

Contribution of excited states to stellar weak-interaction rates in odd-*A* nuclei

P. Sarriguren*

Instituto de Estructura de la Materia, IEM-CSIC, Serrano 123, E-28006 Madrid, Spain

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Weak-interaction rates, including β decay and electron capture, are studied in several odd-*A* nuclei in the *pf*-shell region at various densities and temperatures of astrophysical interest. Special attention is paid to the relative contribution to these rates of thermally populated excited states in the decaying nucleus. The nuclear structure involved in the weak processes is studied within a quasiparticle random-phase approximation with residual interactions in both particle-hole and particle-particle channels on top of a deformed Skyrme Hartree–Fock mean field with pairing correlations. In the range of densities and temperatures considered, it is found that the total rates do not differ much from the rates of the ground state fully populated. In any case, the changes are not larger than the uncertainties due to the nuclear-model dependence of the rates.

DOI: [10.1103/PhysRevC.93.054309](https://doi.org/10.1103/PhysRevC.93.054309)**I. INTRODUCTION**

The relevant role that weak β -decay and electron-capture (EC) processes play in our understanding of the late stages of the stellar evolution has been long recognized [1,2]. In particular, the presupernova stellar structure, as well as the nucleosynthesis of heavier nuclei, are determined to a large extent by those mechanisms. *pf*-shell nuclei are specially important in these scenarios because they are the main constituents of the stellar core in presupernova formations [3] leading to core-collapse (type II) or thermonuclear (type Ia) supernovae.

Type II supernovae are thought to be the final result of the gravitational collapse of the core of a massive star that takes place when the nuclear fuel is exhausted. In the initial stages of the collapse, electrons are captured by nuclei in the iron-nickel mass region, thus reducing the electron-to-baryon fraction Y_e of the presupernova star and correspondingly the degeneracy pressure. At the same time, at typical presupernova densities, the neutrinos generated in those captures can leave the star, reducing the energy and cooling the star. Both effects help to accelerate the stellar collapse. EC processes are therefore essential ingredients to follow the complex dynamics of core-collapse supernova, and reliable estimates of these rates certainly contribute to a better understanding of the explosion mechanism.

Network calculations and astrophysical simulations [4] require nuclear physics input that in most cases cannot be measured directly in the laboratory due to the extreme conditions of densities ρ and temperatures T holding in stellar scenarios. Therefore, nuclear properties, and in particular the Gamow–Teller (GT) transitions that determine to a large extent the decay properties, must be estimated in many cases by model calculations.

A strong effort has been made in the last decades to measure the GT strength distributions of nuclei in the mass region $A \sim 60$. This has been performed by means of (*n, p*) or equivalent higher-resolution charge-exchange reactions such

as (*d, ²He*) and (*t, ³He*) at forward angles [5]. These reactions are the most efficient way to extract the GT strength in stable nuclei [6].

From the theoretical side, the first extensive calculations of stellar weak rates in relevant ranges of ρ and T were done in Ref. [2] under severe assumptions concerning the energy distribution of the GT strength. In Ref. [2] the whole GT strength was assumed to be concentrated in a single resonance at an energy parametrized phenomenologically. The total GT strength was taken from the single-particle model. Since then, improvements in the weak rates have been focused on the description of the nuclear-structure aspect of the problem. Different approaches are found in the literature and can be roughly divided into shell model (SM) [7–10] and proton-neutron quasiparticle random-phase approximation (QRPA) [11–25] categories. Hybrid models using RPA methods on top of a temperature-dependent description of the parent nucleus using a shell-model Monte Carlo approach have also been developed to calculate stellar EC rates [26]. Although QRPA calculations cannot reach the detailed spectroscopic accuracy achieved by present state-of-the-art SM calculations, the global performance of QRPA is quite satisfactory. Moreover, one clear advantage of the QRPA method is that it can be extended to heavier nuclei, which are beyond the present capability of full SM calculations, without increasing the complexity of the calculation.

A systematic evaluation of the ability to reproduce the measured GT strength distributions of various theoretical models based on SM and QRPA was done in Ref. [27]. EC rates were also derived from those models at astrophysical conditions of ρ and T . In Ref. [27] SM calculations using different effective interactions were compared with data and with the QRPA of Ref. [13]. Later, in Ref. [25], the same results were also compared with QRPA calculations using a Skyrme self-consistent mean field and QRPA with residual interactions in both particle-hole (ph) and particle-particle (pp) channels, improving significantly the agreement with experiment.

It is important to realize that there are clear differences between terrestrial and stellar decay rates caused by the effect of high- ρ and - T conditions. One effect of T is directly related to the thermal population of excited states in the decaying

*p.sarriguren@csic.es

nucleus, accompanied by the corresponding depopulation of the ground states. The weak rates of excited states can be significantly different from those of the ground state and a case-by-case consideration is needed. Another distinctive effect comes from the fact that atoms in stellar scenarios are completely ionized, and consequently electrons are no longer bound to the nuclei but form a degenerate plasma that obeys a Fermi–Dirac distribution. This opens the possibility for continuum EC, in contrast to the orbital EC caused by bound electrons in the atom under terrestrial conditions. These two effects make weak-interaction rates in the stellar interior sensitive functions of T and ρ .

In addition to these genuine stellar effects, one has to deal with uncertainties in the extraction of the experimental GT strength due to several causes such as the global normalization of the unit cross section, or to possible interference effects caused by the tensor component of the interaction. One also has to take into account that the GT strength is only measured up to some excitation energy and therefore the rates calculated from it will not include possible contributions from transitions beyond the measured energy range that could have an effect, especially at high T and ρ . The measured GT strength distributions are then strict tests to constrain the theoretical ones under terrestrial conditions, but the rates calculated from the experimental GT strength distributions may still differ significantly from the actual rates operating in stars.

The nuclei under study in this work correspond in most cases to stable pf -shell nuclei, and β^+ decays from their ground states are energetically forbidden. However, as T rises, the thermal population of excited states in the parent nucleus may induce β^+ decays if the energy excitation in the parent nucleus exceeds the Q_β energy. These decays, which are almost independent of ρ and T , might compete with ECs in particular cases. Competition of ECs with β^- decays in somewhat-neutron-rich nuclei in this mass region have also been studied in Ref. [28].

In the case of even-even nuclei studied in Ref. [25] the eventual contributions from excited states could be safely neglected because of the high-energy excitation of the first-excited states, typically 2^+ states beyond 1 MeV that can hardly be excited within the range of temperatures considered in this work. However, low-lying excited states would contribute to the rates in the case of even-even well-deformed nuclei [29], where the rotational states drop easily below 1 MeV, as well as in odd- A nuclei where quasiparticle states are found at very low excitation energies. The main purpose of this work is to study these contributions to the weak rates coming from low-lying excited states in odd- A nuclei.

To perform this study, a set of nuclei has been chosen according to their interest in presupernova models [3,27]. This set of nuclei includes ^{45}Sc , ^{51}V , ^{53}Fe , ^{55}Fe , ^{55}Mn , and ^{57}Fe . They exhibit in most cases rich low-lying spectra with several excited states below 1 MeV, which are displayed in Fig. 1. There is also experimental information [30–33] on the GT strength distributions in ^{45}Sc , ^{51}V , and ^{55}Mn obtained from charge-exchange reactions that will be used for comparison.

