

Description of weak-interaction rates within the relativistic energy density functional theory

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Abstract. A new theoretical framework has been established and applied in the calculation of electron capture (EC) and β -decay rates in stellar environment, characterized by high density and temperature. For the description of the nuclear properties, the finite-temperature Hartree Bardeen-Cooper-Schrieffer (FT-HBCS) theory based on the relativistic derivative-coupling D3C* interaction is employed. In order to describe the charge-exchange transitions, the finite-temperature proton-neutron quasi-particle random-phase approximation is developed (FT-PNRQRPA) which includes both temperature and pairing correlations. In the FT-HBCS calculations, only the isovector pairing is included, while in the residual interaction of the FT-PNRQRPA both the isovector and isoscalar pairing contribute. In this work, results for EC and β -decay rates are presented in the temperature interval $T = 0-1.5$ MeV and stellar density $\rho Y_e = 10^7$ and 10^9 g/cm³. Both allowed 0^+ , 1^+ and first-forbidden transitions 0^- , 1^- and 2^- are included in the calculations. It is shown that interplay between pairing correlations and finite-temperature effects can lead to significant changes in rates. It is also important to include de-excitations, i.e. transitions with negative Q -value, that become increasingly significant at higher temperatures especially for pf -shell nuclei.

1 Introduction

Reactions mediated by the weak force are of significant importance for nuclear and particle physics, as well as nuclear astrophysics, where they specify the dynamics of core-collapse supernovae (CCSNe) and the time-scale of r -process. Electron capture (EC) plays a prominent role in the dynamics of CCSNe, which are mainly determined by two parameters: (i) electron-to-baryon ratio (Y_e) and (ii) the core entropy. An exploding star in the last stages of its life maintains a delicate balance between gravitational pull and degeneracy pressure originating from the Pauli blocking between electrons. The EC reactions remove electrons from

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the system, thus lowering Y_e , while outgoing neutrinos carry out entropy from the core. At certain stages in the collapse, β -decay can compete with EC when temperature is in the range $T_9(K) = 1-10$ ($T_9(K)$ denoting temperature in 10^9 K) and product of stellar density (ρ) and Y_e is $\rho Y_e \geq 10^7$ g/cm³ [1]. Therefore, for a complete understanding of the CCSNe dynamics, we need to study reaction rates of both EC and β -decay in stellar medium. Since the conditions that occur in CCSNe are beyond the experimental reach, simulations of CCSNe have to rely on theoretical predictions. Therefore, it is necessary to develop a robust theoretical framework for the description of key weak force reactions under extreme conditions of density and temperature. First steps toward this direction were made some time ago by Fuller, Fowler and Newman in Refs. [2–5] using the independent particle model. They have recognized the key role played by the Gamow-Teller (GT) resonance. Presently, the theoretical methods can be split into two main categories: (i) based on the shell-model (SM) calculations [6–8] and (ii) based on the random-phase approximation (RPA). Although shell-model calculations can reproduce experimental strength functions with success, they are computationally infeasible for nuclei with $A > 70$ due to the huge configuration space required for the description of nuclear excited states. Compared to the shell model calculations, the RPA method based on the nuclear energy density functionals (EDF) has a solid microscopic basis and the advantage of calculating main nuclear properties and excitations across the nuclide chart. Previously, the finite-temperature RPA (FT-RPA) method based on the relativistic [9] and non relativistic [10, 11] energy density functionals was used in the calculation of the EC rates and cross sections. It was shown that the unblocking effect of temperature in the charge-exchange transitions has a non-negligible effect on the EC results. Unblocking of the Gamow-Teller excitations at finite temperatures and their consequences on the EC and β -decay rates were also studied in the framework of the thermal quasi-particle RPA (TQRPA) which treats thermal excitations in a thermodynamically consistent way [12–14].

