Nuclear Properties at Finite Temperatures in Energy Density Functional Theory

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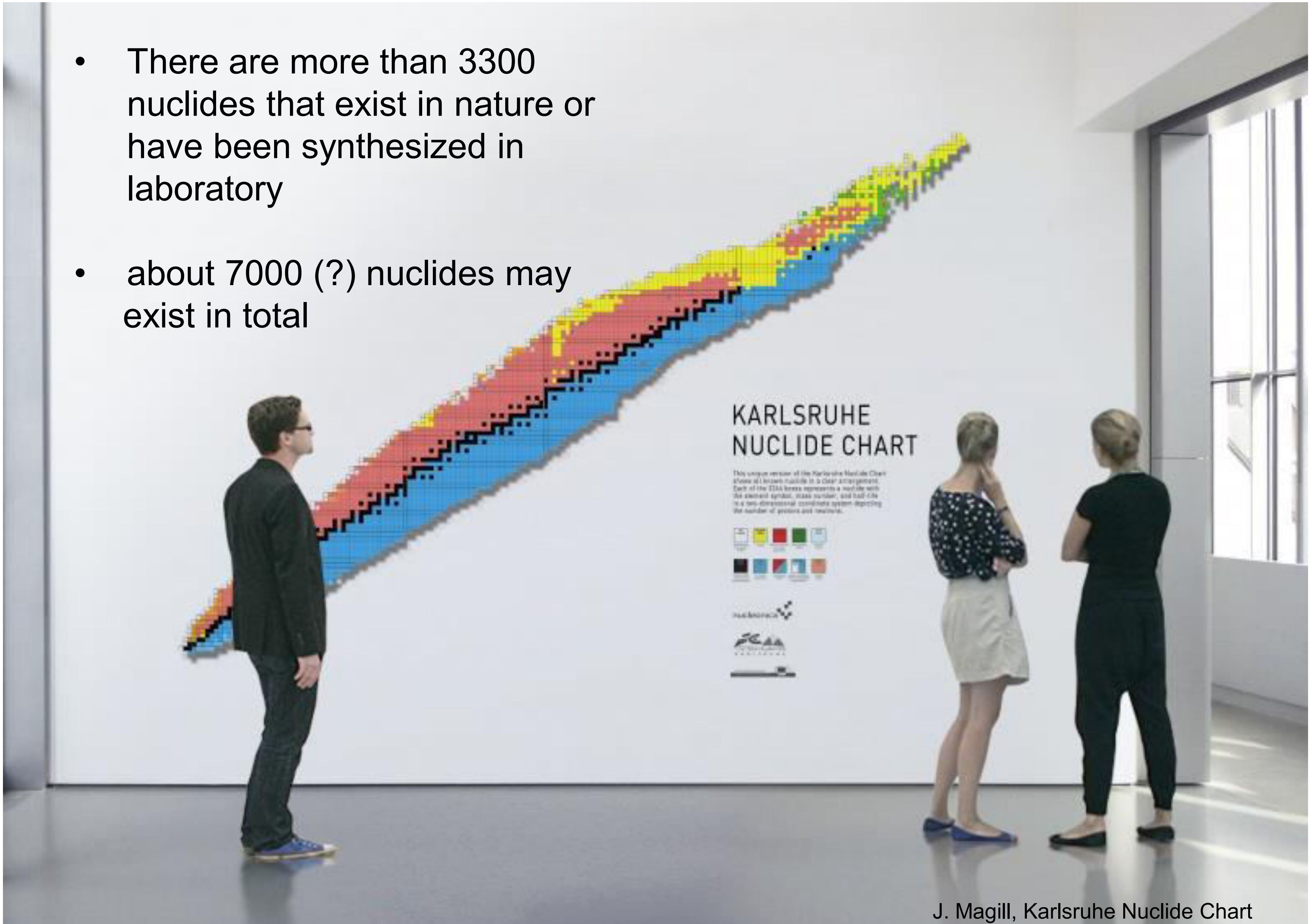
THE CHART OF THE NUCLIDES

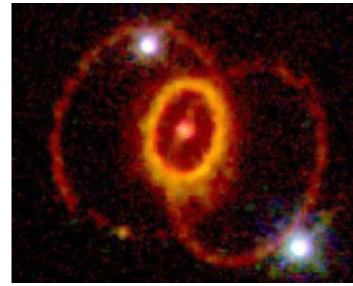
- There are more than 3300 nuclides that exist in nature or have been synthesized in laboratory

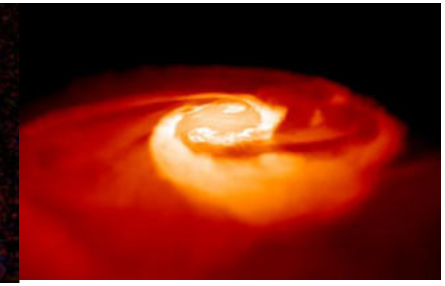
- about 7000 (?) nuclides may exist in total



J. Magill, Karlsruhe Nuclide Chart

INTRODUCTION





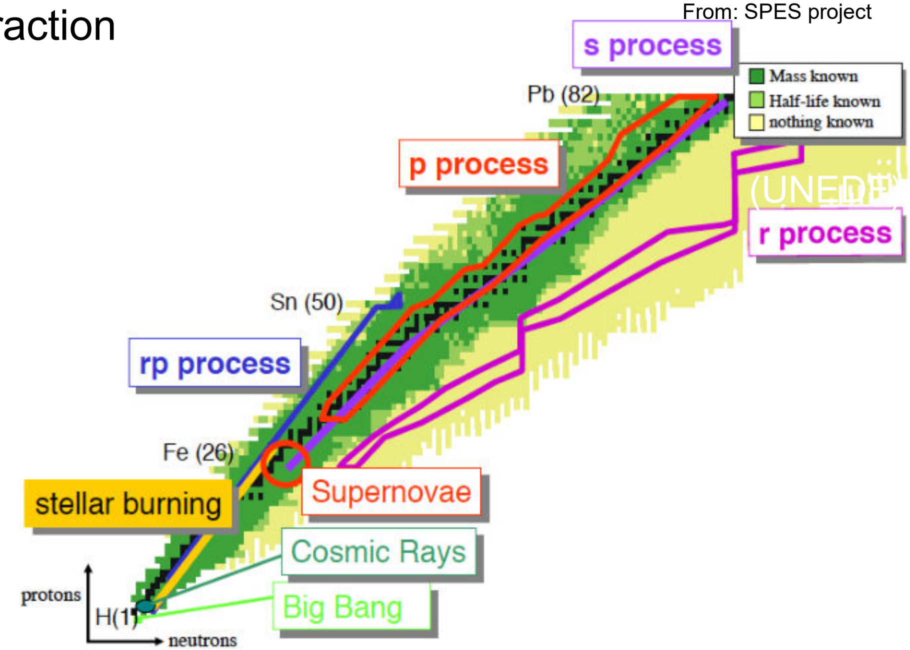
- The properties of nuclei and their processes are important for understanding the evolution of stars and nucleosynthesis

- Astrophysically relevant nuclear processes, e.g.,

    - electron capture
    - beta decay
    - beta-delayed neutron emission
    - neutrino-nucleus reactions
    - neutron capture
    - photodissociation
    - fission
    - …

  (electron capture, beta decay, beta-delayed neutron emission, neutrino-nucleus reactions:) Weak interaction processes

From: SPES project



- Many nuclear properties involved are beyond reach for the experiment. Consistent and universal microscopic theory is required.

NUCLEAR PROPERTIES AT FINITE TEMPERATURE

- In stellar environments nuclei are hot, becoming extremely hot in core-collapse supernovae and neutron-star mergers (e.g. ~10^9 - 10^{10} K)

- Due to theoretical and computational complexity, most model calculations of nuclear properties are performed at zero temperature or limited to a few nuclei

- Finite temperature effects are experimentally challenging

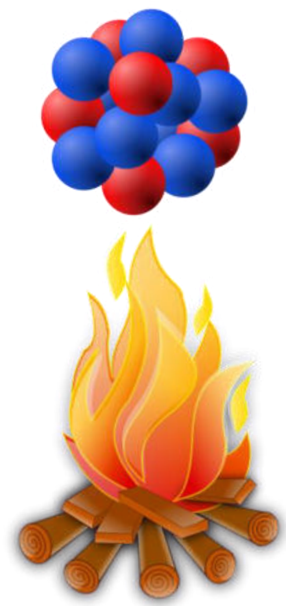
ScienceNews (2020)

Key questions:

How nuclear structure and dynamics change with temperature increase?

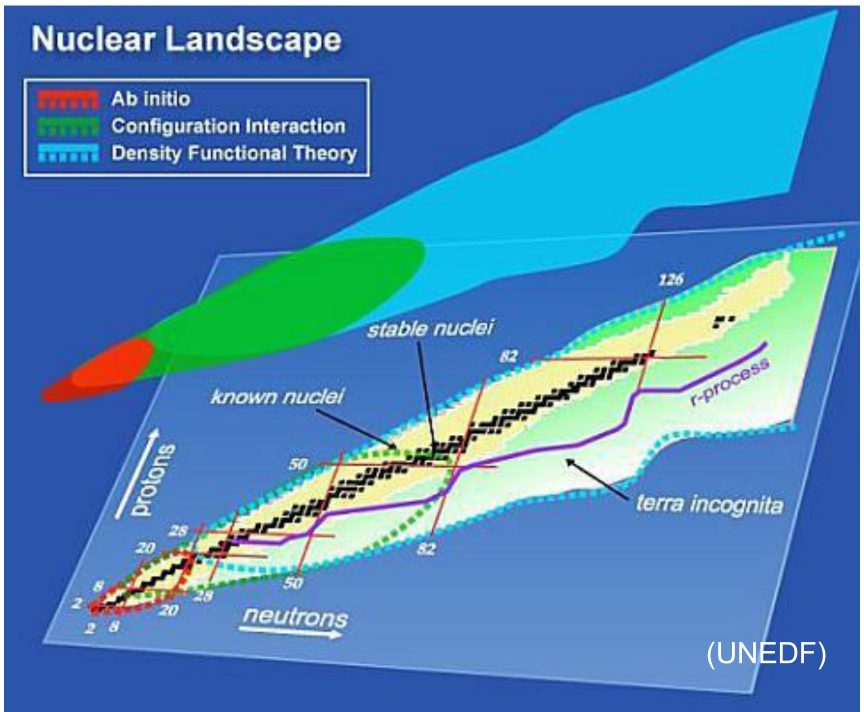
How the nuclear drip lines evolve with temperature?

What are possible implications of the finite temperature effects in nuclei on astrophysically relevant processes?



