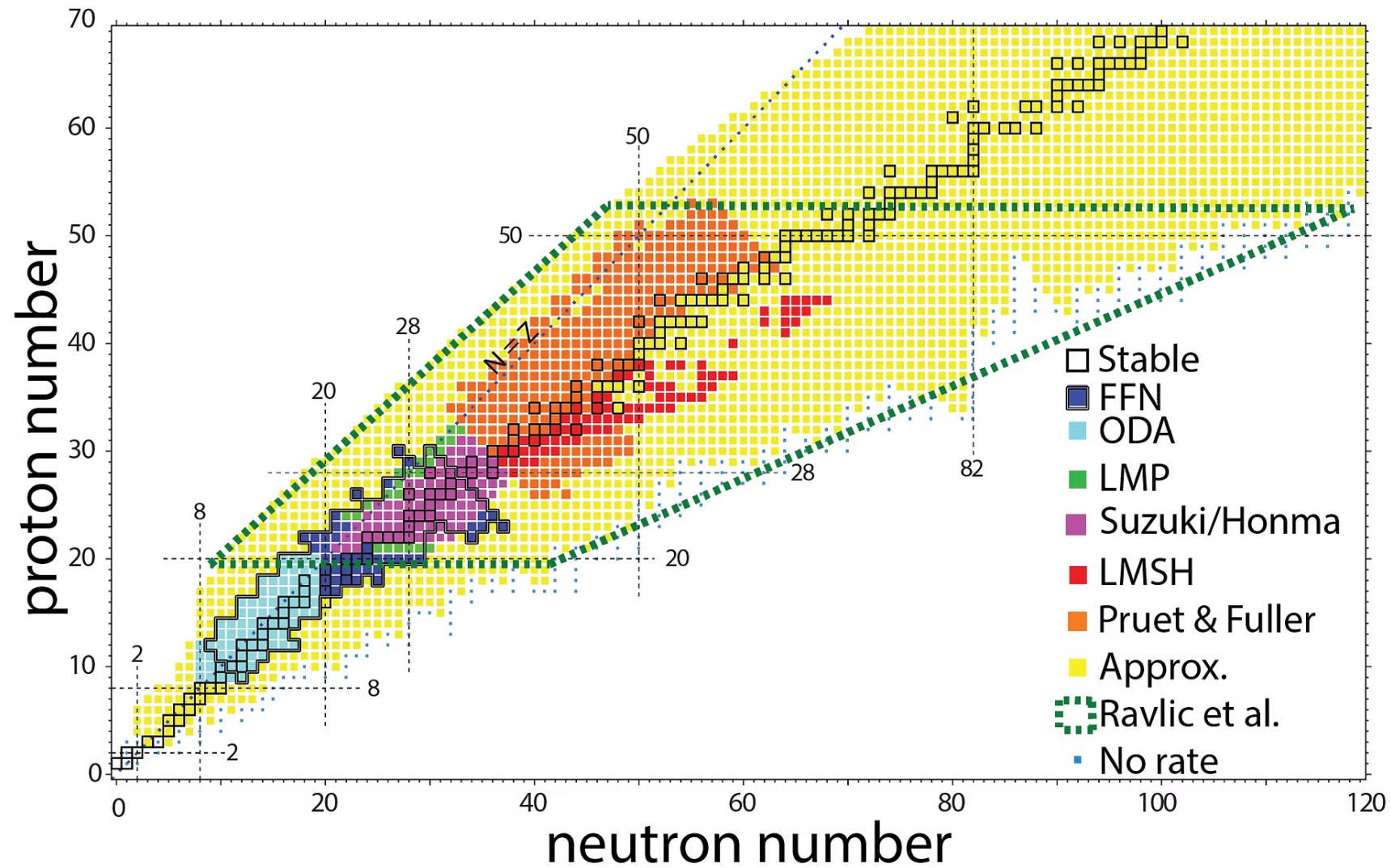
$$Y_e = \frac{\text{\#of electrons}}{\text{\#of barions}}$$

$B(GT)$

$E_{\pi}(\text{MeV})$

[S. Giraud, E.M. Ney, A. Ravlic et al. PRC 105, 055801 (2022).]

