ELECTRON CAPTURE RATES OF MID-fp SHELL NUCLEI FOR SUPERNOVA AND STELLAR EVOLUTION

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Abstract: A detailed model is constructed for the calculation of electron capture rates of some $fp$ shell nuclei for situations prevailing in pre-supernova and collapse phases of the evolution of the core of massive stars leading to supernova explosion. The model uses explicitly the Gamow-Teller strength function obtained through (n,p) reaction studies wherever available. The rates include contribution from the excited states of the mother as well as from the resonant states in equilibrium with the back reaction i.e. the beta decay of the daughter nucleus. Comparisons are made with the shell model results and the earlier calculations by Aufderheide et al. and Fuller, Fowler.
and Newman. For the nuclei $^{56}$Fe, $^{55}$Mn and $^{60}$Ni with negative Q-values one observes large contribution from the excited states.
Weak interactions play a significant role in the evolution of massive stars at the presupernova stage as well as at the subsequent core collapse phase of type II supernovae. The competition between electron capture and beta decay on fp shell nuclei (mostly with $50 < A < 70$) at the late stages of silicon burning and the electron capture during the gravitational collapse, until neutrino trapping sets in, determines the final lepton fraction inside the core, which in turn determines the shock energy at core bounce. Thus a careful evaluation of the electron capture and beta decay rates at presupernova densities and the electron capture rates at higher densities during the core collapse are of utmost importance for the supernova problem. The earlier detailed model of Fuller, Fowler and Newman [FFN,1] had all the important physics aspects incorporated in it. Later it was conjectured [2,3] that some nuclei with $A > 60$ not considered earlier may have significant impact on the deleptonisation and models for the calculations of the electron capture [4] and beta decay [5] rates for these nuclei were developed. Aufderheide et al [4] also identified sets of important nuclei for each density-temperature domain which need to be taken into account. Recently $0\hbar\omega$ shell model calculations in the full fp shell with all the 4 orbits have been carried out for the evaluation of the electron capture and beta decay rates[6]. These rates are based on the allowed beta strength distributions using energy eigenvalues and wavefunctions obtained through very large matrix diagonalisation with a realistic fp shell interaction.
On the other hand (p,n) reaction studies for a number of years and (n,p) reaction studies for the last decade or so carried out on a number of nuclei in this mass range have given us valuable information on the same allowed beta decay and electron capture matrix elements. It is always observed that both for beta decay and electron capture the experimental strength distributions are quenched compared to the best theoretical estimates. The models take account of this by including a quenching factor in the Gamow-Teller (GT) strength distribution, mostly a constant independent of energy.

In an earlier work Kar, Ray and Sarkar [5] had calculated the beta decay rates for a number of important nuclei with $A > 60$ using a statistical model for the GT strength distribution including the effects of excited states and back resonances (coming from the equilibrium of beta decay and the inverse reaction of electron capture between the same two nuclei at typical high pre-supernova (preSN) temperatures). In this letter we extend that to the electron capture sector with the important improvement that the observed (n,p) GT strength distribution is used directly for the evaluation of the rates for the ground state of the mother. So in this work we are concerned with the nuclei for which the (n,p) reaction results are available and we compare our results with those from the shell model calculations and other previous estimates.

The electron capture rate on the nucleus $(Z, N)$ is given by

\[ \text{The electron capture rate on the nucleus (} Z, N \text{) is given by} \]
\[ \lambda_0^{EC}(\rho, T, Y_e) = \ln \left( 2 \sum_{i,j} \frac{(2J_i + 1) \exp[-E_i/k_B T]}{G(Z, N, T)} \frac{f_{ij}(\rho, T, Y_e, Q_{ij})}{(ft)_{ij}} \right) \]

Here \( \rho \) is the matter density, \( T \) the temperature, \( k_B \) the Boltzmann constant and \( Y_e \) is the electron fraction. \( G(Z, N, T) \) is the nuclear partition function at temperature \( T \), \( E_i \) the excitation energy of the mother and \( Q_{ij} \) and \( (ft)_{ij} \) are the Q-value and the ft-value between the i-th state of the mother and the j-th state of the daughter.

\[ Q_{ij} = Q_{g.s} + E_i - E_j \]

where \( Q_{g.s} \) is the ground state Q-value and \( E_i \) is the excitation energy of the i-th excited state of the mother and \( E_j \) is the corresponding energy of the j-th excited state of the daughter and

\[ (ft)_{ij} = \frac{(6250 s)}{(g_A/g_V)^2 B_{ij}(GT)} \]

as for the ground state and the low-lying states there is no contribution from the Fermi strength due to isospin selection rule. \( B_{ij}(GT) = |M_{ij}(GT_\pm)|^2 \) is the usual nuclear matrix element squared of the Gamow-Teller (\( GT_\pm \)) operator.