Recently, we have developed a theoretical framework for the calculation of the nuclear charge-exchange transitions in open-shell nuclei at finite temperatures, based on the relativistic nuclear EDFs. The proton-neutron relativistic quasi-particle RPA (FT-PNRQRPA) has been applied on top of the FT-HBCS to calculate the relevant charge-exchange transitions alongside the EC and β -decay rates [15–17]. In this work, we also use the same model to study the temperature dependence of EC and β -decay rates of selected Ti and Fe nuclei.

2 Theoretical formalism

For the calculation of the nuclear properties, we employ the RMF theory based on the meson-exchange relativistic energy density functional with derivative coupling D3C* [18]. Within this framework, nucleons interact via the exchange of isoscalar-scalar σ meson, isoscalar-vector ω meson and isovector-vector ρ meson, together with the electromagnetic (EM) interaction. The model is formulated starting from the Lagrangian density [18, 19]

$$\mathcal{L} = \mathcal{L}_N + \mathcal{L}_m + \mathcal{L}_{int}, \quad (1)$$

where \mathcal{L}_N is the Dirac Lagrangian for free nucleons, \mathcal{L}_m is the free meson Lagrangian and \mathcal{L}_{int} is the interaction term (see Refs. [18–20] for details). We treat both the mean-field and pairing correlations at finite-temperature within the FT-HBCS theory [21]. At finite temperature, occupation probabilities of single-particle states are given by

$$n_k = v_k^2(1 - f_k) + u_k^2 f_k, \quad (2)$$

where u_k, v_k are the FT-HBCS amplitudes and f_k is the Fermi-Dirac factor, $f_k = (1 + e^{-\beta E_k})^{-1}$, $\beta = 1/k_B T$, T denoting the temperature and k_B is the Boltzmann constant. The quasi-particle

Table 1. The monopole pairing strengths for neutrons(protons) $G_{n(p)}$ (in units MeV/A where A is the nuclear mass number), adjusted to reproduce the empirical neutron(proton) pairing gaps $\Delta_{n(p)}^{5p}$ calculated using the five-point formula [22] for ^{52}Ti and ^{58}Fe . Calculations are performed using the FT-HBCS with D3C* interaction.

Nucleus	Δ_n^{5p} [MeV]	Δ_p^{5p} [MeV]	G_n [MeV/A]	G_p [MeV/A]
^{52}Ti	0.95	1.63	19.40	30.60
^{58}Fe	1.45	1.73	21.60	30.60

(q.p.) energies are given by $E_k = \sqrt{(\varepsilon_k - \lambda)^2 + \Delta_k^2}$, where ε_k is the single-particle energy, λ is the chemical potential for either protons or neutrons and Δ_k is the state-dependent pairing gap obtained by solving the gap equation [21]. In this work, we use a monopole pairing interaction characterized by strength parameters $G_{n(p)}$ for neutrons(protons) which are determined according to the five-point formula [22]. Corresponding parameters $G_{n(p)}$ for ^{52}Ti and ^{58}Fe can be found in Table 1, adjusted to reproduce the five-point neutron(proton) pairing gaps $\Delta_{n(p)}^{5p}$.

The FT-PNRQRPA consists in a small-amplitude limit of the time-dependent FT-HBCS theory. Recently, it was developed and applied to study the charge-exchange transitions in Ref. [15]. The particle-hole (ph) part of the residual interaction is derived self-consistently from the same EDF used in the ground-state calculation. The strength parameter of the Landau-Migdal interaction $g' = 0.76$ is determined by reproducing the experimental excitation energy of GT^- resonance in ^{208}Pb [18]. The particle-particle (pp) part of the residual interaction has both isovector ($T = 1, S = 0$) and isoscalar ($T = 0, S = 1$) components. The isovector component assumes the pairing part of the Gogny D1S interaction [16], while for the isoscalar component a formulation consisting of a sum of two Gaussians is employed