Let's consider "all" nuclei within the FT-PNRQRPA:

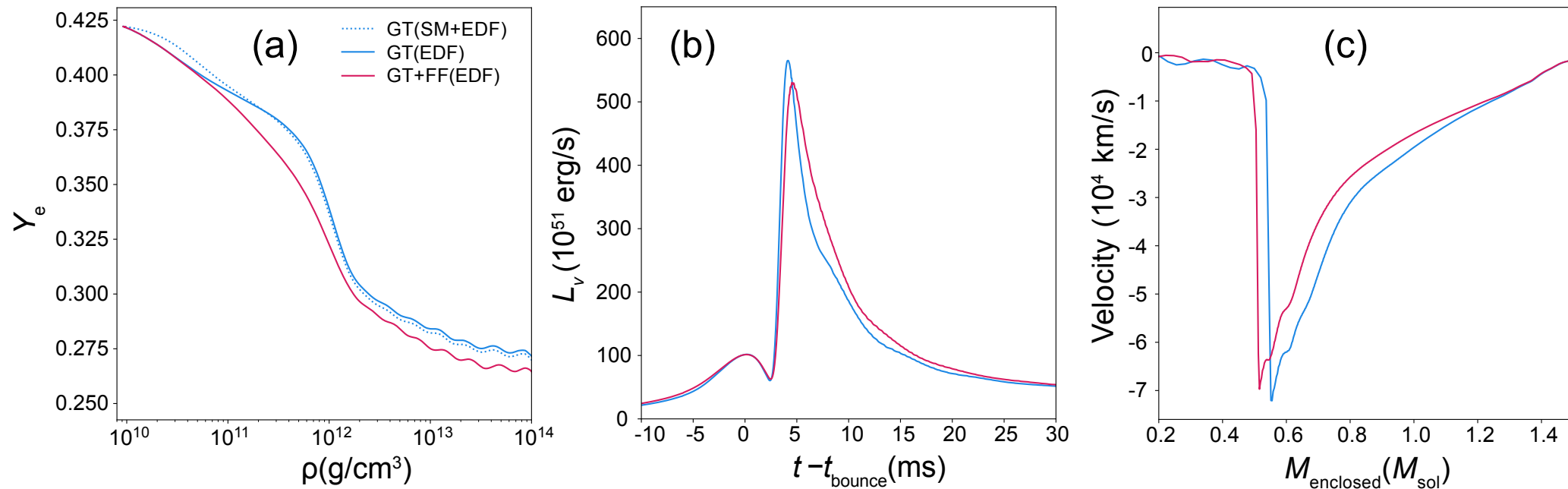


[www.remcozegers.com/weak-rate-library]

