Investigation of Important Weak Interaction Nuclei in Presupernova Evolution

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Abstract

This project aims to investigate the most important weak interaction nuclei in the presupernova evolution of massive stars. To achieve this goal, an ensemble containing 728 nuclei in the mass range of $A = 1$–100 was considered. We computed the mass fractions of these nuclei using Saha’s equation for predetermined values of $T$, $\rho$, and $Y_e$ and assuming nuclear statistical equilibrium. The nuclear partition functions were obtained using a newly introduced recipe where excited states, up to 10 MeV, were treated as discrete. The weak interaction rates (electron capture (ec) and $\beta$-decay (bd)) were calculated in a totally microscopic fashion using the proton–neutron quasiparticle random phase approximation model and without assuming the Brink–Axel hypothesis. The calculated rates were coupled with the computed mass fractions to investigate the time rate of change of lepton to baryon fraction of the stellar matter. We compare our results with the previous calculations reported in the literature. Noticeable differences up to orders of magnitude are reported with previous calculations. These differences may influence the evolution of the star in the later stages of presupernova. We present a list of the top 50 ec and bd nuclei, which have the largest effect on $Y_e$ for conditions after silicon core burning. The competition between the ec and bd rates in the stellar core was investigated and it was found that $Y_e = 0.424$–$0.455$ is the interval where the bd results are bigger than the ec rates.

Unified Astronomy Thesaurus concepts: Nuclear astrophysics (1129); Nucleosynthesis (1131); Stellar physics (1621); Stellar evolution (1599); Stellar abundances (1577); Stellar dynamics (1596); Isotopic abundances (867)

1. Introduction

In the course of evolution of a massive star, weak interaction rates ($\beta$-decay (bd) and electron capture (ec)) play crucial roles. These reactions contribute to the gravitational collapse of the core of a massive star by reducing the electron degenerate pressure, thereby causing a supernova explosion and thus affecting the formation of massive (neutron-rich) nuclei (Bethe et al. 1979; Bethe 1990).

Several attempts have been made for the calculation of weak interaction rates in stellar environment in a bid to have a better understanding of the stellar evolution. Fuller, Fowler, and Newman (FFN; Fuller et al. 1980, 1982, 1985) employed the independent-particle model (IPM) using the then available experimental data and tabulated the weak interaction rates for 226 nuclei with mass in the range 60 $\geq A \geq 21$. Their rates led to a considerable reduction in the lepton to baryon fraction ($Y_e$) throughout the stellar core and significantly contributed to a better understanding of the presupernova evolution of stars (Weaver et al. 1985). In 1994, Aufderheide and collaborators (Aufderheide et al. 1994) studied the influence of weak interaction in evolution of massive stars post silicon burning and searched for the most important ec and bd nuclei in the $Y_e$ range of 0.400–0.500 using the IPM model. They extended the FFN work for heavier nuclei with $A > 60$ and took into consideration explicit quenching of the $GT$ strength. In the same decade, many authors (e.g., Vetterli et al. 1989; El-Kateb et al. 1994; Williams et al. 1995) raised concerns about the systematic parameterization employed by FFN and later adopted by Aufderheide et al. The proton–neutron quasiparticle random phase approximation (pn-QRPA; Nabi & Klapdor-Kleingrothaus 1999, 2004) and shell model (Langanke & Martínez-Pinedo 2000) later calculated weak interaction rates in stellar matter and showed that primarily the misplacement of the $GT$ centroids by FFN in some key nuclei led to disagreement with experimental values. Heger and collaborators (Heger et al. 2001) utilized weak rates in the mass range $A = 45$–65 based on large-scale shell-model (LSSM; Langanke & Martínez-Pinedo 2001) and performed simulation studies during the presupernova evolution. A similar study of the presupernova evolution using the pn-QRPA rates was not performed and was much anticipated.

The aim of the current work is to search for the most important weak interaction nuclei in the presupernova evolution of massive stars using the pn-QRPA model. To achieve this goal, we considered a large pool containing 728 nuclei having atomic number up to 50 and mass number up to 100, in order to cover a decent number of nuclei prevailing in the stellar matter. The nuclei that contribute to the largest change in $Y_e$ values are neither the most abundant nor the ones with the strongest rates, but rather a combination of the two. Thus one must know both the rates and nuclear abundances of nuclei to determine the most important weak interaction (ec or bd) nuclei for given values of $T$ (temperature), $\rho$ (baryon density), and $Y_e$. To compute ec and bd rates for the wide suite of selected nuclei, we employed the pn-QRPA (Hableib & Sorensen 1967) theory, a successful microscopic model frequently used in the past, with reasonable success, to compute the weak rates under terrestrial (Staudt et al. 1990; Hirsch et al. 1993) and stellar conditions (Nabi & Klapdor-Kleingrothaus 1999, 2004). The reliability of the pn-QRPA model was thoroughly discussed earlier (Nabi & Klapdor-Kleingrothaus 2004). A very decent comparison of the pn-QRPA model calculation with experimental data was achieved for more than 1000 nuclei (see Tables E–M and Figures 11–17 of Nabi & Klapdor-Kleingrothaus 2004; for further comparison of the pn-QRPA model with measured data, please see...
The pn-QRPA model is suitable for stellar rate calculations for the important reason that it does not assume the Brink–Axel hypothesis (Brink 1958) for computation of excited state GT strength distributions, as usually done in such calculations. Furthermore a large model space, up to seven major shells, makes the model calculation possible for any arbitrary heavy nucleus. Nuclear abundances were determined using Saha’s equation assuming nuclear statistical equilibrium (NSE). We later investigate the total rate of change of $Y_e$ with changing stellar conditions and also compare our results with previous calculations.