The phase space integral \( f_{ij} \) is of the form [7]

\[ f_{ij} = \frac{1}{(m_e^2/c^2)^5} \int_{E_{min}}^{\infty} E(E^2-m_e^2)^{1/2}(E-\epsilon_0)^2 F_c(Z, E) F D(E-\mu_e) F D C(E-\mu_e-\epsilon_0) dE \]
with \( FD(x) = (1 + \exp(x/k_B T))^{-1} \) and \( F DC(x) = 1 - FD(x) \). Me refers to electron mass, \( \epsilon_0 = -Q_{ij} \) and the lower limit of the integral \( E_{\text{min}} \) is the larger value between \( \epsilon_0 \) and \( m_e c^2 \). For the Coulomb correction factor \( F_c(Z, E) \) we use the form of ref[7].

For PreSN temperatures the reverse reaction on the daughter nucleus, i.e. beta decay of the daughter happens to be in equilibrium with the electron capture. For the ground state or a lowlying state of the daughter the state of the mother that is in equilibrium is not the ground state or other lowlying states, but one that has maximum overlap with the daughter state differing from it by a particle-hole excitation lying a few MeV higher in energy. We include the electron capture rate from this specific resonant state separately and write the electron capture rate as,

\[
\lambda_{\text{EC \ total}}^{EC}(\rho, T, Y_e) = \lambda_0^{EC}(\rho, T, Y_e) + \lambda_{\text{Res}}^{EC}(\rho, T, Y_e)
\]

where \( \lambda_0^{EC}(\rho, T, Y_e) \) is given by eq (1). \( \lambda_{\text{Res}}^{EC}(\rho, T, Y_e) \), the resonance contribution calculated using the model of Fuller, Fowler and Newman [1] is given by,

\[
\lambda_{\text{Res}}^{EC} = \ln 2 \ (6250s)^{-1}(G^d/G^m) \times \\
\left[ \left( \frac{g_A}{g_V} \right)^2 \times \exp(-E_{\text{Res}}(GT)/K_B T) \times | M_{GT} |^2 f(T, \mu, Q_{\text{Res}}(GT)) \right]
\]

\[
+ \exp(-E_{\text{Res}}(F)/K_B T) \times | M_{F} |^2 f(T, \mu, Q_{\text{Res}}(F))
\]
where \( G^d \) and \( G^m \) are the partition functions of the daughter and the mother, \( E_{Res}(GT/F) \) is the GT/F resonance energy in the mother and calculated using the model of FFN as described in ref [1].

\[ Q_{Res}(GT/F) = Q_{g.s.} + E_{Res}(GT/F) \]
for nuclei where the ground state single particle configurations of the daughter can get connected to the resonant state through GT/F transitions, otherwise \( Q_{Res}(GT/F) = Q_{g.s.} \).

\( |M_{GT}|^2 \) is the matrix element of Gamow-Teller operator for the reverse reaction i.e. beta decay [1] and is given by,

\[
|M_{GT}|^2 = Z_n \sum_{r,s} |M_{GT}^{s,p}(r,s)|^2 \times \frac{n_r^p n_h^s}{(2j_s + 1)} \]

(7)

where \( n_r^p \) is the number of neutron particles in orbit ‘r’, \( n_h^s \) is the number of proton holes in orbit ‘s’ (with degeneracy \( 2j_s + 1 \)) and \( M_{GT}^{s,p}(r,s) \) is the single particle GT matrix element between orbit ‘r’ and ‘s’. \( Z_n \) is the quenching factor of the back reaction (taken as 0.6). \( |M_F|^2 = (N - Z) + 2 \) i.e. the difference in neutron and proton numbers of the daughter. \( E_{Res}(F) \) is the excitation energy of the first higher isospin state \( (T_0 + 1) \) in the mother \( (T_0 = (N - Z)/2) \).