NUCLEAR ENERGY DENSITY FUNCTIONAL (EDF)

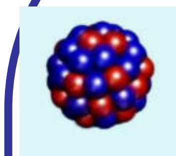
- Hohenberg-Kohn theorem – the exact energy of a quantum many body system is a functional $E[\rho]$ of the local density $\rho(\vec{r})$
- Ground state density and other ground state observables are obtained by minimizing a suitable energy functional $E[\rho]$.
  Optimal EDF is based on some effective nuclear interaction (Skyrme, Gogny, relativistic)



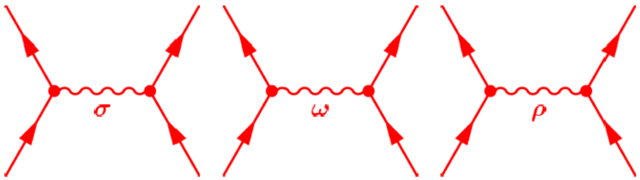
WHY EDF?

- Universal and consistent microscopic theory (the same functional used for all nuclei)
- unified approach to describe at the quantitative level nuclear properties across the nuclide map including exotic nuclei
- systematic calculations are feasible for astrophysically relevant nuclear properties

RELATIVISTIC NUCLEAR ENERGY DENSITY FUNCTIONAL



i) Nucleons are Dirac particles coupled by the exchange mesons and the photon field



ii) Four-fermion contact interaction (Point-coupling model)

- The basis is effective Lagrangian density with relativistic symmetries:

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_m + \mathcal{L}_{int}$$

$$\mathcal{L}_N = \bar{\psi}\left(i\gamma^\mu \partial_\mu - m\right)\psi$$

$$\begin{aligned}\mathcal{L}_m \;=\; & \frac{1}{2}\partial_\mu \sigma \partial^\mu \sigma - \frac{1}{2}m_\sigma^2 \sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2 \omega_\mu \omega^\mu \\ & -\frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2 \vec{\rho}_\mu \vec{\rho}^\mu - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\end{aligned}$$

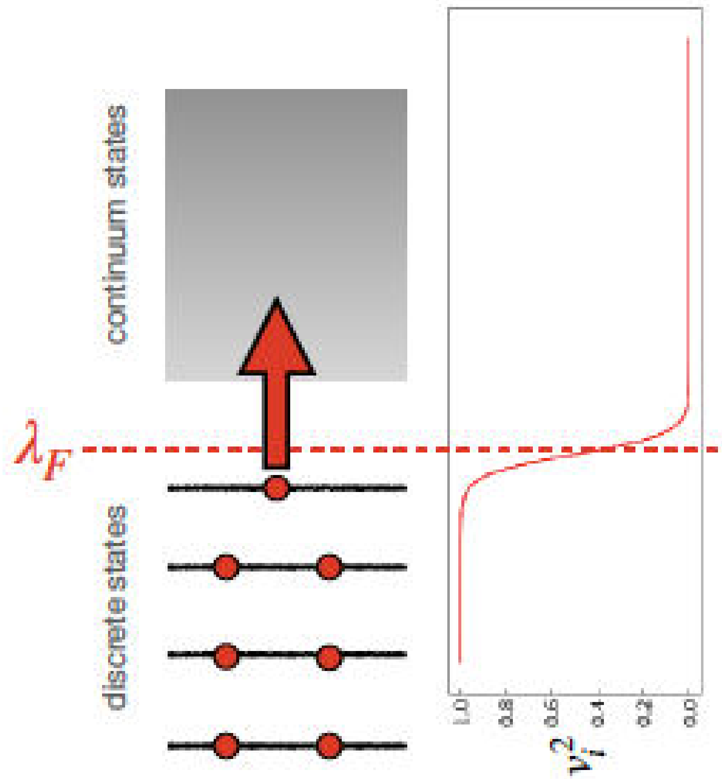
$$\mathcal{L}_{int} = -\bar{\psi}\Gamma_\sigma \sigma \psi - \bar{\psi}\Gamma_\omega^\mu \omega_\mu \psi - \bar{\psi}\vec{\Gamma}_\rho^\mu \vec{\rho}_\mu \psi - \bar{\psi}\Gamma_e^\mu A_\mu \psi.$$

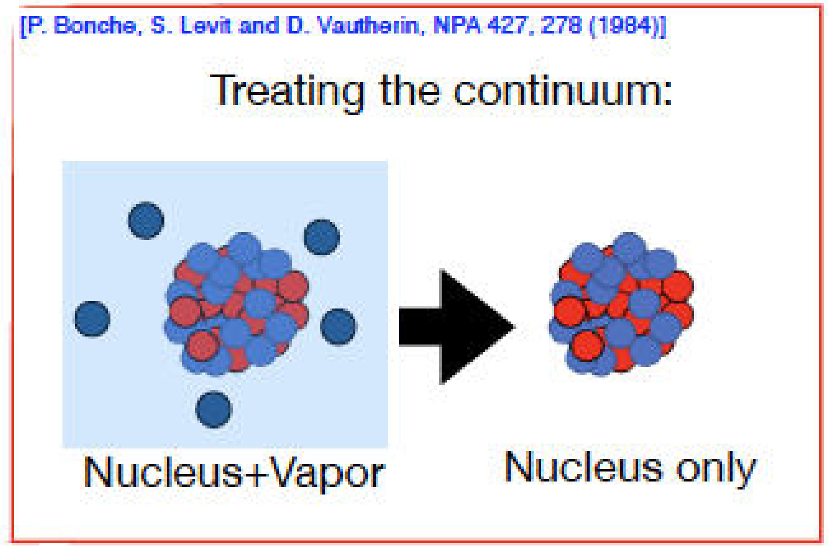
$$\begin{aligned}\mathcal{L} = \; & \bar{\psi}(i\gamma \cdot \partial - m)\psi \\ & - \frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\ & - \frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\ & - \frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma \cdot A\frac{(1-\tau_3)}{2}\psi\end{aligned}$$

- Many-body correlations encoded in density-dependent coupling functions
- The model parameters are constrained directly by many-body observables (masses, charge radii, pseudo-data, excitations, …)

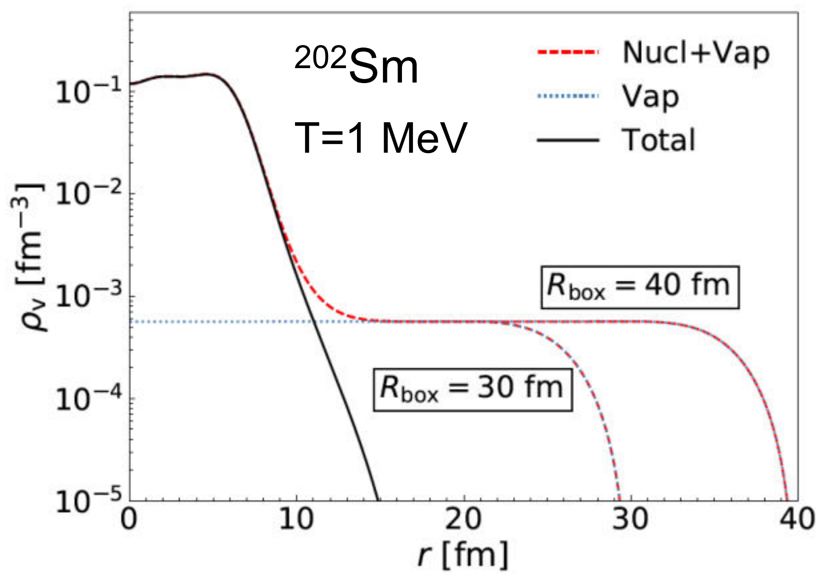
FINITE TEMPERATURE EFFECTS

The nucleons can scatter above the Fermi level, and temperature smears the Fermi surface.





Radial dependence of vector density:



GLOBAL NUCLEAR PROPERTIES AT FINITE TEMPERATURE

How the nuclear properties evolve with increasing temperature across the nuclide chart?

- Finite Temperature Relativistic Hartree-Bogoliubov (RHB) model based on relativistic EDFs
- Includes the nuclear deformation, pairing correlation effects, and treatment of nucleon states in the continuum.

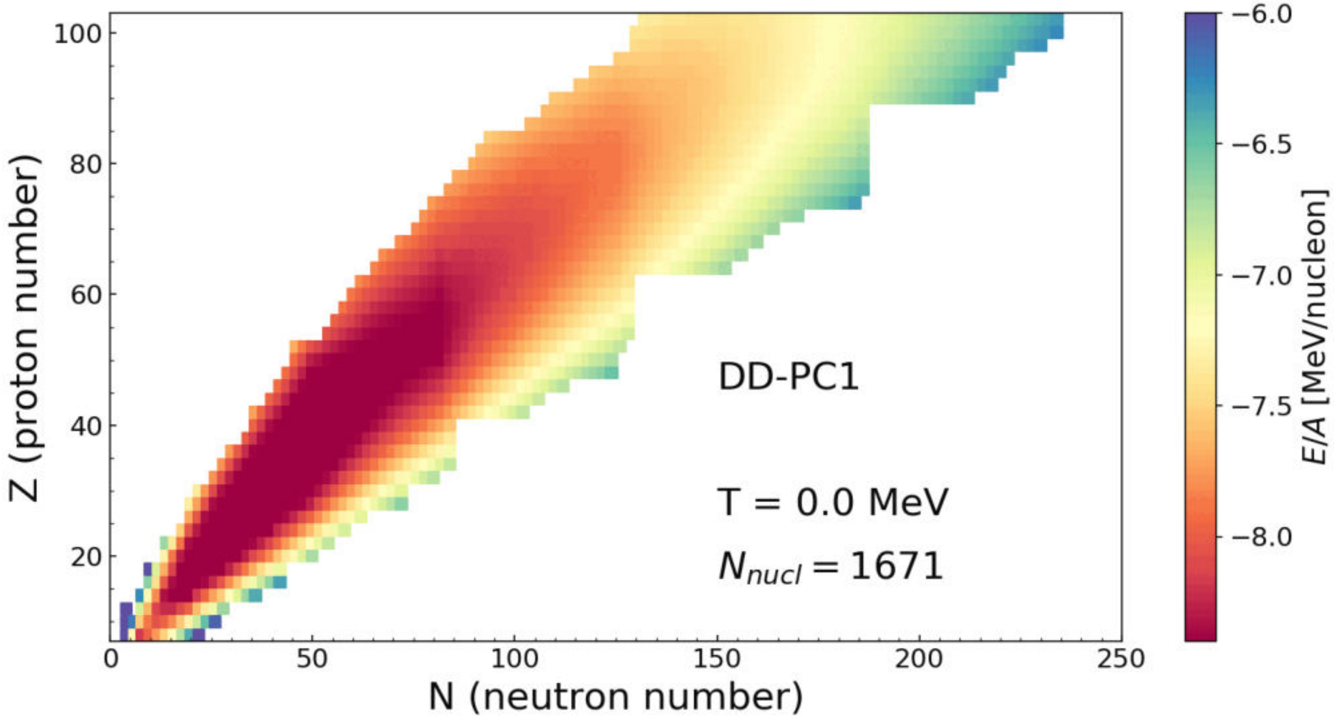
$$\delta E/\delta\rho = 0, \quad \delta E/\delta\kappa = 0$$