The structure of the paper is as follows: After presenting briefly the theoretical framework used to study the weak-interaction rates and the nuclear structure involved in Sec. II, a

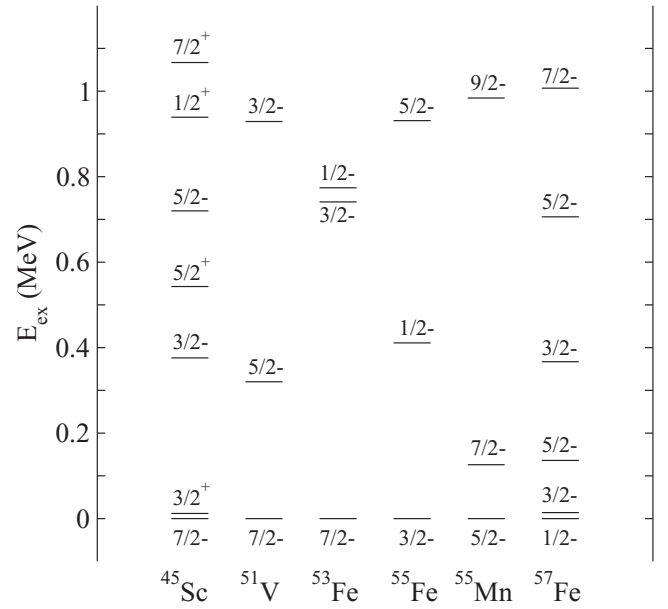


FIG. 1. Experimental energies of the low-lying excited states.

comparison of the results with the available measurements of the energy distribution of the GT strength will be performed in Sec. III A. The weak rates will be evaluated in Sec. III B at various stellar conditions including explicitly the contributions of the excited states. The main conclusions of the work are presented in Sec. IV.

II. THEORETICAL FORMALISM

A. Weak-interaction rates

The weak-interaction rate of a nucleus can be expressed as follows:

$$\lambda = \sum_i \lambda_i P_i(T), \quad P_i(T) = \frac{2J_i + 1}{G} e^{-E_i/(k_B T)}, \quad (1)$$

where $P_i(T)$ is the probability of occupation of the excited state i in the parent nucleus. Assuming thermal equilibrium, it is given by a Boltzmann distribution. $G = \sum_i (2J_i + 1) e^{-E_i/(k_B T)}$ is the partition function and $J_i(E_i)$ is the angular momentum (excitation energy) of the parent nucleus state i . In principle, the sum extends over all excited states in the parent nucleus up to the proton separation energy. However, because of the range of temperatures considered in this work ($T = 1\text{--}10$ GK), only a few low-lying excited states are expected to contribute significantly. The scale of excitation energies to consider is determined by $k_B T$, which for maximum T around 10 GK is given by $k_B T = 0.862$ MeV. Thus, excitation energies beyond 1 MeV are not considered in this work. The experimental energies of the states considered can be seen in Fig. 1. The weak-interaction rate corresponding to the parent state i is given by

$$\lambda_i = \sum_f \lambda_{if} = \frac{\ln 2}{D} \sum_f B_{if} \Phi_{if}(\rho, T), \quad (2)$$

where the sum extends over all the states in the final nucleus that can be reached in the process and $D = 6146$ s. This expression is decomposed into a phase-space factor Φ_{if} , which is a function of ρ and T , and a nuclear structure part B_{if} that contains the transition probabilities for allowed Fermi and GT transitions. In this work we only consider the dominant GT transitions. Fermi transitions are only important for β^+ decay of neutron-deficient light nuclei with $Z > N$. The theoretical description of both Φ_{if} and B_{if} are explained in the next sections.

Dealing with the full sums involved in Eqs. (1) and (2) is in general impracticable, but because our goal is to evaluate the contributions of a few low-lying excited states in odd- A nuclei to the total rates rather than calculating the full rates as a function of temperature, a state-by-state calculation of the sums is feasible. Other alternatives based on equilibrium statistical formulations of the nuclear many-body problem have been explored, giving rise to a temperature-dependent GT strength function. Thus, in Refs. [18,19] a fully self-consistent microscopic framework was used for the calculation of weak-interaction rates at finite temperature based on spherical mean-field models with Skyrme functionals and a finite-temperature RPA. EC was calculated from various Skyrme interactions to estimate the resulting theoretical uncertainty. Differences were found in the EC rates that can be sizable at low temperatures. In Ref. [20] stellar weak-decay rates were studied within a QRPA approach based on a spherical Woods–Saxon potential and separable interactions, extended to finite temperature by the thermofield dynamics formalism. A fully self-consistent relativistic framework was also introduced in Ref. [21] to study EC on nuclei in stellar environments. The formalism was based on a finite-temperature relativistic mean field with charge-exchange transitions described within a self-consistent finite-temperature relativistic RPA.

B. Phase-space factors

In the astrophysical scenarios of our study, atoms are assumed to be fully ionized and continuum ECs from the degenerate electron plasma are possible. The phase-space factor for continuum EC is given by

$$\Phi_{if}^{\text{EC}} = \int_{\omega_\ell}^{\infty} \omega p(Q_{if} + \omega)^2 F(Z, \omega) \times S_e(\omega)[1 - S_\nu(Q_{if} + \omega)] d\omega. \quad (3)$$

We also consider the possibility of β^+ decay, not only because some of the nuclei studied are β^+ unstable, as can be seen from the positive values of Q_{EC} in Table I, but also because excited states in the parent nucleus can be thermally populated and, thus, decay is possible for nuclei which are stable in terrestrial conditions. The phase-space factor for

positron emission β^+ process is given by

$$\Phi_{if}^{\beta^+} = \int_1^{Q_{if}} \omega p(Q_{if} - \omega)^2 F(-Z + 1, \omega) \times [1 - S_{e^+}(\omega)][1 - S_\nu(Q_{if} - \omega)] d\omega. \quad (4)$$

In these expressions ω is the total energy of the electron in $m_e c^2$ units, $p = (\omega^2 - 1)^{1/2}$ is the momentum, and Q_{if} is the total energy available in $m_e c^2$ units:

$$Q_{if} = \frac{1}{m_e c^2} (Q_{\text{EC}} - m_e c^2 + E_i - E_f), \quad (5)$$

with

$$Q_{\text{EC}} = Q_{\beta^+} + 2m_e c^2 = (M_p - M_d + m_e)c^2, \quad (6)$$

written in terms of the nuclear masses of parent M_p and daughter M_d nuclei and their excitation energies E_i and E_f , respectively. $F(Z, \omega)$ is the Fermi function that takes into account the distortion of the electron wave function due to the Coulomb interaction.

$$F(Z, \omega) = 2(1 + \gamma)(2pR)^{-2(1-\gamma)} e^{\pi\gamma} \frac{|\Gamma(\gamma + iy)|^2}{[\Gamma(2\gamma + 1)]^2}, \quad (7)$$

where $\gamma = [1 - (\alpha Z)^2]^{1/2}$; $y = \alpha Z \omega / p$, α is the fine structure constant, and R is the nuclear radius. The lower integration limit in Eq. (3) is given by $\omega_\ell = 1$ if $Q_{if} > -1$, or $\omega_\ell = |Q_{if}|$ if $Q_{if} < -1$.

