Large-scale shell model study of β^--decay properties of N = 126, 125 nuclei along the *r*-process path

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Collaborators:

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[RIBF ULIC mini-WS] Structure of neutron-rich matter revealed by beta decay at RIKEN Tokyo, 29–30 July, 2024

Outline

Nucleosynthesis of heavy elements: competition b/w neutron capture and β decay

The origin of most atomic nuclei with masses heavier than the iron group elements is attributed to **neutron capture** nucleosynthesis

slow neutron capture process (s-process)

neutron capture << beta decay.
– Isotopes near stability are synthesized.

rapid neutron capture process (r-process)

neutron capture >> beta decay.
– Explosive environment!
– High temperatures ($T \approx 10^9\ K$), and neutron densities ($> 10^{20}$ neutrons/cm^3).
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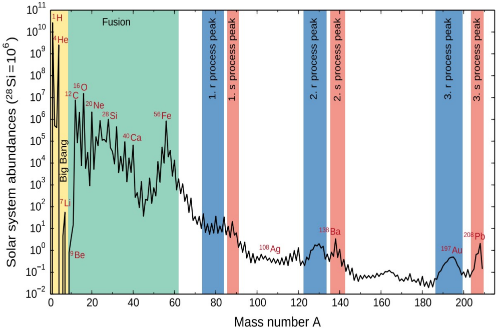

- Fig. taken: A. Arcones et al., Astron Astrophys Rev **31**, 1 (2023).
- T. Kajino et al., Progress in Particle and Nuclear Physics **107**, 109 (2019).

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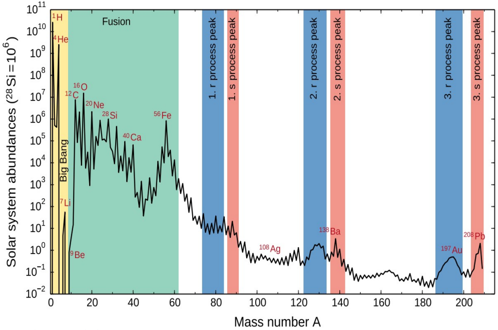

- *About half of the elements heavier than Fe are produced by* **r-process**
- *Lots of neutron-rich nuclei involved around A* ~ 195*, for ex. Au, Pt,...*
- *Poor experimental information about the beta decay around A* ~ 195

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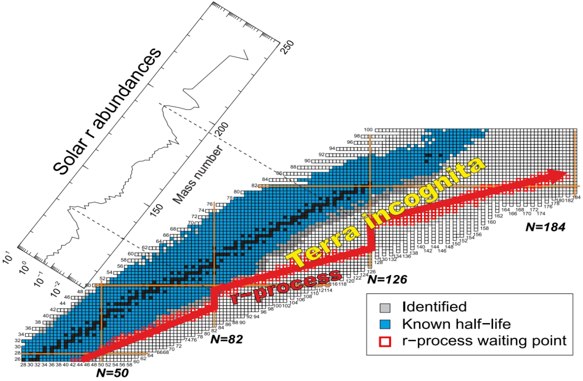
Aim of this study



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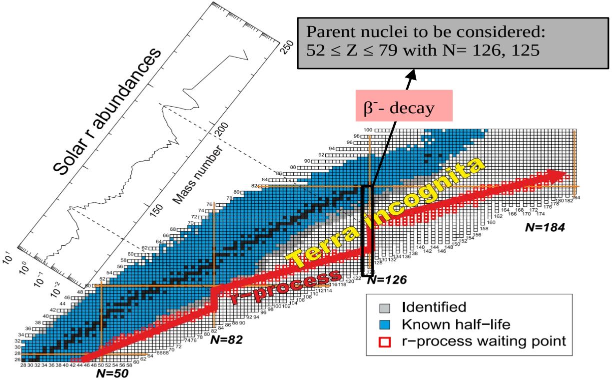

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$52 \leq Z \leq 79$ with N= 126, 125

β^-- decay

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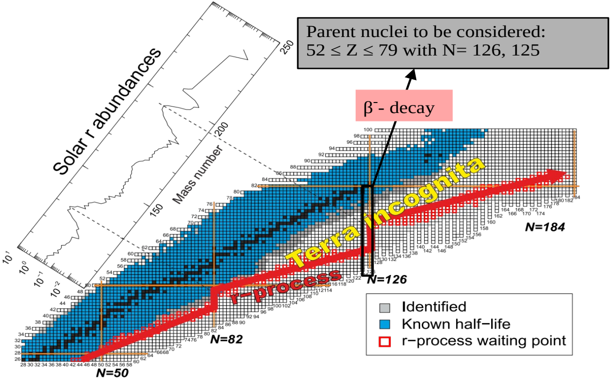