This paper is structured as follows. In Section 2 we briefly introduce the formalism employed to compute weak rates and nuclear abundances. Our results are discussed and compared with previous calculations in Section 3. Finally, concluding remarks are stated in the last section.

2. Formalism

2.1. Weak Interaction Rates

The ec and bd rates from the $i$th state of the parent to the $j$th state of the daughter nucleus in stellar matter is given by

$$\lambda_{ij} = \ln 2 \frac{(fr)_{ij}}{(ft)_{ij}}. \tag{1}$$

In Equation (1), $(ft)_{ij}$ is related to the reduced transition probability $B_{ij}$ of the nuclear transition by

$$(ft)_{ij}^{(cd)} = D / B_{ij}, \tag{2}$$

where

$$B_{ij} = B(F)_{ij} + (g_A/g_V)^2 B(GT)_{ij}. \tag{3}$$

The value of constant $D$ was taken as 6143 s (Hardy & Towner 2009) and the ratio of axial-vector and vector coupling constant was kept as $g_A/g_V = -1.2694$ (Nakamura 2010). $B(F)$ and $B(GT)$ are the reduced transition probabilities of the Fermi and GT transitions, respectively

$$B(F)_{ij} = \frac{1}{2J_i + 1} \left| \sum_{k} t^k_{\pm} |i\rangle \right|^2 \tag{4}$$

$$B(GT)_{ij} = \frac{1}{2J_i + 1} \left| \sum_{k} t^k_{\pm} \sigma |i\rangle \right|^2, \tag{5}$$

where $J_i$ is the spin of parent state, $\sigma$ are the Pauli spin matrices, and $t_{\pm}$ refer to the isospin raising and lowering operators.

The phase space function $(\phi_{ij})$ is an integral over the total energy. For the case of bd, it is given by (here onwards we use natural units, $\hbar = m_e = c = 1$)

$$\phi_{ij} = \int_{\omega = \omega_m}^{\omega = \omega} \omega \sqrt{\omega^2 - 1} (\omega_m - \omega)^2 F(\pm Z, \omega)(1 - G_{-}) d\omega, \tag{6}$$

whereas the phase space for ec is given by

$$\phi_{ij} = \int_{\omega = \omega_1}^{\omega = \omega} \omega \sqrt{\omega^2 - 1} (\omega_m + \omega)^2 F(\pm Z, \omega) G_{-} d\omega, \tag{7}$$

where $\omega$ is the total energy of the electron including its rest mass, $\omega_1$ is the total capture threshold energy for ec, and $\omega_m$ is the total bd energy. $\omega_m = (m_p - m_d + E_i - E_j)$, where $m_p$($m_d$) and $E_i$($E_j$) are the mass and excitation energies of the parent (daughter) nucleus. The $F(\pm Z, \omega)$ are the Fermi functions computed using the recipe of Gove & Martin (1971). $G_-$ is the
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Table 1
The ec Rates for Most Important Nuclei Sorted in Order of $|\lambda_{\psi}^{ec}|$

| $\rho = 1.06E+09$, $T_\psi = 4.93$, $Y_e = 0.430$ | $\lambda_{\psi}^{ec}$ | $\lambda_{\psi}^{ec}$ | $|\lambda_{\psi}^{ec}|$ |
|---|---|---|---|
| $A$ | Symbol | pn-QRPA | IPM | GTh | pn-QRPA | IPM | GTh |
| 67 | Cu | 3.54E−02 | 2.38E−03 | ... | 2.33E−06 | 2.26E−07 | ... |
| 66 | Cu | 4.63E−01 | 6.56E−01 | ... | 1.47E−06 | 1.30E−06 | ... |
| 52 | V | 5.64E−02 | 1.81E−02 | 1.17E−05 | 7.05E−07 | 2.58E−07 | 1.16E−08 |
| 56 | Mn | 7.91E−02 | 2.90E−02 | 2.61E−04 | 5.88E−07 | 2.91E−07 | 1.28E−08 |
| 60 | Co | 7.69E−01 | 2.31E+00 | 4.27E−03 | 5.65E−07 | 3.66E−06 | 1.80E−08 |
| 49 | Sc | 1.94E−03 | ... | ... | 2.63E−07 | ... | ... |
| 65 | Cu | 1.08E−01 | 5.91E−02 | ... | 1.43E−07 | 1.67E−07 | ... |
| 62 | Co | 9.31E−03 | 3.22E−02 | 2.75E−05 | 1.26E−07 | 5.34E−07 | 1.69E−09 |
| 54 | Cr | 6.41E−05 | ... | ... | 7.10E−08 | ... | ... |
| 49 | Ti | 6.41E−02 | 1.70E−02 | ... | 5.67E−08 | 4.09E−08 | ... |
| 53 | Cr | 5.16E−03 | ... | ... | 5.13E−08 | ... | ... |
| 51 | Ti | 1.08E−04 | ... | ... | 5.13E−08 | ... | ... |
| 51 | V | 6.34E−03 | 9.71E−03 | 1.67E−04 | 4.87E−08 | 1.53E−07 | 2.32E−09 |
| 63 | Ni | 1.92E−03 | 3.87E−03 | ... | 4.51E−08 | 8.15E−08 | ... |
| 64 | Ni | 2.10E−05 | ... | ... | 4.25E−08 | ... | ... |
| 48 | Sc | 8.34E−02 | 8.25E−02 | ... | 4.05E−08 | 1.02E−07 | ... |
| 57 | Mn | 5.78E−04 | 4.03E−04 | ... | 3.83E−08 | 6.33E−08 | ... |
| 61 | Co | 1.09E−03 | 2.23E−03 | ... | 3.79E−08 | 2.42E−07 | ... |
| 68 | Cu | 2.18E−03 | 2.62E−02 | ... | 3.66E−08 | 3.21E−07 | ... |
| 55 | Cr | 1.66E−04 | ... | ... | 2.51E−08 | ... | ... |
| 73 | Ga | 4.58E−03 | ... | ... | 2.26E−08 | ... | ... |
| 59 | Fe | 1.36E−04 | 1.83E−04 | ... | 1.92E−08 | 4.51E−08 | ... |
| 53 | V | 2.74E−04 | ... | ... | 1.90E−08 | ... | ... |
| 50 | Sc | 1.03E−03 | ... | ... | 1.83E−08 | ... | ... |
| 72 | Ga | 2.82E−02 | ... | ... | 1.74E−08 | ... | ... |
| 65 | Ni | 4.65E−05 | ... | ... | 1.61E−08 | ... | ... |
| 71 | Ga | 3.45E−02 | ... | ... | 1.53E−08 | ... | ... |
| 55 | Mn | 3.50E−03 | 8.73E−03 | 4.26E−05 | 1.43E−08 | 7.70E−08 | 5.53E−10 |
| 69 | Zn | 1.06E−02 | ... | ... | 1.37E−08 | ... | ... |
| 58 | Fe | 3.27E−05 | ... | ... | 1.27E−08 | ... | ... |