Mean field

Pairing field

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

NUCLIDE CHART AT FINITE TEMPERATURE



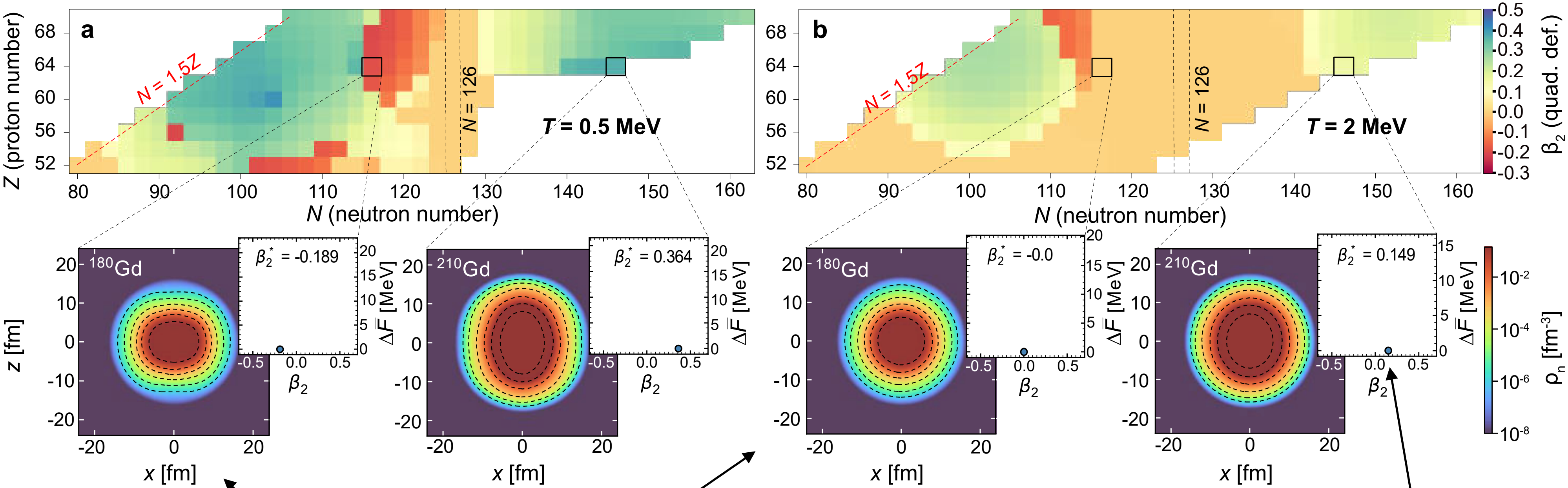
The evolution of nuclear binding energies for temperatures T = 0 - 2 MeV (0 - 2.3*10[10] K)

A. Ravlić, E. Yuksel, T. Nikšić, N.P., Nature Communications 14, 4834 (2023);
A. Ravlić, E. Yuksel. T. Nikšić, N.P., PRC 109, 014318 (2024)

TEMPERATURE EVOLUTION OF QUADRUPOLE DEFORMATION

- quadrupole deformation (β_2) for neutron-rich nuclei in the transition/lanthanide region at temperatures T = 0.5 MeV and T = 2.0 MeV.

$$\beta_2^{p(n)} = \frac{1}{2}\sqrt{\frac{5}{4\pi}}\frac{3}{4\pi Z(N) R_0^2} Q_{20}^{p(n)} \qquad Q_{20}^{p(n)} = \int d^3 r \bar{\rho}_v^{p(n)}(\boldsymbol{r})(2z^2 - r_\perp^2) \qquad \beta_2^{IS} = \beta_2^p + \beta_2^n$$

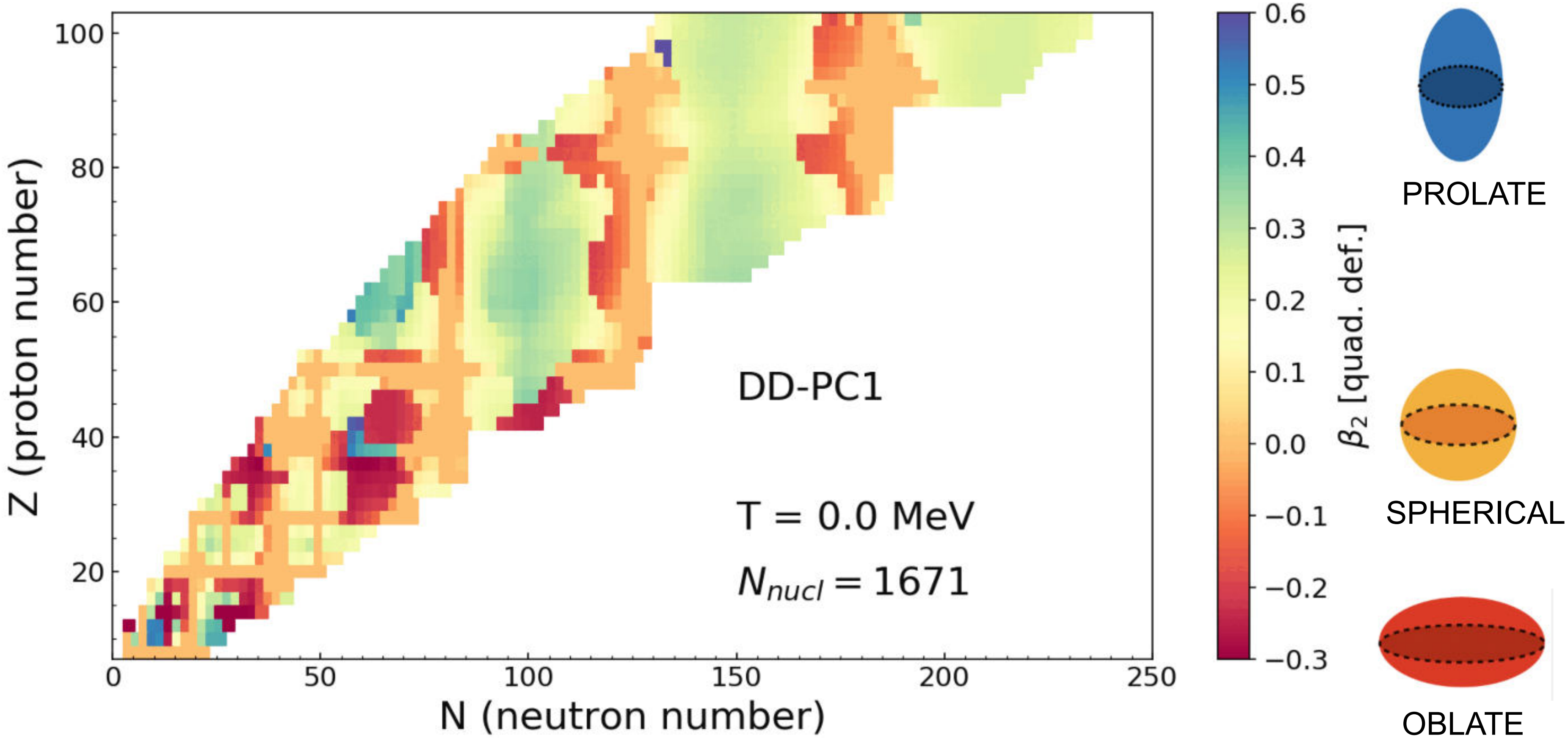


The continuum subtracted neutron density profiles for ^{180}Gd and ^{210}Gd, demonstrating the optimal shapes

Dependence of the relative subtracted free energy (ΔF), on the nuclear shape (β_2), with respect to minimum configuration

TEMPERATURE EVOLUTION OF QUADRUPOLE DEFORMATION

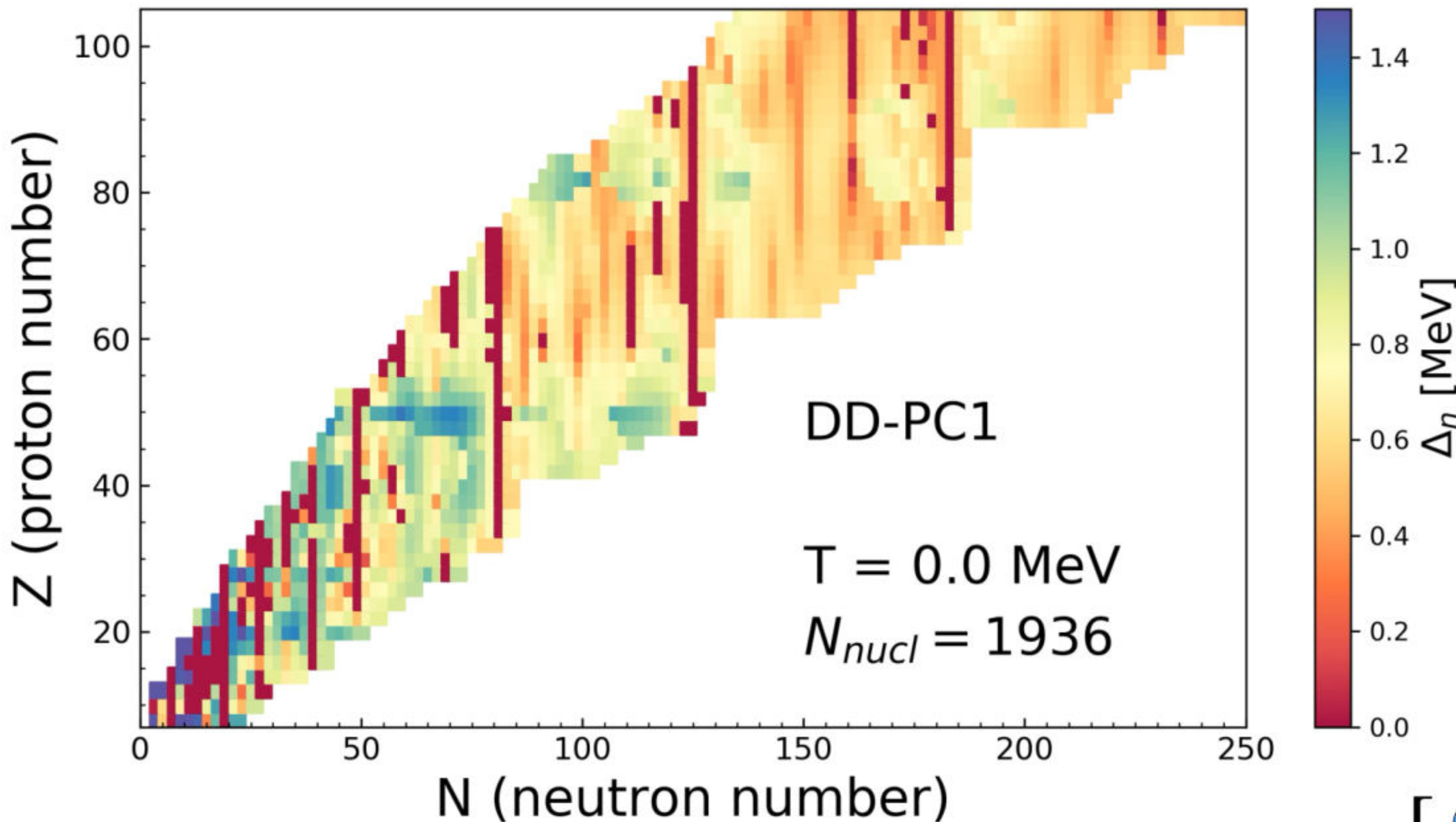
➢ The temperature evolution of the isoscalar quadrupole deformation β_2 for T = 0 - 2 MeV, calculated with the DD-PC1 functional