GT(EDF) – FT-PNRQRPA with Gamow-Teller only

GT+FF(EDF) – FT-PNRQRPA with Gamow-Teller + first-forbidden

GT(SM+EDF) – FT-PNRQRPA with Gamow-Teller + shell-model where available



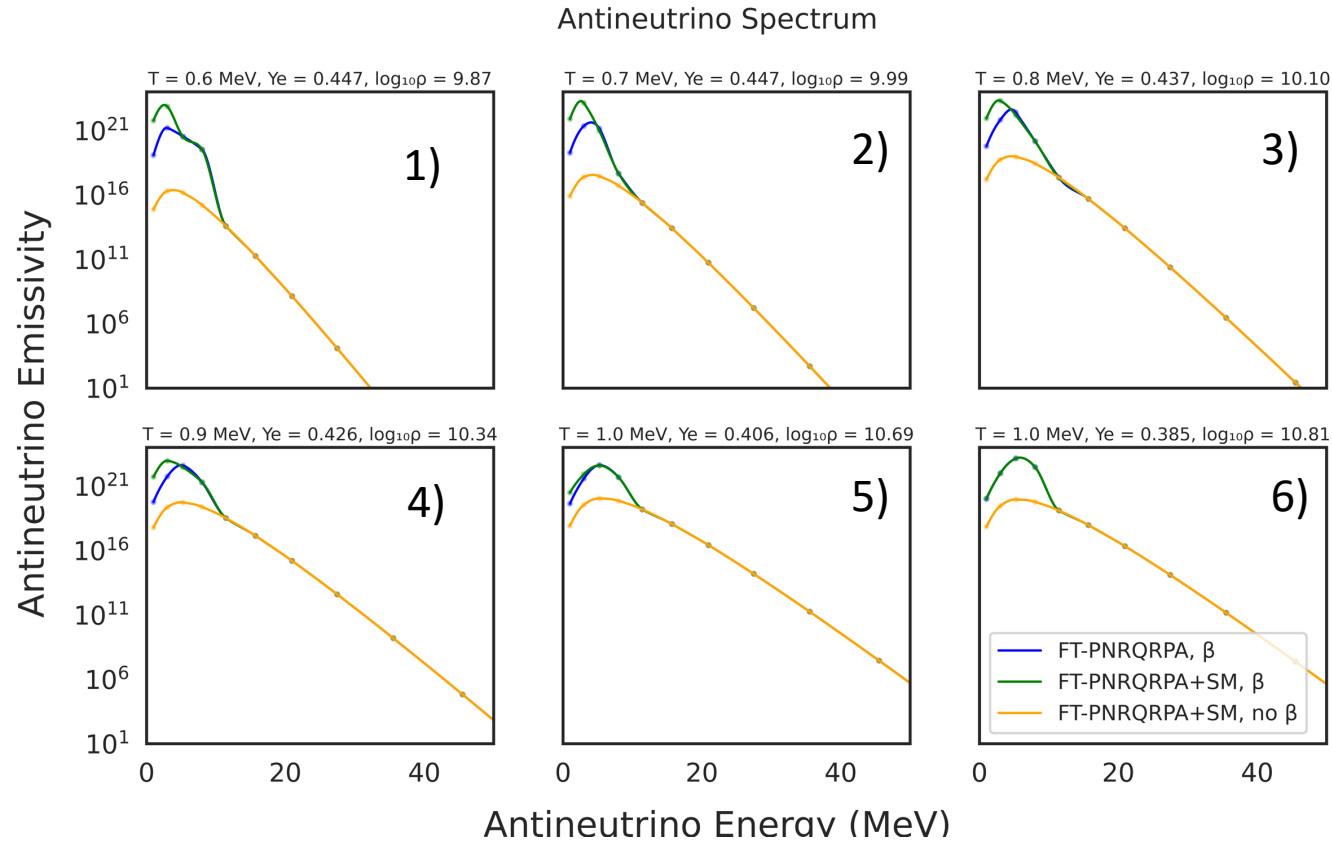
[A. Ravlic, S. Giraud, R. Zegers and N. Paar, PRC 112, L032801 (2025).]

What about stellar β -decay rates ?