$\sum \lambda_{\psi}^{ec} \rightarrow -1.01E-06 -8.21E-06 -4.89E-08$

Note. The rates are compared with IPM and GTh results wherever available. The units of $\rho, T_\psi, \lambda_{\psi}^{ec}$ and $\sum \lambda_{\psi}^{ec}$ are g cm$^{-3}$, GK, s$^{-1}$ and s$^{-1}$, respectively.

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neutrinos produced and energy is channeled out of the system. In such a scenario, the isotopic abundances of nuclei follow simply from the nuclear Saha’s equation for a given \( \rho, T, \) and \( Y_e \) (Hartmann et al. 1985). We treated NSE in the same way it was previously employed by Clifford & Tayler (1965), Kodama & Takahashi (1975), and Hartmann et al. (1985).

According to Saha’s equation, the nuclear abundance of \( k \)th nucleus is given by

\[
\tau_k(A, Z) = \frac{C(A, Z, T) \left( \frac{\rho N_k \lambda_T^3}{2} \right)}{A^{Z+\lambda_T^{-}2}} \times A^{Z+\lambda_T^{-}2} T_p \exp \left[ Q_k(A, Z) / k_B T \right],
\]

(13)

where \( C(A, Z, T) \) is the nuclear partition function of the \( k \)th nucleus, \( N_k \) is the Avogadro’s number, \( \lambda_T = \sqrt{\frac{h^2}{2 \pi m_k \kappa_B T}} \) is the thermal wavelength, \( Q_k \) is the ground state binding energy and \( k_B \) is the Boltzmann constant. \( \tau_n \) and \( \tau_p \) are the mass fractions of the free neutrons and protons, respectively, and can be determined subject to mass conservation

\[
\sum_k \tau_k = 1
\]

(14)

and charge conservation

\[
\sum_k \frac{Z_k}{A_k} \tau_k = Y_e = \frac{1 - \eta}{2},
\]

(15)

where \( \eta \) is the neutron excess. \( \tau_k \) for \( k \)th nucleus can be calculated once \( \tau_n \) and \( \tau_p \) are determined. The time derivative of \( Y_e \) is a key parameter to be monitored during the presupernova evolution and for a \( k \)th nucleus it is given by

\[
\dot{Y}_{e(k)}^{\text{nc(bd)}} = -\frac{(+) \frac{T_k}{A_k} \lambda_{\text{nc(bd)}}}{A_k},
\]

(16)

where the negative sign is for ec and positive for bd, \( A \) is the mass number and \( \lambda_{\text{nc(bd)}} \) was calculated using Equation (12).

While investigating isotopic abundances in presupernova cores, Dimaro et al. (2002) showed that the computed nuclear partition functions showed a deviation of up to 50% when low-lying nuclear states were considered as discrete energy levels as against those assuming a level density function and performing integrations. The authors were able to conduct a summation over states up to 3 MeV. Since the computed nuclear partition function is the cause of one of the biggest uncertainties in calculated mass fractions, Nabi and collaborators (Nabi et al. 2016a, 2016b) recently introduced a novel recipe for an accurate description of nuclear partition functions, which we
follow here. The basic idea is to calculate discrete energy levels up to 10 MeV excitation energies. Beyond 10 MeV, a simple level density function was assumed and integration was performed up to 25 MeV excitation energy. In cases where a few measured levels were missed in the process, they were inserted manually along with their spins in the calculation.