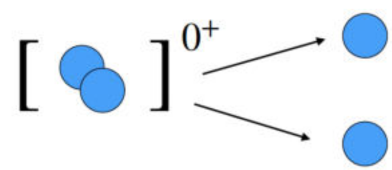


- With temperature increase, shape-phase transitions occur from deformed nuclei toward spherical shapes.

NUCLEAR PAIRING PROPERTIES AT FINITE TEMPERATURE

➢ The temperature evolution of nuclear pairing properties
→ neutron pairing gaps in the temperature range T = 0 – 1 MeV

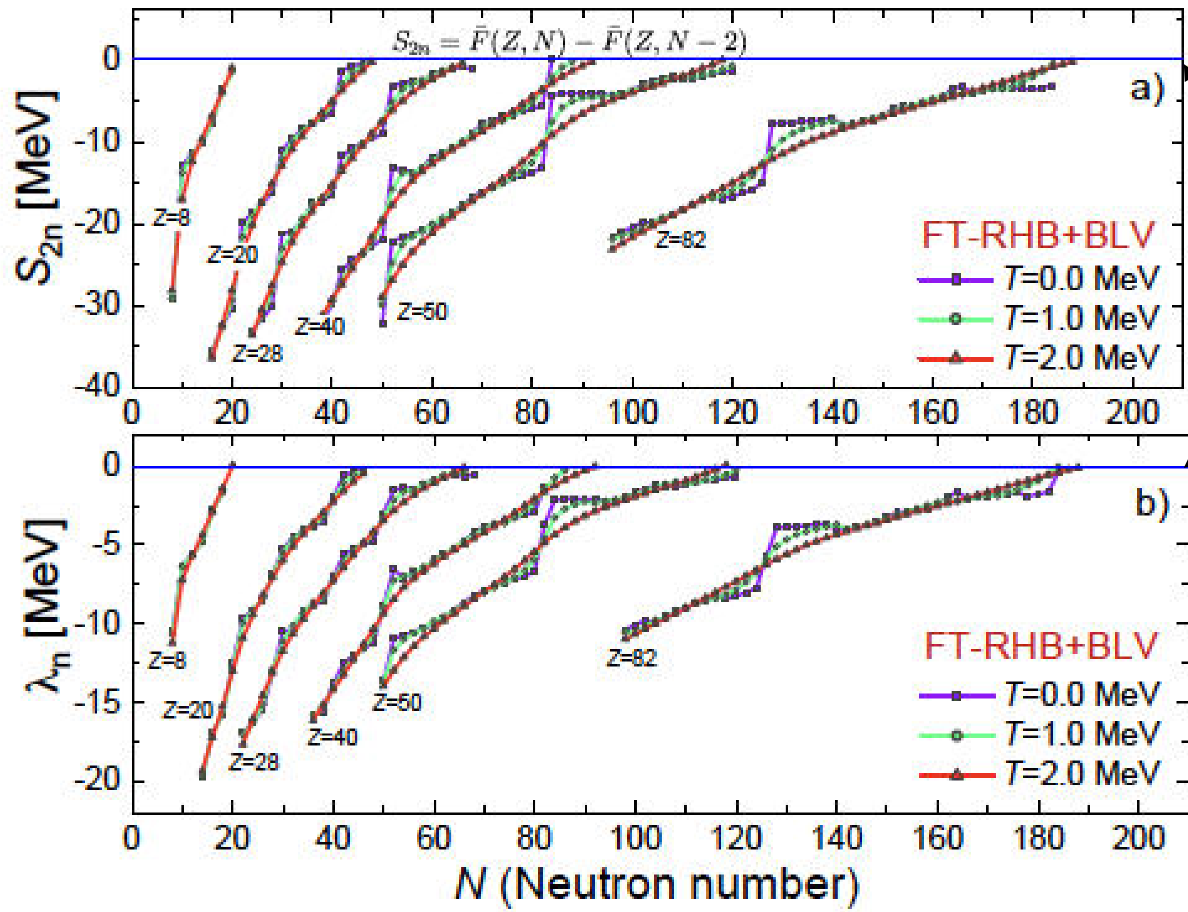




At lower temperatures, interplay of the pairing and temperature effects.
At critical temperature a phase transition occurs from the superfluid to a normal state.

GLOBAL NUCLEAR PROPERTIES AT FINITE TEMPERATURE

➢ Isotopic dependence of two-neutron separation energy S_{2n} (a) and neutron chemical potential λ_n (b) for the selected even-even nuclei



Bound nuclei are determined by the condition $S_{2n} \leq 0$ and $\lambda_n \leq 0$

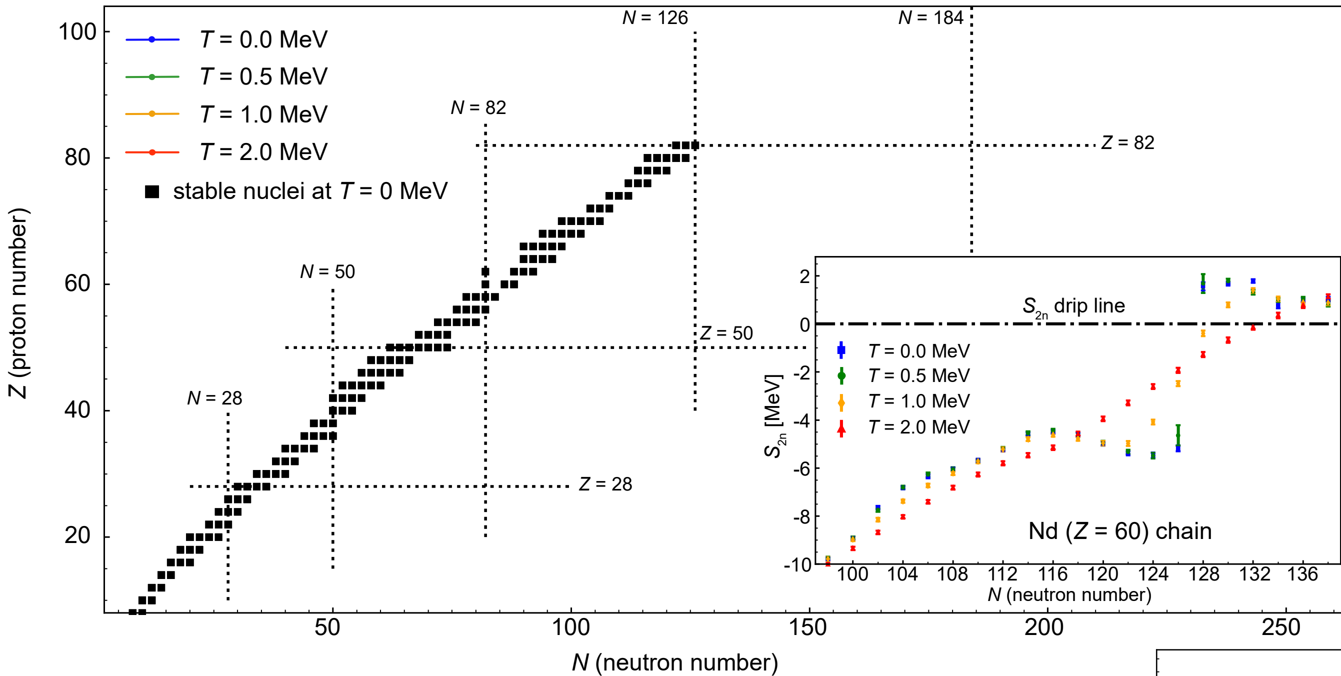
➢ Drip lines

Two-neutron separation energy is obtained from subtracted free energy difference

$$S_{2n} = \bar{F}(Z,N) - \bar{F}(Z,N-2) \geq 0$$

EXPANDING THE LIMITS OF NUCLEAR EXISTENCE WITH TEMPERATURE

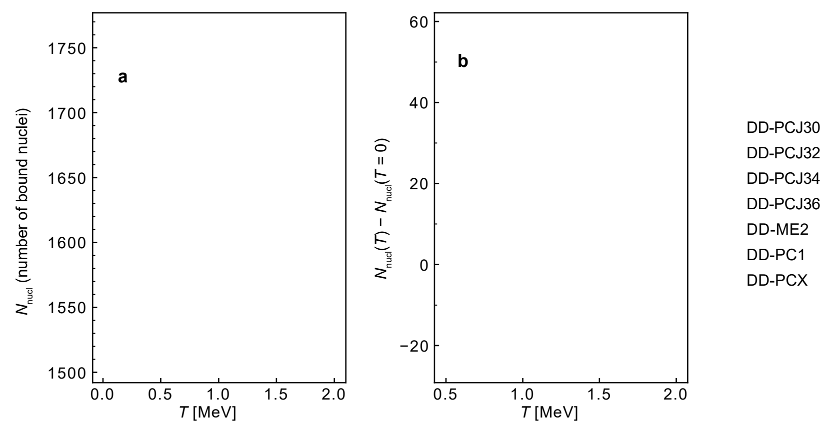
How the nuclear drip lines evolve with temperature?