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β^-- decay

To investigate the β-decay properties like half-lives $(T_{1/2})$ and β-delayed neutron emission probabilities (P_n)

Competition b/w first-forbidden and Gamow-Teller transitions

To discuss the systematic study of Gamow-Teller strength distributions

Recent developments in large-scale shell model calculations like methodology, effective interactions, and the advent of computational resources offer the opportunity to conduct demanding large-scale calculations

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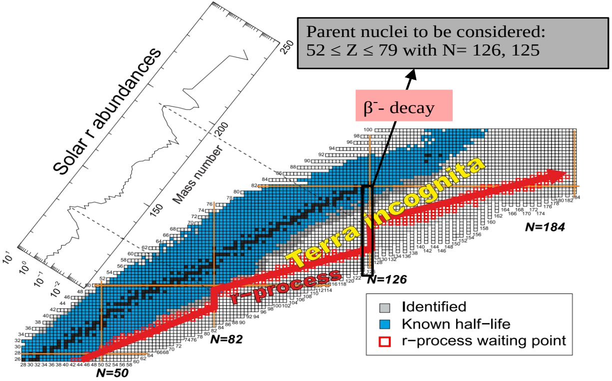

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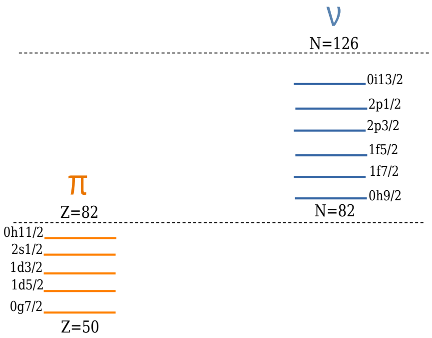
- Many nuclei are particularly important to the *r*-process nucleosynthesis
- The predicted β-decay half-lives play crucial role in determining the *r*-process time scale around the 3^{rd}-peak

▶ Fig. taken: A. Evdokimov et al., "XII International Symposium on Nuclei in the Cosmos", PoS, (2012).

Shell model calculations: Model space

Model space in the present calculation



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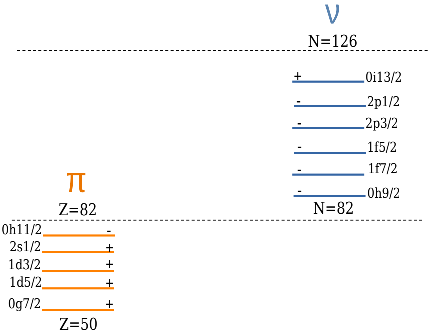

ν
N=126
+ 0i13/2
- 2p1/2
- 2p3/2
- 1f5/2
- 1f7/2
- 0h9/2
N=82

π
Z=82
0h11/2 -
2s1/2 +
1d3/2 +
1d5/2 +
0g7/2 +
Z=50

Inclusion of **first-forbidden** β decay

- For nuclei within this region, protons and neutrons occupy different shells with different parity

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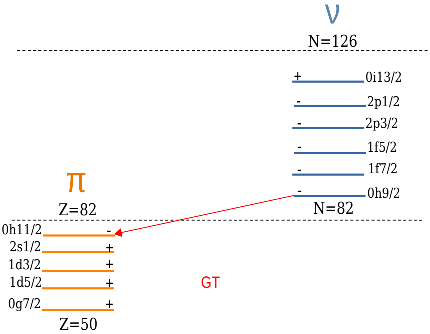

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- When undergoing with β decay, only one Gamow-Teller transition $\nu 0h_{9/2} \longrightarrow \pi 0h_{11/2}$ possible with same parity ($\Delta J = 0, \pm 1$, $\Delta\pi$ = No)

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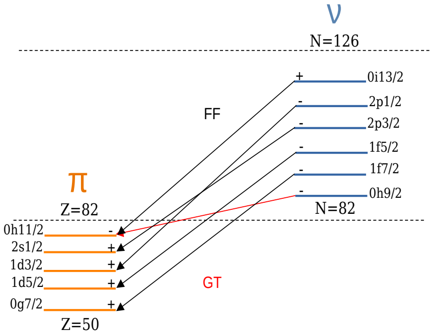

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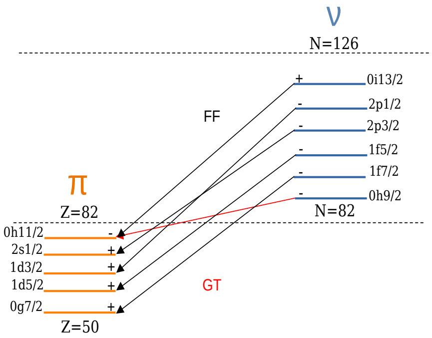

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Hamiltonian

Kuo-Herling hole: KHHE Hamiltonian [1] and modified in [2]

Shell Model code:

KSHELL: MPI + OpenMP hybrid code [3]

- [1] E. K. Warburton et al., Phys. Rev. C **43**, 602 (1991).
- [2] C. Yuan et al., Phys. Rev. C **106**, 044314 (2022).
- [3] N. Shimizu et al., Computer Physics Communications **244**, 372 (2019).