The nuclear partition function was calculated using

\[
C(A, Z, T) = \sum_{\mu=0}^{\mu_{\text{max}}} (2J^\mu + 1) \exp\left[-\frac{E^\mu}{kT}\right] \\
+ \int_{E^{\mu_{\text{max}}}}^{E_{\text{max}}} \sum_{\mu', \pi'} (2J^{\mu'} + 1) \exp(-\epsilon/kT) \times \rho_1(\epsilon, J^\mu, \pi^\mu) d\epsilon, \tag{17}
\]

where \(\mu_m\) labels the last employed (either experimentally available or theoretically calculated) energy eigenstate. The first term in the above equation represents contribution from low-lying states (experimental or pn-QRPA predicted energy eigenvalues) up to \(E^\mu\) and the sum runs over all Boltzmann-weighted states from the ground state to \(\mu_m\). The second term uses process of integration to sum the contribution from continuous states. \(E_{\text{max}}\) was taken as 25 MeV. For details of the formalism we refer to Nabi et al. (2016a, 2016b).

### 3. Results and Discussion

We employed the pn-QRPA model to compute the weak decay rates and mass fractions for our selected pool containing 728 nuclei in the mass range \(A = 1\)–100. It is worth mentioning that our pool of nuclei is significantly larger than the ones considered by previous studies. Recently the Gross Theory (Ferreira et al. 2014) was employed to estimate ec and bd rates under stellar conditions. We compared our calculation with the results of Gross Theory (referred to as GTh throughout the text) and the IPM calculation performed by Aufderheide et al. (1994) and referred to as IPM onwards. Our selected pool of 728 nuclei may be compared with 150, 63, and around 100 nuclei chosen by IPM, GTh, and SM (Langanke & Martinez-Pinedo 2000), respectively. A small pool of nuclei can omit few key nuclei, which may dominate the nuclear composition during the late phases of the collapse before neutrino trapping. The number of nuclei in the stellar ensemble may reach around 2700 species, as reported by the authors in Juodagalvis et al. (2010). According to previous findings (Rauscher & Thielemann 2000; Rauscher 2003), calculation of partition functions is sensitive to the input mass models. All theoretical masses used in this project (including \(Q\)-values) were derived from the recent mass compilation of Audi et al. (2017). For the cases where mass values were not given, we used Möller et al. (2016) to compute the \(Q\)-values.
We estimated the rate of change of the lepton to baryon fraction ($Y_e$) separately for ec (Tables 1–3) and bd rates (Tables 4–6) and sorted the 30 nuclei with the largest contribution to $Y_e$. The ec and bd rates, for all the nuclei listed in Tables 1–6, have been calculated using only allowed GT transitions. Our calculated weak rates and the corresponding $Y_e$ values are most of the time smaller than, sometimes bigger than, and at times comparable to the corresponding results of IPM. For example, our calculated ec rates are smaller than IPM rates by a factor of 4 for $^{50}$V, $^{54}$Fe, and $^{64}$Cu and a factor of 2 for $^{61}$Co, $^{58}$Co, $^{56}$Ni, and $^{60}$Ni (see Tables 1–3). Our bd rates are factors of 3, 4, and 5 bigger than IPM rates for $^{52}$Ti, $^{66}$Co, and $^{65}$Co, respectively (Tables 4–6). The biggest difference between the two calculations were noted for $^{54}$Mn and $^{62}$Cu ($^{58,60}$Co), where our computed ec (bd) rates were found to be 2 (5) orders of magnitude smaller than IPM results. Similar differences were found for $Y_e$ values between the two models. Our computed total $Y_e$ (shown in the bottom of Table 1–6) is always smaller than the IPM value both at low and high ($T_9$, $\rho$) values. Misplacement of GT centroids relative to experimental values led to bigger weak rates in the majority of cases for IPM. When comparing our ec rates with those calculated by GTh, it is noted that all rates and the corresponding $Y_e$ values calculated by our model are bigger by orders of magnitude. Only in very few bd cases ($^{49}$Ca, $^{56}$Mn, and $^{60}$Co), our computed rates and the respective $Y_e$ values are smaller than GTh. The GTh results include transitions only from the ground state, which clearly is a poor approximation to be used for stellar rate calculations. The pn-QRPA model included a huge model space of $\Omega_T$ and is noted to efficiently handle excited states in parent and daughter nuclei. Keeping in view the good comparison of pn-QRPA calculated values with measured data, our ground and excited state GT strength distributions depict a more realistic picture of the proceedings and contribute significantly to the reliability of our calculation. We again remind that the Brink–Axel hypothesis was not used in computation of excited state GT strength functions in our calculation.

Figure 1 shows our computed mass fractions for a few abundant nuclei in NSE as a function of neutron excess ($T_9$) at different temperatures and densities. For the sake of comparison we used the same parameters ($T_9$, $\rho$, and $\eta$) as those used in Figure 1 of IPM. It is noted that the computed mass fractions follow the same behavior in both models with slight variations. The different recipes for nuclear partition functions and different mass models in the two approaches resulted in this small difference. We believe that using our recipe of nuclear partition functions would lead to a more reliable computation of mass fractions (see also Nabi et al. 2016b for a detailed analysis of the comparison between the two computed mass fractions).