S_e , S_{e^+} , and S_ν , are electron, positron, and neutrino distribution functions, respectively. Its presence inhibits or enhances the phase space available. In the stellar scenarios considered here the commonly accepted assumption is that $S_{e^+} = 0$ because electron-positron pair creation becomes important only at higher energies and $S_\nu = 0$ because neutrinos and antineutrinos can escape freely from the interior of the star at these densities. The electron distribution is described by a Fermi–Dirac distribution

$$S_e = \frac{1}{\exp[(\omega - \mu_e)/(k_B T)] + 1}. \quad (8)$$

The chemical potential μ_e as a function of ρ and T is determined from the expression

$$\rho Y_e = \frac{1}{\pi^2 N_A} \left(\frac{m_e c}{\hbar}\right)^3 \int_0^\infty (S_e - S_{e^+}) p^2 dp, \quad (9)$$

in (mol/cm³) units. ρ is the baryon density (g/cm³), Y_e is the electron-to-baryon ratio (mol/g), and N_A is Avogadro's number (mol⁻¹).

The phase-space factor for EC in Eq. (3) is therefore a sensitive function of both ρ and T , through the electron distribution S_e . On the other hand, the phase-space factor for β^+ decay in Eq. (4), under the assumptions $S_{e^+} = S_\nu = 0$, does not depend on ρ and T . The only dependence of the positron decay rates to ρ and T appears indirectly through the population of excited states.

C. Nuclear structure

The nuclear structure part of the problem is described within the QRPA formalism. Various approaches have been developed

TABLE I. Experimental Q_{EC} (MeV) values [34].

⁴⁵ Sc	⁵¹ V	⁵³ Fe	⁵⁵ Fe	⁵⁵ Mn	⁵⁷ Fe
-0.259	-2.472	+3.742	+0.231	-2.603	-2.659

in the past to describe the spin-isospin nuclear excitations in QRPA [11–25]. In this section we show briefly the theoretical framework used in this work to describe the nuclear part of the weak-interaction rates. More details of the formalism can be found in Refs. [22–24].

The method starts with a self-consistent deformed Hartree–Fock mean-field calculation with Skyrme interactions including pairing correlations. The single-particle energies, wave functions, and occupation probabilities are generated from this mean field. The Skyrme force SLy4 [35] is used in this work. It is one of the most successful Skyrme forces and has been extensively studied in the past. The sensitivity of the EC rates to different choices of the Skyrme interactions was studied in Ref. [25] within the same formalism, using SLy4 and SGII Skyrme interactions. The solution of the HF equation is found by using the formalism developed in Ref. [36], assuming time reversal and axial symmetry. The single-particle wave functions are expanded in terms of the eigenstates of an axially symmetric harmonic oscillator in cylindrical coordinates, using twelve major shells. The method also includes pairing between like nucleons in the BCS approximation with fixed gap parameters for protons and neutrons, which are determined phenomenologically from the odd-even mass differences involving the experimental binding energies [34]. Calculations for GT strengths are performed for the equilibrium shape of each nucleus, that is, for the configuration that minimizes the energy.

To describe GT transitions, a spin-isospin residual separable interaction is added to the Skyrme mean field and treated in a deformed proton-neutron QRPA. This interaction contains a *ph* and a *pp* part. By using separable GT forces, the energy eigenvalue problem reduces to find the roots of an algebraic equation. The coupling strengths χ_{GT}^{ph} and κ_{GT}^{pp} are chosen phenomenologically to reproduce GT resonances and half-lives in different mass regions. In previous works [22–24,37] we studied the sensitivity of the GT strength distributions to the various ingredients contributing to the deformed QRPA calculations; namely, to the nucleon-nucleon effective force, to pairing correlations, and to residual interactions. We found different sensitivities to them. In this work, all of these ingredients have been fixed to the most reasonable choices found previously. In particular, to be consistent with previous work in the same mass region [25], we use the coupling strengths $\chi_{GT}^{ph} = 0.10$ MeV and $\kappa_{GT}^{pp} = 0.05$ MeV. The method was successfully applied in the past to the study of the decay properties in different mass regions from proton-rich [29,38,39] to stable [25,37,40] and to neutron-rich nuclei [41].

The GT strength for a transition from an initial state *i* to a final state *f* is given by

$$B_{if}(GT^\pm) = \frac{1}{2J_i + 1} \left(\frac{g_A}{g_V} \right)_{\text{eff}}^2 \langle f | \left| \sum_j^A \sigma_j t_j^\pm \right| | i \rangle^2, \quad (10)$$

where $(g_A/g_V)_{\text{eff}} = 0.7(g_A/g_V)_{\text{bare}}$ is an effective ratio of axial and vector coupling factors that takes into account in an effective manner the observed quenching of the GT strength.

When the parent nucleus has an odd nucleon, the ground state can be expressed as a one-quasiparticle state in which the odd nucleon occupies the single-particle orbit of lowest energy. Quasiparticle excitations correspond to configurations with the odd nucleon in an excited state. In the present study we use the equal filling approximation (EFA), a prescription widely used in mean-field calculations to treat the dynamics of odd nuclei preserving time-reversal invariance [42]. In this approximation the unpaired nucleon is treated on an equal footing with its time-reversed state by sitting half a nucleon in a given orbital and the other half in the time-reversed partner. This approximation has been found [43] to be equivalent to the exact blocking when the time-odd fields of the energy density functional are neglected and then it is sufficiently precise for most practical applications. As we shall see in the next section, because the spin and parity of the ground and low-lying excited states of the nuclei studied are known experimentally, I chose these assignments for the odd nucleons to describe the corresponding states. In all cases the observed states have corresponding calculated states lying in the vicinity of the Fermi energy.

Then, two types of transitions are possible. One type is due to phonon excitations in which the odd nucleon acts only as a spectator. These are three-quasiparticle states (3qp). In the intrinsic frame, the transition amplitudes are basically the same as in the even-even case, but with the blocked spectator excluded from the calculation. The other type of transitions are those involving the odd-nucleon state. These are one-quasiparticle states (1qp), which are treated by taking into account phonon correlations in the quasiparticle transitions in first-order perturbation. The transition amplitudes for the correlated states can be found in Refs. [11,14,24].

In this work we refer the GT strength distributions to the excitation energy in the daughter nucleus. For odd-*A* nuclei we have to deal with 1qp and 3qp transitions. The excitation energies for 1qp transitions in the case of an odd-neutron nucleus are

$$E_{\text{ex},1\text{qp}}[(Z,N-1) \rightarrow (Z-1,N)] = E_\pi - E_{\pi_0}, \quad (11)$$

where E_{π_0} is the lowest proton quasiparticle energy. The excitation energy with respect to the ground state of the daughter nucleus for 3qp transitions is given by

$$E_{\text{ex},3\text{qp}}[(Z,N-1) \rightarrow (Z-1,N)] = \omega + E_{v,\text{spect}} - E_{\pi_0}, \quad (12)$$

where ω is the QRPA excitation energy and $E_{v,\text{spect}}$ is the energy of the spectator nucleon. Similar expressions are obtained for odd-proton nuclei by changing properly protons into neutrons and vice versa.

III. RESULTS

A. Gamow–Teller strength distributions

This section starts with the study of the GT strength distributions corresponding to the ground state and the various excited states considered. The experimental energy spectra below 1 MeV of the nuclei under study can be seen in Fig. 1. The spin-parity assignments of these states can also be seen in the figure. We associate the observed states with the calculated quasiparticle states around the Fermi level having the same

spin and parity or in some instances with rotational states built on them. The experimental excitation energies are adopted to calculate the thermal population of these states. This procedure is valid for the general purpose of estimating the relative contributions from ground and low-lying excited states in the parent nucleus to the weak-decay rates in astrophysical scenarios. However, this approach cannot be implemented in those cases where low-lying excited states are experimentally unknown.