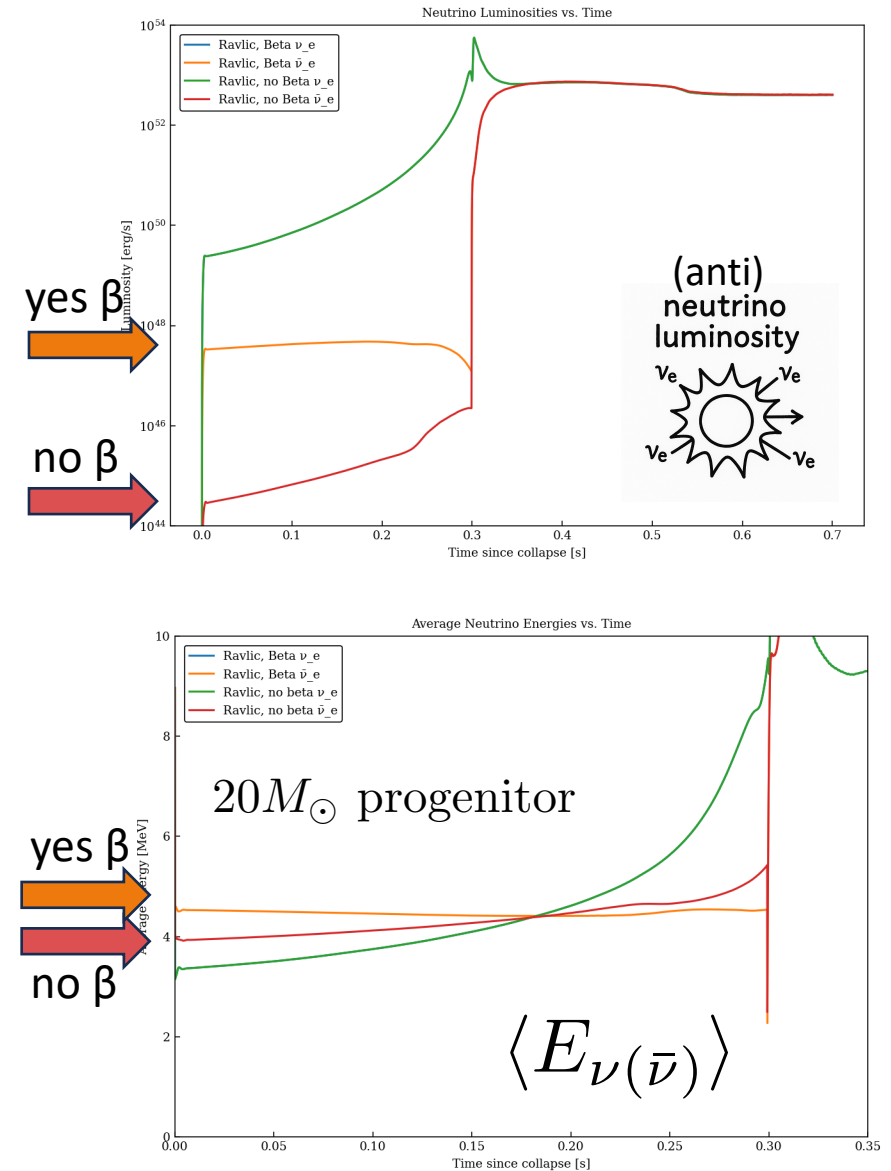
Work by Troy Dasher @ MSU

NuLib + GR1D framework

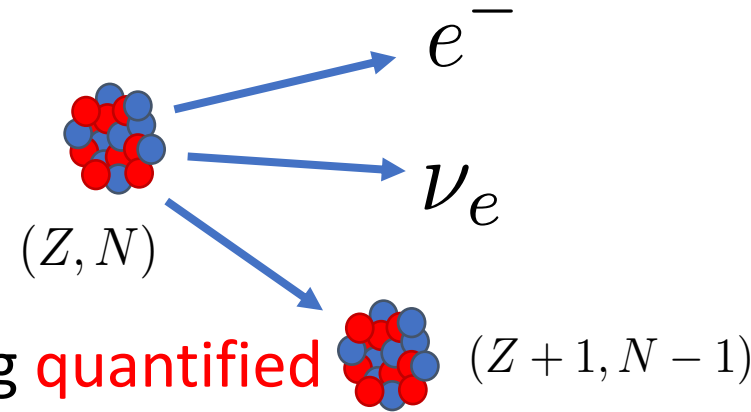
[CQG 27(11), 114103 (2010), Astrophys. J. Suppl. Ser. 219, 24 (2015).]



[T. Dasher, A. Ravlic, S. Lalit, E. O'Connor, in preparation]



Conclusion



- We performed calculations of weak decays in SHEs using **quantified** relativistic DFT
- EC can compete with α -decay and fission for $Z < 109$
- **First-forbidden** transitions dominate weak decay rates $\rightarrow$ more sensitive to details of nuclear structure
- Considering **detailed electronic structure** leads to visible effects in the decay rates for SHEs
- Global calculations of **β -decay rates** for r-process simulations
- Developed **emulators** for the efficient calculation of QRPA observables
- Application to **stellar collapse** $\rightarrow$ extension of QRPA at finite-temp

Thank you for your attention!

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