The drip-lines are changing dynamically with the temperature increase

Increase of the number of bound nuclei with temperature due to thermal quenching of the shell effects

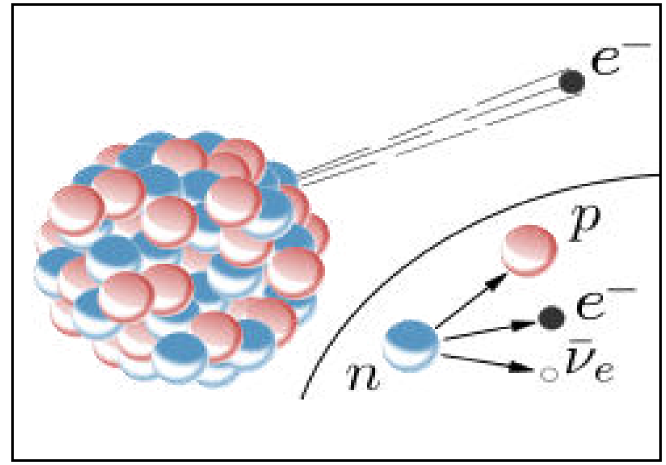
Different than expected for hot nuclei !



A. Ravlić, E. Yuksel, T. Nikšić, N.P., Nature Communications 14, 4834 (2023),

STELLAR BETA-DECAY RATES AT FINITE TEMPERATURE

- β-decay is important in stellar evolution and nucleosynthesis
- **How beta decay rates evolve by varying the temperature *(T)* and density (ρY_e) in stellar environment?**
- Exp. data are mainly limited to T=0 decays
- Theory framework for beta decays based on relativistic energy density functional and FT-PNRQRPA.
  A. Ravlić, E. Yuksel, Y. F. Niu, N. P., PRC 104, 054318 (2021)
- Includes finite temperature and pairing effects



β-decay rates:

Fermi-Dirac distribution for outgoing electrons

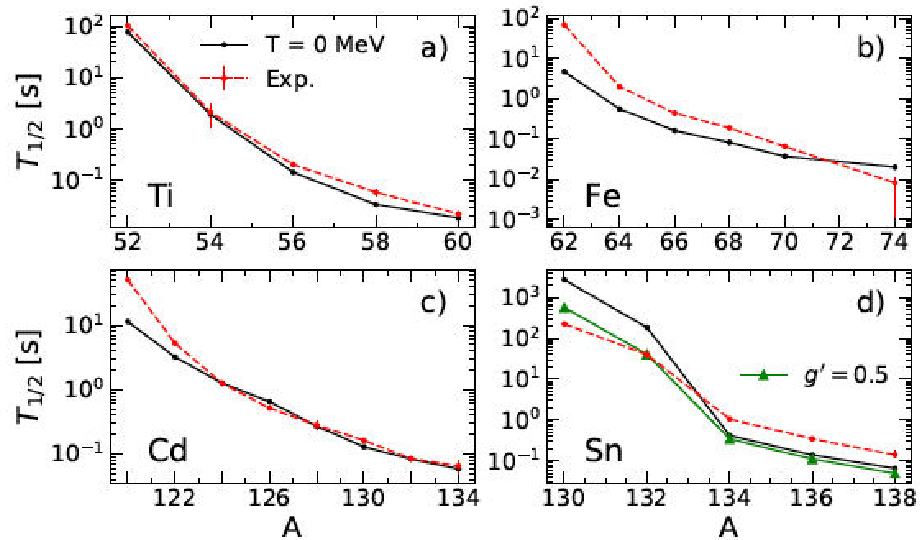
$$\lambda = \frac{\ln 2}{K}\int_0^{p_0} p_e^2\,(W_0 - W)^2\,F(Z,W)C(W)[1-f(W)]dp_e$$

electron energy and momentum

Fermi function

Shape factor (=B(GT) for allowed transitions)

$$T_{1/2} = \frac{\ln(2)}{\lambda}$$ Half-life

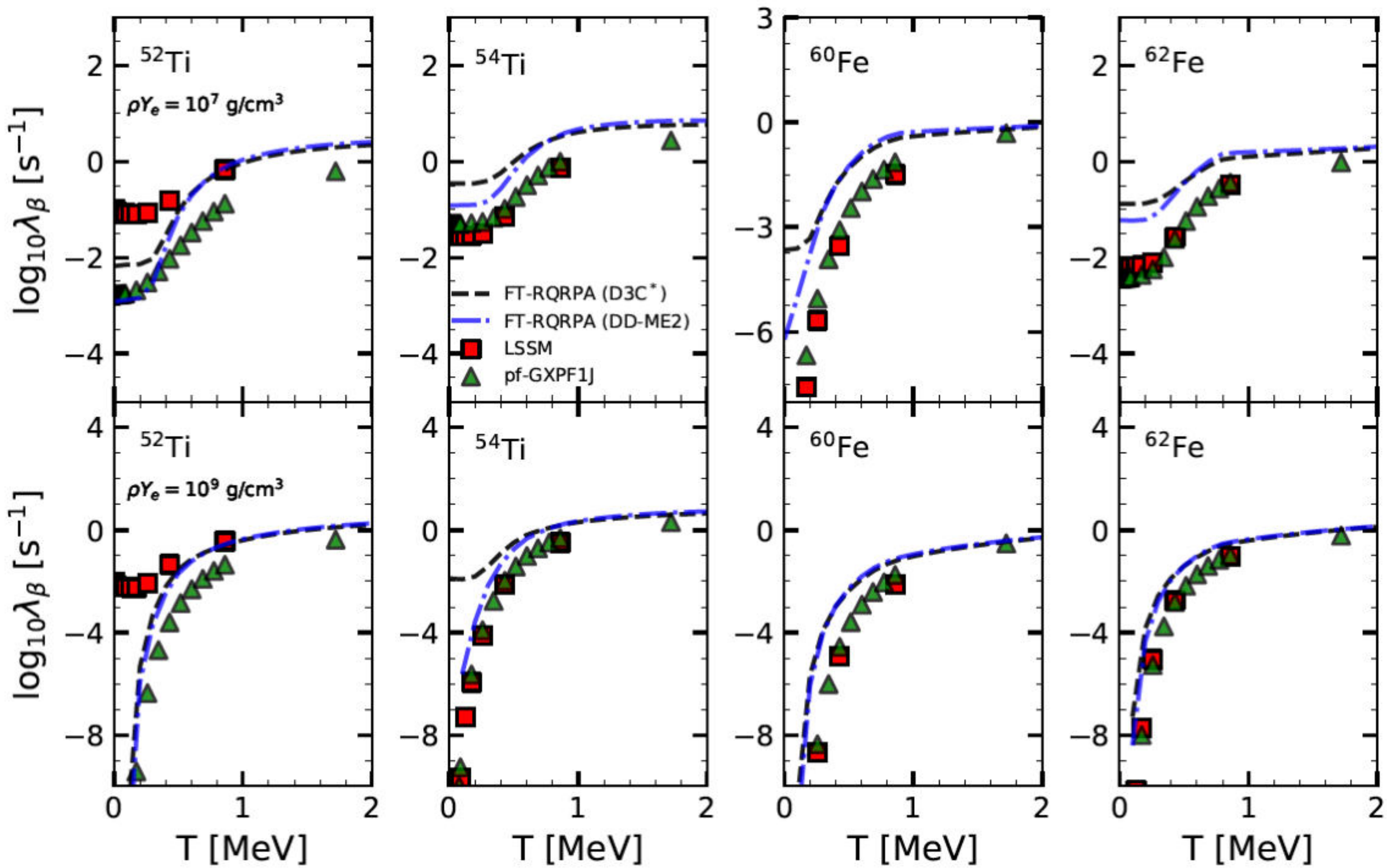


Benchmarking the model with the experimental data at zero temperature.

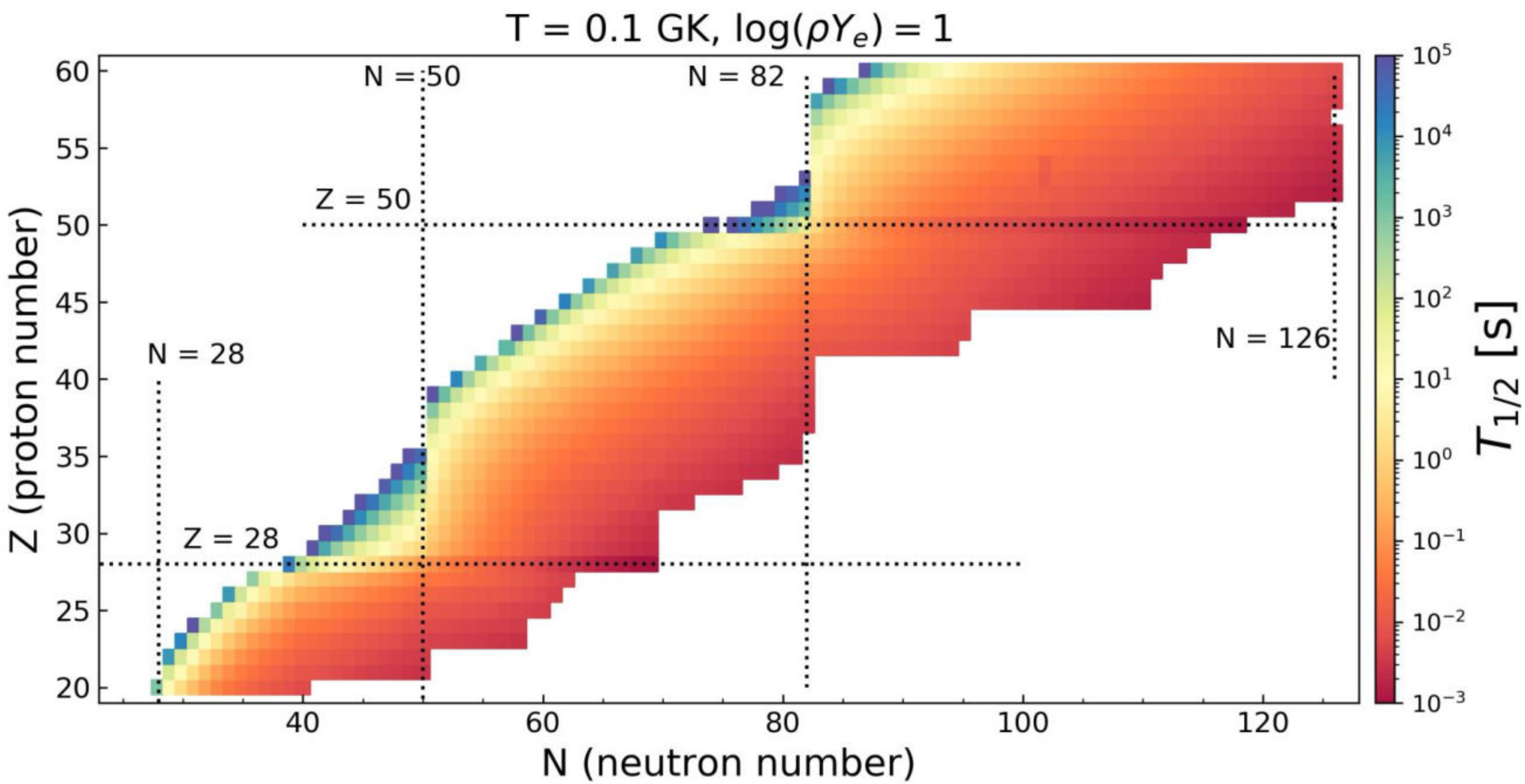
EVOLUTION OF BETA-DECAY RATES IN STELLAR ENVIRONMENT

- Beta-decay rates as a function of temperature for densities $\rho Y_e = 10^7\ g/cm^3$ and $\rho Y_e = 10^9\ g/cm^3$ A. Ravlić, E. Yuksel, Y. F. Niu, N. Paar, PRC 104, 054318 (2021).