$$V_{12} = V_0^{is} \sum_{j=1}^2 g_j e^{-r_{12}^2/\mu_j^2} \prod_{S=1, T=0}, \quad (3)$$

where $\prod_{S=1, T=0}$ denotes projector on $T = 0, S = 1$ states, r_{12} is the relative coordinate, $\mu_1 = 1.2$ fm, $\mu_2 = 0.7$ fm and the strength parameters are set to $g_1 = 1$ and $g_2 = -2$ [23]. The isoscalar pairing strength is constrained using the following functional [24]

$$V_0^{is} = V_L + \frac{V_D}{1 + e^{a+b(N-Z)}}, \quad (4)$$

with values defined in Ref. [17] and adjusted to reproduce all experimental data on β -decay half-lives in the range $8 \leq Z \leq 82$.

The FT-PNRQRPA equation can be written in the matrix form for a well defined angular momentum and parity J^π as [15, 25]

$$\begin{pmatrix} \tilde{C} & \tilde{a} & \tilde{b} & \tilde{D} \\ \tilde{a}^\dagger & \tilde{A} & \tilde{B} & \tilde{b}^T \\ -\tilde{b}^\dagger & -\tilde{B}^* & -\tilde{A}^* & -\tilde{a}^T \\ -\tilde{D}^* & -\tilde{b}^* & -\tilde{a}^* & -\tilde{C}^* \end{pmatrix} \begin{pmatrix} \tilde{P} \\ \tilde{X} \\ \tilde{Y} \\ \tilde{Q} \end{pmatrix} = E_n \begin{pmatrix} \tilde{P} \\ \tilde{X} \\ \tilde{Y} \\ \tilde{Q} \end{pmatrix}, \quad (5)$$

where the excited state energy is determined by the eigenvalue E_n , while the set of eigenvectors $(\tilde{P} \ \tilde{X} \ \tilde{Y} \ \tilde{Q})^T$ is used to calculate the transition strength. Explicit forms of the submatrices $\tilde{A}, \tilde{B}, \tilde{C}, \tilde{D}, \tilde{a}, \tilde{b}, \tilde{a}^T, \tilde{b}^T, \tilde{a}^\dagger, \tilde{b}^\dagger$ can be found in Ref. [25]. Calculations can be performed for both directions of the isospin projection $\Delta T_z = \pm 1$. Finally, the strength function

for the charge-exchange external field operator \hat{F} in the $\Delta T_z = -1$ direction ($n \rightarrow p$) can be written as

$$B(\hat{F})_n = \frac{1}{1 - e^{-\beta(E_n - \lambda_{np})}} \left| \sum_{\pi > \nu} \left[(\tilde{X}_{\pi\nu}^n u_\pi v_\nu + \tilde{Y}_{\pi\nu}^n v_\pi u_\nu) \sqrt{1 - f_\pi - f_\nu} + (\tilde{P}_{\pi\nu}^n u_\pi u_\nu - \tilde{Q}_{\pi\nu}^n v_\pi v_\nu) \sqrt{f_\pi - f_\nu} \right] \langle \pi || \hat{F} || \nu \rangle \right|^2, \quad (8)$$

where $\pi(\nu)$ denote quasi-proton(neutron) states, $\lambda_{np} = \lambda_n - \lambda_p$ is the difference between the neutron and proton chemical potential and summation is performed over states with $E_\pi > E_\nu$. The exponential prefactor $(1 - e^{-\beta(E_n - \lambda_{np})})^{-1}$ appears to relate the FT-PNRQRP strength function to the physical strength function [26]. This implies that not only positive energy transitions with $E > \lambda_{np}$ should be included in the calculation of the strength function but also the negative energy transitions with $E < \lambda_{np}$, i.e. de-excitations. The latter are calculated using the strength function in the $\Delta T_z = +1$ channel (see Refs. [17, 26] for further details).