Previous shell-model studies of β-decay near $N = 126$

T. Suzuki et al.

- $N = 126$ isotones with $Z = 64 - 78$

Previous

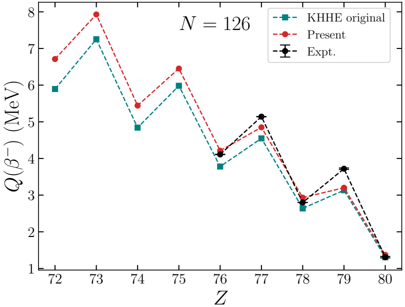
- Utilized original KHHE Hamiltonian
- Truncated model space used for $N = 126$ isotones

Present

- Utilized slightly modified KHHE Hamiltonian by C. Yuan et al.
- Performed full model space calculations for $N = 126$ isotones
- Extend $N = 126$ isotones chain to proton deficient side
- Also included $N = 125$ isotones chain in addition to $N = 126$ isotones
- Discuss the distribution of Gamow-Teller strength

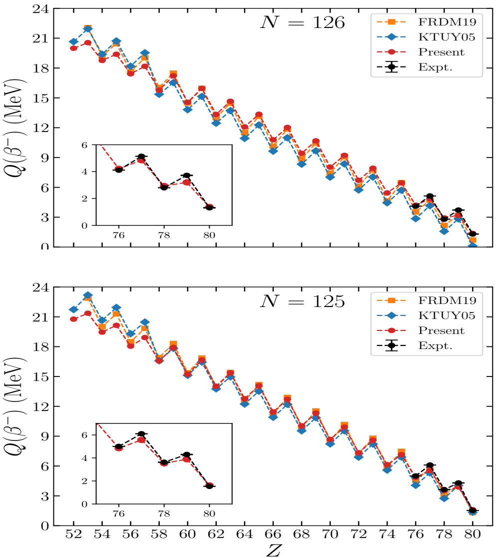
Q. Zhi et al.

- $N = 126$ isotones with $Z = 66 - 73$



- Q. Zhi et al., Phys. Rev. C **87**, 025803 (2013).
- T. Suzuki et al., Phys. Rev. C **85**, 015802 (2012).
- T. Suzuki et al., The Astrophysical Journal **859**, 133 (2018).
- C. Yuan et al., Phys. Rev. C **106**, 044314 (2022).

$Q(\beta^-)$ values of $N = 126, 125$ isotones



Shell model predicted $Q(\beta^-)$ values of $N = 126, 125$ isotones are compared with available experimental data and with different theoretical model calculations

$$Q(\beta^-) = E^{\text{par.}}_{\text{g.s.}} - E^{\text{dau.}}_{\text{g.s.}} + \delta m,$$

where the $\delta m = 0.782$ MeV.

- Shell model excellently reproduced the available experimental values
- Odd-even staggering is also observed similar to that observed in the FRDM19 and KTUY05 models
- Demonstrating a consistent trend with other theoretical models, such as FRDM19 and KTUY05, the predicted values are slightly smaller on the proton-deficient side.

▶ FRDM19: P. Möller et al., Atomic Data and Nuclear Data Tables **125**, 1 (2019).

▶ KTUY05: H. Koura et al., Prog. of Theo. Phys. **113**, 305 (2005).

β-decay Theory

Partial half-life:

$$t_{1/2} = \frac{\kappa}{f}, \quad \text{where} \quad k = 6144 \quad \text{sec},$$

and f is the dimensionless integrated shape function, which can be expressed as

$$f = \int_{1}^{w_0} C(w)(w^2-1)^{1/2} w (w_0 - w)^2 F_0(Z, w) dw,$$

where w is the total energy of the electron and w_0 is the maximum energy of w.
The theoretical shape factor $C(w)$ is defined as

$$C(w) = \sum_{k_e, k_\nu, K} \lambda_{k_e} \Big[M_K(k_e, k_\nu)^2 + m_K(k_e, k_\nu)^2 - \frac{2\gamma_{k_e}}{k_e w_e} M_K(k_e, k_\nu) m_K(k_e, k_\nu) \Big].$$

The shape factor $C(w)$ for the Gamow-Teller transition is defined as

$$C(w) = \frac{|\mathcal{M}_{\mathrm{GT}}|^2}{2J_i + 1}.$$

- H. Behrens, W. Bühring, *Electron Radial Wave Functions and Nuclear Beta-Decay* (Clarendon Press, Oxford, 1982).