- Comparison with the shell model LSSM (K. Langanke et al. ADNDT 79, 1 (2001)) and pf-GXPF1J (K. Mori et al., AJ 833, 179 (2016))

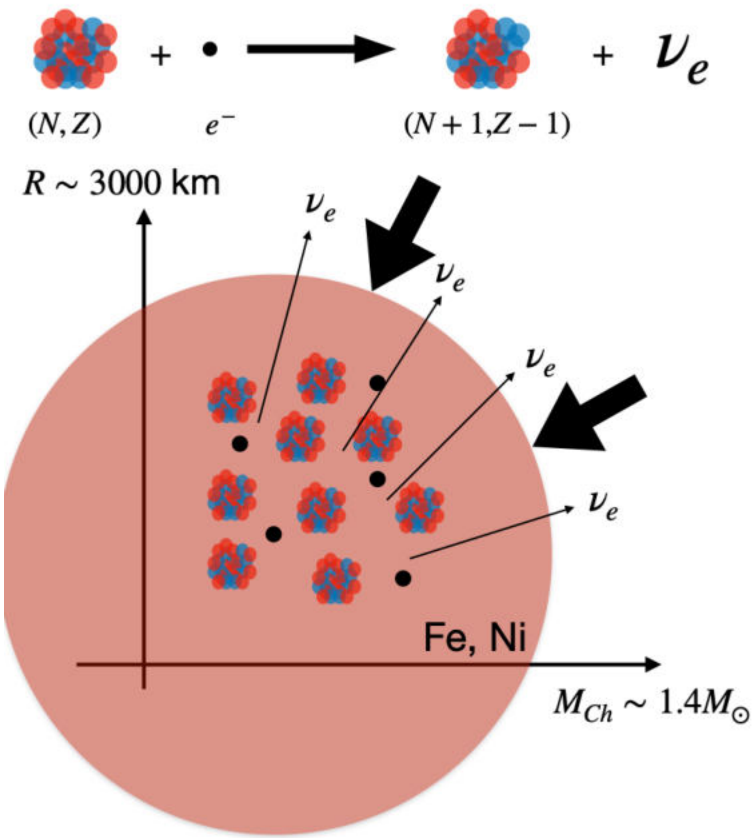


EVOLUTION OF BETA-DECAY HALF LIVES WITH TEMPERATURE INCREASE



- Largest impact of temperature effect on nuclei with long half-lives at T=0
- With temperature increase more nuclei start to decay (initially with long $T_{1/2}$)
- For most of nuclei half-lives decrease with increase of temperature

STELLAR ELECTRON CAPTURE



Initial phase of collapse

$\rho \sim 10^{10}$ g/cm^3, $T \sim 10$ GK

A. Ravlić, E. Yuksel, Y. F. Niu, G. Colo, E. Khan, N. P., PRC 102, 065804 (2020).

- The core of a massive star at the end of hydrostatic burning is stabilized by electron degeneracy pressure
- **Electron capture** (on protons and nuclei) reduces the number of electrons available for pressure support, initiates the gravitational collapse of the core of a massive star, triggering a supernova explosion
- **Weak interaction process**, occurs at finite temperature and at various densities depending on the stage of the stellar evolution

Finite-temperature proton-neutron relativistic QRPA (FT-PNRQRPA) is used for the description of relevant nuclear charge-exchange transitions (Gamow-Teller + forbidden)

⇨ $\sigma(E_e)$ Electron capture cross sections

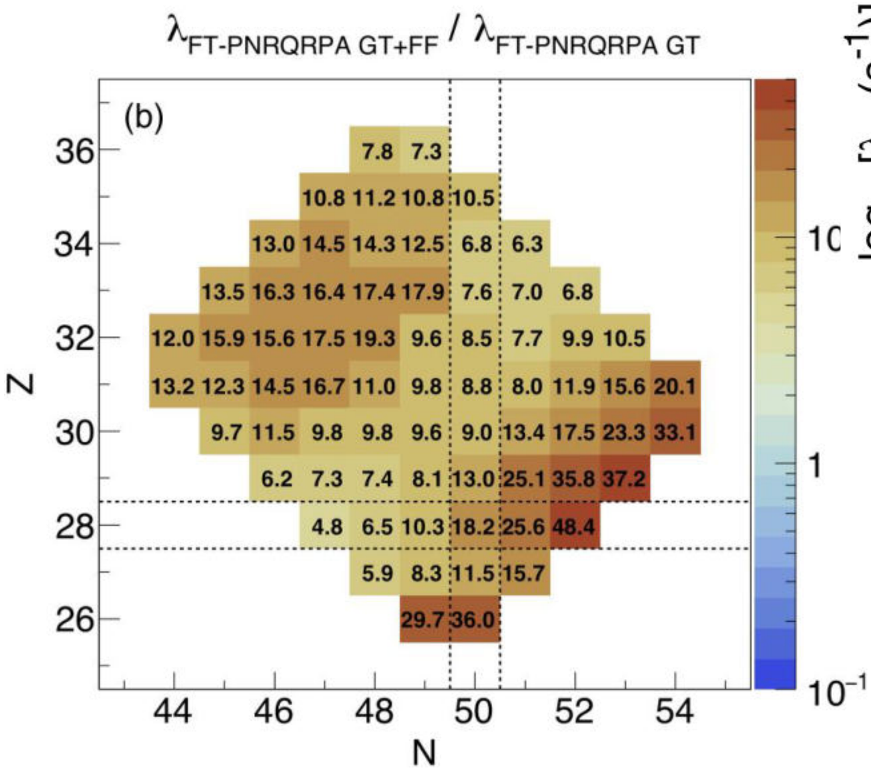
Electron capture rates are obtained by folding the cross section with Fermi-Dirac distribution for electrons

$$\lambda_{ec} = \frac{1}{\pi^2 \hbar^3} \int_{E_e^0}^{\infty} p_e E_e \sigma_{ec}(E_e) f(E_e, \mu_e, T) dE_e$$

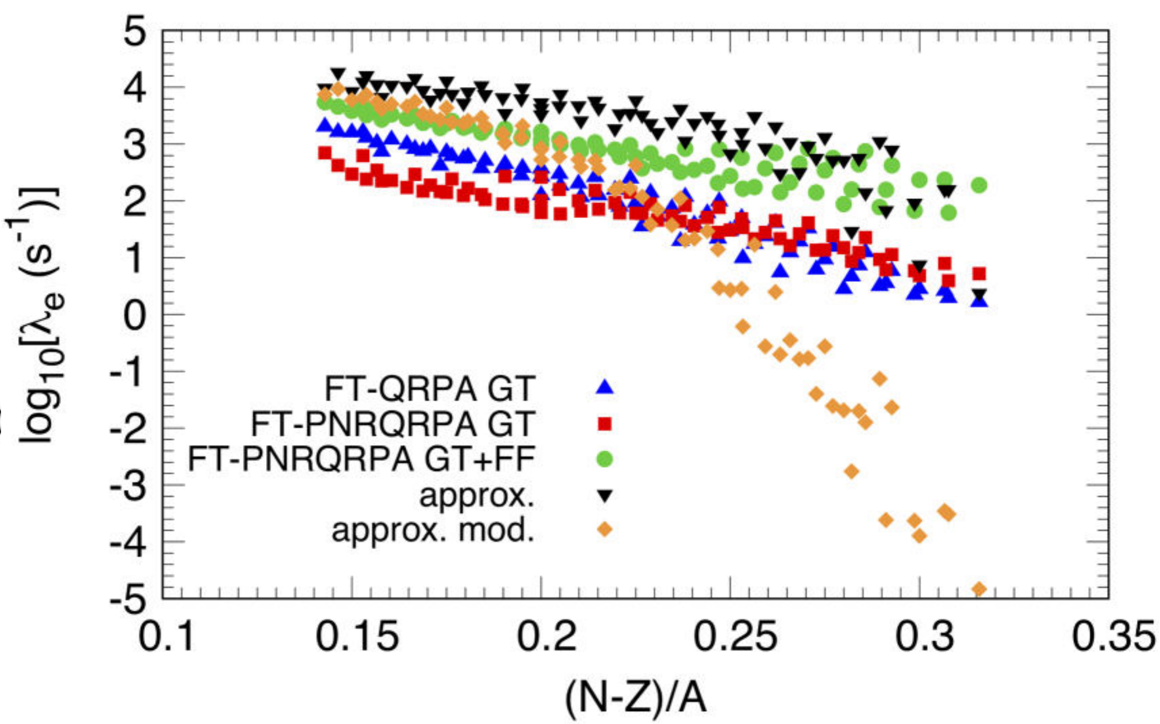
ELECTRON CAPTURE RATES AROUND N=50 SHELL CLOSURE

- Diamond region around N=50 shell closure relevant for core collapse supernova

Complete calculation includes Gamow-Teller and forbidden transitions



➢ S. Giraud, E. M. Ney, A. Ravlić, R. G. T. Zegers, J. Engel, N. P. et al., PRC 105, 055801 (2022)