Practically spherical solutions are obtained in the cases of ^{51}V and ^{55}Fe . The rest of the nuclei appear to be somewhat deformed. The self-consistent quadrupole deformation β_2 of the ground states obtained in our calculations are as follows: $\beta_2 = -0.06$ in ^{45}Sc , $\beta_2 = 0.16$ in ^{53}Fe , $\beta_2 = 0.13$ in ^{55}Mn , and $\beta_2 = 0.18$ in ^{57}Fe .

The correspondence made between the experimentally observed states and the Nilsson asymptotic quantum numbers $[N, n_z, m_\ell]K^\pi$ is as follows: The ground state $7/2^-$ in ^{45}Sc is associated with the $[303]7/2^-$ state. The next excited states, ordered by increasing energies, correspond to $[202]3/2^+$, $[321]3/2^-$, rotational $5/2^+$, $[312]5/2^-$, $[200]1/2^+$, and $[312]3/2^-$. The third excited state, $5/2^+$, is associated with the rotational state $J = 5/2^+$, $K = 3/2^+$ built on top of the band head $[202]3/2^+$, and we deal with it properly in the calculation of the GT strength. In the case of ^{51}V , the ground state corresponds to $[303]7/2^-$, whereas the first two excited states are associated with the asymptotic states $[312]5/2^-$ and $[321]3/2^-$, respectively. Similarly, for ^{53}Fe we have $[303]7/2^-$ as ground state and $[321]3/2^-$ and $[321]1/2^-$ as the two first-excited states. ^{55}Fe has $[312]3/2^-$ as ground state and $[321]1/2^-$ and $[312]5/2^-$ as excited states. In the case of ^{55}Mn only the ground state $[312]5/2^-$ and first-excited state $[303]7/2^-$ are considered. In ^{57}Fe the ground state is associated with a $[310]1/2^-$ state. The first excited state is associated with $[312]3/2^-$ and the next excited state $5/2^-$ is considered to be a rotational state. The next two excited states correspond to $[301]3/2^-$ and a rotational state $5/2^-$ built on it.

Figures 2–7 contain the GT strength distributions $B(\text{GT}^+)$ for the ground and excited states of each nucleus, displayed versus the excitation energy of the daughter nucleus. The calculations correspond to QRPA results with SLy4 Skyrme force. Data from different charge-exchange reaction experiments [30–33] are also shown when available.

One can observe in Fig. 2 quite similar profiles for the GT strength distributions of the negative parity states with a small peak at very low excitation energy, a stronger peak around 7 MeV, and another peak at higher energies. Only the last excited state departs from this pattern. On the other hand, the positive parity states show a rather different profile with a small peak at around 6 to 7 MeV and a stronger one centered at about 12 to 13 MeV. The GT strength distribution of the $7/2^-$ ground state is compared with data [30] extracted from (n, p) charge exchange reactions accumulated in 1 MeV bins. The agreement with experiment is quite reasonable, reproducing the two bumped structure observed, as well as the total strength in the measured energy range. The next three figures (Figs. 3–5) contain the GT strength distributions of the ground state and two first-excited states in ^{51}V , ^{53}Fe , and

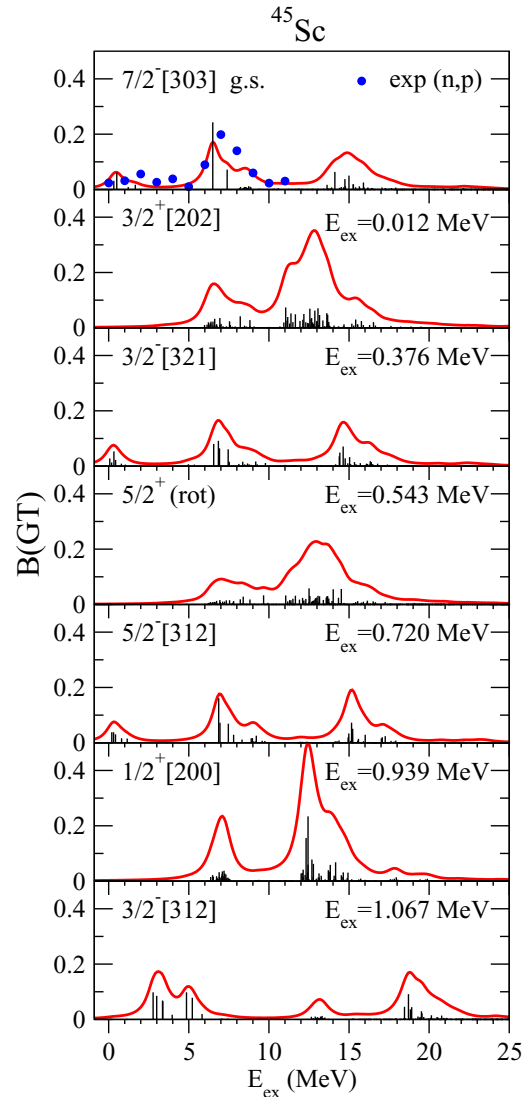


FIG. 2. QRPA Gamow-Teller strength distribution $B(\text{GT}^+)$ for the transition ^{45}Sc to ^{45}Ca plotted versus the excitation energy of the daughter nucleus. Experimental data in the top panel are compared with QRPA results with SLy4 Skyrme force for the decay of the ground state in ^{45}Sc . GT strength distributions for the various excited states in ^{45}Sc are shown in the lower panels. Data extracted from (n, p) reactions are from Ref. [30].

^{55}Fe , respectively. The profiles observed in each case are very similar, with peaks at 6, 10, and 9 MeV, respectively. It is also remarkable the similarity of the GT strength distributions of the various excited states. Experimental measurements from (n, p) [31] and $(d, ^2\text{He})$ [32] reactions are also shown in the case ^{51}V . The GT strength appears concentrated at around 5 MeV, whereas the calculations predict the bump at somewhat larger energies. The total GT strength measured in both experiments is quite similar and agrees with the calculations. In the case of ^{55}Mn (Fig. 6) the GT profile of the ground state shows a broad peak centered a 5 MeV with a two-peaked substructure containing somewhat more strength in the lower one. The GT distribution of the excited state is close to that with the strength

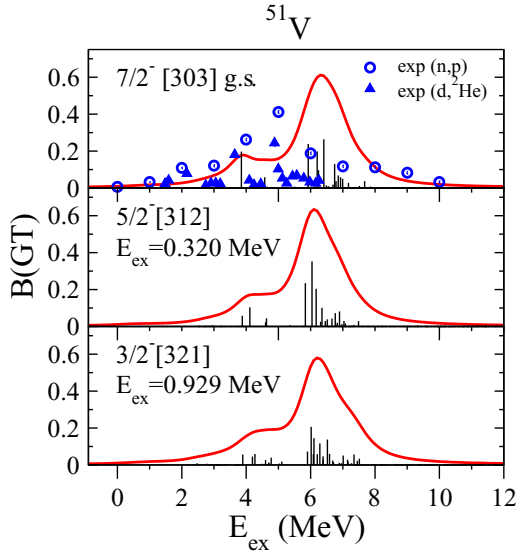


FIG. 3. Similar to Fig. 2 for the transition ^{51}V to ^{51}Ti . Data are from (n, p) [31] and $(d, ^2\text{He})$ [32] reactions.