3 Description of electron capture rates

In presupernova environment, nuclei are assumed to be fully ionized and immersed in electron plasma, described by the Fermi-Dirac distribution of electrons. Such a system is characterized by its temperature T and stellar density ρY_e . To calculate the EC rates including both allowed (0^+ , 1^+) and first-forbidden transitions (0^- , 1^- , 2^-) we use the formalism given in Refs. [27, 28] where the current-current form of the weak interaction Hamiltonian is assumed. By following Refs. [27, 28] the EC cross section σ_{ec} can be expressed in terms of multipole transition operators $\hat{M}_J, \hat{L}_J, \hat{T}_J^{mag}, \hat{T}_J^{el}$, for a well defined J^π . The coupling constant g_A of the axial-vector part of multipole transition operators is quenched from the free-nucleon value $g_A = -1.26$ to $g_A = -1.0$ [16]. Electron capture rates are calculated by folding the cross section σ_{ec} with a Fermi-Dirac distribution of electrons

$$\lambda_{ec} = \frac{(m_e c^2)^3}{\pi^2 \hbar^3} \int_{W_0}^{\infty} p W \sigma_{ec}(W) f_e(W) dW, \quad (7)$$

where the dimensionless electron energy is defined as $W = E_e/(m_e c^2)$, m_e is the electron mass and $p = p_e/(m_e c)$ is the electron momentum. The minimum electron energy W_0 is imposed by the condition on outgoing neutrino energy $E_\nu > 0$. The Fermi-Dirac distribution is defined by the electron chemical potential μ_e and temperature T

$$f(W, \mu_e, T) = \frac{1}{\exp\left(\frac{W m_e c^2 - \mu_e}{k_B T}\right) + 1}. \quad (8)$$

The electron chemical potential μ_e is determined by the charge-neutrality condition [16, 29]. While in Ref. [16] we have performed the sensitivity study of EC rates on the isoscalar pairing strength V_0^{is} , here we constrain it by using the functional form of Eq. (4), with parameters determined by reproducing the experimental β -decay half-lives [17]. In Figure 1, we show the temperature evolution of EC rates for two pf -shell nuclei, ^{52}Ti and ^{58}Fe , at stellar densities $\rho Y_e = 10^7$ and 10^9 g/cm³. The FT-HBCS + FT-PNRQRP calculations with D3C* interaction (blue dashed line) are compared to the large-scale shell model (LSSM) calculations of Langanke *et al.* (red squares) [6] and shell-model calculations based on the pf -GXPF1J interaction (green triangles) [7, 30]. It is seen that EC rates increase with temperature and the

stellar density ρY_e . The former fact is explained by thermal unblocking of q.p. levels at finite temperature and contribution of de-excitations (see Ref. [17] for details), while the latter is a consequence of increasing the lepton phase-space, thus including more transition strength in the EC rate integral of Eq. (7). The present model somewhat overestimates the shell-model rates, however, the overall trends are reasonably reproduced.