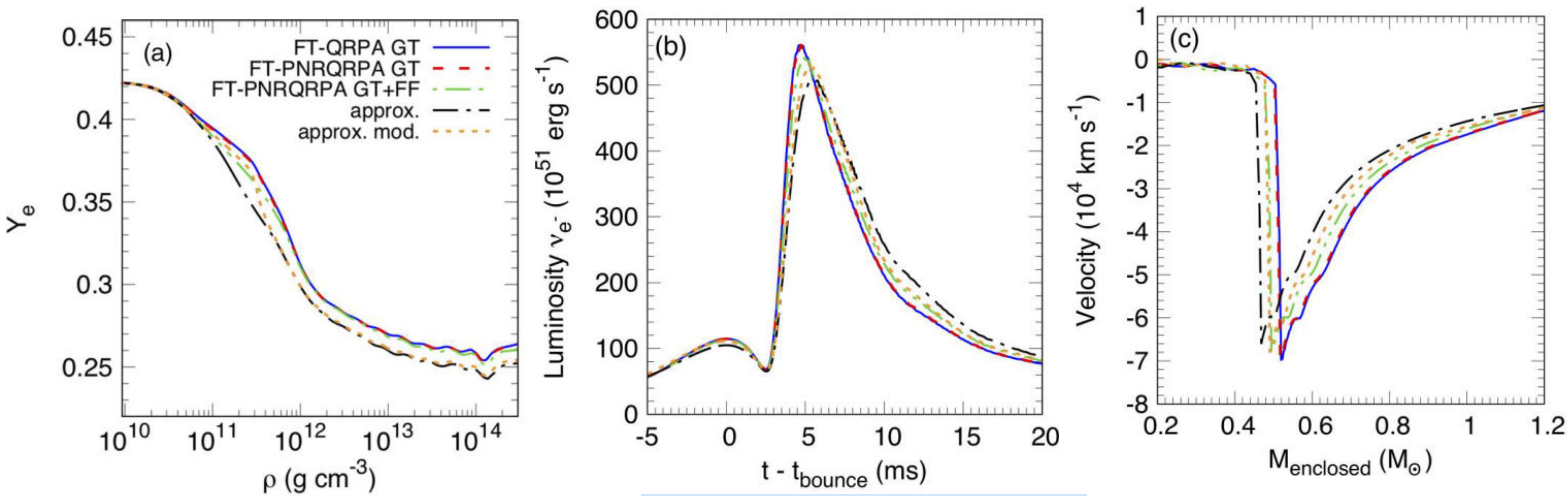


Comparison of the electron capture rates calculated using relativistic and nonrelativistic energy density functionals
→ Only the FT-PNRQRPA calculation is complete (GT+forbidden transitions)

CORE-COLLAPSE SUPERNOVA SIMULATION RESULTS

Initial test case for the new electron capture rates in N=50 diamond region

- core collapse supernova simulation with spherically symmetric code GR1D
  E. O'Connor, Astrophys. J. Suppl. Ser. 219, 24 (2015).
  C. Sullivan, E. O'Connor, R. G. T. Zegers, T. Grubb, and S. M. Austin, Astrophys. J. 816, 44 (2015).
- s15WW95 progenitor S. E. Woosley and T. A. Weaver, Astrophys. J. Suppl. 101, 181 (1995).
- SFHo equation of state A.W. Steiner, M. Hempel, and T. Fischer, Astrophys. J. 774, 17 (2013).



The electron-fraction Y_e as a function of central baryon density ρ

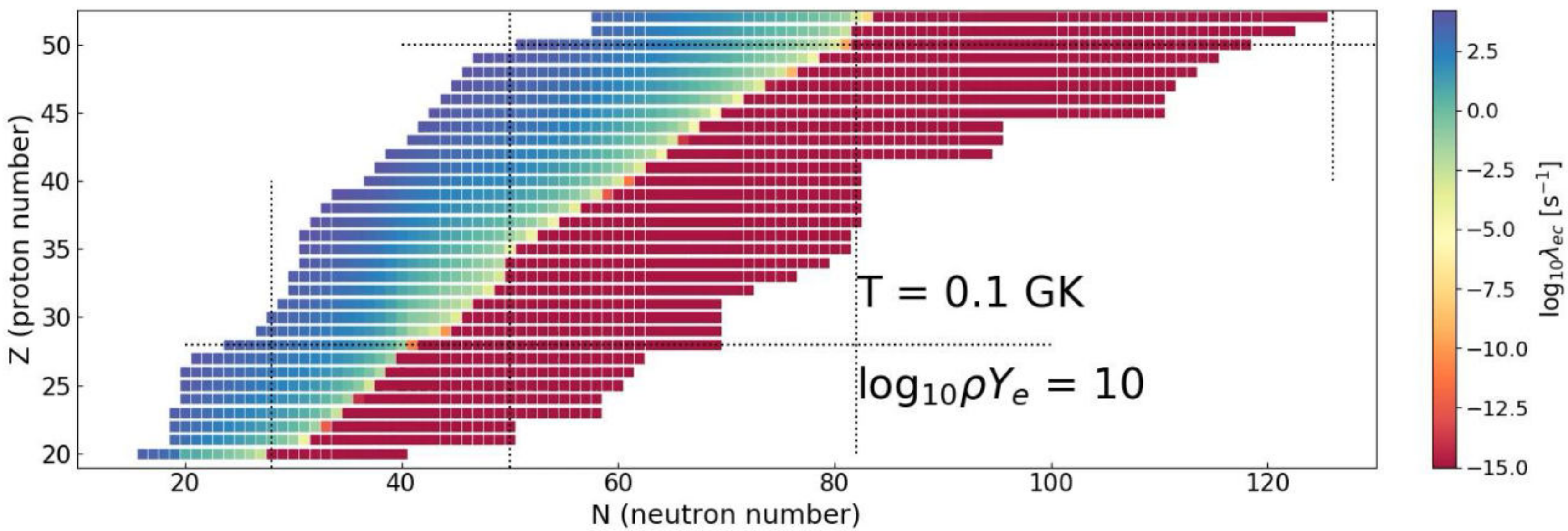
The electron neutrino luminosity at a radius of 500 km as a function of time after bounce,

The central velocity as a function of the enclosed mass.

➢ S. Giraud, E. M. Ney, A. Ravlić, R. G. T. Zegers, J. Engel, N. P. et al., PRC 105, 055801 (2022)

SYSTEMATIC CALCULATIONS OF STELLAR ELECTRON CAPTURE RATES

- Large-scale calculations of electron capture rates (EC) in the relativistic energy density functional approach using the FT-PNRQRPA
- Covering astrophysically relevant range of temperature and densities
- For example, for $\rho Ye=10^{10}$ g/cm^3 , the rates systematically increase

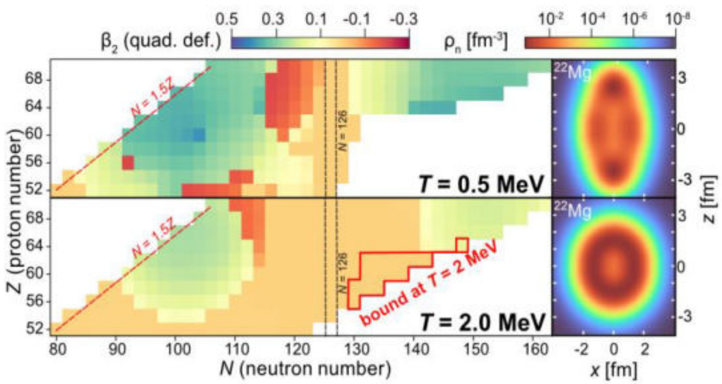


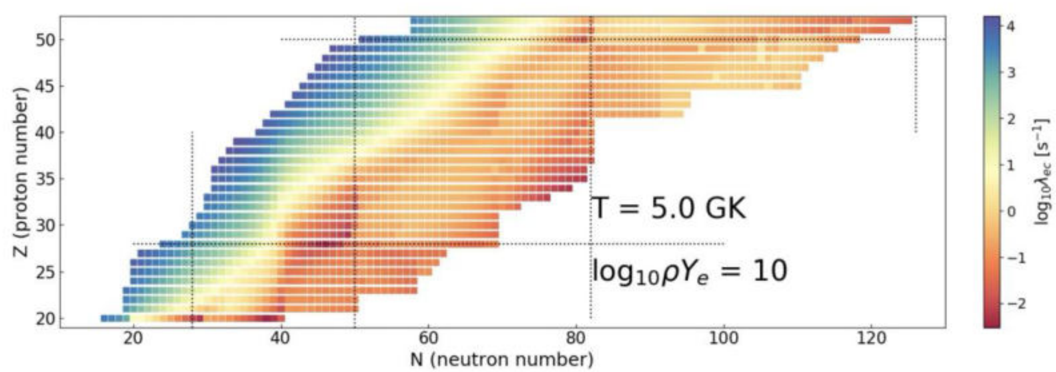
- Possible applications of these EC rates in core collapse supernova simulations

CONCLUDING REMARKS

- New microscopic relativistic framework for the description of nuclear properties and weak interaction processes at finite temperature (FT-RHB, FT-PNRQRPA)
- With temperature increase nuclei exhibit significant changes in their structure, excitation properties and weak processes – the interplay of temperature, pairing, deformation effects
- The nuclear drip lines should be viewed as limits that change dynamically with temperature.
- The beta decay and electron capture rates along nuclide map mainly increase with temperatures