shifted to the peak at higher energy. The GT distribution of the ground state is compared with (n, p) data from Ref. [33]. The measured strength has a broad peak centered at 4 MeV, which is at somewhat lower energy than the calculations. The total measured strength is in agreement with the calculated strength. The GT strength distributions in ^{57}Fe (Fig. 7) exhibit different behavior when comparing the ground state with the excited states. In the ground state we find some strength at 1 MeV and a two-peak structure with centers at 6 and 8 MeV. The first $3/2^-$ excited state and its corresponding rotational state $5/2^-$ show a broad peak at 6 MeV, whereas the second $3/2^-$ excited state and its corresponding rotational state $5/2^-$ show a small

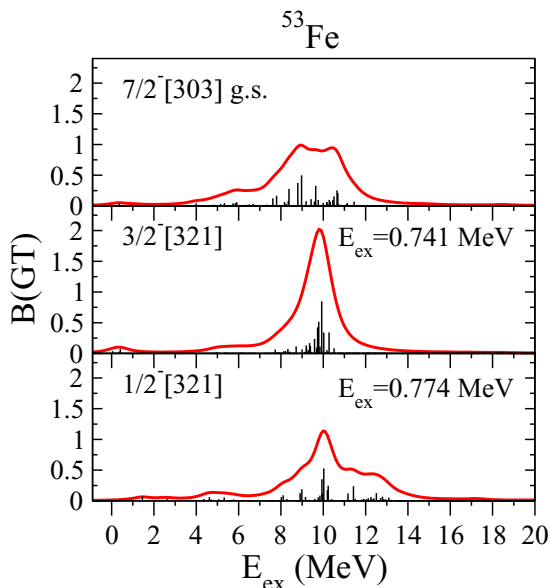


FIG. 4. Similar to Fig. 2 for the transition ^{53}Fe to ^{53}Mn .

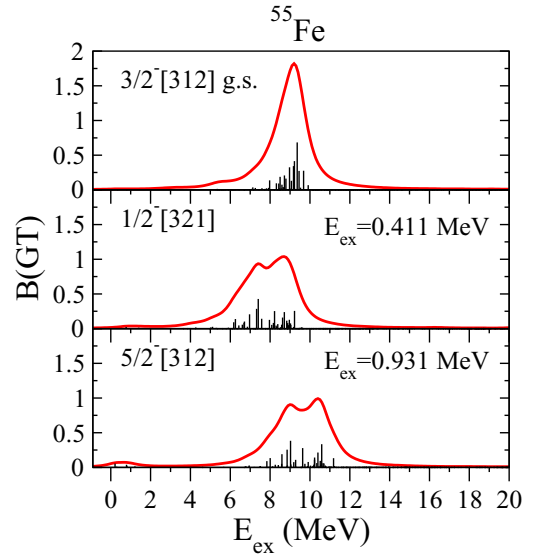


FIG. 5. Similar to Fig. 2 for the transition ^{55}Fe to ^{55}Mn .

bump at 1 MeV and a two-bump structure with peaks at 7 and 10 MeV.

B. Stellar weak-decay rates

In the following figures we present weak-interaction rates for the selected pf -shell nuclei as a function of the temperature and for various electron densities. The range of T considered varies from $T_9 = 1$ up to $T_9 = 10$, in T_9 (GK) units, whereas the range in ρY_e varies from $\rho Y_e = 10^6$ mol/cm³ up to $\rho Y_e = 10^{10}$ mol/cm³. This grid of ρY_e and T includes those ranges relevant for astrophysical scenarios related to the silicon-burning stage in a presupernova star [3] ($\rho Y_e = 10^7$ mol/cm³ and $T_9 = 3$), as well as scenarios related to precollapse of the core [44] and thermonuclear runaway type-Ia supernova [45] ($\rho Y_e = 10^9$ mol/cm³ and $T_9 = 10$).

In these ranges of densities and temperatures, weak-interaction rates are fully dominated by EC. β^+ decays will always contribute for sufficiently high ρ and T because of

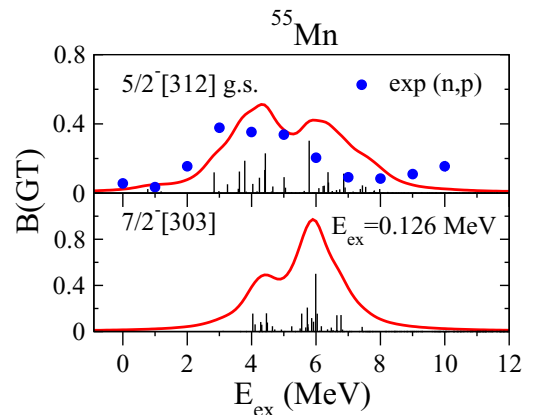
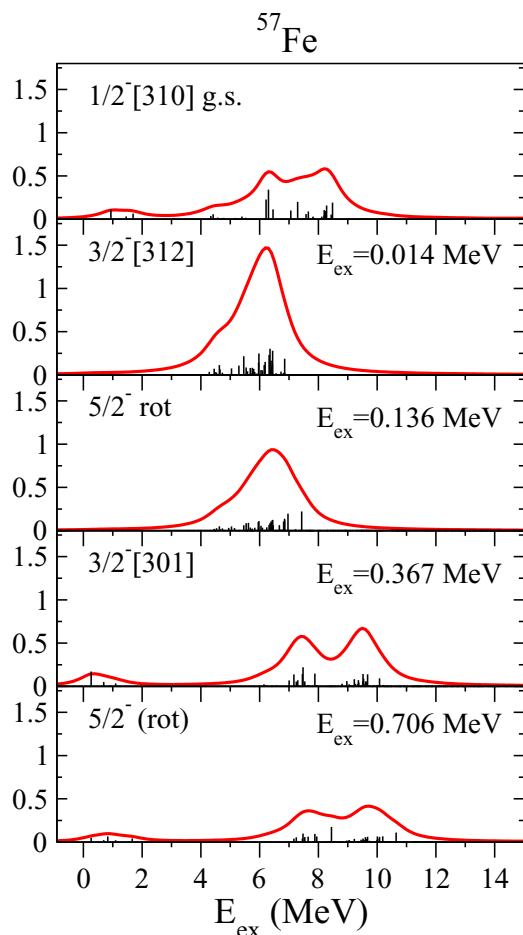
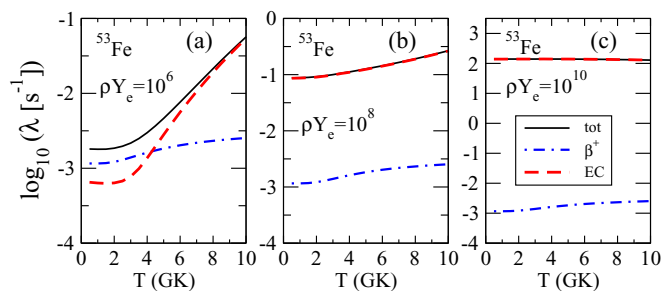
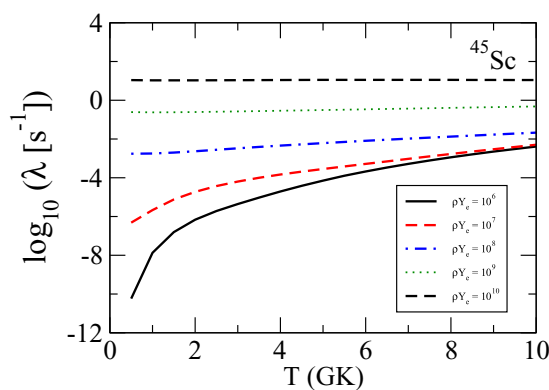


FIG. 6. Similar to Fig. 2 for the transition ^{55}Mn to ^{55}Cr . Data extracted from (n, p) reactions are from Ref. [33].