For the Gamow-Teller strength distribution needed in the calculation of rates we use the results obtained from (n,p) experiments for the ground state of the mother. This is obtained by measuring the (n,p) reaction cross-section on the target and by performing multipole analyses on the resulting spectra. These experimental strength distributions are known to be substantially
quenched with respect to the theoretical predictions and also the shape of the energy distribution is different compared to the theoretical forms. The theoretical forms of strength distribution depend on the model space as well as the realistic interaction used. This is why the experimental strength distribution is the best form to use for the rates wherever available even though there are sometimes large (about 20%) uncertainty in the extraction of the strength. For the nuclei $^{56}$Fe [8], $^{55}$Mn [8] and $^{60}$Ni [9] considered here we use directly the histograms of the GT strength per MeV from (n,p) studies. That is, we use the strength distribution as a function of energy instead of $|M_{ij}(GT_+)|^2$ and replace the summation over the final states in eq(1) by integration over energy.

For the excited states the rates are calculated using Gaussian forms for the $GT_+$ strength distributions based on the spectral distribution theory arguments [10]. The same method was used in the beta decay sector in the model of Kar, Ray and Sarkar [5]. However as the excited states are within 3-4 MeV of excitation we use the ‘Brink hypothesis’ and take for the centroid and width of the strength Gaussian the ground state values obtained from fits to (n,p) data. Thus the centroid of the strength Gaussian corresponding to transition from the i-th excited state is $E_{C}(i) = E_{C}(g.s.) + E_i$. The ground state strength centroid is fixed by the Sutaria-Ray expression [11] which gives a global fit to all known (n,p) data in fp shell as a function of $A$ and $N$. For the widths we use best fit values obtained by Sutaria-Ray for
the specific examples [12].

Table 1 gives the calculated total rates for the nuclei $^{56}$Fe, $^{55}$Mn and $^{60}$Ni with the four representative density grid points log $\rho_{10} = -2.5$, -1.5, -0.5 and 0.5 ($\rho_{10}$ is the density in $10^{10} g/cc$) and five temperatures $T_9$ (in $10^9$ K) = 2, 3, 4, 5 and 6. The rates within parenthesis are the ground state contributions. The quenching factor in our theoretical model is taken as a parameter and fixed by the following procedure: For high density (log $\rho_{10} =$0.5) and low temperatures ($T_9 =$2) when the electron chemical potential is large to see the full GT strength distribution the quenching factor is adjusted to give the ground state rate identical to the one obtained by using the (n,p) data. This quenching factor is then used for all the excited states considered. The rates for all the three nuclei considered (all with negative Q-value for e-capture) show a very rapid fall with decreasing density. This is because though the chemical potential ($\mu_e$) of the electrons is 11.98 MeV at log $\rho_{10} =$0.5 ($T_9$=2,$Y_e =$0.45) it becomes very small i.e. 0.804 MeV at log $\rho_{10} =$-2.5 ($T_9$=2,$Y_e =$0.45) and at this lower density only a very small fraction of the electrons from the tail of the Fermi-Dirac distribution can overcome the Q-value and cause the capture. We also observe that for the highest density tabulated the contribution from the excited states is small (at most about 30% for the highest temperature). But at the lower densities when $\mu_e$ is too small to cause capture on the ground state, the excited states still have a better chance for capture with Q-values higher (and sometimes even positive) and often give
dominant contribution. On the other hand for the back resonances considered though both Fermi and Gamow-Teller can in principle contribute, we find that their contributions even at $\log \rho = 0.5$ is essentially zero (0.10 and 0.00 for GT and Fermi respectively for $^{60}\text{Ni}$ at $T_9 = 6$). For the nuclei $^{56}\text{Fe}$, $^{55}\text{Mn}$ and $^{60}\text{Ni}$ the GT back resonances are at excitations of 5.38, 6.71 and 5.29 MeV respectively (according to the FFN prescription that we use) and these are too high to make any significant contribution to the rates. The back resonance excitation energies for the Fermi are all higher than 10 MeV and here again the exponential factor in eq (6) makes the contributions zero.