➢ Applications in astrophysical simulations and nucleosynthesis calculations





THANKS TO COLLABORATORS

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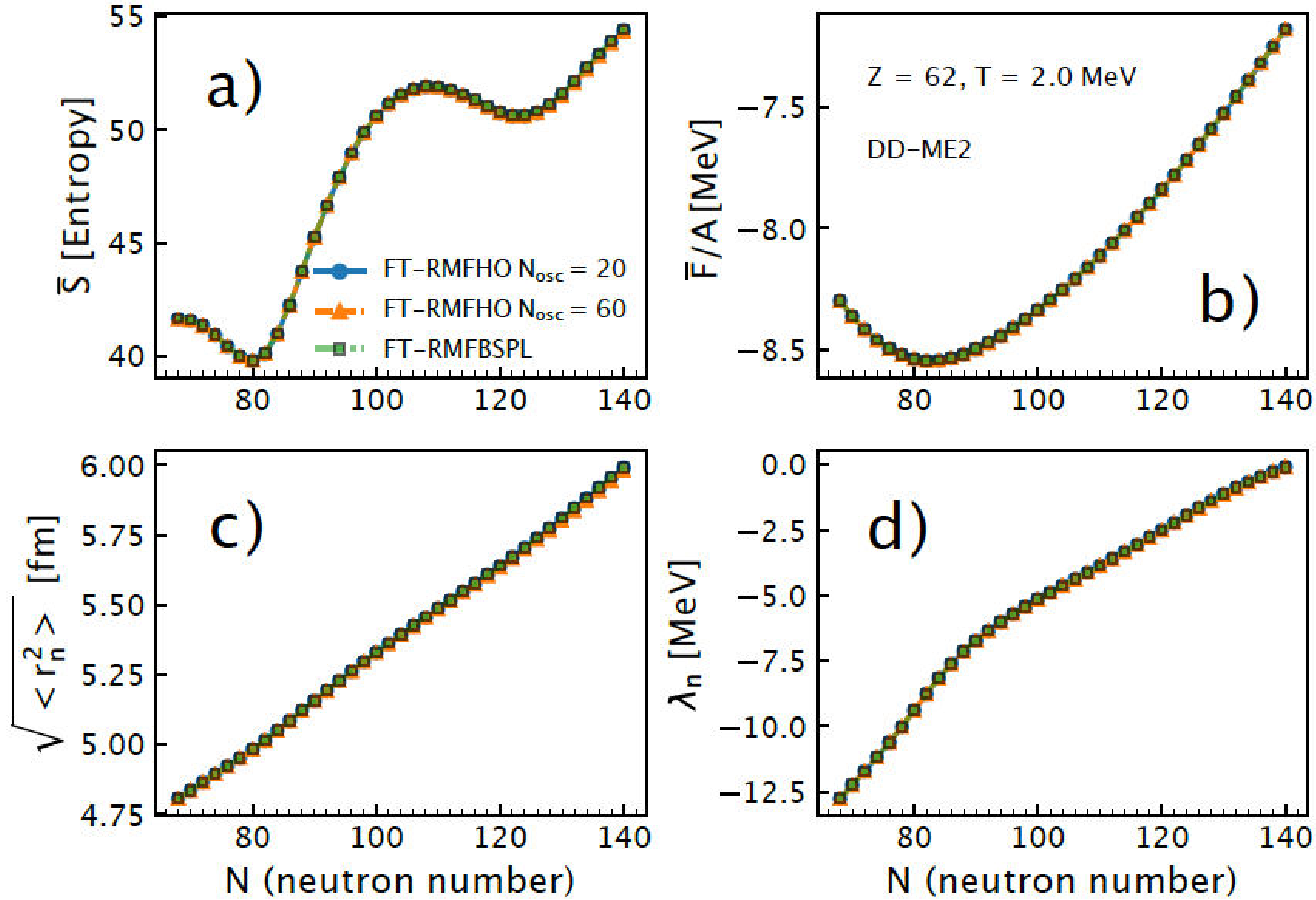
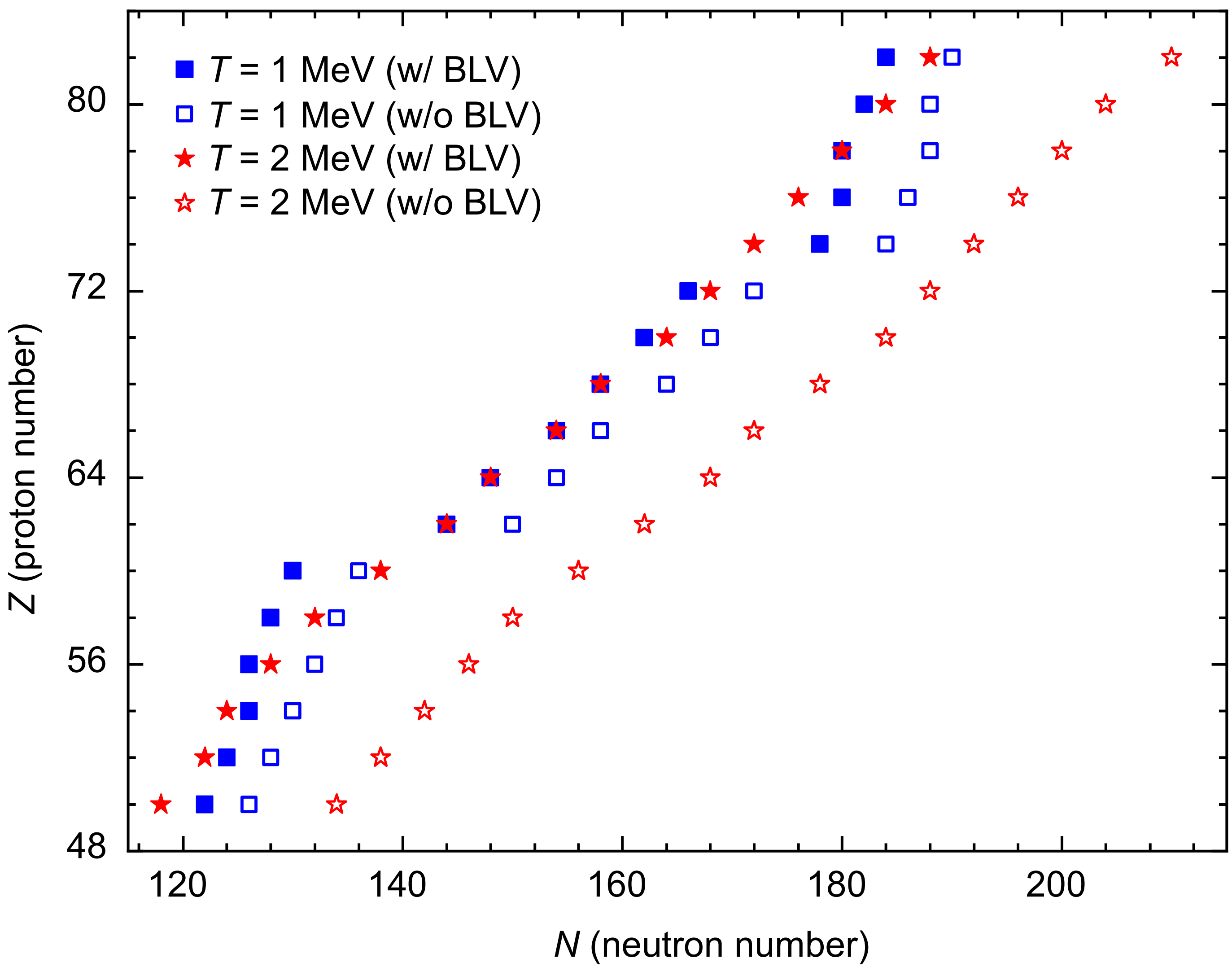
R. G. T. Zegers and S. Giraud (MSU/NSCL/FRIB)

Test of the FT-RMFHO model in comparison to FT-RMFBSPL model

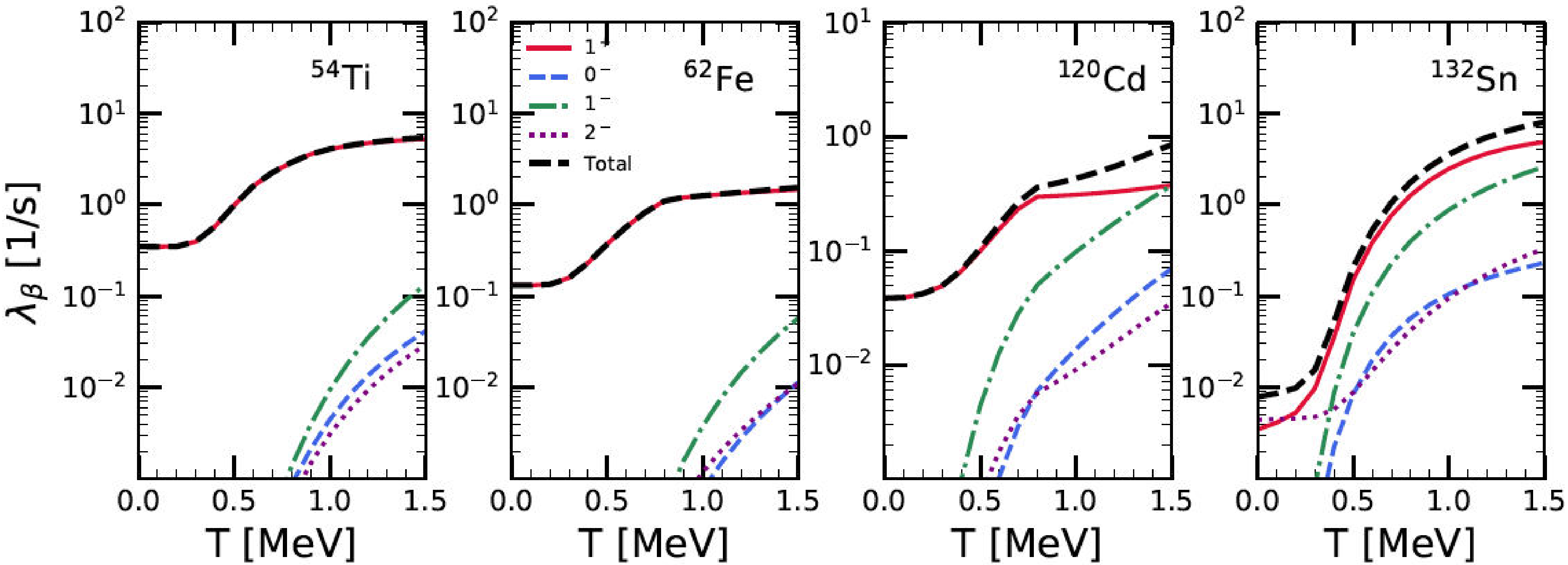


Impact of continuum subtraction on the position of the two-neutron drip-line



EVOLUTION OF BETA-DECAY RATES IN STELLAR ENVIRONMENT

- Temperature dependence of beta-decay rates for allowed (1+) and first-forbidden transitions and their total sum
- Calculations are performed at stellar density $\rho Y_e = 10^7\ g/cm^3$



A. Ravlić, E. Yuksel, Y. F. Niu, N. Paar, PRC 104, 054318 (2021)

STELLAR ELECTRON CAPTURE CROSS SECTIONS AND RATES

Electron capture is nuclear weak interaction process

- Weak interaction Hamiltonian:

$$\hat{H}_W = -\frac{G}{\sqrt{2}} \int d^3x \, j_\mu^{lept}(\boldsymbol{x}) \hat{\mathcal{J}}_\mu(\boldsymbol{x})$$

- Fermi golden rule to obtain the cross section:

$$\frac{d\sigma}{d\Omega} = \frac{1}{(2\pi)^2} \Omega^2 E_\nu^2 \frac{1}{2} \sum_{lept.spin.} \frac{1}{2J_i+1} \sum_{M_i, M_f} \left| \langle f | \hat{H}_W | i \rangle \right|^2$$

- Transition matrix elements are calculated using finite temperature relativistic proton-neutron QRPA (FT-PNRQRPA)

➢ A. Ravlić, E. Yuksel, Y. F. Niu, G. Colo, E. Khan, N. P, PRC 102, 065804 (2020).

Electron capture rates are obtained by folding the cross section with Fermi-Dirac distribution for electrons

$$\lambda_{ec} = \frac{1}{\pi^2 \hbar^3} \int_{E_e^0}^{\infty} p_e E_e \sigma_{ec}(E_e) f(E_e, \mu_e, T) dE_e$$