β-decay Theory

For first-forbidden β decay, the form of the shape factor $C(w)$ can be written in simple way

$$C(w) = K_0 + K_1 w + K_{-1} w^{-1} + K_2 w^2,$$

where, the coefficients $K_n (n = -1,\ 0,\ 1,\ 2)$ depend on the first-forbidden nuclear matrix elements.

Summary of GT and FF nuclear matrix elements, where $\lambda = -g_A/g_V = 1.2701(25)$, $C_1 = \sqrt{4\pi/3}Y_1$, and $C = 1/\sqrt{2J_i + 1}$, $E_\gamma = Q(\beta^-) + \Delta E_C - \delta m$.

Transition	Rank	Notations	Nuclear matrix element (NME)	NME in non-relativistic approximation
GT	0	$\mathcal{M}_{\mathrm{GT}}$	$\lambda\langle f\|\|\boldsymbol{\sigma t}_-\|\|i\rangle$	
FF	0	$\mathcal{M}_0^S$	$\lambda\sqrt{3}\langle f\|\|ir[C_1 \otimes \boldsymbol{\sigma}]^0 t_-\|\|i\rangle C$	
		$\mathcal{M}_0^T$	$\lambda\sqrt{3}\langle f\|\|\gamma_5 t_-\|\|i\rangle C$	$-\lambda\sqrt{3}\langle f\|\|(i/M_N)[\boldsymbol{\sigma} \otimes \nabla]^0 t_-\|\|i\rangle C$
	1	x	$-\langle f\|\|irC_1 t_-\|\|i\rangle C$	
		$\xi' y$	$-\langle f\|\|\boldsymbol{\alpha} t_-\|\|i\rangle C$	$E_\gamma x$
		u	$\lambda\sqrt{2}\langle f\|\|ir[C_1 \otimes \boldsymbol{\sigma}]^1 t_-\|\|i\rangle C$	
	2	z	$-2\lambda\langle f\|\|ir[C_1 \otimes \boldsymbol{\sigma}]^2 t_-\|\|i\rangle C$	

β-decay Theory

To make a comparison conveniently between experiment and theory, we define the average shape factor by

$$\overline{(C(W))} = \frac{f}{f_0} = \frac{6144\ s}{f_0 t}$$

with f_0

$$f_0 = \int_1^{W_0} (W^2 - 1)^{1/2} W (W_0 - W)^2 F_0(Z, W) dW$$

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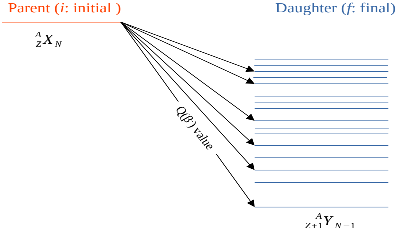
Total half-life

$$\frac{1}{T_{1/2}} = \sum_f \frac{1}{t_{i \to f}}$$



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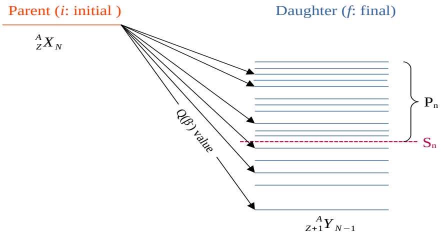
β-delayed neutron emission probabilities:

$$P_n = \left(\sum_{E_f \geq S_n} \frac{1}{t_{i\to f}} \right) \Bigg/ \left(\sum_{\text{all } f} \frac{1}{t_{i\to f}} \right)$$



Lanczos method for strength distribution

- The β-decay half-lives are evaluated by including both the Gamow-Teller and the first-forbidden transitions.
- GT strengths are calculated using the Lanczos strength function method [1].
- The moment

$$S_k = \sum_{\nu} (E_{\nu} - E_i)^k |\langle \nu | \hat{O} | i \rangle|^2$$

  up to a sufficiently large k should be calculated. The Lanczos algorithm guarantees the correct moment up to $k = 2n - 1$ with n Lanczos iteration starting with $\vec{u}_1 = \hat{O}|i\rangle$.
- In this work, the GT strengths calculated with 250 Lanczos iterations to confirm sufficiently converged results for $N = 126, 125$ isotones.