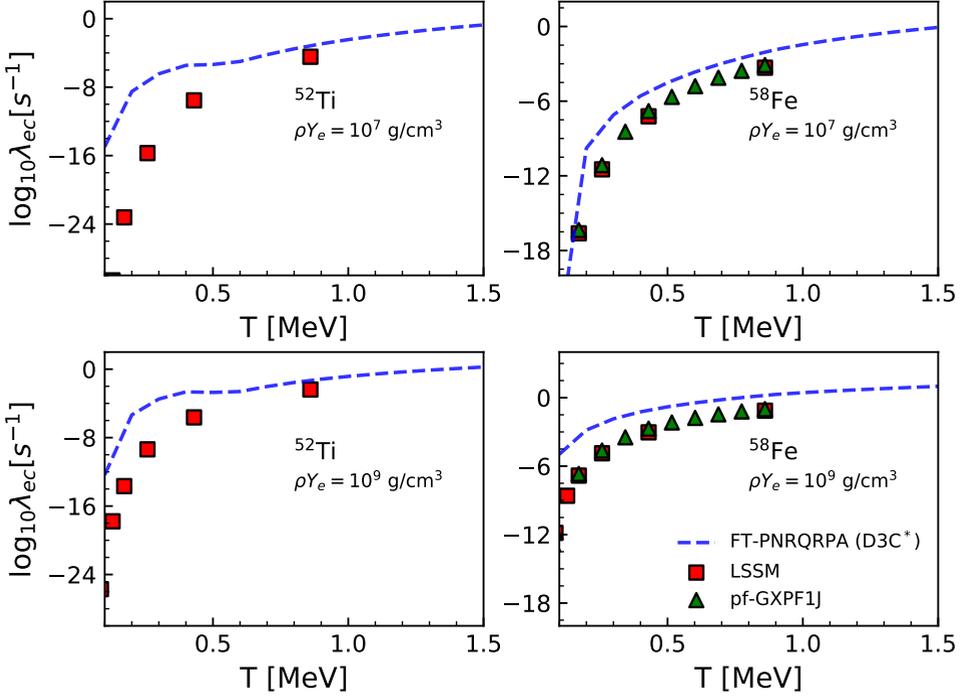


Figure 1. Electron capture rates λ_{ec} for ^{52}Ti and ^{58}Fe for stellar densities $\rho Y_e = 10^7$ and 10^9 g/cm^3 . The FT-PNRQRPA results (blue dashed line) with D3C* interaction are shown together with the LSSM results (red squares) [6], and the shell-model results based on the pf-GXPF1J interaction (green triangles) [7, 30].

4 Description of β -decay rates

Same assumptions of presupernova environment are also applied in the study of stellar β -decay rates. Both allowed and first-forbidden transitions are included in the calculations. The general form of the β -decay rate in stellar conditions is given by [29, 31]

$$\lambda_{\beta} = \frac{\ln 2}{K} \int_0^{p_0} p^2 (W_0 - W)^2 F(Z, W) C(W) [1 - f(W, \mu_e, T)] dp, \quad (9)$$

where W_0 is the maximum electron energy given by the difference between initial and final nuclear mass, and integration is performed up to a maximal electron momentum p_0 . The Fermi function $F(Z, W)$ takes into account distortion of electron wavefunctions [29]. The shape-factor $C(W)$ depends on the quantum numbers of considered transitions, and its functional form can be found in Ref. [31]. The constant K is measured in super-allowed β -decay