Figure 2 compares our computed ec (upper panel) and bd (lower panel) rates as a function of $Y_e$ with the GTh results. The
Table 5
Same as Table 1 but for bd and at Conditions Given Below

| A  | Symbol | pn-QRPA | IPM | GTh | pn-QRPA | IPM | GTh |
|----|--------|---------|-----|-----|---------|-----|-----|
| 67 | Ni     | 2.62E−02| 5.29E−04| 8.52E−06| 1.05E−07| 5.70E−09|
| 49 | Sc     | 3.55E−02|        | 2.00E−06|         |      |
| 63 | Co     | 3.16E−02| 3.52E−04| 1.41E−06| 7.46E−07| 2.00E−08|
| 50 | Sc     | 3.08E−01| 4.10E−02| 1.21E−06| 2.08E−07| 2.04E−07|
| 65 | Co     | 7.46E−01| 1.39E−01| 1.06E−06| 2.02E−08|     |
| 59 | Mn     | 1.44E−01| 5.40E−03| 8.79E−07| 2.89E−07| 3.20E−08|
| 64 | Co     | 2.68E−01| 2.05E−01| 8.62E−07| 5.42E−08|     |
| 58 | Cr     | 4.04E−01| 2.79E−01| 7.47E−07| 2.88E−08|     |
| 69 | Cu     | 3.53E−02|        | 5.90E−07|         |      |
| 61 | Fe     | 1.57E−02| 6.44E−02| 7.45E−04| 5.29E−07| 3.45E−08|
| 51 | Ti     | 1.76E−03| 7.13E−04| 4.32E−07| 1.40E−07|     |
| 57 | Cr     | 1.01E−01| 1.49E−01| 3.66E−07| 2.00E−07|     |
| 62 | Fe     | 2.75E−03| 4.72E−02| 2.70E−07| 2.90E−07|     |
| 51 | Sc     | 8.65E−01| 4.73E−02| 2.37E−07| 6.16E−09| 8.17E−07|
| 55 | Cr     | 2.79E−03| 1.12E−05| 2.19E−07| 2.49E−07| 5.57E−09|
| 71 | Cu     | 7.33E−01|        | 1.45E−07|         |      |
| 63 | Fe     | 5.82E−01| 1.68E−01| 1.12E−07|         | 5.33E−09|
| 53 | Ti     | 3.92E−02| 1.95E−02| 1.02E−07| 1.04E−08| 1.24E−08|
| 49 | Ca     | 1.39E−02| 2.84E−02| 9.42E−08| 7.27E−09| 1.35E−08|
| 54 | V      | 5.38E−02| 3.85E−02| 8.67E−08| 2.04E−07| 1.15E−07|
| 75 | Ga     | 3.21E−02|        | 8.41E−08|         |      |
| 60 | Mn     | 3.82E−01|        | 7.83E−08|         |      |
| 70 | Cu     | 3.34E−01|        | 7.73E−08|         |      |
| 57 | Mn     | 2.37E−03| 5.32E−04| 7.68E−08| 8.02E−08|     |
| 58 | Mn     | 1.14E−02| 1.39E−01| 7.32E−08| 6.30E−07| 8.70E−08|
| 53 | V      | 2.26E−03| 2.98E−03| 6.64E−08| 2.63E−07| 2.05E−08|
| 55 | V      | 5.83E−02| 8.52E−02| 5.19E−08| 1.97E−08|     |
| 54 | Ti     | 1.33E−01|        | 4.41E−08|         |      |
| 65 | Ni     | 1.71E−04| 2.49E−03| 4.22E−08| 5.36E−07|     |
| 56 | Cr     | 8.32E−05| 1.14E−04| 4.17E−08| 2.01E−08|     |

\[ \sum Y_{\rho}^{bd} \rightarrow 2.08E−06 \]

\[ 1.01E−05 \]

\[ 6.39E−07 \]

Table 6
Same as Table 1 but for bd and at Conditions Given Below

| A  | Symbol | pn-QRPA | IPM | GTh | pn-QRPA | IPM | GTh |
|----|--------|---------|-----|-----|---------|-----|-----|
| 55 | Mn     | 1.08E−07| 3.68E−07| 1.78E−13| 1.75E−12|     |
| 57 | Fe     | 3.34E−08| 1.10E−05| 9.45E−14| 5.04E−11|     |
| 58 | Fe     | 2.90E−08| 1.09E−07| 4.14E−14| 1.55E−13|     |
| 52 | V      | 8.71E−03| 1.60E−02| 3.93E−14| 1.33E−13| 2.76E−14|
| 53 | Cr     | 3.75E−08| 5.93E−06| 2.55E−14| 8.22E−12|     |
| 54 | Cr     | 2.02E−07| 2.90E−07| 1.70E−14| 2.46E−14|     |
| 59 | Co     | 3.86E−09| 8.11E−08| 8.90E−15| 7.69E−13|     |
| 61 | Co     | 2.86E−04| 1.36E−03| 5.01E−15| 1.02E−13|     |
| 57 | Mn     | 7.43E−03| 2.97E−05| 4.24E−15| 1.72E−16|     |
| 56 | Fe     | 4.32E−13| 1.19E−10| 4.08E−15| 1.07E−12|     |
| 54 | Mn     | 1.12E−09| 8.81E−06| 3.01E−15| 3.52E−11|     |
| 53 | Mn     | 1.76E−11|        | 2.12E−15| 7.94E−12| 4.23E−13|
| 55 | Cr     | 4.84E−03|    | 1.04E−15| 3.87E−12| 2.17E−13|
| 60 | Co     | 2.03E−06| 4.66E−03| 1.03E−15| 7.94E−12| 2.17E−13|
| 52 | Cr     | 1.48E−12|        | 9.19E−16| 6.66E−16| 2.43E−13| 1.15E−17|
| 57 | Co     | 2.27E−12| 1.34E−09| 3.59E−16| 8.36E−13|     |
| 51 | V      | 5.96E−09|        | 2.87E−16| 6.66E−16| 2.43E−13| 1.15E−17|
| 55 | Fe     | 5.01E−13| 1.30E−10| 2.61E−16| 1.23E−13|     |
ec rates are sensitive to the stellar temperature and density values, showing an increase for higher values of $T_9$ and $\rho$. The behavior of our computed weak rates as a function of $Y_e$ is also in agreement with IPM, i.e., the ec rates approaching higher values when the magnitude of $Y_e$ is reduced ($T_9$ and $\rho$ increased) while there is a decrease in bd rates when the $Y_e$ is decremented. The electron chemical potential increases with rise in stellar density and that is why the ec rates are enhanced.