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- Full model space diagonalized:
  $N = 126$ isotones with $Z = 52 - 79$ and
  $N = 125$ isotones with $Z = 52 - 59$ and $Z = 72 - 79$

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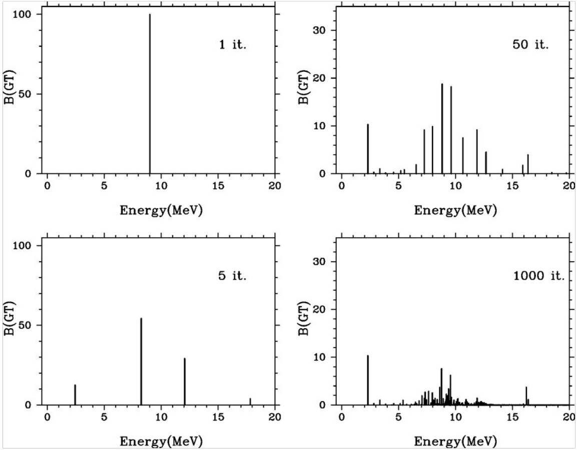
  $N = 125$ isotones with $Z = 52 - 59$ and $Z = 72 - 79$

- Due to the limitation of computational resources, monopole-based truncation is applied on $\boldsymbol{N = 125}$ isotones with $\boldsymbol{Z = 60 - 71}$

Lanczos method for strength distribution: Example ^{48}Ca



- Results from: E. Caurier et al., Rev. Mod. Phys. **77**, 427 (2005).

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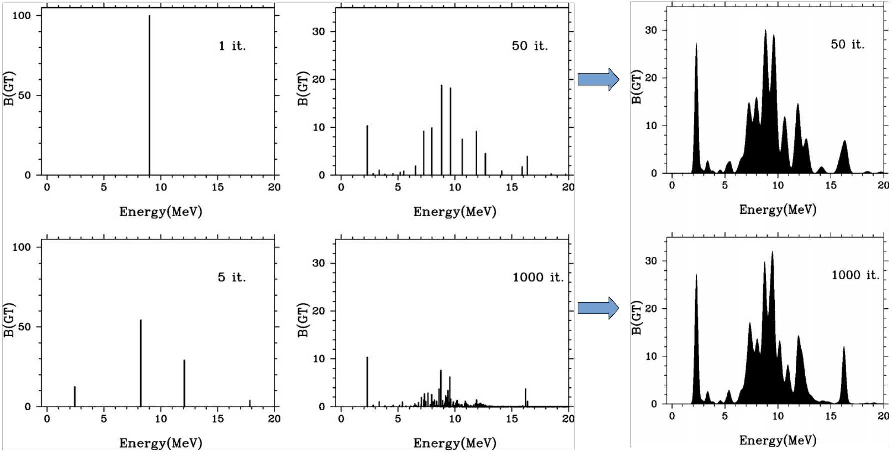


- After 50 iterations, a good distribution is achieved, despite notable variations in individual strengths between 50 and 1000 iterations.
  - Results from: E. Caurier et al., Rev. Mod. Phys. **77**, 427 (2005).

Effective operators: Gamow-Teller

To make a comparison of the shell model calculated β decay rate with the experimental one, we used effective operators in the calculations

$$\hat{O}^{\text{eff}} = q \times \hat{O}^{\text{free}}$$

where, the bare operator $\hat{O}^{\text{free}}$ is multiplied by a scaling factor (a name coined as a **quenching factor** in several earlier studies.)

To address the quenching factor in GT transitions in this study:

GT transitions for quenching factor ($q_{\text{GT}} = 0.54$)

Transition	$\lvert \mathcal{M}_{\text{GT}} \rvert$			$\log f_0 t$		
	Exp.	SM ($q = 1$)	SM ($q = 0.54$)	Exp.	SM ($q = 1$)	SM ($q = 0.54$)
$^{199}\text{Pt}(5/2^-) \rightarrow {}^{199}\text{Au}(7/2^-)$	0.114	0.297	0.160	6.45(1)	5.62	6.16
$^{200}\text{Au}^m(12^-) \rightarrow {}^{200}\text{Hg}(11^-)$	0.349	0.608	0.327	6.1(3)	5.6	6.2

Effective operators: First-forbidden

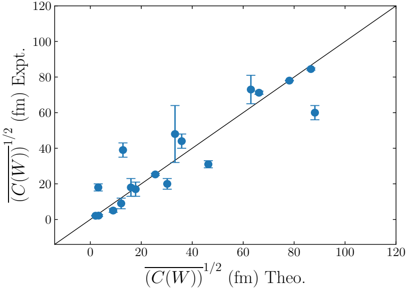
- The operators of rank 0, 1, and 2 in the first-forbidden β decay also required a quenching factor.
- To obtain quenching factors for all FF operators, we have minimized the chi-square function between theoretical and experimental average shape factors by including unique and non-unique first-forbidden transitions (**two unique and sixteen non-unique transitions**).