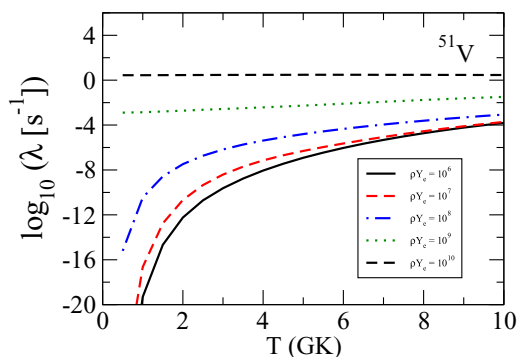

 FIG. 7. Similar to Fig. 2 for the transition ^{57}Fe to ^{57}Mn .

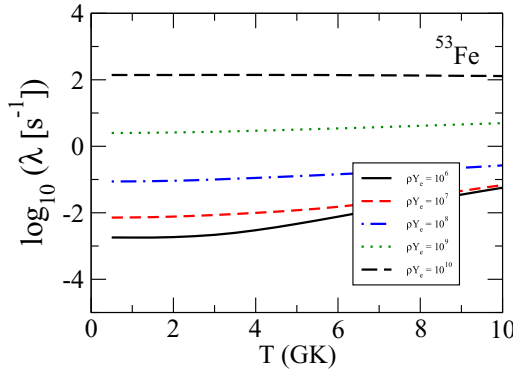
thermal population of excited states beyond Q_{EC} energies. However, for ρ and T values in this work, positron-decay contributions can be neglected. The most-favored cases for β^+ contributions are those with positive Q_{EC} values that correspond to ^{53}Fe and ^{55}Fe . We can see in Fig. 8 the decomposition of the total weak-interaction rates in ^{53}Fe into their EC and β^+ components. At $\rho Y_e = 10^6$ there is a competition between EC and β^+ at low T . At higher T , EC clearly dominates because it increases while β^+ remains almost constant. At higher densities, the electron


 FIG. 8. Weak-decay rates in ^{53}Fe as a function of T , decomposed into their EC and β^+ contributions for (a) $\rho Y_e = 10^6$, (b) $\rho Y_e = 10^8$, and (c) $\rho Y_e = 10^{10}$ mol/cm 3 .

 FIG. 9. Total weak-interaction rates for ^{45}Sc as a function of T for various densities: $\rho Y_e = 10^6$ (solid black), $\rho Y_e = 10^7$ (dashed red), $\rho Y_e = 10^8$ (dash-dotted blue), $\rho Y_e = 10^9$ (dotted green), and $\rho Y_e = 10^{10}$ (dashed black).

chemical potential increases and the electron Fermi-Dirac distribution (8) allows for higher-energy electrons with the result of a remarkably enhanced EC rate. On the contrary, the β^+ phase-space factor in Eq. (3) remains invariant with the density and so does the corresponding β^+ rate. The final result is that β^+ is always very small in comparison with EC and can be safely neglected. The dominant EC determines the total rates in practically all the cases. Therefore, only the total rates will be shown in the following figures.

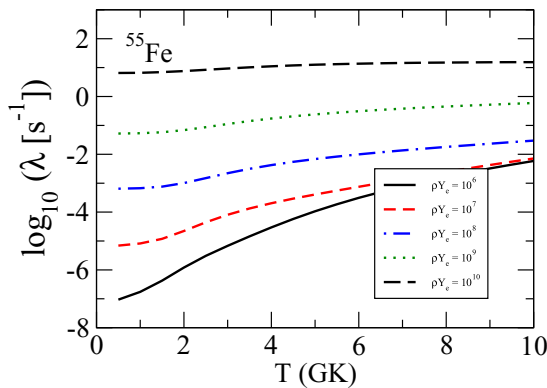
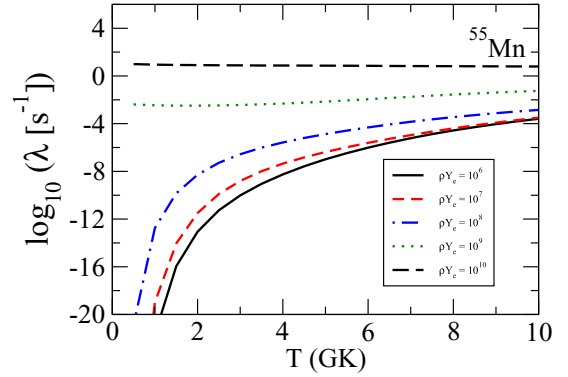
Figures 9–14 show the total rates as a function of the temperature for various densities from $\rho Y_e = 10^6$ up to $\rho Y_e = 10^{10}$ mol/cm 3 . In these figures one can see that the rates always increase when either ρ or T increases. This is a simple consequence of the phase factors that increase accordingly. The sensitivity of the EC rates to the environmental (ρ, T) conditions is obvious. At low ρ (low Fermi energies) and low T (sharp shape of the energy distribution of the electrons S_e), the rates are low and very sensitive to details of the GT strength of the low-lying excitations and therefore to nuclear-structure-model calculations. On the other hand, when ρ increases (larger Fermi energies) and T increases (smearing of the electron distribution functions), EC rates also increase and become sensitive to all the spectrum and, in particular, to the centroids of the GT strength distribution and to the total strength. Then, the whole description of the GT strength


 FIG. 10. Same as in Fig. 9, but for ^{51}V .

FIG. 11. Same as in Fig. 9, but for ^{53}Fe .

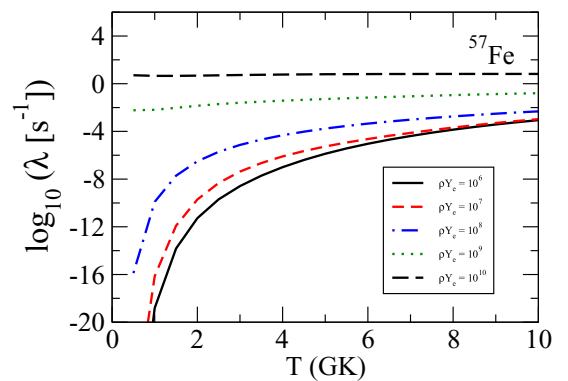
distribution is more important than a detailed description of the low-lying spectrum. This is also the reason why all the rates become flat and roughly independent of T at high ρ . The dependence on the Q_{if} (Q_{EC}) values is also apparent. These energies determine the lower integration limit of the EC phase factor in Eq. (3) and, thus, the minimum energy of electrons in the stellar electron plasma to suffer a nuclear capture. At low densities, where this effect is more pronounced, one can roughly distinguish two types of patterns. Those that start with very low rates at low T and increase rapidly with T , such as the rates in ^{45}Sc , ^{51}V , ^{55}Mn , and ^{57}Fe , and those exhibiting a rather flat behavior with much higher rates, as in the cases of ^{53}Fe and ^{55}Fe . This global behavior can be understood in terms of the Q_{EC} energies. Large negative values, as in the cases of ^{51}V , ^{55}Mn , and ^{57}Fe , lead to very low rates. Q_{EC} energies close to zero as in ^{45}Sc lead to intermediate rates, and positive values of Q_{EC} cause much higher rates. This general behavior and sensitivity of the rates to both density and temperature has been observed in different calculations in this mass region from SM [8–10] to RPA [15,16,18–21] calculations. A comparison of the rates obtained within this formalism and other SM and RPA calculations for even-even pf -shell nuclei can be found in Ref. [25].