Table 6 (Continued)

| $\rho = 3.86E+07$, | $T_9 = 3.40$, | $Y_e = 0.470$ |
|-------------------|---------------|---------------|
| 51 Cr 1.05E−10   | ...           | 1.99E−16      |
| 53 V 6.95E−03    | ...           | 5.39E−17      |
| 49 Ti 1.96E−07   | ...           | 4.94E−17      |
| 61 Ni 5.09E−11   | ...           | 4.36E−17      |
| 51 Ti 2.89E−03   | ...           | 3.68E−17      |
| 63 Ni 4.50E−07   | 3.16E−04      | 3.53E−17      |
| 58 Co 2.96E−11   | 5.67E−06      | 3.22E−17      |
| 50 V 7.87E−09    | 1.89E−05      | 2.38E−17      |
| 49 Sc 8.30E−02   | ...           | 2.31E−17      |
| 62 Ni 7.36E−12   | ...           | 2.07E−17      |

$\sum Y_e^{bd} \rightarrow$ 4.30E−13 1.24E−10 6.68E−13

Figure 2. Comparison of the pn-QRPA and GTh weak decay rates as a function of $Y_e$. 
Figure 3. The pn-QRPA calculated ec rates as a function of $Y_e$ for isotopes of Ni, Co, Cu, and Mn.

Table 7

| A   | Symbol | $R_p$  | A   | Symbol | $R_p$  | A   | Symbol | $R_p$  |
|-----|--------|--------|-----|--------|--------|-----|--------|--------|
| 56  | Mn     | 1.11E+01 | 69  | Cu     | 3.69E−02 | 67  | Ni     | 5.34E−01 |
| 52  | V      | 6.32E−01 | 54  | Cr     | 3.63E−02 | 49  | Sc'    | 1.33E−01 |
| 67  | Cu     | 5.57E−01 | 81  | Ge'    | 3.39E−02 | 65  | Co     | 1.03E−01 |
| 60  | Co     | 4.03E−01 | 78  | Ga     | 3.37E−02 | 63  | Co     | 9.17E−02 |
| 53  | Mn     | 2.51E−01 | 64  | Cu     | 3.22E−02 | 50  | Sc     | 8.56E−02 |
| 49  | Sc     | 2.40E−01 | 57  | Co     | 3.19E−02 | 59  | Mn     | 6.70E−02 |
| 66  | Cu     | 2.09E−01 | 63  | Cu     | 3.04E−02 | 53  | Mn*    | 6.56E−02 |
| 50  | Sc     | 1.75E−01 | 58  | Ni     | 3.02E−02 | 64  | Co     | 6.50E−02 |
| 55  | Fe     | 1.68E−01 | 57  | Fe     | 2.96E−02 | 49  | Ca'    | 6.39E−02 |
| 59  | Co     | 1.53E−01 | 77  | Ge     | 2.88E−02 | 55  | Mn     | 5.64E−02 |
| 79  | Ge     | 1.11E−01 | 64  | Ni     | 2.79E−02 | 58  | Cr'    | 5.47E−02 |
| 77  | Ga     | 7.89E−02 | 58  | Co     | 2.76E−02 | 69  | Cu'    | 3.73E−02 |
| 61  | Ni     | 7.60E−02 | 83  | Se     | 2.73E−02 | 61  | Fe     | 3.66E−02 |
| 78  | Ge*    | 7.46E−02 | 53  | Cr     | 2.62E−02 | 51  | Ti     | 3.54E−02 |
| 83  | As     | 6.85E−02 | 48  | Sc'    | 2.57E−02 | 51  | Sc     | 3.27E−02 |
| 51  | Ti     | 6.78E−02 | 65  | Ni     | 2.48E−02 | 57  | Cr     | 3.08E−02 |
| 67  | Ni     | 6.67E−02 | 65  | Ni     | 2.48E−02 | 57  | Cr     | 3.08E−02 |
| 56  | Ni     | 6.17E−02 | 55  | Cr     | 2.40E−02 | 55  | Cr     | 2.79E−02 |
| 68  | Cu     | 4.62E−02 | 64  | Co     | 2.31E−02 | 62  | Fe     | 2.66E−02 |
| 82  | As     | 4.60E−02 | 57  | Mn     | 2.26E−02 | 57  | Mn     | 2.42E−02 |
| 56  | Fe     | 4.55E−02 | 71  | Cu     | 2.23E−02 | 57  | Co'    | 2.14E−02 |
| 65  | Cu     | 4.48E−02 | 55  | Mn     | 2.07E−02 | 53  | Ti     | 2.12E−02 |
| 55  | Co     | 4.03E−02 | 53  | V      | 2.05E−02 | 52  | V      | 1.80E−02 |
| 75  | Ga'    | 3.83E−02 | 73  | Ga'    | 2.03E−02 | 55  | Fe'    | 1.78E−02 |
| 57  | Ni     | 3.69E−02 | 51  | V      | 1.96E−02 | 67  | Co'    | 1.44E−02 |