Experimentally know β^- first-forbidden transitions

$^{205}\mathrm{Au}\longrightarrow\,^{205}\mathrm{Hg}\longrightarrow\,^{205}\mathrm{Tl}$
$^{206}\mathrm{Hg}\longrightarrow\,^{206}\mathrm{Tl}\longrightarrow\,^{206}\mathrm{Pb}$ (18 first-forbidden transitions)
$^{207}\mathrm{Tl}\longrightarrow\,^{207}\mathrm{Pb}$

Quenching factors adopted in the present study

	FF				
	M_0^S	M_0^T	x	u	z
Present	0.41	1.266	0.51	0.28	0.71
Q. Zhi et al.	0.66	1.266	0.51	0.38	0.42



- E. K. Warburton et al., Phys. Rev. C **44**, 233 (1991).
- Q. Zhi et al., Phys. Rev. C **87**, 025803 (2013).

Result: Half-lives of experimentally known β decay

Shell-model predicted half-lives (sec) in comparison to the existing experimental data

	$N = 125$			$N = 126$	
	^{202}Ir	^{203}Pt	^{204}Au	^{204}Pt	^{205}Au
Present	4.7	20.6	25.4	13.9	23.7
Exp	15(3)	22(4)	37.2(8)	16^{+6}_{-5}	32.5(14)
SM 2018				38.3	

- Exp: A. I. Morales et al., Phys. Rev. Lett. **113**, 022702 (2014).
- SM 2018: T. Suzuki et al., The Astrophysical Journal **859**, 133 (2018).

We introduce r as a measure of deviation

$$r = \log_{10}(T^{\text{calc}}_{1/2}/T^{\text{exp}}_{1/2}),$$

and its mean value and standard deviation can be written as

$$\bar{r} = \frac{1}{n}\sum_{i=1}^{n} r_i,$$

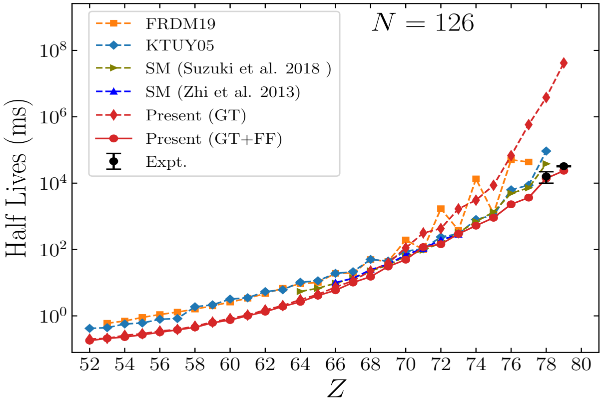
and

$$\sigma = \left[\frac{1}{n}\sum_{i=1}^{n}(r_i - \bar{r})\right]^{1/2},$$

Discrepancies of shell-model half-lives from the experimental ones

$\bar{r}$	σ	$10^{\bar{r}}$	10^{σ}	n
-0.18	0.17	0.66	1.48	5

Result: Half-lives of $N = 126$ isotones



Present shell-model predicted β-decay half-lives for $N = 126$ isotones are compared with different theoretical model calculations and existing experimental data.

- FRDM19: P. Möller et al., Atomic Data and Nuclear Data Tables **125**, 1 (2019).
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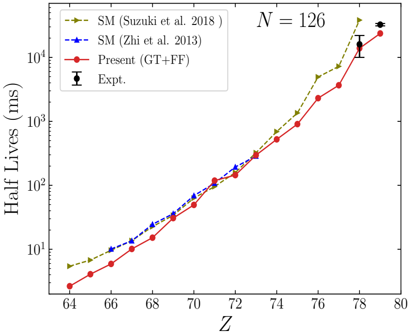
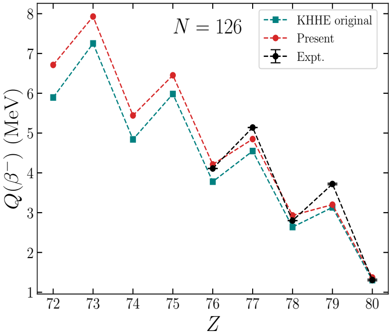
- SM: T. Suzuki et al., The Astrophysical Journal **859**, 133 (2018).
- SM: Q. Zhi et al., Phys. Rev. C **87**, 025803 (2013).
- Exp.: A. I. Morales et al., Phys. Rev. Lett. **113**, 022702 (2014).

Result: Half-lives of $N = 126$ isotones





Present shell-model predicted β-decay half-lives for $N = 126$ isotones are compared with the previous shell model calculated and existing experimental data.