In the next figures, Figs. 15–20, the relative contributions of the ground and excited states to the total rates are studied. In addition, total rates and rates obtained from the ground state with full population labeled “gs only” in the figures, are

FIG. 12. Same as in Fig. 9, but for ^{55}Fe .FIG. 13. Same as in Fig. 9, but for ^{55}Mn .

included. The latter are always larger than the contribution from the ground state at a finite temperature (label 0 in the figures) because of the depopulation of the ground state and both of them converge at zero temperature. As T increases, one would expect a departure of these two curves (0 and gs only) that would be more apparent when very low-lying excited states are present. This is more-or-less the case in ^{45}Sc , ^{55}Mn , and ^{57}Fe (see Fig. 1). The fact that ^{57}Fe shows a stronger effect is due to the angular momentum of the ground state. Whereas ^{57}Fe is a 1/2 state, ^{45}Sc is a 7/2 state, which is more robust against depopulation. Obviously the total contribution (total in the figures) is always larger than the contribution from the state 0, but can be larger or smaller than “gs only,” depending on how the various states become populated. The relative importance of the various excited states is determined by their thermal population at a given T , by the phase factor, and by the structure of the GT strength distribution.

In the case of ^{45}Sc , six excited states have been considered. At low densities ($\rho Y_e = 10^6$ – 10^8 mol/cm 3), the electron chemical potential μ_e is relatively small and the electrons can only excite low-energy states in the daughter nucleus. In this case the contribution from the positive-parity states labeled 1, 3, and 5 are very small because these states show very little GT strength at low energy in Fig. 2. Larger rates are found for the states labeled 0, 2, and 4 that show some GT strength at very low excitation energies. At higher densities ($\rho Y_e = 10^{10}$ mol/cm 3), μ_e is high enough to allow high energetic electrons

FIG. 14. Same as in Fig. 9, but for ^{57}Fe .

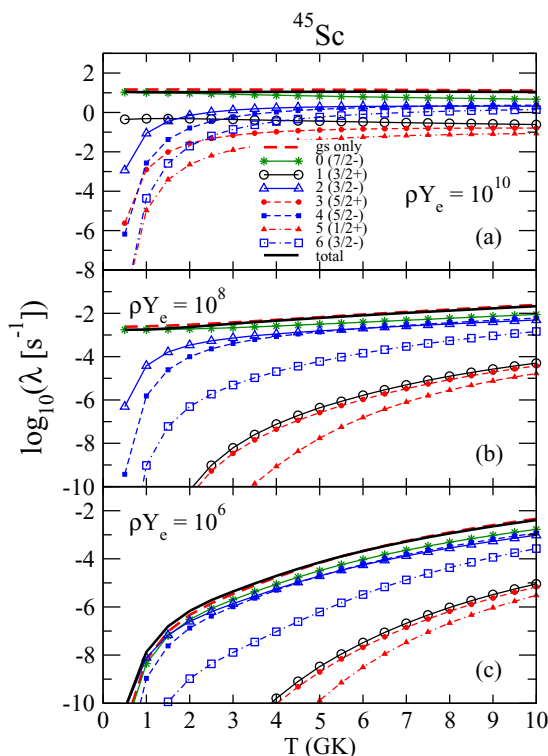


FIG. 15. Weak-decay rates for ^{45}Sc from SLy4-QRPA calculations as a function of T (GK) for densities $\rho Y_e = 10^{10}$, 10^8 , 10^6 mol/cm 3 in panels (a), (b), and (c), respectively. The separate contributions from the ground state and the various excited states below 1 MeV are also shown.

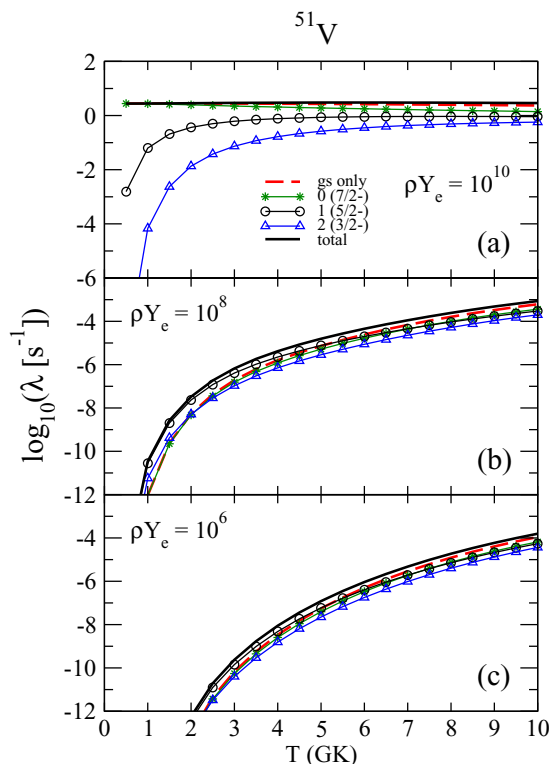


FIG. 16. Same as in Fig. 15, but for ^{51}V .

that excite most of the GT strength distribution. In this case the contribution of the various excited states to the total rates are basically determined by their thermal population, especially at low temperature.

In the case of ^{51}V in Fig. 16 two excited states are considered. The GT strength distributions of the ground and excited states are quite similar and therefore the rates are mainly determined by the thermal population of the states. We find the contributions to the total rate ordered following the excitation energies of the parent nucleus, especially at high densities.

In Fig. 17 for ^{53}Fe the three states studied present also very similar GT distributions. The two excited states appear at a relatively large energy and their thermal population is not significant at these temperatures. The rates are ordered as a function of the population of the states. It is also worth mentioning that the ground-state contribution does not fall at low T , even at low densities, because of the large and positive Q_{EC} energies that allow EC at small electron energies. Similar arguments can be applied to the case of ^{55}Fe with the difference that in this case the rates are lower than the rates of ^{53}Fe mainly because of the smaller Q_{EC} values. Small Q_{EC} values make the rates sensitive to the structure of the GT at low excitation energy. This is the reason why the second excited state, exhibiting some strength at low energy, contributes more significantly to the rate. In the case of ^{55}Mn in Fig. 19 the

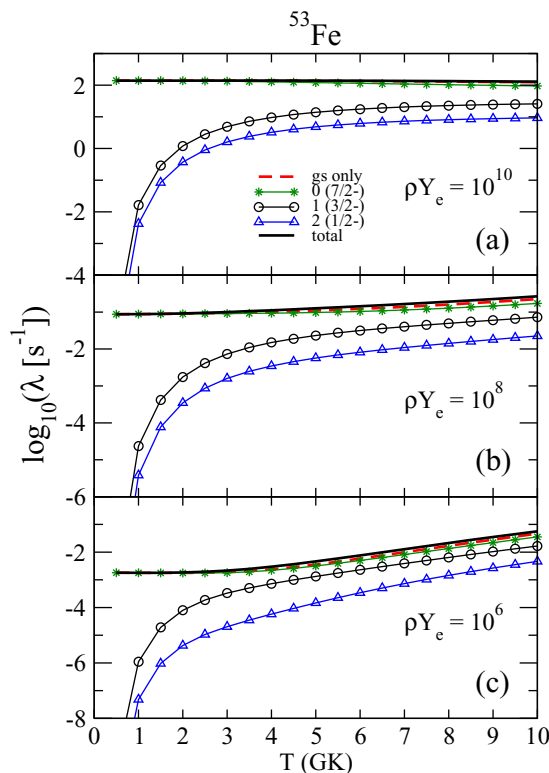


FIG. 17. Same as in Fig. 15, but for ^{53}Fe .