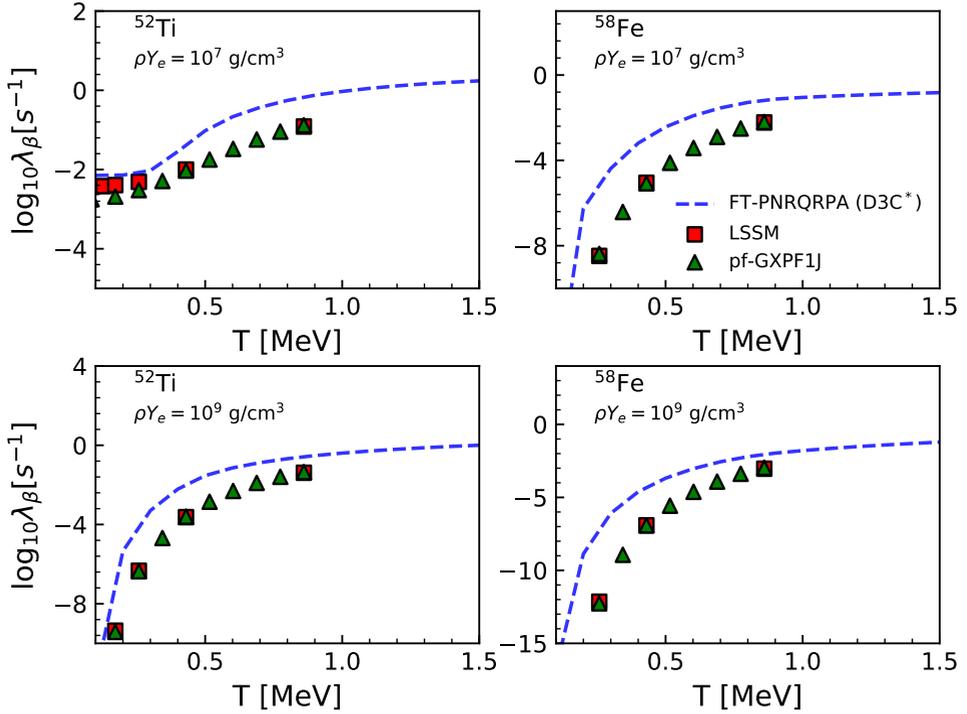


Figure 2. The same as Fig. 1 but for β -decay rate λ_β .

to be $K = 6144 \pm 2$ s [32]. It is important to note that within our model, the same parameters used in EC calculations are applied to the β -decay calculation. Thus, the axial-vector coupling is quenched to $g_A = -1.0$. In Figure 2, the results calculated with the FT-HBCS+FT-PNRQRPA model using D3C* interaction (blue dashed line) are compared to the LSSM results (red squares) [6], and the shell-model results based on the pf-GXPF1J interaction (green triangles) [7, 30] at $\rho Y_e = 10^7$ (upper panels) and $\rho Y_e = 10^9$ g/cm³ (lower panels). Although the shell-model results include only the allowed GT transitions, influence of first-forbidden transitions for pf -shell nuclei is negligible up to $T < 1.5$ MeV [17]. In the case of β -decay, it is observed that rates decrease with increasing ρY_e . This effect is related to the phase-space blocking with increasing electron chemical-potential. As the temperature increases, electron chemical potential is decreased, thus allowing for an increase in the β -decay rate. Also, there are two main reasons for the increase of β -decay rate with temperature: (i) vanishing of pairing correlations and (ii) contribution of de-excitations (check Ref. [17] for more details on de-excitations). With vanishing pairing correlations, low lying strength in the Q_β window gets redistributed to lower excitation energies, thus increasing the rate. Furthermore, with increasing temperature, negative energy transitions (de-excitations) become unblocked and have a dominant contribution to the β -decay rate, especially for pf -shell nuclei near the valley of stability [17]. It is observed that the FT-HBCS+FT-PNRQRPA results have good agreement with two shell-model results, meaning that main trends of the temperature evolution of β -decay rates are reproduced.

5 Conclusions

Recently developed FT-HBCS+FT-PNRQRPA based on the relativistic D3C* derivative coupling interaction has been applied to study both the EC and β -decay rates in presupernova conditions. Our model allows us to study the interplay between finite-temperature and pairing correlation effects, as well as their influence on reactions mediated by the weak force. Rates are characterized by their dependence on temperature T and stellar density ρY_e . In stellar environment, nuclei can be found in highly-excited states, thus the proper treatment of negative energy transitions, i.e. de-excitations is of crucial importance. Model calculations were performed for two pf -shell nuclei ^{52}Ti and ^{58}Fe for EC and β -decay stellar rates and compared with respective shell-model calculations. It is shown that both EC and β -decay rates increase with increasing temperature, however, due to different reasons. The EC rates mainly increase because of the thermal unblocking of q.p. states while the β -decay rates are considerably influenced by the negative energy transitions. For both EC and β -decay rates, vanishing of pairing correlations at critical temperature influences the rates. It is demonstrated that rates based on the FT-HBCS+FT-PNRQRPA model can reproduce the main trends of shell-model rates, with considerably less computational resources. Therefore, our model is instrumental to provide large-scale rate tables of EC and β -decay to be used in astrophysical simulations of interest. Extension of the model from spherical to axially-deformed nuclei is left for future work.

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