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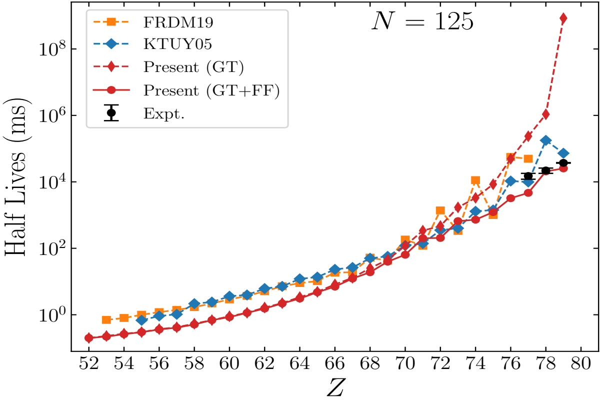
- SM: Q. Zhi et al., Phys. Rev. C **87**, 025803 (2013).
- Exp.: A. I. Morales et al., Phys. Rev. Lett. **113**, 022702 (2014).

Result: Half-lives of $N = 125$ isotones



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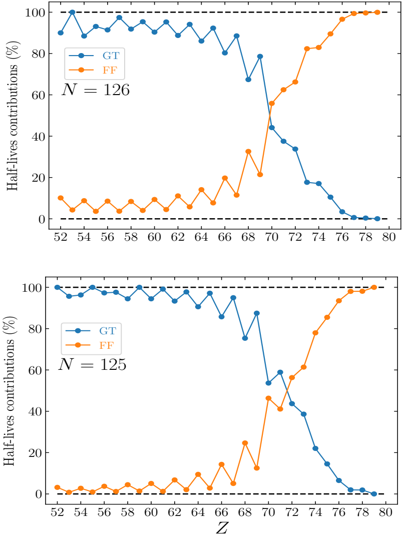
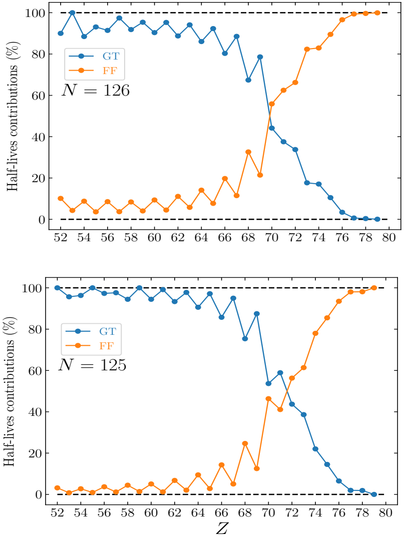
Result: Contribution of GT and FF transitions in Half-lives

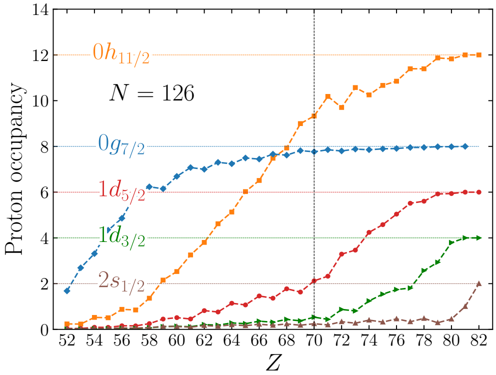


- The effect of first-forbidden transitions in the total half-lives of $N = 126$ **(top)** and $N = 125$ **(bottom)** isotones

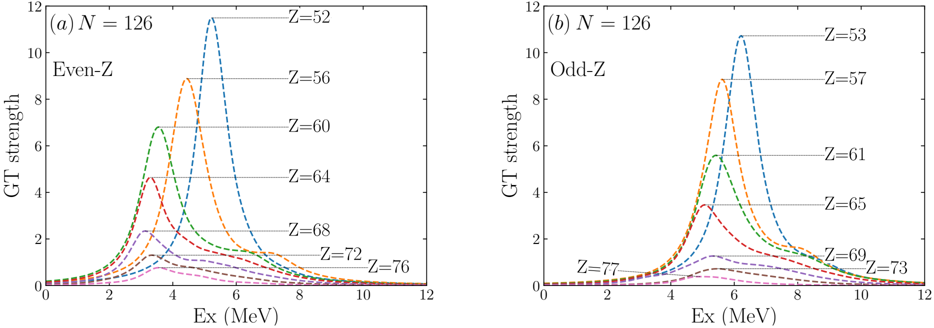
Result: Contribution of GT and FF transitions in Half-lives

- The effect of first-forbidden transitions in the total half-lives of $N = 126$ **(top)** and $N = 125$ **(bottom)** isotones
- GT transition dominated by the $\nu 0h_{9/2} \rightarrow \pi 0h_{11/2}$