Note. The ranking parameter $R_p$ is defined in the text. Nuclei marked with asterisks are new entries not to be seen in the list compiled by IPM.
at lower $Y_e$ values. For higher density, the enhanced chemical potential of electron outside the nuclei impede the bd rates. The major reduction in the density (4E+10 to 1E+9) g cm$^{-3}$ accounts for the sudden increase (decrease) in the bd (ec) rates in the short interval of $Y_e = 0.410-0.430$. The slope of the graph is relatively less steep for higher $Y_e$ values because of the smooth reduction in the $T_e$ and $\rho$ values. Our computed weak rates are bigger by as much as 1–2 orders of magnitude when compared with those of GTh results for the cases shown in Figure 2. The reasons for our bigger rates were discussed above. Figure 3 depicts our computed ec rates, as a function of $Y_e$, for Ni, Co, Cu, and Mn isotopes while Figure 4 shows our bd rates for Fe, Co, Ni, and Mn isotopes.

The evolution of rate of change of lepton to baryon fraction ($\dot{Y}_e$) is shown in Figure 5. Panel (a) depicts 15 nuclei with the largest contribution to the total $\dot{Y}_e$ values for ec, whereas panel (b) shows similar results for 10 nuclei having higher $\dot{Y}_e$ values for bd. Figure 6 shows the sum of $\dot{Y}_e$ values for both ec and bd rates. Here we compare our results with three other models namely IPM, GTh, and SM. It can be seen from Figures 5–6 that the ec rates dominate toward the end values of our chosen range of $Y_e$, while the bd rates win somewhere at the center value ($Y_e \approx 0.440$). At $Y_e = 0.410$, the contribution of $^{67}$Ni, $^{83}$As, and $^{79}$Ge to the total $\dot{Y}_e$ is greater than the contribution of $^{49}$Ca, $^{63}$Fe, and $^{51}$Sc to the $\dot{Y}_e$ and hence the ec rates are dominant at this point. The $\dot{Y}_e$ decreases and $\dot{Y}_e$ increases with rise in $Y_e$ values up to $Y_e \approx 0.422$. However, the ec rates are still dominant. With further increase in the $Y_e$ value beyond 0.422, though the contribution of $\dot{Y}_e^{ec}$ for $^{67}$Cu, $^{56}$Mn, and $^{51}$Ti is bigger, once the shares of other key bd nuclei are summed up, the total $\dot{Y}_e^{ec}$ is smaller than the corresponding $\dot{Y}_e^{bd}$. The increase (decrease) in $\dot{Y}_e^{bd}$ ($\dot{Y}_e^{ec}$) continues until $Y_e = 0.440$ (0.455). Beyond $Y_e \approx 0.440$, where the density is 3.30E+8 g cm$^{-3}$ and temperature is around 4.24E+9 K, the $Y_e^{bd}$ starts to decrease but still dominates up to values of $Y_e \approx 0.455$ due to the main contribution coming from $^{63}$Co and $^{55}$Ti. The decrease in bd continues until the end point ($Y_e \approx 0.500$) whereas the ec continues growing beyond $Y_e \approx 0.455$ with major contribution coming from $^{58}$Fe, $^{76}–^{58}$Ni, and $^{55}$Co. The bd remains dominant over ec for the interval $Y_e \approx 0.424–0.455$, 11% greater than the one proposed by IPM ($Y_e \approx 0.425–0.453$). Our proposed interval was found close to the SM and GTh intervals, which were $Y_e \approx 0.42–0.46$ and $Y_e \approx 0.422–0.455$, respectively. It may be seen from Figure 6 that our estimated total $\dot{Y}_e^{ec(bd)}$ values are smaller in magnitude than IPM results, bigger than GTh estimations and in good agreement with the SM estimation. The end result necessitates the use of a microscopic model for calculation of stellar weak rates.

We finally determined the most important weak interaction nuclei that have the largest effect on $Y_e$ post silicon core burning, by averaging the contribution from each nucleus to $Y_e$ over the entire chosen stellar trajectory. To this effect we introduced a ranking parameter ($\hat{R}_p$) given by

$$\hat{R}_p = \left( \frac{\sum_{\text{ec(bd)}} \dot{Y}_e^{ec(bd)}}{\sum_{\text{ec(bd)}}} \right)^{0.500 > Y_e > 0.400}.$$
Thus, nuclei with the largest contribution to $\dot{Y}_e$ will have the highest value of $R_p$. On the basis of $R_p$, we listed the top 50 ec and bd nuclei for all conditions that follow silicon core burning in Table 7. It is worth noting that 90% (70%) of our most important ec (bd) nuclei are the same as the list provided by IPM. The nuclei marked with an asterisk are the ones missing in the list provided by the IPM.

4. Concluding Remarks

In this work we present the first ever compilation of the nuclei that have the largest effect on $Y_e$ for conditions after silicon core burning using the pn-QRPA model. The use of a fully microscopic model adds to the reliability of calculated weak rates. The pn-QRPA model does not employ the Brink–Axel hypothesis for calculation of excited state $GT$ strength distributions—a feature not available even in the LSSM calculation. We are currently working on quantifying the disadvantages of employing the Brink–Axel hypothesis for calculation of stellar rates and hope to report our findings soon.

The reliability of pn-QRPA results and its decent comparison with measured data were discussed in Section 1. Our computation of mass abundances also used a novel recipe for calculation of nuclear partition functions. We considered all excited states up to 10 MeV as discrete, which may result in a more realistic calculation of isotopic abundances according to a previous study.