In Table 2 we compare our rates with the rates calculated by other models. We find that for the two even-even nuclei our rates are more than an order of magnitude higher than the ones by Aufdeheide et al. [4]. Actually Aufderheide et al. puts the total strength in a single excited state of the daughter nucleus with an effective ‘log ft’ and ref [6] observes that for the even-even nuclei it is put at too high an excitation. For the odd-A nucleus $^{55}\text{Mn}$ however our values are within a factor of 2 higher compared to Aufderheide et al.. Compared to FFN our values are within a factor of 2 on the higher side except for low density ($\rho = 5.86 \times 10^7 \text{g/cc}$ for $^{60}\text{Ni}$) where the FFN value is an order of magnitude lower. But FFN used phenomenological log ft’s concentrated in a giant resonance at a fixed energy whereas we use the observed (n,p) strength distribution. For $^{56}\text{Fe}$ at a density of $10^8 \text{g/cc}$ our ground state rate compares well with that of Martinez-Pinedo et al.[6] but
our total rate is higher by a factor of seven. A more detailed comparison for other densities and other nuclei is needed to understand this.

In conclusion we stress that for a proper comparison of the electron capture rates by different methods a calculation which uses observed experimental ground state GT strength distributions is important and is reported in this letter. We are in the process of extending our calculations to all the nuclei for which (n,p) results are available. We also plan to look at the problem of identifying the sets of important nuclei for the preSN evolution for different densities and temperatures using our rates and the nuclear statistical equilibrium. This may show important differences from the ones prescribed by Aufderheide et al. [4].
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TABLE 1

e\textsuperscript{−} Capture Rates for $Y_e = 0.45$
| Nucleus | Temperature $^0K$ | $\log_{10} \rho_{10}$ |
|---------|------------------|---------------------|
|         |                  | 0.5 | -0.5 | -1.5 | -2.5 |
| $^{56}$Fe | $2 \times 10^9$ | 231.1 | $1.31 \times 10^{-1}$ | $1.65 \times 10^{-7}$ | $8.21 \times 10^{-11}$ |
|         |                  | (227.7) | $(1.22 \times 10^{-1})$ | $(3.72 \times 10^{-8})$ | $(1.13 \times 10^{-11})$ |
|         | $3 \times 10^9$ | 245.8 | $2.06 \times 10^{-1}$ | $2.03 \times 10^{-5}$ | $1.14 \times 10^{-7}$ |
|         |                  | (229.6) | $(1.55 \times 10^{-1})$ | $(3.36 \times 10^{-6})$ | $(1.06 \times 10^{-8})$ |
|         | $4 \times 10^9$ | 268.0 | $3.55 \times 10^{-1}$ | $3.54 \times 10^{-4}$ | $5.76 \times 10^{-6}$ |
|         |                  | (232.6) | $(2.08 \times 10^{-1})$ | $(4.52 \times 10^{-5})$ | $(4.92 \times 10^{-6})$ |
|         | $5 \times 10^9$ | 298.5 | $6.58 \times 10^{-1}$ | $2.41 \times 10^{-3}$ | $7.00 \times 10^{-5}$ |
|         |                  | (236.6) | $(2.84 \times 10^{-1})$ | $(2.63 \times 10^{-4})$ | $(5.87 \times 10^{-6})$ |
|         | $6 \times 10^9$ | 340.5 | $1.22 \times 10^0$ | $9.45 \times 10^{-3}$ | $4.13 \times 10^{-4}$ |
|         |                  | (241.7) | $(3.19 \times 10^{-1})$ | $(9.73 \times 10^{-4})$ | $(3.57 \times 10^{-5})$ |
| $^{55}$Mn | $2 \times 10^9$ | 110.6 | $9.85 \times 10^{-2}$ | $3.13 \times 10^{-6}$ | $1.46 \times 10^{-9}$ |
|         |                  | (108.1) | $(8.03 \times 10^{-2})$ | $(1.61 \times 10^{-6})$ | $(4.00 \times 10^{-10})$ |
|         | $3 \times 10^9$ | 114.3 | $1.28 \times 10^{-1}$ | $4.84 \times 10^{-5}$ | $2.42 \times 10^{-7}$ |
|         |                  | (109.4) | $(9.11 \times 10^{-2})$ | $(1.68 \times 10^{-5})$ | $(5.41 \times 10^{-8})$ |
|         | $4 \times 10^9$ | 121.4 | $1.92 \times 10^{-1}$ | $3.04 \times 10^{-4}$ | $4.40 \times 10^{-6}$ |
|         |                  | (111.3) | $(1.09 \times 10^{-1})$ | $(7.76 \times 10^{-5})$ | $(8.54 \times 10^{-7})$ |
|         | $5 \times 10^9$ | 131.8 | $3.02 \times 10^{-1}$ | $1.15 \times 10^{-3}$ | $3.05 \times 10^{-5}$ |
|         |                  | (113.8) | $(1.36 \times 10^{-1})$ | $(2.48 \times 10^{-4})$ | $(5.56 \times 10^{-6})$ |
|         | $6 \times 10^9$ | 144.4 | $4.62 \times 10^{-1}$ | $3.17 \times 10^{-3}$ | $1.31 \times 10^{-4}$ |
|         |                  | (116.9) | $(1.76 \times 10^{-1})$ | $(6.57 \times 10^{-4})$ | $(2.51 \times 10^{-5})$ |
TABLE 1 (contd.)