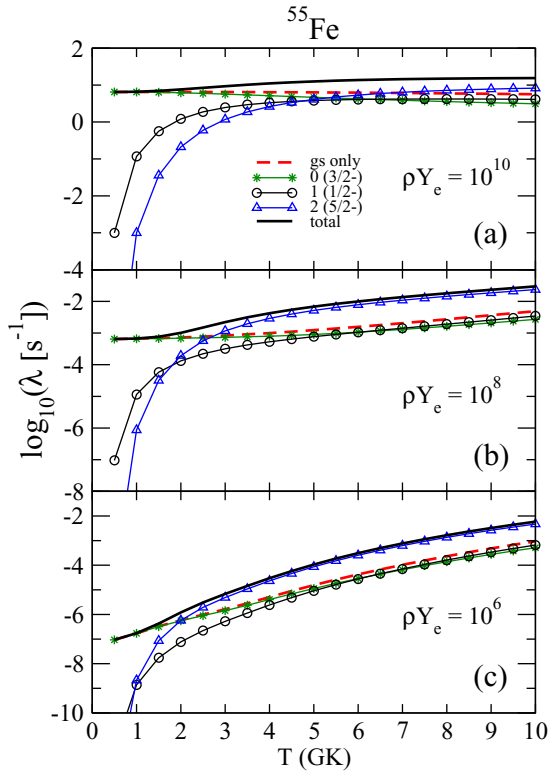


FIG. 18. Same as in Fig. 15, but for ^{55}Fe .

negative value of Q_{EC} makes the rates small with contributions ordered according to the population.

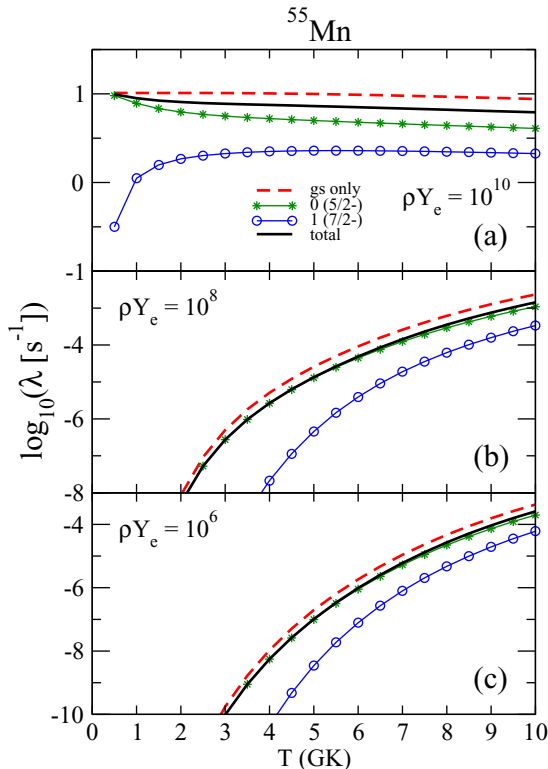


FIG. 19. Same as in Fig. 15, but for ^{55}Mn .

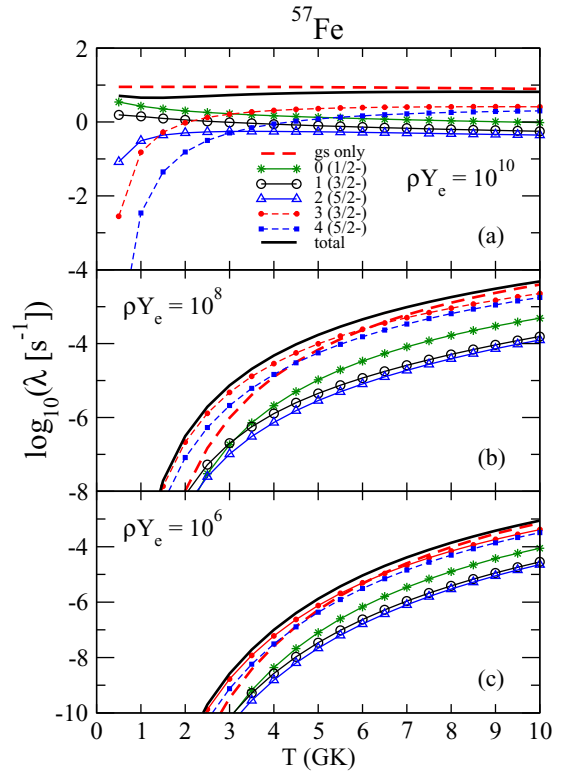


FIG. 20. Same as in Fig. 15, but for ^{57}Fe .

Finally, ^{57}Fe in Fig. 20 shows a competition between the thermal population and the GT strength distribution of the various states. The large negative Q_{EC} value make the rates very small and quite sensitive to the low-lying GT strength, especially at low densities and temperature. Thus, we observe that the contribution of the states labeled 3 and 4, which have some GT strength at low energies, are comparatively large in spite of their lower population.

IV. CONCLUSIONS

In this work we have evaluated weak-interaction rates, which are basically determined by continuum electron-capture rates, at different density and temperature conditions holding in stellar scenarios. This study is performed on a set of odd- A pf -shell nuclei representative of the constituents in presupernova formations (i.e., ^{45}Sc , ^{51}V , ^{53}Fe , ^{55}Fe , ^{55}Mn , and ^{57}Fe). The nuclear structure involved in the calculation of the energy distribution of the Gamow–Teller strength is described within a self-consistent deformed HF + BCS + QRPA formalism with density-dependent effective Skyrme interactions and spin-isospin residual interactions. This formalism has been shown to provide a good description of the decay properties of nuclei by comparing GT strength distributions and half-lives with the measured quantities in the laboratory under terrestrial conditions. Certainly, the calculated rates are subject to uncertainties and there is room for improvement in many theoretical aspects. However, the relative importance of the various contributions to the total rates studied in this paper may still be of great interest.

First, GT strength distributions for ground states and excited states below 1 MeV excitation energies have been studied in those nuclei and compared with the available data from charge-exchange reactions. Second, weak-interaction rates have been calculated for ground and excited states at densities and temperatures holding in astrophysical scenarios of interest, such as silicon burning and presupernova stages. Although ECs are always dominant, positron decays have been also included because some nuclei are unstable $Q_\beta > 0$ and because excited states above Q_β values can be thermally populated. Excited states in the parent nucleus beyond 1 MeV have not been considered because they are not expected to play any role at the temperatures considered.

The contributions of the excited states to the rates depend on the density and temperature through the population of these states and their phase factors, but depend also on their GT structure. All in all, we find quite similar results for the total rates and for the rates considering only the contribution from the ground states fully populated. The reason is that population

of excited states leads to a depopulation of ground states and both effects are compensated to some extent when the GT strength distributions are not very different from each other.

As a general conclusion, we can say that the effect on the rates due to the involvement of the excited states of the parent nuclei is of similar order or smaller than the uncertainties inherent to the nuclear structure. That is, SM versus QRPA calculations, different nuclear interactions, or different treatments in QRPA calculations. Thus, at the densities and temperatures considered, it is relatively safe to use only contributions from ground states, even for odd- A nuclei where quasiparticle states appear at low energy.

ACKNOWLEDGMENT

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