Our results are shown in Tables 1–7, which show rankings of nuclei during several key snapshots of presupernova evolution of massive stars. Specially Table 7 presents an overall ranking for all conditions post silicon burning phase and we compile a list of the top 50 ec and bd nuclei causing the largest effect on $Y_e$. It is to be noted that the list contains 10% of new ec and 30% of new bd nuclei not to be seen in the list of IPM tables. For a nucleus with $A \sim 100$ at $T_9 = 5.39$ GK, the mean nuclear excitation energy is $\sim 3$ MeV and transitions above 10 MeV excitation is in order. Our nuclear partition function (Equation (17)) considers discrete states only up to 10 MeV. Beyond 10 MeV we assumed a level density function and this may bear consequences for the calculated mass fractions. Core-collapse simulators may find this updated list interesting for their future studies. This list can further be extended to the top

Figure 5. Evolution of temporal derivative of $Y_e$ for (a) ec and (b) bd rates.
700 nuclei and may be requested from the corresponding author.

Another key finding of this paper is that we propose an updated interval $Y_e = 0.424 - 0.455$ in which the bd rates dominate the competing ec rates, which is roughly 11% bigger than proposed by IPM and 6% smaller than GTh range. Further, our estimated total $Y_e^{ec(bd)}$ values are in good agreement with shell-model prediction. We plan to extend our pool of nuclei with $A > 100$ and explore role of forbidden transitions (that become important for neutron-rich matter) in the list of nuclei having largest effect on $Y_e$ in the near future.

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References

Audi, G., Kondev, F., Wang, M., Huang, W., & Naimi, S. 2017, ChPhC, 41, 030001.
Auluberheide, M. B., Fushiki, I., Woosley, S. E., & Hartmann, D. H. 1994, ApJS, 91, 389
Bethe, H. A. 1990, RevMP, 62, 801
Bethe, H., Brown, G., Applegate, J., & Lattimer, J. 1979, NuPhA, 324, 487
Brink, D. 1958, RPPh, 21, 144
Clifford, F., & Tayler, R. J. 1965, MNRAS, 129, 104
Dimarco, A., Barbero, C., Dias, H., et al. 2002, JPhG, 28, 121
El-Kateb, S., Jackson, K., Alford, W., et al. 1994, PhRvC, 49, 3128
Ferreira, R., Dimarco, A., Samana, A. R., & Barbero, C. A. 2014, ApJ, 784, 24
Fuller, G., Fowler, W., & Newman, M. 1982, ApJS, 48, 279
Fuller, G., Fowler, W., & Newman, M. 1985, ApJ, 293, 1
Fuller, G. M., Fowler, W. A., & Newman, M. J. 1980, ApJS, 42, 447
Gove, N., & Martin, M. 1971, ADNDT, 10, 205
Halbleib, J. A., Sr., & Sorensen, R. A. 1967, NuPhA, 98, 542
Hardy, J. C., & Towner, I. 2009, PhRvC, 79, 055502
Hartmann, D., Woosley, S., & El Eid, M. 1985, ApJ, 297, 837
Heger, A., Woosley, S., Martinez-Pinedo, G., & Langanke, K. 2001, ApJ, 560, 307
Hirsch, M., Staude, A., Muto, K., & Klapdor-Kleingrothaus, H. 1993, ADNDT, 53, 165
Juedagalvis, A., Langanke, K., Hix, W. R., Martinez-Pinedo, G., & Sampaio, J. M. 2010, NuPhA, 848, 454
Kodama, T., & Takahashi, K. 1975, NuPhA, 239, 489
Langanke, K., & Martinez-Pinedo, G. 2000, NuPhA, 673, 481
Langanke, K., & Martinez-Pinedo, G. 2001, ADNDT, 79, 1
Majid, M., & Nabi, J.-U. 2016, RoRPh, 68, 1447
Majid, M., Nabi, J.-U., & Daraz, G. 2017, Ap&SS, 362, 1
Möller, P., Sierk, A. J., Ichikawa, T., & Sagawa, H. 2016, ADNDT, 109, 1
Majid, M., & Bayram, T. 2020, Ap&SS, 365, 19
Nabi, J.-U., & Bayram, T. 2016, NuPhA, 947, 182
Nabi, J.-U., & Klapdor-Kleingrothaus, H. V. 1999, ADNDT, 71, 149
Nabi, J.-U., & Klapdor-Kleingrothaus, H. V. 2004, ADNDT, 88, 237
Nabi, J.-U., Tawfik, A. N., Ezzelarab, N., & Khan, A. A. 2016a, PhS, 91, 055301
Nabi, J.-U., Tawfik, A. N., Ezzelarab, N., & Khan, A. A. 2016b, Ap&SS, 361, 71
Nakamura, K. 2010, JPhG, 37, 260
Rauscher, T. 2003, ApJS, 147, 403
Rauscher, T., & Thielemann, F.-K. 2000, ADNDT, 75, 1
Staudt, A., Bender, E., Muto, K., & Klapdor-Kleingrothaus, H. V. 1999, ADNDT, 71, 149
Vetterli, M. C., Häusser, O., Abegg, R., et al. 1989, PhRvC, 40, 559
Weaver, T., Woosley, S., Fuller, G., et al. 1985, in Numerical Astrophysics: In Honor of J. R. Wilson, ed. J. Centrella et al. (Portola: Science Book International), 374
Weaver, W., Alford, W., & Brash, E., et al. 1995, PhRvC, 51, 1144

Figure 6. Competition between ec and bd in the evolution of $Y_e$. 

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