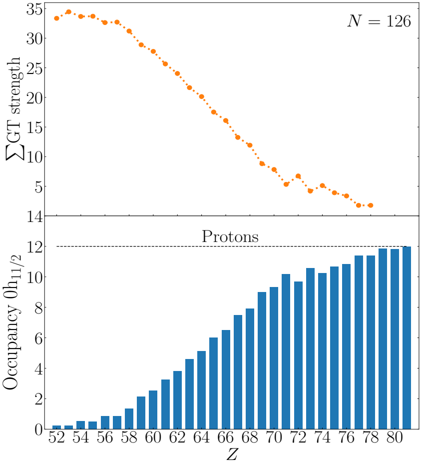


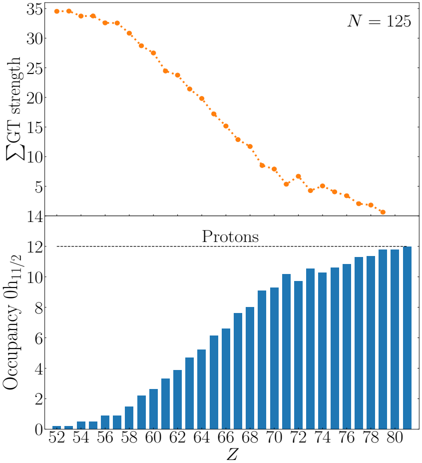
Result: Gamow-Teller strength distributions of $N = 126$ isotones



- The GT strength peaks are observed at low excitation energies between 3-6 MeV and 5-7 MeV for even-Z and odd-Z of parent nuclei, respectively.
- This peak, dominated by the $\nu 0h_{9/2} \rightarrow \pi 0h_{11/2}$ transition, is enhanced on the proton deficient side because the Pauli-blocking effect caused by the occupying the valence proton $0h_{11/2}$ orbit is weakened.

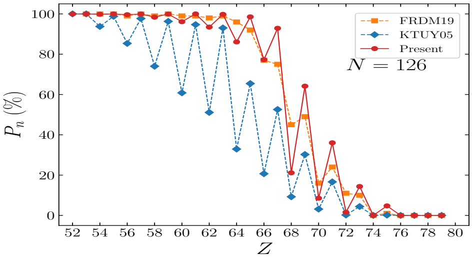
Result: Total Gamow-Teller strength distributions as a function of $\pi 0h_{11/2}$ orbit





- As the proton number increases, the proton $0h_{11/2}$ orbit becomes occupied, and simultaneously, the sum of GT strength decreases due to the **Pauli blocking effect**, reaching almost zero near $Z = 82$.

Result: β-delayed neutron emission probabilities $P_n(\%)$



- No experimental information available about the β-delayed neutron emission probabilities $P_n(\%)$ in this region

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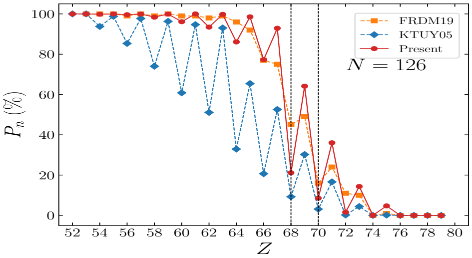

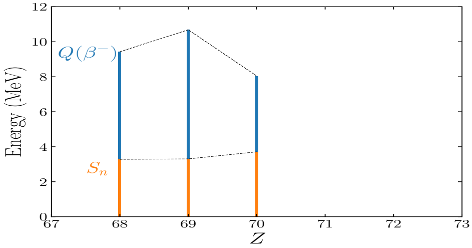

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- Even-odd staggering due to phase space

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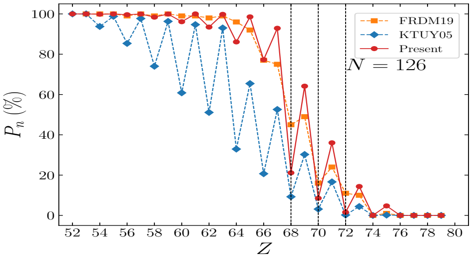

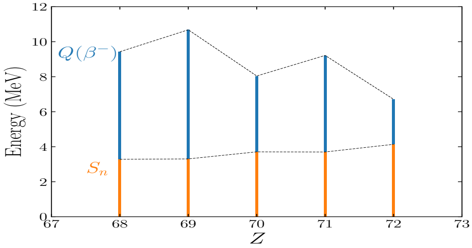

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Future:

- **Further, we will analyze the impact of the present calculated β-decay half-lives and β-delayed neutron emission probability on the r-process abundance distribution (with Nobuya Nishimura).**