$e^−$ Capture Rates for $Y_e = 0.45$

| Nucleus | Temperature $^0K$ | $\log \rho_{10}$ |
|---------|------------------|------------------|
|         |                  | 0.5              | -0.5             | -1.5             | -2.5             |
| $^{60}$Ni | $2 \times 10^9$  | 416.1 (415.5)    | $6.66 \times 10^{-1}$ (6.61) | $7.84 \times 10^{-6}$ (3.66) | $4.99 \times 10^{-9}$ (9.64) |
|         | $3 \times 10^9$  | 426.7 (418.7)    | $8.27 \times 10^{-1}$ (7.56) | $2.51 \times 10^{-4}$ (6.84) | $1.66 \times 10^{-6}$ (2.19) |
|         | $4 \times 10^9$  | 457.3 (423.3)    | $1.25 \times 10^{0}$ (8.96) | $2.45 \times 10^{-3}$ (4.34) | $4.40 \times 10^{-5}$ (4.74) |
|         | $5 \times 10^9$  | 514.8 (429.4)    | $2.14 \times 10^{0}$ (1.09) | $1.18 \times 10^{-2}$ (1.64) | $3.65 \times 10^{-4}$ (3.67) |
|         | $6 \times 10^9$  | 593.2 (437.1)    | $3.45 \times 10^{0}$ (1.35) | $3.55 \times 10^{-2}$ (4.58) | $1.62 \times 10^{-2}$ (1.69) |
TABLE 2

Comparison of our electron capture rates with other model calculations

| Nucleus | Density ($\times 10^7$ g/cc) | Temperature ($\times 10^9$ oK) | $Y_e$ | Our Rate ($s^{-1}$) | Rates ($s^{-1}$) of |
|---------|-------------------------------|--------------------------------|-------|---------------------|---------------------|
|         |                               |                                |       |                     | Aufderheide et al. [4] | FFN [1] | Martinez-Pinedo et al. [6] |
| $^{56}$Fe | 5.86                          | 3.40                           | 0.47  | 2.07E-06            | 6.97E-08            | -       | -                               |
|         | 10.7                          | 3.65                           | 0.455 | 1.42E-05            | 4.68E-07            | 1.0E-05 | 2.1E-06                         |
|         | 14.5                          | 3.80                           | 0.45  | 3.97E-05            | 1.31E-06            | 2.81E-05 | -                               |
| $^{60}$Ni | 5.86                          | 3.40                           | 0.47  | 2.17E-05            | 1.49E-06            | 1.09E-03 | -                               |
|         | 10.7                          | 3.65                           | 0.455 | 1.25E-04            | 7.64E-06            | -       | -                               |
|         | 14.5                          | 3.80                           | 0.45  | 3.18E-04            | 2.74E-05            | 1.39E-04 | -                               |
|         | 33.0                          | 4.24                           | 0.44  | 3.93E-03            | 3.34E-04            | -       | -                               |
| $^{55}$Mn | 10.7                          | 3.65                           | 0.455 | 1.52E-05            | 9.23E-06            | -       | -                               |
|         | 14.5                          | 3.80                           | 0.45  | 3.79E-05            | 2.25E-05            | 2.03E-05 | -                               |
|         | 33.0                          | 4.24                           | 0.44  | 4.55E-04            | 2.64E-04            | -       | -                               |